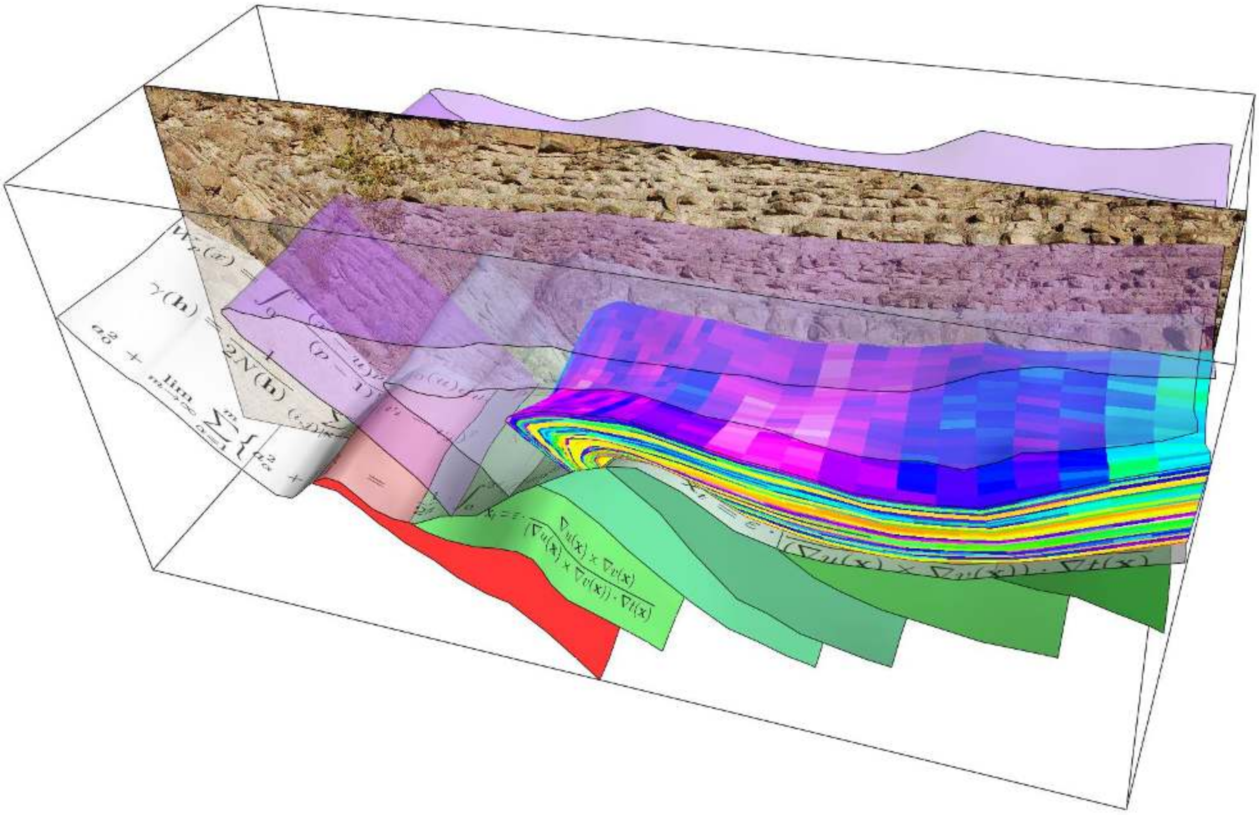
IAMG 2022

The 21st Annual Conference of the
International Association
for Mathematical Geosciences

Abstracts



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August 29-September 3, *Centre Prouvé, Nancy, France*

Foreword

We are very pleased and honored to introduce this book of abstracts of the 21st Annual conference of the International Association for Mathematical Geosciences, held in Nancy from August 29 to September 3, 2022. This is the first time since the 1980 Geological Congress in Paris that the IAMG meeting returns to France, the country where geostatistics and mathematical morphology were formalized by Georges Matheron.

Nancy, a city sitting on Bajocian formations of the eastern Paris Basin, is one of those places in the world where mathematical geoscientists are always welcome. In the 19th and 20th centuries, it exploited the “Minette de Lorraine”, an oolithic iron ore which was eventually used in the *Forges de Pompey* to create the steel of the Eifel Tower in Paris. Nowadays, the Nancy area also hosts active salt mines. As a result, Nancy has become home to one of the largest geoscience communities in France. Nancy is also the birthplace of the French Mathematician Henri Poincaré, who wrote in 1901: “Mathematicians do not study the objects but the relationships between objects” in *La Science et l’hypothèse*. There is no doubt that this statement accurately applies to mathematical geoscientists! Closer to us, two influential mathematical geoscientists studied in Nancy: Andre Journel (at the Nancy School of Mines), and Jean-Laurent Mallet (at the National School of Geology).

The last edition of the IAMG Conference took place in Penn state in 2019 and the pandemic forced us to wait for three long years before reinstating our annual conference. It is a great pleasure to finally introduce this volume of abstracts, which is a proof that the Mathematical Geoscience Community is alive and well!

This volume contains 269 abstracts, organized into one plenary and 24 thematic sessions covering the main topics of mathematical geosciences and their applications, including classical and emerging subfields of statistics and spatial statistics, artificial intelligence, machine learning, geoinformatics, geomodeling and computational methods. We deeply thank all authors, with a special mention to the keynote speakers and IAMG awardees (Philippe Renard, Marie Colette Van Lieshout, Malcolm Sambridge, John Carranza, Qiuming Cheng, Colin Daly and Bruno Lévy) for sharing their insights, work, and ideas. The session conveners also deserve our sincere acknowledgements for their invaluable contribution to the diversity of topics and their help in ensuring the quality of this conference.

We also want to thank the sponsors of IAMG 2022: Schlumberger (Platinum sponsor), TotalEnergies (Silver Sponsor), ANDRA and AspenTech (Bronze sponsors). Their help is very welcome and illustrates the significant role that mathematical geosciences play addressing the societal, environmental and energy transition challenges of today and tomorrow.

We hope you will enjoy reading these abstracts and further enjoy the presentations, social interactions, and scientific exchanges at IAMG 2022, and look forward to the next edition in Trondheim!

Guillaume Caumon
Conference Chair

Pauline Collon
Conference co-chair

Contents

S00 Plenary Session

Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS)

S0001. Multiple-Point statistics for stochastic modeling of aquifers, where do we stand?

Philippe Renard (University of Neuchâtel)
Room: auditorium 2022-08-30 08:40

In the last 20 years, multiple-point statistics have been a focus of much research, successes and disappointments. The aim of this geostatistical approach is to integrate geological information into stochastic models of aquifer heterogeneity to better represent the connectivity of high or low permeability structures in the underground.

Many different algorithms have been and are still proposed. They are all based on the concept of a training data set from which spatial statistics are derived and used in a further step to generate stochastic conditional realizations. While the method clearly succeeded in enabling modelers to generate realistic models, several issues are still the topic of debate both from a practical and theoretical point of view, and some issues such as training data set availability are often hindering the application of the method in practical situations.

In this talk, the aim is to present a review of the status of these approaches both from a theoretical and practical point of view using several examples at different scales and in various geological environment (from pore network to regional aquifer, and from karst to alluvial systems).

S0002. Parametric and non-parametric monitoring of induced seismicity in the Groningen gas field

Marie-Colette van Lieshout (CWI Amsterdam)
Room: auditorium 2022-08-30 13:40

First discovered in 1959, the Groningen gas field is one of the largest in Europe with an estimated recoverable gas volume of around 2,900 billion Normal cubic meters (bcm). Production started in 1963, initially only to accommodate the high demand for gas during the winter months. However, the closure of smaller gas stations in the country led to an increase in production. By 2012, annual production volumes had climbed to over 40 bcm per year.

Increasing production volumes and the resulting depletion of the gas field have led to induced earthquakes in the previously tectonically inactive Northern Netherlands. The most significant event to date, which occurred in August 2012 near Huizinge with a magnitude of 3.6, attracted massive public attention, prompting the Ministry of Economic Affairs to reduce production volumes.

In this talk, I will discuss parametric and non-parametric techniques for monotoring the induced seismicity with specific attention to the relation between seismic hazard and production volumes as well as pore pressure measurements.

This talk is partially based on joint work with Zhuldyzay Baki.

S0003. Optimal transport and Geophysical inversion

Malcolm Sambridge (Australian National University),
Andrew Jackson (ETH Zürich),
Andrew P Valentine (Durham University)
Room: auditorium 2022-08-31 08:30

The field of optimal transport is thought to have originated in the 19th century, when legend has it that Napoleon asked Gaspard Monge to rearrange his sand castles. That started a 200 year story of discovery and re-discovery of the mathematics of how to map, or transport, one curve (or probability distribution on to another). Leonid Kantorovich reformulated Monge's problem in terms of more familiar linear programming which contributed to his winning the 1975 Nobel prize for economics. Cedric Villani pioneered the modern mathematical treatment of the topic and was awarded the 2010 Fields medal.

What has all of this got to do with Geophysics? Here exploration geophysicists have led the way and shown how to exploit OT in Full seismic waveform inversion. It turns out that optimal transport may be used as an alternate to Least squares measures to create a new type of data misfit function. It has been demonstrated that it has significant potential in nonlinear inversion by reducing the presence of local minima in misfit functions which would otherwise by highly multi-modal. Over the past decade this has created a flurry of excitement and activity in Seismic Waveform inversion in exploration geophysics, and a gradual appreciation of the topic more broadly. This talk will introduce OT for geophysical inversion in a more general context, and also discuss some new ideas and open questions which, as always, take the form of how do we best exploit these 'pure' mathematical concepts in an effective manner for practical outcomes.

S0004. Multi-scale Spatial Patterns of Mineral Deposits: Their Exploration Significance

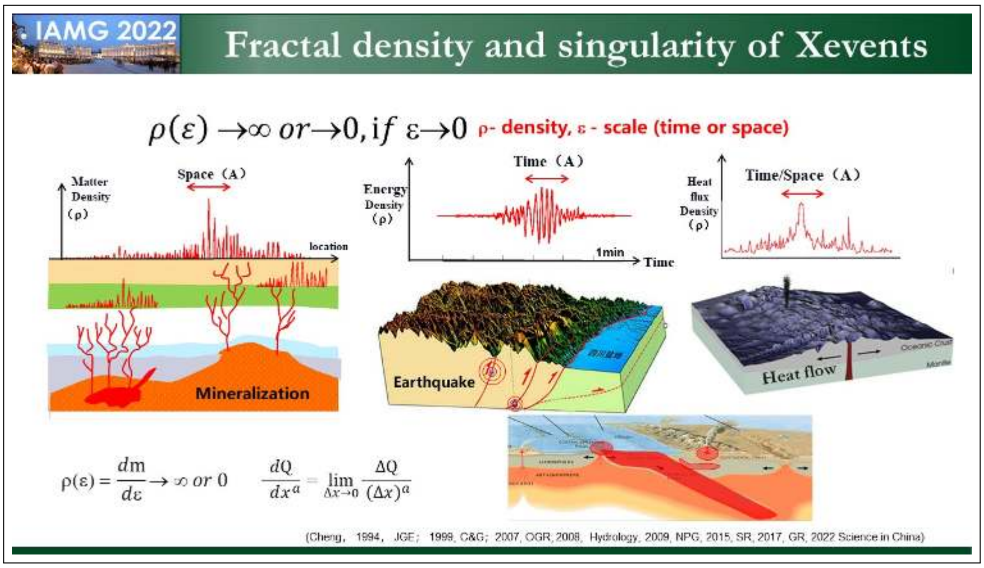
John Carranza (University of the Free State)
Room: auditorium 2022-08-31 13:40

Mineralization and the spatial pattern of its products (i.e., mineral deposits) are due to the interplay of countless processes controlled by the geological setting where they exist. Research in this viewpoint has gradually established that many perceptible processes involved in mineralization exhibit fractal distribution (i.e., they are scale-invariant). It can be intuited, therefore, that, in spite of the discernible intricacy of the spatial pattern of mineral deposits across a range of geographic scales, some orderliness exists in it. If examined properly, this orderly spatial spattern can be informative to various fields relevant to mineral exploration. In this presentation, the spatial pattern of iron oxide-copper-gold deposits in the world-class Carajás Mineral Province of Brazil is examined at the regional-scale (as point locations on a regional map), local-scale (as ore bodies on a mine-scale map) and micro-scale (as ore minerals in thin sections). It is shown that the spatial pattern of ore minerals at the micro-scale is largely non-random, displays fractal distribution and exhibits discernible trends that mimic those of ore bodies at local-scale and deposit locations at regional-scale. Therefore, the fractality of the spatial pattern of mineral deposits is largely because of structural controls on mineralization, as certain geological structures are major controls on fluid flow. Hence, that the key factor that governs the perceived fractal nature of the spatial pattern of mineral deposits is permeability, which is largely linked to multi-scale geological structures. The analyses presented offer insights to the fractal nature of mineral deposit controls, new multi-scale methods to examine structural controls on mineralization and innovative techniques for mineral prospectivity modeling.

S0005. Quantitative simulation and prediction of extreme geological events

Qiuming Cheng (Sun Yat-Sen University/China University of Geosciences (Beijing))
Room: auditorium 2022-09-01 08:30

The systematic study of extreme geological events (such as plate collision and subduction, extreme cold and extreme hot events, biological extinction and revival, earthquakes, volcanoes, mineralization, and oil accumulation) that occurred during the evolution of the earth is essential not only for understanding the "abrupt" changes in the evolution of the earth, but also for an in-depth investigation of the co-evolution of material-life-environment of the livable earth. However, due to the temporal and spatial anomalies and complexity of extreme geological events, classical mathematical models cannot be effectively applied to quantitively describe such events. Comparative studies of many types of geological events suggest that such extreme geological events often depict "singular" characteristics (abnormal accumulation of matter or massive release of energy in a small space or time interval). On this basis, the author proposes a unified definition of extreme geological events, a new concept of "fractal density" and a "local singularity analysis" method for quantitative description and modeling of extreme geological events. Applications of these methods to several types of extreme geological events are introduced to demonstrate that the singularity theory and methods recently developed can be used as general approaches for the characterization, simulation, and prediction of extreme geological events.



S0006. Interpolations, realizations and scenarios - using ML spatially without big data

Colin Daly (Schlumberger)
Room: auditorium 2022-09-02 08:30

A typical geostatistical problem might only have sparse observations of the target variable, sometimes accompanied by (a possibly large) number of densely observed secondary data variables. The geostatistical approach constructs a spatial model using a random function (RF), with hypotheses such as stationarity, and uses this model to make predictions. As well as predictions, realizations of the RF are used to understand ‘typical’ behaviour of the target variable, often as Monte Carlo samples for further spatial nonlinear analysis, such as fluid flow. When there is too much uncertainty in the geoscience to focus on a single type of RF, scenarios are constructed by varying model type or significant parameters to cover the meaningful uncertainty. Some problems are that the RF models are difficult to manipulate with multiple auxiliary variables, the stationarity hypothesis is too simple and constructing scenarios can be very time consuming.

In contrast, a stereotypical view sees machine learning as strong when there is a significant amount of data to train with. Deep Learning approaches, which are well established for classification are less developed when used in regression type problems with few training data, the terrain of the Geostatistical model. Problems for the Deep Learning approach so far are the lack of appropriate training data, lack of associated RF and hence uncertainty management.

A class of models that have proved useful in mapping, and increasingly popular, are those based on random forests (or similar). Many published variants of this are only poorly spatially aware. This presentation will show how one approach, developed originally for 3d geological modelling in the oil industry, leverages geostatistical models. It has a simple, yet sufficiently rigorous, statistical interpretation to allow construction of realizations to study the behaviour of the target variable. Using ideas of Structural Equation Models and Interventions from Causal modelling, it is easy to intervene on a realization to emphasise particular features (e.g seismic features or user interpretations). This parametric route easily, and rapidly, allows a wider set of ‘scenarios’ than standard geostatistical models.

S0007. Computational optimal transport

Bruno Lévy (Inria Nancy Grand-Est research)

Room: auditorium 2022-09-02 13:50

I will give an introduction to optimal transport, a mathematical theory that makes it possible to measure distances between functions (or distances between more general objects), to interpolate between objects or to enforce mass/volume conservation in certain computational physics simulations. Optimal transport is a rich scientific domain, with active research communities, both on its theoretical aspects and on more applicative considerations, such as geometry processing and machine learning. I will summarize the main principles behind the theory of optimal transport, introduce the different involved notions, and more importantly, how they relate, with the aim of giving an intuition of the elegant theory that structures them. Then we will consider a specific setting, called semi-discrete, where a continuous function is transported to a discrete sum of Dirac masses. Studying this specific setting naturally leads to an efficient computational algorithm, that uses classical notions of computational geometry, such as a generalization of Voronoi diagrams called Laguerre diagrams.

S01 Beyond Gaussianity: what is the status of the GANs, MPS, Cumulants or Copula approaches?

Julien Straubhaar (University of Neuchâtel),
Thomas Mejer Hansen (Aarhus University),
Philippe Renard (University of Neuchâtel)

In this session, we invite authors to show their latest research in the field of non multi-Gaussian random fields. This includes for example Generative Adversarial Neural networks, Multiple-Point Statistics, High-order Cumulants, and Copula approaches. All aspects from new theoretical developments to practical applications, comparison of methods, success or failure stories are welcome.

S0101. Multiple-point based simulation and estimation with uncertain data

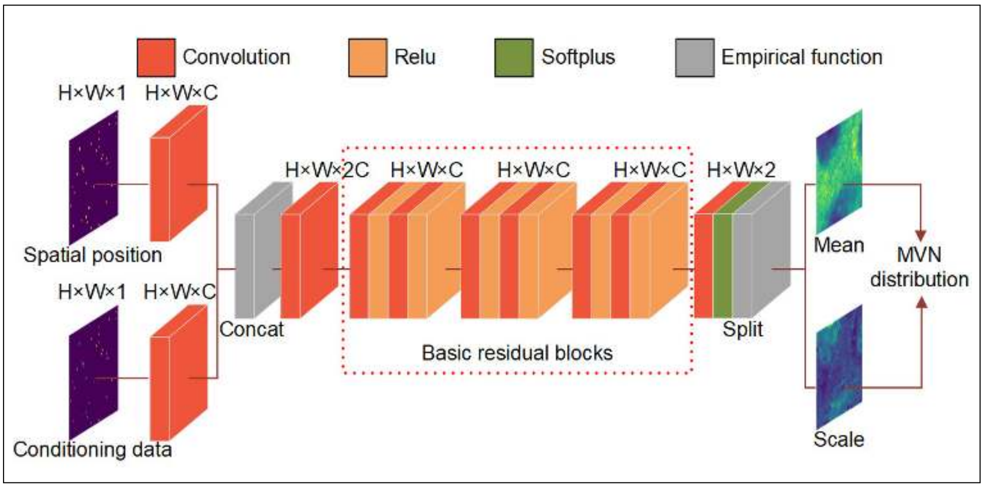
Oli Johannsson (Aarhus University),
Thomas Mejer Hansen (Aarhus University)
Room: 106 2022-09-01 09:50

The initial development of 2-point based geostatistics focused on estimation (of the conditional distribution) and accounted for conditional data both with and without uncertainty. Later more focus was on simulation, conditioning to co-located uncertainty data. When the use of multiple-point statistics (MPS) was first popularized, it was with a focus on simulation and conditioning to uncertain data was in practice limited to co-located uncertain data. Initially, we argue that the use of only co-located data with MPS can be problematic both in case using sparse uncertain data (from e.g. borehole information), and densely available uncertain information. In principle, uncertain data should be considered on par with certain conditional data. Then we will discuss a set of alternative methods that allow for non-co-located soft information with MPS simulation. We discuss the limitations due to computational requirements. Finally, we will demonstrate how one can use these methods to perform both MPS simulation and estimation.

S0102. Characterization of subsurface hydrogeological structures with convolutional conditional neural processes on limited training data

Zhesi Cui (China University of Geosciences),
Qiyu Chen (China University of Geosciences),
Gang Liu (China University of Geoscience)
Room: 106 2022-09-01 10:15

One of the main issues in the application of statistical-learning-based methods to the characterization of hydrogeological phenomena is the lack of connectivity of spatial structures. With the development of deep learning technique, the difficulty of obtaining enough training data and generating multiple-scale structures hinder the applications of deep learning-based methods in hydrogeological modeling. It is found that hydrogeological modeling problems can be regarded as stochastic processes, and stochastic processes based on meta-learning have been proposed. One of these approaches, convolutional conditional neural processes (ConvCNP) is introduced and adapted to modeling subsurface structures in earth sciences. In this work, ConvCNP is used to reconstruct the entire spatial structures of subsurface hydrological facies and channels from a limited amount of conditioning data. To extend 3-D applications of original approach, 3-D ConvCNP is proposed according to the spatial distribution characteristics of 3-D conditioning data. Compared to other deep learning-based methods, we use a small amount of training data and obtain positive model generalization capabilities. Four datasets of categorical and continuous hydrogeological structures are exploited in the experiments. Various validation tests including variograms, connectivity functions, and multi-dimensional scaling map (MDS) are used to evaluate the quality of generated realizations. The proposed approach is able to significantly reduce training consumption and improve the performance of realizations compared to a set of different benchmark tests. The experiments confirm that the ConvCNP model can extract heterogeneous patterns by using meta-learning from limited training data and reconstruct multiple-scale hydrogeological structures.



S0103. Multiple-point statistics in unstructured grids

Julien Straubhaar (University of Neuchâtel),
Philippe Renard (University of Neuchâtel),
Tatiana Chugunova (TotalEnergies)
Room: 106 2022-09-01 10:40

Unstructured grids are often used for modeling physical processes, because they allow to represent properties more accurately in areas of interest using small cells, and to follow specific geometries by adapting the shape of the cells. Numerical methods can solve physical equations on such grids. To quantify uncertainty, geostatistical tools are needed for populating these unstructured grids with properties. The challenge is that the spatial statistics are scale dependent (support effect). As covariances between points and blocks (volumes) can be computed analytically or numerically, two-point statistics algorithms can be applied on unstructured grids for generating multi-Gaussian simulations. On the contrary, multiple-point statistics (MPS) is a non parametric approach consisting in borrowing pattern from a training image (TI) and then the change of support can not be handled straightforwardly.

In this work, we propose a new MPS technique for simulating directly a property in the cells of an unstructured grid. The algorithm uses a multi-scale representation of the TI defined in a regular grid, i.e. composed of rectangular parallelepiped cells. The first step consists in defining for every simulation grid cell the dimensions of a box having the same volume and respecting the size ratios along each axis, then in selecting a fixed number of representative scales (box dimensions) and assigning one scale to each unstructured cell. Then, the TI property is defined for each of theses scale (upscaling) by accounting for the support effect (moving averages in the case of an additive variable). Finally, the MPS simulation is done following a direct sampling strategy where multi-scale patterns are retrieved from the simulation grid and searched for in the multi-scale TI. The results compares well with the simulation on a fine grid followed by upscaling on the unstructured grid, but the proposed method saves time and memory.

S0104. Downscaling tomographic models using multi-point statistics

Thomas Bodin (Univ. Lyon),
Navid Hedjazian (Univ. Lyon),
Gaspard Larrouturou (Univ. Montpellier),
Yann Capdeville (Univ. Nantes)
Room: 106 2022-09-01 11:05

The level of resolution in tomographic models obtained by full waveform inversion is related to the minimum wavelength of the observed wavefield. Since seismograms are band limited, scales smaller than the minimum wavelength such as sharp discontinuities are often not resolved in tomographic images. For example, a stack of fine layers will be imaged as a smooth anisotropic medium. In this way, tomographic models only depict a long wavelength effective medium that cannot be directly interpreted geologically.

Here we propose a downscaling approach to combine small-scale geological information extracted from training images with long-wavelength tomographic information. Our approach is based on a multi-point statistics algorithm. This is made possible by using an effective medium theory called non-periodic elastic homogenization, that gives some equivalence between models of different scales in terms of waveform fitting. We use a geostatistical simulation to construct a model represented by 2 types of variables representing small and large scales. During the simulation, the statistics of small scales are required to be compatible with training images, whereas the large scales are required to fit a smooth tomographic image. We show examples of applications on typical subsurface imaging problems.

S0105. Downscaling of digital elevation models by using a multiple-point statistics approach

Guanghui Hu (Nanjing Normal University & University of Lausanne),
Gregoire Mariethoz (University of Lausanne)
Room: 106 2022-09-01 11:30

Digital elevation models (DEMs) have been widely used in geomorphology, hydrology, geology, glacier science, and planetary science. Although coarse resolution DEM can express the Earth surface on a large scale, they are not suitable for modelling surface processes at scales smaller than their spatial resolution. Downscaling of DEMs, also called super-resolution DEMs, has been developed in recent years and aims to reconstruct the terrain in a finer resolution. To this end, techniques have been proposed based on deep learning, however, the limited availability of fine-resolution DEMs are challenging the requirement for massive training datasets in deep learning. In this research, we develop a multiple-point statistics approach for downscaling of DEMs using only a limited fine resolution training DEM dataset. In our algorithm, we first decompose the target coarse DEM into a deterministic trend component and a stochastic residual component. A training image is constructed by choosing a geomorphologically similar fine resolution DEM and computing its residual component. Next, the fine resolution of the target residual DEM is simulated with an open-source multiple-point simulation framework named QuickSampling. In this process, the coarse target residual DEM is used as conditioning data to ensure local accuracy. Finally, we add the interpolated fine resolution trend to the simulated fine resolution residual to obtain the final downscaled DEM. Case study areas of the Tibet Plateau in China, the Chokai volcano in Japan, and the Jura Mountain in Switzerland are used to validate the proposed approach. In addition, the proposed algorithm is benchmarked against a two-point statistics simulation method and a deterministic interpolation technique. Results show that the proposed approach maintains the statistical properties of the fine-scale DEM as well as its spatial details.

S0106. Can FPGAs speed up MPS?

Mathieu Gravey (Utrecht University)
Room: 106 2022-09-01 11:55

Yes ! Even significantly.

Multiple-point statistics (MPS) is increasingly used in Earth and environmental applications due to its capacity to produce stochastic simulations with realistic complex structures. However, the computational efficiency has remained a major issue for a large-scale adoption. Early algorithmic improvements were focused on computation time and memory footprint reduction (e.g., using search tree and then lists, and the use of multigrids). In the last decade, research has shifted to improving flexibility and simulation results, popularizing continuous and multivariate simulations with algorithms such Direct Sampling or QuickSampling.

Although recent algorithms are very versatile, from a computational point of view they are still not as efficient as early approaches for simple settings. For example, generating categorical models with limited number of categories can potentially be faster with earlier algorithms such as SNESIM or IMPALA. Therefore, these algorithms are still widely in use until this day. However, since their original development, technologies have significantly evolved, allowing the transition from a single sequential computation with high computational cost to multi-core vectorized computations which is only capped by the memory bandwidth limitation. Recently hardware accelerators, such as GPUs, have changed the rules by pushing further performance for computations as well as memory.

Field-programmable gate array (FPGA) is a technology relying on programming the hardware, i.e. designing circuits that tailored to do the expected computation. While CPUs can run any computation slowly and GPU can run faster graphical computation, FPGAs will run even faster, but only the very specific problem for which it was set up. Furthermore, FPGAs are known to have a much lower energetic footprint than CPUs or GPUs.

Here we propose to revisit early simulation algorithms, in particular Impala, and take advantage of FPGAs to get several orders of magnitude speed up (> 50x)!

S0108. Lessons learned from simulating fluvial deposits using process-based models and generative adversarial networks

Guillaume Rongier (TU Delft),
Luk Peeters (CSIRO Land and Water)
Room: 106 2022-09-01 15:00

Reproducing the architecture and heterogeneity of sedimentary deposits while conditioning to data remains one of the biggest challenges in subsurface modeling. Over the recent years, generative adversarial networks or GANs have made headlines for generating images of mesmerizing realism. Could they achieve similar results with sedimentary deposits? A first hurdle arises even before exploring GANs' abilities: how to find the large amount of 3D images required to train them? While methods requiring training images have gained momentum over the last decade, options to generate such images remain scarcely explored. To go beyond the object-based simulations traditionally used, we have turned to a landscape evolution model, the Channel-Hillslope Integrated Landscape Development model (CHILD), to simulate fluvial deposits over geological times based on simplified physical models. By simulating 20000 3D images with varying meandering histories, we peek at the diversity of spatial distributions of fluvial deposits. Having a training set driven by geological processes includes more physics into stochastic simulations, even though GANs themselves only reproduce patterns. Once trained on those images, GANs reproduce the non-stationarity and extent of the channel belt, as well as some meanders, even though some details are lost. But our experience shows that GANs are difficult to set up due to their unstable training. While many solutions have been developed to overcome this issue, they are mostly empirical and require some testing to determine which one(s) might work for a given network architecture and training set. And while the realism of GANs' samples is constantly improving, this often comes from increasingly complicated architectures, falling short of the initial promises of deep learning. The openness of its community has turned deep learning into a fast-moving field, which leads to amazing opportunities in geoscience, but makes it harder to keep up with the latest developments.

S0109. What can GAN learn from depositional patterns to build 3D facies models?

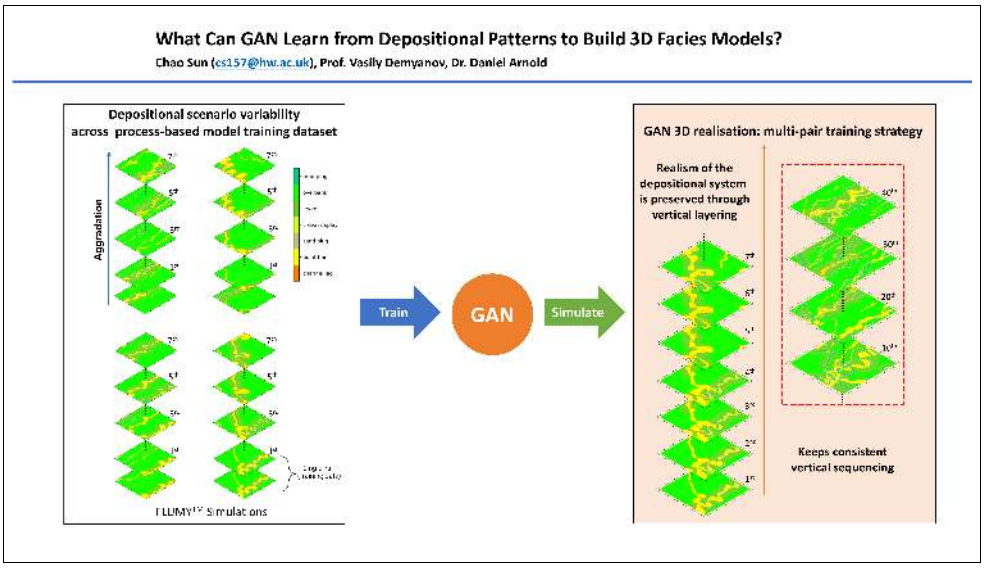
Chao Sun (Heriot-Watt University),
Vasily Demyanov (Heriot-Watt University),
Daniel Arnold (Heriot-Watt University)
Room: 106 2022-09-01 15:25

This paper proposes a new way to generate 3D geological models using generative adversarial networks (GANs) by building the 3D volume from a set of associated 2D images. To replicate natural depositional systems, the GAN must capture the complex sequences of facies and their spatial correlation patterns, e.g., the distribution of channels and point bars in a fluvial system. There has been some success in 2D, however 3D modelling remains challenging due to the complexity of geological patterns, increased model size and added computational burden when training with 3D patterns.

Our novel GAN training strategy builds the model upwards layer by layer, realistically mimicking a depositional process, making it more computationally efficient than the geological models on which it is trained and GANs trained with 3D samples (entire 3D facies models). Each new layer is created, conditioned to the facies distribution in the layers below, preventing the GAN simulations from gradually losing realism vertically, while honouring how the channel system could evolve. The results indicate the trained generator can create unconditional 3D fluvial simulations with any thickness (number of layers) without loss of geological consistency through vertical layering, without retraining.

We trained the GAN on an ensemble of complex geologically realistic models of a meandering fluvial system, created using a processes-based tool. This training data set represents more realistic facies associations (channels, point bars, levees, overbank) and geometries under the variability within the fluvial depositional scenario than those used in previous GAN studies, which typically tackle three or fewer facies.

The work will discuss the advantages and limitations of our GAN approach in preserving the key geological patterns and show how to lessen the prevalence of geologically unrealistic features and artifacts.



S0110. Deep-learning spatial generation of geological facies

Ferdinand Bhavsar (Mines Paris Tech),
Thomas Romary (Mines Paris Tech),
Fabien Ors (Mines ParisTech - PSL Université),
Nicolas Desassis (Mines Paris Tech)
Room: 106 2022-09-01 15:50

Deep learning methods applied to geological facies modelling for heterogeneous reservoir simulations is getting more and more attention. Indeed, when the quantity and the complexity of data is high, those algorithms display impressive results in terms of inference cost, flexibility and quality of generated facies simulations. The most popular methods use generative adversarial networks (GAN) where two neural networks are trained competitively to reach a Nash Equilibrium. This framework outputs a spatial probabilistic model, the generator, allowing to generate images.

In this work, we are faced with realistic and fast geological facies generation and the subsequent task of conditioning, which is the fitting of the model to field data. We are focusing on using Flumy, a stochastic process-based modelling tool, to generate non conditional simulations which are then used to train a faster and more flexible deep-learning based proxy.

The results are evaluated based on visual realism, uncertainty quantification, and consistency of various descriptive metrics (e.g. facies connectivity and inference speed). We will showcase the different tested neural networks architectures, among which a promising fully convolutional multi-scale approach, trained using various metrics (e.g. Wasserstein metric). An efficient variational Bayesian method for the conditioning to various data types (e.g boreholes, seismic information,...) will also be proposed. We will finally discuss the results and shortfalls of these methods.

S0111. Should we use Machine Learning to get Geostatistical realization?

Mathieu Gravey (Utrecht University)
Room: 106 2022-09-01 16:15

No! Unless you are sure of what you're doing!

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S0112. Three-dimensional Geological Structure Reconstruction with Multiple- point Statistics Method Guided by ANN: A Case Study of Metro Station in Guangzhou, China

Hou Weisheng (Sun Yat-sen University),
Hengguang Liu (Sun Yat-sen University),
Yonghua Chen (Guangzhou Metro Design & Research Institute Co. Ltd.),
Yanhua Li (Sun Yat-sen University),
Chengjun Liu (Guangzhou Metro Design & Research Institute Co. Ltd.),
Dian Wang (Guangzhou Metro Design & Research Institute Co. Ltd.)
Room: 106 2022-09-01 16:40

Economic development has prompted the rapid expansion of cities, which results in many problems like traffic congestion and shortage of land resources. Developing subway traffic is an alternative option to solve these problems. It is an important for the design and construction of metro engineering to establish a reasonable 3D geological structure to clarify the geological conditions along the subway.

Compared to the two-point statistics (TPS) method, multiple-point statistics (MPS) reproduces spatial characteristics from Training Image (TI) and conditional data, in which spatial structures of geological bodies are extracted and reconstructed with a moving template. However, it is difficult to reproduce global spatial relationship between geological objects with local continuity of ovelapped area.

In the field of 3D geological modeling, deep learning (DL) methods have been directly applied to build 3D models, of which some methods also attempt to combine MPS algorithm. The DL-based algorithms are adopted to judge the stratigraphic attributes according to the location, without considering the spatial relationship between multiple points in local space. When GAN architecture is simply applied to reconstruct 3D geological model, the demand of cross-dimensional data for training network is still a key problem.

In this study, a novel 3D reconstruction method combining deep artificial neural network (DANN) and MPS is proposed. The DANN is constructed and used to extract and simulate the global characteristics of geological structures. An initial model is bulit with the process of sequential simulation and stratigraphic sequence calibration. The final result is output arfter an iterative MPS simulation process with a multi-scale strategy. With several cross-sections used as modeling dataset, a concrete examples of constructing 3D geological structures in a metro station in Guangzhou, South China is given. The result illustrated that the presented method can build a reasonabl 3D geological structures with high precision effectively.

S0113. Copula-Based Geostatistics: Recent Developments and Geo-Hydrological Applications

Claus Haslauer (University of Stuttgart),
Sebastian Hörning (The University of Queensland),
András Bárdossy (University of Stuttgart, LHG)
Room: 106 2022-09-02 14:40

Mulitvariate copula-based geostatistical methods enable (i) the description varying degrees of dependence in various quantiles and (ii) facilitate a meaningful uncertainty quantification. Furthermore, these models enable to incorporate secondary data both in categorical and numerical form. These secondary data may have a different influence depending on the quantile and/or on the location. Simulation strategies based on FFTMA allow the generation of the fields with these prescribed dependences for the primary and secondary variables. Through an effective simulation with conditioning both expected values and uncertainties can be assessed.

A key practical application of copulas is the operational evaluation of the state of Baden-Württemberg's (a state of Germany) groundwater quality for about 200 solutes.

We demonstrate that when the degree of the deviation from normal dependence is incorporated into the geostatistical model used for the simulation of spatially distributed fields of hydraulic conductivities, then this leads to a more realistic representation of solute transport characteristics.

S0114. A Multiple-Point Statistical Descriptor Measuring High-Order Spatial Data Consistency

Lingqing Yao,
Roussos Dimitrakopoulos (McGill University)
Room: 106 2022-09-02 15:05

High-order spatial statistics fully characterize non-Gaussian random fields used to model pertinent attributes of natural phenomena. The latter attributes typically exhibit non-Gaussianity in terms of their probability distributions as well as nonlinear, complex features in their spatial structures. Contrary to the conventional second-order spatial statistics that only capture pairwise correlations of the related attributes, high-order spatial statistics delineate complex spatial patterns and multiple-point interactions, thus providing a more realistic featuring of the corresponding natural phenomena. The integration of high-order spatial statistics is also essential in uncertainty quantification framework under high-order stochastic simulation; the inference of the probability distribution in high-order simulation approaches, relies on experimentally computed high-order spatial statistics, instead of fitting parameterized models. A multiple-point statistical descriptor is proposed herein as a new mathematical alternative to quantify high-order spatial statistics. The statistical descriptor is built upon the concept of spatial Legendre moments, consisting of the moments of certain order n corresponding to different combinations of random variables within a m-point spatial template, and thus extracting the wealth of information beyond the multi-point simulation approaches that partially utilize the multi-point statistics associated to the presence of a full template. In addition, this statistical descriptor can be extended to a kernel function as a similarity index to measure the spatial data consistency of different patterns. Lastly, the conventional covariance model can be simply incorporated as a lower-order descriptor while the high-order statistical information can be complemented from additional sources if needed, and thus bridges the conventional second-order simulation to high-order simulation and improves the spatial data consistency. A case study is carried out for verification.

S0115. Porous media reconstruction conditioned to well information using multi-modal generative adversarial networks (GANs)

Zihan Ren (The Pennsylvania State University),
Sanjay Srinivasan (The Pennsylvania State University)
Room: 106 2022-09-02 15:30

The flow and transport of fluids in the subsurface ultimately occurs at the pore scale. To characterize the heterogeneity of multiphase flow properties at field scale, it is often necessary to obtain large amount of representative porous media images in different geo-spatial locations. Although generative models such as DCGAN had been developed to generate porous images of different rocks, the generation algorithm is uncontrolled and unconditional to physical variables such as porosity, connectivity etc., which are key reservoir properties that can be inferred from well logs at the field scale. We present a modified physical driven GAN structure called PCGAN which can incorporate heterogeneous multi-modal physical information into the Gaussian space and image space through attaching different embedding layers to generator and discriminator to construct a hierarchical representation of different physical properties. Besides the adversarial loss function, new physical loss functions have been added to PCGAN to further optimize the generation process.

We have demonstrated our approach for reconstructing Micro CT images of synthetic pore structures as well as well for reconstructing pore spaces in Berea and Bandera Gray sandstones and compare the reconstructed physical properties with input ‘conditional’ physical properties. Results indicate that the generation process in PCGAN not only can be controlled and conditioned to physical information (such as porosity, connectivity etc.), but also represent the residual uncertainty. The balance between representation of uncertainty and conditioning to physical factors during the generation process can be tuned by modifying the noise vectors and weights of physical loss functions. This result provides a solid foundation to characterize the heterogeneity of multiphase flow behavior at field scale, because the physical properties that are used to control and condition PCGAN generation are all common properties that can be inferred at the well/inter-well scale.

S0116. Direct Sampling Strategy for Extensive Hard Data-based Training Image

Sangga Rima Roman Selia (Helmholtz Institute Freiberg for Resource Technology), Raimon Tolosana-Delgado (Helmholtz Institute Freiberg for Resource Technology, HZDR), van den Boogaart K. Gerald (Helmholtz Institute Freiberg for Resource Technology, HZDR)

Room: 106 2022-09-02 15:55

Extensive hard data could potentially replace the training image in doing MPS. However, direct use of the the standard MPS Direct Sampling algorithm will typically not produce proper results, owing to the absence (or at least, sufficient replication) of every necessary data pattern in the data set. As a result, during the step of training image scanning, there will be a reduction of the conditional data neighbourhood in the simulation grid data event, generating inconsistencies of neighbourhood size in simulating each point. Here, we propose to use a spatial tolerance in extracting the training image data events. This has long been used to obtain experimental variogram in two-point geostatistics, and is also common in high-order cumulant based methods.

A synthetic case study of a fluvial depositional environment will be presented, together with a comparison of the usage of various types of training images (e.g. hard data, complete training image, multiple training images). This framework can also be extended to MPS for the purpose of estimation rather than simulation. This is achieved by obtaining marginal conditional probabilities by storing potential simulated values during the training image scanning step for each grid cell, conditioning only to hard data. This could be a time saver for users interested only in the point-wise statistics of the realizations without having to generate multiple realizations.

S02 Recent developments in machine learning techniques and quantum computing for geoscience applications

Teeratorn Kadeethum (Cornell University),
Daniel O'Malley (Los Alamos National Laboratory),
Hongkyu Yoon (Sandia National Laboratories),
Hamid M. Nick (The Danish Hydrocarbon Researc)

Recent advancements in machine learning techniques and quantum computing have made their way into geoscience research. These approaches have been adopted and proposed to tackle long-standing challenges in geoscience or an enhancement of classical methods that have been used in this field. This mini-symposium invites presentations on advances within areas of machine learning and/or quantum computing in geoscience research. Topics include, but are not limited to,

- machine learning algorithms and applications for model-reduction, optimization, inverse problems, uncertainty quantification, highly parameterized problems (e.g., parametrization of heterogeneous fields), and efficient dimensionality reduction of nonlinear operators and
- quantum computing applications in geoscience research; for instance, seismic inversion with quantum annealing, quantum-computational hydrologic inverse analysis, or quantum optimization.

The mini-symposium will bring together researchers working on fundamental and applied aspects of machine learning and quantum computing to provide a forum for discussion, interaction, and assessment of their presented techniques.

S0201. A novel quantum machine learning approach for enhancing sweep efficiency mapping

Klemens Katterbauer,
Marko Maucec (Saudi Aramco),
Sara Abu Al Saud (Saudi Aramco),
Abdallah Al Shehri (Saudi Aramco)
Room: 105 2022-08-30 10:00

Artificial intelligence and 4IR technologies have led to a significant transformation. Advanced artificial intelligence (AI) algorithms are deployed to improve production forecasts. A major challenge in the maximization of sweep efficiency is the determination of saturation around and far from the wellbores from resistivity and associated logs. This challenge to quantify accurately sweep efficiency has been only partially addressed with conventional technologies. Semi empirical relationship, such as Archie's law, allow the estimate of water saturation, knowing rock formation porosity and electrical resistivity.

In this work, we present a quantum machine learning approach to determine the saturation in the near-wellbore region of a reservoir, taking into account the uncertainty in the acquired data. Quantum machine learning allows incorporating directly the state of the data and corresponding logging responses as sampled from the underlying probability (density) functions. This allows to overcome some of the estimation and classification challenges arising from the uncertainty in the interpreted training data. The work we present focuses on utilizing the principles of quantum physics for dealing with data, utilizing the probabilistic nature of a state in order to represent the data, irrespective of whether a quantum computing machine is utilized.

The training data are utilized for the training of the quantum machine learning neural network as incorporated into a feedback (reinforcement learning step) process that enhances the robustness of the trained model and improves the estimation quality. This framework was examined on a reservoir box model with strong heterogeneity and uncertainty in the well log measurements. The framework performed rather well, allowing to provide reliable estimates of saturation in the wellbore surrounding.

In challenging fractured carbonate reservoirs, this method may also be extended, broadly incorporating the uncertainty of the fracture network distribution, by means of models of discrete fracture network as framework constraints.

S0202. Identification of groundwater contaminant source characteristics through artificial neural network

Daniele Secci (Università degli Studi di Parma),
Laura Molino (Università degli Studi di Parm),
Andrea Zanini (Università degli Studi di Parma)
Room: 105 2022-08-30 10:25

The needs of the modern man have given rise to economies based on intensive agriculture and industrial production in which water is both a resource and a waste product. Limited water resources address the problem of its sustainable use and without causing environmental consequences or groundwater pollution. In this sense is essential to have a tool that can reduce the computational burden of a numerical model, preserving the reliability of the results. Artificial Intelligence, and in particular neural networks, can be employed in this context as data-driven surrogate models to solve forward and inverse problems.

In this work, a groundwater contaminant source reconstruction problem is investigated through feedforward artificial neural network (FFWD-ANN). Different cases have been analyzed and the Latin Hypercube Sampling has been used to randomly generate the training dataset. Firstly, the release history at two contaminant sources with known location has been used as input data to train the network for solving a forward transport model. In the process, the ANN is able to well estimate the pollutant concentrations in 7 monitoring wells, at different times. Then, the surrogate model has been trained to deal with inverse transport problem related to different application cases: 1. estimation of the release history at one contaminant source with known location; 2. simultaneous estimation of the release history and location of one contaminant source; 3. estimation of the release history at two contaminant sources with known location; 4. simultaneous estimation of the release history and error on observations. The obtained results, compared with literature data, show that neural networks represent an efficient approach in contaminant source reconstruction problems.

S0203. On the application of NLP techniques to French geological descriptions

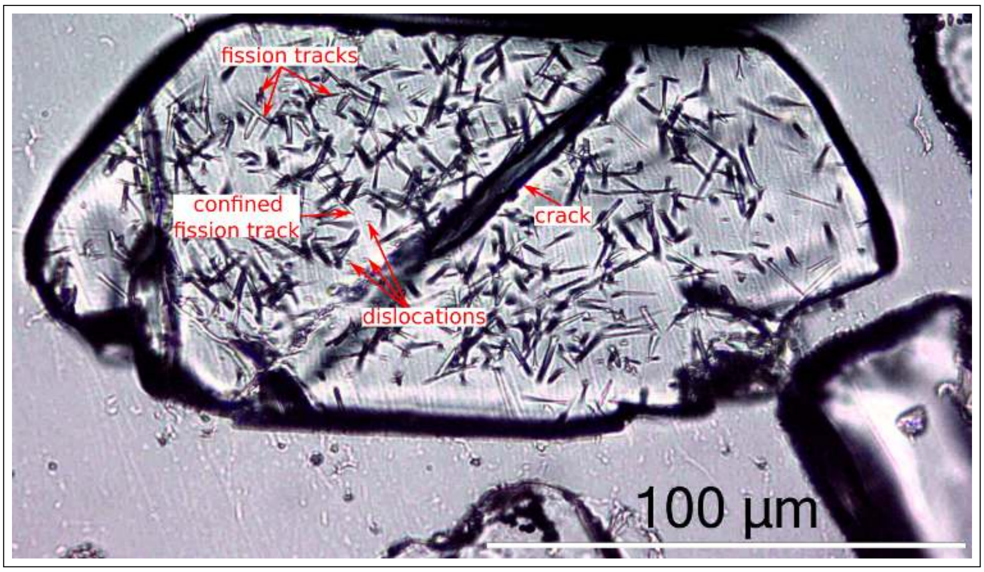
Musaab Khalid (BGRM),
Cécile Gracianne (BGRM),
Maelys Galant (BGRM),
Romain Darnault (BGRM),
Christelle Loiselet (BRGM),
Vincent Labbé (BGRM)
Room: 105 2022-08-30 11:44

S0204. FTAIGE: Opportunities and pitfalls in machine-learning-based fission-track analysis

Robert Arato (Georg-August University, Göttingen),
Nils Keno Lünsdorf (Georg-August Universität, Göttingen)
Room: 105 2022-08-30 10:50

Fission-track dating is a well-established thermochronological method, which is based on the counting and length measurement of nuclear damage trails (i.e. fission tracks) in minerals by means of optical microscopy. Due to the complexity of microscopic images (Fig. 1) and objects to be studied, the operator-based manual counting remains the most widely applied approach until these days. However, the manual approach has serious limitations especially with respect to the number of grains being dated as well as the comparability and reproducibility of the results. This study is an attempt to automatize large parts of the slow and tedious manual procedure. We combine fission-track dating with artificial-intelligence-assisted image analysis exploiting the capability of convoluted neural nets (CNN) to be 'taught' to detect user defined objects in an image. Sub-tasks include the recognition of datable grains in etched strew mounts, detection of fission tracks in datable grains, length measurement of track openings and the length measurement of confined tracks. We employ various neural network architectures within the PyTorch framework using a set of apatite standards. The dataset includes grains with various track densities and a varying amount of disturbing optical effects (e.g. dislocations). For the different sub-tasks we optimize the necessary set of raw reflected light/transmitted light microphotographs and their combination. We test various CNNs (e.g. Mask R-CNN, Unet, Feature Pyramid Networks, etc.) and define various object classes to discriminate features in a datable grain relevant for fission-track dating, which are, for instance, flat tracks, confined tracks and dislocations. We present the state of our progress in each of the sub-tasks including an extensive comparison of various neural network setups with manual counting/length measurement results.

Fig. 1: Etched apatite crystal with fission tracks and some typical disturbing effects.



S0205. Machine learning clinopyroxene thermobarometry – a solution for mafic-alkaline systems

Corin Jorgenson (University of Geneva),
Oliver Higgins (University of Geneva),
Maurizio Petrelli (University of Perugia),
Guido Giordano (University of Roma Tre),
Luca Caricchi (University of Geneva)
Room: 105 2022-08-30 11:15

Our understanding of the physical and thermal structure of volcanic plumbing system is essential to unveil relationships between pre-eruptive processes and duration and intensity of volcanic events. Crystals within volcanic rocks provide valuable information regarding the magmatic history of a volcano, allowing us to reconstruct pressure (P) and temperature (T) of the crust and reconstruct the past. Clinopyroxene mineral chemistry is strongly dependent on P and T, and there are many studies which use thermodynamic constraints to model P-T dependencies on the clinopyroxene chemical composition using major elements (Masotta et al., 2013; Putirka et al., 2008). These models, while rooted in thermodynamics, are limited in compositional space and assume end-member purity which is rarely the case in complex natural systems. Here we present developments in a machine learning approach to thermobarometery using a random forest algorithm (available at https://github.com/corinjorgenson/RandomForest-cpx-thermobarometer). We have applied our method to clinopyroxene crystals of Colli Albani – a mafic and alkaline volcano whose composition is so unique it cannot be used in any current clinopyroxene based thermobarometer. Colli Albani is a volcano of notable significance as it is located only 20 km away from Rome and has produced large volume explosive eruptions in the past. Additionally, we present a unique advantage of this thermobarometer compared to existing calibrations, which uses the interquartile range of random forest voting distributions to give a degree of confidence for each individual estimate. Results show that clinopyroxenes crystallise between 1-5 kbar and 800-1200 C (SEE 3.1 kbar, 71.9 C), in agreement with present day geophysical findings (Bianchi et al., 2008). Such agreement lends weight to using random forest to identify loci of magma storage beneath active volcanoes.

Masotta, M., Mollo, S., Freda, C., Gaeta, M., & Moore, G. (2013). Clinopyroxene–liquid thermometers and barometers specific to alkaline differentiated magmas. Contributions to Mineralogy and Petrology, 166(6), 1545–1561. https://doi.org/10.1007/s00410-013-0927-9

Putirka. (2008). Thermometers and barometers for volcanic systems. Reviews in Mineralogy and Geochemistry, 69, 61–120. https://doi.org/10.2138/rmg.2008.69.3

Bianchi, I., Piana Agostinetti, N., de Gori, P., & Chiarabba, C. (2008). Deep structure of the Colli Albani volcanic district (central Italy) from receiver functions analysis. Journal of Geophysical Research, 113(B9), B09313. https://doi.org/10.1029/2007JB005548

S0206. Quantum Computing for Open-Pit Optimization

Malte Leander Schade (RWTH Aachen),
Denise Degen (RWTH Aachen),
Florian Wellmann (RWTH Aachen)
Room: 105 2022-08-30 11:40

The optimized development of open-pit mines based on underlying geologic models greatly influences their maximal runtime and profitability.

Considering all influential parameters and restrictions that arise in real-world mining operations, this proves to be a mathematically complex problem to solve for classical computers. Recent advancements in the construction of quantum computers and the discovery of new quantum algorithms could lead to new optimization techniques for mine planning that reduce the computational runtime and increase the possible input model complexity.

In this work, we evaluate how basic concepts of quantum computation and their differences to standard computation can help with this classical optimization problem, considering a complex-theoretical approach. Open-pit mine development is set up as a Traveling-Salesman-Problem, a combinatorial optimization problem of finding the shortest Hamiltonian path through interconnected nodes, and a quantum phase estimation algorithm is used to solve it as a proof of concept. Furthermore, in cooperation with Rheinkalk GmbH (Lhoist Germany), the restrictions, parameters, and problems in real-world open-pit mine planning and current optimization techniques are assessed.

The experimental results show that an open-pit mining optimization problem can be solved with quantum phase estimation and is executable on real-world quantum computers today - though only at a limited scale to date, with verifiable results.

S0207. A geothermal heat flow model of Africa based on Random Forest Regression

Magued Al-Aghbary (TU Bergakademie Freiberg),
Mohamed Sobh (TU Bergakademie Freiberg),
Christian Gerhards (TU Bergakademie Freiberg)
Room: 105 2022-08-30 11:42

In this study, we implement a hybrid model of Random Forest regression to model the Geothermal Heat Flow (GHF) in Africa. To this end, we train the model with preprocessed observables from global and regional datasets to improve data quality. After tuning the hyperparameters of the algorithm, the trained model relates the GHF to various geophysical and geological observables, such as Moho depth, Curie depth, gravity/geomagnetic anomalies, and seismic wave velocities. As a result, the predicted GHF map of Africa has good performance indicators and is consistent with existing GHF maps of Africa. This model not only represents the GHF of Africa in its entirety but also indicates GHF anomalies and could help in GHF exploration.

S0209. Estimation of Sill Thickness by Classifier Algorithms Using Measurement While Drilling (MWD) Data

Ozge Akyildiz (Norwegian University of Science and Technology),
Hakan Basarir (Norwegian University of Science and Technology),
Veena S. Vezhapparambu (Amrita Center for Wireless Networks and Applications),
Steinar Løve Ellefmo (Norwegian University of Science and Technology)
Room: 106 2022-08-30 14:35

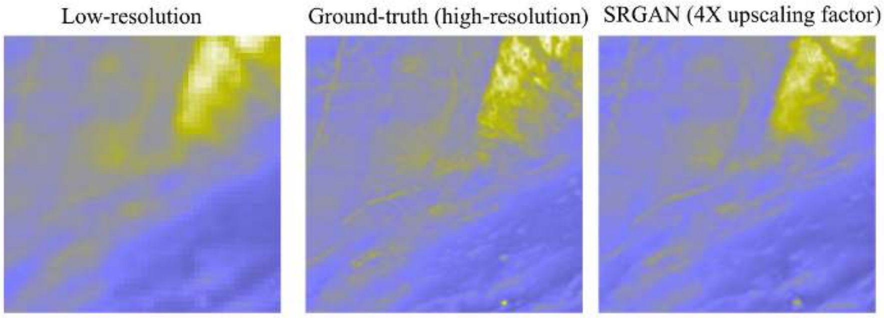
Drilling and blasting activity in quarries and open pit mines is carried out in a series of processes, including the determination of blast design parameters depending on the rock mass characteristics. In the studied industrial mineral open pit mine, the holes are first drilled through the sill or highly disturbed rock occurring due to the previous blasting. After this weak and loose formation, a more compact zone, unaffected from the previous blast, is drilled. In the mine the normal practice is to avoid charging the sill formation to improve the safety. In addition to the safety aspects, charging the sill leads to the escape of the explosive gases providing effective energy in the fragmentation process. Moreover, when the sill is relatively thin and constant thickness is assumed then large boulders requiring hammering may occur due to undercharged hole. Therefore, it is important to predict the sill thickness beforehand not only to avoid the safety issues but also to improve fragmentation process and cut costs for hammering.

In this study, the sill thickness was predicted using logistic regression, random forest and support vector machine as classifier modelling algorithms. For model construction, a previously published database including MWD data from the drilling rigs and measured sill thickness, via the use of OTV images from boreholes, was used. The performance of the models was investigated through performance indicators such as confusion matrix, accuracy score and R2. The model constructed using random forest classifier algorithm presented the highest performance. It is suggested that the developed model can be used for the assessment of sill thickness, leading to safer and more cost-efficient blast design.

S0210. SRGAN domain adaptation for super-resolving low-resolution aeromagnetic map: A case study in Québec, Canada

Mojtaba Bavandsavadkoohi (Centre Eau Terre Environnement (INRS-ETE)),
Matthieu Cedou (Centre Eau Terre Environnement (INRS-ETE)),
Martin Blouin (Geostack company),
Erwan Gloaguen (Centre Eau Terre Environnement (INRS-ETE)),
Shiva Tirdad (Geological Survey of Canada),
Bernard Giroux (Centre Eau Terre Environnement (INRS-ETE))
Room: 106 2022-08-30 15:00

For decades, aeromagnetic data have been acquired to guide mineral exploration as a cost-effective approach. These data are routinely used to enhance geological interpretations. Over the last decades, technological improvements allowed increasing the sensitivity of data acquisition systems and accuracy of navigation instrumentation, which resulted in higher resolution (HR) maps. Such higher resolution implies close lines of flight, which typically implies smaller area coverage. On the other hand, the vintage aeromagnetic surveys have high coverage but a much lower resolution. Geological interpretation for regions where only low-resolution aeromagnetic data (LR) are available remains a challenging task. Hence, we trained a deep neural network to address this problem by learning the statistical relations between collocated LR and HR airborne magnetic data. This trained network permits generating high-resolution images at locations where only LR magnetic data are available. This novel workflow relies on two practical machine learning components, which complement one another. First, we trained a Super-Resolution (SR) network based on Generative Adversarial Networks (GANs) in the source (training) domain for mapping LR images to HR images. Second, given this trained network, we apply domain adaptation, a subcategory of transfer learning, to generate HR images in the target (testing) domain where only LR images are available. We trained the network using HR images and their measured LR counterparts. Therefore, there are less discrepancies across source and target domain distributions. We evaluated the generalization of our SRGAN model on several regions of the Québec province aeromagnetic maps by comparing super-resolved GAN outputs with ground truth high-resolution aeromagnetic images. We computed the Structural Similarity Index (SSIM) to assess the spatial similarity between generated super-resolved images and HR ground truth images. The experimental results demonstrate that the SRGAN can generate super-resolution images up to 0.93 SSIM with HR ground truth in the cross-domain test.


Low-resolution
Ground-truth (high-resolution)
SRGAN (4X upscaling factor)

S0211. Speeding up the solution of the Richards equation through reduced order modeling

Teeratorn Kadeethum (Cornell University),
Daniel O'Malley (Los Alamos National Laboratory),
Hongkyu Yoon (Sandia National Laboratories)
Room: 106 2022-08-30 15:25

The Richards equation to model unsaturated water flow in porous media is highly nonlinear and contains complex relative permeability and capillary pressure relations. This high nonlinearity makes it very challenging to achieve the fast and stable numerical solutions of the Richards equation. To make the problem even more challenging, heterogeneous subsurface structures could cause a sharp discontinuity, resulting in difficulties in solving such a highly nonlinear system. In this work we propose the use of data-driven reduced order modeling developed by Kadeethum et al. [1] to speed up a nonlinear solver used for solving Richards' equation. We use a predicted state variable from the ROM as an initialization for the nonlinear solver. Our results show that our proposed approach could reduce the computational burden by approximately 60%.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

[1] Kadeethum, T., O'Malley, D., Fuhg, J. N., Choi, Y., Lee, J., Viswanathan, H. S., & Bouklas, N. (2021). A framework for data-driven solution and parameter estimation of PDEs using conditional generative adversarial networks. Nature Computational Science, 1(12), 819-829.

S0212. Feature subset selection for lineaments detection

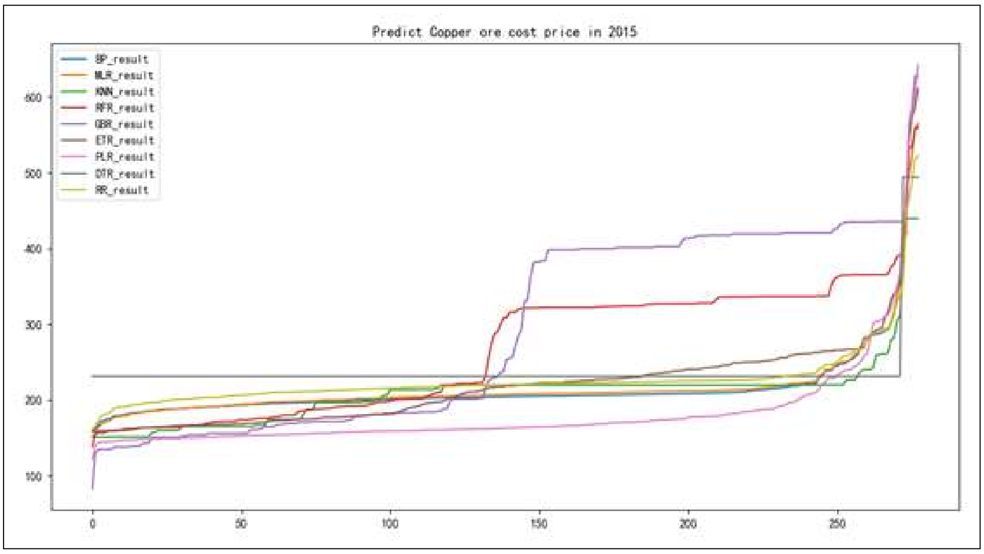
Bahman Abbassi (University of Quebec),
Li Zhen Cheng (Université du Québec en Abitibi-Témiscamingue)
Room: 106 2022-08-31 15:00

Geological lineament detection is a crucial task in mineral exploration. Conventionally, the process is time-consuming and demands challenging field geological operations in the regions with limited outcrop exposures. Interpretation of satellite imagery and geophysical data complement the detection of lineaments and add value to the structural geology of an area and subsequent mineral explorations. However, manual digitization of linear features is subjective to human errors and therefore lacks reproducibility. This study proposes an automated feature subset selection algorithm for geological lineament detection through machine learning and multi-objective optimization. The program integrates multiple satellite and geophysical datasets and extracts numerous features for subsequent lineament feature subset selection. We used a bi-objective optimization based on a Non-dominated Sorting Genetic Algorithm (NSGA-III) for machine learning optimization to simultaneously regularize the neural network structure and the number of input features. The results help geologists predict the lineaments from geophysical images in large areas with limited geological understanding.

S0213. Prediction of China's Copper Availability through a Machine Learning Framework

Yongguang Zhu (China University of Geosciences),
Jinqi Fan (China University of Geoscience),
Deyi Xu (China University of Geoscience)
Room: 106 2022-08-31 15:25

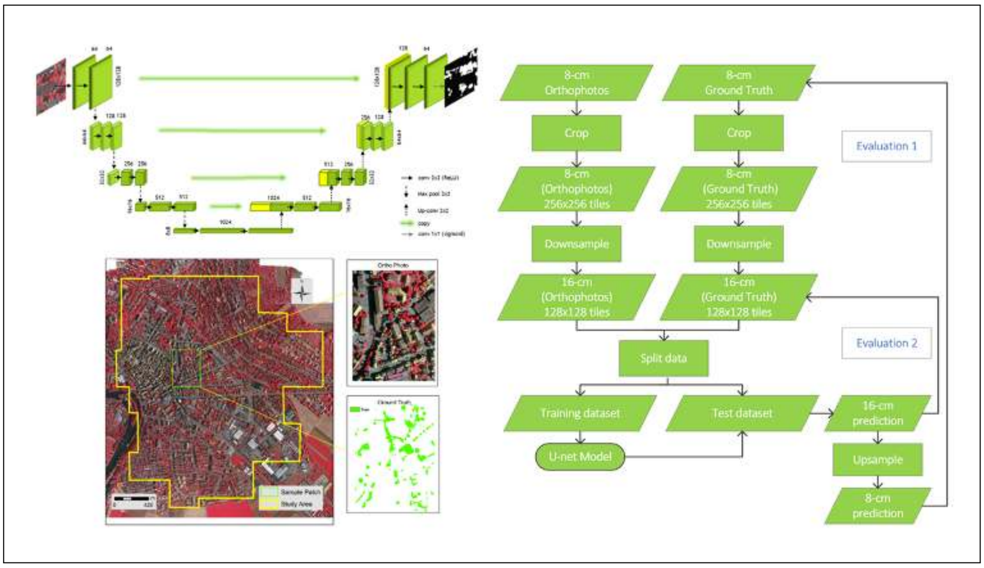
Copper is a kind of critical metal in great demand in the process of energy transition. The availability of copper is an important factor affecting energy transition. The traditional mineral resources availability evaluation needs to know the cost data of all mines. In fact, it is difficult to obtain cost data for all mines. In this paper, we propose a prediction method of mineral resources availability based on machine learning methods. The main innovation of this method is to predict the availability of all mines through a small number of samples based on the analogy idea of machine learning. We make an empirical study on the data of copper mines in China. Firstly, 12 indicators are selected from 57 indicators through random forest algorithm to predict China's copper availability. Then, nine kinds of machine learning methods are used to predict the availability of copper in China. Finally, the validity of the results is tested by KS and JS divergence.



S0214. Application and Evaluation of a Deep Learning Architecture to Urban Tree Canopy Mapping

Zhe Wang (University of Idaho)
Room: 106 2022-08-31 15:50

Urban forest is a dynamic urban ecosystem that provides critical benefits to urban residents and the environment. Accurate mapping of urban forest plays an important role in greenspace man-agement. In this study, we apply a deep learning model, the U-net, to urban tree canopy mapping using high-resolution aerial photographs. We evaluate the feasibility and effectiveness of the U-net in tree canopy mapping through experiments at four spatial scales—16 cm, 32 cm, 50 cm, and 100 cm. The overall performance of all approaches is validated on the ISPRS Vaihingen 2D Se-mantic Labeling dataset using four quantitative metrics, Dice, Intersection over Union, Overall Accuracy, and Kappa Coefficient. Two evaluations are performed to assess the model performance. Experimental results show that the U-net with the 32-cm input images perform the best with an overall accuracy of 0.9914 and an Intersection over Union of 0.9638. The U-net achieves the state-of-the-art overall performance in comparison with object-based image analysis approach and other deep learning frameworks. The outstanding performance of the U-net indicates a possibility of applying it to urban tree segmentation at a wide range of spatial scales. The U-net accurately recognizes and delineates tree canopy for different land cover features and has great potential to be adopted as an effective tool for high-resolution land cover mapping.



S03 Random patterns and shapes in spatio-temporal data

Aila Sarkka (Chalmers University of Technology),
Radu Stoica (Université de Lorraine)

This session aims to bring together specialists in point processes, spatial statistics, and stochastic geometry, who have a common research question: characterisation and detection of patterns and structures in spatio-temporal data. The complexity of the available data today requires rigorous stochastic methodologies based on probabilistic modelling, simulation algorithms, and Bayesian inference, in order to obtain reliable and interpretable results. The purpose of this session is to present some new mathematical methods which have been developed for answering questions in environmental sciences, forestry, image analysis, stereology, astronomy and other fields, and which can be valuable additions in the methodological toolbox for the statistical analysis of geological data.

S0301. Nonparametric testing of the covariate significance under the presence of nuisance covariates for a spatial point pattern

Tomas Mrkvicka(Faculty of Economics, University of South Bohemia, Czech Republic)
Room: 105 2022-08-30 14:35

Determining the relevant spatial covariates is one of the most important problems in analyzing point patterns. The parametrical methods may lead to a wrong result (the statistical tests can be liberal), especially when the model of interaction between points is wrongly chosen. Also, the choice of the parametric form of the point pattern intensity can influence the selected significant covariates. Therefore, we propose a fully nonparametric method for identifying significant covariates. We also propose a semiparametric method that uses the parametrical form of the intensity but does not assume any model for the point interaction, which we believe is the more serious issue. Our methods maintain the apriori chosen significance level (even the semiparametric one in a case of a wrong parametric model), and their powers are comparable with the powers of parametrical methods in cases of correct use of the parametrical models. When the parametrical model for the intensity is incorrectly chosen, they reach higher powers.

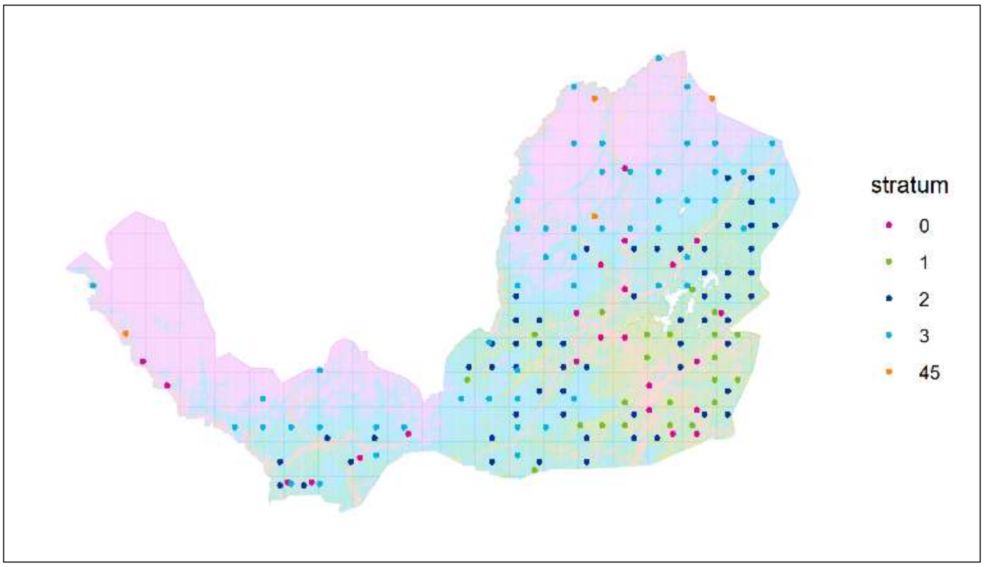
The methods are based on the newly introduced covariate weighted residual measure and the Monte Carlo tests. We also define a correlation coefficient between a point pattern and a covariate and a partial correlation coefficient with the presence of nuisance covariates in order to quantify the level of spatial correlation.

S0302. Spatial two-phase systematic cluster sampling with stratification

Juha Heikkinen (Natural Resources Institute Finland (Luke))
Room: 105 2022-08-30 15:00

Spatially systematic cluster sampling can be highly cost-efficient in large-scale surveys of the environment. If population-level auxiliary data is available prior to sampling, it may allow further improvements in efficient allocation of field measurements. Stratified sampling is a robust way to utilize auxiliary data, and with Neyman allocation higher sampling intensity can be allocated to more variable parts of the survey region. However, it is not a trivial task to combine the three – systematic sampling grid, clustering of sampling points, and stratification – without sacrifices. For example, how to stratify without breaking the clusters? A way to do this is presented in this talk, in the context of national forest inventory. The efficiency is compared to the more straightforward approach, which replaces systematic sampling with spatially balanced sampling (Grafström et al. 2012).

Grafström, A., Lundström, N.L.P. and Schelin, L. (2012), Spatially Balanced Sampling through the Pivotal Method. Biometrics, 68: 514-520. https://doi.org/10.1111/j.1541-0420.2011.01699.x



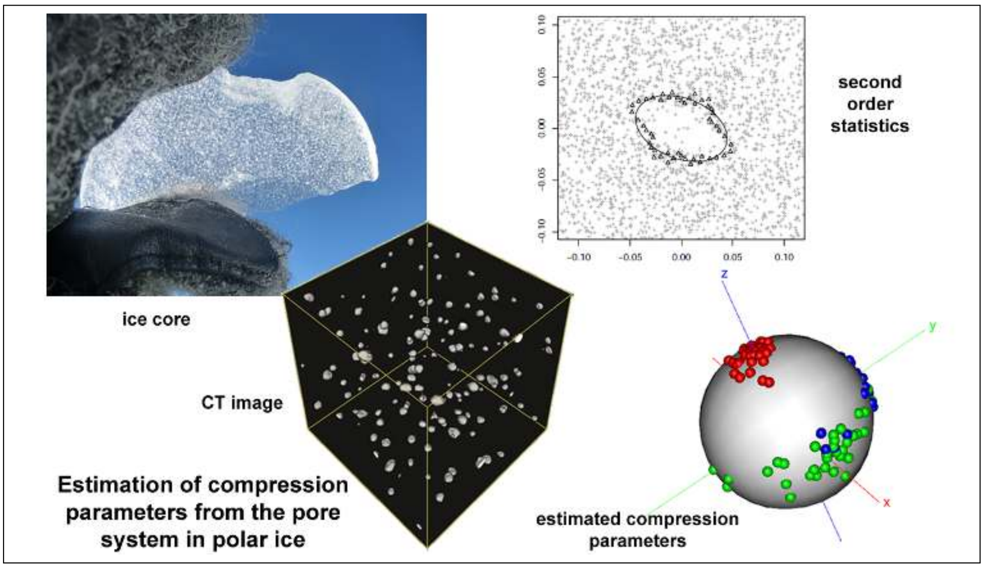
S0303. Estimation of compression parameters from the pore system in polar ice

Claudia Redenbach (TU Kaiserslautern),
Johannes Freitag (Alfred-Wegener Institute for Polar and Marine Research),
Martina Sormani (TU Kaiserslautern),
Tuomas Rajala (Natural Resources Institute Finland),
Aila Särkkä (Chalmers University of Technology)
Room: 105 2022-08-30 15:25

We discuss statistical methods for the analysis of anisotropic point processes which are motivated by the investigation of the pore system in polar ice cores. These cores are drilled from the Antarctic and Greenlandic ice sheets and consist of compacted snow. During the compression process, air pores are isolated within the ice. The system of these pores can be analysed based on 3D image data obtained by micro computed tomography.

We study the 3D point patterns formed by the center locations of air bubbles. Interpreting the system of bubble centres as a realisation of a regular point process subject to geometric anisotropy, preferred directions and strength of compression can be estimated. For this purpose, second order methods from spatial statistics are applied.

In this talk, we will illustrate the approach and present a depth profile of compression parameters obtained for the RECAP (REnland ice CAP project) ice core from Greenland.



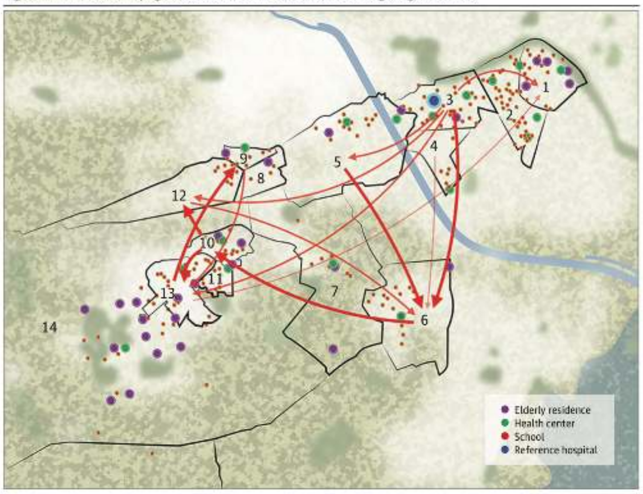
S0304. Trends in Incidence and Transmission Patterns of COVID-19 in Valencia, Spain

Adina Iftimi (University of Valencia)

Room: 105 2022-08-30 16:30

Studies have described SARS-CoV-2 transmission based on online public data, but limited information is available on local COVID-19 transmission patterns. We present a single-center epidemiological cohort study of patients with COVID-19 from the start of the pandemic on February 19 until August 31, with SARS-CoV-2 carried out at University General Hospital in Valencia. The study includes all consecutive 2020. The primary outcome was the characterization of dissemination patterns and connections among the 20 neighborhoods of Valencia during the outbreak. To recreate the transmission network, the inbound and outbound connections were studied for each region, and the relative risk of infection was estimated. This study of local dissemination of SARS-COV-2 revealed nonevident transmission patterns between geographically unconnected areas. The results suggest that tailor-made containment measures could reduce transmission and that hospitals, including testing facilities, play a crucial role in disease transmission. Consequently, the local dynamics of SARS-CoV-2 spread might inform the strategic lockdown of specific neighborhoods to stop the contagion and avoid a citywide lockdown.

Figure 4. Functional Propagation Network and Interactions Among Neighborhoods



The thickness of an arrow indicates the strength of the propagation link; thicker arrows represent stronger links, whereas thinner arrows represent weaker links.

S0305. Statistical learning for point processes

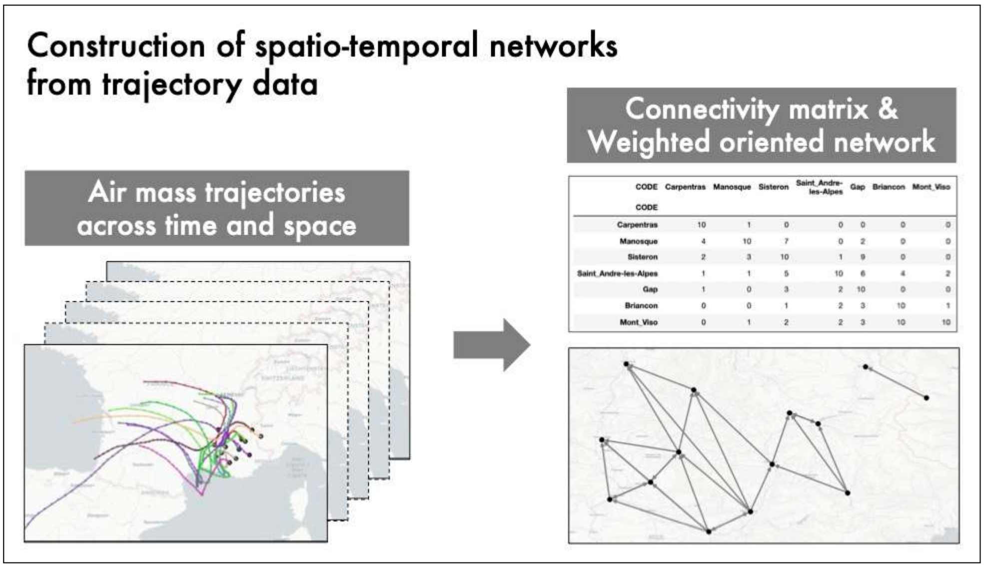
Ottmar Cronie (Chalmers University of Technology),
Mehdi Moradi (Public University of Navarra,),
Christophe Biscio (University of Aalborg, Denmark)
Room: 105 2022-08-30 16:55

In this talk we present the first general statistical learning framework for point processes in general spaces. Our approach is based on the combination of two new concepts, namely: i) point process prediction errors, which are measures of discrepancy/prediction-accuracy between two point processes, and ii) point process cross-validation (CV), which we here define through point process thinning. The general idea is to carry out fitting by predicting CV-generated validation sets using the corresponding training sets; the accuracy is measured by means of the prediction errors. Here we will discuss various theoretical properties of our approach and discuss different settings to which it may be applied. We restrict ourselves to the case where the CV procedure is obtained through independent thinning and we apply our statistical learning methodology to a typical spatial statistical estimation setting, showing numerically that our statistical learning approach significantly outperforms the state of the art in terms of mean (integrated) squared error.

S0307. Construction of spatio-temporal networks from trajectory data - Application to infer tropospheric networks

Samuel Soubeyrand (INRAE - BioSP)
Room: 105 2022-08-30 17:45

Tropospheric movements can be represented by three-dimensional trajectories of air masses connecting distant areas of the Earth. Such connection between distant areas is essential to infer and predict the dispersal of entities that air masses may carry, e.g., volcanic ash, dust, radioactive chemical elements and micro- or small-biological organisms. We proposed a mathematical formalism to construct spatial and spatiotemporal networks where the nodes represent the subsets of a partition of a geographical area and the links between them are inferred from sampled trajectories of air masses passing over and across them. We proposed different estimators of the intensity of the links, relying on different bio-physical hypotheses and covering adjustable time periods. This construction leads to a new definition of spatiotemporal networks characterized by adjacency matrices giving, e.g., the probability of connection between distant areas during a chosen period of time. Once the network is inferred, its properties can be derived, it can be used as input in models of propagation of airborne pathogens for example, or it can be used as explanatory variables for understanding random spatial and spatio-temporal patterns. Beyond the construction of tropospheric networks, our approach could be applied to other types of trajectories, such as animal trajectories, to characterize connectivity between different components of the landscape hosting the animals.



S0308. False discovery rate envelopes with local spatial correlation and other applications

Mari Myllymäki (Natural Resources Institute Finland (Luke))
Room: 105 2022-08-31 09:50

Recently, we developed a global envelope test which provides a global envelope, i.e. the acceptance region for testing with a functional test statistic, under the control of family-wise error rate (FWER). The direct visualization of the test results through the acceptance region shows the reasons for the rejection of the tested global null hypothesis and helps to interpret the results in details. This method is based on resampling and allows for a very general application while controlling FWER. It has been used already in many applications. However, in functional tests, it is often essential to obtain not only if the global test is significant but also to estimate the whole domain which is responsible for the rejection, i.e., the local inference. A popular and powerful control for local inference is the false discovery rate (FDR). Also under the control of FDR, it is of great practical importance to visualize the functional test statistic together with its rejection or acceptance region. Therefore, we propose a graphical envelope that controls FDR and detects the outcomes of all individual hypotheses by a simple rule, similarly as the FWER envelopes: the hypothesis is rejected if and only if the empirical test statistic is outside of the envelope. The FDR envelopes are explained and illustrated through applications, particularly for studying local spatial correlations in soil data. The talk is based on joint work with Tomáš Mrkvička.

S0309. Marked point processes for astronomical applications

Elmo Tempel (UT Tartu Observatory)
Room: 105 2022-08-31 10:15

I will present the Bisous model, a novel marked point process with interactions to detect and characterize structures in the input data.

We have appliced the marked point processes model to the galaxy redshift surveys to detect the cosmic filaments. The developed model is compared with other methods in the field and it is found to be one of the best methods for observational data. The detected filamentary structures have been used in many astrophysical studies. One of the latest discovery was the largest rotating system in the Universe which was published in Nature Astronomy.

Additionally we have used similar marked point process model to optimize the observing tiling pattern for the upcoming astronomical surveys. This was specifically developed for the upcoming 4MOST survey, which is one of the next generation astronomical surveys.

In my talk I will shortly present the developed marked point process model and describe the applications in astrophysical context.

S0310. Object-valued marked point processes

Matthias Eckardt (Humboldt-Universität zu Berlin)
Room: 105 2022-08-31 10:40

The analysis of marked spatial point processes, where discrete-, interger- or real-valued additional information is available for each event of a random point constellation has become a highly attractive field of research in different disciplines. Due to the immense technological progress and increase in storage capacities, researchers are now facing an ever-increasing amount of even more complex spatial point process scenarios, where the points and/ or the marks live on more complex domains. While extensions of spatial point processes to to different settings, i.e. network structures or the sphere, have been proposed in recent years, extensions of spatial point process scenarios where the marks themselves are data objects living on more complicated spaces (i.e. object-valued marks) rather than scalar-valued quantities, remain extremely limited. In particular, there is a lack of suitable summary characteristics which account for the specificity and nature of the marks.

This talk will introduce different example of spatial point process with object-valued point attributes and discuss suitable mark characteristics to such non-scalar mark scenarios.

S0311. DRlib: a C++ library for point processes simulation and inference

Didier Gemmerle (Université de Lorraine),
Radu Stefan Stoica (Université de Lorraine),
Christophe Reype (Inria)
Room: 105 2022-08-31 11:05

In this poster we will present a C++ library whose goals are on the one hand to implement the generation of realizations of Strauss and Area Interaction type point processes with the Markov Chain Monte Carlo method of Metropolis-Hasting and on the other hand to implement the ABC Shadow method.

Our architecture is composed of three concepts : a ”model”, a ”sampler” and a ”realization”. These three concepts constitute the mother classes of our class diagram. From these parent classes are derived specialized classes that take into account the specifics of the Strauss, Area Interaction and ABCshadow algorithms.

Our poster will present examples of instantiations of our specialized classes StraussFixedRadius, StraussRandomRadius, AreaInteractionFixedRadius, AreaInteractionRandomRadius and the parameters to be used.

Results for different values of intensities and interaction parameters will be presented in the form of realization images as well as their statistics. Our library supports constant or random ray processes and allows the manipulation of point configurations of several thousand points.

Our poster will present the use of the ABCshadow method to estimate the parameters of supposed realizations from a Strauss process, an areainteraction process or a mixture of both.

A very simplified class diagram of our library will give an overview of the classes and their dependencies.

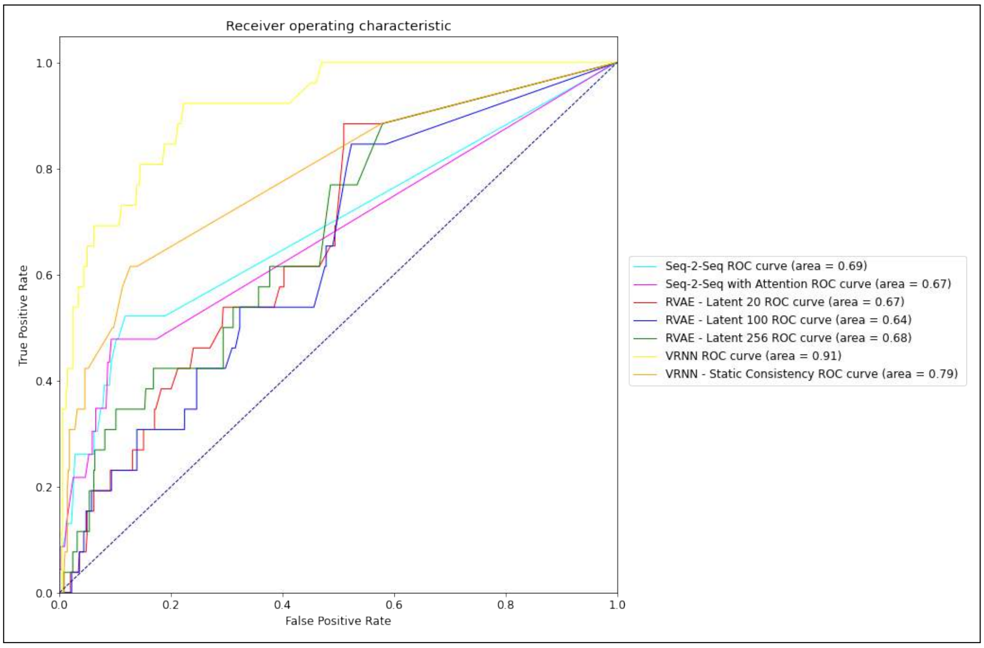
This work constitutes the reliable base on which a part of our future work can be based. Perspectives on our future developments concerning optimizations will be briefly presented.

This work enriches and further develops of the ideas proposed by the MPPLIB C++ library and the R spatstat package built by M. N. M. van Lieshout and A. J. Baddeley together with their co-authors, respectively.

S0312. Detecting Abnormal Maritime Trajectories with Recurrent Neural Networks

Kristoffer Vinther Olesen (Technical University of Denmark),
Line Katrine Harder Clemmensen (Technical University of Denmar),
Anders Nymark Christensen (Technical University of Denmar)
Room: 105 2022-08-31 11:07

Increasing worldwide maritime traffic makes maritime safety and security of growing importance. Surveillance operators monitor and predict emerging critical situations based on a wide range of data sources from many vessels within a large sea area. This makes operators prone to mistakes due to cognitive overload, time pressure, fatigue, ect. To support operators, methods and systems capable of performing anomaly detection have received increased attention. Lately, a few methodologies applying Deep Learning techniques have been proposed for analyzing maritime trajectories. In this work, we compare the performance of unsupervised anomaly detection based on reconstruction/prediction using four different Recurrent Neural Network architectures. We compare Seq-2-Seq methods trained for trajectory prediction, Recurrent Variation AutoEncoder (RVAE), and Variational Recurrent Neural Network (VRNN) trained for trajectory reconstruction. We evaluate the performance, measured by AUC, using trajectories extracted from Automatic Identification System (AIS) data around the Danish island of Bornholm from December 13th 2021. On this day, there was a collision accident that caused a few vessels to make abnormal route deviations as well as Search-and-Rescue operations involving several ships. We find poor performance of all suggested approaches for detection of real-life anomalies. VRNN methods significantly outperform Seq-2-Seq and RVAE methods, but still suffer from too many false positives to be practical in operational use. VRNN methods detect outliers related to Search-and-Rescue operations but struggle to detect ships deviating from the regular route or simply sailing in a straight line. However, these kinds of behaviors are among the first detections for RVAE methods. We illustrate that the poor performance is likely due to the latent encodings mainly focusing on global behavior like the chosen route through the Region of Interest. These global behavior encodings can be achieved in VRNN by introducing recently proposed static consistency enforcing losses at the cost of reduced performance.


Receiver operating characteristic
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
Seq-2-Seq ROC curve (area = 0.69)
Seq-2-Seq with Attention ROC curve (area = 0.67)
RVAE - Latent 20 ROC curve (area = 0.67)
RVAE - Latent 100 ROC curve (area = 0.64)
RVAE - Latent 256 ROC curve (area = 0.68)
VRNN ROC curve (area = 0.91)
VRNN - Static Consistency ROC curve (area = 0.79)

S0313. Detecting large-scale structure of the Universe using photometric data with the Bisous model

Moorits Mihkel Muru (Tartu Observatory),
Elmo Tempel (UT Tartu Observatory)
Room: 105 2022-08-31 11:09

The mass in the Universe forms a dynamical large-scale structure that consists of high-density clusters of galaxies, curvilinear filaments between clusters, and large, almost empty voids. As there is no standard definition for these elements of large-scale structure, there are many different approaches for finding them. The Bisous model is a stochastic method that uses a marked point process and applies geometric rules to detect filaments from observational data. This model has been shown to work well with spectroscopic data, i.e. data with precise positions for galaxies. There are about 100 times more available photometric data, i.e. data with considerable uncertainty in the distance measure. We show that including photometric data improves the cosmic web detected by the Bisous model. In this study, we create a mock catalogue of photometrical targets from dark matter-only simulation by adding random shifts to the galaxies' distances and assigning uncertainties. We compare the Bisous model results using different spectroscopic, photometric, and mixed samples. Including photometric data improves the recall compared to the reference values and has a false discovery rate $<5\%$. Using mixed datasets of spectroscopic and photometric galaxies to obtain higher galaxy number density improves the completeness of the filamentary network detected by the Bisous model.

S0314. Pattern analysis and estimation of parameters for the HUG point process in order to characterize sources in hydrochemical data

Christophe Reype (Inria),
Antonin Richard (Université de Lorraine, CNRS, GeoRessources),
Madalina Deaconu (Université de Lorraine, CNRS, GeoRessources),
Radu Stoica (Université de Lorraine)
Room: 105 2022-08-30 17:20

Groundwaters are often a mixture of several sources. However determining the composition of sources from hydrochemical data is challenging. This determination is a pattern detection problem in a highly multidimensional space of hydrochemical parameters. The HUG model is a point process able to detect sources in such data. This is done via a simulated annealing procedure maximising a posterior law that combines the HUG model distribution with prior knowledge of the model parameters. The prior model was integrating chemical knowledge, it was tunned on simulated data and finally applied on real data, embedded within the posterior model. The simulated annealing is based on a Metropolis Hastings within Gibbs dynamics in order to deal with the multidimensional character of the problem. The purpose of this work is to present the performances of the Approximate Bayesian Computation (ABC) Shadow algorithm in order to improve the quality of the prior embedded within the posterior model. Results on synthetic and real data are shown. Conclusions and perspectives are also presented.

S04 Inverse problems

Thomas Bodin (Univ. Lyon),
Kerry Gallagher (Univ. Rennes)

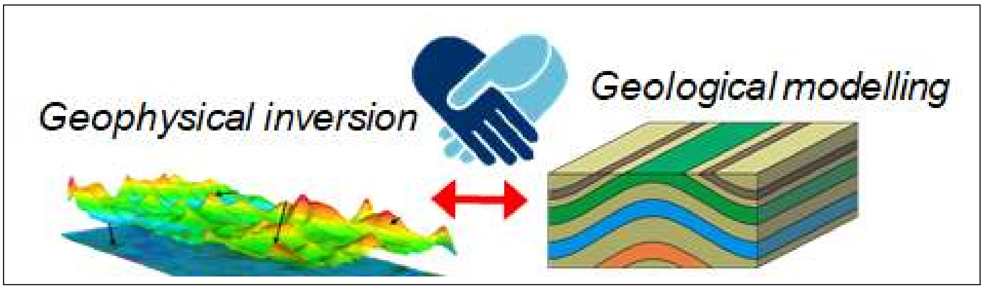
Numerous advances in the Earth sciences are driven by innovative inverse modelling techniques, and the ever-increasing power of computational resources. To promote further progress, this session offers a platform to discuss and learn about current and future approaches to solve (nonlinear) inverse problems in the geosciences. Examples of novel applications are also very welcome. Of particular interest are contributions focusing on:

- Seismic tomography and full-waveform inversion at all scales,
- Uncertainty analysis,
- Bayesian inference,
- Optimization methods,
- Joint inversion of disparate datasets,
- Multi-scale, multi-parameter inversion,
- Strategies for exploiting massive data volumes,
- Effective medium theory, downscaling, and inverse homogenization.

S0401. An iterative inversion scheme to reconcile implicit geological models and geometric geophysical inverse problems

Jeremie Giraud (RING, GeoRessources / ENSG, Université de Lorraine),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS),
Lachlan Grose (Monash University),
Paul Cupillard (Univ. Lorraine)
Room: auditorium 2022-08-31 09:50

The quantitative reconciliation between geological and geophysical data is an essential but often overlooked aspect to reduce subsurface uncertainty and increase the predictivity of geomodels. We present a method that integrates implicit geological modelling in a geometrical geophysical inversion process which considers each petrophysical interface as a level set. Our objective is to encourage geological plausibility in the results of deterministic geophysical inversion to recover the geometry of interfaces between rock units. By interleaving geophysical inversion steps and geological model updates, we explore two possibilities to reach this goal. Firstly, we introduce a geological correction term to reduce geological inconsistencies at each iteration based on the current geophysical inversion result. This is achieved by calculating the geological model that is closest to the model obtained by geophysical inversion by adding the interfaces of the geophysical model to the set of geological interpolation data. Secondly, we incorporate a geological modelling component directly into the objective function of the geophysical inverse problem. In this fashion, geological constraints become an integral part of geophysical inversion. This allows geophysical inversion to combine geological concepts and measurements together with geophysical data. After introducing the main theoretical aspects of the proposed approach, we investigate synthetic cases illustrating the capability of the method. Results indicate that our approach effectively steers inversion iteratively towards geologically consistent models and may therefore be applied to field data. They also suggest that while the use of a geological correction term is efficient at removing comparatively fine-scale geological inconsistencies, using geological modelling in the definition of the inversion's objective function is more effective to enforce geological rules at coarser scales.



S0402. New opportunities for Monte Carlo inversion from generative models

Matthias Scheiter (Australian National University),
Andrew Valentine (Durham University),
Malcolm Sambridge (Australian National University)
Room: auditorium 2022-08-31 10:15

In geophysics, available data are generally sparse, incomplete, and ambiguous. When inferring models from these data, this results in unfavourable model properties such as high uncertainties and significant non-uniqueness. These challenges can be overcome by ensemble-generating inversion methods such as Markov chain Monte Carlo. The goal is to build a large collection of suitable models that together characterise uncertainty and non-uniqueness of the properties of interest. Though powerful, Monte Carlo methods have significant drawbacks such as long computational times and a large amount of digital outputs. The generation, handling, and distribution of model ensembles is challenging and new approaches are necessary to improve the user experience with Monte Carlo methods.

Generative models, a family of machine learning models that have attracted much attention in recent years, are one way out. They have the ability to build a parametric representation from a collection of samples, thereby enabling compression and enhancement of an ensemble. This leads to manifold advantages such as improved solution of numerical integrals which are ubiquitous in Monte Carlo inversion, and suggests possibilities to overcome the curse of dimensionality. In addition to these opportunities in dealing with existing ensembles from Monte Carlo studies, generative models offer several potential avenues during the ensemble-building process itself. These include the potential for convergence assessment during the sampling process and the possibility for building adaptive proposal distributions to make the sampling process more efficient. Many different generative models exist, and care has to be taken in the choice of a particular type, architecture, training strategies, and other hyperparameters. When overcoming these challenges, generative models promise to revolutionise the way that Monte Carlo studies in geophysical inversion are conducted in the future. This presentation explores the interaction between ensemble-based methods and generative models, and demonstrates progress towards more efficient strategies for Monte Carlo inversion.

S0403. Inverting an Object Based geostatistical facies model with Ensemble Smoother Mutiple Data assimilation technique.

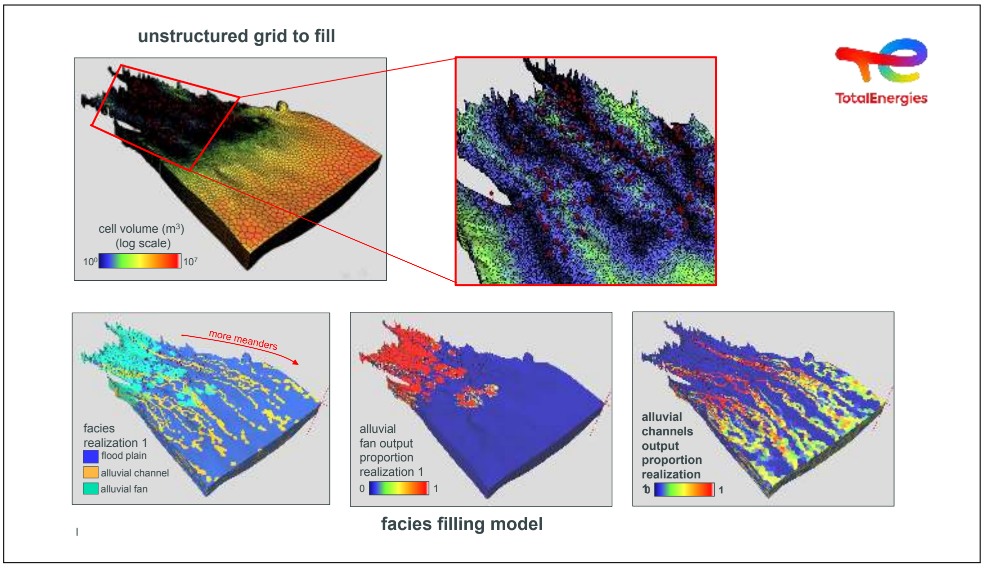
Pierre Biver (TotalEnergies),
Augustin Gouy (GeoRessources - Université de Lorraine),
Ahanita Abadpour (TotalEnergies),
Jessica Franco (TotalEnergies),
Abbas Zerkoune (TotalEnergies)
Room: auditorium 2022-08-31 10:40

During the last decade, new inversion techniques (Ensemble Kalman filters, Ensemble Smoother, ...) have emerged which can be very useful for assisted history match of complex problems. They are based on an ensemble of geo-models. These geo-models are simulated dynamically (initial state) and the mismatch regarding dynamic observations is calculated. Subsequently, the link between geo-models' parameters and dynamic mismatch is defined with a Kalman gain matrix computation. Then geo-models underlying parameters are updated and a new state is computed. By repeating the procedure (called dynamic data assimilation), we can converge to a set of calibrated models.

Concerning facies modeling, these inversion techniques are very efficient with truncated gaussian related facies models. For this kind of models, the underlying gaussian fields are updated with the Kalman gain matrix and the corresponding facies model is rebuilt from these updated underlying gaussian fields. However, for other facies models and specifically object-based facies models, the update is not so trivial and problematic. This fact strongly limits the application domain of assisted history match techniques based on Kalman gain.

In the paper, an innovative method is presented to actualize an object-based facies model in the framework of this assisted history match techniques. The idea is relatively simple: each individual object of one realization is coupled with its homolog in another realization; by doing so we can invert object coordinates and sizes (thickness and width) with Kalman gain matrix. The tricky aspects are to preserve conditioning data and to be able to invert the model on a limited area if required. The method is applied on a synthetic five spot example. Results are very encouraging.

Conclusions are future works are proposed based on this first experiment results.


unstructured grid to fill
TotalEnergies
cell volume (m³)
(log scale)
10⁰
10⁷
more meanders
facies
realization 1
flood plain
alluvial channel
alluvial fan
alluvial
fan output
proportion
realization 1
0
1
alluvial
channels
output
proportion
realization
0
1
facies filling model

S0404. Stochastic joint inversion to improve model uncertainty quantification in Quaternary aquifers

Alexis Neven (University of Neuchâtel),
Ludovic Schorpp (University of Neuchâtel),
Philippe Renard (University of Neuchâtel)
Room: auditorium 2022-08-31 11:05

Estimation of uncertainty when dealing with (hydro)-geological models has become capital. These models are often based on different data, such as prior knowledge, typical parameters databases, geophysical data, or hydrogeological measurements. However, classical data integration usually occurs in successive steps, usually with a separate geophysical and hydrological inversion, with poor uncertainty propagation. Moreover, the final model can even sometimes disagree with data integrated at an earlier step. In this study, we combine a stochastic hierarchical geological model generator with joint stochastic inverse algorithms. The geological and parameter models are first generated using a hierarchical geostatistical approach allowing to respect sedimentological principles. We then investigate the advantages of performing an inversion relying only on geophysical data, only on hydrological data, and on the combination of both through a joint inversion. All 3 combinations of data and three different stochastic inversions are compared. This study demonstrates how aggregating different data types through joint inversion can significantly reduce the uncertainty on the final model. Furthermore, this approach has the strong advantage to account directly for the various types of uncertainties coming from the different data types and prior information. This methodology is agile, easy to implement, open-source, and could be applied to a wide range of situations. We believe that such improvements could greatly improve decision-making when dealing with hydro-geological problems.

S0405. Implementation of a Markov-Chain Monte Carlo algorithm for high temperature thermal history inversion using the Fast Grain Boundary model

Guillaume Siron (University of Bologna),
Chloe Bonamici (University of Wisconsin-Madiso)
Room: auditorium 2022-08-31 11:30

Retrieving time-tempearture (t-T) histories of metamorphic rocks is vital to understanding the geodynamics of orogens and subduction zones. While many thermochronological systems have been developed for low to medium temperatures (< 400 °C), retrieving t-T histories at higher temperature remains complicated. Here we present a new Markov chain Monte Carlo (MCMC) algorithm for inversion of the Fast Grain Boundary model1, which couples equilibrium fractionation of oxygen isotopes between minerals and intragrain oxygen isotope diffusion within minerals. The MCMC approach uses a Metropolis-Hastings sampler that randomly selects a point in the t-T history and then randomly modifies that temperature using a normal distribution centered on 0 with a standard deviation of 1, multiplied by a scale factor. A uniform prior is assumed and computed as the inverse of the temperature span for the thermal history. The number of iterations has been set to 2000 with 1000 iterations for the burn-in. The scale factor has been set to 50. These parameters were selected by testing the MCMC algorithm for synthetic data, either computed from a linear cooling t-T history or a linear cooling t-T history with a superimposed heating spike. The starting profile with the greatest deviation from the actual cooling history converged after >600 iterations, necessitating the burn-in of 1000 iterations. The model successfully reproduces linear t-T histories and identifies the presence of a heating spike, though not always at the correct temporal location of the spike, especially for starting profiles far from the actual t-T history. FBG inversion with MCMC can improve reconstructions of high temperature thermal evolution, and thus our understanding of the earliest stages of exhumation of deep orogenic rocks and subducted rocks.

[1] Kropf, Bonamici, Borchers (2021) Computers & Geosciences 151, 104753.

S0406. Efficient inversion with complex geostatistical priors using neural transport

Shiran Levy (University of Lausanne),
Eric Laloy (Belgian Nuclear Research Center),
Niklas Linde (University of Lausanne)
Room: auditorium 2022-08-31 11:55

We study the combination of a neural transport routine consisting of inverse autoregressive flows (IAF) and variational inference (VI) on the latent variables of deep generative models. This approach may offer an efficient alternative to Markov chain Monte Carlo (MCMC) sampling and more appropriate uncertainty quantification compared with classical gradient-based deterministic inversions. Variational inference seeks to approximate a target distribution parametrically for a given family of distributions by solving an optimization problem. Recent studies show that the approximate distribution, which is limited by the chosen parameterized family of distributions, can become more flexible by parametrizing it using a neural network in the form of a series of transport maps (also referred to as flows). In our study we use IAFs as our neural transport map to push samples from a standard normal distribution through a series of invertible transformations onto a variational density approximating the unnormalized posterior of interest. The parameters of the IAFs are learned by minimizing the Kullback-Leibler divergence between the variational density and the unnormalized target posterior distribution. We consider inference in the context of two different deep generative models: generative adversarial network (GAN) and variational autoencoder (VAE) whose realizations depend on their low-dimensional latent variables. Previous attempts to perform gradient-based deterministic inversion on the latent variables of GANs of the same architecture were proven unsuccessful as the learned GAN-transform is highly nonlinear with complex topology. Our results obtained on channelized subsurface models and a nonlinear geophysical forward solver suggest that the combined IAF-VI approach recovers the true model reliably, particularly when using VAE, and needs a few hundred up to one thousand iterations. It also provides an uncertainty quantification as a representation of the posterior probability density function is learned compared to deterministic gradient-based methods and at a much lower computational cost compared to MCMC sampling.

S0407. Hydrogeological multiple-point statistics inversion by adaptive sequential Monte Carlo

Macarena Amaya (University of Lausanne),
Niklas Linde (University of Lausanne),
Eric Laloy (Belgian Nuclear Research Center)
Room: auditorium 2022-08-31 11:57

Markov chain Monte Carlo (MCMC) methods may fail to properly explore the posterior probability density function (PDF) given realistic computational times, especially when the inverse problems are strongly non-linear and high-dimensional. Particle methods present an alternative, we focus on adaptive sequential Monte Carlo (ASMC), which is an extension of annealed importance sampling (AIS). These methods approximate the posterior PDF together with the evidence (the key quantity in Bayesian model selection) using the states and weights of a population of evolving particles. To do so, they rely on importance sampling performed over a sequence of intermediate distributions, known as power posteriors, that link the prior and posterior PDF. The advantages of ASMC over AIS is that it adaptively tunes the tempering schedule and performs resampling of particles when the variance of the particle weights becomes too large. We consider a challenging synthetic groundwater transport inverse problem with a categorical channelized 2D hydraulic conductivity field designed such that the posterior facies distribution is bimodal. Conditional multi-point statistics (MPS) simulations are used to iteratively propose new models. We focus on the ability of ASMC to explore the posterior PDF and compare results with those obtained with parallel tempering (PT), a state-of-the-art MCMC inversion approach that runs multiple interacting chains targeting different power posteriors. For a similar computational budget, the ASMC implementation outperforms the results obtained by PT as the models fit the data better and the reference likelihood value is contained in the ASMC sampled likelihood range, while this is not the case for the PT results. Moreover, we show that ASMC partly recovers both posterior modes, while none of them is recovered by PT. Additionally, we demonstrate how the power posteriors obtained by ASMC can be used to visualize the influence of the assumed data errors on the posterior means and variances.

S0408. CoFI - Linking geoscience inference problems with tools for their solution

Jiawen He (Australian National University),
Hannes Hollmann (Australian National University),
Malcolm Sambridge (Australian National University),
Juerg Hauser (CSIRO, Deep Earth Imaging Future Science Platform),
Andrew P Valentine (Durham University)
Room: auditorium 2022-08-31 11:59

Inference problems in the geosciences vary significantly in size and scope, from 1D regression of geochemical data, to building 3D models of Earth's interior structure. As such, the combination of datasets and the approaches used for solving are often highly problem-specific. Some researchers develop inversion and parameter estimation algorithms that suit their needs and wonder where else they could be applied. Others focus on developing new and flexible forward models of Earth phenomena and want a complementary inversion algorithm that fits their needs. Many more of us have data and questions to answer and need both.

Our aim with CoFI, the Common Framework for Inference, is to build a community collaboration using open-source platform agnostic infrastructure to interface geoscience inference problems with the tools required to solve them. In addition by creating an extensive set of demonstration problems and worked examples, we hope to support education at all levels in this space. CoFI will initially take the form of a Python package able to interface with inference algorithms from different sources. In addition, we are building an Inversion Test Suite which collects examples from many disciplines within geoscience and elsewhere. The connection points between the two is a common standard that is flexible and capable enough to accommodate a variety of inference problems which can be recognised by various solvers that comply with this same common framework.

Having the basic setup and several examples in place already, we hope to encourage more forward examples and inversion algorithms to be developed and be contributed to this modular designed framework, with the lowest possible barriers to participation.

S0409. Overcomplete Tomography: A sparsity constrained approach to inversion

Buse Turunctur (Research School of Earth Sciences, Australian National University),
Andrew Valentine (Durham University),
Malcolm Sambridge (Australian National University)
Room: auditorium 2022-08-31 15:00

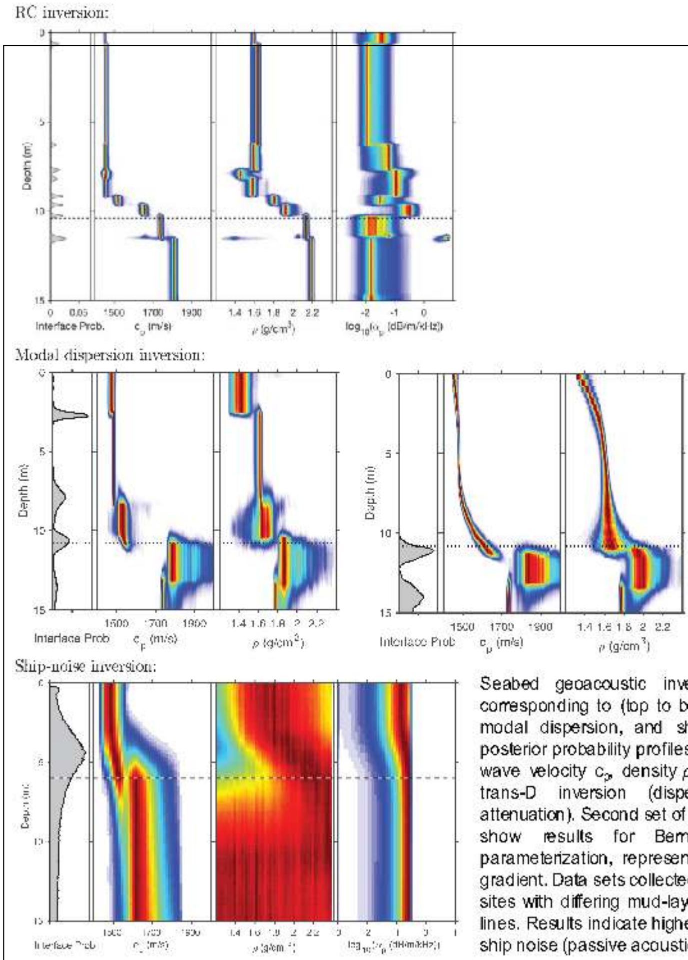
In tomographic problems, a preferred method to construct parametrized models of the indirectly constrained physical property is the regularised least-squares inversion. However, it has a few drawbacks, such as: (i) the regularization imposed during the inversion tends to give a smooth solution, which will fail to reconstruct a multi-scale model well or detect sharp discontinuities, (ii) it requires finding optimum control parameters, (iii) it does not produce a sparse solution. It was recently proved with the approach 'compressive sensing' that if the model is sparse, i.e., has only a few non-zero coefficients, it can be recovered with high-resolution with fewer but randomly chosen samples by minimizing the L1 norm of the recovered model.

We introduce 'overcomplete tomography,' a novel method that adapts the concept of compressive sensing to inverse problems and finds a sparse representation of the model using an 'overcomplete basis'. We demonstrate our method with a synthetic and a real X-ray tomography example. The results show that we can reconstruct a multi-scale model and detect sharp discontinuities with a very small number of randomly sampled data. It can also successfully separate the local and global parts of the model in a respective basis. We compare our results with the least-squares inversion and show that our method enables excellent recovery. We also explore several intriguing geophysical applications, such as low-artifact imaging of systems containing features at multiple scale lengths.

S0410. Bayesian inversion and uncertainty quantification in seabed geoacoustics

Stan Dosso (University of Victoria),
Jan Dettmer (University of Calgary),
Charles W. Holland (Portland State University),
Julien Bonnel (Woods Hole Oceanographic Institution),
Dag Tollefsen (Norwegian Defence Research Establishment),
Yong-Min Jiang (University of Victoria)
Room: auditorium 2022-08-31 15:25

This paper considers uncertainty quantification for seabed geoacoustic profiles estimated by Bayesian inversion of ocean-acoustic data. Several types of acoustic data are considered, including broadband seabed reflection coefficients, dispersion of water-borne acoustic modes, and complex ship-noise spectra across an array of sensors (hydrophones). Several approaches to quantitative model selection are presented including: trans-dimensional (trans-D) inversion, which parameterizes the seabed as an unknown number of uniform layers; Bernstein-polynomial (BP) inversion, which represents seabed profiles as smooth gradients with the polynomial order determined via the Bayesian information criterion; and hybrid parameterization with a BP gradient over trans-D layers. All approaches employ Markov-chain Monte Carlo sampling with parameter perturbations based on principal-component (PC) decomposition of the unit-lag parameter covariance matrix; that is, the covariance estimated from successive parameter changes along the Markov chain. The PC proposal is initiated from a linearized estimate that is subsequently updated with a nonlinear estimate from the on-going sampling (a diminishing adaptation). The acceptance rate of parameter perturbations and trans-D steps is improved by parallel tempering, based on a series of interacting Markov chains with successively tempered (relaxed) likelihoods. The PC proposals are adapted individually to the tempering of each Markov chain, which significantly improves sampling efficiency. The data-error model assumes multivariate Gaussian errors with correlations represented by an autoregressive (AR) process. The parameters of zeroth- and first-order AR processes are sampled in the inversion, with trans-D sampling over AR order to avoid over- or under-parameterizing the error model. Inversion results (marginal posterior probability profiles) are compared between data types and parameterization approaches, and compared to co-located core measurements.

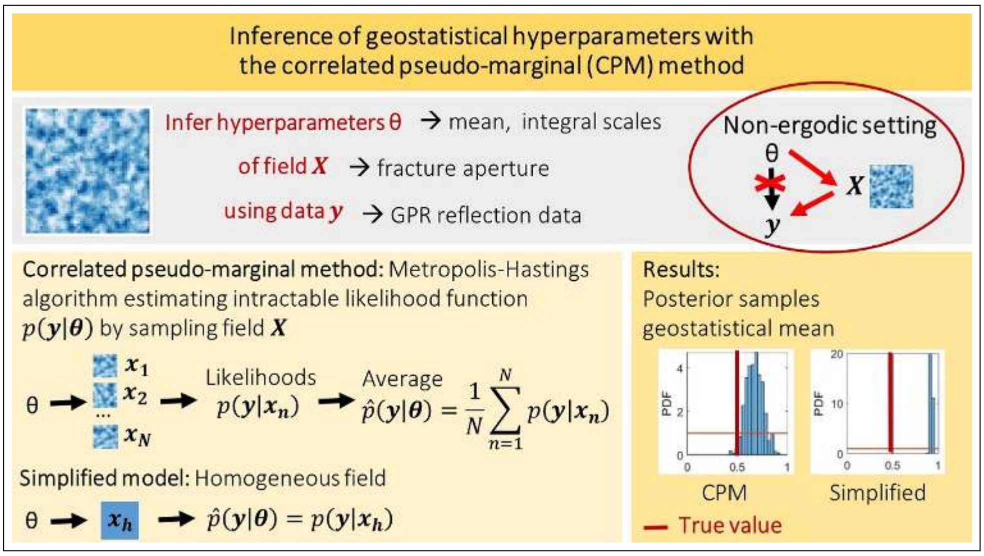


Seabed geoacoustic inversion results for acoustic data corresponding to (top to bottom): reflection coefficients (RC), modal dispersion, and ship noise. Panels show marginal posterior probability profiles for interface depth, compressional-wave velocity c_p, density ρ, and attenuation α computed via trans-D inversion (dispersion data do not constrain attenuation). Second set of panels (on right) for dispersion data show results for Bernstein polynomial over trans-D parameterization, representing the upper layer as a smooth gradient. Data sets collected on the New England Mud Patch at sites with differing mud-layer thicknesses indicated by dashed lines. Results indicate highest resolution from RCs, lowest from ship noise (passive acoustic data).

S0411. Inference of geostatistical hyperparameters with the correlated pseudo-marginal method

Lea Friedli (University of Lausanne),
Niklas Linde (University of Lausanne),
David Ginsbourger (University of Bern),
Alejandro F. Visentini (University of Lausanne),
Arnaud Doucet (Oxford University)
Room: auditorium 2022-08-31 15:50

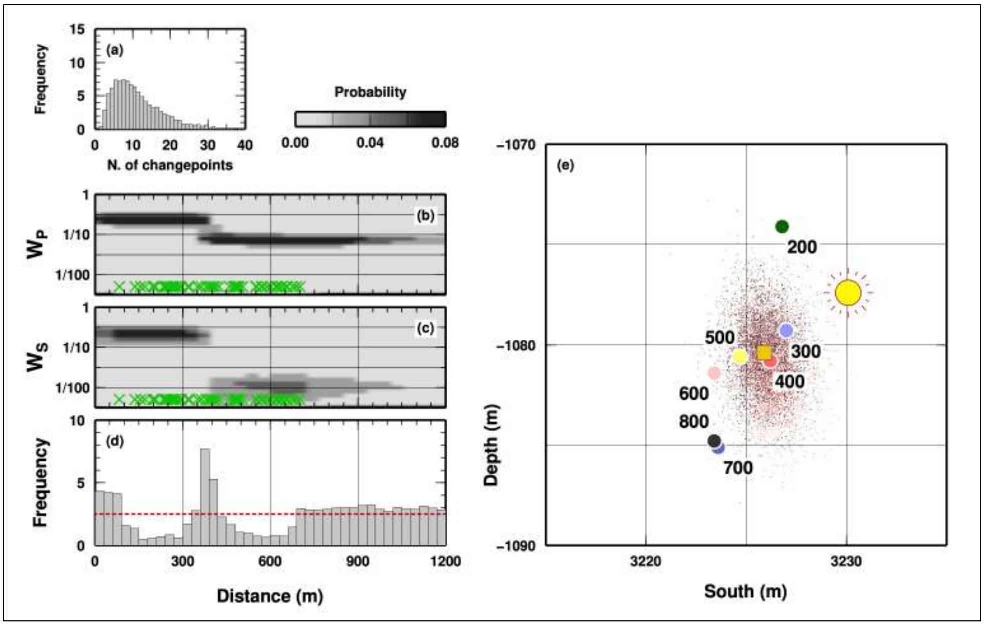
We consider non-linear Bayesian inversion problems to infer the (geostatistical) hyperparameters of a random field describing hydrogeological or geophysical properties by inversion of hydrogeological or geophysical data. This type of problem is of particular importance in the non-ergodic setting as no analytical upscaling relationships exist linking the data to the hyperparameters, such as, mean, standard deviation, and integral scales. Full inversion of the hyperparameters and the "true" realization of the field (typically involving many thousands of unknowns) brings substantial computational challenges, such that simplifying model assumptions (e.g., homogeneity or ergodicity) are typically made. To prevent the errors resulting from such simplified assumptions while circumventing the burden of high-dimensional full inversions, we use a pseudo-marginal Metropolis-Hastings algorithm that treats the random field as a latent variable. In this random effect model, the intractable likelihood of observing the hyperparameters given the data is estimated by Monte Carlo averaging over realizations of the random field. To increase the efficiency of the method, low-variance approximations of the likelihood ratio are ensured by correlating the samples used in the proposed and current steps of the Markov chain and by using importance sampling. We assess the performance of this correlated pseudo-marginal method to the problem of inferring the hyperparameters of fracture aperture fields using borehole ground-penetrating radar (GPR) reflection data. We demonstrate that the correlated pseudo-marginal method bypasses the computational challenges of a very high-dimensional target space while avoiding the strong bias and too low uncertainty ranges obtained when employing simplified model assumptions. These advantages also apply when using the posterior of the hyperparameters describing the aperture field to predict its effective hydraulic transmissivity.



S0412. Geophysical data-mining using trans-dimensional algorithms: the case-study of earthquakes location

Nicola Piana Agostinetti (Università degli Studi di Milano-Bicocca)
Room: auditorium 2022-08-31 16:15

Geophysical investigations are generally developed in the "model-space", i.e. geophysical data are exploited to improve our knowledge about the physical properties of the Earth. Less attention has been paid to investigate the geophysical data-space, i.e. to improve our knowledge about the data structures (e.g. the relation between data uncertainties and geometry of data sampling, the existence of highly correlated noise in the portion of the data accessible to the scientists). Here we illustrate how data-space can be explored using trans-dimensional algorithms, an information technology specifically developed to investigate the model-space. We apply a trans-D algorithm to explore the data-space and find volumes of the data-space not consistent with our starting hypothesis. Recasted in the low-dimensional geophysical inverse problem of locating an earthquake in an elastic half-space, our algorithm will be able to map out data un-consistent with the hypothesis of straight-line ray-path (i.e. data that need 3D heterogeneities to be modelled in a compelling way). The parsimonious behaviour of trans-D algorithm will allow to find only volumes of data un-consistent with the hypothesis strictly dictated by the data themselves, without imposing any pre-defined (user-defined) idea about the data structures. Results indicate that our approach is equivalent to standard procedures based on expert-opinion when simple data-structures are present, and demonstrate the feasibility of using trans-dimensional algorithm to explore the data-space.



S0413. Time-lapse seismic AVO inversion method by using Gradient descent optimization

Nisar Ahmed (University of Stavanger),
Wiktor Waldemar Weibull (University of Stavanger),
Dario Grana (University of Wyoming),
Tuhin Bhakta (NORCE Norwegian Research Centr)
Room: auditorium 2022-08-31 16:40

Pre-stack AVO inversion technique is being widely used for seismic reservoir characterization and geofluids discrimination by estimating the subsurface petro-elastic properties from the offset/angle gathers. We have presented a nonlinear least-squares approach based on the gradient descent optimization algorithm to predict the time-lapse reservoir changes e.g., water saturation and pressure either due to hydrocarbons production or fluid injection. This inversion method comprises on seismic forward model, an objective function defining the distance between real and modelled seismic data and nonlinear minimization algorithm. The adjoint-state numerical method and chain rule of derivative are applied to compute the gradients of the objective function with respect to the reservoir dynamic changes and to obtain the possible best optimized model by minimizing the objective function iteratively, we used limited-memory BFGS. Furthermore, the developed inversion method has been applied on a real well log based 1D synthetic data and 2D real field 4D seismic AVO data obtained from the two North Sea oil fields. The inversion scheme has been tested on various reservoir 4D conditions. The results demonstrate the accuracy of inversion algorithm with very good convergence rate.

S0414. Using deep learning to model gravity and seismic datasets with different spatial coverage

Mahtab Rashidifard (The University of Western Australia),
Mark Jessell (The University of Western Australia),
Jeremie Giraud (RING, GeoRessources / ENSG, Université de Lorraine),
Mark Lindsay (CSIRO Australian Resources Research Centre)
Room: auditorium 2022-08-31 17:05

Integrated geophysical inversion approaches are recognized for their efficiency and have become common tools for recovering the 3D structure of the subsurface. Gravity and seismic datasets have been commonly integrated as they provide high lateral and vertical resolution images from their respective geophysical responses. However, integrated inversion of these two datasets is not straightforward and involves computationally expensive forward modeling and inversion algorithms. Many studies in recent years have proposed to predict geological structures from seismic datasets using deep learning techniques. However, these approaches have seldom been used to integrate seismic with other geophysical datasets for recovering geological model parameters.

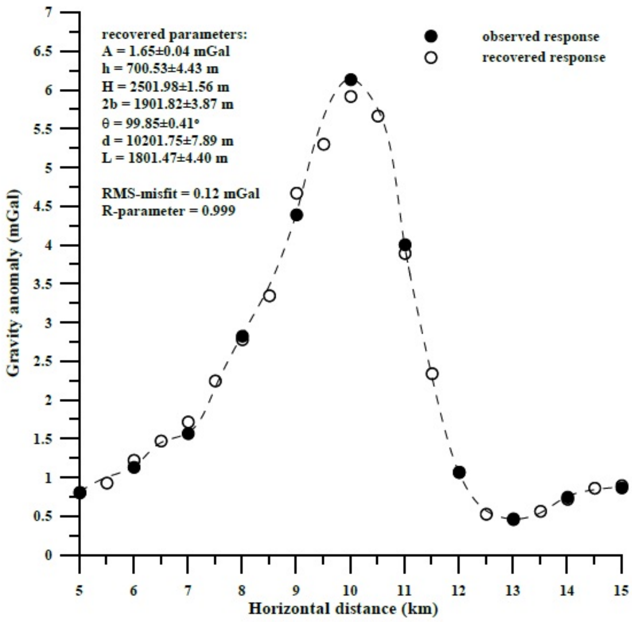
To mitigate this, we use 1 million of publicly available 3D geological models generated by the Noddy software. These models are automatically generated by defining different series geological histories. For each model, we generate the corresponding 2D surface gravity responses as well as 2D seismic sections and store them as 2D images. In this research, we introduce a new technique that utilizes deep learning to predict the event history of these models using gravity and seismic datasets with different surface coverage. We utilize a multi-view deep learning approach to train the network on a large portion of the synthetic models. We then validate the trained network on the remaining synthetic models. The validation process shows high accuracy in predicting the historical events of the geological models. In order to test the algorithm, we perform a case study in Mt Isa in Queensland, Australia. The preliminary results of this application case suggest that the predicted models from the deep learning algorithm partly agrees with existing interpretations of the area and can be used in support of more traditional modelling techniques.

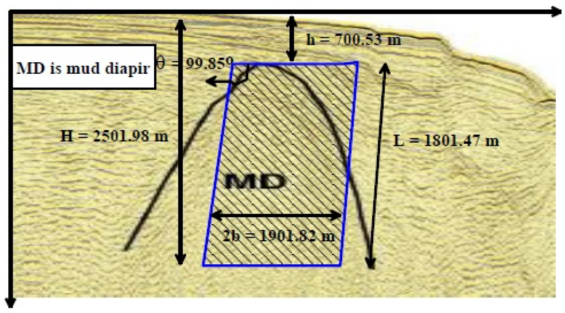
S0415. A full interpretation applying a metaheuristic particle swarm for gravity data of an active mud diapir, SW Taiwan

Khalid Essa (Professor),
Yves Géraud (GeoRessources Laboratory, University of Lorraine),
Marc Diraison (GeoRessources Laboratory, University of Lorraine)
Room: auditorium 2022-08-31 17:07

An interpretation for the gravity anomalies is essential to visualize the horizontal and vertical extension of the subsurface intrusion such as mud diapirs resembling dike-like geologic bodies. Therefore, the use of simple-geometrical resembling models helps in the validation of the subsurface targets. A particle optimization algorithm is one of the recently established metaheuristic algorithms, which is utilized to various geophysical applications and allows discovering and explaining the parameters of the buried geologic-targets (Biswas et al. 2017; Essa and Géraud 2020). We were interpreted gravity response profiles for mud diapir, which close an expected two-dimensional (2D) inclined using the particle optimization algorithm. The stability this study were checked on numerical examples. Moreover, it tested on a gravity response for mud diapir from SW Taiwan and validated by seismic interpretation. The obtained results declared that the suggested algorithm works well even in the presence of noise. Furthermore, Gravity profile for mud diaper, SW Taiwan, which this areas is characterized by activation of mud diapirs, mud volcanoes and gas emitting (Chen et al. 2010; Doo et al. 2015). After that the particle optimization algorithm was utilized to this residual gravity anomaly using probable search ranges of all characteristic parameters. The best interpretative model parameters are corresponding to the minimum objective function (RMS-misfit), which equals 0.12 mGal and the recovered parameters are the corresponding best obtained interpretive target parameters are: A = 1.65 ± 0.04 mGal, h = 700.53 ± 4.34 m, H = 2501.98 ± 1.56 m, 2b = 1901.82 ± 3.87 m, = 99.85 ± 0.41o, d = 10201.75 ± 7.89 m, and L = 1801.47 ± 4.40 m with correlation coefficient (R-parameter) equals 0.999. The results of real case model are found in good agreement with the available geological and seismic interpretation as mentioned in Doo et al. (2015).

Graphical Abstract

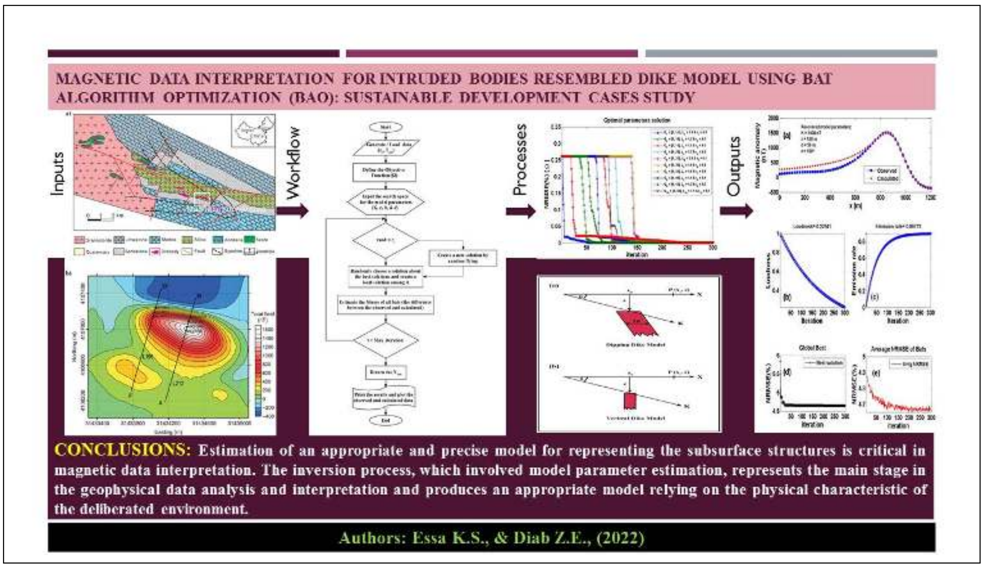




S0416. Magnetic data interpretation for intruded bodies resembled dike-model using Bat algorithm optimization (BAO): sustainable development cases study

Khalid Essa (Professor),
Zein A. Diab (Cairo University)
Room: auditorium 2022-08-31 17:09

Metaheuristic techniques are increasingly being applied as a global optimal approach in the inversion and modeling of magnetic data. We proposed a bat algorithm optimization (BAO) technique, a new metaheuristic optimization algorithm based on bat echo-location behavior, to interpret magnetic data by finding the global optimum solution. The best-estimated source parameters that correspond to the minimum of the objective function are obtained after achieving the global optimum (best) solution. The suggested BAO technique does not require any prior information and provides an effective global tool for scanning the full space of data to estimate the source's appropriate model parameters. The BAO technique is applied to magnetic data in the class of 2D dipping and vertical dikes magnetic profiles to estimate the dimensional source parameters that include the depth to top, origin location, amplitude coefficient, index angle of magnetization, and width of the dipping dikes. The BAO technique has been applied to single and multiple dikes structures comprising both dipping and vertical dikes. The accuracy and stability of the BAO technique are achieved on different synthetic examples including the effect of noise and multi-cases. Furthermore, the presented BAO technique has been effectively applied to three field examples from China and Egypt for iron ore deposits and metavolcanics basalt rock investigation. Overall, the BAO technique's recovered inversion findings are in good agreement with borehole, geology, and published literature data. Finally, according to findings, the offered metaheuristic BAO technique is a simple, rapid, accurate, and powerful tool for magnetic data interpretation.



S05 Knowledge graphs in the cyberinfrastructure ecosystem of geosciences

Xiaogang Ma (University of Idaho),
Chengbin Wang (China University of Geoscience)

Vocabularies, schemas and ontologies have been increasingly created and applied in geosciences in the past decades, and have always been a topic of interest in geoinformatics. Inspired by the recent success of knowledge graphs in industry, the academia is beginning to use knowledge graph as an umbrella topic for works on vocabularies, schemas, and ontologies. In the geoscience community, we have seen many successful applications of knowledge graph in data curation and integration in the past decades, such as the global geologic map sharing enabled by OneGeology. Recently, there were also applications of knowledge graph together with machine learning algorithms to improve the quality of data analytics, such as those in hyperspectral remote sensing image processing, extension to mineral taxonomy, and petroleum exploration. Together, knowledge graphs have shown promising contribution to data science applications in geosciences, and more innovative developments are undergoing. This session welcomes submissions of all the topics mentioned above, to provide a venue for knowledge graph practitioners to share their results and experience, learn best practices, and discuss visions and potential collaborations for future work.

S0501. Temporal topology in the deep-time knowledge base and applications in geoscience

Xiaogang Ma (University of Idaho)
Room: 101 2022-08-30 14:35

Deep time (i.e., geologic time) has received increasing attention in recent data-driven geoscience studies. Although deep time is a fundamental framework for studying the evolution of the Earth, many existing open geoscience data facilities are short of clear and structured vocabularies and knowledge graphs for deep time concepts. In our work of a deep-time knowledge base (deeptimekb.org), we have leveraged existing community standards to build a formal framework for various deep-time concepts, including those from both global and regional geological time scales. Another highlight is the incorporation of temporal topology into the framework to enable reasoning capabilities. We are currently collaborating with geoscientists in mineralogy and paleobiology to use the knowledge base for retrieving and synthesizing data from multiple sources, with the goal of supporting scientific discoveries in their corresponding fields. This presentation will introduce the functionality of the deep-time knowledge base and illustrate a few successful applications of it in geoscience research. This work is supported by the National Science Foundation (NSF OAC #1835717).

S0502. Metallogenic prediction based on Knowledge Graph – Taking pangxidong area in western Guangdong as an example

Zhang Qianlong (Sun Yat-sen University),
Yongzhang Zhou (Sun Yat-sen University),
Feng Han (Sun Yat-sen University)
Room: 101 2022-08-30 15:00

As earth science enters the era of big data, artificial intelligence technology is contributing to solving earth science problems. As one of the core technologies in the field of artificial intelligence, knowledge graph has a wide range of applications in the field of earth science. This paper takes the Pangxidong mining area in South China as the research object, and constructs a geochemical knowledge graph based on geochemical data. Geochemical elements were semantically queried in the knowledge graph, combined with thermal matrix analysis, three sets of geochemical element assemblages in this area were obtained, and finally the prospecting potential areas were indicated according to the element assemblages. This data science method is simple and efficient to mine the frequency characteristics and spatial characteristics of geochemical data, and has a good application prospect in exploration geochemical research.

S0503. A metadata and data entry and editing tool using ontologies for knowledge graph creation

Leon Steinmeier (Helmholtz Institut Freiberg / Helmholtz Metadata Collaboration), Karl Gerald van den Boogaart (Helmholtz Institute Freiberg), Florian Rau (Helmholtz Institute Freiberg), Theresa Schaller (Helmholtz Institute Freiberg)
Room: 101 2022-08-30 15:50

Making research reproducible and FAIR (Findable, Accessible, Interoperable, and Reusable) often requires more information than what is commonly published within scientific articles. There is a growing number of repositories for publishing additional material like data or code. However, articles are still at the center of most scientific work and thus efforts on gathering information which is important for reproducibility but not for the article itself are often only started at a later stage. This usually makes the collection more tedious, error-prone, and less comprehensive.

In order to lower the barrier for recording all relevant information directly when it is generated, we propose a design for a data and metadata entry and editing tool. It should allow researchers to create metadata for the files and assets which they already have and offer a possibility for structured entry of new data. To support consistent (meta)data entry over time, the user will be able to create forms which can enforce comprehensiveness and correctness. Furthermore, data FAIRness is supported through the automated usage of established ontologies for (meta)data annotation. This will be done by a background process so the user isn´t involved in these technologies. Nevertheless the tool will grant further possibilities to those who are aware of ontologies used in their domain. Resources can be referenced consistently across (meta)data sets of many stakeholders through identifiers provided by central sources. In conjunction, the usage of these common identifiers and ontologies forms large knowledge graphs of the data recorded with our tool.

This contribution will be a discussion of the various components of such a tool, potentially used metadata standards, possible variations, important features, and most relevant: How it can be useful for your work!

S0504. A Multi-granularity Geological Objects (Multi-GeoO) Knowledge Representation Framework

Wenjia Li,
Xiaogang Ma (University of Idaho),
Zhong Xie (China University of Geoscience),
Liang WU (China University of Geoscience)
Room: 101 2022-08-30 15:52

Geology research has accumulated a large amount of unstructured data so far, such as text, graphics, images, audio, video, etc. Among them, text data is an integral part of geoscience big data. These massive text data contain the rich expert experience and domain knowledge. How to effectively manage and fully utilize this knowledge, expand the cognitive space of geology, and improve the intelligent and complete cognitive ability of geology is the inevitable trend of current geology research. Therefore, this paper explores the modeling and object representation methods of geologic phenomena in unstructured data, using geological texts as data sources and aiming at the spatio-temporal analysis and visualization of the evolutionary process of the Earth. Considering the diversity of knowledge granularity and geological objects at spatio-temporal scales, a multi-granularity geological object (Multi-GeoO) knowledge representation framework is developed to comprehensively and holistically describe geological objects and their interactions in unstructured texts. In addition, based on this framework, a multi-granularity stratigraphic knowledge base is constructed in this paper using relevant information from the open literature to augment the performance of the Multi-GeoO framework for spatio-temporal analysis and visualization at different granularities. The experimental results show that the granulated geological objects have more advantages for showing the differences between different geological objects, which is important for deeper understanding and utilization of existing geological knowledge.

S0505. Impact of complex geological setting on the Hydrodynamic modeling Case of the Gabes aquifer system, SE Tunisia

Mohamed Amine Hammami,
Hayet CHIHI (Georesources Laboratory, Centr),
Imen Mezni (Center for Water Research and),
Mohamedou Ould Baba Sy
Room: 101 2022-08-30 15:25

Modeling is practice approached and applied differently in every discipline of geoscience. There are distinct differences between these models, but also plenty of similarities according to their application fields. For instance, geological modeling, and groundwater modeling, have the construction conceptual model in common. A conceptual hydrogeological model is the description of the groundwater flow system. The development of such a model is actually synonymous with the sub-terrain characterization.

The construction of a conceptual groundwater flow model relies on prior knowledge of lithology and structural configuration and processes provided by geo-logical modelers. However, groundwater modelers channel all their efforts into the study of groundwater flow mechanisms and aquifer parameters. Despite the advances of modeling in both domains, efforts of connecting the geological modeling and the groundwater modeling's stronger assets are not widely practiced.

In our work, we contribute to the efforts of groundwater characterization in the Gabes aquifer system by providing a hydrogeological model that reflects the impact of the geology of the area on the groundwater flow. We demonstrate the importance of a reliable geometrical model on the understanding of the Gabes's groundwater evolution after decades of overexploitation and diminishing recharge rates through a juxtaposition and comparison of the results of the 3D geometrical model with the results of the Hydrodynamic model.

S06 Fractured geological media and fracture networks: flow, graphs, morphology

Rachid Ababou (Institut de Mecanique des Fluides de Toulouse),
Israel Cañamón Valera (Universidad Politécnica de Madrid)

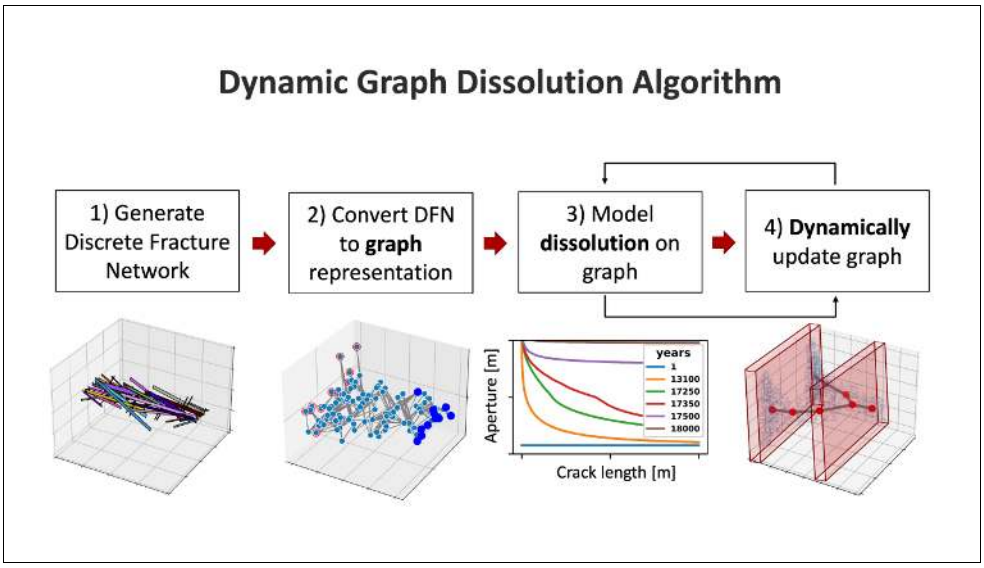
"Fractured geological media and fracture networks: flow, graphs, morphology."

This session is an opportunity to present various approaches for analyzing geometrical, topological, and hydraulic properties of 3D Discrete Planar Fracture Networks (DPFN), or their 2D counterpart (e.g., discrete flow networks represented by intersecting segments in the plane), or other discrete sets of Boolean objects (conductors, barriers, cavities, etc.). These generalized geological "networks" may be described deterministically or statistically (e.g. as random Boolean objects), and/or, based on graph theory concepts. Extensions to other mechanisms focusing on morphology and structure of discrete fracture networks are also welcome (e.g., two-phase flow, mechanical deformation, electrical conduction…). This topic is also related to upscaling issues in fractured media and networks : these are relevant to this session in connexion with morphology and structure. Overall, this session focuses on mathematical and algorithmic approaches for characterizing geological media and/or discrete fracture networks, in terms of topology, morphology, hydraulic/conduction properties, based on field observations as well as models.

S0601. Stochastic Geomodelling of Karst Morphology by Dynamic Graph Dissolution

Rayan Kanfar (Stanford University),
Tapan Mukerji (Stanford University)
Room: 105 2022-09-02 09:50

Cave networks are excellent groundwater and hydrocarbon reservoirs. Cave geometry, spatial distribution, and interconnectivity is critical for developing production and contaminant remediation strategies. Geologically realistic stochastic models for simulating karst are essential for quantifying the spatial uncertainty of karst networks given geophysical observations. Dynamic Graph Dissolution, a novel physics-based approach for three-dimensional stochastic geomodelling of telogenetic karst morphology is introduced. The cave evolution is modelled through dissolution of fractures over geologic time based on a graph representation of discrete fracture networks, which can be informed by field observations. The graph is initially represented based on fracture intersections. We update the graph representation over time using the Mapper algorithm with density-based spatial clustering to account for overlapping enlargements. This modelling approach enables modelling a priori different geologic scenarios of karst formation at tractable computational cost. In order to validate the model, generated models are compared with real cave geometries using topological graph theory metrics such as central point dominance, assortativity, and howard's parameters. Topological metrics of generated models are shown to fall within the distributions of known caves.



S0602. Exact algebraic approach to flow calculation and permeability upscaling in 2D fracture networks using graph operators

Rachid Ababou (Institut de Mecanique des Fluides de Toulouse),
Philippe Renard (University of Neuchâtel)
Room: 105 2022-09-02 10:15

Exact algebraic approach to flow calculation and permeability upscaling in 2D fracture networks using graph operators

ABABOU Rachid (IMFT, Toulouse), RENARD Philippe (Centre d'Hydrogéologie et Géothermie, Neuchâtel)

We present an exact algebraic approach for calculating the detailed flow and the equivalent tensorial permeability for 2D fracture networks, or possibl,y 3D conduit networks. We focus here essentially on irregular bond networks made up of intersecting fracture segments on the plane. Single phase flow in each fracture is calculated using Poiseuille law (analogous to Darcy), with steady mass conservation implemented at the nodes (connections). An exact algebraic relation between the mean flux vector (Q) and the mean hydraulic gradient or total pressure gradient (J) is developed, through a mathematical analysis of the network flow problem, based on concepts from graph theory. The detailed flow problem is formulated on the graph representing the network, using discrete versions of the Divergence and Gradient operators (difference operators on the graph) as in Strang (1988); see also Ababou & Renard (2009, 2011). An equivalent permeability is then obtained algebraically for the entire network, for given boundary conditions and upscaling procedures. The resulting permeability Kij is analyzed. It is shown to be a 2nd rank tensor, not necessarily symmetric and not necessarily positive-definite. It is explicitly expressed given the geometric properties of the network (fracture lengths and apertures), and the topological graph structure (adjacency and incidence matrices). We detail the case of « gradient immersion » boundary conditions (linearly varying boundary pressures), combined with Volume Average Flux (VAF) upscaling, which always leads to symmetric tensorial Kij (unlike some other upscaling procedures).

Acknowledgments. The first author acknowledges useful exchanges along the years with B. Noetinger on various mathematical approaches to fracture network permeability.

Keywords: Fracture networks ; Bond networks ; Graphs ; Difference operators ; Equivalent tensorial permeability

S0603. Statistical analysis and stochastic simulation of Fracture Networks

Francois Bonneau (Université de Lorraine, CNRS, GeoRessources), Radu S. Stoica (Université de Lorraine)

Room: 105 2022-09-02 10:40

Fracture networks (FN) are systems of complex mechanical discontinuities in rocks. Such networks dramatically impact fluid flow acting as a drain or a barrier. This work proposes to build a stochastic mathematical model and to use it as a tool for fracture characterization.

For a few decades, the mathematical framework of marked-point process has been successfully used to study fracture networks. In this work, we will also use this approach to approximate FN with a collection of straight-line segments. Each object is then represented by a marked-point. The “point” locates the geometrical center of the segment and holds two real valued “marks” standing for segment length and strike azimuth. Geologists commonly use first-order characterization to access a statistical description of the object geometry, i.e. their density and their mark distributions. More recently, second-order characteristics have been used to characterize inner correlation and spatial variability of objects. Investigating stochastic models that are known to produce realizations presenting similar first and second order characteristics may be the key of a final understanding of FN.

In this work, we built a mathematical model to produce stochastic realizations of marked point process that considers and reproduces such observations. Also, we investigated the optimization of model parameters in the light of a natural FN pattern. This work may open the path to a thinner classification of FN and a more realistic stochastic simulator.

S0604. TOP 3D: Topological analysis of 3D fracture networks, graph representation, and percolation

Israel Cañamón Valera (Universidad Politécnica de Madrid),
Tawfik Rajeh (Institut de Mecanique des Fluides de Toulouse (IMFT)),
Rachid Ababou (Institut de Mecanique des Fluides de Toulouse),
Manuel Marcoux (Institut de Mecanique des Fluides de Toulouse (IMFT))
Room: 105 2022-09-02 11:05

We present a computer toolbox (TOP3D) to analyze geometrical, topological and hydraulic properties of 3D Discrete Fracture Networks (DFN) and to estimate their properties near percolation threshold. Efficient algorithms were developed to perform geometrical and topological analyses upon 3D networks of planar fractures with various shapes (circular, elliptical). The TOP3D toolbox is capable of (i) calculating all intersections and resulting trace lengths and other geometrical attributes of the 3D network; (ii) extracting percolating clusters and eliminating dead-end clusters; and (iii) constructing the graph of the 3D planar fractures network. All calculations were validated by direct simulations. The graph representation of the DFN enables implementation of broad-purpose algorithms inspired by graph and percolation theories. It is demonstrated that the TOP 3D toolbox as a pre-treatment tool can considerably reduce CPU time of network flow/transport simulations (pre-treatment involves extracting the percolation network, eliminating all dead-end fractures and clusters, and searching for shortest paths). The gain on CPU time was several orders of magnitude for thousands of fractures. TOP3D's computational efficiency permits a broad study of percolation phenomena in 3D planar fracture networks. The results of this work concern two main developments: (1) a new procedure for numerical determination of the critical percolation density (based on the concept of marginal percolation); and (2) an enhanced formula with low sensitivity to fracture shape, orientation, and size distribution, is proposed for estimating the critical percolation density. This work was recently published by the authors in Computers and Geotechnics 142 (2022) 104556, https://doi.org/10.1016/j.compgeo.2021.104556

Keywords: Discrete Fracture Networks, Fractured rocks, Connectivity, Percolation clusters, Excluded volume, Graphs

S0605. Modelling realistic fracture networks in a mechanically multilayered sequence: constraints from field observations and numerical modelling

Andrea Bistacchi (Università degli Studi di Milano-Bicocca),
Mattia Martinelli (Università degli Studi di Milano-Bicocca),
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Stefano Casiraghi (University of Milan - Bicocca),
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Giovanni Dal Piaz (LTS - Land Technology & Services SRL, Treviso),
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Davide Bertolo (Regione Autonoma Valle d'Aosta)
Room: 105 2022-09-02 11:30

Improving our understanding of fracturing processes thanks to observations on outcrop analogues and mechanical modelling can help modelling fracture networks in reservoirs of geofluids.

Here we investigate a counterintuitive behavior in mechanically layered sequences of different rocks where we observed a more intense fracturing, both in terms of fracture density/intensity and number of fracture sets, in more competent layers. In the Island of Gozo (Malta) we have characterized fault zones in porous carbonates, and we found that, in the relatively softer units, the thickness of damage zones is about 1/30, and fracture intensity is about 1/10 (at the same distance to the fault core). In metamorphic rocks in the Alps we have observed a strikingly similar situation in uniformly fractured rocks far from major faults, with an inverse correlation between mechanical and fracturing parameters.

Simulations with a geomechanical finite element code show that, during horizontal extension of a multilayer with variable elastic properties, deviatoric stresses build up much more quickly in stiffer rocks. This is because all the different layers are subject to the same strain (horizontal stretching), and stress is controlled by the elastic moduli, resulting in higher deviatoric stresses in more rigid layers. At some point, brittle failure (simulated as plastic yield in continuous FEM codes) takes place in the stiff layers, well in advance with respect to failure in the soft ones. At this point, the simulation reveals a situation where fracturing is confined in the stiff layers. As horizontal stretching continues, failure can occur also in the soft layers, but always in a more limited way.

This mechanical behavior, observed in very different tectonic environments and lithological units, can be of general relevance and might result in a reevaluation of paradigms used to predict fracturing and hydraulic properties of mechanically layered reservoirs.

S0606. Optimization of boreholes positions to maximize flux rate in a 3D Discrete Fractured Medium

Israel Cañamón Valera (Universidad Politécnica de Madrid),
Borja Brasero Zabalete (Universidad Politécnica de Madrid),
Paola Cruz Amores (Universidad Politécnica de Madrid)
Room: 105 2022-09-02 11:55

We present in this study a methodology to statistically model a 3D Discrete Fractured Medium (DFN) and optimize the location of prospective boreholes in order to maximize the flux between them. We use machine learning to obtain 3D geometrical parameters of the DFN from 2D and 1D statistical geological information (tracemaps and boreholes), and we apply a fast intersection algorithm and graph approach to describe the connectivity between the fractures. The Bounding-Box and Sweeping Line algorithm described in [Dong et al, 2018] has been ameliorated in 3D, and applied to the TOP3D toolbox [Canamon et al, 2022] to increase computational efficiency. Then, this toolbox has also been adapted to analyze the connectivity between several vertical boreholes, and an optimization technique has been implemented to optimally determine the location of those boreholes in order to get a maximum flux rate between them. This methodology has been tested with synthetic DFNs, and its performance has been evaluated, giving promising results for its application to real scope industrial applications like petroleum, water or gas geological prospection.

Reference.

Canamon I., T. Rajeh, R. Ababou, M. Marcoux (2022): Topological analysis of 3D fracture networks: Graph representation and percolation threshold. Computers and Geotechnics 142 (2022) 104556. https://doi.org/10.1016/j.compgeo.2021.104556

Shaoqun Dong, Lianbo Zeng, Peter Dowd, Chaoshui Xu, Han Cao (2018) : A fast method for fracture intersection detection in discrete fracture networks. Computers and Geotechnics 98 (2018) 205–216. https://doi.org/10.1016/j.compgeo.2018.02.005

Keywords: Discrete Fracture Networks, Machine Learning, Bounding-Box, Sweeping Line, Connectivity, Graphs, Optimisation, Borehole

S0607. Fracture and karst modeling: an embedded workflow including fracture abutting and permeability enhancement with karst.

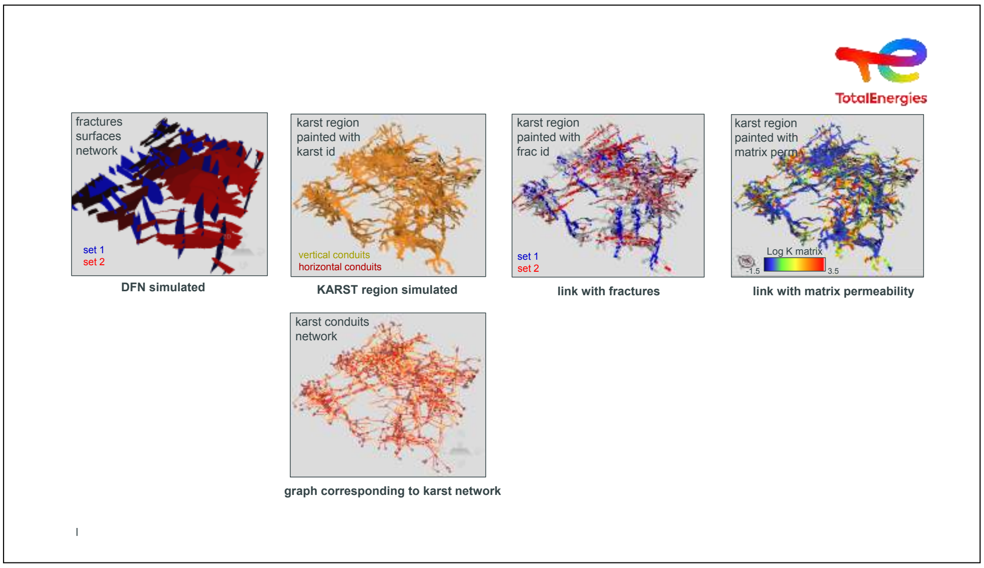
Pierre Biver (TotalEnergies),
Alan Irving (TotalEnergies),
Patrick Henriquel (TotalEnergies),
Nadège Vilasi-Marmier (TotalEnergies)
Room: 105 2022-09-02 14:40

In carbonate reservoirs, an important concern is to model secondary porosity and permeability. In effect, fracturing and karstification produce high permeability streaks that significantly modify the behavior of the reservoir (earlier water breakthrough for secondary hydrocarbon recovery or contaminant transport).

In this paper, we present a full workflow to handle both fracture and karst modeling. A discrete fracture network (DFN) is modelled by a classical marked point Boolean process. We introduce an original modification, however, to model chronological relationships between fractures, or abutting. Once the DFN is built, the equivalent permeability is computed with analytical formulas (Oda, 1985; Rajeh et al., 2019).

The subsequent karstification process is built by propagating conduits (see Biver et al., 2012 for a detailed description). Using the fracture equivalent permeability field, we can ensure the conduits follow preferential paths in zones of high permeability and therefore fractures. The final equivalent permeability is computed by adding the karst conduits' contribution, computed with an analytical formula (modified Poiseuille law with a correction factor for turbulence).

We illustrate the methodology on a realistic synthetic case, on which we obtain very consistent results. Finally, some conclusions are given regarding the application domain.



S0608. Graph-based scenario-testing of fluid pathways in 2D & 3D

mark jessell (The University of Western Australia),
Guillaume Pirot (The University of Western Australia),
Vitaliy Ogarko (The University of Western Australia),
Uli Kelka (CSIRO),
Mark Lindsay (CSIRO Australian Resources Research Centre),
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Stephane Perrouty (Laurentian University)
Room: 105 2022-09-02 15:05

Whilst fluid-mechanical simulations may provide the most complete approach to understanding fluid pathways in natural systems, they are computationally intensive. Graph representations of geological maps and 3D models allow summary analysis of the tectonic setting, as well as providing a pathway to understanding pathways in complex geometries.

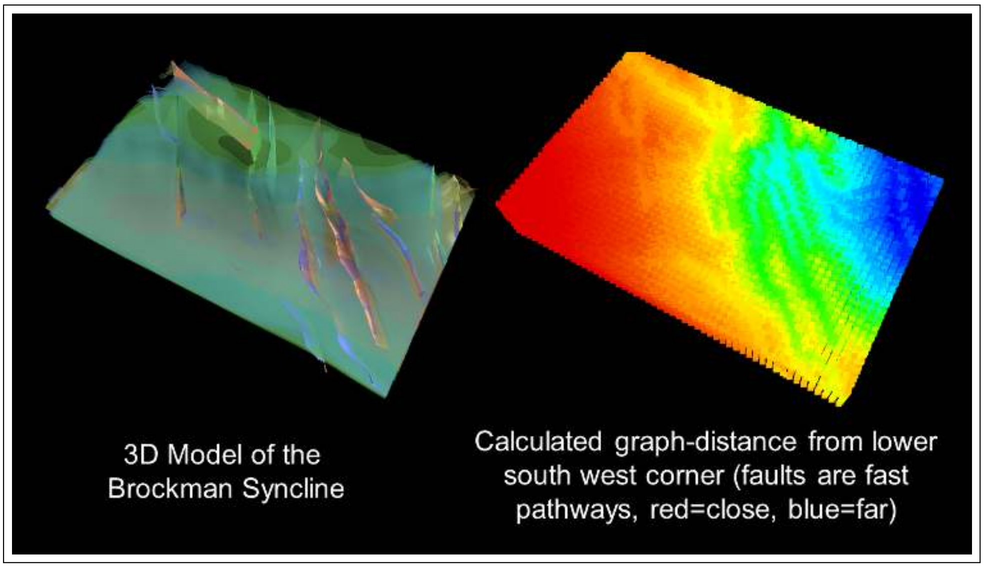
The description of geology as graphs pre-dates routine GIS analysis and allows us to analyse stratigraphic and fault relationships in a single representation (Burns, 1975). This can be extended to analysing potential preferred fluid pathways in fault networks (Ghaffari et al., 2011) and anisotropic distance metrics in folded strata (Boisvert & Deutsch, 2011). In this study we extend graph analysis to consider 3D connectivity of systems with potential permeability pathways following both faults and stratigraphic units using add-ons to the Loop modelling system (https://loop3d.github.io/). The graphs consist of nodes, representing small surfaces of fault or small volumes of a stratigraphic unit. Graph edges represent the connectivity between fault segments, between adjacent stratigraphic volumes, and between fault surfaces and stratigraphic volumes. Both nodes and edges can be assigned weights according to the local nature of the geological feature, and minimum pathways can be calculated on the resulting graphs.

This approach allows us to compare a wide range or different tectonic scenarios and fault and stratigraphic behaviours in 2D and 3D, and to analyse not just the pathways but also the chemical environments the fluids may interact with along their paths. Whilst still just a proof of concept, this approach provides new avenues for the interpretation of complex alteration patterns in multiply deformed systems such as orebodies and may improve our understanding of the transport behaviour of natural faults.

Boisvert, J.B., Deutsch, C.V. 2011. Computers Geosciences 37, 495–510.

Burns, K.L. 1975. Math. Geology, 7, 295-321.

Ghaffari, H.O., Nasseri, M.H.B. and Young, R.P. 2011. arXiv:1107.4918


3D Model of the
Brockman Syncline
Calculated graph-distance from lower
south west corner (faults are fast
pathways, red=close, blue=far)

S07 Computational Petrology and Geochemistry

Pierre Lanari (University of Bern),
Marion Garçon (Université Clermont Auvergne),
Paolo Sossi (ETH Zurich)

Numerical modeling has become a critical aspect of modern research, especially in Earth Sciences as physical and chemical processes occurring in planetary interiors are not always directly observable from the surface. In petrology and geochemistry, a large variety of computational models have been developed to simulate and study these processes. To be realistic, computational experiments commonly rely on an algorithmic or mechanistic approach rather than deriving a mathematical analytical solution to the problem. In addition, the increase in the amount of geochemical data from state-of-the-art instruments (e.g. ICP-MS, microprobe, SIMS) has fostered the development of advanced software solutions for data reduction and interpretation. The ever-increasing size and availability of these datasets has, in turn, opened up new avenues for extracting statistical information on geological processes. The main goal of this session is to bring together geochemists, petrologists and data scientists who are either developing, using and/or applying numerical tools to understand geological processes. Topics of interest include (but are not limited to) geochemical and petrological modeling for fluids, melts and solids using major/trace elements or isotopes, thermodynamics and kinetics, thermo-mechanical simulations of petro/geochemical processes, provenance analysis, optimization and testing of databases. Model developers using machine learning, big data or minimization/inversion routines as well as those developing new techniques and tools for data visualization are particularly encouraged to submit an abstract.

S0701. Deducing the composition of Archean continents with a simple model for sediment geochemistry

Alex Lipp (Imperial College London),
Oliver Shorttle (University of Cambridge),
Sediment Geochem. and Paleoenv. Project Weathering Working
Room: 106 2022-08-30 10:00

The composition of the earliest continents remains a matter of debate. This uncertainty is a challenge for constraining the geodynamics of early Earth, in particular the onset of plate tectonics. Here, we use the major-element composition of Archean sedimentary rocks to constrain the geochemistry of the first continents. The composition of a sediment holds information about the composition of its protolith, but modified by chemical weathering. We formalise this observation by describing sediment compositions as existing on a 2D plane (in log-ratio space) which contains vectors defining trends of igneous evolution and chemical weathering. By projecting compositions onto this plane we are able to describe any major-element composition in terms of the intensity of weathering experienced, and the composition of its protolith, as well as a residual term. Uniquely, this method allows us to reverse the compositional effect of weathering to reconstruct the original protolith for a sediment. We apply this method to the major new sedimentary geochemical compilation produced by the Sedimentary Geochemistry & Paleoenvironments Project. We thus deduce that the Archean continents were dacitic in composition, similar to the modern continents with a similar level of heterogeneity. We suggest that our method represents a novel and generic approach for extracting information from multivariate geochemical data.

S0702. Statistical optimization for geochemical classification of Precambrian igneous rocks

Rebecca Montsion (Laurentian University),
Stéphane Perrouty (Laurentian University),
C Michael Lesher (Laurentian University),
Mark D Lindsay (CSIRO),
Mark W Jessell (The University of Western Australia)
Room: 106 2022-08-30 10:25

Geochemical classification diagrams provide a framework for comparing samples, discriminating composition, and inferring geological processes. However, most are poorly suited for use with metasomatized Precambrian rocks and in applications with a wide range of compositions (i.e., ultramafic to felsic). The configuration of many commonly used diagrams was constrained by pristine samples from modern geological environments and/or were defined using statistically unoptimized element ratios for axes. In an effort to refine current practices for Precambrian igneous rocks, a new classification scheme was defined using Principal Component Analysis (PCA) and k-means Cluster Analysis (CA). These statistical tools were applied to samples from greenstone belts in the southern Abitibi and western Wabigoon subprovinces of the Archean Superior Province in Canada. Using selected major elements and least mobile trace (including HFSE and REE) in a PCA, element ratios that maximize spread between compositional groups along diagram axes were identified. CA was used to identify compositionally similar sample clusters and aid in defining classification fields. The resulting, statistically optimized classification scheme indicates a broad range of sample compositions (i.e., ultramafic to felsic) independent of alteration and texture. It can also be used to discuss trends related to igneous processes (partial melting, accumulation, crustal interaction, assimilation, and fractional crystallization). In using a statistically driven approach to define a new classification scheme for Precambrian igneous rocks, protolith compositions may be more reliably identified.

S0703. Development of a Python GUI application to automate EQ3/6 computations.

Guillaume Siron (University of Bologna),
Alberto Vitale-Brovaronne (BiGEA, University of Bologna),
Simon W Matthews (University of Iceland)
Room: 106 2022-08-30 10:50

Fluid-rock interactions are one of the most important processes on Earth and play an important role in many metamorphic systems. Nevertheless, even if thermodynamic data for mineral and fluid species are easily accessible though many software packages, in most metamorphic studies, the fluid phase is usually reduced to a simple system, either pure H2O or a H2O-CO2 mixture. Yet, we know that dissolved elements can play a major role in many metasomatic reactions. Here we present a Python application with a user-friendly graphical user interface that allows automation of EQ3/6 thermodynamic fluid speciation modeling.

The application enables EQ3 computations and then automation of two designs of batch EQ6 computations. The first option computes batches of EQ6 calculations with different fluid-rock ratios set by the user. The user can then plot the resulting compositional variables, i.e., mineral modes, end-member proportions of solid solutions, dissolved elements, and fluid species concentrations. Again, the UI allows several plotting possibilities, either 2D plots such as either reaction progress or fluid-rock ratios for a specific reaction progress versus one or more compositional variable(s) or in 3D where up to 2 compositional variables can be represented as surfaces in function of the fluid-rock ratio and the reaction progress. The second option allows the user to batch process EQ6 computations with different proportions for 3 minerals at a set fluid-rock ratio. Three different resolutions are accessible with one point every 10%, (66 computations) 5% (231) and 2.5% (861), respectively. As for fluid-rock ratio batch computations, the results can be displayed inside the ternary diagram using a color scale for each run, where the user can choose which variable and which reaction progress is displayed.

We believe that user-friendly applications such as the one presented here will allow more petrologists to introduce fluid speciation into their metamorphic projects.

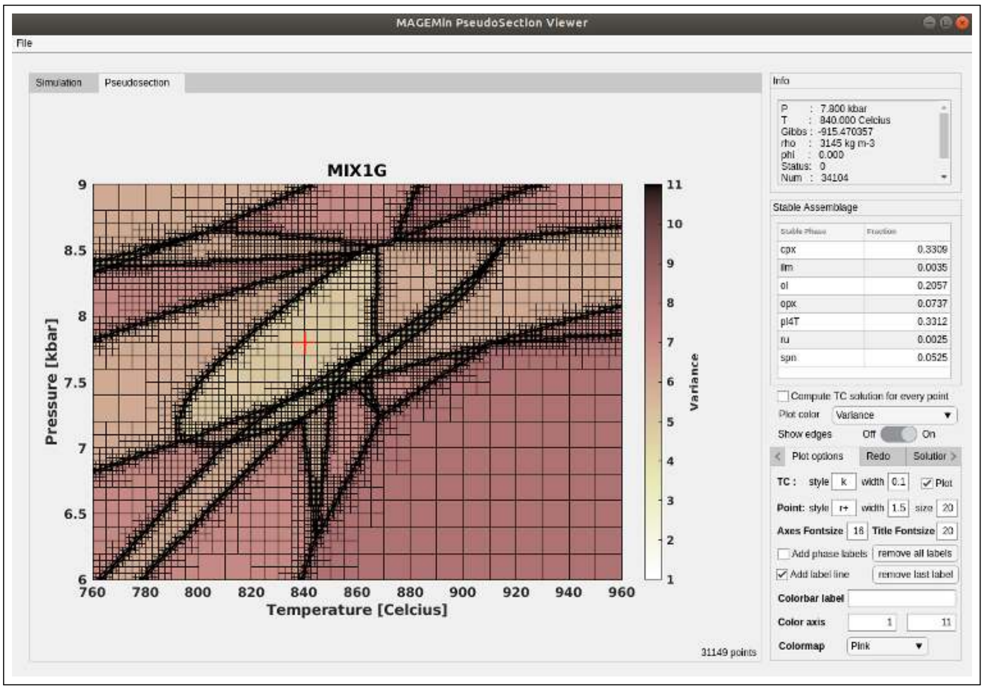
S0704. MAGEMin, a new and efficient Gibbs free energy minimizer: application to igneous systems

Nicolas Riel (Johannes Gutenberg University, Mainz),
Boris J.P. Kaus (Johannes Gutenberg-University),
Eleanor C.R Green (The University of Melbourne),
Nicolas Berlie (Johannes Gutenberg-University)
Room: 106 2022-08-30 11:15

Modelling stable mineral assemblage is crucial to calculate mineral stability relations in the Earth's lithosphere e.g., to estimate thermobarometric conditions of exposed rocks and to quantify the fraction and composition of magma during partial melting. Accurate prediction models of stable phase are also fundamental to model trace element partitioning and to extract essential physical properties such as, fluid/melt/rock densities, heat capacity and seismic velocities. This thus forms a crucial step in linking geophysical observations with petrological constraints.

Here, we present a new Mineral Assemblage Gibbs free Energy Minimizer (MAGEMin). The package has been developed with the objective to provide a minimization routine that is easily callable and fulfilling several objectives. Firstly, the package aims to consistently compute for single point calculations at given pressure, temperature and bulk-rock composition with no needed a priori knowledge of the system. Secondly, the package has been developed for stability, performance and scalability in complex chemical systems. Finally, the code is fully parallel and we directly translate THERMOCALC formulation of solution models which yields easier and faster updates, less prone to implementation mistakes.

As a proof of concept we apply our new approach to the thermodynamic dataset for igneous systems of Holland et al. (2018). The database works in the NCKF-MASHTOCr chemical system and has been updated to account for the new plagioclase model Holland et al. (2021).



S0705. GeoPS: an efficient visual computing tool for thermodynamic modeling of phase equilibria

Hua Xiang (Chinese Academy of Geological Sciences)
Room: 106 2022-08-30 11:40

The availability of thermodynamic data for geologically relevant phases has made practical the calculation of stable phase relations throughout the mantle and crust of terrestrial planets. GeoPS (http://www.geops.org) is a program designed for this purpose in which both input and output are done through an intuitive graphical user interface. GeoPS provides a wide range of phase equilibrium calculations based on a novel Gibbs energy minimization algorithm. The algorithm provides for exceptionally robust and computationally efficient solution to the phase equilibrium problem by successive alternation between a linear programming step to identify stable phase compositions and a non-linear programming step to refine the compositions estimated during the linear programming. It can accomplish a phase diagram section in a few minutes even if the computation involves complex solution models, the speed is up to orders of magnitude faster than Perple X and Theriak-Domino. For calculations from the same thermodynamic dataset and models, results from GeoPS are consistent with those obtained with other popular software, e.g. THERMOCALC. Applications include calculation of various types of phase diagrams and path-dependent phase fractionation. By combining an easy-to-use graphical user interface with a robust and efficient solver, GeoPS makes phase equilibrium modeling accessible to users with any level of expertise and provides a powerful tool for understanding natural phase relations and for planning experimental work.

The main interface of GeoPS

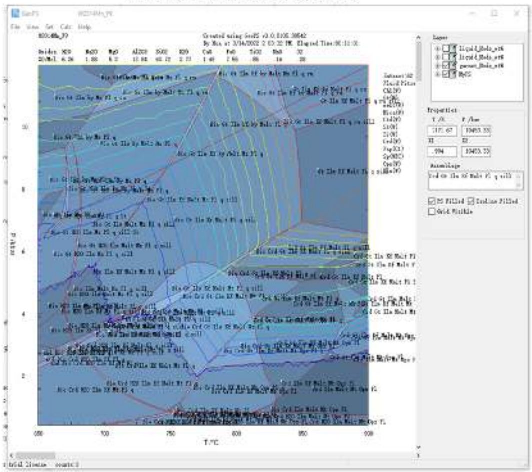
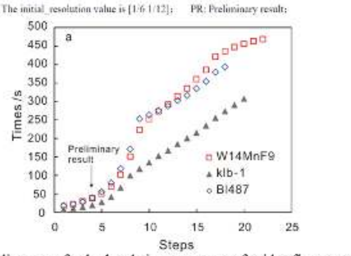


Table 1 Computing time for several phase diagram sections using different software.

Fig.	a-x models	GeoPS computer II	Perple_X v6.9.0 [a]	Domino [b]
W14MnF9	Same with the Fig 9 of White et al., 2014b	7m17s; PR: ~50s	26m53s	1h12m19s
BL487a	Same with the Fig 6a of Green et al., 2016	6m31s; PR:<1m	14h35m [b]	2h00m25s
BL487b	Amph(DHP), No melt Others are Green et. al., 2016	1m10s PR: 20s	9m29s	
KLB-1	Jennings (2015)	3m41s; PR: ~30s	20m18s	

a: The initial_resolution value is [1/8 1/16], All other option values at default.
b: The initial_resolution value is [1/6 1/12]; PR: Preliminary result;



A diagram of calculated time vs. steps of grid refinement

S0706. A Convolutional Neural Network to classify garnet grains in 3D

Philip Hartmeier (University of Bern),
Thorsten Andreas Markmann (University of Bern),
Pierre Lanari (University of Bern)
Room: 106 2022-08-30 12:05

Quantifying the spatial variations of grain shapes in crustal rocks remains exceptionally challenging since imaging and chemical analysis are usually performed on thin sections. Micro-computed tomography (µCT) allows determination of the 3D distribution of minerals based on their physico-chemical properties. Whilst this technique can visualize individual grains, whose shapes then can be recognised by eye, robust statistics on several thousand grains are required to differentiate between distinct populations of a mineral based on grain geometry.

To address this limitation, we present an automated machine learning approach, which can recognize and classify grain shapes from 3D data. The algorithm is an application of image classification using a Convolutional Neural Network to µCT data. 3D voxel arrays of single grains are fed into the model, where they are converted to 2D raster images by integrating over the coordinate axes to preserve the information contained in the three-dimensional grain shape. These images are then classified using a deep neural network consisting of convolutional and fully connected layers. We focused on garnet grains, since this metamorphic mineral is widely used for thermobarometry and can be dated, making it thereby a valuable source of information for reconstructing the past pressure–temperature–time evolution of metamorphic rocks.

The algorithm for example successfully identifies atoll garnets, which exhibit resorption in their interior. Their distribution indicates the extent of fluid infiltration during exhumation at the sample scale. Preliminary results obtained on a retrogressed eclogite from the Zermatt-Saas-Zone in the Swiss Alps suggest a pervasive fluid flow during exhumation that is not controlled by prior heterogeneities such as compositional layering. Our findings also indicate potential that this algorithm is applicable to other minerals and rocks.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 850530).

S0707. Classification of chemical maps in XMapTools – Part 1: algorithms and strategy

Pierre Lanari (University of Bern),
Mahyra Tedeschi (Programa de Pós-graduação em Geologia da Universidade Federal de Minerais, Centro de Pesquisas Manoel Teixeira da Costa)
Room: 106 2022-08-30 12:07

The use of maps depicting the chemical composition of minerals drastically increased the amount of data used in recent petrological investigations. It is today straightforward to collect such maps with standard instruments, such as the electron probe micro-analyzer (EPMA) and the Laser Ablation Inductively Coupled Plasma Mass Spectrometer (LA-ICPMS). Combined with the availability of software solutions for data reduction, the mapping technique has become very popular in petrology and beyond. However, one critical and still challenging aspect is the classification of the chemical maps for generating maps of mineral distribution. In this presentation, we describe the implementation of a set of machine learning algorithms (Random Forest, Discriminant Analysis, Naive Bayes, Support Vector Machine, Classification Tree, k-Nearest Neighbor, k-means) for classification of various types of chemical maps in the open-source software solution XMapTools. The graphical user interface provides a user-friendly environment for selecting training data. The input data and the hyper-parameters of each algorithm were tuned to improve performances and accuracy of the results. We show that the Random Forest algorithm is the most powerful technique for classification of complex datasets containing millions of analyses and multiple elements (between 10 and 40). A probability of successful classification is calculated for each pixel and can be used to detect mixing pixels, i.e. pixels having a mixing composition between two or more minerals.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 850530).

S0708. Classification of chemical maps in XMapTools – Part 2: performance evaluation and application examples

Mahyra Tedeschi (Programa de Pós-graduação em Geologia da Universidade Federal de Minerais, Centro de Pesquisas Manoel Teixeira da Costa),
Pierre Lanari (University of Bern)
Room: 106 2022-08-30 12:09

The use of maps depicting the chemical composition of minerals drastically increased the amount of data used in recent petrological investigations. It is today straightforward to collect such maps with standard instruments, such as the electron probe micro-analyzer (EPMA) and the Laser Ablation Inductively Coupled Plasma Mass Spectrometer (LA-ICPMS). Combined with the availability of software solutions for data reduction, the mapping technique has become very popular in petrology and beyond. However, one critical and still challenging aspect is the classification of the chemical maps for generating maps of mineral distribution. In this presentation, we apply the Random Forest algorithm implemented in XMapTools to several datasets. The three case studies include (i) a high-pressure rock from Latto Hills (Togo) containing strongly zoned epidote formed after the destabilization of lawsonite; (ii) a chloritoid-staurolite-garnet schist from Southern Brasília orogen (Brazil); and iii) a garnet–biotite gneiss from the Canadian Grenville Province. The results of the classification algorithm are evaluated and compared with previous results on the same samples. This study demonstrates that the application of supervised machine learning algorithms significantly improves the classification, affecting other results for the sample, including: the local-bulk composition determinations, pressure and temperature estimates, and the determination of the mineral structural formula.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 850530).

S0710. Numerical advection schemes for an accurate and efficient modeling of magma ascent

Hugo Dominguez (University of Bern),
Pierre Lanari (University of Bern),
Nicolas Riel (Johannes Gutenberg University)
Room: 106 2022-08-30 16:30

Although recent developments in geodynamic modelling allow us to better capture the coupled dynamics of two-phase systems, quantifying the chemical processes at play remain a very challenging task. This is mostly due to

the high computational cost of phase equilibrium calculation and to the limitations of the available numerical techniques in charge of transporting the chemical information.

A commonly used approach to transport material properties is the Lagrangian Particle-In-Cell (PIC) technique. On one hand, this method is always stable and has no numerical diffusion. On the other hand, PIC technique is inherently non-conservative, and due to large particle population, phase equilibrium calculation cannot possibly be computed for every particle with realistic run-time.

Alternatively, Eulerian advection schemes such as the upwind scheme are conservative by essence and have for advantage to be computed at the grid resolution. However, they are usually highly diffusive or oscillatory on sharp gradients which constitutes a critical drawback when applied to magma transport.

In this study, we present two Eulerian alternative strategies based on high-order numerical techniques: a Weighted Essentially Non-Oscillatory scheme (WENO) and a Conservative Quasi-Monotone Semi-Lagrangian scheme (CQMSL). The WENO scheme is a non-linear Eulerian advection scheme. It is locally conservative, shows very small numerical diffusion and is non-oscillatory. The CQMSL scheme is a scheme that takes advantages of both Eulerian and Lagrangian frameworks, being always stable and globally conservative. These two schemes were implemented to compare their advantages and drawbacks using analytical solutions in 1D and 2D for constant and non-constant velocity fields. We then applied the WENO and CQMSL advection schemes to a realistic 2D case study of magma flow in a porous solid matrix.

The results show that these 2 schemes are conservative. They are good alternative to the classical PIC technique and allow to drastically decrease the thermodynamic computational load.

S0711. Numerical modeling of formation of a porphyry-copper ore shell: implications for the mechanism of metal enrichment

Fan Xiao (Guangdong Provincial Key Lab of Geological Process and Mineral Resource Survey),
Weilin Chen,
Kaiqi Wang (Sun Yat-sen University)
Room: 106 2022-08-30 16:55

Porphyry copper deposits (PCDs) are the most important sources of copper and molybdenum, providing about 75% of the world's copper resources, more than 50% of the metal molybdenum resources, formed by precipitation of metal sulphides from hydrothermal fluids released by magmatic intrusions that cooled at depth within the Earth's crust. The metals are typically concentrated in confined ore shells within vertically extensive vein networks. In this contribution, the finite-element method was used to simulate the fluid migration, heat transmission and mineralization of PCD formation process. Numerical modeling results show that hydrothermal flow is the main factor controlling the mineralization. Dynamic permeability responses to magmatic fluid expulsion can stabilize a metal precipitation above the magma chamber, forming a crescent-shaped metal enriched shell. The metallogenic duration as well as temperature gradient controls the most important economic characteristics of ore shell including shape, aggregation and ore grade. The validity of numerical model is verified in the Dexing porphyry copper deposit, which confirms the results of the coupled model in the field of emerging computational geoscience and provides insights into the mineralization process.

S0712. Petro -geochemical modelling of subduction zone metamorphism: Interplays between rock and aqueous fluids

Thorsten Andreas Markmann (University of Bern),
Pierre Lanari (University of Bern)
Room: 106 2022-08-30 17:20

The release of aqueous fluids within the crust and interactions with surrounding rocks are fundamental processes on Earth especially in subduction zones. Examining the mineral record of high-pressure rocks exhumed to the surface can elucidate the pathways of aqueous fluids during metamorphism. Fluctuations in the 18O composition of fluids are recorded in the oxygen isotopes of minerals from blueschist and eclogite facies rocks. In these settings, the breakdown of minerals can trigger pervasive fluid flow because metamorphic reactions modify the rock volume. Documenting such triggers is critical for understanding the shift between closed and open system behaviours and how aqueous fluids flow at high-pressure conditions. Important aspects are: (1) mineral reactions and their impact on system properties (2) reaction overstepping which can delay metamorphic reactions.

The petro-geochemical model presented herein simulates rock dehydration and fluid extraction at equilibrium via metamorphic reactions along typical subduction pressure-temperature-time gradients. For several rock types, the model uses Gibbs Energy minimization coupled with a physical model for fluid extraction and oxygen isotope fractionation. It shows that changes in mineral assemblages and mineral modes are important for creating fluid-filled porosity in subducting rocks. For example, the lawsonite out and garnet in reaction for a subducted metasediment at 550 °C and 2.4 GPa can easily reach one volume percent of fluid-filled porosity accompanying a change in density of 20 kg/m3. The effects of reaction overstepping on the generation of fluid-filled porosity and the conditions of the main extraction steps (continuous or episodically) were also investigated. Efforts are made to predict overstepping based on changes in the total energy of the system.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 850530).

S0713. Presentation of Thermotopes-COH, a software for isotopes calculations of C bearing species, and fluid speciation of COH-fluid

Antoine Boutier (Laboratoire de géologie de Lyon : Terre, Planètes, Environnement),
Alberto Vitale Brovarone (BiGEA, University of Bologna),
Isabelle Martinez (Institut de Physique du Globe de Paris, Sorbonne Paris Cité),
Isabelle Daniel (Université Claude Bernard Lyon)
Room: 106 2022-08-30 17:45

The carbon cycle is a central topic of the Earth-system sciences, linking geological and biological processes and shallow to deep energy. In particular, carbon is omnipresent in geologic fluid, either in small amounts in aqueous fluid or dominant in CO2-rich or hydrocarbon-rich fluids. The isotopic evolution of a redox-sensitive element like carbon is strongly related to the thermodynamics of the considered geologic system. The COH thermodynamic system has long been used to assess the evolution of carbon-bearing fluids as a function of pressure (P), temperature (T), and redox state (e.g., fO2; XO). It also provides a solid thermodynamic basis to reconstruct the isotope evolution of molecular carbon-bearing fluid species (mainly CH4 and CO2) and graphite/diamond as a function of the considered P-T-redox variations. Thermotopes-COH is a python-based software allowing modeling of conventional carbon isotopic exchanges and more advanced thermodynamic and isotopic processes in the C-O-H system and in the 300 - 900 °C and 1 - 50 kbar pressure-temperature range. The software allows user-friendly modeling and graphical visualization of five major functions: (1) Carbon isotope equilibrium between two phases, (2) Carbon isotope fractionation modeling, (3) C-O-H fluid speciation, (4) Multi-component diamond/graphite precipitation, and (5) Diamond/graphite precipitation/dissolution. The software is available for Windows or MacOS. Data produced by the software can be saved as .txt file and .svg file.

S0714. Protocol for improving reproducibility and image acquisition quality for deep learning application in mineralogy

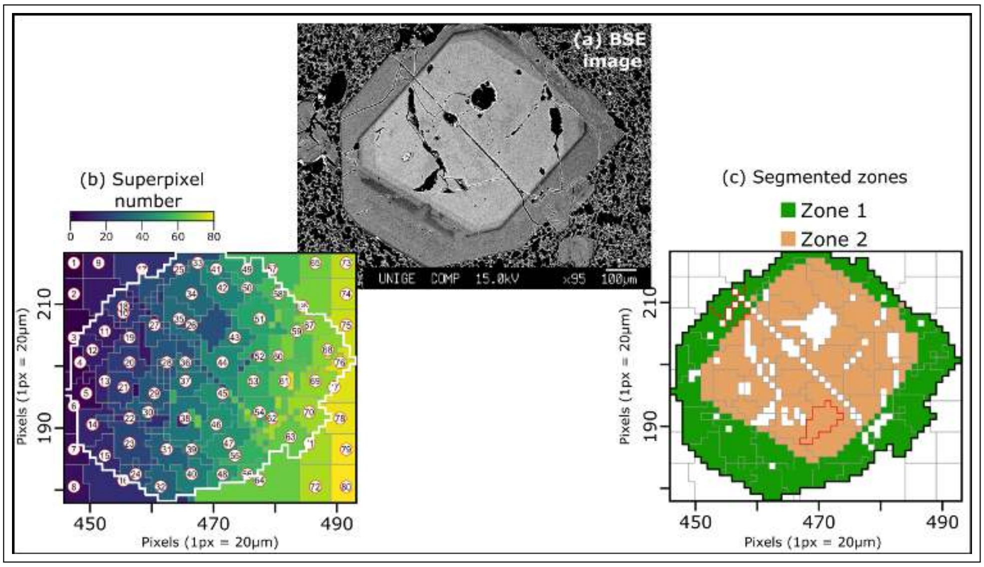
Arnaud Back (UQAC),
Paul L. Bédard (UQAC),
Julien Maitre (UQAC),
Ghazanfar Latif (UQAC),
Kevin Bouchard (UQAC)
Room: 106 2022-08-31 09:50

Mineral identification is essential for geology, mining exploration, environmental science, and engineering. Machine learning based on photographs or photomicrographs offers a fast, cost-effective, and reliable means of mineral identification. Although there has been a rapid increase in the number of papers detailing mineral recognition using machine-learning algorithms, little research has addressed the image acquisition part of these processes. Artificial intelligence requires reproducible, high-quality data to perform complicated tasks such as mineral identification. To address this requirement, we propose a practical image acquisition protocol for optical microscopes. Our protocol focuses on two main objectives: (1) ensuring reproducibility and (2) enhancing mineral image quality. In terms of reproducibility, this study details how to manage camera errors and provide standard utilization and experimental parameters, such as external light and temperature. For image enhancement, we specify the lighting choice and its impact on algorithm accuracy, lens selection, and white-balance calibration. We test our protocol using a case study of mineral recognition from till sample photomicrographs and a machine-learning algorithm. The study sample is a heavy mineral concentrate of till comprising about 15 mineral species. This protocol will ensure the reliability of data acquisition and increase the image quality for multiple photomicrographic deep-learning applications such as mineral recognition.

S0715. Segmentation and correlation of zoned crystals from 2D chemical compositional maps

Tom Sheldrake (University of Geneva),
Oliver Higgins (University of Geneva),
Luca Caricchi (University of Geneva)
Room: 106 2022-08-31 10:15

In nature, many crystals exhibit chemical zonation that reflects changes in the state of the local environment from which they grew. To understand the genesis of an individual crystal, it is important to compositionally characterise each of these different chemical zones and their relationship to each other. Whilst the human eye is adept at identifying 2D zonation, automation of this process is complicated by chemical variability within distinct zones. By adapting a series of algorithms primarily designed for image segmentation, we characterise chemical zonation in 2D chemical maps containing hundreds of crystals. This permits statistical comparison and correlation of mineral zonation both within and between multiple geological samples. Such a feat has proved difficult via an array of 1D and 2D approaches, especially when it is not possible to control the plane of a crystal which is cut and polished. Ultimately, our tool allows us to intimately track chemical variability both temporally and spatially in geological systems. We show this by correlating plagioclase zonation in a stratigraphic sequence of volcanic deposits on the island of St. Kitts.



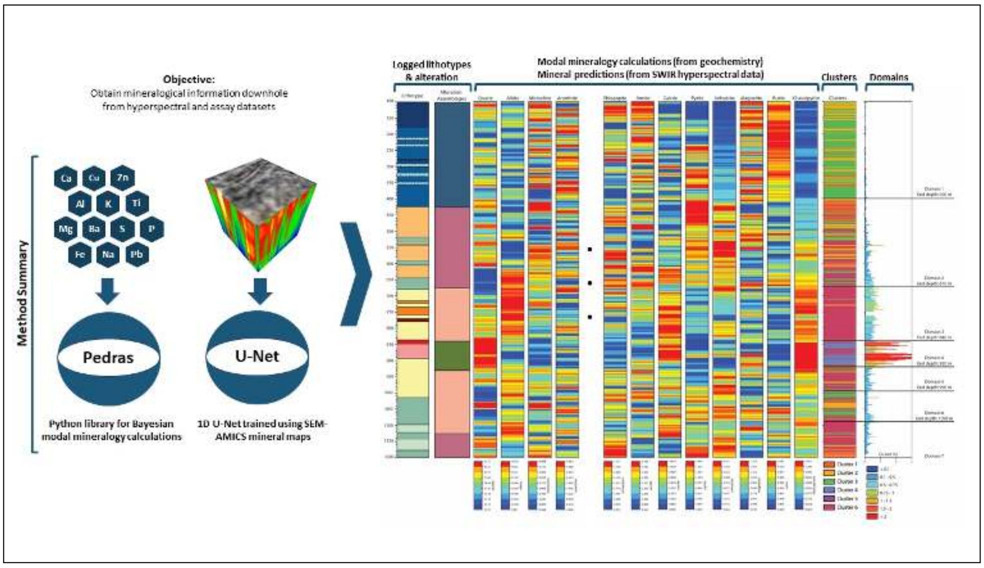
S0716. Machine supported mineralogical interpretations from hyperspectral and geochemical datasets

Angela Rodrigues (Monash University),
Laurent Ailleres (Monash University),
Lachlan Grose (Monash University),
Robin Armit (Monash University),
Matthew Cracknell (University of Tasmania),
Mehrtash Harandi (Monash University),
Angela Escolme (University of Tasmania),
Scott Halley (Mineral Mapping Pty),
Himashi Peiris (Monash University)
Room: 106 2022-08-31 10:40

The combination of hyperspectral and geochemical datasets provides valuable insights about the mineral distribution within a porphyry copper deposit, since variations in mineralogy reflect variations of lithotypes, hydrothermal alteration and mineralization. While visual core logging is a commonly used technique to co-register these variables downhole, the process suffers from some limitations, as it is a manual, time-consuming and subjective technique.

Shortwave infrared hyperspectral data and whole-rock geochemical data are an industry standard of downhole data collection, and can be used as a rapid proxy for mineralogy, which, in turn, can guide the process of core logging, and provide invaluable insights on the deposits' paragenesis. This contribution introduces a workflow that allows the upscaling of information contained in hyperspectral and geochemical datasets into mineralogical domains from drill-core data.

More specifically, the workflow shows how modal mineralogy calculations (via Bayesian inference applied to assay data) and mineral classifications (via a convolutional neural network from hyperspectral data) can be used to domain drill-hole data. Both methods are applied to datasets obtained from a drill hole within the Wainaulo porphyry copper deposit, located in the Republic of Fiji. Seven major mineralogical domains downhole are obtained, reflecting different types of lithotypes, alteration and mineralization patterns. These mineralogical domains be used to objectively guide the process of core-logging. The modal mineralogy outputs also provide invaluable insights of mineral associations that vector towards mineralization: for the case of Wainaulo, it has been described that iron-rich chlorite is associated with copper mineralization; this correlation is corroborated by our downhole modal mineralogy calculations.


Objective:
Obtain mineralogical information downhole from hyperspectral and assay datasets
Method Summary
Ca
Cu
Zn
Al
K
Ti
Mg
Ba
S
P
Fe
Na
Pb
Pedras
U-Net
Python library for Bayesian modal mineralogy calculations
1D U-Net trained using SEM-AMICS mineral maps
Logged lithotypes & alteration
Modal mineralogy calculations (from geochemistry)
Mineral predictions (from SWIR hyperspectral data)
Clusters
Domains

S0717. Supported development and application of machine-learning models on mineral X-ray maps: the software X-Min Learn

Alberto D'Agostino (University of Catania),
Gaetano Ortolano (University of Catania),
Roberto Visalli (University of Catania),
Michele Zucali (University of Milan)
Room: 106 2022-08-31 11:05

Over the recent years, the use of machine learning (ML) algorithms has spread over many industrial and scientific fields. Due to the great amount of data that can be extracted from rocks thin sections through EDS and WDS X-ray maps, one of the geoscience fields that may potentially benefit from ML algorithms is mineralogy (and petrology consequently). Nevertheless, often the lack of programming skills represents a gap that prevent geoscientists to make the most out of ML libraries potential. Our proposal is to try to fill such gap through the development of a new ML-oriented software (X-Min Learn) for mineral X-ray maps analysis.

X-Min Learn is developed to stepwise guide users towards the creation of customized supervised ML models adapted to their specific needs, starting from the creation of training datasets up to the selection of the hyper-parameters to obtain an optimal training. This, in turn, can lead the operator to develop a greater knowledge of the potential and operational functioning of ML.

The software provides a friendly environment to test well-known supervised and unsupervised algorithms to predict the mineral mode and composition from input X-ray maps. Several statistical scores and graphics can be extracted to evaluate the performance of each prediction; morphological image processing algorithms can be applied to reduce the noise of the output, allowing a full control of the operator on the final result. The algorithms can be recursively repeated to identify potential mineral zoning patterns as well as to extract mineral reaction boundaries.

X-Min Learn is under development, but can already be used to process X-ray maps data in a pixel-oriented fashion. Under construction is a procedure for quantitative mapping and calibration of the data, fundamental step to be taken to extract useful and reliable information from the input maps.

S0718. Two-dimensional thermodynamic forward model of water transport in subduction zones to calculate the globally subducted water – a tool to quantify and visualize differences in thermodynamic datasets and equations of state

Nils Benjamin Gies (University of Bern),
Matthias Konrad-Schmolke (University of Gothenburg)
Room: 106 2022-08-31 11:30

The deep water cycle in subduction zones is of significant importance for numerous geological, petrological and geophysical processes from the Earth's surface to the mantle. In particular, subduction of the hydrated lithospheric mantle and water release are important parameters for the transfer of water, in volcanic arcs and to depths greater than 350 km. Thus, the interplay of the thermal structure, the initial hydration intensity and the stability of hydrous phases within the subducted slab controls slab dehydration and the amount of water transported into the deeper mantle.

We have created a numerical model that calculates the effects of different thermodynamic data sets and equations of state on the Earth's deep water cycle. We use a combination of MATLAB and Perple X to quantify the water budget in the slab. Using a gridded two-dimensional thermodynamic forward model, which takes the migration of fluids within the slab into account, the effects of different thermodynamic databases and equations of state, thermal and geometric patterns of subduction zones, and chemical compositions can be benchmarked and quantified.

Using the example of phase A and Mg-sursassite in the hydrated lithospheric mantle of the subducted plate, we show the differences in the migration of fluids within the plate and the different dehydration.

This reveals an increase of 150 °C in the potential stability boundary of the hydrous phases. This implicates that the potential water transport in a partially hydrated oceanic mantle lithosphere to greater depths in moderately hot subduction zones is significantly increased and holds the potential to allow water transport into the mantle transition zone.

Our model has the potential to be extended including trace element and fluid chemistry modelling and allows to quantify the resulting differences of new thermodynamic, geometric or thermal datasets and provides a relatively simple insight into water transport in subduction zones.

S0719. From data to model: Microstructure aware models for reactive transport in granitoid rocks

Solveig Pospiech (Institute for Resource Ecology, HZDR),
Raimon Tolosana-Delgado (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Vinzenz Brendler (Institute of Resource Ecology, HZDR),
Kai Bachmann (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Joachim Krause (Helmholtz Institute Freiberg for Resource Technology, HZDR),
K. G. van den Boogaart (Helmholtz Institute Freiberg for Resource Technology, HZDR)
Room: 106 2022-08-31 11:55

Safety of nuclear waste repositories in crystalline host rocks depends on realistic predictions of radionuclide migration in undisturbed geologies beyond the geotechnical barrier. There, fluids will migrate - in absence of large scale connectivities like fissures, fault systems and joints - along weakzones like microcracks, alterations and grain boundaries. The retention potential of crystalline rocks is thus not only controlled by its modal mineralogy but also by the (heterogeneous) distribution of mineral grains and the contact area of different mineral surfaces to migration paths. Until now, reactive transport models assume homogeneous and isotropic distribution of minerals in the host rock. Including the spatial correlation of transport and mineralogy, especially the modal mineralogy along fluid migration paths in the various scales, would significantly improve the estimation of radionuclide retention potentials.

In this contribution we focus on the small scale correlation in the microstructure. We present a workflow from (real) samples to microstructure aware retention models, and discuss challenges of input data uncertainties, how they affect the model, and whether these models can be used for upscaling. Our approach is based on the idea that models for heterogeneous distribution of mineral phases can be derived by estimating spatial co-occurrences from measured microstructures. Our workflow requires analytical spatially distributed data, which a) provide information about mineral composition including voids and b) allow to detect migrations paths and the mineral surface types with related areas. Here, information from gneissic samples is used to train a structure simulation model. The resulting variability of "accessible" mineral surfaces then allows to derive (by geochemical speciation codes) the variability of contaminant distribution coefficients based on sorption data and pore water composition. Finally, the lithological predictions are applied in reactive transport models to calculate the effective radionuclide retention within a representative rock volume.

S0720. Presenting a new tool for working with spatial spectroscopic data

Nils Benjamin Gies (University of Bern),
Jörg Hermann (University of Bern),
Pierre Lanari (University of Bern)
Room: 106 2022-08-31 11:57

Spectroscopic data are an essential component of modern Geosciences. In the past years there was a significant shift in petrology and crystallography from using single-spot analysis to 2-dimensional mapping. Differences in signal through different areas can help to reveal patterns in a sample which would be not detected with single point measurements. Filtering and extracting signal information from multiple pixels can help to improve the signal to noise ratio and thus the quality of data.

In this contribution, we present a software solution for preparing, editing extracting and comparing spatial spectral datasets. The extraction of spectra from chosen regions of interest represents a quick and efficient way to compare signals between different areas in datasets and to prepare these spectra for further calculations. Deconvolution of a large number of complex spectra allows the investigation of relations between the peak position (or shape) and location within the sample. These maps can then be exported, which makes it possible to apply statistical tools and find correlation between the spectral dataset and quantified chemical data of the same area.

Application examples based on Fourier Transform Infrared Spectroscopy (FTIR) data will be presented, especially for imaging the distribution of trace amounts of H2O in clinopyroxene. The water absorption spectrum of clinopyroxene is composed of many different overlapping peaks representing different point defects of H2O incorporation. Due to the monoclinic crystal symmetry of clinopyroxene, absorption bands vary in intensity depending on the orientation and polarization angle of the IR light. In order to be able to assign these peaks to defects and coupled substitutions in the crystal lattice, a spatial correlation of deconvoluted peaks in different maximum polarizations is necessary.

The program can also handle any data type containing a map of wavenumber, energy, frequency, wavelength and intensity.

S0721. Quantitative compositional mapping by LA-ICP-MS: a software solution for multi-phase application

Thorsten Andreas Markmann (University of Bern),
Pierre Lanari (University of Bern),
Francesca Piccoli (University of Bern),
Mona Lüder (University of Bern)
Room: 106 2022-08-31 11:59

The analytical technique of LA-ICP-MS is largely used in the geosciences for in-situ determination of the chemical composition of minerals with a high spatial resolution. Geological materials can host textures in elemental and isotopic compositions that are otherwise not perceptible to the naked eye. Mapping and imaging of such patterns is a major step helping geoscientist to understand the formation of geological products. Acquiring two-dimensional, quantitative and meaningful data from LA-ICP-MS mapping experiments is not trivial. It requires an analytical procedure and an adapted data reduction scheme including pixel allocation and multi-phase calibration.

In this work, we present a software solution that covers data reduction and image generation of multi-element mapping experiments using LA-quadrupole-ICP-MS. The tool is implemented in the open-source software XMapTools. Instrumental conditions have a direct effect on the image quality and so have the pixel allocation strategies. Rendering to quadratic pixels by interpolation outperforms averaging where one pixel comprises several sweep times. To benchmark the LA-ICP-MS imaging tool a digital sampling model was applied to an annulus of fixed concentration. Depending on the texture size analysed, the spot size together with the scanning direction can lead to a shift in composition depending on the size and orientation of the measured feature.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement No 850530).

S08 Analyzing compositional data in geosciences

Jennifer McKinley (Queen's University Belfast),
Karel Hron (Palacky University),
Alessandra Menafoglio (Politecnico di Milano)

Compositional data analysis deals with vectors whose components show the relative importance of parts of a whole. This type of data appears in many geological applications commonly expressed as percentages, ppm, or the like. Since the log-ratio approach to compositional data analysis was introduced back in the 1980s, steady progress has been made in methodological approaches, visualization techniques, data modelling and applications. Submissions that cover these topics for analyzing compositional data in geosciences are welcomed, with particular emphasis on the problems related to earth resources and the environment.

S0801. Deviations from compositional equilibria

Vera Pawlowsky-Glahn (University of Girona),
Juan José Egozcue (Technical University of Catalo),
Antonella Buccianti (Universitá degli Studi di Fire)
Room: auditorium 2022-08-30 14:35

The law of mass action states that for a chemical reaction mixture that is in equilibrium, the ratio between the powered concentrations of reactants and products is constant. Other well-known examples include chemical equilibria regulated by stoichiometry in mineralogy. These equilibria appear as a restriction in the sample space of compositional data. For example, olivine crystals have stoichiometry that corresponds to a non-linear equilibrium. This non-linearity is caused by the possible substitution of magnesium (Mg) atoms by iron (Fe) atoms and vice versa. A compositional approach to model this aspect in a set of samples is presented. It consists of a linearisation, which is achieved by adding terms to the original composition. In the case of olivine crystals a term, computed as the addition of the measured atom concentrations of Mg and Fe, is added to the original composition. The deviation to the equilibrium locus is shown to be the Aitchison distance between an observation and its orthogonal projection on that locus.

S0802. Prediction of the rock mass class with machine learning models trained on synthesised data.

Alla Sapronova (Graz University of Technology),
Paul Johannes Unterlas (Graz University of Technology),
Thomas Dickmann (Amberg Technologies AG),
Jozsef Hecht-Méndez (Amberg Technologies AG),
Thomas Marcher (Graz University of Technology)
Room: auditorium 2022-08-30 15:00

Geological risk assessment during the construction of an underground structure (e.g., tunnel) is based on available information describing the rock mass that will be excavated. At present, engineering equipment can obtain massive in-situ data at runtime, and this opens a possibility for data-driven prediction of geological conditions for effective proactive risk management.

Recent progress in data science and the development of machine learning opens a possibility to predict the geological conditions ahead of the tunnel face. The development of reliable methods capable of yielding an accurate prediction is highly dependent on the quality of the data. One of the main difficulties in developing accurate machine learning-based models is the extreme sparseness and imbalance of engineering data. However, the oversampling procedure could help to overcome the limitations arising from training the machine learning models using an imbalanced dataset. The main question remains whether and to what extent the synthesized data can be used in classification and regression tasks as a substitution for real observations to train the machine learning models in geoengineering.

We used available geological information and seismic data from Gotthard Base Tunnel, Switzerland, and Rogfast Tunnel, Norway that exhibited various degrees of imbalance between mass classes. We applied two oversampling techniques, SMOTE and ADASYN, to gain more training samples for the underrepresented rock mass classes. The synthesized data was used to train a classifier to predict the rock mass class.

In this work, we targeted not only improving the classifiers' accuracy with oversampling but also checking whether the oversampled data can be used to substitute the missing observations. By assessing the quality of generated data, we can determine the extent to which the oversampled data can mirror real-world observations. In case of success, the oversampling can be further utilized to predict extremely rare events.

S0803. Soil organic carbon mapping combining environmental and depth information

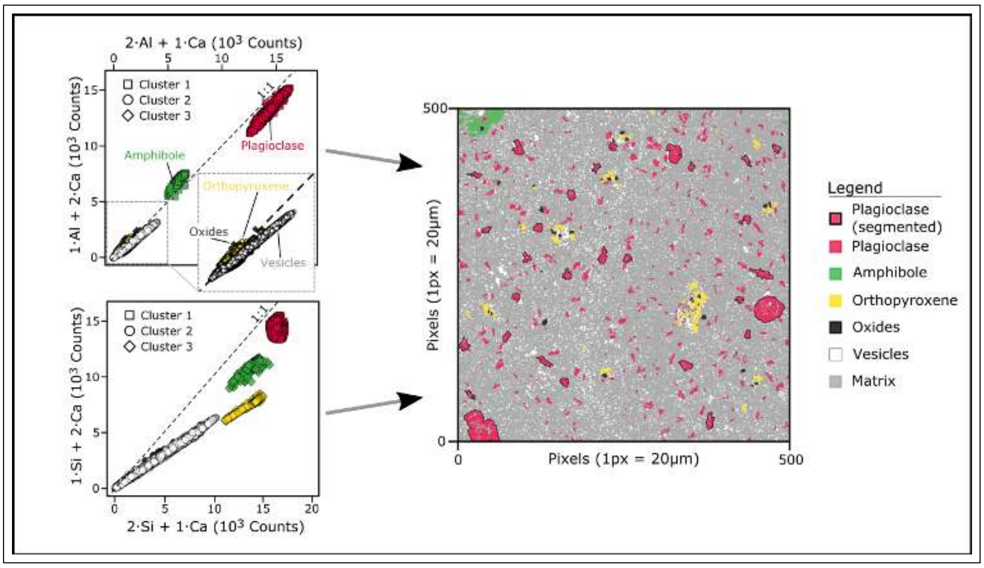
Mo Zhang,
Wenjiao Shi,
Yong Ge
Room: auditorium 2022-08-30 15:25

Soil organic carbon (SOC) is vital to the global carbon cycle and ecological balance. More accurate and detailed spatial prediction of multilayer soil organic carbon density (SOCD) can help gain a better understanding of the changes in multilayer SOC stocks and carbon dynamic processes. However, previous mapping technique still have their limitations, such as ignoring the relationship between and interaction of different depths and not fully utilizing statistical analysis of soil samples and surface classification information, leading to lower accuracy and greater uncertainty. Here, we propose new methods based on the proportional allocation of soil depth for multilayer mapping using log-ratio transformation. We compared the methods that use the exponential and equal-area spline functions, as well as independent modeling without depth information. The generalized linear model and random forest were used to produce predictive models of the Sanjiang Plain, northeastern China. The results demonstrated that the model using the exponential function overestimated the predicted values and performed poorly, indicating that the blind use of depth information increased the prediction error, and thus further classification was necessary. The proportional allocation methods performed better than other sperate modeling methods for accuracy and interpretability, especially for the middle and bottom layers. The generalized linear model generated more aggregated predictions than the random forest model, losing the distribution pattern of the original data. We also calculated the SOC stocks in the Sanjiang Plain using our new methods, which were more reasonable compared with those of previous studies and had the advantages of in-depth information, environmental variable selection, and model optimization. Our findings can provide not only other perspectives for SOCD mapping, with more fully integrated depth information and more accurate assessment of multilayer SOC stocks, but also can provide guidance for the evaluation of land quality, farmland, and ecological environmental management.

S0804. Classification of mineral grains using finite mixture models

Tom Sheldrake (University of Geneva),
Oliver Higgins (University of Geneva)
Room: auditorium 2022-08-30 15:50

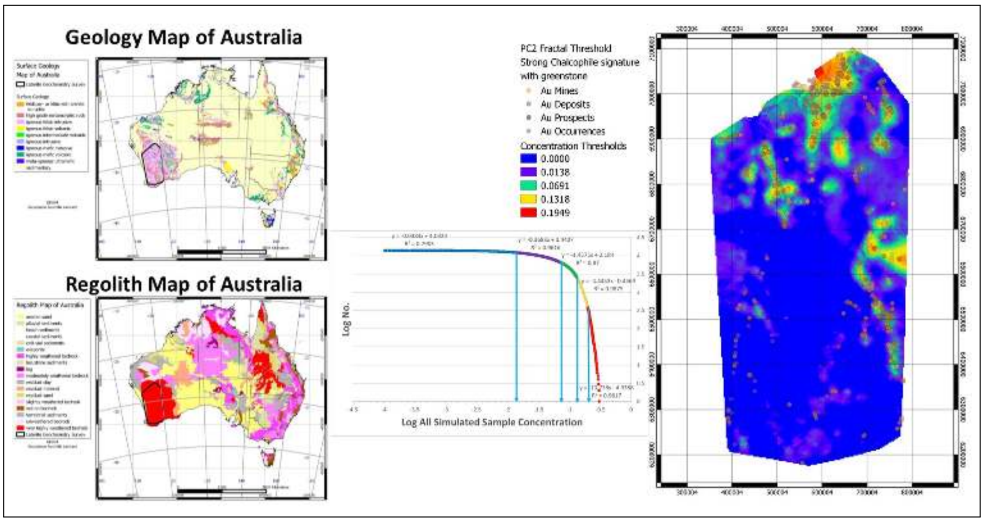
The combination of machine learning techniques with geochemical compositional maps has led to automated mineral recognition in thin sections. Such an approach provides rapid quantitative data to calculate statistics such as modal abundances, which can be used to classify and compare geological samples. Recently, a developing field of research has looked to use these geochemical maps for more demanding tasks such as crystal segmentation, barometry, or thermometry. Such tasks, however, require careful calibration of the machine learning techniques to ensure individual pixels are correctly classified, especially along grain boundaries or where small mineral inclusions may exist. Driven by a goal to segment individually zoned crystals, we have developed a novel mineral recognition method using finite mixture models. This approach can correctly identify pixels that constitute complex mixtures of different mineral and/or non-mineral phases. This is important to ensure the accuracy of further analysis of 2D geochemical maps once minerals phases have been classified.



S0805. Compositional-Category-Based modeling: a new insight for geochemical anomaly classification

Behnam Sadeghi (EarthByte Group, School of Geosciences, University of Sydney), Eric Grunsky (University of Waterloo)
Room: auditorium 2022-08-30 15:52

In regional mineral exploration, we strongly need to consider the target element concentration through a multivariate point of view using compositional data analysis and to study the geochemical samples in individual groups, based on the host rocks from which the samples have been collected. This helps with a better geological insight over the samples. In this research, both factors were studied together to study the Yilgarn region, in Western Australia, which is a rich polymetallic area, specifically for gold mining. There are lots of active mining projects in this region along with many new exploration projects. To come up with a better insight into this region and its gold potential deposits, this research aims to review the available data (including 820 lithological samples) based on the above-mentioned factors. To do so, the category-based fractal (CBF) model was applied to the principal components (mainly PC2), obtained based on centered log-ratio transformed and opened data, to study the Cu-Ni-Zn-Co-Mn-Au commodity. To apply the CBF model, 7 main rock types were taken into account, including meta-igneous felsic intrusive, metamorphic protolith unknown: gneiss, igneous granitic, meta-igneous ultramafic volcanic or undivided, igneous mafic volcanic, sedimentary siliciclastic, and several others generally classified as unknown rock types. Because the number of the samples per bedrock is not similar due to some limitations such as lack of access, time, and topography, in the CBF model, Monte Carlo Simulation is applied to each bedrock's samples to homogenize their number to a large simulated group of values. In the end, the CBF fractal model was applied to the whole simulated values to classify them from background to anomalies. Based on the final map created using the defined thresholds obtained by the CBF model, the main gold anomalies in Yilgarn are concentrated in the northern and central-eastern parts of the region.



S0806. Compositional scalar-on-function regression with application to sedimentary geochemistry

Karel Hron (Palacky University),
Tomas Matys Grygar (Institute of Inorganic Chemistry of the Czech Academy of Sciences)
Room: auditorium 2022-08-30 16:30

The chemical composition of sediments is controlled predominantly by the sediment grain size, and thus evaluating their relationship is an important task in sedimentary geochemistry. The grain size is characterized by the respective particle size distribution, which can be expressed as a probability density function. Because of the relative (compositional) character of densities, the Bayes space methodology need to be employed to build a regression model between a real response and a density function as a covariate, here the chemical composition and the particle size density. For practical computations, density functions are expressed in the standard L2 space using the centred logratio transformation and spline approximation of the input discretized densities is utilized by respecting the induced zero-integral constraint. In the contribution a simulation study, supporting the relevance of the proposed regression model, will be presented and the new methodology will be applied to examine the relationship between sediment grain size and geochemical composition, with samples being obtained in the Czech Republic in the Skalka Reservoir and in the Ohre River floodplain upstream of the reservoir, to reveal proper grain size proxies.

S0807. Compositional MAF and random forest analysis of geochemical data to reveal geochemical signatures for sustainable resource availability and environmental resilience

Jennifer McKinley (Queen's University Belfast),
Ute Mueller (Edith Cowan University),
Eric Grunsky (Department of Earth and Enviro),
Ray Scanlon (Geological Survey Ireland),
Vincent Gallagher (Geological Survey Ireland),
Laura Smith (Geological Survey Ireland),
Mairead Fitzsimons (Geological Survey Ireland),
Mark Cooper (Geological Survey of Northern Ireland,)
Room: auditorium 2022-08-30 16:55

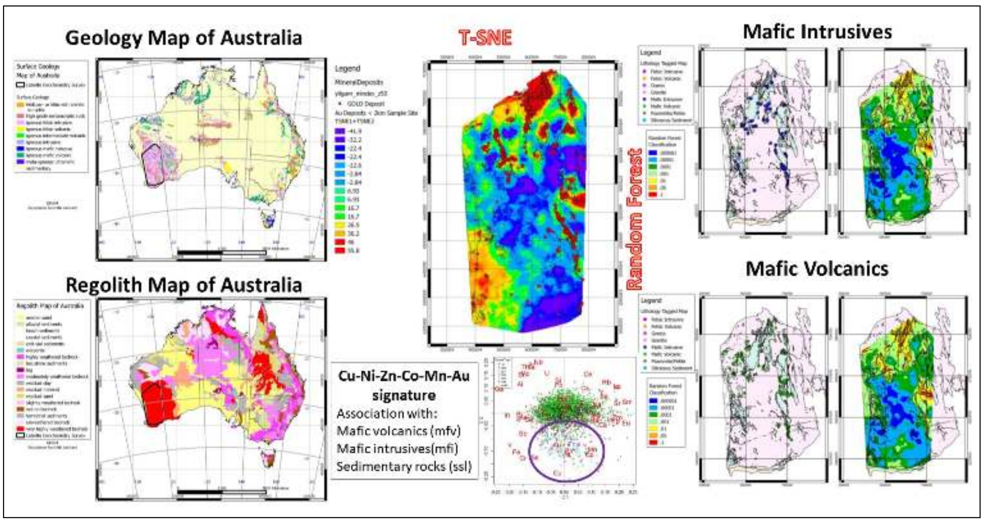
Sub-continental and national scale surveys provide high-resolution, spatially-located geochemical open-access datasets. However, these big datasets are still currently underutilized for informing critical land use planning decisions, especially with regards to mitigating and adaptation to the expected impacts of climate change on resource availability and environmental resilience. National surveys funded by major government and European investment to gather geochemical data across the island of Ireland include the Tellus Project (a Department of Environment (DfE)-funded programme) for Northern Ireland (NI), Tellus Border (EU INTERREG IVA-funded a joint programme between NI and Republic of Ireland (RoI)) and the current Tellus Programme (a RoI national programme). Datasets such as geochemical survey data pose many challenges for exploratory data analysis and any subsequent geostatistical analysis. Compositional data analysis (CoDA) methods are frequently used to extract information from geochemical data by treating log ratio or equivalently transformed data instead of analysing the raw constant sum values. Using the Tellus soil geochemical database this study investigates compositional multivariate techniques including minimum/maximum autocorrelation factor (MAF) analysis that uses the spatial relationships of the data to assess natural resource availability. The MAF components for each sample site are merged based on the nearest mineral occurrence/prospect/deposit and specific commodities, using a distance threshold (2500m for this study). A training set is established by selecting sample sites with mineral occurrences within the threshold distance limit and test data represent sample sites outside the threshold distance. A Random Forests classification/prediction procedure is applied to test the prediction of commodities of the training and test datasets. Geospatially coherent maps of the posterior probabilities define the predicted extent of the selected commodities. Such an approach has the potential to focus exploration on areas with the highest potential to host natural resources.

S0808. Predictive Lithologic Mapping and Prediction of Potential Mineral Resources using a Probabilistic Approach with Multivariate Methods: a case study in Western Yilgarn, Australia

Behnam Sadeghi (EarthByte Group, School of Geosciences, University of Sydney), Eric Grunsky (University of Waterloo)

Room: auditorium 2022-08-30 17:20

The use of multi-element geochemistry and geospatial analysis of rocks, soil, stream/lake sediments, regolith, and weathered materials can be very effective in the prediction of mineral resources and underlying bedrock lithologies. Such applications assist with rendering interpretable results and provide patterns that describe geochemical/geological processes associated with underlying lithologies and potential ore mineralization. These patterns can be expressed in qualitative and quantitative terms at regional scales, e.g., >1:250,000. The results obtained can be presented in a probabilistic framework thereby assigning levels of confidence/risk in predictive mapping and resource identification. Multi-element geochemical data contains information about the source (protolith) and subsequent modifications through a range of processes (alteration, mineralization, weathering). In this research, the Western Yilgarn region in Western Australia was studied with the main intent of mapping and identifying the different laterite types that are associated with weathering, climate, and geology. The prediction of the geology is fairly evident, but the relationship of the laterite type with climate and weathering is less clear. Therefore, compositional data analysis in terms of application of centered-logratio (clr), and metrics including principal component analysis (PCA: PC1-PC2), in addition to random Forrest and t-distributed stochastic neighbor embedding (t-SNE: t-SNE1+t-SNE2) machine learning algorithms were applied to the whole dataset to provide associations and patterns that enable Process Discovery/Validation, mainly focused on Au deposits.



S0809. Case studies based on CoDA and ML

BingLi Liu (Chengdu University of Technology)
Room: auditorium 2022-08-30 17:45

Mineral resources assessment relies on Multi-resources data and the related data analysis methods. Geochemical data analysis and geochemical mapping for mineral prospectivity mapping stay in the frontier of Geosciences. At present, more and more experts recognized that geochemical data is compositional data. The Composition Data Analysis (CoDA) approach to geochemical data analysis typically uses knowledge- and data-driven data processing frameworks. The knowledge-driven framework is based on expert knowledge (e.g., knowledge of the geology and geochemistry of a study area) to identify geochemical patterns within a dataset. In comparison, the data-driven framework is based on mathematical solutions (e.g., hierarchical clustering) to identify geochemical associations. Machine learning and deep learning approaches including random forest, decision tree, convolutional neural network and so on, are also powerful tools to geochemical signatures identification. Some study cases from our research team based on CoDA and machine learning/ deep learning show significantly important evidences to regional or at-depth mineral resources prediction.

S09 Filters and smoothers. Filters or smoothers?

Jaime Gomez-Hernandez (Research Institute of Water and Environmental Engineering, Universitat Politècnica de València),
Liangping Li (South Datoka School of Mines and Technology)

Are you working with the Kalman filter, or the ensemble Kalman filter, or the ensemble smoother, or the extended Kalman filter, or the unscented Kalman filter, or the particle filter, or the diffuse Kalman filter, or the unscented particle filter, or the cubature Kalman filter, or the Gauss-Hermite quadrature filter, or the iterative ensemble Kalman filter, or the singular evolutive extended Kalman filter, or the iterative ensemble maximum likelihood filter, or the singular evolutive interpolated Kalman filter, or the error subspace transform Kalman filter, or the normal-score ensemble Kalman filter, or the restart ensemble Kalman filter, or the ensemble adjustment Kalman filter, or an square root Kalman filter, or the ensemble smoother with multiple data assimilation, or the iterative ensemble Kalman smoother? If so, this session is for you. Submit your abstract and explain your choice.

S0901. An open-source software package for the solution of generic inverse problems implementing ES-MDA

Valeria Todaro (University of Parma),
Marco D'Oria (University of Parma),
Maria Giovanna Tanda (University of Parma),
J. Jaime Gómez-Hernández (Technical University of Valencia)
Room: auditorium 2022-08-30 10:00

This work presents the development of an open source software package for the solution of inverse problems by means of ensemble Kalman filter methods. The Ensemble Smoother with Multiple Data Assimilation (ES-MDA) was considered as reference method. The ES-MDA is a data assimilation method that updates unknown parameters of the forward model assimilating the same system state data multiple times. The software package, named GENES-MDA, is written in the Python programming language and is designed with a flexible workflow that can be easily adapted for other variants of the Ensemble Kalman filter and, more importantly, to be applied for the solution of generic inverse problems. The code provides several functionalities to implement alternative configurations of the algorithm suited for the specific problem at hand. In particular, the GENES-MDA presents tools for the solution of inverse problems aimed at identifying forcing terms that are variable in time, a novelty for ES-MDA applications. The software package has been tested in several synthetic examples in the context of surface and subsurface hydrology. For

instance, the solution of the reverse flow routing problem for the estimation of the inflow hydrograph to a river reach based on observed water levels downstream and on a calibrated routing model of the system. Or, in the context of groundwater, the estimation of the hydraulic conductivity field using piezometric observations and a known forward flow model. Or the estimation of the release history of a contaminant spill in an aquifer based on measured concentration data and a calibrated flow and transport model. The good results of all tests demonstrated the capabilities of the ES-MDA and the flexibility of the software package to solve different types of inverse problems.

S0902. Ensemble Smoother Multiple Data Assimilation in hydrogeological modeling

Thomas Beraud (INRS-ETE),
Maxime Claprood (INRS-ETE),
Erwan Gloaguen (INRS-ETE)
Room: auditorium 2022-08-30 10:25

Ensemble methods are a type of data assimilation algorithms used in many geoscientific fields to update numerical models with spatio-temporal data. Most recent papers show efficiency in ensemble data assimilation method for 2D and 3D model with a lot of observations versus the number of parameters state to update. But in environmental studies, the characterization budget is limiting the amount of available information to build reliable numerical model.

In this example, we shown that data assimilation process is still reliable in hydrogeological modeling with only few observations. We applied our workflow to a synthetic 3D salt intrusion in a pumping well. We used FEFLOW for the modeling part and hydraulic heads and salt concentration time series to update the hydraulic conductivity field.

In our study, 6 temporal series were assimilated at 3 wells to update 68940 hydraulic conductivity elements. The classic assimilation method described in literature allow a mean improvement on RMSE of 20% on hydraulic head and salt concentration. Our method, with an approach based on well by well and parameter by parameter assimilation reach an improvement of 50%. Our method was also able to better improve the ensemble hydraulic conductivity field, reaching a log10 permeability RMSE of 0.532 versus 0.547 for the classic assimilation.

Our results are promising, showing that ensemble assimilation methods could be brought to hydrogeological studies with lor characterization budget.

S0903. Model-based ensemble Kalman filter

Håkon Tjelmeland (Norwegian University of Science and Technology),
Håkon Gryvill (Norwegian University of Science and Technology),
Margrethe Kvale Loe (Norwegian University of Science and Technology)
Room: auditorium 2022-08-30 10:50

The ensemble Kalman filter (EnKF) is used for data assimilation according to a state-space model. In EnKF the available knowledge about the conditional distributions is represented by an ensemble of (approximate) realisations. An iteration of EnKF consists of two steps, prediction and update (analysis) steps. The prediction step is exact, whereas the update step involves approximations. Several versions of the update step has been suggested in the literature. We propose to base the update on an assumed joint Bayesian model for the prediction ensemble elements and the newly observed data.

In the assumed Bayesian model for updating ensemble element number m, say, the prediction ensemble elements and the unobserved true state are assumed independent and Gaussian, and a conjugate prior is adopted for the mean vector and the covariance matrix. A linear Gaussian likelihood function is assumed for the new data. We then develop an updating procedures consistent with this assumed Bayesian model. The updating consists of two parts. First the parameters of the Gaussian distribution is generated from the resulting posterior distribution conditioning on the data and all prediction ensemble elements except number m. One should note that the prediction ensemble element that are to be updated is not used in this part, which is different from what is usual in standard EnKF procedures, but a necessary consequence of the assumed Bayesian model. The second part of the updating is to generate the updated ensemble element. For this a class of Gaussian distributions, all consistent with the assumed Bayesian model, is possible. Within this class of possible updating distributions we identify a procedure that us robust against the model choices in the assumed Bayesian model. Using the proposed EnKF in simulation exercises, the most striking property is that the inbreeding problem occurring in standard EnKF procedures is essentially eliminated.

S0904. Structural Geologic Modelling and Restoration by Ensemble Kalman Inversion

David Oakley (University of Stavanger),
Nestor Cardozo (University of Stavanger)
Room: auditorium 2022-08-30 11:15

Restoration using kinematic principles of fault-related folding is a valuable and widely used tool in structural geology. Data inversion methods can be employed to find the best-fitting model and estimate uncertainty, but their use in structural restoration has been limited to relatively simple models. In this work, we address the problem of inverting for complex, three-dimensional, kinematically restorable structural models, for which we use Ensemble Kalman Inversion (EKI), an iterative method based on the Ensemble Kalman Filter (EnKF), which is ideally suited to data inversion problems that involve large numbers of model parameters. We develop a workflow in which fault geometry, the distribution of slip on a fault, and the geometry of folded horizons are all modelled using EKI. The models are constrained by observations of faults and horizons in the present deformed state together with the expectation that horizons should restore flat. We test two modelling approaches: one in which the model is built in the deformed state and then restored, and one in which the model is built in the restored state and then forward modelled to match present-day data. We first test these methods on a synthetic model involving a single fault, demonstrating their use in both dense and sparse data cases, and we then apply them to a real-world example, the Emerald field, involving five faults. Both the restoration- and forward modelling-based methods work well, but forward modelling shows some advantages. We find that models are prone to ensemble collapse, which results in underestimation of uncertainty at small ensemble sizes. We employ localization and covariance inflation to help mitigate this issue. While some challenges remain, EKI shows promise as a tool for building complex, restorable structural models, and it holds the potential for integration of fault kinematics with other EKI- or EnKF-based workflows in subsurface modelling.

S0905. Ensemble-Smoother with Multiple Data Assimilation for Assisted History Matching of Geological Facies using Multi-Point Statistics Pyramid: a Case Study of Turbiditic Multi Facies System

Alireza Nahvi (Research Associate EMEARC Gas & LNG),
Anahita Abadpour (TotalEnergies),
Jessica Franco (TotalEnergies),
Abbas Zerkoune (TotalEnergies)
Room: auditorium 2022-08-30 11:40

One of the main challenges in the history matching processes is that artificial changes should be made to fit simulation results to field observations. Despite a good match of production profiles, the model does not respect geological realism, and it might be invalidated by new measurements. This paper presents a tailored version of the newly introduced method for assimilating field measurements data into categorical properties of groundwater flow models. In this approach, a multi-resolution Multi-Point Statistics (MPS) geomodelling simulation is coupled with Ensemble Assimilation Methods for assisted history matching. Because of the importance of underlying geological features that control the spread of petrophysical parameters, we update the facies distribution throughout the reservoir. We study 2 inverted five-spot synthetic cases by focusing on a quaternary facies system in the field as oppose to two-facies models.

For all initial steps, we build an ensemble of realizations with multi-resolution MPS. All these models are constrained to the prior geological information contained in the training image. The low-resolution models, where categorical properties are transformed into the continuous domain, are retrieved and used in the conditioning loop after being applied a Normal Score Transform (NST) filter. At each iteration in the conditioning loop, a new fine-grid ensemble is created ensued from assimilating the field observations to the NST images, and the updated coarse resolution models are kept for the next assimilation loop. This is another difference compared to the original work that uses part of updated coarse model used for building the fine grid models. This tailor made approached proposed in the original work would be cumbersome to implement for real size industrial utilization. We lay out the result of our case studies showing advantages and caveats of the mentioned technique and discuss the further necessary steps in maturing the workflow.

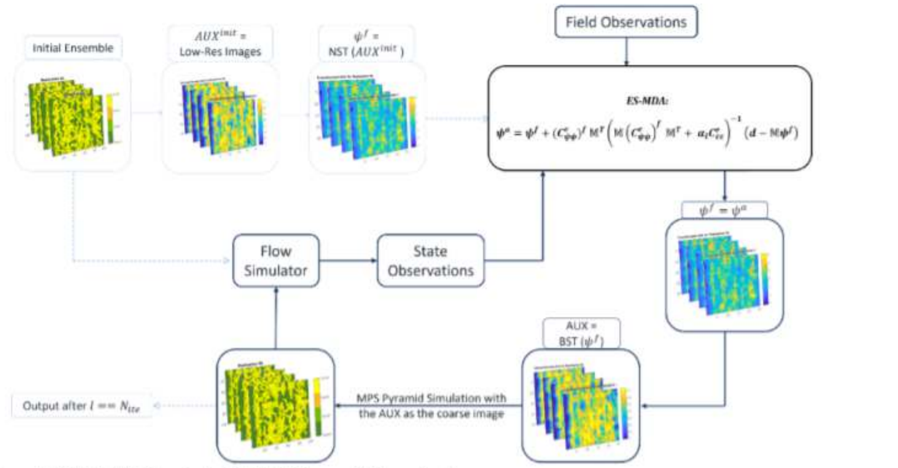


Figure (2) ES-MDA Coupled with MPS Pyramid Flowchart

S0906. Coupling optimization and the ensemble Kalman filter for multiple source contaminant identification

Alicia Sanz-Prat (IIAMA-UPV),
J. Jaime Gómez-Hernández (Research Institute of Water and Environmental Engineering, Universitat Politècnica de València)
Room: auditorium 2022-08-30 12:05

Identifying where, when, and how much contaminant has been discharged into an aquifer is difficult in sites where sparse observation networks are the only tool to know the status of the aquifer. The main objective of this study is to answer such questions using the ensemble Kalman Filter (EnKF) for transport inverse modeling assuming a multisource discharge. We propose merging the EnKF with mixed-integer nonlinear optimization (MINLO) to fit observed and predicted breakthrough concentrations. The EnKF starts with initializing the model parameters, followed by iterated steps of (i) prediction of the state variables by direct modeling from time k = 0 and (ii) updating the estimated values of the parameters from the deviations between observations and predictions. Parameters and corrected variables serve as input data in the next iteration at time k + 1. The novelty of this work lies in mixing an integer parameter (the number of sources) with continuous ones (hydraulic flow and transport model parameters) into the vector parameter. The method is demonstrated in numerical scenarios in two dimensions of increasing complexity subject to coupled nonlinear physicochemical processes and dynamic environmental conditions.

S10 Mining geostatistics, optimization and geometallurgy

Jörg Benndorf (TU Freiberg),
Julian M. Ortiz (Queen's University (Kingston)),
Raimon Tolosana-Delgado (Helmholtz Institute Freiberg for Resource Technology, HZDR),
K. Gerald van den Boogaart (Helmholtz Institute Freiberg for Resource Technology, HZDR)

The sessions aims to bring together all aspects of mining-relevant mathematics. The session integrates all mining related geomathematical methods: from microstructure characterization to an integrated spatiotemporal decision making for mining and processing including real time information updating. Important areas are: Potential Mapping, Microstructural Modelling and Observation, Geostatistics of Geometallurgical Variables, High Order Geostatistical Simulation, Structural Modelling with Uncertainty, Stochastic Mine Planning, Real Time Mining updating, and Predictive Process Optimization. Contributions from all fields of application or development of geomathematical methods for mining are welcome.

S1001. High-Order Block-Support Simulation and its Benefits to the Simultaneous Stochastic Optimization of Mining Complexes

Joao Pedro De Carvalho (COSMO lab - McGill University),
Roussos Dimitrakopoulos (McGill University)
Room: 102 2022-08-31 09:50

Mineral deposit modelling is driven by the underlying uncertainty and variability associated with the spatial distribution of geological attributes, quantifying the supply materials in industrial mining complexes. These uncertain attributes are traditionally modelled using geostatistical simulations, where Gaussian-based methods are typically used. Given the limitations of Gaussian simulation methods, a distribution-free high-order statistics-based framework has been developed to better reproduce non-linear and spatially complex multiple-point geological patterns. Within this framework, a direct block-support high-order simulation method has been proposed to efficiently generate mineral deposit realizations. A mining complex is an integrated business that extracts supply materials from the mines and transforms them through different processing steps until products are sold at the mineral markets. The supply materials are critical inputs to the simultaneous stochastic optimization of mining complexes, aiming to generate production plans that maximize net present value (NPV). To investigate the impact of the simulation approaches, the present work compares the traditional sequential Gaussian simulation (Case 1) versus the high-order direct-block support simulation method (Case 2) when applied at a gold mining complex. An initial comparison between the sets of simulated realizations generated by each method demonstrates that connectivity of high-grade values is better reproduced by the high-order-based approach. Subsequently, each set of simulated realizations is used as the input into the production schedule stochastic optimization model, allowing the comparison of production forecasts. The results show that the optimization in Case 2 provides a life-of-asset production schedule with 5% higher NPV compared to Case 1. Additionally, the extraction sequence obtained in Case 2 is notably driven towards zones where the high-grade mining blocks are better connected in space, which is a direct effect of the more-informed high-order simulation approach. Not only higher-grade material is fed to the processor, but also the overall extraction is more efficient generating less waste.

S1002. Future Knowledge in Geometallurgical Mining Optimization

K. Gerald van den Boogaart (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Raimon Tolosana-Delgado (Helmholtz Institute Freiberg for Resource Technology, HZDR)
Room: 102 2022-08-31 10:15

Mining and processing involves a lot of decision making, on capacity building, mine scheduling, blending, process parameters, and contracted sales. Traditionally stochastic mine planning and

predictive Geometallurgy use stochastic knowledge provided e.g. by conditional geostatistical simulations of the conditional distributions of ore properties to infere optimal decisions through

stochastic optimization. Stochastic knowledge is however no fixed fact, but can rather increase by later aquisition of information, automatically as a direct consequence of the operation itself, and optionally through additional exploration.

The contribution shows with simple and easy to comprehend sand box examples how and why such future knowledge and even the option to obtain future knowledge already changes, what is an optimal decision even before this knowledge is obtained. In case of optional knowledge, the decision to obtain it and when, becomes an integral part of the decision problem. This radically changes what algorithms can be feasibly used to compute optimal decissions. Straight forward stochastic optimization is not yet computationally feasible, for situations with increasing knowledge. The state of the art for models

using increasing information is to use reinforcement learning based heuristics.

This contribution explores the idea of making a stochastic optimizating possible by exploiting certain structures of the mining related increasing knowledge optimization problem. Possible speedup are based on 1) inequality relations in stochastic optimization allowing for advanced branch and bound techniques, 2) exploiting the fact that certain values are equivalent in different branches which

simplifies comparisions and precomputation, and 3) explicit computation of conditional expectations in a partial separation of the processing optimization and the scheduling optimization.

S1003. Geostatistics and Machine Learning for anticipation of production impairments An application to the Grande Côte Operations HM deposit, Senegal.

Christophe Bessin,
Pierre Boszczuk (Eramet Ideas)
Room: 102 2022-08-31 10:40

Grande Côte Operations (GCO) is a Senegalese subsidiary of the Eramet Group that specializes in the recovery of Heavy Minerals (HM): ilmenite, rutile, and zircon. GCO's mineral sands concession stretches 106 km along the Atlantic coast and 4 km inland.

Two of the mining facilities - the dredge and the floating Wet Concentration Plant (WCP) – are constantly moving, travelling around 7 to 13 km a year.

As the dredge moves the input HM grade varies due to the geological morphology of the deposit. These variations cause changes in the WCP output flow rate. Since 2019, reductions of the input throughput of the WCP have occurred because of HM concentrate flow rate exceeding the capacity of the HM concentrate pumping circuit. These events are mainly related to local HM grade peaks in the deposit that the WCP is not able to smoothen.

For long term planning, we predict the occurrence of these throughput impairments using a set of geostatistical and Data Science methods:

- Detailed sequencing of the mine operations of the past and coming years,
- Kriging and Uniform Conditioning of the deposit to get insights on the frequency of HM peaks,
- Deterministic modelling of the theoretical maximum output HM concentrate flow rate, given the input HM grades and throughput,
- Machine Learning model for the prediction of throughput impairment based on historical throughput impairments data, input HM grades, proportions of input HM above a set of values and theoretical throughput suggested by the deterministic model.

A software was developed to allow the testing of different nominal throughput hypotheses and to give help in the decision-making process to justify debottlenecking investments.

This hybrid method mixing Geostatistics and Machine Learning was able to predict future throughput impairments of the dredge with a satisfying error.

S1004. Geostatistical Domaining accounting for Geological Knowledge and Rock Quality in a Copper Porphyry Deposit

Nasser Madani,
Mohammad Maleki (Universidad Católica del Norte)
Room: 102 2022-08-31 11:05

The concept of domaining has been always an important issue in mineral resource estimation. Conventionally, either using geological variables or grade shells are realizing identification of homogenous estimation domains. For instance, in a metalliferous deposit, the former can be alteration, mineralization, and/or rock types, and in the latter, grade variability controls such spatial domaining. However, currently, machine-learning algorithms showed better recognition of these domains. Those based on clustering such as Geostatistical Hierarchical Clustering (GHC) are the best fit for this purpose. This method is capable of producing clusters (e.g., domains), by using both geological variables and the grades of interest. This clustering technique offers more flexibility to obtain the contiguous and compact clusters that are both in agreement with geological concept and grades distributions. Indeed, the compactness and contiguity of the estimation domains (signifying the homogeneity), are of paramount importance in further geostatistical analysis. In this study, we applied GHC to obtain the estimation domains in a Cu-Mo-(Au) copper porphyry deposit, where mineralization, alteration, rock types and Cu, Mo, and Au are inputted into the algorithm. However, this domaining is mainly suitable for splitting the region into the homogenous clusters where at most the low- to high-grade zones can be identified. Although this technique is proper for the mine planning purposes, but it does not show any geotechnical properties of the domains. To circumvent this problem, another continuous variable, Rock Quality Designation (RQD) is added to the input variables. The resulting domains showed a satisfying compatibility with grades, geological variables, and rock quality. These domains, not only can be used for resource estimation, but they can also be used later for geotechnical designs in mine planning and design steps. The geostatistical tools are also used to model the Cu, Mo, Au, and RQD in the specified domains.

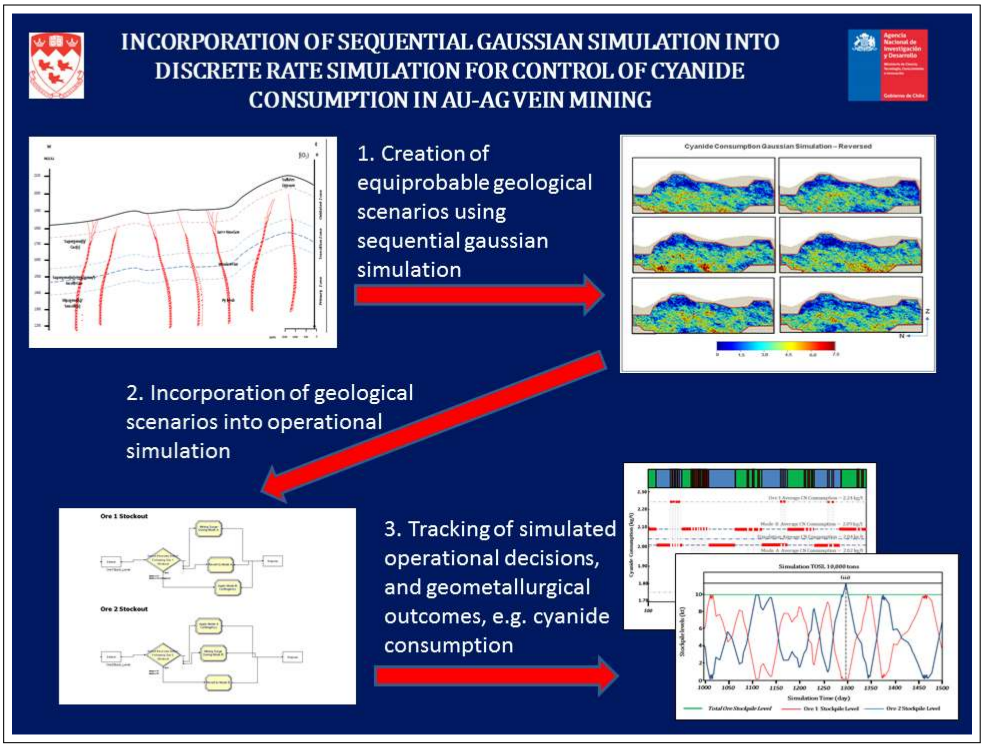
S1005. Incorporation of Sequential Gaussian Simulation into Discrete Rate Simulation for Control of Cyanide Consumption in Au-Ag Vein Mining

Javier Órdenes (McGill University),
Felipe Peña-Graf (Universidad Católica del Norte),
Samuel Cantor (Minerva Intelligence),
Alessandro Navarra (McGill University)
Room: 102 2022-08-31 11:30

Epithermal deposits of low sulphidation Au-Ag consist of quartz-adularia accompanied by ore minerals such as electrum (mostly 40-60 % by weight Au), native gold, Ag sulphides and sulfosalts and base metal sulphides, mainly Pb-Zn-Cu. Notably for gold extraction, chalcopyrite is refractory to cyanidation and closely related to the hypogenic zone, whereas other Cu-bearing sulphides are cyanicidal to varying degrees and are a challenge to geometallurgical controls. Comprehension of the occurrence of supergene Cu-bearing sulphides (e.g. chalcocite, digenite, covellite) is indeed a major operational challenge for the gold industry, as it is a major factor in cyanide consumption.

Significant variability is caused by the interaction of the orebody with other features such as the water table, topography, emplacement depth, up-lift/exhumation artifacts and younger faults, resulting in post-depositional mineralogical changes; these are manifest both as discontinuities as well as gradients. The problematic supergene Cu-bearing sulphides occur in the upper limit of the water table, and are linked to spikes in cyanide consumption due to their high cyanide solubility; indeed, the cyanide reacts with these minerals instead of gold, so that gold recoveries can only be maintained through increased cyanide rates. In contrast, the shallower portions of the orebody (above the paleo water table) are entirely oxidized.

Robust operational policies to stabilize cyanide consumption, while maintaining mine production levels, can be evaluated by integrating geostatistical techniques (e.g. Sequential Gaussian Simulation) into operational simulations. The current paper features Discrete Rate Simulation which is a comparatively simple approach to dynamic mass balancing, including spikes in cyanide consumption. The resulting framework demonstrates the attenuation of such spikes through a balancing of feeds from zones having more or less supergene Cu-bearing sulphides.


INCORPORATION OF SEQUENTIAL GAUSSIAN SIMULATION INTO DISCRETE RATE SIMULATION FOR CONTROL OF CYANIDE CONSUMPTION IN AU-AG VEIN MINING
1. Creation of equiprobable geological scenarios using sequential gaussian simulation
Cyanide Consumption Gaussian Simulation – Reversed
2. Incorporation of geological scenarios into operational simulation
Ore 1 Stockout
Ore 2 Stockout
3. Tracking of simulated operational decisions, and geometallurgical outcomes, e.g. cyanide consumption
Simulation Time (day)
Total Ore Stockpile Level
Ore 1 Stockpile Level
Ore 2 Stockpile Level

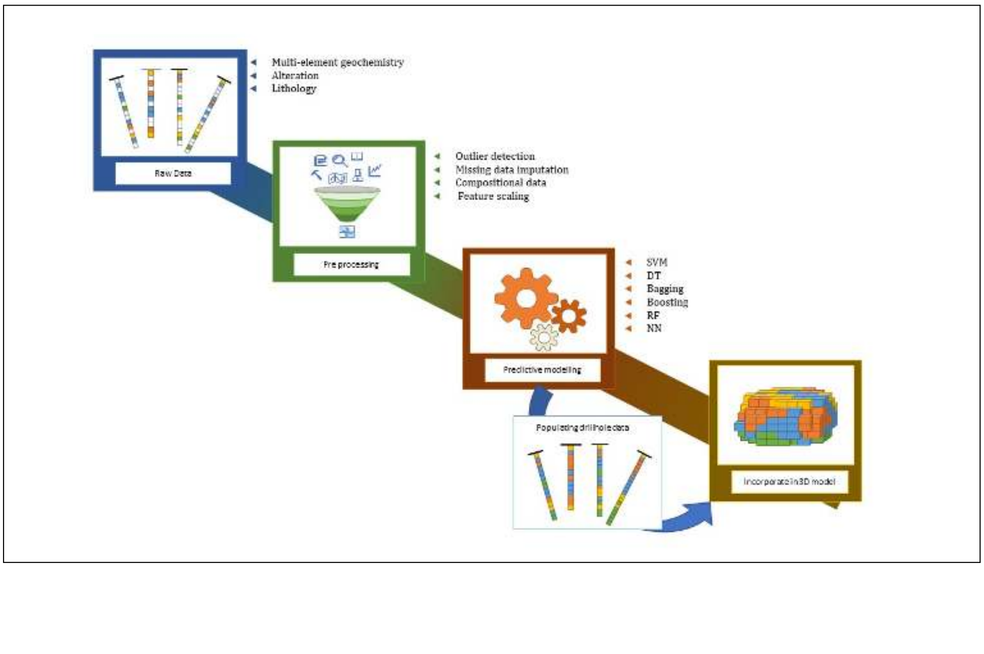
S1006. Application of machine learning to predict gold recovery at the Sari-gunay deposit, Iran

Zahra Nourizenouz (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Max Frenzel (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Jens Gutzmer (Helmholtz Institute Freiberg for Resource Technology, HZDR)
Room: 102 2022-08-31 11:55

The Sari-gunay gold deposit in northwest Iran represents an epithermal volcanic-hosted gold deposit. The gold is largely refractory and occurs as fine-grained submicroscopic inclusions or as invisible solid solution gold within pyrite and arsenopyrite. However, supergene oxidation of the sulphide ore to depths of 20 to 150 m has liberated a significant percentage of the gold and allowed for conventional cyanide leach extraction protocols, which achieve an average recovery of 70%. Thus, understanding the relationship between ore type and gold recovery is considered to be a critical aspect.

Metallurgical factors are non-linearly controlled by a large number of complex variables making the modelling challenging. Differences in scale, type and distribution of features, occurrence of censored/missing values and compositional data characteristics further complicate this procedure. In this contribution, we investigate the application of different machine learning algorithms for handling complex multivariate data in predictive modelling.

Geochemical and geological data of 91 drillcores from the Sari-Gunay gold mine were applied to predict the variability of gold recovery as a classification problem. Required preprocessing included outlier detection and removal, imputation of missing values and log ratio transformation of compositional data were carried out prior to modelling. Calibration of the predictive models was achieved by using the gold recoveries from 5425 bottle roll tests. Algorithms ranging from SVM, decision trees, random forest, and neural networks were adopted to find the best fit. All models were adjusted and hyperparameters were tuned carefully to achieve the highest accuracy while maintaining bias and variance to avoid over and underfitting. Results show accuracies above 80% for all the utilized methods. The same workflow is applicable to other geometallurgical studies.



S1007. Predicting hardness in iron ore blast holes using MWD

John Zigman (Australian Centre for Field Robotics, The University of Sydney),
Katherine Silversides (DARE Centre, University of Sydney),
Rami Khushaba (Australian Centre for Field Robotics, The University of Sydney)
Room: 102 2022-08-31 11:57

Hardness is a material's quality to withstand localised deformation and is an important characteristic for both blast control and downstream material processing. Hardness is usually derived from material types manually logged by site geologists and thus is not directly measured. As material type data is sparse, with only a small proportion of holes being logged, no hardness information is available for most production holes, posing limitations on subsequent mining processes. Additionally, as the logging process is manual, variability is imposed due to the subjective nature of the geologists logging materials and the diversity in mineralization and geology. Therefore, automating the hardness estimation can increase the amount of information available for blast planning and give an indication of the probable location of problematic material types.

To overcome the limitations, we report a pilot study to automate hardness estimation based on measure-while-drilling (MWD) data provided by autonomous drill systems. A hypothesis is developed that the application of machine learning algorithms can infer the necessary information for hardness estimation from MWD data without the need for extensive material type logging, i.e., to enable the use of MWD as a proxy for hardness. Specifically, we use a hardness proxy derived from logged material-type data, apply signal filtering/pre-processing to MWD data and extract a set of features from those MWD signals including: Hjorth parameters, mean, sample entropy, empirical CDF, and DASDV. Cross-validation (and repeated runs) using Random-Forest (RF) regression was used to model and predict hardness. The experiments utilized MWD data from automated drills in a banded iron formation-hosted mine in the Hammersley Province of Western Australia. The produced estimations were within 15% of the derived hardness values for over 81% of the holes tested. This can greatly increase our understanding of the variations in hardness across a bench using only information routinely collected.

S1008. Modelling microstructures with flexible Laguerre Mosaics

Raimon Tolosana-Delgado (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Sebastian Avalos (Queen's University (Kingston)),
K. Gerald van den Boogaart (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Max Frenzel (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Julian M. Ortiz (Queen's University (Kingston)),
Lucas Pereira (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Alvaro Riquelme (Queen's University Kingston)
Room: 102 2022-08-31 11:59

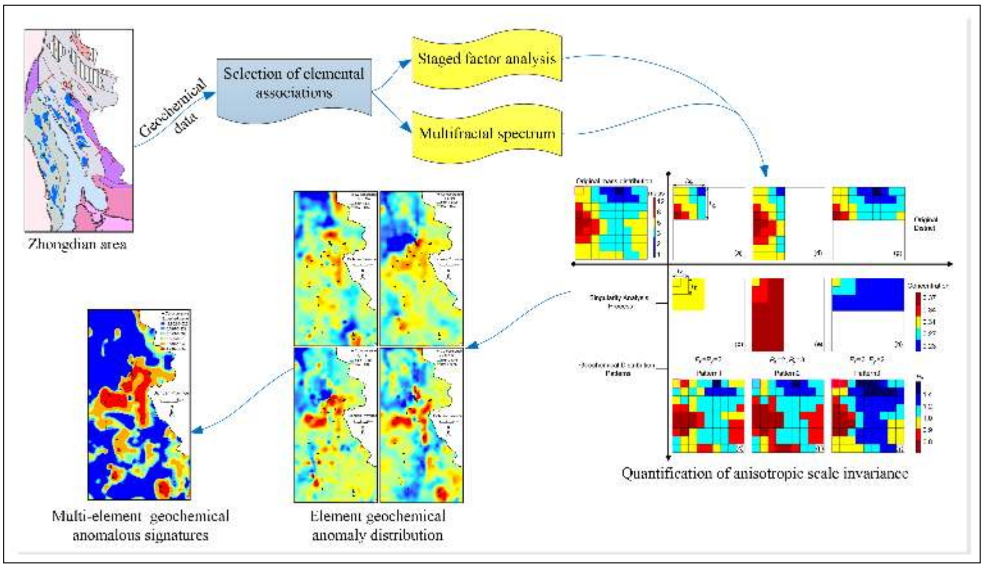
Particle-based process models offer a promising avenue towards greater predictability in geometallurgy, i.e., the ability to predict the outcomes of specific mineral processing routes from the mineralogical and microstructural ore characteristics. While the particle-based prediction of separation processes is already possible with acceptable levels of accuracy, the ability to predict the outcomes of comminution processes is currently limited to particle size distributions. Expanding comminution modelling tools to include particle microstructures would enable the full particle-based modelling of mineral processing flowsheets. As a step towards the inclusion of microstructure in comminution modelling, Laguerre tessellations are proposed to represent both the microstructure and the successive comminution steps. In contrast to the PARGEN library of simulated particles, our goal is to provide a low-parametric, dynamic, and efficient generator of parent and progeny material to inform forward and backward modelling efforts.

The idea is to follow a hierarchical decision structure in the simulation procedure. We first define an intensity field in 3D for the occurrence cell nuclei, which are then realised by a marked Poisson process. The first mark corresponds to realisations of a multinomial variable, and defines the mineral of each potential cell. Conditional on the mineral, the second mark follows a normal distribution, defining the weight of each cell, related to its size. A communition step is defined by a Voronoi mosaic, with a (t+1)-step exhibiting a higher intensity of its Poisson process than the previous t-step. To model preferential breakage, we inhibit some of the potential breakage surfaces with a probability depending on the weighted average hardness and the cleavage quality of the minerals that each surface cuts. Two consecutive comminution steps generate the corresponding parent and progeny particles, Each independently cut by a random plane to generate the equivalent of a 2D SEM-based automated mineralogy dataset.

S1009. A Hybrid Method for Quantifying Anisotropic Scale Invariance of Geochemical Anomalies and Identifying Multi-element Anomalous Signature of Cu–Polymetallic Deposits in Zhongdian, Yunan Province

Mengyu Zhao (School of Earth Resources, China University of Geosciences)
Room: 102 2022-08-31 15:00

The complex spatial and frequency distribution characteristics of exploration geochemical data are the result of the superposition of a series of geological processes at different spatio-temporal scales, which induces the non-stationarity and nonlinearity of spatial distribution of geochemical elements. How to effectively identify and extract element geochemical anomalies under complex geological conditions, comprehensively analyze the association signatures of multi-element geochemical data, and extract ore-forming geochemical anomalies is of great significance for prospecting breakthroughs. To describe the spatial non-stationarity that arises from direction differences, an improved fractal density model was proposed by introducing the parameter Pc based on "general fractal topography", so as to reveal the anisotropic scale invariance of geochemical anomalies. However, the Cu anomaly uncertainty assessment presented in Zhongdian area (China) shows that there are about 33% copper occurrences in low probability areas, indicating that there is still great uncertainty in these areas. Therefore, the multifractal analysis method and staged factor analysis were utilized to identify multi-element associations signature related to Cu mineralization, and two elemental associations Cu-Zn and Mo-Pb were recognized. Then, the expected value function based on singularity data was adapted to generate an enhanced multi-element geochemical anomalous signature for delimiting exploration targets. And the relevance of the enhanced multi-element geochemical signature on mineralization was validated by comparing it with the performance of the fuzzy sum operator. Finally, a binary geochemical map was produced by a prediction-area(P-A) plot based on the stronger geochemical evidence layer, and the high potential area can be considered as a reference in further exploration.



S1010. Utilising local varying anisotropy in the multivariate conditional simulation model of Olympic Dam deposit

Ilnur Minniakhmetov (BHP Geoscience Centre of Excellence),
David Clarke (BHP Olympic Dam)
Room: 102 2022-08-31 15:25

The Olympic Dam deposit is truly a world-class Cu-U-Au-Ag deposit. It is the world's fourth-largest deposit of copper and the world's largest uranium deposit. Traditional and non-traditional estimation methods have been used to accurately model the geology and mineralisation of the Olympic Dam deposit. While conditional simulation models have been used as the most robust method for estimating risk and uncertainty in mine planning decisions at other mines, they are now in only the second year of use at Olympic Dam.

There have been a number of challenges associated with simulating the Olympic Dam deposit at a selective mining unit size sufficient for underground mining purposes. These include:

- the size of the deposit;
- the disseminated sulphide mineralisation (chalcocite, bornite, chalcopyrite, pyrite) which is strongly zoned across the deposit; and
- the direct relationship of the relative abundances of the sulphide minerals (Cu:S is a proxy) which are crucial to the Olympic Dam smelter performance.

It is essential that the simulation model honour the distribution of the copper sulphide minerals in the deposit as the abundance of sulphides and the Cu:S ratio are critical mine plan inputs.

Three key techniques used in the Olympic Dam conditional simulation models are:

1) projection pursuit multivariate transform to decorrelate the main elements before simulation;

2) pluri-gaussian domain estimation for the sulphide non-sulphide contact; and

3) local varying anisotropy, which has been used to help guide simulation around the complex geology of the margins of the barren hematite quartz breccia which are excellent targets for high-grade mineralisation.

S1011. Comparison of multiGaussian transforms in multivariate geostatistical simulation

Sultan Abulkhair (University of Adelaide),
Peter Dowd (University of Adelaide),
Chaoshui Xu (University of Adelaide)
Room: 102 2022-08-31 15:50

Geostatistical modelling of two or more continuous variables is a common requirement in mining applications. In these applications, it is essential to consider the spatial correlation of each variable and the cross-correlations among them. For example, conventional cokriging and cosimulation methods use a linear model of coregionalization to account for univariate and multivariate spatial correlation. However, variogram inference becomes more complex as the number of variables increases. An alternative is to use decorrelation methods by transforming the original values into decorrelated factors and then simulating them individually. As a result, the back-transformation of simulated values restores the multivariate relationships between coregionalized variables. To date, several linear and multiGaussian transformation methods have been developed to deal with different types of bivariate relationships such as linear, non-linear, heteroscedastic and geologically constrained. This study compares the following multiGaussian transforms: rotation-based iterative gaussianization, projection pursuit multivariate transform, flow transformation, and their combination with spatial decorrelation. Different case studies with bivariate complexities are used to evaluate and compare the realizations of transformed values. For this purpose, commonly used geostatistical validation metrics are applied, including multivariate normality tests, reproduction of bivariate relationships, histogram and variogram validation.

S1012. Multivariate morphing transformation: Fundamentals and challenges

Sebastian Avalos (Queen's University),
Julian M. Ortiz (Queen's University (Kingston)),
Oy Leuangthong (Corporate Consultant (Geostatistics), SRK Consulting Inc.)
Room: 102 2022-08-31 16:15

Transforming a multivariate dataset into a multi-Gaussian distribution is a prevailing need in geostatistical modeling. The transformed variable can be fully characterized by an expected value and covariance matrix assuming a multi-Gaussian random function approach. Values at unsampled locations are then simulated by geostatistical methods. The resulting values are back-transformed into their original units. Challenges arise on high-dimensional datasets in terms of finding an adequate transformation between the original and multi-Gaussian spaces, variogram model characterization, and computational implementation. A decorrelation strategy can be applied to work on a decorrelated multi-Gaussian space. However, preserving relevant information is an additional challenge, reflected in the reproduction of statistical and spatial relationships on the original units.

In this work, we provide the fundamentals and challenges of a multivariate morphing transformation approach. A mapping function between the original multivariate space and a decorrelated multi-Gaussian space is computed by means of space landmark points. The spatial structures of the random Gaussian variables can then be modeled independently, and values are simulated at unsampled locations using any univariate Gaussian simulation method. Simulated values are projected into the original units by the inverse mapping functionº. We discuss the potential of the method as well as challenges related to the landmark points selection, landmark points pairing, and modeling the mapping function. The discussion is supported with a multivariate dataset from an iron ore deposit where we show the performance of the method.

S1013. Application of SPDE method to a continental-fluvial uranium ore body and comparison with classical methods

Marie-Cécile Febvey (Orano),
Nicolas Desassis (Mines Paris Tech),
Didier RENARD (Mines Paris Tech)
Room: 102 2022-08-31 16:40

Big data management is a concern for most businesses and the mining industry is no exception. To boost productivity, a risk analysis associated with mineral resource estimation is often required and an assessment of the uncertainty is compulsory. Conditional simulations bring an appropriate answer but the traditional methodologies (e. g. Turning Bands method, with the conditioning kriging) may lead to a prohibitive computing time and the need to choose a moving neighbourhood, which is a conundrum.

Most of the Geostatistical standard procedures suffer from severe limitations in the presence of large data sets and numerous target sites. The Stochastic Partial Differential Equation (SPDE) approach offers an innovative way of calculating Kriging and Geostatistical Simulations, which departs from the traditional geostatistical workflow by working directly on the precision matrix (inverse of the covariance matrix) instead of the dense covariance matrix. This precision matrix is directly computed from the model by using the link between a certain class of random functions and solutions of a SPDE [Whittle, 1954] [Lindgren, 2011] and by approximating the solution with the finite elements method.

The SPDE approach leads to a very significant gain in performance of Estimation and Conditional Simulations. It enables to deal with large set of inequalities through an efficient Gibbs sampling procedure. As it can handle a huge amount of data, it gets rid of concepts such as the Moving Neighbourhood. The algorithm initially developed for 2D dataset was adapted for 3D context. This approach naturally allows to use varying anisotropies in a global consistent model by making variable the operator involved in the stationary SPDE.

This paper summarises the key points of the methodology and its implementation in 3D. Then, the SPDE method is applied to a uranium ore body to compare these results with the ones obtained by the “classical” methods.

S1015. Use of the specific surface to measure the efficiency of grids of drillholes and classify the resources of a set of 2D mineral deposits.

Marie-Cécile Febvey (Orano),
Jacques Rivoirard (Mines Paris Tech)
Room: 102 2022-08-31 17:05

The hole spacing is an essential element that controls the precision of estimated resources, hence their categorisation. Generally, with a regular sampling grid, the smaller the grid cell, the better the precision. However, for a given grid, the precision also depends on the spatial continuity, typically the variogram of the target variable. The specific surface (specific volume in 2D) has been designed to measure the efficiency of a grid cell, depending on this variogram. This further allows to approximate the precision of the resources contained in volumes made by blocks centered on the grid and having the size of the grid cell. Classification of resources can be deduced by considering a number of blocks corresponding to a nominal, for example annual, production. It provides an objective method to evaluate the level of confidence of resources, then to make comparison of different projects.

This concept of specific surface has been used by Orano, a leader of uranium mining industry, for the classification of the resources of a set of deposits at various stages of regular sampling. The present paper illustrates the methodology in the example of one such deposit. It also shows how the method can be used to make a synthetic comparison of different projects at the level of a mining company.

S1016. Geoscience workflows using ioGAS Software

Putra Sadikin (Imdex Ltd),
Rob Wall
Room: 102 2022-08-31 17:07

ioGAS software is used to rapidly undertake geochemical analysis, as many standard techniques co-exist in one software package, such as: Principal components analysis, Mahalanobis distance calculations, Discriminant projection analysis, Auto domain classification, Classification and regression trees, Self-organising maps, Regression analysis, K-means clustering, Tukey outlier identification, t-SNE.

Results can be displayed live in other environments (such as geographic information system software and geology modelling packages) including QGIS.

Recent work allows workflows to be automated and shared in a team. This talk will present some practical examples of using ioGAS workflows for exploratory data analysis to find anomalies and identify patterns in geochemistry data.

Recorded workflows can be used for knowledge sharing of best-practices in data interpretation between geoscientists. Another use of the workflow engine is in automating the process of classifying data points into geological groups.

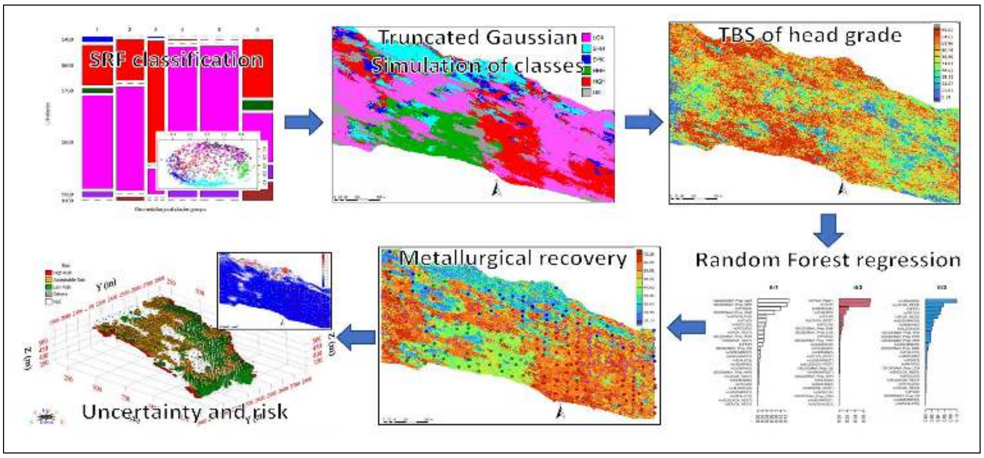
This could be run as a 1/2 day course, or condensed into a 20 minute talk.

See https://reflexnow.com/product/iogas/

S1017. Modelling of Unequally Sampled Geometallurgical Properties using Geostatistical Simulations and Machine Learning

Will Patton (BHP Iron Ore),
Ute Mueller (Edith Cowan University),
Hassan Talebi (Edith Cowan University),
Ilnur Minniakhmetov (BHP Geoscience Centre of Excellence)
Room: 102 2022-09-01 15:00

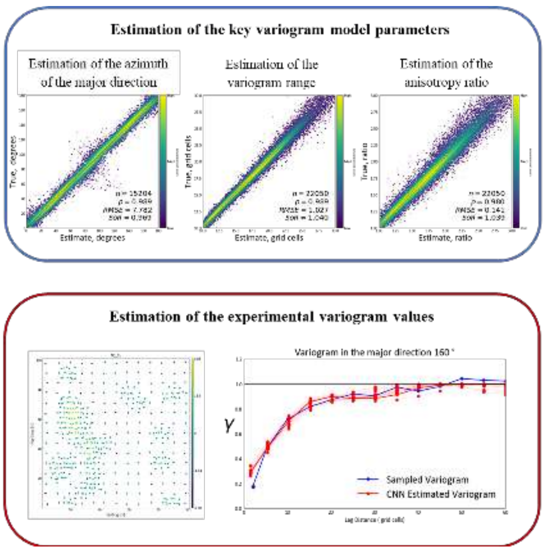
Important orebody characteristics that determine viability of the mineral resource and ore reserve potential such as physical properties, mineralogical and geochemical compositions often vary substantially across an ore deposit. Geometallurgical models capture the spatial relationships between mineral compositions and physical properties of ores and their responses to industrial processes. Challenges include the high-dimensionality of data, limited availability of metallurgical test results acquired on larger support and the non-additive nature of some properties such as metallurgical recoveries. Modelling of spatially and statistically homogeneous geometallurgical classes is demonstrated at Orebody H; a complex stratabound Bedded Iron Ore deposit in Western Australia's Pilbara. Supervised and unsupervised learning via the spatial random forest algorithm was used to define geometallurgical classes from geometallurgical test work data (oxide grades, mineral concentrations and associated recoveries). The layout of geometallurgical categories and variabilities of associated rock properties are mapped with hierarchical truncated gaussian simulation and head grades via turning bands simulation. Geometallurgical properties in the form of size fraction recoveries are then predicted using machine learning regression. Finally, uncertainties are quantified to assess risk following a confidence interval based framework. This could be used to identify zones of high uncertainty where collection of additional data might help mitigate or minimise risks and in turn improve forecast production performances.



S1018. Automatic Variogram Inference Using Convolutional Neural Networks (CNN)

Abdelkerim Mokdad (University of Alberta),
Behrang Koushavand (Cenovus Energy),
Jeff Boisvert (University of Alberta)
Room: 102 2022-09-01 15:25

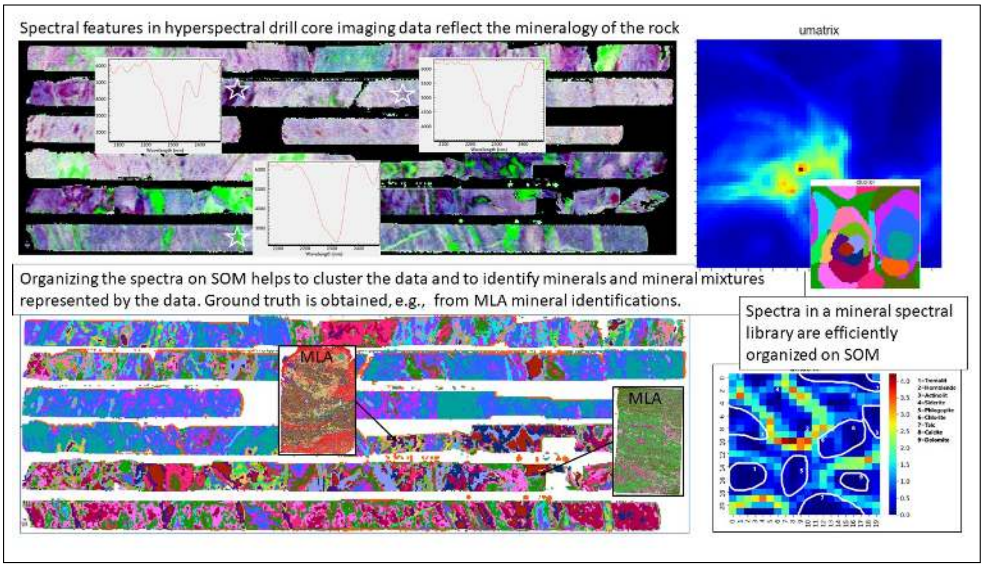
To assist with variogram modeling, this work develops an automatic variogram inference workflow based on Convolutional Neural Networks (CNN) to model the variogram by estimating its key parameters (range, azimuth, nugget effect, and anisotropy ratio), using the sparsely sampled data as input. Training data for the proposed technique consists of a large set of unconditional Sequential Gaussian Simulation (SGS) realizations with different variogram parameters. To reproduce a realistic modelling situation, a data set is sampled from "the simulated truth". Training a CNN directly on sampled data was not effective so each data set is modeled using inverse distance; kriging was also implemented but did not result in better variogram prediction after applying the CNN, the minimal number of input parameters for inverse distance is attractive. Two workflows are considered (1) train a CNN to predict variogram model parameters and (2) directly predict the azimuth and variogram values at specified lag distances. The loss function considered in training is the difference between the true and estimated variograms. When applying the CNN to data sets, data augmentation (rotation) is performed to obtain a set of variogram predictions that improves prediction robustness and can be used to examine variogram uncertainty. The workflows are applied to the Walkerlake data set to validate variogram prediction. The prediction of variogram model parameters is limited by a fixed number of variogram structures and the second workflow involving predicting values at lags performs better without limiting the number of variogram structures. The CNN results in a smooth experimental variogram prediction that can be easily fit with automated variogram algorithms to generate the final modeled variogram. The final variogram prediction has an r2 of 0.96. The proposed workflow is fully automated, once the CNN is trained, the only user input is the sparse sample data.



S1019. Self-organizing maps in analyzing hyperspectral drill core imaging data

Johanna Torppa (Geological Survey of Finland),
Samuli Haavikko (Geological Survey of Finland),
Markku Korhonen (Geological Survey of Finland),
Juha Köykkä (Geological Survey of Finland),
Kati Laakso (Geological Survey of Finland),
Maarit Middleton (Geological Survey of Finland),
Vesa Nykänen (Geological Survey of Finland),
Jarmo Rauhala (Geological Survey of Finland),
Akseli Torppa (Geological Survey of Finland),
Tuomo Törmänen (Geological Survey of Finland)
Room: 102 2022-09-01 15:50

Hyperspectral (HS) drill core imaging is a way to quickly acquire data that contain high spatial resolution information on drill core mineralogy. In the Hyperspectral Lapland (HypeLAP) project, we investigate how the unsupervised self-organizing maps (SOM) clustering method can be used in extracting this mineral information from the data. We use HS imaging data of 500 meters of drill core representing two gold prospects and a Cu-Zn volcanogenic massive sulphide prospect in northern Finland. The data were acquired in the visible – near infrared – short-wave infrared (400-2500 nm) and long-wave infrared (8000 -12000 nm) regions of the electromagnetic spectrum. Since the HS image pixel size of appr. 1.5 mm exceeds the scale of the mineralogical variation, most of the pixels represent mixed spectra of two or more minerals with varying abundances, complicating the task of mineral identification. By organizing the spectra on a 2D SOM, we have studied the HS data structure for finding the best clustering scheme for it. Our preliminary results show that the spectra of different minerals are well separated on SOM and spectra of a single mineral forms a homogenous region in the SOM network. We have investigated how SOM computation of mainly mixed spectra can be guided by using training spectra of pure minerals. To interpret the SOM results and define the mineralogy of each cluster, we use endmember spectra extracted from the HS data, ground truth mineralogy from MLA mineral identifications, and external spectral libraries. SOM computations are carried out with the GisSOM software that was recently developed in the Horizon 2020 project New Exploration Technologies (NEXT).


Spectral features in hyperspectral drill core imaging data reflect the mineralogy of the rock
umatrix
Organizing the spectra on SOM helps to cluster the data and to identify minerals and mineral mixtures represented by the data. Ground truth is obtained, e.g., from MLA mineral identifications.
Spectra in a mineral spectral library are efficiently organized on SOM
MLA
MLA

S1020. Inferring parameters of 3D particles microstructures from 2D sections using statistical learning

Julian M. Ortiz (Queen's University (Kingston)),
Sebastian Avalos (Queen's University (Kingston)),
Max Frenzel (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Lucas Pereira (Helmholtz Institute Freiberg for Resource Technology, HZDR),
Alvaro Riquelme (Queen's University Kingston),
Raimon Tolosana-Delgado (Helmholtz Institute Freiberg for Resource Technology, HZDR),
K. Gerald van den Boogaart (Helmholtz Institute Freiberg for Resource Technology, HZDR)
Room: 102 2022-09-01 16:15

Understanding and modeling comminution processes is key to automate and control mineral processing performance. Particle breakage depends on multiple factors, including the mineralogical composition, mineral associations and grain size distribution of the ore prior to breakage. While current comminution models are limited to predicting the size distributions of progeny particle with limited compositional information, the ability to forecast microstructure properties of individual progeny particles would allow to model the downstream separation processes in higher detail.

In this contribution we propose a statistical learning methodology that reconstructs 3D particle microstructures from 2D sections. The idea is to apply this methodology to automated mineralogy 2D cross sections of comminuted material, to predict the actual 3D particle microstructure of an ore prior to breakage. However, as a first step, we develop the method for a simulated material defined from Laguerre tessellations with particular mineralogical compositions, which are then used to simulate the breakage. The resulting 3D particles are then randomly intersected by planes to simulate 2D sections similar to those obtained by automated mineralogy.

The algorithm feeds the number, shape and surface of the 2D fragments as well as the raw sections into an ensemble of neural networks trained to infer the parameters of the Laguerre tessellation. From these, relevant statistical features of the 3D data can be inferred, such as grain size distributions and mineral associations.

S1021. Pedras 1.0.0: A Python library for modal mineralogy calculations from routine assay data

Angela Rodrigues (Monash University),
Lachlan Grose (Monash University),
Laurent Ailleres (Monash University),
Scott Halley (Mineral Mapping Pty),
Angela Escolme (University of Tasmania),
Robin Armit (Monash University),
Mehrtash Harandi (Monash University),
Matthew Cracknell (University of Tasmania)
Room: 102 2022-09-01 16:40

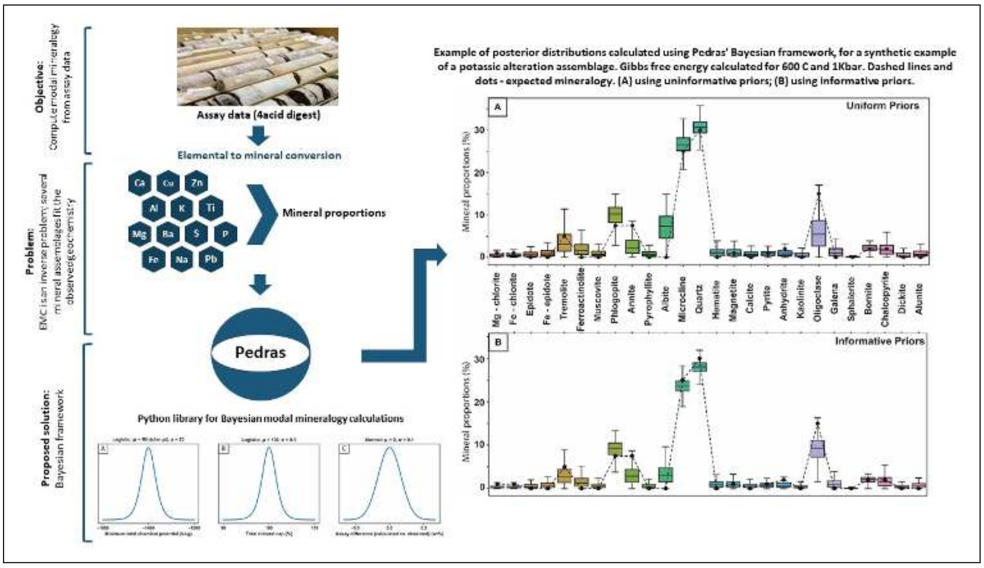
The evaluation of modal mineralogy is critical to understand a deposit's mineralogy, estimate its size, and enable efficient ore beneficiation. Elemental-to-mineral conversion techniques (EMC) applied to geochemical datasets are a commonly chosen method to estimate a sample's modal mineralogy.

EMC techniques are designed with the basic underlying principle that the bulk chemistry of a sample is proportional to the product of its modal mineralogy with the mineral elemental composition, which corresponds to a mathematical inverse problem: the solution (modal mineralogy) is approximated given the problem's consequence (measured geochemistry).

An inverse problem suffers from information deficit, and therefore several solutions fit the observations: the same geochemical information can yield a multitude of possible mineral assemblages. This ambiguity can be resolved by the objective introduction of additional information in the modelling stage, and Bayesian methods offer great potential in this space.

In this work, we present a probabilistic framework to infer modal mineralogy from compositional data, compiled into a Python library – Pedras 1.0.0. We build upon the works of Escolme et al. (2019) and Berry et al. (2011), an EMC method that uses linear programming to minimize coefficients representing the energy required to generate a given mineral assemblage. The minimization constraint implies thermodynamic equilibrium, which is rarely the case for hydrothermal environments. The new probabilistic framework defines the thermodynamic coefficients as a probability distribution function centred at the mineral assemblage's equilibrium with a scale factor of 100 KJ/g, which relaxes the thermodynamic coefficient's minimization.

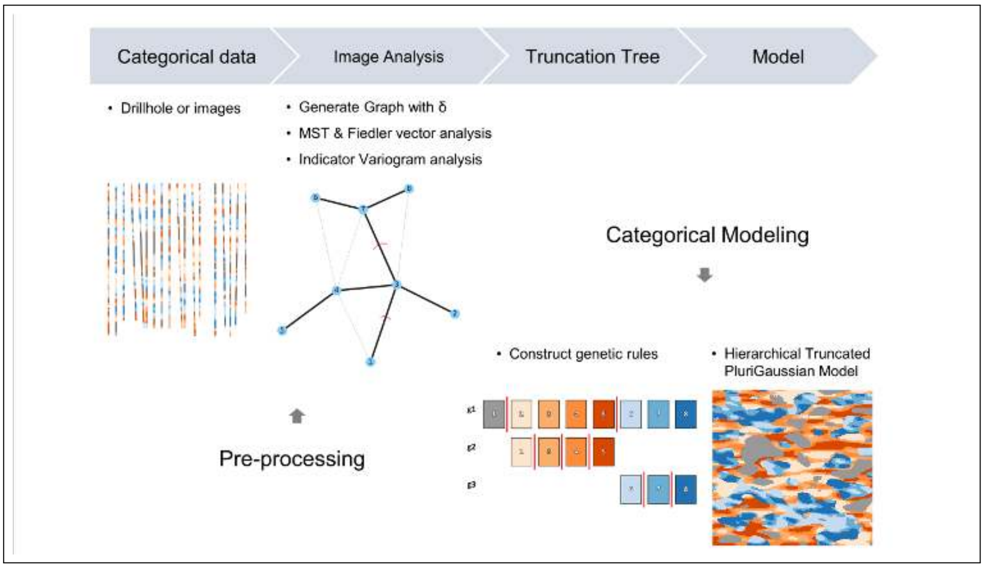
We test this framework on synthetic alteration assemblages within a porphyry copper deposit. Our results show that by relaxing thermodynamic minimization constraint, accurate modal mineralogy can be approximated at different stages of hydrothermal alteration in porphyry copper deposit systems. The method's accuracy is enhanced when prior knowledge is objectively included in the modelling stage.


Objective:
Compute modal mineralogy from assay data
Problem:
EMC is an inverse problem; several mineral assemblages fit the observed geochemistry
Proposed solution:
Bayesian framework
Assay data (4acid digest)
Elemental to mineral conversion
Ca
Cu
Zn
Al
K
Ti
Mg
Ba
S
P
Fe
Na
Pb
Mineral proportions
Pedras
Python library for Bayesian modal mineralogy calculations
Example of posterior distributions calculated using Pedras' Bayesian framework, for a synthetic example of a potassic alteration assemblage. Gibbs free energy calculated for 600 C and 1Kbar. Dashed lines and dots - expected mineralogy. (A) using uninformative priors; (B) using informative priors.
A
Uniform Priors
Mineral proportions (%)
0
10
20
30
Mg - chlorite
Fe - chlorite
Epidote
Fe - epidote
Tremolite
Ferroactinolite
Muscovite
Phlogopite
Annite
Pyrophyllite
Albite
Microcline
Quartz
Hematite
Magnetite
Calcite
Pyrite
Anhydrite
Kaolinite
Oligoclase
Galena
Sphalerite
Bornite
Chalcopyrite
Dickite
Alunite
B
Informative Priors
Mineral proportions (%)
0
10
20
30

S1022. Graph Theory Tools for Hierarchical Analysis of Rock Types

Harold Velasquez (University of Alberta),
Clayton C.V.D. Deutsch (University of Alberta)
Room: 102 2022-09-02 09:50

Drillholes represent a reliable source of categorical data from the subsurface. In the past, interpretations from drillholes have been focused on the analysis of transition matrices and stacking patterns. A Graph Theory approach could be used as a means to encode geometric and hierarchical relationships of objects within an image such as contiguity or precedence of categorical domains. Facies modeling aims to preserve these relationships in the final output; however, there are a vast combinatorial of genetic rules. This work presents an application of undirected weighted graphs and its associated algebraic techniques to determine a genetic interpretation of categories compatible with truncation trees required in Hierarchical Truncated Pluri-Gaussian Simulation. The methodology is based on a novel measure of distance between categories based on the distinct intervals between pairs to establish the initial graph. Minimum Spanning Tree Clustering and Spectral Partitioning are applied on the graph to infer suitable trees. The approach is tested in examples with known trees to assess its performance. Consistent results are obtained in stationary and non-stationary environments. The measure of distance and the level of information in drillholes determined by its spatial orientation highly influenced the inferred trees. Overall, a reduced set of possible trees are obtained. They closely match the true underlying tree in cases where the reference truth is known.



S1023. Mineral and lithology classification on Ernest Henry Au-Cu deposit using hyperspectral and RGB data

Shaoqiu Zheng (Australian Centre for Field Robotics, The University of Sydney),
Katherine Silversides (DARE Centre, University of Sydney),
Mehala Balamurali (Australian Centre for Field Robotics, The University of Sydney)
Room: 102 2022-09-02 10:15

Automated processing of hyperspectral data can provide an efficient, non-destructive and reproducible method of identifying the mineral in exploration drill core. However, the texture or lithology of the rock that is visible in the cores can provide additional information about the zonation and alteration present in the deposit. These are important when interpreting the structure and shape of a deposit, but cannot be interpreted from line-scan hyperspectral data. Our study considers the Ernest Henry Cu-Au deposit in Northern Queensland, Australia. Hyperspectral visible near-infrared (VNIR) to short-wave infrared (SWIR) and thermal infrared (TIR) scans, along with corresponding RGB images of the drill cores, were taken using the HyLogger system. These were made available by AuScope and National Virtual Core Library. The availability of both the line-scan hyperspectral data and the RGB images provides the opportunity to create a combined mineral and lithology classification. Two forms of convolution neural network, AlexNet and MobleNet v2, are implemented for mineral and textural classification. A validation accuracy of 97% was achieved for mineral classification using the VNIR-SWIR and TIR data. Lithology classification by from RGB achieved a maximum validation accuracy of 94% with AlexNet. When texture prediction was performed on drill cores without ground truth, the results demonstrated a sensible and consistent classification. This study demonstrated that both mineralogical and textural information can be obtained automatically from HyLogger scanned drill cores. This provides a fast, consistent way of gaining additional information that can be used in interpreting and understanding a deposit.

S1024. Definition of Geological Domains with Ensemble Support Vector Classification

Kasimcan Koruk (Queen's University (Kingston)),
Julian M. Ortiz (Queen's University (Kingston))
Room: 102 2022-09-02 10:40

Uncertainty is an inherent characteristic of resource models since they are built using limited information. To better evaluate mineral resources, uncertainties can be quantified using traditional approaches, such as geostatistical simulation methods. However, exploration datasets may contain rich geochemical information that can be used to search for alternative approaches for the definition of geological domains. Today, machine learning algorithms not only stand as strong alternatives to the traditional geostatistical methods, but they can also support any stage of resource models since they can easily incorporate large and multivariate datasets to reach flexible results.

In this study an ensemble learning approach is proposed to define geological domains and their uncertainty. The study starts with an unsupervised binary clustering method to label the data, and continues with supervised machine learning, which makes use of the labelled data to build an uncertainty model. Unsupervised clustering is performed considering particular subsets of the geochemical elements available and using certain distributional assumptions. To define the two distinct clusters, three steps are followed: (1) exploratory data analysis to determine the most relevant geochemical variables, (2) optimization of parameters defining their distribution and (3) domain assignment according to the optimum distributions found in (2). The domain assignments obtained are used to inform the supervised machine learning method. An ensemble support vector classification (SVC) approach is proposed to assign each location in the block model to one of the two domains. This is done by repeatedly applying SVC with subsets of training samples (bagging) and with subsets of geochemical variables to build weak classifiers. These weak classifiers then are combined to define a stronger classifier. We demonstrate the proposed method with an application to a real database from a porphyry copper deposit.

S11 Preserving realistic geology in statistical and mathematical geomodels

Ingrid Aarnes (Norwegian Computing Center),
Jacob Skauvold (Norsk Regnesentral /Norwegian),
Carl Jacquemyn (Imperial College London)

In this session, we invite authors to share their research on how to represent realistic geology in statistical and mathematical geomodels. This could be for example stochastic facies models, process-based/process-mimicking models, implicit and surface-based representations or other statistical and mathematical solutions that ensure geological validity of models. The aim of the session is to bring together researchers working on translating geology into statistical and mathematical geomodels and learn from each other across scales, disciplines and applications. We welcome contributions from a wide range of approaches where the main aim is for numerical models to realistically represent geology as seen in outcrops and analogues.

S1101. Checking for geological truth in our 3D models; a knowledge based approach

Marion Parquer (University of Lorraine),
Eric A de Kemp (Geological Survey of Canada),
Boyan Brodaric (Geological Survey of Canada)
Room: 101 2022-09-02 09:50

3D geological modelling technologies are providing the geosciences community with sophisticated applications, able to generate numerous multi-parameter realizations. Despite the success of the technology to fit mathematical and geometrical constraints, the results can be meaningless to geological experts, as models do not always respect accepted geological norms. As the output models from these applications will be used for downstream characterization, it is important, to verify this geological reasonableness before proceeding down the modelling pipeline. As a start in this process, we limit the verification of geological reasonableness, termed 'geological consistency' in this study, to the spatial, temporal and relevant geological entity relationships that come from the knowledge component of 3D geological models.

In order to deal with this problem, we propose a clearing house approach that can quickly identify models that are geologically inconsistent, directly after their construction, and highlight these inconsistencies. This tool relies firstly on the formalization of geological rules and norms into computer readable documents. This information is stored into matrices detailing accepted geological relations between any two geological entities in terms of temporality, spatiality and polarity called ”truth tables”. As 9 distinct geological entities have been counted (i.e. depositional unit, intrusion, extrusion, metamorphic unit, fault, erosion surface, fold volume, linear and planar fabric), 45 truth tables have been created.

For a given case study, critical geological features are classified along with their polarity. Temporal information is transformed into binary temporal relations between each geological entity pair and the 3D geological model is explored for extracting actual binary spatial relationships between all geological entities.

Finally, by confronting model entity relations with corresponding truth tables, the model is declared consistent or not. If the geological model is not valid, the inconsistency is noted, and can be dealt in subsequent model runs until the model passes the consistency test.

S1102. Constrained, process-based, stochastic, explicit revervoir modelling - One step at a time.

Jean-Claude Dulac (Next-shot @ geomodeling)
Room: 101 2022-09-02 10:15

Reservoir modeling techniques have not fundamentally changed in the past 30 years. Nevertheless, it has been shown many times that reservoir models tend to overestimate recoverable volume for two main reasons: lack of lateral heterogeneity and thin flow barriers that disappear or become discontinuous.

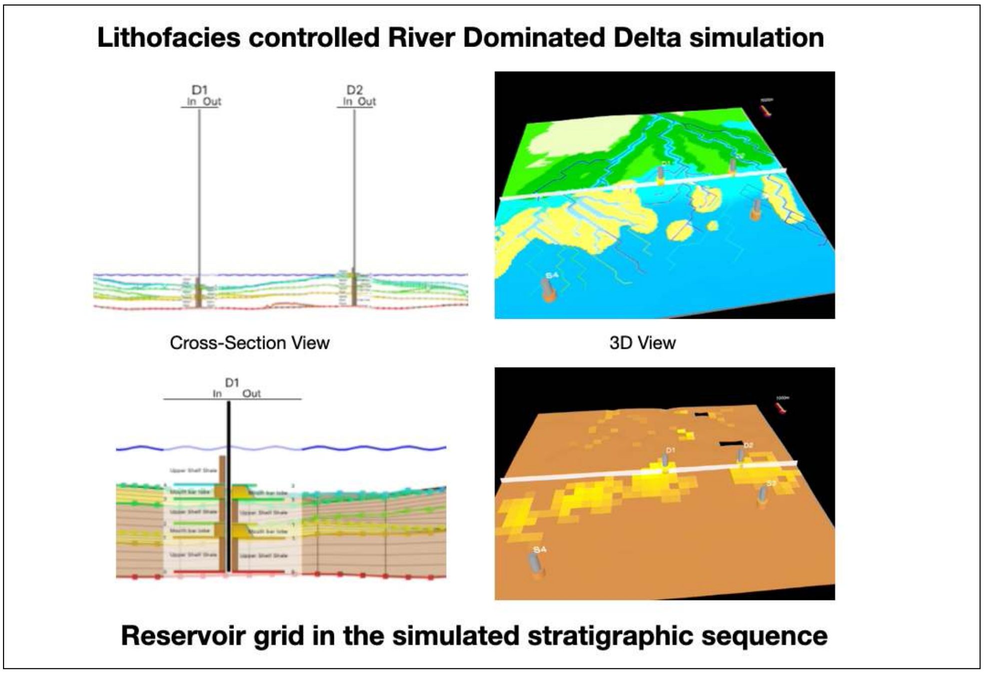
The first problem with the current method is the independent creation of the grid and the rock properties, leading to the misrepresentation of thin shale layers. The second problem is that creating a realistic geological model with geostatistics is difficult.

We propose a new method using a constrained, process-based model to create realistic geobodies fitting the well's data. The body's explicit boundaries will be the support for the reservoir grid. The body's intrinsic properties will guide the rock properties distributions. In input, we need wells in a restored/flattened position, interpreted lithofacies, a depositional environment with associated geometrical constraints, and a eustatic sea-level curve correlated with parasequences.

Unlike traditional modeling techniques that force the end-user to map geology into variogram models, the modeling burden is moved to the developer to implement geologic concepts. Each depositional environment requires the specific implementation of simulation objects, processes, and constraints. For example, in the case of a river-dominated delta, a percolation type process generates an object that represents the terminal distributary channels of the delta front and mouth-bars. Lithofacies intervals are transformed into bathymetry range constraints and channel/mouth-bar constraints. Intervals' thickness and the channel network control the aggradation process.

Unlike classical process-based methods, we see the simulation problem as the generation of a series of snapshots associated with discrete lithofacies intervals on each well. We also look at the simulation as a grid creation problem that constrains the discretization schema. A by-product of the simulation will be correlated well's interval.

We will illustrate our work on a river-dominated delta simulation.


Lithofacies controlled River Dominated Delta simulation
D1
In Out
D2
In Out
Cross-Section View
3D View
D1
In Out
Reservoir grid in the simulated stratigraphic sequence

S1103. A rule-based reservoir stacking model with effective well conditioning

Oscar Ovanger
Room: 101 2022-09-02 10:40

Rule-based geological reservoir modeling can capture depositional patterns realistically by mimicking physical processes. This can be seen as a more complex version of object models, where the objects are added sequentially in depositional order, and thus influence each other much more than usual in such models. Another way of looking at it is as a simplification of process-based models, where we speed up the process by simplifying physical processes into geological rules, thus allowing for faster realizations and conditioning. Bayesian statistics is a natural way of doing rule-based reservoir modelling and data conditioning. Here, realistic geometry and reservoir properties are part of the prior distribution, while well data is part of the likelihood model.

The main goal is then to assess the posterior distribution which is constrained by both rule-based reservoir modeling and the reservoir specific well observations. In this work we focus on shallow marine geometries, where we have a natural ordering of stacked objects within the area of interest. This hierarchical structure enables us to make many conditional independence assumptions by forming the model structures in a sequential manner. We introduce a rule-based model that relies on conditional sampling from Gaussian Random Fields (GRF). We model the boundaries that separate objects in the reservoir, and condition on data between boundaries. The prior GRF model has trends resembling the structure of typical outcrop boundaries.

As presented, the model is a useful first approximation to a more general solution, producing easily interpretable results. However, the model presented here would have to be extended before it could be applied to more complex geological systems. In particular, going beyond the conditional independence assumptions. Nevertheless, the sequentially updating of GRFs allows for analyzing complex well patterns and provides an approximation of the mass function for well configurations, which is otherwise infeasible.

S1104. Conditional simulations of process-based reservoir models using particle filtering: application to Loranca basin, Spain

Alan Troncoso (MINES-ParisTech),
Xavier Freulon (MINES ParisTech),
Christian Lantuejoul (MINES ParisTech),
Fabien Ors (Mines ParisTech - PSL Université),
Jacques Rivoirard (MINES ParisTech)
Room: 101 2022-09-02 11:05

In oil and gas industries, as well as in environmental studies (CO 2 storage or geothermal energy), geological reservoirs are often simulated, conditionally on field data, to better understand their geometry and their connectivity. Reservoirs formed by channelized meandering systems can be notably modeled using a process-based approach that mimics three interacting sedimentary processes, namely migration, aggradation, and avulsion. This process-based approach allows reproducing the genesis of the reservoir at geological time scale. This presentation describes an iterative procedure, called particles filtering, which addresses the difficult task of constraining the reservoir simulations to well data. This new conditioning approach assimilates the data sequentially while building the reservoir by stacking horizontal layers of deposited facies from bottom to top. At each iteration, a proposition step firstly extends the set of simulations (or so-called particles) by filling the current layer non-conditionally. Secondly, a resampling step aims at selecting the particles that are the most apt to match the data and discarding the others. Finally, a replication step leads to keep the number of particles constant over the iterations. When all layers have been processed, one particle is randomly picked up as the final conditional simulation. This approach is illustrated by a case study on the channelized meandering system of the Loranca basin (Spain) using the FLUMY process-based model. The results are presented and compared to those yielded by the current FLUMY conditioning approach, which consists in running a single simulation directly constrained to well data by adapting the physical processes at work.

S1105. Discrete karst network simulations: application to the Barrois limestones

Augustin Gouy (GeoRessources - Université de Lorraine),
Pauline Collon (Université de Lorraine, CNRS, GeoRessources),
Vincent Bailly-Comte (BRGM, Univ. Montpellier),
Philippe Landrein (Andra, Centre de Meuse / Haute)
Room: 101 2022-09-02 11:30

Like most of the carbonate formations, the Barrois Limestones (South-east of the Paris Basin, France) are prone to karstification. At local scale, several penetrable conduits are known close to the main karst outlets, but little is known for smaller karst drainage systems. At the scale of the recharge area, tracer tests and many surface and subsurface karst features reveal a large extension of the karst drainage system governing flow and transport in the whole aquifer, but its exact geometry is also unknown. This lack of information is the main factor limiting the use of physically-based models of flow and transport for most karst aquifers. A method able to simulate possible karst network geometries accounting for uncertainties at different scales is thus required. While several methods have been proposed in the literature, none of them have been tested on a well-documented site like the Barrois Limestones. Indeed, this case study is characterized by a large amount of pluri-disciplinary data used to build a 3D comprehensive and integrative conceptual model of the whole karst aquifer, including stratigraphic and geological models, cave topographies and speleogenetic concepts, land markers of karsts, well logging and hydraulic tests, surface observations of fractures, geochemistry, tracer tests, etc. In this work, we aim at explicitly generating a set of possible geometries for the Barrois karstic network using a stochastic approach constrained by the pluridisciplinary information stored in the 3D conceptual model. After presenting the site, we propose a brief review of karstic networks simulation methods. Their applicability is discussed regarding the different scales at which we want to study the area, the corresponding data and the objectives of the associated flow simulation. First results are shown on a kilometric-scale karst subsystem in the south of the Meuse department.

S1106. Three dimensional modelling of igneous sills: application to the Tasmanian dolerites in the Hobart district

Fernanda Alvarado Neves (Monash University),
Laurent Ailleres (Monash University),
Lachlan Grose (Monash University),
Alexander Cruden (Monash University),
Robin Armit (Monash University)
Room: 101 2022-09-02 11:55

A recently proposed method to build 3D geological models of igneous intrusions has enabled the reproduction of realistic intrusion shapes while honouring the input data. This method involves a parametrization of the propagation and growth of intrusions constrained by field measurements and knowledge of host rock anisotropies. Host rock anisotropies are incorporated depending on whether they played a role during intrusion emplacement. Geometrical conceptual models are then parameterized using the propagation and growth directions and used to stochastically simulate the intrusion geometry in three dimensions (3D).

We applied this method to model the Tasmanian dolerites in the Hobart region and we explored how pre-intrusion structures influenced the spatial distribution and geometry of the dolerite sills. Our approach was to build a series of 3D geological models constrained using contact points picked from geological maps and anisotropy of magnetic susceptibility (AMS) measurements collected within the sills. The difference between each model is due to the set of anisotropies that were adopted to parameterize the intrusion geometry. A similarity comparison between the 3D models and geological maps was carried out to assess those host rock anisotropies that most likely affected the geometry and spatial distribution of the intrusions. The results suggest some segment connectors between sills may be controlled by pre-intrusion structures, while others most likely formed during the coalescence of sill segments that propagated and grew at different stratigraphic levels.

S12 Spatial Associations

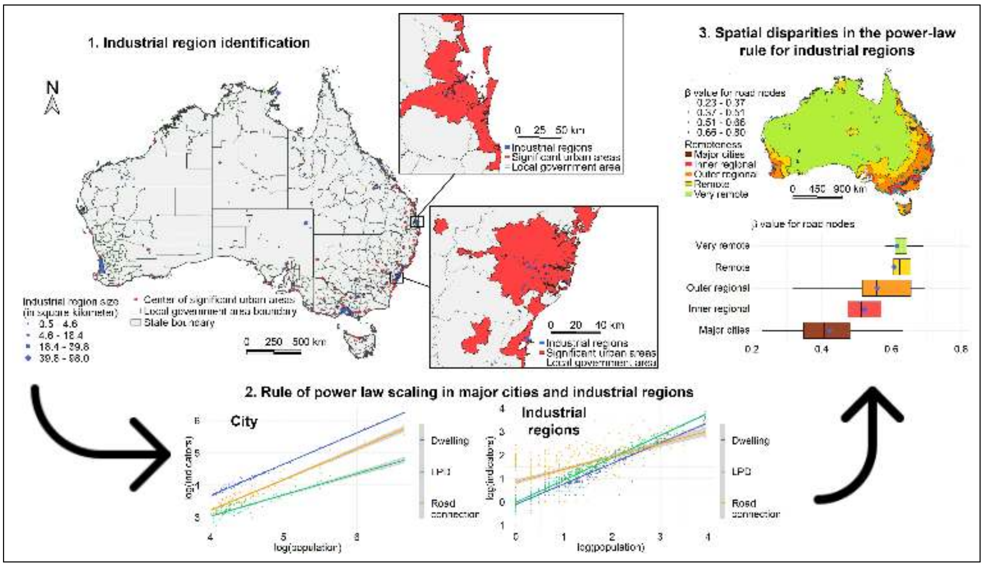
Yongze Song (Curtin University),
Qiuming Cheng (Sun Yat-Sen University/China University of Geosciences (Beijing))

This session aims to invite researchers from multiple fields to present their latest methods and applications about the identification of spatial associations. In geosciences, spatial associations are generally explored based on spatial dependence, similarity, heterogeneity, singularity, and other structures of spatial data. In recent a few years, geospatial artificial intelligence provides more opportunities for more accurate and in-depth understanding of spatial associations. In this session, we encourage authors to submit papers in following areas: innovative methods of spatial associations; advanced applications of spatial associations; spatial statistics for spatial associations; and geospatial artificial intelligence for spatial associations.

S1201. Identifying Spatial Disparities of Power-law Scaling in Nation-wide Industrial Regions

Zehua Zhang (Curtin University),
Yongze Song (Curtin University)
Room: 101 2022-09-01 15:00

Urban and regional expansion follows the rule of power-law scaling. This rule of development demonstrates a quantitative understanding of regional resilience, population growth and infrastructure design, and provides opportunities for sustainable future planning. The spatial disparity phenomenon is ubiquitous for geographical objects, especially urban and social attributes, and no exception for the rule of power-law. However, current studies have limited discussions of spatial disparities in power-law scaling. Therefore, this research was designed to investigate power-law scaling rules and relevant spatial disparities in Australian industrial regions, with population density, dwelling and road connection as indicators, using power-law geographically weighted regression (PL-GWR). To achieve ultimate goals, we analyzed Australian national census and OpenStreetMap big data, and tested power-law scaling models for industrial regions and urban areas in Australia. This research discovered two facts that: (1) Population density and road connection scaling relationships had differences between industrial regions and urban areas. (2) The longer industrial regions' distance to major cities was the higher scaling exponent would be. In terms of methodological design, this research made a first trial on identifying spatial disparities in power-law scaling for nation-level land use research using PL-GWR. In terms of outcomes, research findings could help urban planners design better human settlements when facing city expansion challenges.



1. Industrial region identification
N
0 25 50 km
Industrial regions
Significant urban areas
Local government area
0 20 40 km
Industrial region size (in square kilometer)
0.5 - 4.6
4.6 - 18.4
18.4 - 39.8
39.8 - 98.0
Center of significant urban areas
Local government area boundary
State boundary
0 250 500 km
3. Spatial disparities in the power-law rule for industrial regions
β value for road nodes
0.23 - 0.37
0.37 - 0.51
0.51 - 0.66
0.66 - 0.80
Remoteness
Major cities
Inner regional
Outer regional
Remote
Very remote
0 450 900 km
β value for road nodes
Very remote
Remote
Outer regional
Inner regional
Major cities
2. Rule of power law scaling in major cities and industrial regions
City
Industrial regions
Dwelling
LPG
Road connection
log(indicators)
log(population)

S1202. Reconstruct the Fine-resolution Urban Apparent Temperature (Humidex) Combined with Canopy Parameter

Xilin Wu (Institute of Geographic Sciences and Natural Resources Research, CAS),
Yong Ge,
Qingsheng Liu,
Daoyi Gong
Room: 101 2022-09-01 15:25

The “felt temperature” is the preferred measure of hotness or coldness expressed to depict human sensory rather than other temperature concepts. However, to date, our perception of its spatial pattern with fine spatiotemporal data remains incomplete, especially lacking datasets with clear physical mechanisms. Here, we demonstrated an empirical statistical approach incorporating atmospheric dynamics theory with aerodynamic parameters capable of developing hourly datasets at a high spatial resolution (0.01 x 0.01). This fusion mechanism model, named the Humidex Reconstruction Model based on Numerical Simulation Data (HRMNSD), employed reanalysis data and satellite data for both near surface temperature(Tair) and the dew point temperature(Tdew) to combine their respective advantages in the correct representation of a turbulent exchange between the surface and the atmosphere and good spatial performance. To explain the physical constraints, we also mixed aerodynamic parameters (roughness length for a natural surface and urban geometric characteristics for an artificial surface) into the Tair downscaled model. We showed the good performance of this model in each season using the Yangtze River Delta, China as an example. The root mean square errors (RMSEs) of the Humidex were 2.47°C (in winter), 2.49°C (in spring), 2.80°C (in summer) and 2.56°C (in autumn), respectively, where the correlation coefficient (r2) was 0.83 (in winter), 0.90 (in spring), 0.74 (in summer) and 0.66 (in autumn). Furthermore, we found a diverse spatial pattern between the near surface temperature and the Humidex (in seasons such as winter and summer), suggesting that water vapor is a strong weather component of the temperature “felt“ by humans that merits more attention.

S1203. Holographic Digital Earth

Shoutao Jiao (Development Research Center of China Geological Survey),
Yueqin Zhu (Development Research Center of China Geological Survey),
rongmei liu (Development Research Center of),
Zhenji Gao (Development Research Center of China Geological Survey),
Lingling Yuan (luckyy1103@163.com)
Room: 101 2022-09-01 15:50

Holographic digital earth is a new generation of spatiotemporal information infrastructure. It is based on earth system science, and aims to reveal the changing laws of the Earth system and the interaction between human activities and global changes. It is a general term for the collection, processing and application of digital Earth information. Its core is to build a data system set that covers the global scope and truly reflects the distribution, characteristic attributes and transformations of global spatiotemporal phenomena, and enables these data systems to have the ability to timely and accurately collect, process, store and distribute the global spatiotemporal information. This paper introduces some ideas of holographic digital earth, including the collection, processing and application of holographic digital earth data, the construction of holographic digital earth basic framework, the construction of geophysical digital benchmark, the construction of holographic digital earth data engineering, the construction of holographic digital earth visualization engine and equipment. As well as the construction of high-performance cloud service clusters of holographic digital earth, it provides support for the construction of a new generation of full information infrastructure.

S1204. Understanding spatially varying relationships in environmental studies

Chaosheng Zhang (NUI Galway)
Room: 101 2022-09-01 16:15

The relationships between environmental variables are "spatially varying", meaning that they are different at different spatial locations which deserves proper investigation to better reveal their controlling factors. With growing databases available at regional, national, and global scales, new opportunities arise for the exploration of such relationships. The geographically weighted regression (GWR) offers new opportunities to explore the relationships between environmental factors at the local level. In this presentation, examples are provided to demonstrate the power of GWR in revealing the spatially varying relationships in geochemical databases.

It was found that in urban soils of London, the generally positive relationships between Pb and Al was disturbed in the city center areas with weakened correlations, while in the suburban area in the north London, the relationship even became negative due to the significantly elevated Pb concentration in areas close to the city center. Meanwhile, in large green areas in the city center, the positive relationships between Pb and Al still remained. The relationships between soil organic carbon (SOC) and elevation in Ireland exhibit strong spatial variation which are related to the type of peat. In the mountainous areas, positive relationships were found between SOC and elevation, which was in line with the distribution of blanket peat. In the central area of Ireland where basin peat was formed, the relationships between SOC and elevation became negative, as basin peat was formed in areas of low elevation.

The spatially varying relationships provides new insight into the complicated relationships between environmental variables.

S1205. Key Technologies of Multiscale 3D Geological Model Database for Resource and Environment Big Data Integration and Sharing

Chen Genshen (China University of Geosciences),
Gang Liu (China University of Geoscience),
Qiyu Chen (China University of Geoscience),
Xuechao Wu (China University of Geoscience)
Room: 101 2022-09-01 16:40

3D geological model data is the basis of analysis and calculation of complex problems in the field of resources and environment. However, there are some difficulties in the integrated application of massive multi-source 3D geological model data, such as different scales and storage structures, difficult data scheduling and inefficient sharing services. Aiming at the multiscale and data structures of massive multi-source 3D geological model data, we propose a metadata organization structure and integrated expression model. We design different metadata organization structures for three application scenarios: visualization, thematic analysis and application, comprehensive information mining. By analyzing the organization mode of 3D geological model data from various sources, we established an integrated expression mode considering spatial relationship and semantic relationship, and constructed the multiscale 3D geological model database through the distributed file system. We proposed relational and non-relational data integrated storage scheme based on distributed storage structure to solve the difficulty of data scheduling. We adopted the distributed interval data index structure and multi-level spatio-temporal data cache structure, to establish a distributed index for large-scale and multiscale complex 3D geological objects. It has improved the retrieval and scheduling ability of 3D geological objects and related attribute data. To eliminate the limitations of data integration and sharing service, a data conversion and service interface based on Geo3DML is provided to realize the integrated management of different types of 3D geological models. We have developed a prototype system of 3D geological model database for big data storage and management. The system has realized the integrated management and rapid scheduling of multiscale 3D geological model data in 3D visualization environment. And it verified to be feasible with the basic geological survey results of the Yangtze River Basin, the Three Gorges Reservoir area 3D geological disaster model data and the basin urban geological survey results.

S13 Structural modelling: Parametrisation and Interpolation of Sub-Surface Architectures

Gautier Laurent (ISTO-Univ.Orleans),
Lachlan Grose (Monash University),
Simon Lopez (BRGM)

This session is dedicated to new advances and remaining challenges in the field of geomodelling: the reconstruction of sub-surface architectures (e.g., stratigraphic layering, faults, folds, intrusions) from sparse and ambiguous spatial observations. This is a complex data assimilation problem, which is facing the hurdle of both aleatory and epistemic uncertainties. This problem has long been formalised as an interpolation process, with various mathematical implementations, but it generally remains dependent on expert inputs for adding geological controls or counterbalancing mathematical artefacts. This session welcomes presentations that illustrate this problem in original applications and/or propose original solutions, in particular - but not limited to - topics covering:

- Limitations of numerical interpolation schemes and ways forward,
- Formalisation of geological objects and concepts,
- Knowledge integration within interpolation schemes,
- Aleatory vs. epistemic uncertainties,
- Original formalisms and modelling schemes.

S1301. Advances in Implicit 3D Geological Modelling using Implicit Neural Representations

Michael Hillier,
Florian Wellmann (RWTH Aachen),
Boyan Brodaric (Geological Survey of Canada),
Eric de Kemp (Geological Survey of Canada),
Karine Bedard (Geological Survey of Canada)
Room: 101 2022-08-30 10:00

Neural networks that parameterize implicitly defined functions are emerging as a powerful framework for learning 3D shape representations. These types of neural networks, known as implicit neural representations, can be used effectively to perform implicit geological modelling given appropriately designed loss functions are employed during training. Using neural networks for this purpose provides unique advantages over existing implicit modelling methods in terms of scalability and flexibility in incorporating constraints. An implicit neural representation network-based modelling method is developed that exploits these advantages to help address the problems of existing implicit methods – namely, the issues with producing geologically reasonable models in complex settings and with computational scalability as the number of constraints increases. Advances in implicit geological modelling using implicit neural representation networks are presented that include: (1) an improved loss function for interface data that produces modelled interfaces that are both qualitatively (more geologically representative) and quantitively (smaller errors) better to what is produced using commonly used loss functions, (2) the incorporation of unconformities into the geological model, and (3) a better efficiency enabling a scaling for big datasets. These advances provide an efficient modelling method to support national scale 3D geological modelling from massive point-based datasets – modelling initiatives which are becoming increasingly common at Geological Survey Organizations. The developed method's capacity to support such initiatives is demonstrated by modelling a provincial scale geological model of the Western Canadian Sedimentary Basin in Saskatchewan, Canada. The point dataset used to train the network contains over 500,000 noisy points sampling top markers and intraformational picks of 49 geological formations. Results show that the method can efficiently produce reasonable 3D geological models of sedimentary basins containing numerous unconformities from massive noisy point datasets. Moreover, the large variations in formation thickness between sampled interfaces is well represented and fitted in the model.

S1302. 3D structural geomodelling of complexly deformed basement units: the Aosta Valley case study (Western Alps, Italy)

Gloria Arienti (University of Milano-Bicocca),
Andrea Bistacchi (Università degli Studi di Milano-Bicocca),
Giorgio Vittorio Dal Piaz (Accademia delle Scienze di Torino),
Giovanni Dal Piaz (LTS - Land Technology & Services SRL, Treviso),
Bruno Monopoli (LTS - Land Technology & Services SRL, Treviso),
Davide Bertolo (Regione Autonoma Valle d'Aosta),
Gabriele Benedetti (Università degli Studi di Milano-Bicocca)
Room: 101 2022-08-30 10:25

The North-Western Alps represent one of the best-known orogenic playgrounds worldwide, exposing a complexity of polyphase ductile and brittle structures that makes this area also one of the richest in terms of deformation styles.

Here we present preliminary results of a new 3D structural model of a large area (1300 km2). Input data are represented by structural surveys and detailed geological mapping, defining a truly 3D dataset that compensates for the absence of subsurface data thanks to important differences in elevation of 3-4 km, from valley floors to mountain summits. Our modelling workflow is based on a first step of conceptual modelling in vertical cross-sections, based on classical and sound structural concepts, followed by interpolation with implicit and explicit surface algorithms.

In our area, geological complexity is given by several finite faults, internal to the model, that intersect each other as the result of multiple brittle deformation events. The basement units are also interested by polyphase ductile tectonics: isoclinal and cuspate-lobate folds, polyphasic folds, and other structures that produce great thickness variations of the lithological bodies outcrop.

In this setting, the geological legend needs to be conceived as a complex conceptualization of surfaces organized in a hierarchical structure. The most consistent contacts (e.g. between different Alpine domains) are first order surfaces, second order is given to surfaces that divide different tectonic units and following down to the lithological boundaries (the least order of importance).

In this contribution we focus our attention on areas that are very explicative of the complex metamorphic nature of the basement. We present the adopted geomodelling solutions while performing a comparison on how different software packages (both licensed and open-source) perform when modelling this challenging structural setting, in order to obtain a model that properly fits the geological interpretation of the area.

S1303. A field sampling workflow for Fold Geometry modelling

Rabii Chaarani (Monash University),
Lachlan LG Grose (Monash University),
Laurent LA Ailleres (Monash University),
Robin Armit (Monash University),
Laurent Gautier (ISTO-Univ.Orleans)
Room: 101 2022-08-30 10:50

The main objective of structural mapping is to elucidate the 3D geometry and the history of the studied structures. This objective is only achieved if the structural map contains a representative sample of structural data. Due to varying outcropping conditions, the collected structural data may not represent the studied structures. The purpose of our study is to build a field sampling workflow that addresses structural data representativeness for fold structural mapping. To do so, we use the new open-source modelling engine LoopStructural to study the sampling requirements to recover the observed fold geometries. LoopStructural models folds within a fold coordinate system (i.e. the fold frame). The axes of the fold frame correspond roughly to the axes of the finite strain ellipsoid associated with the local geometry of folds. Two angles are defined within the fold frame and are used to constrain fold geometry: (1) The fold axis rotation angle is the angle between the fold axis and Y-axis of the fold frame; (2) The fold limb rotation angle is the angle between the normal to the folded foliation and the Z-axis. Then, a Fourier series is fitted to fold rotation angles observations using unconstrained least squares to constrain 3D fold models. An experimental workflow is used to assess the sampling locations that reproduced models similar to a synthetic reference model. These experiments show that folds should be sampled at the inflexion line to produce models similar to the reference model. If geologists cannot sample the inflexion line, we propose a series of constraints that incorporate indirect observations into the curve fitting process that fit field observations. This workflow will allow geologists to sample effectively fold geometry in a time-efficient way.

S1304. Knowledge-guided process for Semantic geological structure detection and representation

Imadeddine Laouici (BRGM/ISTO),
Gautier Laurent (ISTO-Univ.Orleans),
Christelle Loiselet (BRGM),
Yannick Branquet (Univ. Orléans, CNRS, BRGM, IST)
Room: 101 2022-08-30 11:15

This contribution introduces a knowledge-based approach to geological structure detection and representation that simulates the human cognition process. Geological structures (e.g., faults and folds) are present in different kind of data sources (Well-data, cross-sections, and geological maps), but their expression is generally ambiguous and calls for expert interpretation. Experts seek to explicitly apply their held knowledge in the procedure of detecting and representing these structures, which exposes the work to subjectivity as they dependent on their backgrounds and working habits. In the proposed approach, expert's knowledge is expressed through an ontological model. In this model, the geometrical descriptions of the structures are formalized in combination of relevant contextual geological concepts. The proposed ontological model has for its top layer the GSO (GeoScience Ontology) specially designed for representing the various shared geological concepts as they are defined in reality. This combination allows independent formal description and defining of the structures' attached qualities and in-depth link with their geological frame. Thus, granting an exhaustive objective expression of relevant knowledge related to their identification and representation. We argue that this knowledge-based paradigm is effective as it requires less human interplay and does not necessitate resting on large initial datasets that are not always available but required for data-based algorithms that use other artificial intelligence techniques like machine learning. As the proposed ontology uses the OWL ontology language, it is compatible not only with the GSO but with other domain ontologies and standard web technologies.

S1305. Combinatorial and topological considerations for conducting angular distance measurements between geological interfaces

Michal Michalak,
Filip Turoboś (Lodz University of Technology),
Paweł Gładki (University of Silesia in Katowice)
Room: 101 2022-08-30 11:40

When considering a number of sub-conformable geological interfaces, it is possible to measure angular distance between them. This may serve to assess the degree of parallelism between the top and bottom of these interfaces and detect possible unconformities. However, from a computational perspective, it is of vital importance to realize the relationship between the number of input surfaces and the resulting angular distance distributions. These distributions may be subsequently used to create derivative distributions, for example arithmetic differences. These combinatorial problems are discussed along with an important topological question about these workflows. Namely, whether the proposed angular distance function is a metric. Specifically, we are interested if the triangle inequality holds for the function used. A positive answer would be welcomed since it would imply that there exists no optimization profit of replacing direct measurements with a sum of indirect measurements. This potential result would testify about the validity of conducting direct measurements. This study was suported by National Science Centre, Poland, 2020/37/N/ST10/02504.

S1306. A Bayesian framework for the inversion of geological maps for fault geometry

Lachlan Grose (Monash University),
Laurent Ailleres (Monash University)
Room: 101 2022-08-30 12:05

Recent developments in 3D geological modelling allow for fault kinematics (slip vector and displacement magnitude) to be incorporated into the model description. However, fault geometries and kinematics are often not recorded geological maps or poorly understood. Estimating the fault geometry from a geological map is an inverse problem, where the geologist needs to interpret the fault surface geometry and kinematics that best explain the observed geology. The interpreted fault geometry is usually a single non-unique solution with little to no indication of the associated confidence/uncertainty. Using LoopStructural, faults can be modelled from a combination of parameters describing the fault surface geometry, fault slip direction, fault ellipsoid geometry and fault displacement magnitude. Faults are added to the implicit function that represents the faulted geological objects by un-faulting the observations of the faulted object and allowing the geological object to be interpolated without the fault. In this study, we adapt the fault model used by LoopStructural as a forward model and define a geological misfit function for a likelihood function to determine how well the fault describes the un-faulting of the observations. A forward gravity model is also calculated using the geometries defined by the fault model. A geophysical misfit function is determines how well the modelled geophysics match the observed geophysics. We use The likelihood function is incorporated into a Bayesian inversion scheme where the geologist's knowledge can be used to constrain the prior distributions of the fault parameters. We apply our approach to estimating the geometry and kinematics of faults from the Preliminary results from the Hamersley region in Western Australia and demonstrate that show comparable map patterns can be produced for a range of parameter combinations – e.g. decreasing the displacement magnitude as the fault slip vector becomes more horizontal.

S1307. On some comparison metrics between 3D implicit structural models.

Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS)
Room: 101 2022-08-30 12:07

During the last two decades, several implicit structural modeling approaches have flourished to automatically build 3D models of complex geological structures from sparse structural data. The essential idea of implicit modeling is to use one or several three-dimensional scalar fields, each of them representing one or several conformable geological interfaces as iso-surfaces (or level sets). In detail, the various implicit methods use different numerical representations of the scalar field and different formulations of the interpolation / extrapolation problem. Consequently, from the same input data, two different implicit methods may lead to different 3D models. In addition to theoretical analyzes, numerical benchmarks are important to better understand these behaviors in multiple geological settings. For such benchmarks, a first approach is to extract the individual surfaces corresponding to the target geological interfaces and then compute the distance between these surfaces. However, for implicit stratigraphic models where a conformable stratigraphic series is modeled at once by one single scalar field, such comparison does not capture variations for horizons corresponding to iso-values not present in the data. A difficulty is also that the absolute scalar field values may be scaled differently from one model to the other. Therefore, we propose, to compare normalized scalar field gradients as a global measure. Inspired by persistent homology, we also use some measures which characterize the topology of the scalar fields. These measures also open interesting perspectives to detect similarities between stochastic structural models and cluster realizations in structural uncertainty studies.

S1308. Subsampling Structural Data for Multiscale 3D Geological Modelling

Ranee Joshi (The University of Western Australia),
Mark Jessell (The University of Western Australia),
Mark Lindsay (CSIRO),
Tim Ivanic (Geological Survey of Western Australia)
Room: 101 2022-08-30 12:09

Multiscale three-dimensional (3D) geological models allow us to maximize the analysis of multiple datasets, avoid losing information content and utility, reduce assumptions from data imputation and better answer specific scale-dependent geological questions. To visualize meaningful geological information as multiscale 3D geological models, properly subsampling of geological data is critical. We investigate the implications of different subsampling techniques in order to develop workflows best suited to subsampling structural data (0D: point observations, 2D: fault lines and fold axes).

In this contribution, we present the findings of subsampling 1:500,000 knowledge-rich structural data and their implications to the Ninghan Syncline 3D geological models. The Ninghan Syncline is a mineralized, lithologically diverse and structurally complex area with regions of sparse and clustered sampling. This dataset gives the opportunity to test the effectivity and limits of these subsampling workflows. The structural measurements are subsampled depending on the scale of interest, concentration of measurements and consistency of the orientation of these measurements. The subsampled data are used as inputs into a geomodelling engine, in this case, LoopStructural. The resulting 3D geological models are compared and assessed for the effects of subsampling on their geometries and the associated uncertainties from subsampling. In these comparisons, we do not suggest what the better or "correct" model is. Instead, we use these comparisons to demonstrate the relationship between the subsampled orientations and the similarity of the resulting models. The results show that subsampling methods using geological rules more effectively select and identify structural measurements, particularly for areas with sparse geological data and complex geology.

S1309. A spline-based regularized method for the reconstruction of geological models from sparse data

Belhachmi Ayoub (Schlumberger),
Bernard Mourrain (INRIA),
Azeddine Benabbou (Schlumberger)
Room: 101 2022-08-30 16:30

The construction of a geological numerical model is a key step in the study and exploration of the subsurface. These models are constructed from seismic or well data. Often the available data are sparse and noisy, which makes this task difficult, mainly for reservoirs where the geological structures are complex with distinct discontinuities and unconformities.

In this paper, we propose a new method to compute an implicit function of the stratigraphic layers. In this method, the data are interpolated by piecewise quadratic C1 Powell-Sabin splines and the function is regularized via a diffusion partial differential equation PDE. The method is discretized in finite elements on a triangular mesh conforming to the geological faults.

Compared to classical interpolation, the use of piecewise quadratic splines on a mesh has three major advantages. First, a better handling of stratigraphic layers with strong curvatures. Second, a reduction in the resolution of the mesh, allowing a considerable gain in computation time. Third, a local adaptivity to the geometry of the data, taking faults into account.

The regularization of the function is the most difficult component of any implicit modeling approach. Often, classical methods produce inconsistent geological models, in particular for data with high thickness variation, and bubble effects are generally observed. To address these problems, we propose a new scheme in which a diffusion term is introduced and iteratively adapted to the shapes and variations of the data, while minimizing the fitting error.

S1310. Building on 50 years of geomodelling: walking a tightrope between tradition and clean slate

Nicolas Clausolles (BRGM),
Thomas Janvier (BRGM),
Simon Lopez (BRGM)
Room: 101 2022-08-30 16:55

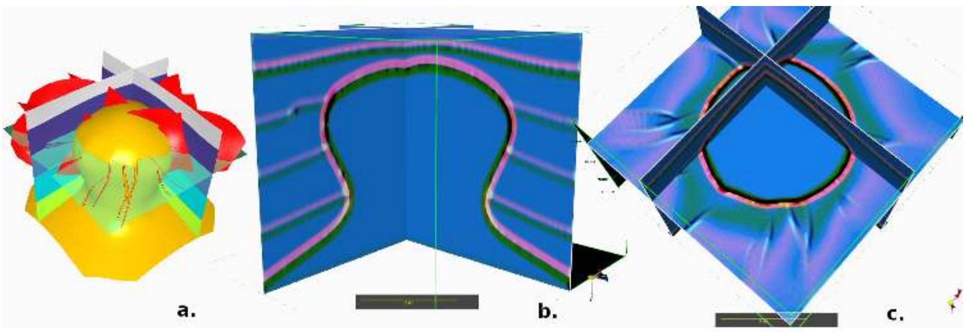
Geological surveys are facing the transition from systematic 2D mapping of national territories to more versatile – possibly cross-border – 3D models. BRGM has produced geological models for several decades in a project driven approach implying specific goals, hypotheses, scales, modeling tools... In such an approach, a few experts' choices may constrain the final deliverable and hamper interdisciplinary contributions. Our talk will detail practical challenges that is currently facing BRGM in redesigning its set of existing modelling tools into an open modeling platform based on modular software components that will ideally combine both proven legacy and newer methodologies to overcome existing tools limitations and promote true interdisciplinary experience.

Starting from the observation that several tools share common concepts, a first step is to clearly identify and generalize these underlying concepts (e.g. geological pile/architecture to express relations between geological interfaces). Nevertheless, there is still a considerable gap between the geologist's dream tool and the modeling experience that have been offering geological software for the last twenty years – mainly consisting in popularizing the "implicit" modeling approach. Though some fields of research are promising, as are many technological devices, the feeling is that we still need a breakthrough that would change the daily life of geological model producers and represent a clear alternative to old monolithic software. As a survey, our position, either individually or more collectively (e.g., European geological surveys) still needs to be found between two major trends: the replacement of proprietary commercial suites by web-service based cloud platforms and the rise of many open-source initiatives. Though promising, the latter does not benefit from a mature structured global community support yet, as it can exists in other communities (e.g., for GIS), which would make us take the next step.

S1311. Hypersurface curvatures of seismic attributes

Anne-Laure Tertois (AspenTech),
Igor Ravve (Emerson Automation Solutions),
Zvi Koren (Emerson Automation Solutions)
Room: 101 2022-08-30 17:20

Reflector-normal vectors and reflector-curvature parameters are the principal geometrical attributes used in seismic interpretation for characterising the orientations and the shapes of geological reflecting surfaces. The input dataset for their computation consists of fine 3D grids of scalar fields representing the seismic-driven or model-driven reflectivities. Conventionally, computation of curvature parameters at each grid point analyses the potential existence of a local reflecting surface. This assumption can break down for subsurface points in the vicinity of complex reflecting surfaces and/or sharp/discontinuous geological features. We present a novel method that better characterises the shapes of these complex geological features by extending the assumption of 2D local surfaces in 3D space into 3D local hypersurfaces in 4D spaces, with their corresponding principal curvature parameters. The proposed approach does not assume the existence of a specific local surface associated with the grid points. It is formulated for any n-dimensional space as a smooth hypersurface in a space of a higher dimension n+1. For n=2, only the minimum and the maximum principal curvatures exist; for n=3, (hypersurface in 4D space), there is an additional medium-valued principal curvature. The fourth dimension is the studied scalar parameter, which may be seismic reflectivity, wave velocity, impedance, relative geological time, or any other scalar field. We show that this type of curvature computation can be reduced to the eigenvalue problem. This leads to a straightforward algorithm to compute the three stationary curvatures of the hypersurface and their corresponding principal directions and makes it possible to characterise non-surface-like geological features, like faults and fractures. The figure accompanying this abstract shows the three principal hypersurface curvatures applied to the velocity field (Figure a) of a salt dome with radial faults, mapped to the RGB channels to create a blended picture (Figures b and c).



Hypersurface curvatures applied to a salt dome with radial faults.
A velocity scalar field is initialized based on the geometry of the structural model shown in Figure **a.** with four layers of increasing velocity with depth, a salt dome and induced radial faults. Figures **b.** and **c.** show our three principal hypersurface curvatures computed from this velocity field, each mapped to one of the R, G, B channels to create a blended picture.
As well as delineating the major structural interfaces such as the horizons and the salt dome, the blended curvatures also highlight the steep salt flanks, faults and the singular points where horizons are connected to the salt body.

S1312. Loop - An open-source, integrative 3D geological modelling platform

Laurent Ailleres (Monash University),
Lachlan Grose (Monash University),
Mark W. Jessell (The University of Western Australia),
Gautier Laurent (ISTO-Univ.Orleans),
Robin Armit (Monash University)
Room: 101 2022-08-30 17:45

To improve the efficiencies of mining requires the ability to better predict subsurface geology at multiple scales. Geologically consistent mine models should equate to better resource models and mining/processing optimisation for the extraction of our green-future-dependent metals. We present the current state of the Loop project, an open-source interoperable, integrative, probabilistic 3D geological modelling platform. We have implemented the use of all structural geological data (fault kinematics, fold axial surfaces, fold axes, overprinting relationships). We have automated the topological analysis maps and geological history building. As a proof of concept, users can now draw a polygon on a map and generate 3D models in just a few minutes using map2loop and LoopStructural libraries (github.com/Loop3D). We are integrating geophysical constraints as early as possible in the modelling workflow. The main outcome of the development of the structural modelling method (LoopStructural) is the definition of structural frames which allow the definition of a curvilinear and conformable to layering, rectangular coordinate system throughout the models. We present the concept for LoopResources, our proposed property modelling library. Using this deformed cartesian coordinate system, we propose to adapt geostatistical and interpolation methods to curvilinear coordinate systems using classical XYZ-UVW transformations. This will ensure that lithological anisotropies are enforced during resource estimation and property modelling.

Loop is a OneGeology initiative, initiated by Geoscience Australia and funded by Australian Territory, State and Federal Geological Surveys, the ARC and the MinEx CRC. The project is led by Monash University and involves research groups from the University of Western Australia, the RING consortium at the Universite de Lorraine, Nancy, France and RWTH Aachen in Germany. In-kind research is also provided by Natural Resources Canada (Geological Survey of Canada), Geoscience Australia and the British Geological Survey. Other partners include AuScope and the USGS.

S14 Machine learning-based mineral prospectivity mapping

Renguang Zuo (China University of Geosciences),
John Carranza (University of the Free State)

Mineral prospectivity mapping as a computer-based approach to delineate targeted areas for a specific type of mineral deposit has changed from being knowledge driven to data driven to today's big data analytics. There are increasing applications of machine learning algorithms in mapping mineral prospectivity and identifying geochemical anomalies association with mineralization. The session welcomes the following submissions:

- machine learning (such as logistic regression, random forests, support vector machines, and extreme learning machines),
- deep learning (such as convolutional neural networks, deep autoencoder networks, recurrent neural networks, and generative adversarial networks,
- simulation, and
- case studies for identifying geochemical anomalies or mapping mineral prospectivity.

S1401. Machine learning in Prospectivity Modeling: Feature Engineering, Selection and Integration

Alok Porwal (Indian Institute of Technology Bombay)
Room: 105 2022-08-31 15:00

Recent advances in machine learning, particularly the proliferation of deep learning algorithms in recent years have led to wide-spread interest in the applications of these techniques to mineral prospectivity modeling. This contribution aims to present a comprehensive, but critical, review of applications of the machine-learning paradigm in general, and deep-learning approaches in particular, to mineral prospectivity mapping. The inputs to "shallow" machine learning algorithms are hand-crafted predictor features that are identified using a mineral systems mode and typically derived by geoprocessing of regional-scale public domain data. Given the same inputs, all models are likely to generate similar outputs, irrespective of the model used. New models for data integration are not likely to make a significant difference. As a matter of fact "classical" algorithms such as weights-of-evidence are likely to return outputs that are comparable to the outputs of machine-learning algorithms. This has been amply demonstrated by a number of case studies on comparison of different integration techniques. Furthermore, most machine learning algorithms consider pixels as independent and identically distributed, an assumption that ignores spatial autocorrelation and neighborhood dependencies. Deep learning algorithms such as convolution neural networks (CNN) accommodate spatial neighborhood relationships; however, these algorithms require far too many training samples. It has been shown that, with limited training samples (which is typically the case in mineral prospectivity modeling), simpler models outperform deep learning models. However, the power of deep-learning algorithms to accommodate the spatial neighborhood relationships can be harnessed for feature engineering in unsupervised learning mode. In this presentation, I make a strong case for focussing on unsupervised machine learning algorithms for automating feature engineering. New research in prospectivity modeling should focus on automated feature extraction, complementing the knowledge-driven feature engineering. A paradigm shift from data integration to feature engineering is required for future progress in prospectivity modeling.

S1402. Automated regional-scale exploration targeting of REEs in western Rajasthan, northwest India.

Malcolm Aranha (Indian Institute of Technology Bombay),
Alok Porwal (Indian Institute of Technology Bombay)
Room: 105 2022-08-31 15:25

Mineral prospectivity modelling traditionally requires a consistent availability of robust geoscientific datasets that are manually filtered and processed to map desirable mineralising processes that are identified using a conceptual generalised mineral systems model. The identification of mineralisation processes and the conceptual mineral systems model are subject to bias due to the subjective preference of the expert geologist. As a result, the entire process is time-consuming, labour-intensive and subject to uncertainty.

This contribution applies self-organising maps (SOM), a neural network-based unsupervised machine learning clustering algorithm, to unprocessed gridded geophysical and topographic datasets to automate the process of prospectivity modelling and delineate regional-scale exploration targets for carbonatite-alkaline complex related REE deposits in western Rajasthan in northwest India. This study used no interpreted or manually generated geological data such as bed-rock or surface geological maps and mapped structures; and relies solely on the algorithm to identify crucial features and delineate targets. The ideal number of clusters, obtained as a direct result of the size of the SOM network, is a dilemma in such an algorithm. Too many clusters would isolate individual features of the individual datasets, leading to over classification. Too few clusters result in broad, generalised clusters covering large spatial areas. Statistical indices such as the Davies Bouldin index can be used in virgin areas, whereas known deposit points can guide this decision in partially or well-explored regions. The obtained results of this study were compared with those obtained from a previous supervised knowledge-driven study for validation and were found to be comparable. Therefore, unsupervised machine learning algorithms can reliably automate manual mineral prospectivity modelling studies, providing robust, time-saving alternatives to traditional knowledge-driven or supervised data-driven prospectivity modelling. These methods would be particularly effective in unexplored terrains with limited geological knowledge, where conventional prospectivity modelling cannot be applied.

S1403. Exploration targeting at the Rajapalot Au-Co project in Finland – Application of machine learning methods for identification and prioritization of drilling targets at the prospect scale.

Bijal Chudasama (Geological Survey of Finland),
Johanna Torppa (Geological Survey of Finland)
Room: 105 2022-08-31 15:50

This study presents the results of gold prospectivity modeling at the Rajapalot project area in the northern Fennoscandian Shield in Finland. The study area comprises epigenetic-hydrothermal high-grade gold-cobalt mineralization. Ground exploration, ore-resources estimation and ore-body delineation activities are in progress at Rajapalot. This area, therefore, provides an ideal opportunity to test the effectiveness of prospectivity modeling methods (which are largely 'predictive tools' at regional- and belt-scales) as a targeting aid at the scale of a deposit where extensions of mineralization are usually the target for exploration drilling.

The workflow implemented in this study comprised of (i) mineral system modeling, (ii) the formulation of geological hypotheses and creation of corresponding evidence layers, (iii) statistical testing of each geological hypothesis, and (iv) mineral prospectivity modeling. Different statistical and machine learning methods were implemented for detailed prospectivity modeling in the study area. The mathematical modeling methods used were unsupervised self-organizing maps and supervised artificial neural networks and fuzzy inference systems (FIS). Additionally, the FIS were optimized using (i) Monte Carlo Simulations, and (ii) the gradient descent algorithm. The results from this study identified three important drilling targets at high confidence levels. Hence, we conclude that collective implementation of unsupervised and supervised (knowledge- and data-driven) methods, can help to (i) identify mineralization-related patterns in feature space from the input data without the use of training data, (ii) delineate prospective areas based on conceptual understanding of mineralization processes using the knowledge-driven approach, and (iii) recognize mineralization features represented in the training data using data-driven models. Advanced machine-learning based pattern recognition and prospectivity modelling routines can therefore be used for guiding exploration activities at the smaller target scale. The knowledge-driven methods are efficient at modeling mineralization processes, and the data driven methods are effective at identifying geological attributes related to mineral deposits and occurrences.

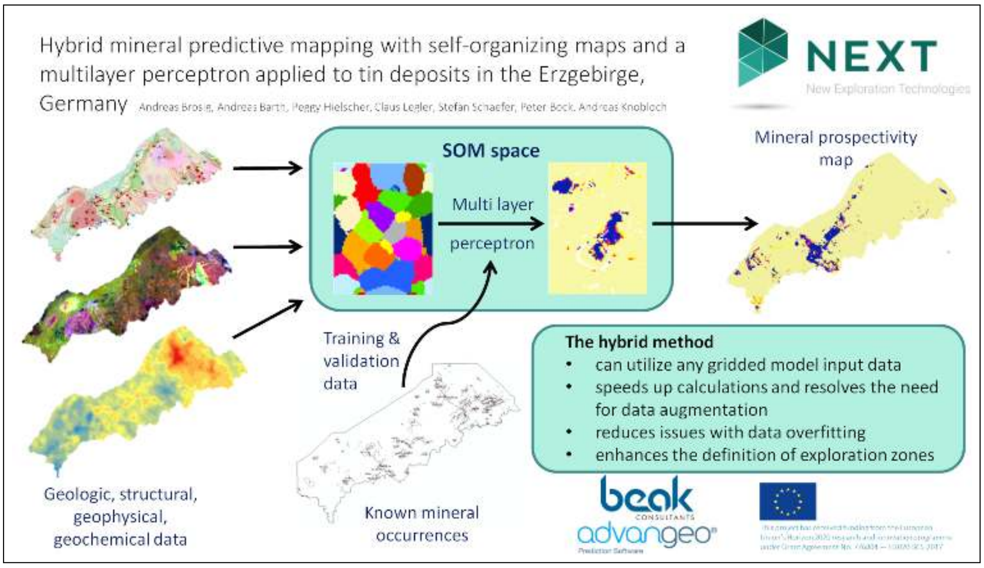
S1404. Hybrid mineral predictive mapping with self-organizing maps and a multilayer perceptron applied to tin deposits in the Erzgebirge, Germany

Andreas Brosig (Beak Consultants GmbH),
Andreas Barth (Beak Consultants GmbH),
Peggy Hielscher (Beak Consultants GmbH),
Claus Legler (Beak Consultants GmbH),
Stefan Schaefer (Beak Consultants GmbH),
Peter Bock (Beak Consultants GmbH),
Andreas Knobloch (Beak Consultants GmbH)
Room: 105 2022-08-31 16:15

Self-organizing maps (SOM) are a useful tool to analyse and interpret gridded datasets like potential field or stream sediment geochemistry data. The data are transformed from geographic space to SOM space where they can be clustered according to overall similarity. By transforming the clusters back to geographic space, geological interpretation of the clusters is facilitated. We present the application of a multilayer perceptron (MLP) in SOM space to produce mineral predictive maps. The reduced number of grid cells in SOM space greatly enhances the performance of the MLP and the tolerance to noise in the input data, compared to an application of the MLP to the original data. By clustering the training data locations with the most similar locations (in terms of model input data) in the same codebook vector of the SOM grid an elegant solution for data augmentation is realized within the workflow.

The method is applied to tin skarn deposits in the German part of the Erzgebirge. The training and validation data required for the MLP are compiled from mining and exploration records. The input data for the SOM are reprocessed gravimetric, magnetic, stream sediment geochemistry, geologic and tectonic data sets. Potentially ore-controlling spatial relationships, such as the distance to different types of partly covered granite intrusions, are derived from a regional scale 3D geological model. The resulting mineral prediction map allows the definition of exploration zones for detailed studies. In particular a linear, probably tectonically controlled zone near Schwarzenberg with little previous skarn exploration is recognised as a new target for further work.

The paper has been compiled in the frame of ”NEXT - New EXploration Technologies” project. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 776804.


Hybrid mineral predictive mapping with self-organizing maps and a multilayer perceptron applied to tin deposits in the Erzgebirge, Germany
Andreas Brosig, Andreas Barth, Peggy Hielscher, Claus Legler, Stefan Schaefer, Peter Bock, Andreas Knobloch
NEXT
New Exploration Technologies
SOM space
Multi layer
perceptron
Mineral prospectivity map
Training & validation data
The hybrid method
• can utilize any gridded model input data
• speeds up calculations and resolves the need for data augmentation
• reduces issues with data overfitting
• enhances the definition of exploration zones
Geologic, structural, geophysical, geochemical data
Known mineral occurrences
beak
advangeo

S1405. Predictivity modelling from multivariate environments coupling Disc-Based Association and Random Forest analyses

Alex Vella (BRGM),
Guillaume Bertrand (Bureau de Recherches Géologiqu),
Bruno Tourlière (Bureau de Recherches Géologiqu),
Eric Gloaguen (Bureau de Recherches Géologiqu),
Vincent Labbé (Bureau de Recherches Géologiqu),
Charles Gumiaux (Institut des Sciences de la Terre d'Orléans),
Stanislas Sizaret (Institut des Sciences de la Terre d'Orléans)
Room: 105 2022-08-31 16:40

Mineral prospectivity mapping (MPM) aims at outlining areas with the highest mineralization hosting likelihood. The outcome of data-driven MPM approach highly depend on the spatial resolution and precision of the input cartographic datasets. Besides, the geological map has the inherent specificity of displaying 3D structures on a 2D surface map view; some structural configurations can usually lead to a misestimation of the relative proportion of the geological units, the faults or other features displayed in the map. From the Cell-Based Association (CBA), we develop here a new approach – the "Disc-Based Association" (DBA) – analyzing neighboring associations of cartographic features. First, disks entities are generated over a regular node grid covering the study area. Each disk discretize the overlapped data layers by integrating their information into a multivariate spectrum. Then, a Random Forest (RF) predictive model classify the multivariate spectrum from both mineralized nodes (e.g. whose associated disk contain a mineralization) and non-mineralized ones. As mineral concentration processes are inherently rare natural phenomena, we argue that all nodes except the mineralized one can be regarded as non-mineralized and thus used in the classification process. Predictivity scores are computed over the area based on the multivariate spectrum classification. This approach could allow the identification of several signature spectra associated to mineralization; which could be interpreted as several distinct metallotects / mineralization processes forming deposits in the study area. To test and evaluate its consistency, this new methodology is applied to prospectivity mapping of Sb along the Ibero-Armorican Arc (Western European Variscan Range). We infer this new data-driven approach applied to natural cases will improve prospectivity mapping and automatic recognition of new metallotects while giving new insights on the genetic processes forming deposits.

This Ph.D research work is funded by the ERA-MIN2 AUREOLE project (ANR-19-MIN2-0002, https://aureole.brgm.fr).

S1406. Artificial Intelligence (AI) based Exploration Targeting for Small Scale Gold Mining Operations in the Dunkwa Area, Ghana

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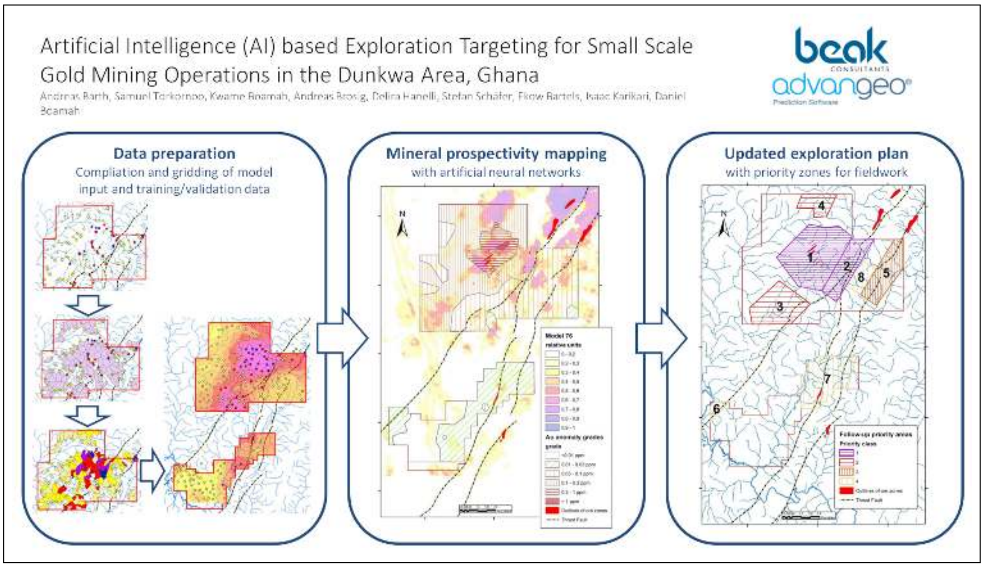
Samuel Torkornoo (Torkornoo and Associates),
Kwame Boamah (Beak Consultants GmbH),
Andreas Brosig (Beak Consultants GmbH),
Delira Hanelli (Beak Consultants GmbH),
Stefan Schaefer (Beak Consultants GmbH),
Ekow Bartels (Ministry of Lands and Natural),
Isaac Karikari (Ministry of Lands and Natural),
Daniel Boamah (Ghana Geological Survey Authority)
Room: 105 2022-08-31 17:05

About 35 % of Ghana´s annual 142 t gold production is produced by artisanal and small-scale mining (ASM) operations. Thus, they contribute substantially to Ghana´s mining industry generated national income and are an important factor of poverty reduction and national development. Because of declining production figures, exhausting resources, and enormous ASM related environmental damages the Government of Ghana generated the World Bank financed program "Ghana Artisanal and Small-Scale Mining Formalisation Project (GASMFP)" executed under the Management of the National Ministry of Lands and Natural Resources, and accompanied by the Ghana Geological Survey Authority. Among others, the generation of new exploitation targets suitable for ASM activities is one of the key tasks of this program. The here presented methodology and results are thought to be a case study and guideline for further similar activities throughout the country. They can be used as guidelines for similar activities in other countries as well.

Within just 6 months a multicomponent program allowed to evaluate both the placer and the hard rock gold potential in the 115 km2 survey area. Placer occurrences have been evaluated as not economic, while the hard rock gold potential was recommended for further detailed exploration. The prospective mineralisation style was identified as low thickness and high-grade quartz veins hosted by phyllites.

The implemented multistep artificial neural network (ANN) based exploration targeting technology in combination with a streamlined field work program was very successful. It allowed to minimise exploration expenditure and to speed-up the target identification process. The methodology can be recommended for further application throughout the country.


Artificial Intelligence (AI) based Exploration Targeting for Small Scale Gold Mining Operations in the Dunkwa Area, Ghana
Andreas Barth, Samuel Torkornoo, Kwame Boamah, Andreas Brosig, Delira Hanelli, Stefan Schäfer, Ekow Bartels, Isaac Karikari, Daniel Boamah
Data preparation
Compliation and gridding of model input and training/validation data
Mineral prospectivity mapping
with artificial neural networks
Updated exploration plan
with priority zones for fieldwork

S1407. Data integration and machine learning applications on the unconformity-related uranium mineral system of Athabasca basin

Marion Parquer (University of Lorraine),
Patrick Ledru (University of Lorraine),
Anthony Le Beux (Orano Mining),
Rémy Chemillac (University of Lorraine)
Room: 105 2022-08-31 17:07

Decades of uranium exploration and production in the Athabasca basin allowed companies to gather a very rich geological, petrophysical and geophysical database. Indeed, data from around 1000 drillholes covering themes such as lithology, structures, alteration, geochemistry, gamma probing or spectral clay analyses have been collected along with regional interpretative geological maps and geophysical surveys (e.g. magnetic, electromagnetic, gravity, radiometrics, resistivity studies). In addition, Orano Canada constructed several 3D structural geological models of their exploration assets within the Athabasca basin.

In order to increase the performance of its uranium exploration, Orano Mining, in collaboration with Université de Nancy have launched a project to test new concepts and tools covering data science and artificial intelligence. The area of interest for this project has been restricted to the Orano exploration asset named Waterbury Cigar.

The first stage of the project consisted in analyzing and controlling data in order to remove unnecessary information and to ensure data compatibility between the various data sources. Indeed, variations can be observed according to the company, the period of time, the working team. Integration of drillholes data (i.e. lithology, structures, geochemistry, gamma probing, spectral clay) with geological maps was performed with the package Geosciences INTEGRATOR & Geoscience ANALYST developed by MIRA Geosciences. It allows for spatial visualization and analysis and therefore facilitates controls to ensure data consistency with a unique template. It also permits to integrate and combine a very large range of data types with is valuable in such a multidisciplinary project. Through this integration data test, we aim the integration of geological data and geophysical models in a 3D geometrical model as well as the reproducibility of such workflow.

In a second stage, integrated data will permit to apply more advanced spatial analyses and artificial intelligence techniques on the area of interest.

S1408. Developing a Unified Exploration Model using a Bayesian hierarchical framework

Ehsanollah Baninajar (University of Exeter)
Room: 105 2022-08-31 17:09

The mineral prospectivity mapping is a process of combining geoscientific data to rank target areas according to their potential of hosting a particular type of mineral deposits. However, the traditional approaches of mineral prospectivity mapping only calculate "relative" prospectivity of targets and often fail to fully appreciate all the available information (e.g., geologists' opinion, exploration intensity maps, etc). This study aims to develop a unified probabilistic prospectivity model to deal with shortcomings of traditional prospectivity analysis. The proposed method calculates real prospectivity which is the probability of occurrence for deposits of different magnitude. Additionally, by combining the real prospectivity and exploration model, the unified exploration model can assess the probabilities of eventual outcomes from different exploration stages and quantifying their uncertainty.

A novel machine learning approach is developed to extract the priors for critical components of the mineral system model. Using a hierarchical Bayesian framework, the prior expectations are then updated with mineral deposit data and intensity of different exploration stages which results in a prospectivity map. In practice mineral occurrences are only observed via the different stages of the exploration process. As each exploration stage has a different hit rate with regards to eventual mineral occurrence or deposit discovery, the probability of gold occurrence, non-occurrence and deposit size is inferred from exploration information and deposit data through the proposed hierarchical Bayesian model. The final probabilities represent real probabilities of discovery for deposits of different magnitude. The Gold deposits of the Yilgarn region are used as a test case due to relative exploration maturity and the richness of data in this region.

The Unified Exploration Model is a powerful tool for ground selection, explore/defer/drop/deal decisions and capital allocation which not only provides more reasoned and accurate project valuations, but also quantify and profile exploration uncertainty.

S1409. Entity and Relationship Extraction From Geological Document Based on The Method of Deep Learning

Feng Han (Sun Yat-sen University),
Guangliang Cheng (Sun Yat-sen University),
Jing Bian (Sun Yat-sen University),
Qianlong Zhang (Sun Yat-sen University),
Yongzhang Zhou (Sun Yat-sen University)
Room: 105 2022-08-31 17:11

As a key step and important component in information extraction, natural language understanding and information retrieval, entity and relation extraction can extract semantic relationship between entity pairs from text. In recent years, the application of deep learning in joint learning, remote supervision and other aspects has made abundant achievements in relation extraction study.

Geological document like geological exploration reports, research article, geodesic monographs and other texts material contain rich knowledge in the field of geology, which is of great significance to geological information services. The relationship between conceptual entities is an important part of geological knowledge. It is of great significance to geological disaster warning and metallogenic prediction. In view of the sparse structure of Chinese text in geological texts, the original word-based feature representation has limited effect. Therefore, from the perspective of feature selection, a feature learning method based on deep learning is proposed to further abstract the limited context features. In the experiment, deep sparse automatic coding is used to rerepresent the vector representation of entity context, so as to get more abstract and more recognizable meaning

The characteristics of meaning. Experiments demostrated that the deep learning feature rerepresentation method used in this paper has significantly improved the recall rate of recognition compared with the baseline experiment.

S1410. Mineral Prospectivity Mapping Using a Combination of Cell-Based Association and Gradient Boosting Methods: Investigating Gold Occurrences in French Brittany

Hugo Breuillard (BGRM),
Vincent Labbé (BGRM),
Jan Mortier,
Bruno Tourlière (BRGM),
Alex Vella (BRGM),
Guillaume Bertrand (Bureau de Recherches Géologiqu)
Room: 105 2022-08-31 17:13

Mineral prospectivity mainly focuses on measuring the statistical link between a mineral occurrence data (points) and a geological map (polygons) to point out favorable zones in terms of mining potential. However, usual favorability methods may not yield satisfactory results due to input data quality (e.g., clustered or scarce points, approximate location) or some assumptions that are considered unreasonable (e.g., map areas relevance, conditional independence). To address this issue, the Cell-Based Association (CBA) method has been developed by Tourlière et al. (2015). It consists in replacing polygons of geological units with a square cell grid, each cell recording the presence (1) or absence (0) of lithological units. The synthetic map of lithological associations can then be coupled to the mineral occurrence data set to generate a favorability map. In this study, we combine the CBA method with a supervised machine learning technique based on an ensemble of decision trees (gradient boosting) to investigate gold occurrences in French Brittany. We compare the performance of this approach with a baseline model based on the classical Weight of Evidence method. We show that the use of such machine learning approach 1) significantly improves the predictivity of the model and 2) eases the process of adding valuable information (e.g., faults, streams, etc.) that increases further its performance.

S1411. A geologically-constrained deep learning algorithm for mapping mineral prospectivity

Renguang Zuo (China University of Geosciences),
Yihui Xiong (China University of Geosciences)
Room: 105 2022-09-01 09:50

Mineral prospectivity mapping is a computer-based approach to delineate targeted areas for a specific type of mineral deposit. The application of machine learning and deep learning algorithms in mapping mineral prospectivity and identifying geochemical anomalies association with mineralization is increasing. The integration of expert and domain knowledge into deep learning algorithms (DLAs) is a challenging task in geosciences which can not only improve the consistency and credibility of the DLAs but also incorporate the generalization and interpretation of the geological models. In this study, we introduced geologically-constrained DLAs for identifying geochemical anomalies and mineral prospectivity mapping. A nonlinear relation between an ore-forming controlling feature and locations of mineral deposits was built as a loss function for constructing geologically-constrained DLAs. Two case studies were presented with the aim of demonstrating the necessity and importance of geologically-constrained DLAs in enhancing geological consistency and interpretability in the field of geochemical prospecting and mineral prospectivity mapping. In the future, we will focus on constructing a hidden layer of DLA in terms of metallogenic dynamics to increase the ease of interpretation of the DLA.

S1412. Research on metallogenic prediction method based on multi-scale 3D fine geological model and big data mining

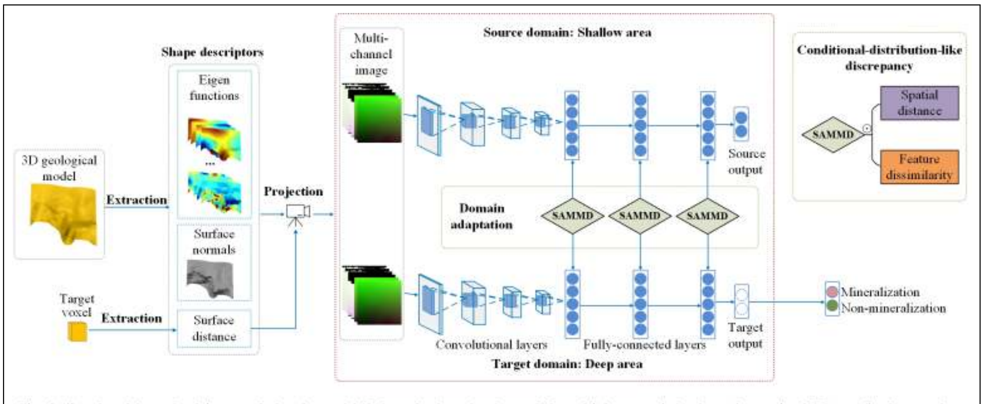
Xuechao Wu (China University of Geosciences),
Gang Liu (China University of Geoscience)
Room: 105 2022-09-01 10:15

The traditional two-dimensional comprehensive information prospecting method can not directly describe the spatial form and characteristics of the geological body, and has limitations in the analysis of ore-controlling elements and ore-forming conditions, so it is not suitable for the prediction of concealed ore and deep ore. A metallogenic prediction method based on multi-scale 3D fine geological model and big data mining is proposed to mine and extract ore-controlling factors in 3D space, providing important information support for 3d deep prediction and target delineation. Firstly, based on the knowledge driven multi-scale 3D geological modeling technology, the outer and deep strata and structural structure of the mining area are reconstructed accurately.Then, based on the structural model, the kriging geostatistical interpolation method is used to construct a three- dimensional comprehensive geology-geophysical-geochemical model of the mining area. Finally, the big data mining method combined with a variety of machine learning methods is adopted to quantitatively extract 3d ore control information such as fault structure buffer zone and geological interface buffer zone based on the comprehensive model, and the ore control factors are mined and extracted by combining with geophysical and geochemical exploration information. Taking the Wuzhishan lead-zinc deposit in Zhijin County, Guizhou Province as the study area, the above techniques and methods improved the prediction accuracy of peripheral and deep lead-zinc deposits, effectively reduced the risk of target area delineation, and verified the reliability of the method through drilling.

S1413. Spatial-associated deep transfer learning for three-dimensional mineral prospectivity modeling in deep-seated areas

Yang Zheng (MOE, School of Geosciences and Info-Physics, Central South University),
Hao Deng (Key Laboratory of Metallogenic),
Jin Chen (CSU),
Xiancheng Mao (Key Laboratory of Metallogenic)
Room: 105 2022-09-01 10:40

Carrying out three-dimensional (3D) mineral prospectivity modeling in deep-seated areas is a challenging and work-intensive task. The deep-seated areas, compared with the shallow ones, are featured by the scarcity of sampled data and the difference of ore-forming regularity. Inspired by successful applications of deep networks in learning transferable representations, we present a spatial-associated deep transfer learning method for 3D mineral prospectivity modeling, which ensures the deep networks to learn transferable mineralization-associated representations mainly from shallow areas where the training data is relatively sufficient. Specifically, we devise the spatial-associated maximum mean discrepancy metric to narrow the information discrepancies between the shallow and deep-seated areas. This results in an effective learning objective that considers both the feature consistency and the spatial proximity to extract transferable representations. We compare the prediction performance with other state-of-the-art mineral prediction methods, demonstrating that our model has significant advantages in extending the shallow ore-controlling information to model mineral prospectivity in deep-seated areas.



The pipeline of spatial-associated deep transfer learning model. To input the shape descriptors of 3D models into convolutional neural networks (CNNs), we first leverage the perspective projection to reorganize the shape descriptors into multi-channel images. The deep network part transitions shape descriptors from general to specific. Specifically, convolutional layers extract relatively general features shared by shallow and deep areas, while fully-connected layers are designed to fit our mineral prospectivity task. The core of our approach is spatial-associated maximum mean discrepancy, SAMMD, a metric that simultaneously considering the factors of spatial distance and feature dissimilarity. This results in an effective learning objective that allows to narrow the information discrepancies between the shallow and deep areas and thus ensures the CNN to learn mineralization-associated representations for deep-seated areas.

S1414. Geochemical Anomaly Detection Based on Auto-encoder Network

Sheng Chang (Beijing Normal University),
Tao Huang (Beijing Normal University),
Yunzhen Chang (Institude of Geological and Mineral Resources Survey),
chongyang li (Institude of Geological and Mineral Resources Survey),
Xinglin Gao (Beijing Normal University),
Ruiqing Yan (Beijing Normal University),
Xianchuan Yu (Beijing Normal University)
Room: 105 2022-09-01 11:05

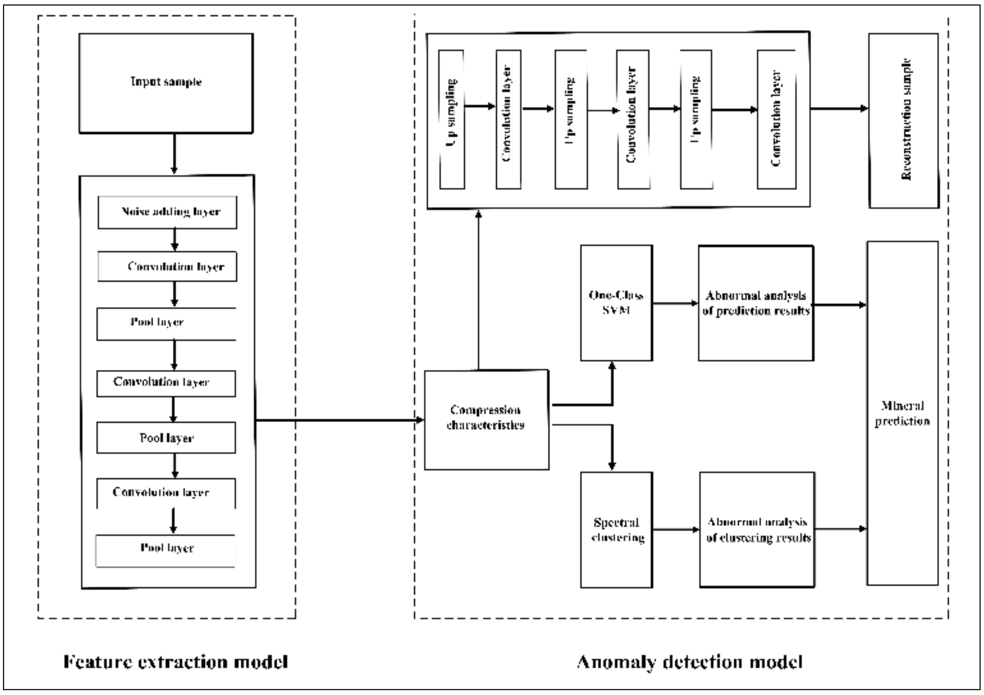
Traditional methods of geochemical anomaly detection often requires a large number of artificial feature engineering design, but the recent generation of artificial intelligence technology does not need to do so. We take 12 elements of the 1:10,000 pedogeochemistry data and 1:50,000 stream sediment data in the Xiaoshan area of Henan Province, China as an example to carry out our research, and the results show that the method can effectively detect the information anomalies of 12 geochemical elements and their combinations in the research area. Our contributions are listed as follows:

(1) Aiming at the problem of unclear probability distribution of geochemical data, we propose an anomaly detection method for one-dimensional convolutional noise reduction auto-coding network. In this method, the samples collected in the mine-free area are regarded as normal samples, and the samples containing mineralization information are regarded as abnormal due to the large reconstruction error.

(2) In view of the risk of manual label selection of geochemical data, we propose an anomaly detection method that combines auto-encoding network and spectral clustering. The method learns the deep features of the data through a auto-encoding network, and then performs spectral clustering analysis on these features to obtain a spatial spread of geochemical elements, in which clusters are rare or appear in a special shape in planar space are considered abnormal.

(3) Aiming at the problem that the proportion of sampled geochemical data is sparsely labeled, we propose an anomaly detection method that combines the auto-encoding network and the One-Class SVM. This method performs deep feature extraction through a auto-encoding network, and then adopts the One-Class SVM method to extract the data by a single class, and data samples which is not extracted is regarded as abnormal.

Keywords: geochemical anomaly detection, auto-encoding networks, spectral clustering


Input sample
Noise adding layer
Convolution layer
Pool layer
Convolution layer
Pool layer
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Pool layer
Up sampling
Convolution layer
Up sampling
Convolution layer
Up sampling
Convolution layer
Reconstruction sample
Compression characteristics
One-Class SVM
Abnormal analysis of prediction results
Spectral clustering
Abnormal analysis of clustering results
Mineral prediction
Feature extraction model
Anomaly detection model

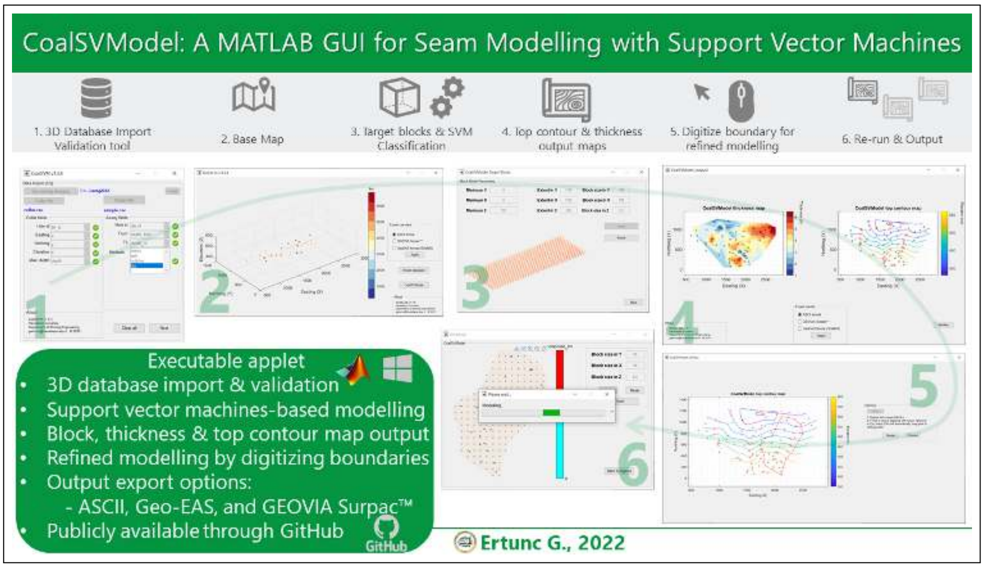
S1415. CoalSVModel: A MATLAB GUI for Coal Seam Modelling with Support Vector Machines

Gunes Ertunc (Hacettepe University)
Room: 105 2022-09-01 11:30

In this study, Graphical User Interface (GUI) called CoalSVModel is presented. The main objective of this executable program is to generate lignite block model with support vector machines (SVM) methodology. The outputs of the application are thickness map, top contours of the lignite seam, and block centroids which can be exported in various formats. CoalSVModel is coded with MATLAB programming language and made executable with Compiler application.

Separating the lignite seam from other strata is a classification problem. SVM algorithm with radial basis function kernel is coded and merged in the GUI. The hyper-parameters' selection is automated with k-fold validation.

CoalSVModel starts with import and validation of the database files. The program requires total of 4 files as an input. User inputs are as follows: three files (MS Excel *.xlsx or *.csv) are related to the database (collar, assay -or lithology-, and survey) and one digital elevation model point cloud in ASCII (*.txt) format. CoalSVModel does not utilize raw data as it is. In order to use them as an SVM input, data is processed before modelling phase. This process is adaptation of geostatistical compositing which can be described as creating equi-length binary input. Program proceeds with defining the user-defined classification target space. The classification results based on SVM can be exported in ASCII, Geo-EAS, and GEOVIA Surpac™ format. Additionally, user may digitize boundary over solution and re-run by excluding the certain boreholes.



S1416. Study on metallogenic prediction method based on multi-scale three-dimensional fine geological model and big data mining——Taking Wuzhishan lead zinc mine in Guizhou Province as an example

Xuechao Wu (China University of Geosciences),
Gang Liu (China University of Geoscience)
Room: 105 2022-09-01 11:55

The traditional two-dimensional comprehensive information prospecting method can not directly describe the spatial form and characteristics of the geological body, and has limitations in the analysis of ore-controlling elements and ore-forming conditions, so it is not suitable for the prediction of concealed ore and deep ore. A metallogenic prediction method based on multi-scale 3D fine geological model and big data mining is proposed to mine and extract ore-controlling factors in 3D space, providing important information support for 3d deep prediction and target delineation. Firstly, based on the knowledge driven multi-scale 3D geological modeling technology, the outer and deep strata and structural structure of the mining area are reconstructed accurately.Then, based on the structural model, the kriging geostatistical interpolation method is used to construct a three- dimensional comprehensive geology-geophysical-geochemical model of the mining area. Finally, the big data mining method combined with a variety of machine learning methods is adopted to quantitatively extract 3d ore control information such as fault structure buffer zone and geological interface buffer zone based on the comprehensive model, and the ore control factors are mined and extracted by combining with geophysical and geochemical exploration information. Taking the Wuzhishan lead-zinc deposit in Zhijin County, Guizhou Province as the study area, the above techniques and methods improved the prediction accuracy of peripheral and deep lead-zinc deposits, effectively reduced the risk of target area delineation, and verified the reliability of the method through drilling.

S1421. The behavior of hydrothermal mineralization with spatial variations of the fluid pressure

Yihui Xiong (China University of Geosciences),
Renguang Zuo (China University of Geoscience)
Room: 105 2022-09-01 15:00

Spatial variability is an inherent natural property of pore fluid pressure, which should be fully considered in the study of the formation and evolution mechanism of fault controlled by fluid pressure. This study constructed a cellular automaton model of mineralization by taking the spatial variability of fluid pressure into consideration. The spatial structure of the three patterns varies from (a) essentially spatially random (a relative nugget of 100%) to (b) partially structured (a relative nugget of 50%) to (c) a strong spatial structure (a relative nugget of 0%) are representative of the data used for simulating and exploring the influence of the spatial variability of fluid pressure on fault evolution and the enrichment of ore-forming elements. It is found that as the spatial correlation of fluid pressure increases, the larger the scale of fracture occurs, the fluid pressure relief will induce the large-scale ore-forming material precipitation, leading to the higher spatial correlation of ore-forming elements. This provides a new understanding of the constraints of spatial distribution pattern of the fluid pressure on the migration and enrichment of ore-forming elements.

S1422. Deep Auto-encoder applied to mapping prospectivity for Ag-Au deposits

Xiaotong Yu,
Yongzhang Zhou (Sun Yat-sen University)
Room: 105 2022-09-01 15:25

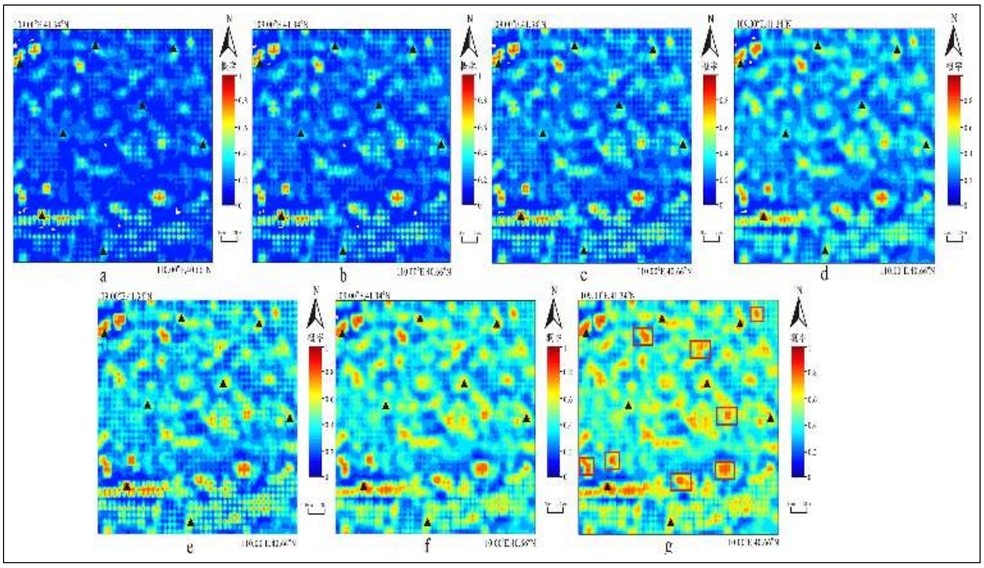
Deep Auto-encoder is a powerful tool to find features which are hidden in amounts of data.

According to previous studies, mineralization is constrained by many factors which are different sources and structures. As long as these geological data such as strata, lithology, tectonics, and geochemistry can be integrated into the same structure, deep Auto-encoder is a quick and convenient way to mapping prospectivity for Ag-Au deposits. In this study, we deploy some methods to convert unstructured data into structured data for applying deep Auto-encoder. Firstly, faults were processed by weight of evidence method. Then, strata and lithology were handled by one-hot coding. Besides, all the data are combined in the same coordinate system. In order to validate the deep Auto-encoder in this study, 3 typical Ag-Au deposits are labled. After deep Auto-encoder processing, result shows that AUC value of this model is 0.82, which illustrates that the model is effective in this study. MSE values were adopted to characterize the mineralization possibility. The map of MSE values suggest Ag-Au mineralization significance in geological map. Overall, the proposed methods not only effectively recognize the mineralization factors hidden in geological data, but also indicate the prospecting targets for further exploration.

S1423. Extraction of Weak Geochemical Anomalies Based on Multiple-Point Geostatistics and Local Singularity Analysis

Wenyao Fan (China University of Geosciences),
Gang Liu (China University of Geoscience),
Qiyu Chen (China University of Geosciences),
Laijun Lu (School of Earth Science, Jilin University)
Room: 105 2022-09-01 15:50

The traditional interpolation might cause smoothing effect on the geochemical elements' concentration due to its moving weighted average properties. Meanwhile, it cannot describe the elements' spatial variability if the data's distribution is sparse, which could cause uncertainties when inferring the unsampled locations' information. Since the Multiple-Point Geostatistics (MPS) is a stochastic simulation based on the statistical characteristics of the pattern conducted by spatial multiple points, it can reduce the smoothing effect and describe the spatial variabilities and uncertainties. The Local Singularity Analysis (LSA) could identify the weak geochemical anomalies more effectively due to its statistical self-similarity. Therefore, we proposed a new method combing the advantages of both MPS and LSA for improving the identification of the weak anomalies and quantifying the uncertainties distribution. We firstly treated the geochemical raster data as the Training Images (TIs) and then the Direct Sampling (DS) algorithm was used to perform elements spatial distribution. The LSA with different sliding-windows' size and information fusion were finally adopted to obtain the probability map of geochemical anomalies. We used partial 1:200,000 stream sediment data and 8 alter Fe deposits in the Wula Mountain to verify the experience and a satisfactory performance was obtained. Specifically, the anomalous fields identified by the MPS-based method were smaller than the Kriging-based ones, and it had a better spatial consistency and accuracy with these Fe deposits. In addition, Kriging-based methods only use the spatial neighborhood points relatively to infer the undetermined ones instead of stochastic simulation, which cannot make accurate prediction for the unsampled regions. According to the ROC curves' analysis, this method performed better results than the traditional ones and its anomalous fields were consistent with these Fe deposits, which can help us have a clearly understanding for the metallogenic backgrounds and the element distribution patterns.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S1424. Positive and unlabelled bagging for mineral prospectivity mapping

Ehsan Farahbakhsh,
R. Dietmar Muller (EarthByte Group, University of Sydney)
Room: 105 2022-09-01 16:15

Most supervised machine learning algorithms require both positive and negative training samples to create a model. Mineral occurrences are considered positive samples while using supervised machine learning algorithms to create mineral prospectivity maps. However, there are usually insufficient or unreliable labels for the negative class, i.e., barren regions. A few efficient machine learning methods have recently been developed in the category of positive and unlabelled learning (PUL), requiring positive and unlabelled samples for training a model. PUL is a semi-supervised binary classification method that recovers labels from unknown samples. It does this by learning from positive samples and applying what it has learned to relabel unknown samples. Therefore, these methods can be considered a potential solution to a classic challenge in mineral prospectivity mapping. Our study applies a PUL method called positive and unlabelled bagging (PUB) to create mineral prospectivity maps of different ore deposit types in the Gawler craton, South Australia. Various exploration datasets were used as input features, including geological, geochemical, and geophysical data. We used known mineral occurrences as positive samples and created different sets of random samples throughout the study area as unlabelled samples. According to the results and different evaluation metrics, the performance of the model is stable. The PUL methods can be used as wrappers of any supervised machine learning algorithm and generate reliable positive and negative samples. We used the random forest (RF) method as the main classifier and compared the combination of a standard RF and random negative samples with PUB and RF. Based on the results, the PUB method improves the accuracy of the maps on average by nearly ten percent. The PUB-RF map shows a strong spatial correlation between high probability values and known mineral occurrences and even predicts potential regions with few or no known mineral occurrences.

S15 Time series analysis in Geosciences: an homage to Professor Walther Schwarzacher

Jennifer McKinley (Queen's University Belfast),
Eulogio Pardo-Igúzquiza (Instituto Geologico y Minero de Espana)

Time series analysis is widely used in cyclostratigraphy, paleoclimatology, hydrology, geophysics, environmental geosciences, etc. The main objective of this session is the presentation of methodologies and cases studies dealing with the analysis of times series in Geosciences. New theoretical developments, new algorithms implementing known methodologies, new strategies for dealing with classical problems or classical methodologies dealing with new problems as well as case studies are appropriate for this special session. The session will be an homage to Professor Walther Schwarzacher a pioneer in mathematical geosciences in general and cyclostratigraphy in particular. Topics of special interest, among others, are:

- Time series analysis in quantitative stratigraphy
- Spectral analysis of uneven time series and categorical data
- Uncertainty evaluation of the estimated power spectrum
- New methodologies of spectral analysis
- Time series analysis of compositional data
- Soft-computing and learning machine methods in time series analysis
- New developments in wavelets analysis of time series

S1501. A comparison of gap filling methods: a study case in Northern Italy

Camilla Fagandini (University of Parma),
Valeria Todaro (University of Parma),
Maria Giovanna Tanda (University of Parma),
Andrea Zanini (Università degli Studi di Parma)
Room: 101 2022-08-31 09:50

The lack of data in hydrometeorological datasets is a common problem. There may be various reasons for missing values, e.g., sensor malfunction, errors in measurements, faults in data acquisition from the operators and so on. Finding efficient methods to deal with this problem is an important issue because it is necessary to have complete time series to carry out reliable hydrological analyses. In this research, the performance of two gap-filling approaches – FAO's linear regression and Kriging interpolation – are compared. The FAO procedure fills the gaps using data collected at the gap time in other stations. The approach proceeds as follow: aiming at filling the missing data of a certain monitoring station, the correlation coefficients with the other existing stations, having an appropriate common recording period, are computed. Then, the station with the highest correlation is considered to estimate the parameters of a regression equation, which is used to obtain the missing value of the interested station. The Kriging approach, instead of considering time series at a specific location, analyses the spatial distribution of hydrometeorological data at a certain time. As a result, to fill each gap at a monitoring station, the approach requires: recognition of the stations with available data, computation of the variogram and interpolation of the missing data at a specific location through the Kriging approach. The FAO method requires little computational effort, even if it is suggested in case of small number of gaps. Whereas Kriging can manage more intensive processes, but it involves the use of a large amount of monitoring stations. Pros and cons of the two approaches are discussed considering precipitation records in a large area in Northern Italy.

S1502. Maximum entropy cross-spectral analysis of compositional time series in cyclostratigraphy

Juan Jose Egozcue Rubi (Technical University of Catalonia),
Eulogio Pardo-Iguzquiza (Instituto Geologico y Minero de Espana),
Vera Pawlowsky-Glahn (University of Girona)
Room: 101 2022-08-31 10:15

One of the methodologies frequently used in cyclostratigraphy is spectral analysis of time series in order to unveil periodicities hidden in stratigraphic sequences. Those periodicities can be correlated with physical cycles like the Milankovitch orbital ones, as notoriously advocated by Professor Walther Schwarzacher. In this sense, maximum entropy spectral estimation has been frequently used due to its advantages of having a high spectral resolution and its good efficiency with short time series frequently appearing in cyclostratigraphy.

Additionally, many stratigraphic sequences are compositional and require a treatment using log-ratio coordinates. This methodology avoid the spurious covariances between the raw series.

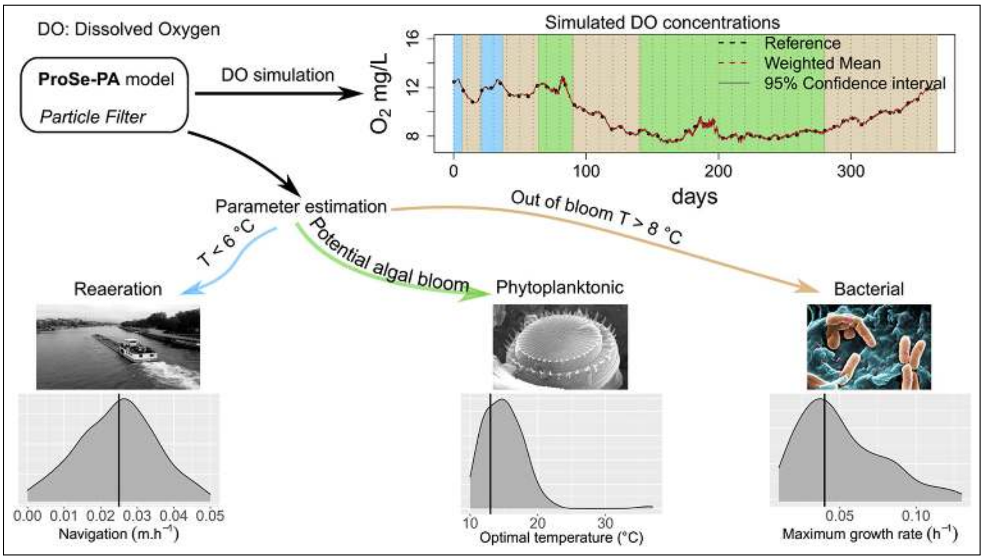
Based on Geostatistical ideas for regionalized compositions like the variation variograms, cross-spectral densities are computed from auto-spectra of differences of log-components, thus avoiding fitting cross-covariances.

Maximum entropy spectral estimation is then applied to univariate series of log-differences. The appropriate combination of these univariate spectral estimations provide the cross-spectral analysis of a compositional cyclostratigraphic series and their coherence.

S1503. Oxygen data assimilation in river systems

Thomas Romary (Mines Paris),
Shuaitao Wang (Sorbonne Université),
Masihullah Hasanyar (Mines Paris Tech),
Nicolas Flipo (Mines Paris Tech)
Room: 101 2022-08-31 10:40

The coupling of high frequency data of water quality with physically based models of river systems is of great importance for the management of urban socio-ecosystems. The hydro-biogeochemical model Prose has been under development for several decades in Mines Paris center of geosciences. It consists of three modules: hydrodynamics, transport and biogeochemistry, and simulates the metabolism of river systems. In the meantime, a high frequency sensors network measuring the dissolved oxygen (DO) concentration in the Seine River has been deployed. The calibration of the Prose model to the DO data is made difficult by the large number of, possibly dynamic, parameters involved. These parameters are both physical and related to micro-organisms (reaeration coefficient, photosynthetic parameters, growth rates, respiration rates and optimal temperature). Focusing on the most influential parameters, selected through a sensitivity analysis of the biogeochemical module C-Rive, we develop a sequential data assimilation approach based on a particle filtering algorithm. It is able to reproduce the observed DO concentrations while characterizing the dynamics of the parameters governing the Seine river metabolism. In particular, we show that the physical, bacterial and phytoplanktonic parameters can be retrieved properly.



S1504. Seismicity since 1500 in Hunan Area China

Bateer Wu (The Institute of Disaster Prevention),
ShuQi Hu (The Institute of Disaster Prevention)
Room: 101 2022-08-31 11:05

The Hunan area is located in the Seismic belt which in the middle and lower reaches of the Yangtze River and it is also located in the transition area from strong earthquake area of north China to moderate earthquake area of south China. The weak level of modern seismicity in Hunan and the long period and low frequency of destructive earthquakes, it is difficult to combine modern small earthquakes with historical destructive earthquakes in the study of seismicity. However, the surface effect in Hunan is relatively strong, and the seismic intensity is strong. There are geological conditions and backgrounds for strong earthquakes.Therefore, according to the geographical environment, geological background, and major fault structures in Hunan Province, the temporal and spatial distribution characteristics and seismicity are analyzed. The spatial distribution, activity cycle and time series of earthquakes in Hunan are discussed, and post-earthquake trends are discussed. Judging and predicting the trend of seismicity in Hunan in recent years, and based on the results of the judgment and the detailed investigation data collected, it will propose countermeasures and opinions for future earthquake prevention and reduction work.

S1506. Sorting signals recorded during EDX experiments

Sadeg Said (Université de Lorraine),
EL Hadi Djarmoun (Université de Lorraine),
Cecile Fabre (Université de Lorraine),
Jean Cauzid (Université de Lorraine)
Room: 101 2022-08-31 11:30

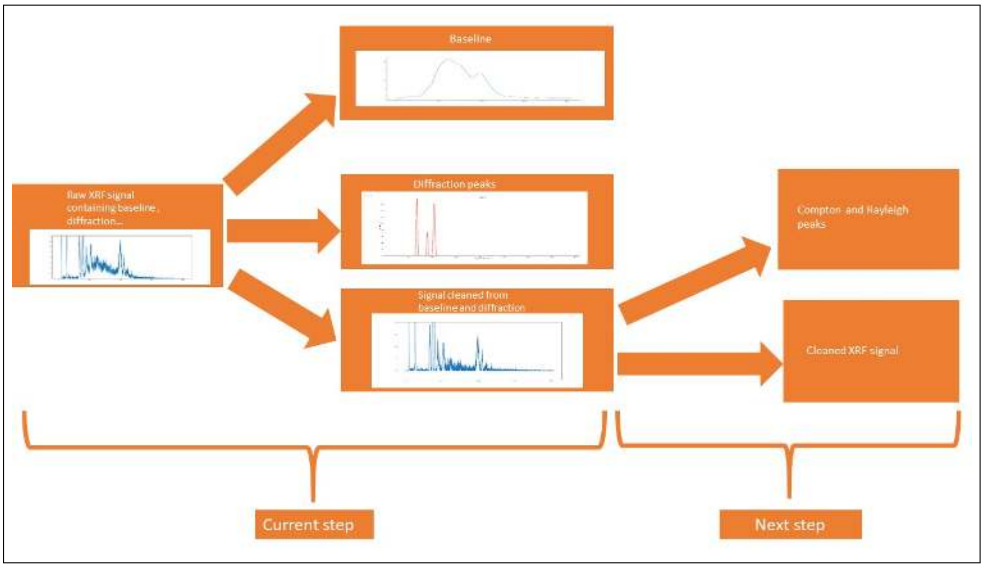
Energy Dispersive X-Ray Spectroscopy (EDX) is a subset of X-Ray Fluorescence (XRF), which provides geochemical information about the elemental composition of a sample. The EDX detector records all X-rays emerging from the sample. The elemental information arises from the specific emission lines emitted by the sample. However, the sample can also scatter the signal from the X-Ray tube itself. Three scattering signals may occur: elastic and inelastic scattering of the specific emission lines of the tube material, elastic and inelastic scattering of the bremsstrahlung and coherent elastic scattering from the periodic atomic organization in crystals. The first scattering manifests as extra peaks (Compton and Rayleigh) on the recorded spectrum, the second as a baseline and the third as X-Ray Diffraction (XRD) peaks. These spectra are superimposed with XRF stricto sensu. Each of these four signals contains useful geochemical information.

EDX is in our study applied as an imaging technique. This means that an image of up to several million pixels contains a full EDX spectrum in each pixel, providing a 3D data cube, with two spatial dimensions and one spectral dimension. The objective of this work is to extract, from a data cube, the previous elementary signals to generate four data cubes, each containing only one type of signal for later use.

To this end, we follow the steps below:

1. Spatial binning on the pixels to obtain signals with improved signal to noise ratios.
2. Baseline processing with various methods to choose the best one
3. Processing of the diffraction peaks by jointly exploiting the two signals from two detectors
4. Extracting the spectral range containing the Compton and Rayleigh peaks

The work is currently focusing on steps 2 and 3



S16 Reservoir/Petroleum Geostatistics

Juliana Leung (University of Alberta),
Sanjay Srinivasan (The Pennsylvania State University)

Traditionally, geostatistics has been applied in the petroleum industry for generating multiple geomodels conditioned to well, seismic and other reservoir-specific information. These models are subsequently used for flow modelling and recovery analysis. We are soliciting abstracts that showcase recent advancements in uncertainty quantification, characterization of complex reservoirs, integration of multifaceted data from diverse sources recognizing the scale and precision of such data, upscaling of flow/transport properties and coupling of artificial intelligence with traditional modelling workflows. Interesting case studies (including for oil and gas extraction, CO2 sequestration, hydrogen storage, geothermal reservoirs), as well as novel theoretical and computational developments, are welcome.

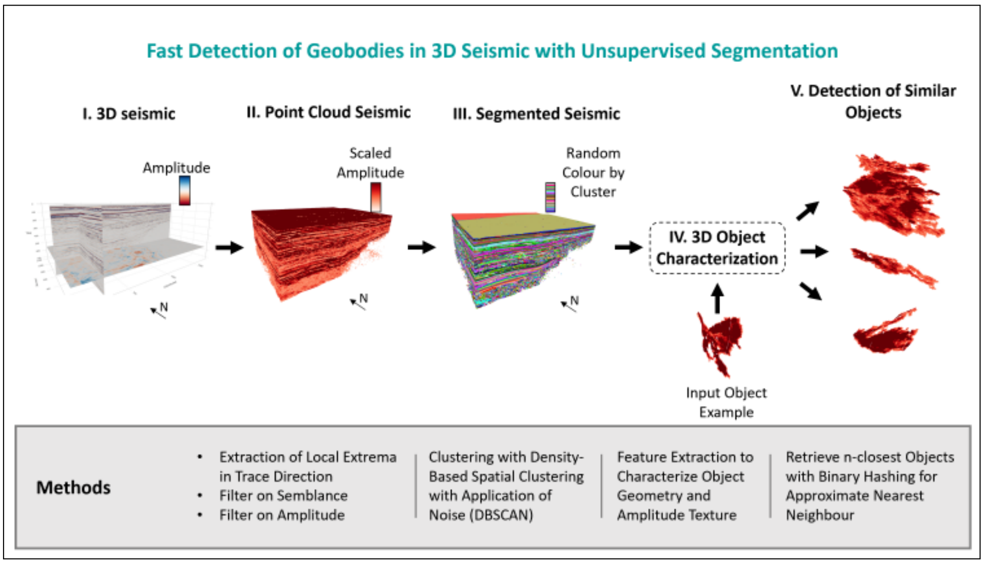
S1601. Fast Detection of Geobodies in 3D Seismic with Unsupervised Segmentation

Quentin Corlay (Heriot-Watt University),
Dan Arnold (Heriot Watt University),
Dave McCarthy (British Geological Survey),
Vasily Demyanov (Heriot-Watt University)
Room: auditorium 2022-09-01 09:50

Seismic interpretation is a time-consuming task and is particularly subject to interpreter bias. In order to address these challenges we present a novel fully data-driven automated approach to the detection of geobodies in 3D seismic reflection data. Geobodies in seismic refer to geometric, structural or stratigraphic features such as channels, turbidite fans, salts, etc. Their detection and delineation are important for improved understanding of the subsurface and to build a range of conceptual models.

In this contribution, a point cloud-based segmentation approach is applied to identify complex stratigraphic features within large volumes of 3D seismic data. The step change of this workflow is that the 3D seismic cube is converted to 3D seismic point cloud, reducing the volume of data to analyse. The 3D point cloud is obtained by filtering the seismic reflection volume using different seismic attributes. In the proposed method, each point of the seismic point cloud is segmented into different clusters. The clustering is performed using the unsupervised Density-Based Spatial Clustering of Applications with Noise (DBSCAN). The segmentation allows an individualization of the structures present into individual segmented objects, which are then characterized with features based on their 3D shape and spatial amplitude distribution. Finally, the method allows the selection of a specific geobody and can retrieve geobodies that have been identified as very similar.

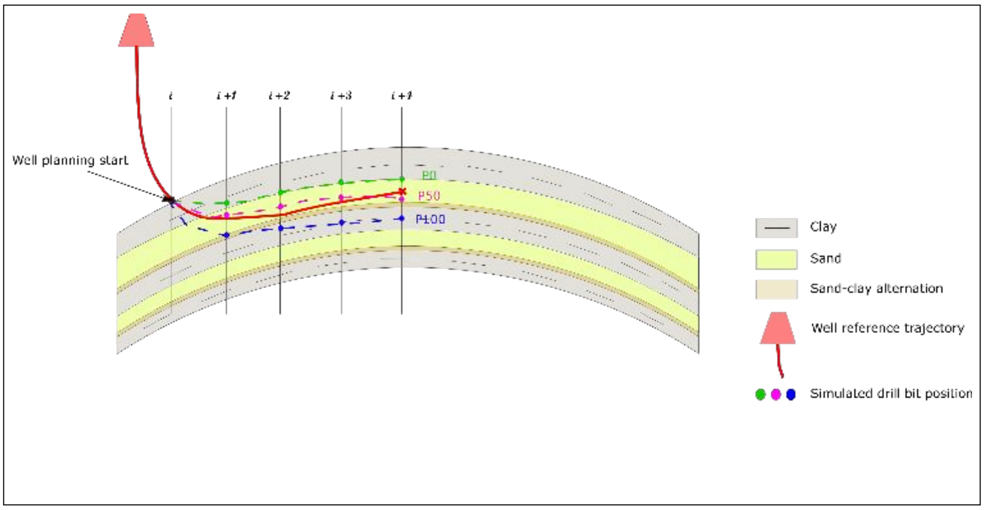
The method has been applied to a modern 3D seismic dataset to successfully detect geobodies, which have been interpreted as turbidite fans. The results indicated that the method was able to segment the seismic into spatially consistent clusters and to identify the turbidite fans in an automatic manner and with high computational efficiency. So this approach can be used to quickly scan through an entire 3D seismic looking for geobodies of interest, saving time and providing unbiased results.



S1602. A Bayesian methodology for real-time updating of well trajectory in depositional space

Julien Herrero (GeoRessources - Université de Lorraine),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS),
Paul Baville (Université de Lorraine - GeoRessources)
Room: auditorium 2022-09-01 10:15

Horizontal drilling is useful to target subsurface formations for injection or recovery of fluids in subsurface reservoirs. However, drilling with a low angle relatively to the stratigraphic dip can be a significant cause of targeting error and sub-optimal drilling process. Real-time consistency between the drill bit and the subsurface model is, therefore, essential for the drilling engineers. We propose a dynamic Bayesian updating of the positioning of a well relatively to a geological model, which accounts for: (1) A prior probabilistic model for petrophysical properties in the vicinity of the well being drilled. (2) The prior well geometric uncertainty based on deviation survey parameters. (3) Logging while drilling (LWD) measurements which can be compared to the prior geological model. Such models have recently been proposed in the literature, but they often consider a one-dimensional "type-log", which is limited to represent lateral petrophysical variations. They also use relatively simplified geometric settings, making isopach layer assumptions. In this project, we consider the updating problem in depositional coordinates and a three-dimensional prior petrophysical model as derived from geostatistical reasoning. We demonstrate the proposed framework on a synthetic case study, both deterministically to find the most likely well trajectory or stochastically to generate possible trajectories, and discuss its potential towards implementing a model updating operator for geosteering. Results highlight that the process allows to rapidly update relative well trajectories honoring prior information and suggest that the method could be used to automatically detect some unseen geological objects such as faults not visible on seismic images.



S1603. A model selection workflow for assimilating time-lapse seismic data in models for point bar geologic system.

Ismael Dawuda (The Pennsylvania State University),
Sanjay Srinivasan (The Pennsylvania State University)
Room: auditorium 2022-09-01 10:40

Point bar geology is frequently observed in many target reservoirs that are used for large-scale injection and storage of CO2. To reliably assess the containment of the injected CO2 within the reservoir, model calibration algorithms have been developed to reduce the uncertainty associated with characterizing the geologic heterogeneity in point bar reservoirs. However, due to the complex geologic heterogeneity exhibited by point bar reservoirs, there can be a significant amount of residual uncertainty even after model calibration. This can affect the reliability in predicting the reservoir storage capacity and future migration of the CO2 plume. In this study, we develop a model selection algorithm that refines an initial suite of calibrated models for a point bar reservoir, to create a posterior set of models that reflect time-lapse seismic information, based on observed dynamic response. In the model selection algorithm, we: (1) compute discrete Fréchet distances to quantify the similarity in post-injection seismic responses obtained from a large prior ensemble of models, (2) combine multidimensional scaling with k-means clustering, to partition the models into subgroups based on their seismic responses, (3) apply Bayes' rule in the reduced model space, to select the subgroup of models that yield response closest to the observed seismic information, and (4) iteratively sample the posterior models, to further refine the selection of the model clusters. The final ensemble of the selected refined models can be used to assess the uncertainty in predicting the future displacement of CO2 plume. The applicability of the workflow to a real field scenario is demonstrated, using the CO2 injection dataset for the Cranfield in Mississippi. The proposed model selection workflow has the potential to efficiently map the CO2 plume migration and assess the uncertainty in CO2 migration paths.

S1604. Bayesian Seismic Rock Physics Inversion Using the Local Ensemble Transform Kalman Filter

Mina Spremic (Norwegian University of Science and Technology),
Jo Eidsvik (Norwegian University of Science and Technology),
Per Avseth (Norwegian University of Science and Technology)
Room: auditorium 2022-09-01 11:05

We study the challenge of quantifying uncertainty in seismic amplitude versus offset (AVO) inversion. We perform inversion in a Bayesian manner, as it provides a natural framework for modeling and uncertainty quantification in the posterior solution. To solve the nonlinear inversion problem, we are using a Local Ensemble Transform Kalman filter (LETKF). The approach starts by generating prior ensembles of continuous reservoir parameters such as fluid saturations; brine, oil and gas, porosity and clay content. They are modeled on the two-dimensional grid defined via inline and crossline coordinates at the top-reservoir. In the modeling, the depth or traveltime at each grid cell is assumed known. The prior ensembles are then taken through the likelihood model defined by the non-linear rock physics relations to provide simulated seismic AVO coefficients. The hierarchical structure of the rock physics relation allows for accounting of, among others, cementation and non-uniform stress distribution. The goal lies in modeling the reservoir parameters of the Alvheim reservoir unit, capturing their realistic uncertainties and in conditioning on the data using the localized ensemble-based method to approximate posterior calculations. We present results and potential future challenges of the method for the case of Alvheim field.

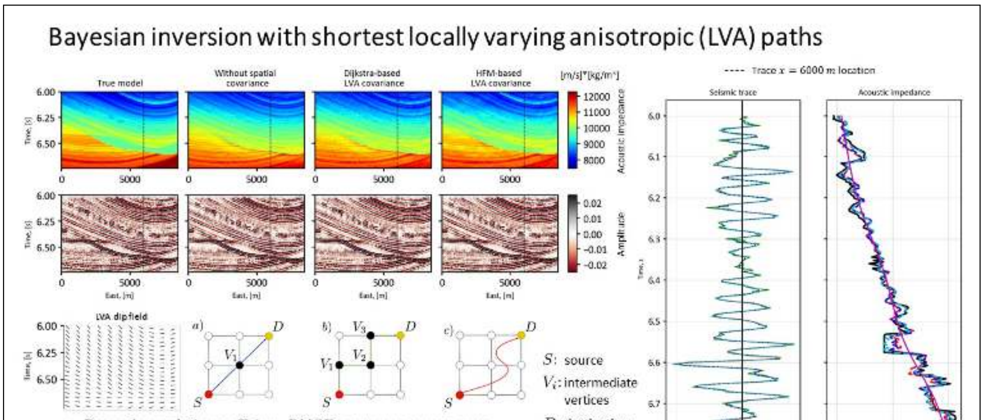
S1605. Bayesian inversion with shortest locally varying anisotropic (LVA) paths

Jeff Boisvert (University of Alberta),
Anton Bogrash (University of Alberta),
Mauricio Sacchi (University of Alberta)
Room: auditorium 2022-09-01 11:30

We present a Bayesian spatially coupled post-stack inversion method for estimating acoustic impedance. The proposed workflow incorporates non-Euclidean shortest path distances (SPD) to define a prior covariance matrix that honors spatial coherency and locally varying geometric anisotropy (LVA) field.

For complex geological settings where stratigraphic coordinate transformation is not feasible, the proposed approach overcomes the conventional geostatistical assumption of constant geometric anisotropy across the domain of study and estimates a more accurate covariance. A Hamiltonian Fast Marching (HFM) algorithm is used for the SPD calculation to enhance the geological realism of prediction.

Robust estimation of spatial covariance requires redundant measurements in all directions. However, typical petroleum exploration problem have insufficient data points for robust spatial covariance estimation in the horizontal direction. Local dips and anisotropy ratios along the major and minor continuity directions constituting the LVA field are estimated directly from seismic stacked data. The latter alleviates the issue with data scarcity in the lateral direction. Post-stack inversion for acoustic impedance is used to demonstrate the benefits of the proposed methodology; however, the proposed workflow is valid for other inversions, such as the inversion of perturbations of elastic parameters and density from preconditioned amplitude-vs-angle gathers. Since non-Euclidean distances capture geological structures better than straight Euclidean paths, the resulting impedance estimate is more accurate and follows geological continuity along the locally varying anisotropic features.



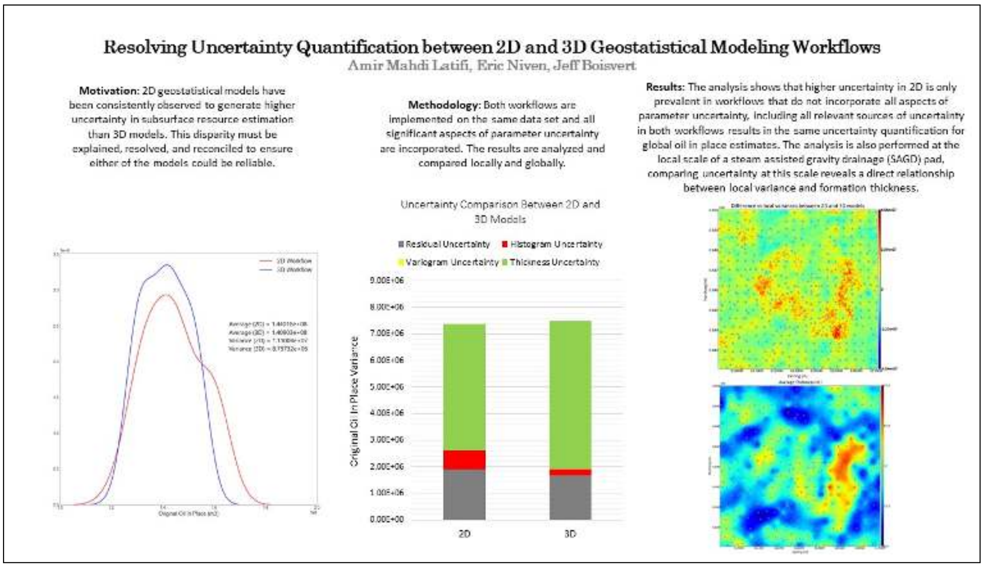
ρ : Pearson's correlation coefficient, $RMSE$: root mean square error.

Inversion method	Acoustic impedance RMSE	Acoustic impedance ρ	Seismic RMSE	Seismic ρ
Without spatial covariance	251.56	0.98	0.0032	0.978
Dijkstra-based LVA covariance	229.91	0.98	0.0031	0.979
HFM-based LVA covariance	188.47	0.99	0.0031	0.979

S1606. Comparing Uncertainty Quantification Between 2D and 3D Geostatistical Modeling Workflows

Amir Mahdi Latifi (University of Alberta),
Eric Niven (Suncor Energy),
Jeff Boisvert (University of Alberta)
Room: auditorium 2022-09-01 11:55

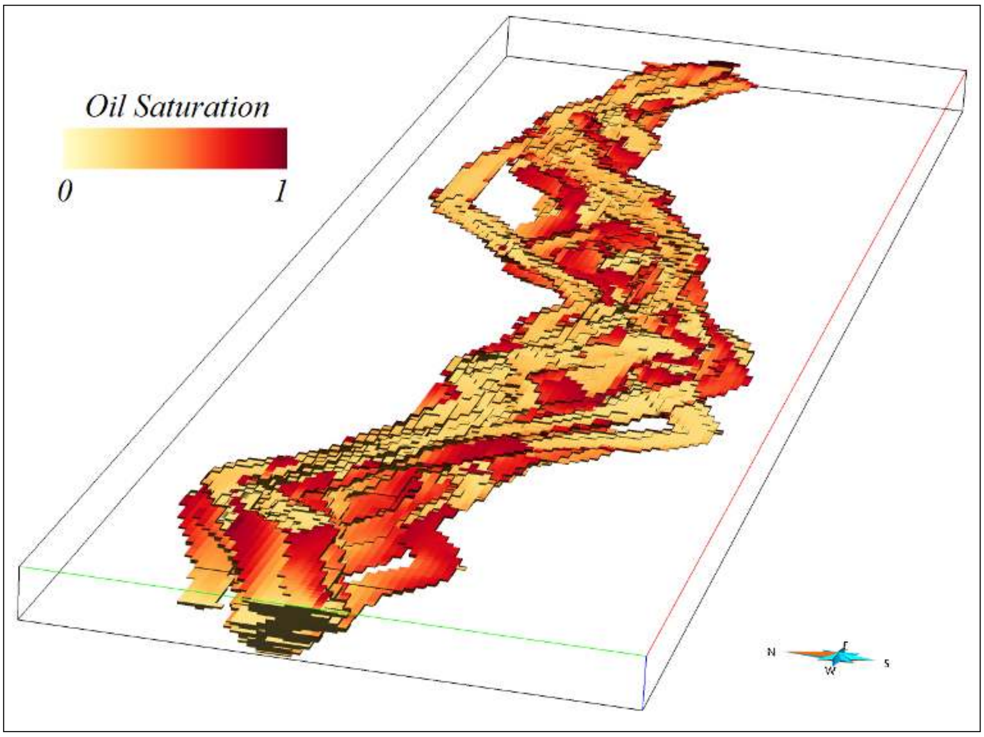
In most geostatistical workflows the goal is a 3D model of a targeted subsurface domain that contains valuable minerals or hydrocarbons; however, 2D modeling is less complex and is often easier to implement, especially when considering uncertainty quantification. 2D modeling workflows generate accurate resource estimations in some domains and can be a reasonable alternative to full 3D modeling. While the results generated by 2D and 3D workflows are similar when considering resource estimation, differences have been observed in terms of uncertainty quantification with 2D modeling generating more uncertainty; this is disconcerting and casts doubt on both workflows as it is difficult to objectively determine which model of uncertainty is correct, it is important to understand why this disparity exists. This research reconciles the quantification of uncertainty between 2D and 3D modeling by considering all relevant aspects of uncertainty in typical geospatial modeling workflows. A large domain the McMurray formation in Northern Alberta, Canada is considered. The analysis shows that higher uncertainty in 2D is only prevalent in workflows that do not incorporate all aspects of parameter uncertainty, including all relevant sources of uncertainty in both workflows results in the same uncertainty quantification for global oil in place estimates. The analysis is also performed at the local scale of a steam assisted gravity drainage (SAGD) pad, comparing uncertainty at this scale reveals a direct relationship between local variance and formation thickness. Finally, the contribution of each source of uncertainty to global uncertainty is quantified: uncertainty in the distribution of porosity, saturation, and facies accounts for 8.23% of the global uncertainty; uncertainty in thickness accounts for 68.73% of the global uncertainty; uncertainty in the variogram accounts for 0.07% of the global uncertainty; the remaining 23.46% of uncertainty is attributed to ergodic and stochastic fluctuations; uncertainty in the trend for porosity, saturation, and facies is found to be negligible. The apparent differences in uncertainty quantification between 2D and 3D modeling confuses the application of appropriate modeling workflows, explaining these differences is a valuable lesson for all geospatial modelers. Understanding the nature of differences in uncertainty quantification within these workflows allows modelers to make informed choices on the type of modeling workflow they want to choose and which workflow is most appropriate for a project.


Resolving Uncertainty Quantification between 2D and 3D Geostatistical Modeling Workflows
Amir Mahdi Latifi, Eric Niven, Jeff Boisvert
Motivation: 2D geostatistical models have been consistently observed to generate higher uncertainty in subsurface resource estimation than 3D models. This disparity must be explained, resolved, and reconciled to ensure either of the models could be reliable.
Methodology: Both workflows are implemented on the same data set and all significant aspects of parameter uncertainty are incorporated. The results are analyzed and compared locally and globally.
Results: The analysis shows that higher uncertainty in 2D is only prevalent in workflows that do not incorporate all aspects of parameter uncertainty, including all relevant sources of uncertainty in both workflows results in the same uncertainty quantification for global oil in place estimates. The analysis is also performed at the local scale of a steam assisted gravity drainage (SAGD) pad, comparing uncertainty at this scale reveals a direct relationship between local variance and formation thickness.
Uncertainty Comparison Between 2D and 3D Models
Residual Uncertainty
Histogram Uncertainty
Variogram Uncertainty
Thickness Uncertainty
Original Oil In Place Variance
9.00E+06
8.00E+06
7.00E+06
6.00E+06
5.00E+06
4.00E+06
3.00E+06
2.00E+06
1.00E+06
0.00E+00
2D
3D

S1607. Dynamic connectivity measures on turbidite channel complex architectures

Enrico Scarpa (GeoRessources, University of Lorraine),
Pauline Collon (Université de Lorraine, CNRS, GeoRessources),
Irina Panfilov (Lemta, CNRS),
Christophe Antoine (GeoRessources, Universite de Lorraine),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS)
Room: auditorium 2022-09-01 11:57

Channelized submarine systems are often gathered into complexes and display various stacking patterns. Their internal architectures represent one of the fundamental properties of a reservoir because they impact the connectivity of sand-rich bodies and affect hydrocarbons recovery. Some works have analyzed the static connectivity of various stacking patterns; however, few have qualitatively evaluated the dynamic implications of different stacking patterns on fluid flow circulations. For this reason, we analyze the hydrodynamic responses of several stacking patterns considering a set of many stochastic realizations grouped into three categories, where each category considers one particular stacking pattern setting. To study the hydrodynamic responses, we set a two-phase system containing oil and water, quantify the oil recovery efficiency, the water breakthrough time, and we compute the dissimilarities between the saturation maps at a specific time equal to 0.5 the injected pore volume. The metrics and dissimilarities are then visualized using heat maps and two-dimensional representations based on multidimensional scaling. This approach facilitates the comparison among flow simulations and quantitatively evaluates the differences of stacking patterns in a channelized submarine meandering reservoir. Moreover, our method permits us to estimate the relation between static and dynamic metrics descriptions.



S1609. How to capture high-resolution continuous facies geobodies across wells in a geomodeling workflow? Example from an outcrop and from a subsurface dataset from the Western Canadian Sedimentary Basin

Thomas Jerome (GMDK, University of Calgary),
Carolyn M. Furlong (University of Calgary),
Simon S.P. Poirier,
Per K. Pedersen (University of Calgary)
Room: auditorium 2022-09-01 11:59

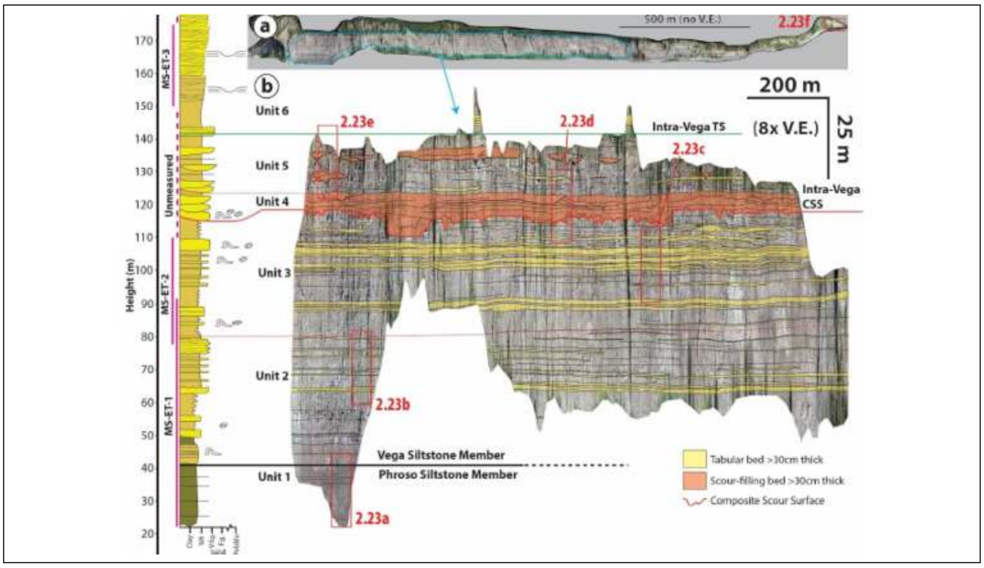
In many reservoirs, wells are so far apart one from the other that it is difficult if not impossible to correlate high-resolution stratigraphic details from well to well. The geobodies observed at one well often have too short lateral extension to be observed at the surrounding wells. In geomodeling, it leads us to be satisfied in using geostatistical algorithms to populate between the wells.

In the Western Canadian Sedimentary Basin (WCSB), it is not uncommon to have vertical wells drilled every kilometer over large areas. It is a high-enough well density to correlate even thin changes in marine or coastal environment for example. How can such details be incorporated in a geomodeling workflow? An outcrop study and a high-resolution sequence stratigraphy study will be used to illustrate the challenges.

Poirier built a digital outcrop model of the 1.5km by 100m high Evan-Thomas Creek outcrop, in Alberta, Canada. The Sulphur Mountain Formation visible there is an analogue to the Lower Triassic Montney Formation, a prolific unconventional oil and gas reservoir in Western Canada. Poirier described tabular and scour-filling beds, some just a few 10s of centimetres thick, continuous over the whole 1.5km length of the outcrop. How do we model these?

Furlong focused on the Sunset Prairie Formation, in British Columbia, Canada. The studied area shows the high-density of vertical wells typical of the WSCB. The high-resolution sequence stratigraphy correlation shows that high-resolution GR variations can be tracked over many kilometers. It is the case not only in the studied formation but also in the underlying Montney Formation. Again, how shall we capture this?

The goal of this presentation is to raise awareness about the problem as it is the authors' experience that many geomodels ignore such correlation. Some solutions to this problem will be presented.


a
500 m (no V.E.)
2.23f
b
200 m
(8x V.E.)
25 m
Unit 6
Unit 5
Unit 4
Unit 3
Unit 2
Unit 1
2.23e
2.23d
2.23c
2.23b
2.23a
Intra-Vega TS
Intra-Vega CSS
Vega Siltstone Member
Phroso Siltstone Member
Height (m)
MS-ET-1
MS-ET-2
MS-ET-3
Unmeasured
Tabular bed >30cm thick
Scour-filling bed >30cm thick
Composite Scour Surface

S1610. Facies modeling using unstructured grid, a groundwater field case: the Roussillon coastal aquifer.

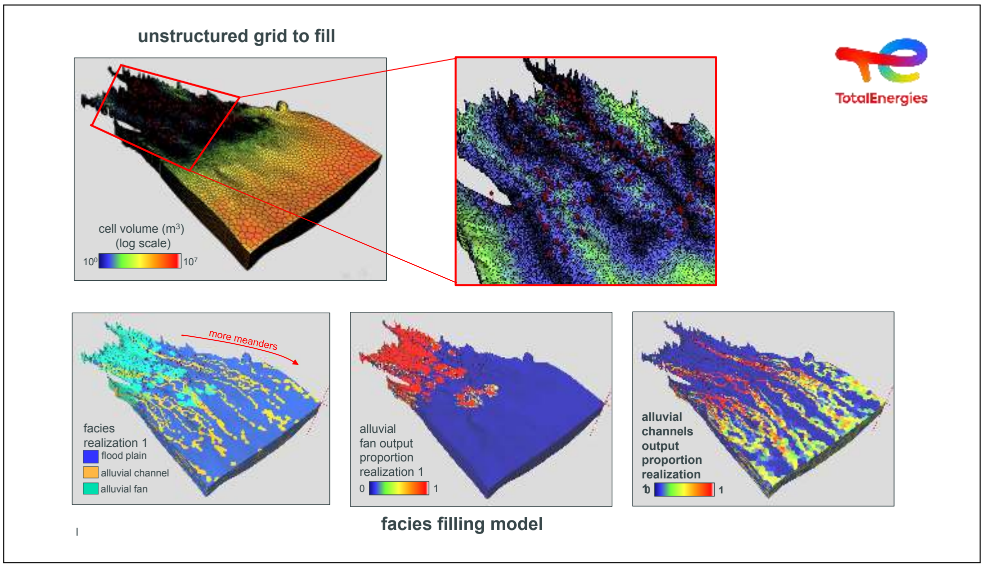
Pierre Biver (TotalEnergies),
Francis Morandini (TotalEnergies),
Philippe Renard (University of Neuchâtel),
Yvan Caballero (BRGM),
Valentin Dall'Alba (University of Neuchatel)
Room: auditorium 2022-09-02 09:50

Unstructured grids are useful because they allow adapting locally the model resolution to ensure solving the physical problem under consideration accurately while being parsimonious in the number of cells and saving computing time. Such grids are frequently used in hydrogeology, but the simulation of petrophysical properties on these grids while accounting for the support effect is rarely done.

In a pair of previous publications, a new geomodelling workflow has been proposed to populate directly unstructured grids with lithologies (facies or rock-types) and petrophysical attributes (namely porosity and permeabilities) [Biver et al. 2019; Mourlanette et al. 2020].

In this paper, we illustrate the effectiveness and applicability of the workflow for facies modeling in an environmental application. The study site is the Roussillon coastal aquifer located in the south of France [Dall'Alba et al. 2020]. The groundwater model of this aquifer requires a fine resolution around the pumping wells and along the rivers where active groundwater exchanges are occurring. A coarse resolution is sufficient far away from the wells and from the present coastline where the salinity boundary conditions can be expressed more globally. A dedicated unstructured Voronoï grid has been constructed based on these requirements

Subsequently, the facies model is built using all the available well data. Two methods are presented: the Pluri-Gaussian simulation and an object-based technique. In both cases, azimuth and input proportions trends are used. Facies are simulated at integration points inside the cells. For small cells, a single point is used; for larger cells, larger number of points are simulated and averaged (proportions of each facies and most likely facies are computed). With this procedure, the support size effect is handled, and facies mixing is allowed in large cells. The results demonstrate the applicability and efficiency of the method.



unstructured grid to fill
cell volume (m³) (log scale)
TotalEnergies
more meanders
facies realization 1
flood plain
alluvial channel
alluvial fan
alluvial fan output proportion realization 1
alluvial channels output proportion realization
facies filling model

S1611. GANSim-3D for conditional geomodelling: theory and field application

Suihong Song (Curtin University),
Tapan Mukerji (Stanford University),
Jiagen Hou (China University of Petroleum),
Dongxiao Zhang (Southern University of Science)
Room: auditorium 2022-09-02 10:15

Based on our previous research, we present a Generative Adversarial Networks (GANs)-based 3D reservoir simulation framework, GANSim-3D, where the generator (a Convolutional Neural Network, CNN) is progressively trained to capture geological patterns and relationships between various input conditioning data and output earth models and is thus able to directly produce multiple 3D realistic and conditional earth models from given conditioning data. Conditioning data can include 3D sparse well facies data, probability maps, and global features like facies proportion. Because only including 3D convolutional layers, once trained on training dataset consisting of small-size data cubes, the generator can be used for geomodelling of 3D reservoirs of large arbitrary sizes by simply extending the inputs. To illustrate how GANSim-3D is practically used and to verify GANSim-3D, a field karst cave reservoir in Tahe area of China is used as an example. The 3D well facies data and 3D probability map of caves obtained from geophysical interpretation are taken as conditioning data. First, we create a training dataset consisting of 64×64×64-size 3D cave facies models integrating field geological patterns, 3D well facies data, and 3D probability maps. Then, the 3D generator is trained and evaluated with various metrics. Next, we apply the pretrained generator for conditional geomodelling of two field cave reservoirs of size 64×64×64 and 336×256×96. The produced reservoir realizations prove to be diverse and consistent with the field geological patterns and the field conditioning data. The noise in the probability map is suppressed. Each realization with 336×256×96 cells only takes 0.988 seconds using 1 GPU.

S1612. Generation of Synthetic Compressional Travel Time using Well-Logging-Learning Model and Its Application to the Ulleung Basin Gas Hydrate Field, Republic of Korea

Minsoo Ji (Ewha Womans University),
Seoyoon Kwon (Ewha Womans University),
Kyungbook Lee (Kongju National University),
Sungil Kim (Korea Institute of Geoscience),
Baehyun Min (Ewha Womans University)
Room: auditorium 2022-09-02 10:40

This study utilizes a deep-learning-based model to output synthetic compressional travel time from well-logging data. Logging parameters such as gamma-ray, neutron porosity, bulk density, and photoelectric absorption are selected as input variables of the learning-based model. We compare the estimation performance of Long Short-Term Memory (LSTM) and Artificial Neural Network (ANN) with application to the Ulleung Basin Gas Hydrate in the East Sea, Republic of Korea. Sensitivity analysis on the number of hidden neurons is performed to obtain an efficient structure of each deep-learning model. Our results indicate that the LSTM-based model outperforms the ANN-based model by preserving the geological sequence of well logging data. The results of 10-fold cross-validation reveal the consistency of the LSTM-based model with an average coefficient of determination greater than 0.8. The estimation performance of the LSTM-based model is satisfactory for gas hydrate deposited in a less-consolidated formation. It is anticipated that the generation of synthetic well-logging via deep learning can estimate missing logging data for the characterization of gas hydrate-bearing sediments.

S1613. Quantifying Uncertainty in 3D Facies Modeling Using MCRF with Lateral Gradational Fields

Jonas Kloeckner (UFRGS),
Zhen Yin (Stanford University),
Paulo R. M. Carvalho (Petrobras),
Diego M. Marques (Universidade Federal do Rio Grande do Sul),
João Felipe C. L. Costa (Universidade Federal do Rio Grande do Sul),
Jef Caers (Stanford University)
Room: auditorium 2022-09-02 11:05

Building high-resolution 3D facies models is important for subsurface reservoir forecasting, but it is subject to considerable geological uncertainty. This study develops a 3D Markov Chains Random Fields simulation (MCRF) approach to quantify facies model uncertainty using high-resolution borehole samples and 3D seismic data. The proposed geostatistical method will use transiograms to model cyclicity and rhythmicity, for facies models in carbonate and siliciclastic reservoirs in a subsalt environment. Traditional geostatistical methods (such as sequential indicator simulation) generate facies successions that are identical along one direction and its opposite, thus, symmetrical. Transiograms, on the other hand, are capable to impose asymmetrical relationships for spatial phenomena. These transiograms are modeled using well logs, resulting in vertical direct and cross transiograms. The challenge is estimating the lateral transiogram when limited boreholes are available. Onto overcome this problem, we rely on Walther's law of facies. By using lateral gradational fields, it is possible to laterally replicate the vertical transiograms models. The lateral gradational fields use corrected distances to impose 3D transitional probabilities. The lateral gradational fields are generated using seismic data. Furthermore, to take into account the uncertainty, probability fields of the vertical proportion curves for each facies are used. At the end, with the modeled transiograms and lateral gradational fields, we generate multiple realizations of high-resolution 3D facies models to quantify the geological uncertainty of high-resolution geological models. The method will be tested on a case study of subsalt carbonate from Santos Basin, Brazil offshore.

S1614. Sequential Determination of Well Placements using Multi-modal Convolutional Neural Network for the Optimal Primary Recovery at an Oil Reservoir

Seoyoon Kwon (Ewha Womans University),
Minsoo Ji (Ewha Womans University),
Min Kim (Ewha Womans University),
Baehyun Min (Ewha Womans University)
Room: auditorium 2022-09-02 11:30

This study develops a multi-modal convolutional neural network (M-CNN) to sequentially determine the locations of oil production wells for maximizing the field oil production during primary recovery at a hydrocarbon reservoir. This M-CNN inputs near-wellbore static (e.g., permeability and porosity) and dynamic (e.g., pressure and saturation) properties and outputs cumulative oil production at a candidate well location. The M-CNN learns how to correlate the petrophysical spatial data and temporal oil productivity. Multi-modal learning is employed to simultaneously import static and dynamic properties for feature extraction in the M-CNN. The proposed M-CNN is tested to the modified UNISIM oil reservoir model. The problem is designed to install up to four oil production wells in sequence with the same time interval. The results of the M-CNN show in good agreement with those of the full-physics reservoir simulator. Also, the M-CNN outperforms a multi-layered neural network for qualified well locations. This study highlights the efficacy of the M-CNN in the multi-well-placement optimization problem, revealing the balance between accuracy and savings at the computational cost.

S1615. Multifractal-based Quantitative Characterization of Micropore Structures in Burial Dissolution of Carbonate Reservoirs

Jiayi Ma (China University of Geosciences),
Shuyun Xie (State Key Laboratory of Geological Processes and Mineral Resources (GPMR), Faculty of Earth Sciences, China University),
Cunli Jiao (Research Institute of Explorat),
Min She (PetroChina Hangzhou Institute),
Tianfu Zhang (PetroChina Hangzhou Institute),
Zhiwei Kuang (State Key Laboratory of Geological Processes and Mineral Resources)
Room: auditorium 2022-09-02 11:55

Fluid-rock interactions play an important role in the generation of porosity in carbonate reservoirs. It is of great significance for the further development of carbonate reservoir to clarify the pore evolution law in the process of burial dissolution. Fractal and multifractal theory have been widely used in the study of pore structure as an effective method for quantitative characterization of irregular objects. While, there is still a lot of work to be done in combination with the quantitative characterization of micropore structure and the dissolution law of reservoirs. In this study, batch dissolution experiments were carried out with water bath instrument, rotating disk reactor and high-temperature and high-pressure reactor. Pore microstructure and elements distribution images were obtained by X-ray computed tomography and environmental scanning electron microscopy. multifractal analysis was used to quantify the structure and composition heterogeneity in two-dimensional (2D) and three-dimensional (3D) space.

The results show that the 2D/3D spatial distribution patterns of micro-pore structures before and after dissolution are of multifractal characteristics. Porosity and permeability are closely related to the box-counting dimensions and corresponding multifractal parameters, which demonstrates that the microstructure morphological characteristics control the porosity and permeability to a certain extent. The microscopic morphology and multifractal parameters revealed that microcracks and micropores are areas of preferential dissolution, dissolution reduced the irregularity and singularity of pores. Further, the dissolution mechanism of carbonate reservoirs was innovatively explained from the perspective of element distribution patterns on the microscopic scale. It indicated that carbonates with higher spatial singularity of Ca and Mg are more likely to dissolve. In summary, local topography, local mineral arrangement and element singularity will affect the evolution of micropore spaces in burial dissolution of carbonate reservoirs. Furthermore, dissolution reduce the microscopic heterogeneity of the complex pore system, which is significant for further development of carbonate reservoirs.

S17 Spatiotemporal Geostatistics

Dionissios Hristopulos (Technical University of Crete),
Sandra De Iaco (University of Salento)

The development of spatiotemporal models is at the forefront of current research in Geostatistics. Flexible and realistic models that can capture the complex behavior of dynamic processes are crucial for improved prediction of spatiotemporal processes and for reliable evaluation of the uncertainties involved. Significant modeling challenges involve topics such as the increasing size, heterogeneity, multivariate dependence, multiple correlation scales and non-Gaussian probability distribution of modern spatiotemporal data.

This session seeks contributions that will advance spatiotemporal Geostatistics by proposing novel concepts and methodologies, computational algorithms, and innovative applications or studies that focus on spatiotemporal data analysis. A non-exhaustive list of topics includes the development of novel space-time covariance functions (e.g., non-separable models, models on the sphere and on manifolds, multivariate dependence, complex-valued models), covariance-free approaches (e.g., models based on stochastic partial differential equations and explicit precision operators), innovative simulation methods, computational advances and applications to interesting or challenging spatiotemporal datasets, as well as approaches for non-Gaussian space-time data and multiscale models. Contributions that combine Geostatistics with current developments in applied mathematics (e.g., uncertainty quantification and multifidelity frameworks), as well as in machine learning (e.g., hierarchical models, sparse and multiscale Gaussian process regression) are also welcome.

S1701. Blind source separation for multivariate stationary space-time data

Christoph Muehlmann (Vienna University of Technology),
Sandra De Iaco (University of Salento),
Klaus Nordhausen
Room: 102 2022-08-30 10:00

Multivariate spatio-temporal data is increasingly common and when modeling such data the dependencies between the variables and in space and time need to be considered, which is a quite challenging task.

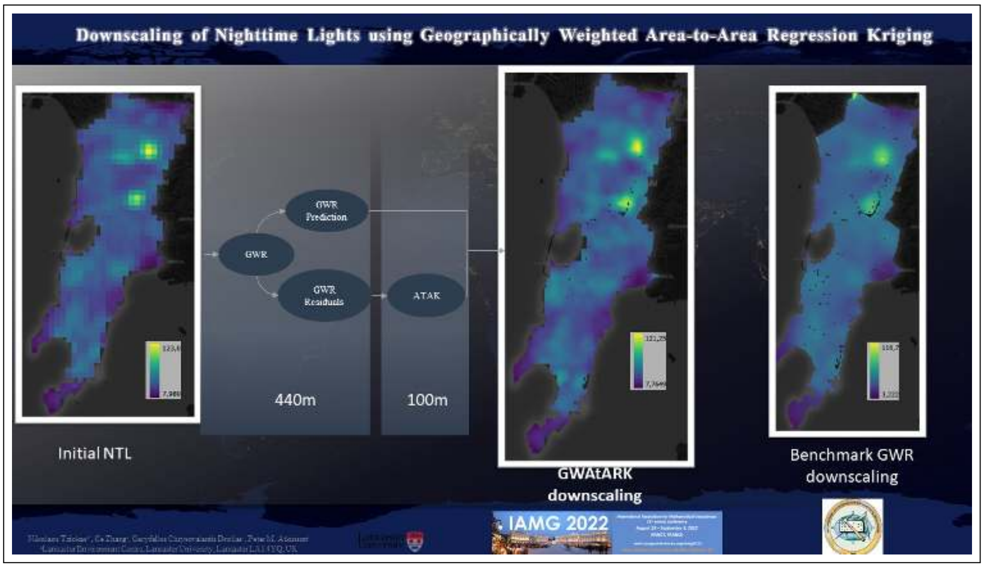
In this presentation we suggest a blind source separation model for multivariate stationary space-time data. Follwing the model the observed process is a linear mixture of uncorrelated unobservable stationary space-time components and the goal is estimate these components based on the observed process alone without specifying their covariance functions. These components can then help interpretations and allow univariate modeling and dimension reduction. We suggest two different approaches, stAMUSE and stSOBI, for the estimation of the components which are both based on the joint diagonalization of local autocovariance matrices. We investigate statistical properties of the new methods and show how the model relates to the space-time linear model of coregionalization.

The performance of stAMUSE and stSOBI is investigated in a simulation study and investigated in a real data example using environmental space-time data.

S1702. Downscaling of Nighttime Lights using Geographically Weighted Area-to-Area Regression Kriging

Nikolaos Tziokas (Lancaster University),
Ce Zhang (Lancaster University),
Garyfallos, G/Ch Drolias (Lancaster University),
Peter, P/M Atkinson (Lancaster University)
Room: 102 2022-08-30 10:25

Satellite nighttime light (NTL) Observations offer a timely and geographically explicit measurement of human activities, facilitating a variety of applications such as tracking urbanisation and socioeconomic dynamics, assessing military conflicts, mapping light pollution etc. The Day/Night Band (DNB) of the Visible Infrared Imaging Radiometer Suite (VIIRS) collects low-light imaging data globally and provides crucial indication of settlements and human activities. The coarse spatial resolution (450m) of NTL observations, however, severely restricts its practical applications to capture fine-grained details. One of the most common approaches for acquiring fine spatial resolution images is the spatial downscaling of satellite sensor data. This has been widely employed in daytime satellite images such as MODIS, Landsat and Sentinel-2, while seldom used in NTL images. In this study, we used Geographically Weighted Area-to-Area Regression Kriging (GWATARK) for downscaling of NPP-VIIRS NTL, together with fine spatial resolution ancillary variables being incorporated, including Landsat 8 OLI/TIRS imagery and population density from WorldPop. The GWATARK, as a geostatistical approach, is designed to address challenges caused by spatially local heterogeneity, which cannot meet the underlying condition of stationarity within ATARK. Our case study in Mumbai, India, using GWATARK demonstrates strong capability for downscaling to produce 100m NTL predictions from eight 440m NTL raw images monthly in 2016. The method achieved an average Pearson's correlation coefficient of over 0.98 in the majority of months, far better than other benchmark approaches, such as Geographically Weighted Regression (GWR) downscaling, Spline interpolation using hybrid Machine Learning. Our further work is to test the spatial downscaling of NTL using GWATARK in wider geographical regions and to identify the vast potential for real-world applications.



S1703. Generating large spatiotemporal precipitation fields moving across a region

Sofia Nerantzaki (PhD Student),
Dionissios T. Hristopulos (Technical University of Crete),
Simon Michael Papalexiou (University of Calgary)
Room: 102 2022-08-30 10:50

Precipitation at fine spatiotemporal scales is a complex process characterized by strong dependence, anisotropy, and advection, following the movement patterns of the weather system. Being the primary factor affecting surface and underground hydrological processes, precipitation is the main input variable in most water management and risk assessment studies. Effective stochastic simulation of such complex environmental flows in space and time is therefore of utmost importance. Here, we use the Complete Stochastic Modeling Solution (CoSMoS) framework to simulate random fields (RFs) with complex patterns and motion resembling the movement of rainfall storms. The approach preserves any non-Gaussian marginal distribution, any spatiotemporal correlation structure, the locally varying anisotropy, and the general advection given by velocity fields with locally varying speed and direction. Real-world applications (e.g., large-scale applications of hydrologic models) need simulated fields of large dimensions. However, there is a limit in the size of RFs that can be generated. To achieve a fast interpolation for the densification of the moving RFs in space, we incorporate the stochastic local interaction (SLI) model. In the latter, local interactions in terms of near neighbors are used. The interaction strength and the neighborhood size are defined by kernel functions and local bandwidths, allowing to create sparse and explicit precision (inverse covariance) matrices for spatial dependence. In SLI, the requirements for storage are modest, since a matrix inversion is not required, thus enabling the production of large fields with advection when combined with CoSMoS. The study provides a modeling framework for the simulation of large moving rainfall fields which can be used as input to large-scale hydrological studies.

S1704. Simulation of Complex Multivariate Relationships Based on a Non-Stationary Coregionalization Model

Alvaro Riquelme (Queen's University),
Julian M. Ortiz (Queen's University (Kingston))
Room: 102 2022-08-30 11:15

The geostatistical analysis of continuous attributes often benefits from related secondary information, which helps improving accuracy in estimation results and reduces uncertainty. However, the process of including secondary information may be challenging when data shows complex relations among variables. Managing the non-linear behavior on the multivariate probability distribution is not always a straightforward procedure.

In this work, we propose a method to disaggregate the global non-linear behavior among data attributes into the spatial domain in a piece-wise linear fashion. We demonstrate that multivariate complexities on geochemical variables can be reproduced by looking at the local linear correlations between variables at sample locations, inferred in a local neighborhood, and interpolating this local dependency of the coregionalized variables using a non-stationary version of the Linear Model of Coregionalization.

These local correlations defined at sample locations can be interpolated on the spatial domain by mapping them into the space of correlation matrices, which form a Riemannian manifold. As Euclidean distances are no longer a suitable metric on this Riemannian space, the main challenge is to find an appropriate metric to measure closeness among correlation matrices, with the purpose of interpolating between known correlations. This task is addressed by using tools from Riemannian Geometry. A detailed application of the procedure is shown in a real case study, focusing on the essential steps of the methodology. This example demonstrates how the proposed methodology honors the multivariate configuration of data in the probability space, as well as agreeing with spatial experimental features such as cross-semi-variograms.

S1705. A general geospatial interpolation framework with locally varying anisotropy

Zhanglin Li,
Xialin Zhang (China University of Geoscience),
Rui Zhu (University of California, Santa Barbara),
Zhengping Weng (China University of Geoscience),
Zhiting Zhang (China University of Geoscience),
Gang Liu (China University of Geoscience)
Room: 102 2022-08-30 11:40

Kriging in the presence of locally varying anisotropy (LVA) is a typical solution to express complex geological structures such as folds and fractures. The realistic shortest path distance (SPD) associated with curvilinear features in geology are crucial to geostatistical modeling when LVA is present. However, the SPD is not always in a straight line, and thus cannot be easily incorporated into classical kriging. For such cases, this paper proposes a general geospatial interpolation framework, termed as direct kriging, in which a straightforward incorporation of the SPD in kriging estimation with LVA is achieved. In this method, minimization of the error variance is treated as an optimization objective to acquire an optimal linear unbiased estimate. For demonstration, a genetic algorithm is employed to implement this optimization process. This method developed is illustrated and evaluated using a case study with two synthetic datasets. Compared with classical solutions, the proposed method not only produces more accurate estimates but also preserves more realistic geology, especially for the underlying curvilinear structures

S1706. Stochastic Local Interaction Models for Gap Filling of Gridded Datasets

Dionissios Hristopulos (Technical University of Crete),
Emmanouil A. Varouchakis (Technical University of Crete),
George P. Petropoulos (Harokopio University of Athens)
Room: 102 2022-08-30 12:05

Gridded datasets are common in remote sensing. Images often have gaps due to incomplete coverage, noise contamination, sensor malfunction, and cloud obscuration. Interpolation methods, in either space or time, are used often in conjunction with other approaches (e.g., combination of images from more than one satellites) to fill such gaps.

Stochastic local interaction (SLI) models can capture spatial and space-time correlations between neighboring points and they can provide computationally efficient estimates of missing values [1,2]. They involve a small set of parameters that control the correlations. They can easily incorporate anisotropic dependence by means of directionally dependent parametrization, and they can be used either as global or as local models. In the first case, the same parametrization is applied to the entire dataset, while in the second case the parametrization is allowed to change locally. For randomly missing data values, a version of the SLI model which is equivalent to a Gaussian Markov random field with a specific interaction structure is used. In the case of contiguous areas of missing data, a different version of the SLI model which involves kernel functions is more suitable. The kernel functions implement spatially extended interactions between points, which enable the model to capture correlations between sites in a controlled, finite-size neighborhood. We present the SLI model, discuss its main features, and test its gap filling performance using cross validation on synthetic and real datasets.

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S1707. Spatio-temporal modeling with stochastic partial differential equations: simulation and inference

Lucia Clarotto (Mines Paris Tech),
Denis Allard,
Nicolas Desassis (Mines Paris Tech),
Thomas Romary (Mines Paris)
Room: 102 2022-08-30 16:30

In the task of predicting spatio-temporal fields in environmental science, statisticians have a great interest in introducing models inspired by the physics of the underlying phenomena. On the one hand, the abundance of space-time datasets calls for new numerical methods to efficiently process these large datasets. On the other hand, the richness of the datasets opens the possibility to relax some restrictive hypotheses on the models. The Stochastic Partial Differential Equation (SPDE) approach has proven to be effective for the estimation and the prediction (kriging) in a spatial context. By varying the coefficients of differential operators of a given SPDE, this method allows defining new space-time models and prediction methods.

Here, we present the advection-reaction-(hyper)diffusion SPDE with first order derivative in time. In this large class of spatio-temporal models, the spatial trace is characterized by the Matérn covariance function. The simulation of this class of models is based on the numerical solution of the SPDE, obtained by discretizing the temporal derivative with a finite difference method (implicit Euler) and, at each time step, by solving the purely spatial SPDE with a Finite Element Method (Continuous Galerkin). Stabilization techniques need to be introduced when the advective term dominates the diffusive term in the SPDE. Computationally, efficient methods based on sparse computations are required to infer the parameters of this SPDE and to predict the spatio-temporal field by kriging.

S1709. A comparative analysis among the spatio-temporal complex covariance functions for vectorial data

Claudia Cappello (University of Salento),
Sandra De Iaco (University of Salento),
Sabrina Maggio (University of Salento)
Room: 102 2022-08-30 16:55

In the spatio-temporal geostatistical literature, an increasing attention to the theory of complex-valued random fields for describing phenomena, which can be naturally decomposed in modulus and direction, can be recognized.

The first contributions in the framework of complex analysis date at the end of the last century, where some parametric classes of covariance models were proposed as well as practical aspects regarding the fitting procedure and the related computational difficulties were faced in the spatial domain. Thanks to the potentiality of this area of research, it is also in great demand the development of tools for space–time complex analysis. Recently, new families of spatio-temporal complex covariance models, for second order stationary spatio-temporal complex-valued random fields, based on different techniques have been introduced. One of the first contributions has been obtained by extending the spatial complex covariance model to a space–time domain, where the imaginary part was derived as convolution of the real part. Another class of complex-valued spatio-temporal covariance models has been generated starting from Bochner's characterization of a real-valued covariance function and translating the even spectral density function. Finally, a new class of complex-valued spatio-temporal covariance models obtained through positive mixture of the class based on the translated spectral density function has been proposed.

Hence, after an introduction of the complex-valued random fields in space–time and the presentation of the classes of spatio-temporal complex covariance models, some details on parameters estimation and modeling will be discussed through an application on data related to wind provided by the Global Forecast System (GFS) of the USA's National Weather Service and a comparison among the different classes available for spatio-temporal complex covariance will be proposed.

This contribution is supported by the Project "Rigenerazione Sostenibile dell'agricoltura nei territori colpiti da Xylella fastidiosa"

S1710. Modeling and predictions of spatiotemporal environmental data

Claudia Cappello (University of Salento),
Monica Palma (University of Salento)
Room: 102 2022-08-30 17:20

The whole process of assessing and forecasting the outdoor air quality over an area of interest requires the implementation of complex procedures which involve explorative analysis tools, as well as modeling and prediction techniques of huge amount of data collected for several air pollutants at the sites of the monitoring network and for several time-points.

The scientific community has proposed multivariate spatiotemporal models which are able to synthesize the hazardous variables under study by capturing the main features of the behavior of the basic hidden components which are common to the same variables. One of the most flexible multivariate models in space-time is the linear coregionalization model firstly proposed in the spatial context and successively extended to the spatiotemporal case.

Initially, the applications of the space-time linear coregionalization model (ST-LCM) proposed the use of the same covariance models for the basic hidden components, actually the product-sum model. In the last years, the ST-LCM fitting process has been further developed and improved to comply with the main characteristics shown by the variables, in terms of symmetry, separability/non-separability, type of non-separability. In particular, proper statistical tests have been formulated with the final aim to allow the researcher the identification of the most apt covariance models for the different basic components.

In this paper, the based-tests procedure of fitting a ST-LCM will thoroughly apply to a multivariate space-time environmental data set. The performance of the fitted ST-LCM will be assessed through a comparison with the ST-LCM based on only product-sum models. Finally, the model will be used to make cokriging spatiotemporal predictions of the observed variables.

This contribution is supported by the Project “Rigenerazione Sostenibile dell’agricoltura nei territori colpiti da Xylella fastidiosa”

S1711. Stochastic Local Interaction Models for Space-Time Processes

Dionissios Hristopulos (Technical University of Crete)
Room: 102 2022-08-30 17:45

The construction of valid (permissible) space-time models which provide realistic representations of the interactions between spatiotemporal correlations remains an ongoing research topic of practical importance. Classical approaches rely on the use of space-time covariance functions.

For the processing of large datasets, the use of covariance functions with infinite support can lead to insurmountable computational difficulties resulting from the inversion of very large covariance matrices. Stochastic local interaction models (SLIs) can overcome the computational costs [1]. SLI models lead to sparse precision (inverse covariance) matrices which can be used to interpolate and simulate space-time processes at a faction of the cost necessary for covariance-based methods (e.g., kriging). This is due to the fact that the predictive equations used in SLI interpolation and simulation scale linearly with the size of the dataset, compared to the third-power exhibited by covariance–based methods [2].

This presentation focuses on recent progress in SLI models focusing on the definition of space-time distance. Covariance functions employ different types of space-time distances: in separable models spatial and temporal components are disconnected; non-separable models use composite distances by extending the Euclidean formalism to the 4D space-time domain; composite distances are also obtained by positing specific forms for the spectral density. In the SLI framework, space-time distances enter in interaction kernels which control the correlations between different space-time points. By construction, it is straightforward to impose permissibility (non-negative definiteness) conditions in SLI models. This enables exploring novel space-time distance functions which can better capture space-time interactions. We test these ideas using synthetic and real datasets.

References

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2. Hristopulos, D.T.; Agou, V.D. Stochastic local interaction model with sparse precision matrix for space–time interpolation. Spatial Statistics, 2020, 40, 100403.

S18 Uncertainty Modeling

Florian Wellmann (RWTH Aachen),
Clare Bond (University of Aberdeen)

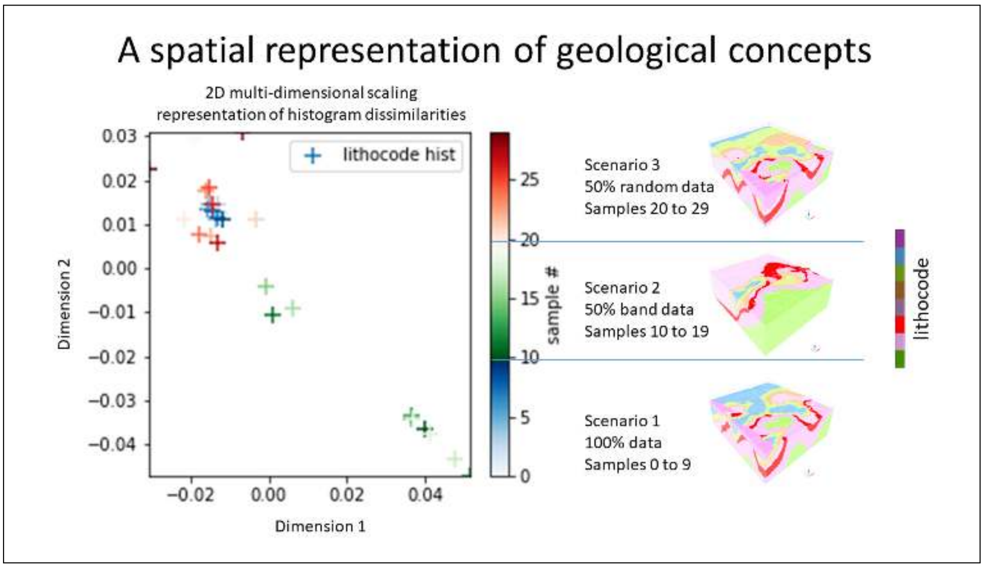
Uncertainties are prevalent in many geoscientific studies: from geostatistics and 3-D geological modelling to coupled process simulations. In this session, we invite contributions covering aspects of uncertainty estimation, modelling and visualisation in geosciences. A special focus will be on (1) methods to estimate uncertainties in data sets, expert elicitation and the analysis of bias (2) approaches to propagate uncertainties through modelling and simulation, including surrogate modelling, probabilistic programming and machine learning approaches, and (3) the quantification and visualisation of uncertainties in temporal and spatial domains. We encourage contributions both addressing theoretical and methodological challenges, as well as applications to geoscientific problems.

S1801. Can we parameterize geological conceptual models in a continuous space?

Guillaume Pirot (The University of Western Australia),
Mark W Jessell (The University of Western Australia),
Mark D Lindsay (CSIRO)
Room: 102 2022-09-01 09:50

Proper uncertainty quantification for geoscience applications such as the exploration of natural resources like groundwater, minerals and geothermal energy, relies on the exploration of an ensemble of geological models. Out of convenience, or perception bias, this exploration is often limited to a single concept or even a single geological interpretation. Moreover, when several conceptual models are considered, the risk that they are not fit for applications using real data remains high. Indeed, initial scenarios can suffer from errors, notably bias and a too narrow scope, as they are built with limited knowledge and data and are subject to interpretation bias. Here, we propose to build a continuous parameter space representation of conceptual models from a discrete and finite set of initial geological scenarios. The approach relies on statistical dissimilarities between models, and scenario representatives. It allows us to explore additional locations of the conceptual model parameter space to build scenarios that are compatible with collected geological data and it allows us to quantify uncertainty around the initial scenarios. To illustrate our approach, we use several subsets from an ensemble of one million synthetic geological models with complete tectonic histories (from https://github.com/Loop3D/noddyverse) and uncertainty indicators based on (geo-) statistical, connectivity and topological dissimilarities (from https://github.com/Loop3D/loopUI).

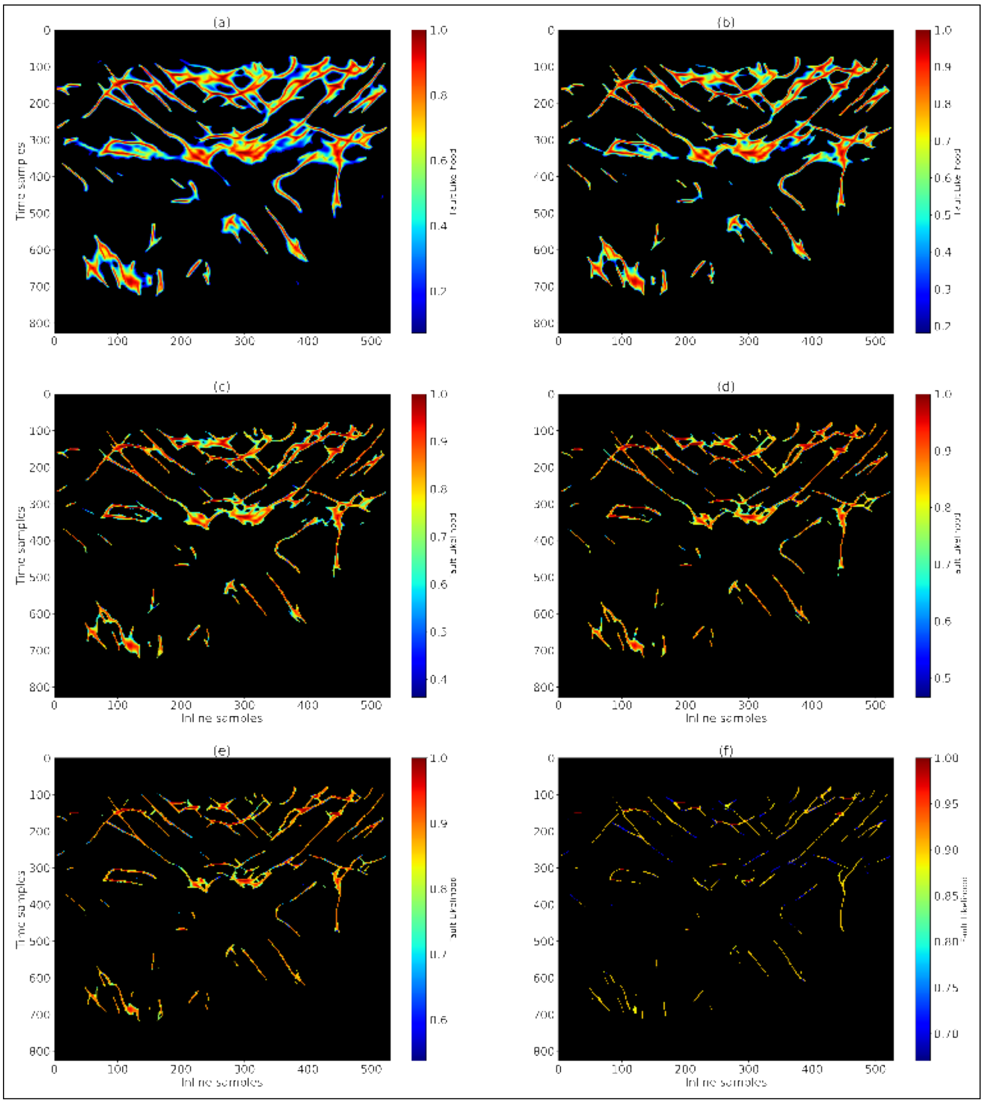
We acknowledge the support from the ARC-funded Loop: Enabling Stochastic 3D Geological Modelling consortia (LP170100985) and the Mineral Exploration Cooperative Research Centre. This is MinEx CRC Document 2022/10.


A spatial representation of geological concepts
2D multi-dimensional scaling
representation of histogram dissimilarities
lithocode hist
Dimension 1
Dimension 2
sample #
Scenario 3
50% random data
Samples 20 to 29
Scenario 2
50% band data
Samples 10 to 19
Scenario 1
100% data
Samples 0 to 9
lithocode

S1802. Two dimensional seismic fault network interpretation using marked point processes

Fabrice Taty Moukati (GeoRessources - Université de Lorraine),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS),
Radu Stefan Stoica (Université de Lorraine),
François Bonneau (Université de Lorraine, CNRS, GeoRessources)
Room: 102 2022-09-01 10:15

Seismic fault interpretation is an important input to structural models. Since in seismic images the dominant features are reflection events corresponding to horizons, fault interpretation can be achieved by computing a fault probability image. Such an image highlights fault presence while suppressing reflection events. Many methods like Machine Learning approaches have been proposed to produce probability images with good resolution. However, current approaches extract the 'best' fault network from the fault probability image (e.g., by thinning). The goal of this paper is to quantify the uncertainties related to the number and connectivity of faults honoring a given probability image, as all the possible fault networks can yield different outcomes in terms of subsurface behavior (e.g., reservoir flow). In this paper, we propose a rigorous approach to assess seismic fault network uncertainty. We use a mathematical framework that originates from stochastic geometry modeling, called marked point processes. Seismic fault networks can be seen as realizations of such processes. Therefore, a probability density needs to be defined that characterizes a marked point process. Such a probability density is built thanks to an energy function that is required for fault detection and description. This energy function is composed of two terms including a data term, necessary for fault localization, and an interaction energy for fault relationships. We use a simulated annealing framework based on Metropolis-Hastings algorithms, which makes it possible to find the global maximum of the probability density, built in the form of a Gibbs density. We apply the methodology to a 2-D seismic cross-section extracted from the Volve seismic cube provided by Equinor.


(a)
(b)
(c)
(d)
(e)
(f)

S1803. Linking Implicit Geometric and Kinematic Modeling of the Eastern Alps for Uncertainty Estimation

Sofia Brisson (RWTH Aachen),
Florian Wellmann (RWTH Aachen),
Christoph von Hagke (Paris Lodron Universität Salzburg),
Josefine Ziegler (RWTH Aachen),
Jan von Harten (RWTH Aachen),
Nils Chudalla (RWTH Aachen)
Room: 102 2022-09-01 10:40

In order to understand the influence of mantle-related processes on mountain building in the Eastern Alps, it is important to resolve the time-temperature evolution of the Alpine foreland basin, where foreland basin dynamics are linked to the exhumation history of the orogen. Models linking the exhumation history with cooling over time are commonly referred to as thermokinematic models. Most of the time, however, thermokinematic modeling relies on prescribed geometric and kinematic models at depth without considering their uncertainty. This does not allow for the quantification of the relative contributions of different drivers to the exhumation signal.

The aim of this work is to combine probabilistic structural modeling with thermoklinematic forward simulations to investigate the related uncertainties. For this purpose, 3D implicit geological modeling of the Bavarian Subalpine Molasse zone was carried out and combined with a systematic random sampling approach to automatically generate an ensemble of geometric models in the range of assigned uncertainties. The uncertainties were then visualized using probability and entropy plots, to observe how entropy behaves as a function of data availability and density and in areas of high structural complexity.

In addition, several 2D kinematic reconstructions are constructed as a basis for a probablistic 3D kinematic forward model. A link can then be obtained between kinematic model parameters and present-day geometry in comparison with field observations at the surface and also in comparison to the range of geometric uncertainties in the 3D geological model. In a next step, these models will be combined with a thermokinematic forward model to integrate thermochronological measurements from sampling campaigns in the Subalpine Molasse to obtain an integrated picture of foreland evolution and associated uncertainites over space and time.

S1804. Assessment of geophysical monitoring strategies for CO2 storage using ensemble-based methods and value of information analysis

Susan Anyosa (Norwegian University of Science and Technology),
Jo Eidsvik (Norwegian University of Science and Technology),
Dario Grana (University of Wyoming)
Room: 102 2022-09-01 11:05

Underground CO2 storage projects require geophysical monitoring to optimize injection strategies such as whether to continue with the CO2 injection or to stop the operation in case of risk of leakage. Associated with monitoring surveys, some questions arise related to which data are to be collected, such as acquisition and processing of seismic data or electromagnetic data, and the time of the surveys. In this work, we present a methodology to conduct value of information analysis for assessing the expected gained knowledge from these data. The approach is using geostatistical modeling and multiple reservoir simulations for the CO2 plume characteristics. Ensemble-based methods are used for uncertainty quantification and data conditioning, and it forms the basis for the value of information analysis based on how the ensemble weights change with data assimilation. The evaluation considers the possibility of performing surveys at different times during the CO2 storage project. We present a case study based on the Smeaheia reservoir model that considers a decision-making problem for CO2 injection strategies. The results show that the value of the different data depends on the time after injection, and optimal data acquisition strategies can be assessed based on the value of information of geophysical data.

S1805. Stochastic velocity modeling for structural uncertainty assessment during migration: application to salt body imaging

Nicolas Clausolles (BRGM),
Pauline Collon (Université de Lorraine, CNRS, GeoRessources),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS),
Modeste Irakarama (Université de Lorraine, CNRS, GeoRessources)
Room: 102 2022-09-01 11:30

Variations in the migration velocity model directly impact the position of the imaged reflections in the subsurface. Deterministically building an adequate velocity model - either by manual iterative updating and remigration or by solving a large inverse problem - does not allow, however, to investigate the structural uncertainties that stem from velocity uncertainty. To assess these uncertainties, we propose to use stochastic structural modeling to generate a set of velocity models and to analyze the set of seismic images that are obtained after remigration.

We apply it to a 2D synthetic example of salt diapir. We use a recently published method to generate a large set of salt structural interpretations having varying geometries and topologies. These interpretations are then combined with an adaptive background sediment velocity model to obtain the set of migration velocity models. The corresponding perturbed seismic images are obtained by performing a reverse time migration (RTM). We analyze the structural variability of the image set using various measures. The first ones are the mean seismic image and its standard deviation. They provide both qualitative and quantitative information about the sensitivity of the seismic data to variations in the migration velocity model. Results show that "stacking" the different seismic images emphasizes the model parts where the seismic response is consistent from one realization to another, providing insights about the structures at depth. In order to also account for sediment velocity variations, we then investigate the use of post-stack seismic attributes to characterize the structural variations by the changes in the seismic image texture, which is more robust to vertical phase shifts.

S1806. Accounting for uncertainties in soil pollution simulation by metamodeling

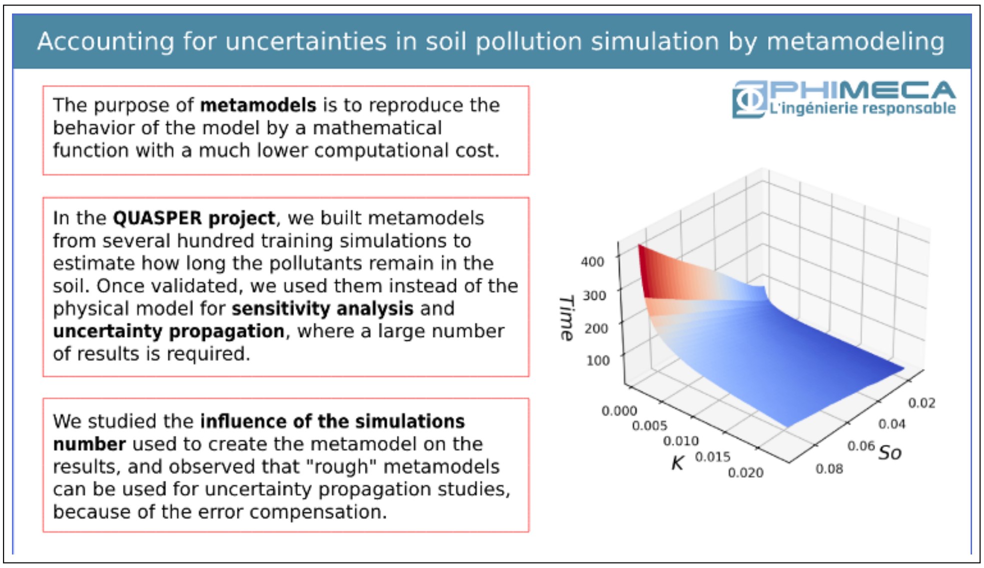
Raphaël Périllat (Phimeca),
Claire-Eleuthèriane Gerrer (Phimeca),
Sylvain Girard (Phimeca),
David Pitaval (Ginger-BURGEAP),
Juliette Chastanet (Ginger-BURGEAP)
Room: 102 2022-09-01 11:55

Estimation of the lifespan of NAPL (Non Aqueous Phase Liquid) source in soil is invaluable for deciding between competing management scenarios. Modelling and simulation in the short, medium and long term provide quantitative elements to guide the choice and the design of management solutions.

The QUASPER project, a partnership between Ginger-BURGEAP, GeoRessources and Phimeca, aims at improving and securing the modelling results. In particular we focus of the quantification of key parameters driving the evolution of pollution source areas and the quantification of uncertainties in pollution models. But these methods are often expensive in terms of computation time and the use of metamodels can facilitate their use.

The purpose of a metamodel is to reproduce the behavior of a model by a mathematical function with a much lower computational cost. They are built from several training simulations and the estimation error depends on the number of simulations used. Once built and validated, it can be used *instead of the physical model* when a large number of results is required, for example for sensitivity analysis or uncertainty propagation.

In our study, we observe that the simulations used to create the metamodel have a strong influence on the results. A prior knowledge of the model allows to use less simulations and thus to obtain metamodels more quickly in an operational context. Also, using hundreds of simulations allows to obtain very accurate metamodels but is computationnally expensive. For uncertainty propagation studies, ”rough” metamodels, built using few simulations, can however be used, because the set estimation errors compensate and the results obtained are very similar to those obtained with very accurate metamodels.



S1807. Automated hierarchical 3D modeling of Quaternary aquifers - the ArchPy approach

Ludovic Schorpp (University of Neuchâtel),
Julien Straubhaar (University of Neuchâtel),
Alexis Neven (University of Neuchâtel),
Philippe Renard (University of Neuchâtel)
Room: 102 2022-09-01 11:57

When modeling groundwater systems in Quaternary formation, one of the first steps is to construct a geological and petrophysical model. This is often repetitive because it relies on multiple manual steps which include geophysical interpretation, construction of a structural model, identification of geostatistical model parameters, facies and property simulations. Those steps are often carried out in different software, which makes the automation intractable or very difficult. A non automated approach requires a lot of time and makes the model critical to update when new data is available.

To address these issues, we propose a new approach and a Python module, ArchPy, to automatically generate realistic geological and parameter models. One of its main features is that the modeling operates in a hierarchical manner. The input data consists of a set of borehole data and a stratigraphic pile. The stratigraphic pile describes formally and in a compact manner how the model should be constructed. It contains the list of the different stratigraphic units and their order in the pile, their conformability (eroded or onlap), the surface interpolation method (e.g. kriging, sequential Gaussian simulation (SGS), multiple-point statistics (MPS), etc.) and the filling method for the lithologies (e.g. MPS, sequential indicator simulation (SIS), etc.) and the petrophysical properties (e.g. MPS, SGS, etc.). Then, the procedure is automatic. In a first step the stratigraphic unit boundaries are simulated. Secondly, they are filled with lithologies and finally the petrophysical properties are simulated inside the lithologies. All these steps are straightforward and automated once the stratigraphic pile and its related parameters have been defined. Hence, this approach is extremely flexible. The automation provides a framework to generate end-to-end stochastic models and then the proposed method allows for uncertainty quantification at any level and may be used for fully inversion.

S1808. A Geocognitive Approach to Epistemic Uncertainty Exploration

Gautier Laurent (ISTO-Univ.Orleans),
Lachlan Grose (Monash University),
Imadeddine Laouici (University of Orleans, BRGM)
Room: 102 2022-09-02 14:40

As in other sciences of interpretation, geological uncertainty is subject to the dichotomy that separates aleatory and epistemic uncertainties. The aleatory component pertains to all the variations that are accidentally recorded when documenting the Earth. It corresponds to the variability that would be observed if the same observation was made several times. The epistemic component is the remaining – it corresponds to the lack of knowledge that prevents from filling with certainty the gap between observations. Ultimately, this component would disappear if a complete observation was made. When it comes to geological uncertainty modelling, epistemic uncertainty is the hidden part of the iceberg: it is both the most difficult part to tackle and, in most cases, the biggest one. Our ability to explore the space of possible alternative representations of subsurface architectures is bound to the way models are parameterised. The panel of existing modelling methods can be analysed with respect to their use of data, more particularly localised data that corresponds to direct rock observations. In this analysis, it is unsettling to realise that most advanced modelling techniques are centred on – and often even parameterised by – localised observations, whereas epistemic uncertainty is mainly about geological knowledge and concepts. We advocate that this contradiction is at the core of current method limitations to explore geological uncertainties, which calls for developing methods that are more intrinsically based on structural concepts. However, it remains difficult to appreciate or communicate this contradiction because, in practice, we do not have access to the full extent of possible architectures of the subsurface. In this contribution, we transpose the space of possible geological models into a simpler discrete geological version that allows to consider that the global set of possible models is known.

S1809. Combination of hierarchical clustering and geostatistical simulation for delineating Au rich zones and interpretating ore generation process in an epithermal vein-type deposit

Vitor de Sá (Kyoto University),
Toshiki Muraoka (Kyoto University),
Shohei Albert Tomita (Kyoto University),
Koike Katsuaki (Kyoto University)
Room: 102 2022-09-02 15:05

Epithermal vein-type deposits are main sources of Au and Ag over the world, accurate 3D modeling of vein structure and extraction of rich zones are uppermost important to resource exploration and reserve assessment. However, spatial modeling of vein structure and rich zones poses a nuisance and time costly obstacle due to heterogeneity of geologic structure and the scarcity of available data mostly obtained by drilling. For this problem, we aim to develop an efficient and reliable workflow not to only clarify spatial distribution of Au-rich veins in detail but also shed light on the mechanisms of transport and deposit of ore fluids by selecting an Au-Ag low-sulfidation epithermal deposit in the Philippine archipelago. This archipelago is known to host manifold world-class epithermal Au-Ag deposits, which can be typified by veins, stockworks and disseminations. In the selected deposit, the mineralization was hosted in open veins and breccias that are vertically continued. To attain our purpose, this study integrates whole-rock geochemical data obtained by fire assay and atomic absorption spectrometry as well as lithological information through visual core descriptions and X-ray diffraction with hierarchical clustering analysis (HCA) and conditional geostatistical methods: turning bands simulation (TBSIM) and truncated-gaussian simulation (TGSIM). TBSIM is applied to simulate the Au grade distributions and interpret the generation process of mineralization. By the ore fluid properties, Au and Ag occurrences are correlated with linear correlation coefficient 0.69 and causal in this vein-type deposit and therefore, HCA is employed to classify similar grades into clusters and the cluster distribution is simulated by TGSIM. As the result, hydrothermally mineralized and altered zones with rich Au are specified in detail. This spatial model can be linked efficiently with field works to identify ore-rich zones caused by rock fracturing and ascent of hydrothermal fluids.

S1810. Uncertainty Quantification of depositional and structural properties with Generative Deep Learning and Graph Convolutions

Gleb Shishaev (Heriot-Watt University),
Vasily Demyanov (Heriot-Watt University),
Daniel Arnold (Heriot Watt University)
Room: 102 2022-09-02 15:30

This abstract introduces a novel approach to construct reservoir models and estimate uncertainty of depositional and structural properties with Variational Autoencoders (VAE) based on Graph Convolutions. The work demonstrates how to parameterize depositional and structural scenarios with Generative Deep Learning to provide more efficient ways for geomodel construction and uncertainty quantification (UQ).

Our Graph Variational Autoencoder (GVAE) addresses the non-uniform gridding nature of reservoir models, unlike earlier works that utilises the concept of latent space with Convolutional Neural Networks for regular grids. The latter is limited in representing structural uncertainties and irregularities in flow behavior. Our approach provides more accurate representation of structural uncertainty in geomodels via latent space, which extends the Generative Deep Learning capability for geomodel parametrization and UQ.

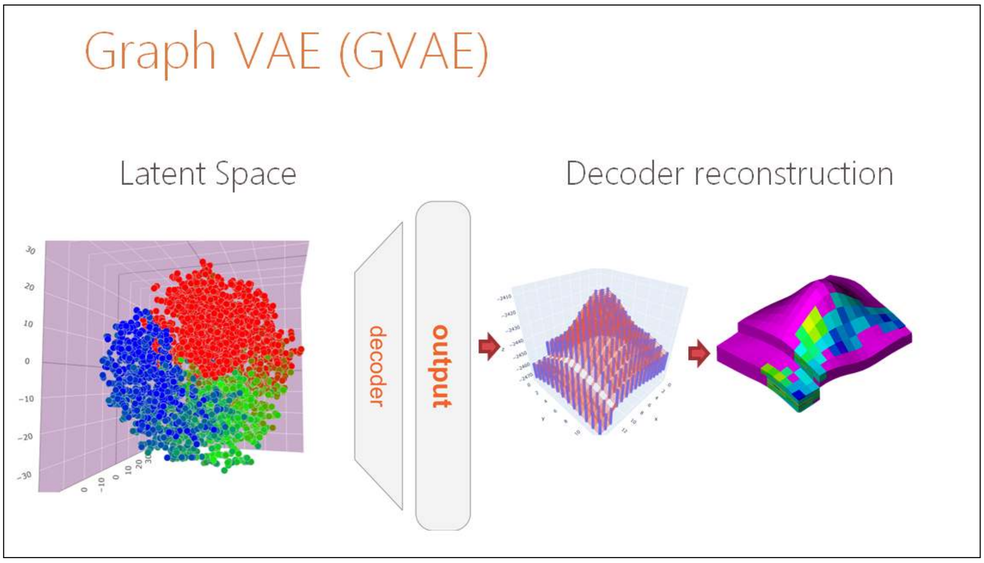
Geometric deep learning is a general term for emerging techniques attempting to generalize “regular” deep neural nets to non-regular domains, such as graphs, and perform convolutions on connected topological graph data. In general, grid-based geological models could be treated as graphs, and hence graph convolutions can be performed on it to account for non-regular geological features. Every node of a graph represents a vector of reservoir properties (e.g., porosity, permeability), while the connections between the nodes are adjusted according to the structure (e.g., faults, unconformities, etc.).

Trained GVAE can generate new geomodels through latent space representation that covers both depositional and structural uncertainties.

In the Application part we outline two experiments on synthetic channelized 3D grids:

· We show that GVAE can reliably reproduce depositional and structural settings from the latent space of decreased dimensionality

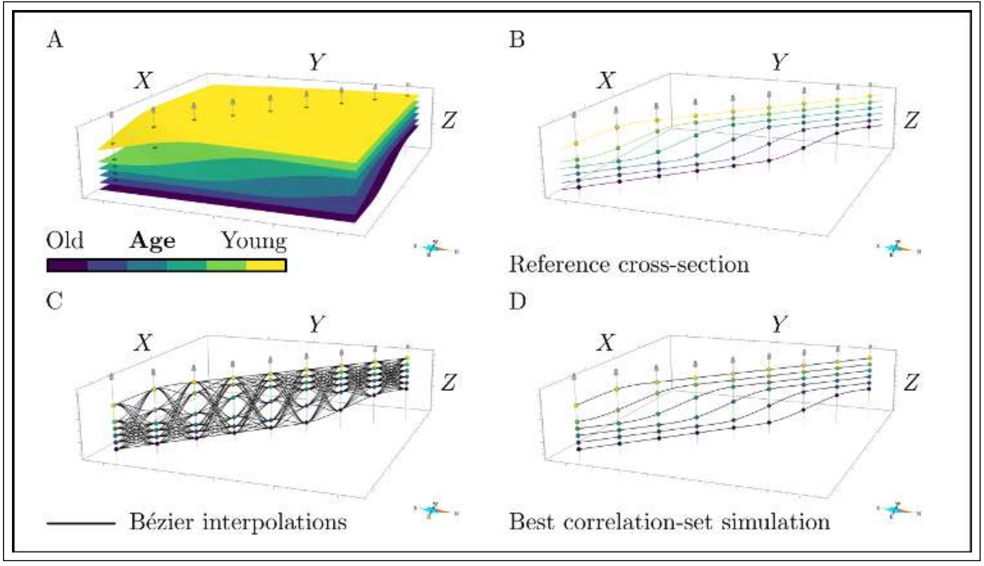
· The latent space of GVAE depicts variation of geological concepts in interpretable and controllable manner.


Graph VAE (GVAE)
Latent Space
Decoder reconstruction
decoder
output

S1811. Computer-assisted stochastic multi-well correlation: Depositional surface interpolation versus theoretical depositional profile

Paul Baville (Université de Lorraine - GeoRessources),
Marcus Apel (Equinor ASA),
Silvan Hoth (Equinor ASA),
Dirk Knaust (Equinor ASA),
Christophe Antoine (GeoRessources, Universite de Lorraine),
Cédric Carpentier (GeoRessource, Université de Lo),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS)
Room: 102 2022-09-02 15:55

Assisted well correlation aims at complementing sedimentological expertise with computational rigor to increase automation, improve reproducibility and assess uncertainties during stratigraphic correlation. In this work, a computer-assisted method is proposed to automatically generate possible well correlations based on facies interpretation, dipmeter data and prior knowledge about depositional environments. Facies interpretation and dipmeter data may be used to interpolate three-dimensional surfaces using the three-dimensional Bézier cubic curves between pairs of well markers and triangular Bézier cubic patches between triplets of well markers. These curves and surfaces are compared to a theoretical depositional profile generated from depositional environment knowledge by computing the area between the curves and the profile, or the volume between the patches and the profile. The main principle of correlation used in this method assumes that these areas and volumes may be linked to the likelihood of each possible correlation: the higher the area or the volume, the lower the correlation likelihood. Well correlations are computed using correlation costs between all possible marker combinations aggregated by the Dynamic Time Warping Algortihm. The proposed method produces consistent stratigraphic well correlation with respect to the data set. However, this approach is highly sensitive to the well order of correlation because of the Dynamic Time Warping Algortihm.



S19 Up-Scaling of Flow and Transport Models

Benoit Noetinger (IFPEN),
Marco Dentz (CSIC)

Despite the continuous improvement of the computing power, up-scaling remains a major step allowing to pass fluently from a detailed description of subsurface, to an effective flow model. Up-scaling is essential to address subsurface uncertainties and to effectively explore parameter spaces having large number of dimensions.

Up-scaling can help to understand the large-scale behavior of the system at hand and to capture the most relevant parameters. That allows building a tractable model working in a lower dimensional space of parameters. This session welcomes contribution on recent advances in up-scaling research, from stochastic to homogenization theories, from heterogeneous to fractured media, from single to multiphase flows.

S1901. Reservoir characterization by graphs.

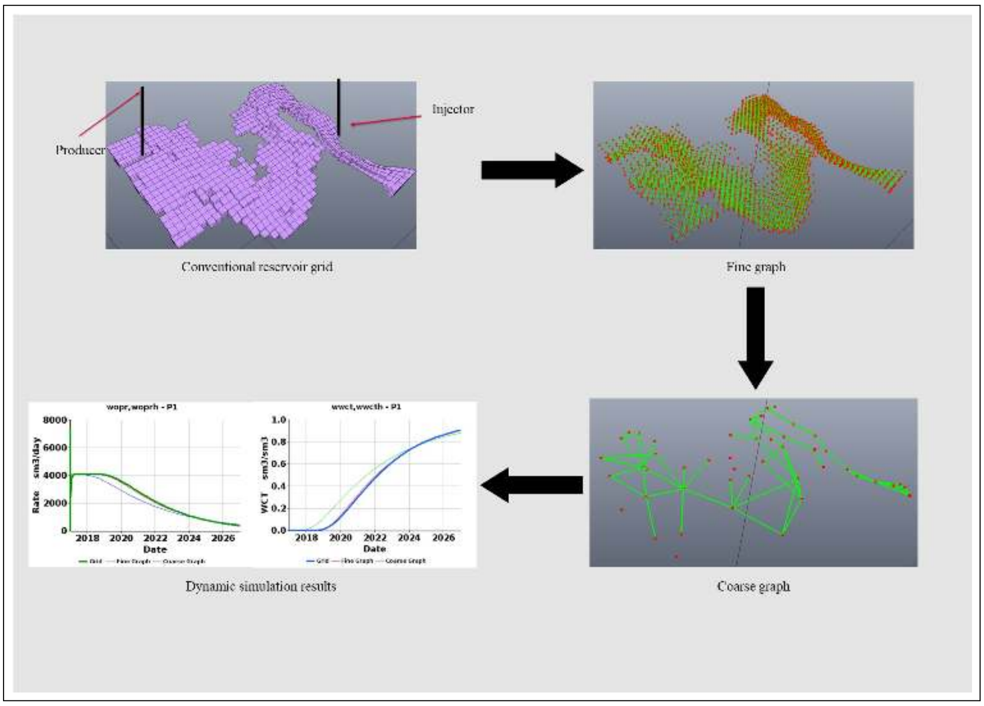
Tatiana Chugunova (TotalEnergies),
Mohammad Sajjad Moradi (TotalEnergies),
Maël Simon (EISTI, TotalEnergies)
Room: 106 2022-09-02 09:50

The reservoir model is generally defined on a structured grid where cells contain a pore volume and a hydrocarbon saturation. To predict the dynamic behavior of such reservoirs, finite volumes algorithms are generally applied. This conventional approach has its limits: the contrasted media would induce convergency problems, small and sharp heterogeneities would require the increase of the number of cells. Adding the uncertainties on static and dynamic parameters would lead to a high dimensional model, intricate to solve optimization problems.

The smarter discretization of the reservoir with an unstructured grid may improve the situation: only the zones of high impact and/or of small-scale heterogeneities are supposed to be finely discretized. It allows keeping a modeling precision with fewer cells. However, the unstructured grid is constructed before populating the heterogeneities, but the heterogeneities displace from one realization to another. Hence, the discretization is never adapted to a given realization's heterogeneity.

To push forward reservoir heterogeneities representation in an optimal way, we propose here a reservoir characterization by a graph. This approach converts a conventional realization on a grid to a graph that compresses the information where it is possible and keeps fine heterogeneities where it is needed. Such an approach optimizes the number of discreet units for dynamic modeling and provides a flexible discretization of the model which follows main heterogeneities.

In this work, we illustrate the transfer from the conventional reservoir model to the graph representation and the method of compressing the graphs based on spectral clustering. The characteristics of the graphs before and after compressing are calculated and compared. We also juxtaposed the dynamic results between grid, fine graph, and a reduced graph showing the preserving of dynamic profiles. We illustrate the results on the set of synthetic cases and the island karst caves model.



S1902. Upscaling permeability from unstructured meshes to non-matching structured grids. First results

Mustapha Zakari (CNRS-OTELO),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS)
Room: 106 2022-09-02 10:15

Numerical models are powerful tools to study aquifers and subsurface reservoirs. In these numerical models, geological grids can approximate the subsurface geometry with structured or unstructured meshes. Because structured grids lead to relatively simple and efficient algorithms, they have become the industrial standard to approximate geometries in reservoir modeling. Unstructured grids can produce more accurate geometrical approximations of complex geological features and are more flexible to mesh the simulation domain adaptively than Cartesian or corner point grids (CPG). However, explicitly accounting for fine-scale heterogeneity leads to a number of grid cells too large to be directly manageable by flow solvers. Upscaling methods were developed to coarsen geological grids in order to produce manageable grids for flow simulations. Most upscaling methods were developed for structured grids. Here we propose a new upscaling strategy to upscale unstructured grids to non matching structured grids. It combines a control volume finite element (CVFE) method to compute fine scale pressure values and an incremental mesh intersection algorithm to upscale flow information to a non matching coarser structured grid. The intersection algorithm is inspired from computational geometry algorithms. We introduce upscaling methods and present our CVFE solver and
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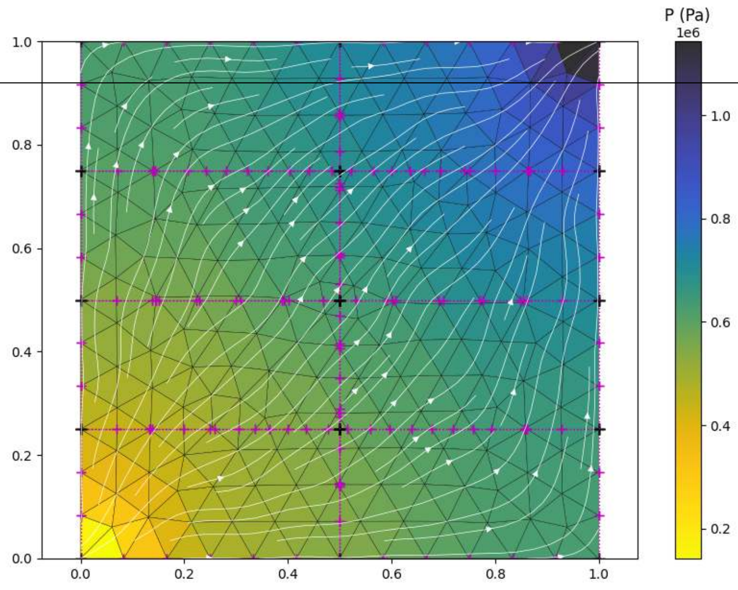


S1903. Comparison between ECPM and DFN approach for fractured media flow and transport simulation.

Quentin Courtois (Univ. Rennes, CNRS, Géosciences Rennes, UMR 6118),
Romain L.G. Le Goc (ITASCA Consultants S.A.S),
Philippe D. Davy (CNRS),
Caroline D. Darcel (ITASCA Consultants S.A.S),
Benoit P. Pinier (ITASCA Consultants S.A.S)
Room: 106 2022-09-02 10:40

Discrete fracture network (DFN) models are the most accurate representation of fractured systems and the geologic context and are capable of handling its inherently highly heterogeneous and anisotropic nature. However, they rely on significant computational resources, which limits the scale and size of the models. ECPM (Equivalent Continuous Porous Medium) methods consider the medium of interest as a continuum, allowing for fast and efficient modeling of flow and transport processes, even for fine discretization.

ECPM methods are used to evaluate the properties of fractured media by upscaling the flow properties of fractured media, based on an equivalent hydraulic conductivity tensor. The upscaling process can be performed in different ways, either analytically or numerically, with different results. Here we explore the upscaling methods and compare flow and transport simulations using both ECPM and DFN to assess the validity and accuracy of ECPM representations. We show that for coarse discretizations, ECPM is a good way to model the average behavior of fractured media but not their complete characteristics. When the discretization becomes finer and the ECPM starts to reproduce the geometry and organization of the DFN, the ECPM approach diverges from the DFN. Thus, the formulation of the ECPM for simulating flow in a fractured medium must be carefully defined based on the processes of interest, the expected results, and the amount of information available.

S1904. About non-linear diffusion in porous and fractured1 media: Early- and late-time regimes

Benoit Noetinger (IFPEN),
Noetinger Benoit (IFPEN),
Sina MOMENI (IFPEN),
Frédéric Douarche (IFPEN),
Benjamin Braconnier (IFPEN),
Michel Quintard (INPT)
Room: 106 2022-09-02 11:05

Studying non-linear diffusion phenomena in porous media is a generic problem which is often encountered in particular for applications involving displacement of non-aqueous phase liquid (NAPL) by water. In this paper, we revisit the problem by presenting two exact asymptotic solutions valid for short and long times. In the latter, a complete analytical solution is presented. In the time domain, it involves a simple Ansatz, under the form of a power law time decay of the NAPL saturation. On the spatial domain, that solution is an eigenvector of the non-linear diffusion operator driving the saturation, with Dirichlet boundary conditions. If the diffusion coefficient varies as a power law of the

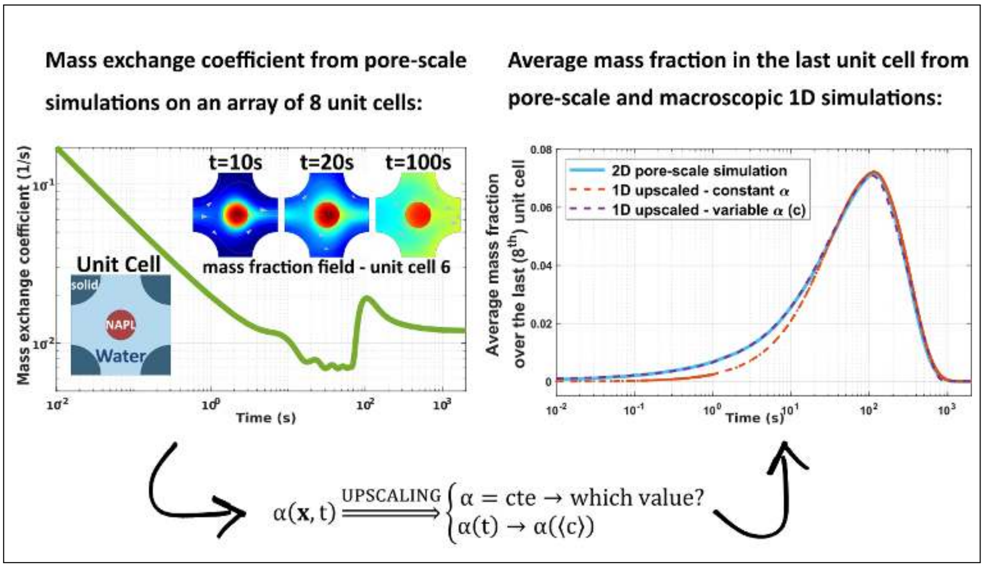
NAPL saturation, the spatial variations of the solution is given analytically. The solu tion is in very good agreement with results of numerical simulations involving various realistic sets of input transport parameters. It agrees also with previous findings of other authors based on other approximations.

S1905. Non-Aqueous Phase Liquid Dissolution in Porous Media: Upscaling the Mass Exchange Coefficient

Narges Dashtbesh (Université de Lorraine),
Fabrice Golfier (Université de Lorraine, CNRS, GeoRessources),
Anne-Julie Tinet (Université de Lorraine, CNRS, GeoRessources),
Constantin Oltean (Université de Lorraine, CNRS, GeoRessources),
Michel Quintard (INPT)
Room: 106 2022-09-02 11:30

Understanding and modelling contaminant transport is necessary to assess the lifetime of pollution sources and their severity and optimize the remediation strategies. The transfer of contaminants from the NAPL (Non-Aqueous Phase Liquid) phase to the aquifer is a multi-scale problem with different transport mechanisms within the various phases and at the interfaces. This two-phase flow problem is, in particular, driven by mass transfer between both phases, and is generally described by local non-equilibrium models. Such models at the macroscopic scale include transport equations for each phase which are coupled through one or several mass exchange coefficients. While these coefficients, which integrate the impacts of different pore-scale features (pore geometry, phase distribution, flow velocity), play a key role in the fate of the pollution source, it is usually approximated, for a given phase saturation, by a constant value estimated from empirical correlations. However, it generally shows a transient behaviour and can evolve with NAPL phase composition and relative solubilities, which remains poorly studied.

In a theoretical framework, this parameter can be estimated from the solution of boundary value closure problems on some representative unit cells using the method of volume averaging. In this work, we upscale numerically this effective property from 2D pore-scale numerical simulations. We study the impact of different factors on the form and behaviour of the mass exchange coefficient in the presence of a multi-component NAPL source depending on whether the internal mass transfer is limiting. The solubility of each component is governed by Raoult's law so that the solubilities evolve in a complex and coupled way as a function of the molar fractions of the component considered, themselves dependent on time. The potential implications of replacing this time-and-space-dependent mass transfer coefficient with a constant and unique value are discussed and regime diagrams are proposed.


Mass exchange coefficient from pore-scale simulations on an array of 8 unit cells:
Average mass fraction in the last unit cell from pore-scale and macroscopic 1D simulations:
t=10s
t=20s
t=100s
mass fraction field - unit cell 6
Unit Cell
solid
NAPL
Water
Mass exchange coefficient (1/s)
Time (s)
Average mass fraction over the last (8th) unit cell
2D pore-scale simulation
1D upscaled - constant α
1D upscaled - variable α (c)
α(x, t) UPSCALING α = cte → which value? α(t) → α(⟨c⟩)

S1906. Numerical assessment of thermo-hydraulic properties of Sphagnum moss, lichen and peat from a permafrost-dominated Arctic wetland.

Simon Cazaurang (Institut de Mécanique des Fluides de Toulouse),
Manuel Marcoux (Institut de Mecanique des Fluides de Toulouse (IMFT)),
Oleg S. Pokrovsky (Laboratoire Géosciences Environnement Toulouse),
Sergey V. Loiko (BIO-GEO-CLIM Laboratory),
Artem G. Lim (BIO-GEO-CLIM Laboratory),
Stéphane Audry (Laboratoire Géosciences Environnement Toulouse),
Liudmila S. Shirokova (Laboratoire Géosciences Environnement Toulouse),
Laurent Orgogozo (Laboratoire Géosciences Environnement Toulouse)
Room: 106 2022-09-02 11:55

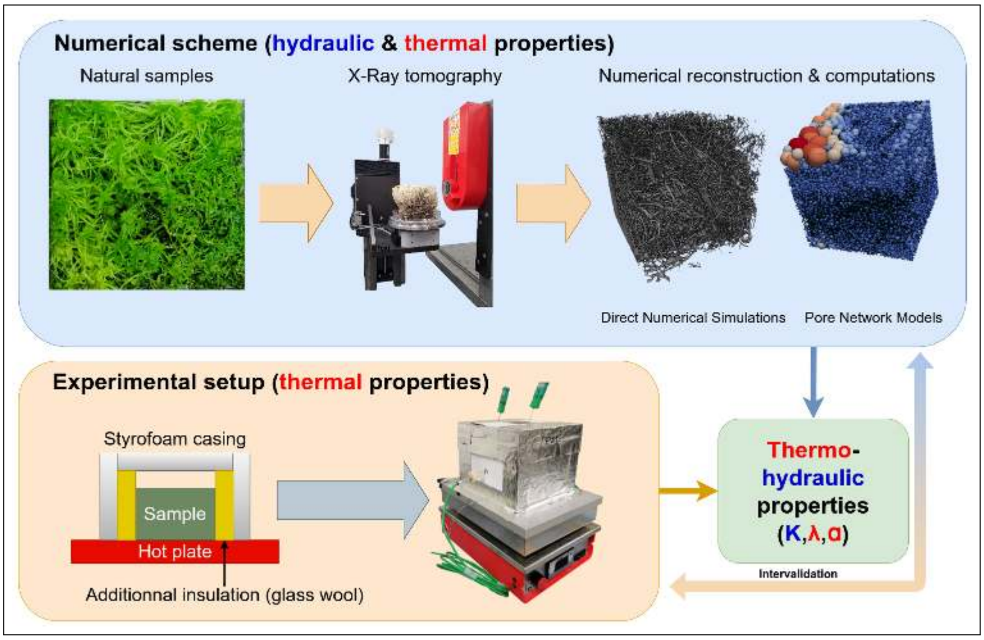
Boreal regions dynamics are strongly driven by perennially frozen soil (permafrost) physical properties. Sphagnum moss, lichen, and peat are widely present in these regions, forming a complex biological patchwork covering millions of km^2. In such regions, energy and mass transfers mainly occur via evapotranspiration, involving both vegetation's hydraulic and thermal properties.

The latest IPCC reports show that arctic regions are highly vulnerable to climate change. Therefore, a thorough study of arctic vegetation cover's thermo-hydraulic properties is needed to create a numerical model of this biological boundary layer. In this work, arctic vegetation cover is pictured as a complex fibrous porous media. Based on this assumption, some methods used for porous media properties' assessment (upscaling, representative elementary volume and homogenization) are developed hereafter.

To this end, 12 dried samples extracted from Khanymey Research Station (Western Siberian Lowlands) are studied in conjunction with their X-ray tomographical reconstructions. These samples consist of eight Sphagnum moss samples, two lichen samples and two peat samples.

First, a Representative Elementary Volume study associated with Direct Numerical Simulations is carried out to quantify porosity and hydraulic conductivity. For non-homogeneous samples, numerical simulations are made on generated pore network models. Then, thermal diffusivity and thermal conductivity are assessed using two techniques: signal and image processing results based on a modified Guarded Hot-Plate Method and direct numerical simulations associated with a pore network modeling.

Results validate the assumption to consider this vegetation cover as a porous media. Some Representative Elementary Volumes are found for most samples concerning porosity and for homogeneous samples for hydraulic conductivity. For thermal properties, ongoing studies confirm strong insulation capabilities, joining previous conclusions made in the literature. Further work will be devoted to quantify the coupling between water content and state inside these peculiar biological porous media with their hydraulic and thermal properties.


Numerical scheme (hydraulic & thermal properties)
Natural samples
X-Ray tomography
Numerical reconstruction & computations
Direct Numerical Simulations
Pore Network Models
Experimental setup (thermal properties)
Styrofoam casing
Sample
Hot plate
Additionnal insulation (glass wool)
Thermo-hydraulic properties
(K,λ,α)
Intervalidation

S20 Meshing and simulation of subsurface processes

Christian Boehm (ETH Zürich),
Tara LaForce (Sandia National Laboratories),
Jeanne Pellerin (TotalEnergies)

Nearly all fields in geoscience leverage numerical simulations to study subsurface processes, whether to infer unknown parameters, or to predict possible future evolution of a dynamical system. The widespread availability of massively parallel supercomputers enables researchers to create digital representations of the Earth with ever-increasing resolution and physical complexity.

Representing subsurface structure in those numerical models is a key ingredient that can have a significant impact on the accuracy and efficiency of the simulations. Meshing the location and geometry of material interfaces, cavities, fault lines, infrastructure, etc., can be challenging, and the complexity of mesh generation algorithms often trade-off with the efficiency and accuracy of the numerical solvers.

This session aims at discussing recent advances in (1) mesh generation algorithms and strategies to discretize complex Earth structure, (2) numerical methods to simulate subsurface processes and (3) case studies of applications in the geosciences. Examples include, but are not limited to, geodynamics, single and multi-phase geophysical flow and reservoir modeling, CO2 sequestration, nuclear waste disposal and seismic wave propagation.

S2001. Local 3D meshed geomodel updating: geometry and topology

Capucine Legentil (GeoRessources - Université de Lorraine),
Jeanne Pellerin (TotalEnergies),
Paul Cupillard (Univ. Lorraine),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS)
Room: 101 2022-08-31 15:00

In the course of subsurface modeling projects, one often needs to revise an existing interpretation, integrate new spatial data, and perturb a geomodel to reflect subsurface uncertainty and to ultimately reduce this uncertainty using inversion methods. One way to solve an inverse problem is to use physical simulations that are performed on a meshed model. The computation time and the results of the physical simulations are strongly impacted by the mesh quality and usually updating a geomodel involves rebuilding the entire mesh. In this work, we propose to address model updating challenges by exploring a mesh-based approach to modify a particular region of the model. Our approach is based on the level-set discretization method, developed by the MMG community, that generates high-quality meshes conformable to an implicit surface embedded in a 3D volume.

The input tetrahedral meshed model is conforming to geological structures. The 3D meshed model is locally updated, which means that only the mesh around the future inserted interface is modified. This interface is defined by a scalar field iso-value. A range of scalar field values determines the remeshed model subset that is modified during the interface insertion. After this first remeshing step, we introduce a buffer zone around the intersection with existing surfaces (e.g. model boundaries or geological horizons) to preserve the initial mesh quality. Unlike implicit/level-set methods, most explicit surface insertion methods require a mesh simplification step before running the physical simulation. By using an implicit definition of the surface, local modifications of the scalar fields make it possible to limit the reduction of mesh quality. The mesh quality impact is here assessed by running physical simulations with GEOSX.

S2002. Quadrangular adaptive meshing for wave simulation in homogenized media

Marius Rapenne (RING),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS),
Paul Cupillard (Univ. Lorraine),
Corentin Gouache (Caisse Central de Réassurance)
Room: 101 2022-08-31 15:25

Geological objects are complex due to their geometry and the abrupt changes in physical property which may occur between them. This complexity often makes them difficult to mesh while honoring their properties. As a result, the obtained meshes contain extremely small elements which drastically increase the computation cost of dynamic process simulations. In seismic wave simulation, a way around it is by using the homogenization method. This method allows us to compute a smooth equivalent model to the geological medium. The homogenized medium prevents meshing difficulty, allowing the use of a coarse mesh which decreases the computation cost of the simulation. In this work, we consider spectral element method (SEM) simulations. In order to take full advantage of the SEM, an adaptive quadrangular meshing algorithm which adapts to the local smooth S-wave velocity is proposed. The algorithm relies on the octree-based method introduced by Maréchal (2009). After the octree decomposition, a smoothing is applied to further optimize the size of the elements, which leads to a higher global time-step and, consequently, faster simulations. To test our method, we consider a 2D section of the homogenized SEG-EAGE overthrust model.

S2003. Application of time reversal simulation with an homogenized velocity model: Case of Groningen gas field.

Zoe Renat (GeoRessources - Université de Lorraine),
Paul Cupillard (Univ. Lorraine),
Guillaume Caumon (GeoRessources - ENSG, Universite de Lorraine, CNRS)
Room: 101 2022-08-31 15:50

It is essential to locate and characterize the earthquakes because it helps us to understand the origin of the seismicity and the risks for the population. To do so, we here consider the time reversal method. This method is based on the backpropagation of the recorded signals from a closed surface of receivers. In such an ideal setting and assuming a good velocity model, the backpropagated wavefield focuses at the source location. A good velocity model means proper wave velocity values as well as accurate positions of the discontinuities (e.g. horizons and faults). When the mirror is incomplete, such discontinuities help in improving the focalisation. However, geological discontinuities often show a complex geometry which can be challenging for meshing algorithm and lead to extremely small elements. In wave propagation simulation, such elements imply a huge computation cost. A solution to overcome this issue is to homogenize the velocity model. The principle of homogenization is to filter the small scales which lie in a model in a way that is relevant for wave propagation. The obtained model is smooth so it can be meshed with coarse elements which make the computational cost of wave simulations tractable. In this work, we present an application of time reversal in the homogenized velocity model of the Groningen gas field (Netherlands). Setting up an incomplete mirror, we show that the backpropagated wavefield focuses properly, meaning that the discontinuities are correctly taken into account in the homogenization.

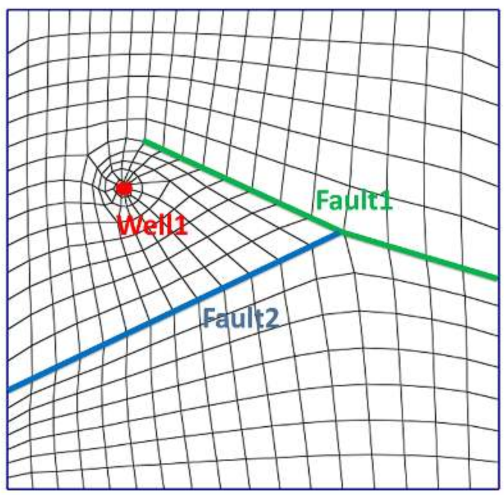
S2004. Hexahedral grid honoring complex faults and wells for coupled flow-geomechanics simulations

Wan-Chiu LI (Tessael),
Cedric Borgese (Tessael),
Alexandre Benedicto (Tessael),
Nicolas Ray (Pixel, Universite de Lorraine),
Dmitry Sokolov (Pixel, Universite de Lorraine)
Room: 101 2022-08-31 16:15

We propose a method of building full hexahedral grids that honors different prescribed geologic and geometric constraints such as complex fault networks, well trajectories and horizontal wells. Such a grid is built by extruding along the stratigraphy an unstructured quadrilateral grid constructed on the horizons of the geological model.

Our method uses a pair of parameterizations for the UV coordinates that can have local frame transformations (rotation + translation). Thus, offering additional degrees of freedom during the gridding process to honor the geometry of the faults and wells. These transformations are defined by transition functions that “glue” the local parameterizations back into a global one in a non-trivial way, called Global Parameterization. A hexahedral grid built this way might have singular vertices, which have valence not equal to eight. The grid can be considered as locally structured when there is no singular vertices in the vicinity.

We present the main steps of the grid building process and results of flow and geomechanical simulations conducted on such a grid. Then, we discuss the important advantage of this new hexahedral grid in the development of coupled flow-geomechanics simulation techniques by offering a unique support for integrated multi-physics analysis.



S2005. Optimal hybrid mesh for flow simulations

Margaux RAGUENEL (TotalEnergies),
Wan-Chiu LI (Tessael),
Cédric Borgese (Tessael),
Antoine Mazuyer (TotalEnergies)
Room: 101 2022-08-31 16:40

The development of CO2 capture and storage projects is a major challenge that we face in the coming years on the road to carbon neutrality. To tackle this challenge, the precise 3D modeling and monitoring of the physical phenomena occurring during CO2 injection and sequestration are crucial. The desire (need?) to represent several phenomena (flow, thermal effects, geomechanical effects) on the same model calls for the use of a unique mesh as a support for the multi-physical simulations. Hybrid meshes, consisting of different predefined types of cells (hexahedra, tetrahedra and pyramids), built in an optimal and adaptive way with respect to the geological constraints of the input reservoir models, appear to be a good choice in terms of flexibility and performance, compared to classic tetrahedral and structured grid solutions, to run such simulations.

In this work, we propose to build such hybrid meshes as well on synthetic cases as a real application. The global workflow used from the building of the mesh to the physical simulations is presented. We show that flow simulations of CO2 injection have been successfully conducted on the meshes and the results are detailed and discussed.

S2006. High-order homogenization for simulating local effects of small-scale structures on seismic waves

Paul Cupillard (Univ. Lorraine),
Wim Mulder (Shell Global Solutions International B. V., Delft University of Technology)
Room: 101 2022-08-31 17:05

For performance reasons, most of the seismic wave equation solvers rely on explicit time-schemes. The downside of such schemes is the CFL stability condition, which makes the global time-step proportional to the minimum local space-step. When handling small geological scales, this dramatically degrades the performance of the solvers. To circumvent this critical issue, long-wavelength equivalent media can be used. In the last fifteen years, non-periodic homogenization proved to be an efficient theory to compute such media. Zeroth-order solutions were proposed in 2D and 3D models of the subsurface such as Marmousi and the SEG-EAGE overthrust, respectively. In the present work, we consider this latter as a case-study to analyse the benefit of taking higher-order terms into account. We show that such terms are able to model local, non-propagating effects of small-scale structures on the seismic wavefield. In some contexts (e.g., ground motion simulation), the correct account of these effects is key.

S2007. Hybrid pressure approximation for coupled flow and transport in heterogeneous porous media

Jumanah Al Kubaisy (Imperial College London),
Pablo Salinas (Imperial College London),
Matthew D. Jackson (Imperial College London)
Room: 101 2022-08-31 17:07

Control volume finite element methods provide a flexible framework for modeling coupled flow and transport in complex geological subsurface models using unstructured meshes. The combination of the finite-element (FE) based flow solution with the the mass conservative, control-volume (CV) method to resolve the transport solution provides an appropriate sequential solution algorithm that addresses many simulation challenges. The FE approach discretizes the pressure and velocity degrees of freedom on the element mesh, while the transport problem is discretized on the CV dual mesh. The control volumes are node centered and span element boundaries. In the presence of sharp material interfaces, the continuous CV approach introduces numerical leakage in the transport solution. Recently, a discontinuous pressure method was implemented and shown to circumvent this issue by introducing discontinuous control volumes (Salinas et al., 2018). Despite the effectiveness of the approach in preventing numerical leakage, discontinuous approximations are computationally expensive due to the additional degrees of freedom requirement per element applied globally to the domain.

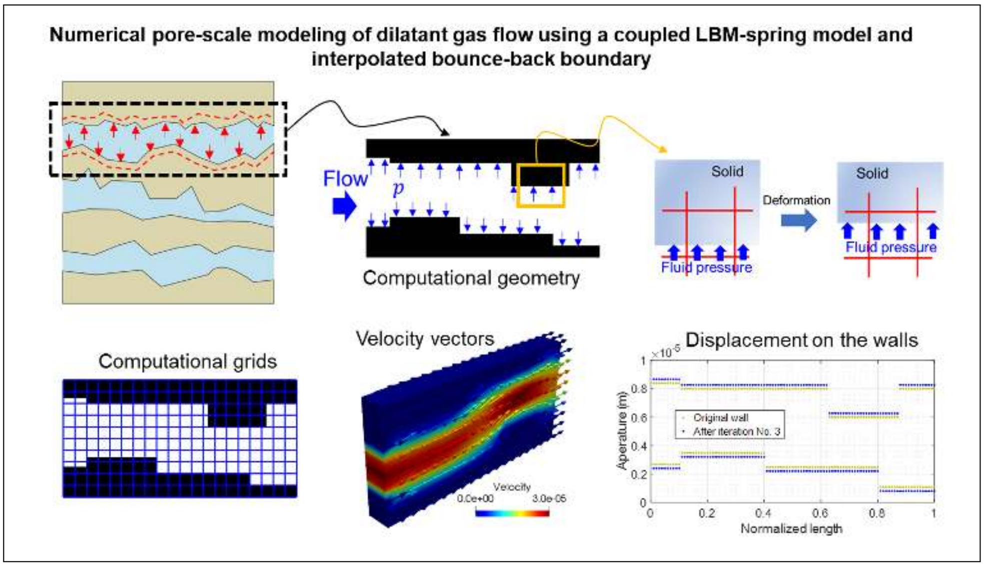
In this work, we propose a hybrid pressure formulation represented by the element pair $P0, DG - P1, H$ which denotes a constant, element-wise, discontinuous Galerkin velocity vector approximation and a hybrid (continuous/discontinuous) Galerkin first-order pressure scalar approximation of the flow solution. We exploit the efficient, continuous approach in homogeneous regions while the discontinuous approximation is applied locally along material discontinuities. This enables CVs to be continuous in smooth regions while preventing them from spanning element boundaries only at material discontinuities. Consequently, the hybrid transport solution captures the accuracy of discontinuous approximations with minimal computational cost. The hybrid formulation addresses both robustness and accuracy, challenges often encountered while modeling coupled flow and transport in highly heterogeneous porous media.

Salinas et al., J. Comp. Phys. 352, 602-614 (2018)

S2008. Numerical pore-scale modeling of dilatant gas flow using a coupled LBM-spring model and interpolated bounce-back boundary

Luyu WANG,
Anne-Julie Tinet (Université de Lorraine, CNRS, GeoRessources),
Fabrice Golfier (Université de Lorraine, CNRS, GeoRessources),
Constantin Oltean (Université de Lorraine, CNRS, GeoRessources)
Room: 101 2022-08-31 17:09

Previous studies have proven that, in geological environment, the coupled hydro-geomechanical processes have significant effects on the features of the rock matrix. In clay rocks, if the pore pressure is high enough, fluid flow at pore-scale may produce an expansion of the pore-throats. With a continuous pore pressure, the damage and degradation of the rock matrix could occur. Modelling of fluid-solid interaction at pore-scale provides a powerful tool for investigating this issue. This study focuses on the role of coupled hydro-geomechanical processes in nanoporous rock materials, and more particularly on the effect of pore pressure on deformation of the localized fractures walls. To this end, a mesoscopic model based on the multiple relaxation time Lattice Boltzmann Method (MRT-LBM) and the spring model is proposed, in which the interpolated bounce-back (IBB) boundary is applied to capture the exact displacement of the deformable pore walls with irregular shapes. First, we validate the use of IBB method on a single fracture. We propose a numerical assessment of this non-conforming method, coupling IBB and LBM model, by comparing with the reference solution obtained on the boundary-conforming grid. The impact of grid resolution on solution accuracy is discussed and comparisons for single- and two-phase flow conditions are presented. In a second step, fluid-solid interaction is considered assuming elastic behavior of pore walls. The choice of the equivalent pore pressure used in the calculation of pore walls displacement is investigated, especially in two-phase flow and application of the model to representative pore-throat geometries is presented.



S2009. Automated Meshing for Simulations of Subsurface Contaminants

Tara LaForce (Sandia National Laboratories),
William K Eymold (Sandia National Laboratories)
Room: auditorium 2022-09-01 15:00

A common issue when meshing complex geological structures is the flexing of grid cells to conform to the geological structure. As a result, the accuracy and efficiency of complex numerical simulations of subsurface fluid flow is decreased by nonuniformity in grid cell size or shape. Voronoi meshes allow for flexibility in mesh grid cell size throughout a model domain without incurring issues with non-orthogonal fluxes when grid cells are small or skewed. Voronoi meshes can be produced with VoroCrust, a meshing software which allows for fully automated creation of unstructured random meshes of complex geological systems based on water-tight interior and exterior surfaces.

We generate Voronoi simulation models clipped out of a geological framework model created using the geological mapping software RockWorks17. Tracer simulations for flow from a hypothetical nuclear waste repository due to natural subsurface fluxes are run using the finite volume multiphase flow and reactive transport simulator PFLOTRAN. Our geologic models include six layers composed of distinct limestone, sandstone, shale, and siltstone formations and the waste repository is emplaced in a shale layer. Mesh resolution varies across the 3D model space, with higher resolution cells implemented near the waste repository and coarser cells near the base of the model. We present multiple realizations of our simulations which start at the time the tracer begins to migrate and evaluate tracer concentrations at monitoring points down stream where connections to the biosphere could be possible.

Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2022-2373 A.

S2010. Evaluation of mesh quality for CO2 geological sequestration

Antoine Mazuyer (TotalEnergies),
Jeanne Pellerin (TotalEnergies),
Margaux RAGUENEL (TotalEnergies)
Room: auditorium 2022-09-01 15:25

Modeling and simulating CO2 geological sequestration is a multi-disciplinary effort involving coupled physical phenomena. In this study, we focus on a fully coupled approach involving a coupling between geomechanics flow. The fully coupled method means that both mechanical and flow simulations are solved at the same time, using the same mesh as a support. Because of the geological complexity, we use unstructured grids. They bring the flexibility to represent the geological structures such as faults and horizons. Numerical methods used to solve the problem are the Finite Element Methods for the geomechanics and the Finite Volume Method, with TPFA and hybrid schemes for the flow. To provide reliable results, there are some quality requirements for the mesh to follow as a bad quality element can make the simulation fail. Metrics are given as an input of the meshing tools. We propose to use specific metrics to generate a mesh and constrain the shape, the size ratio and the cell orientations of the mesh elements. We then explore the relationship between tetrahedron mesh quality and the results of the multiphysics simulation on a real case of a full field reservoir model.

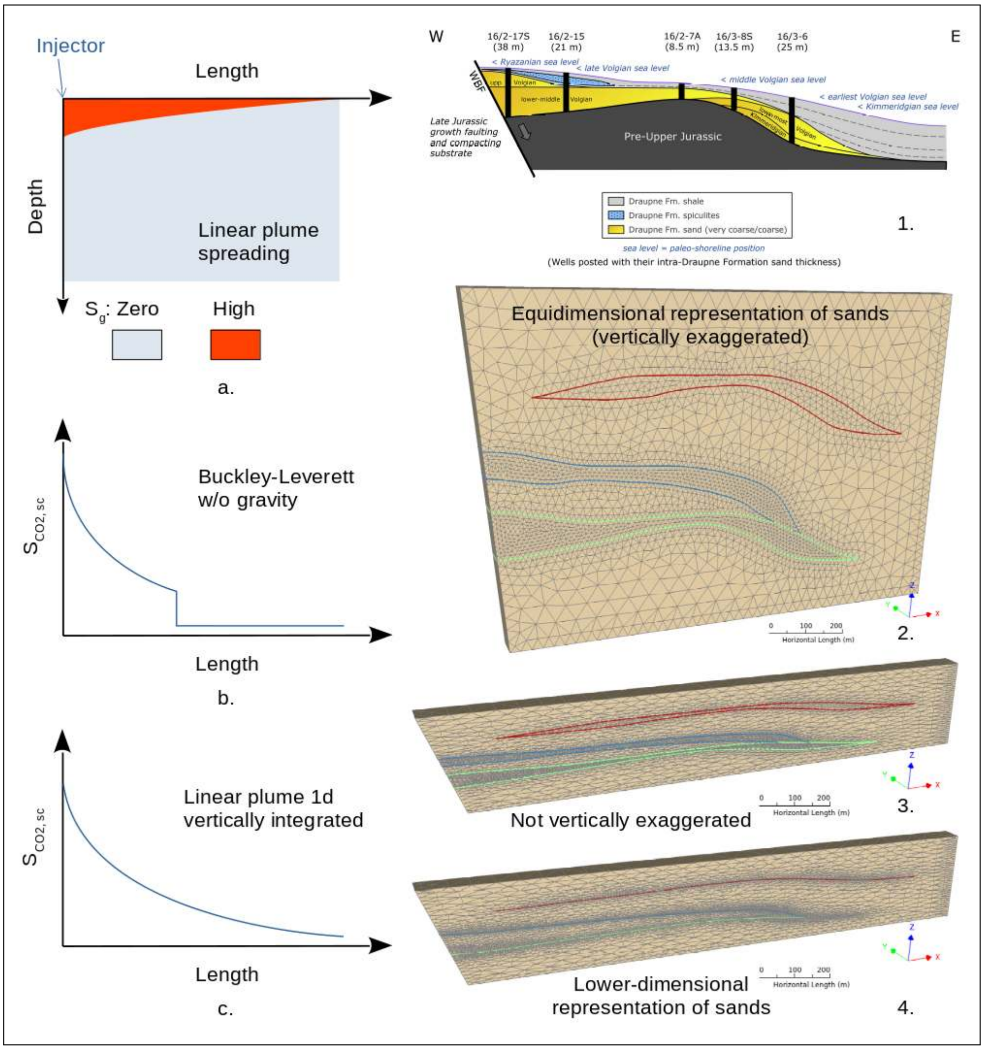
S2011. Reduced-Order Modelling of Tabular Sand Bodies for Performance Assessment Simulations of CO2 Storage Sites

Stephan Matthai (Melbourne University),
Anne-Laure Tertois (Emerson Automation Solutions)
Room: auditorium 2022-09-01 15:50

Potential CO2 storage formations often show pronounced layering: “reservoir” sandstone alternates with non-reservoir mudstones, and the thickness of individual highly permeable and porous sandstone beds is often less than a few meters, although they may be traceable for kilometres. Evidence from the field and laboratory experiments indicates that supercritical CO2, injected into such narrow sands is likely to gravitationally override formation water. This is due to the CO2‘s buoyancy and extremely low viscosity, giving rise to unstable displacement. When reservoir engineers model such narrow sand units with just a few layers of simulation grid cells, gravity override becomes impossible to resolve. Instead, their simulations will indicate more favourable “piston”-type displacement, simply because there are not enough degrees of freedom in this discretisation to resolve CO2 overriding brine. Yet, even if single-cell layers are used, models resolving individual sand units may be prohibitively detailed.

In this study we address this discretisation problem using a two-pronged approach: 1) instead of using large aspect ratio grid cells to minimise the number of cells needed to resolve the sands, we employ lower-dimensional shell elements with thickness attributes. These are allowed to intersect to capture the connections between sand units. 2) A reduced-order multiphase flow model is applied to these surface representations of the sand bodies, using an analytic gravity current model to forecast the position of the saturation front and the vertically integrated flow rate, without explicitly resolving small-scale saturation variations (Fig. 1). The rest of the simulation grid is retained volumetric.

Initial results indicate that the proposed lower-dimensional discretisation combined with reduced-order modelling, simplifies geomodelling, reduces computational cost and delivers an increased solution accuracy / appropriate flow-rate sensitivity for the drainage of the sheet sands.



Injector
Length
Depth
Linear plume spreading
S_g: Zero
High
a.
Buckley-Leverett w/o gravity
$S_{CO2, sc}$
Length
b.
Linear plume 1d vertically integrated
$S_{CO2, sc}$
Length
c.
W
E
Pre-Upper Jurassic
Draupne Fm. shale
Draupne Fm. spiculites
Draupne Fm. sand (very coarse/coarse)
(Wells posted with their intra-Draupne Formation sand thickness)
1.
Equidimensional representation of sands (vertically exaggerated)
2.
Not vertically exaggerated
3.
Lower-dimensional representation of sands
4.

S2012. Numerical modeling of gas drainage and drying in nanoporous media by SPH method

Nathan Amrofel (Université de Lorraine),
Magdalena Dymitrowska (Institut de Radioprotection et de Sûreté Nucléaire (IRSN)),
Amaël Obliger (Institut des Sciences Moléculaires (ISM)),
Anne-Julie Tinet (Université de Lorraine, CNRS, GeoRessources),
Fabrice Golfier (Université de Lorraine, CNRS, GeoRessources)
Room: auditorium 2022-09-01 16:15

A full understanding of the migration behavior of corrosion gases in clay rock is of fundamental importance for the reliability of scenarios predicting the long-term evolution of geological repositories. Due to the low permeability of host clay rock, the produced gas will accumulate as a distinct phase until the pressure becomes large enough. The high pressure generated will desaturate the surrounding clay rock by displacement of pore water far along gas paths, but also by the diffusion of water vapor through the gas.

In order to better understand the impact of key transport processes occurring in gas flow in clay material, a pore-scale numerical study taking into account the capillary-dominated two-phase flow, the diffusion of water vapor in the gas phase and specific features of nanoporous materials such as kelvin effect is proposed. The work has been carried out using the Smoothed Particle Hydrodynamics (SPH) method, a Lagrangian and meshless method which has emerged as an efficient and reliable tool for simulating complex fluid flows. A drying algorithm with Kelvin effect, which drives the thermodynamic equilibrium between the fluid phase and the gas phase at nanoscale, has been implemented in a two-phase flow SPH code, initially developed at IRSN.

A study on a 2D isolated pore will first be presented. Different flow conditions with and without capillary effect, and/or Kelvin effects will be investigated and results will be compared against analytical solutions. Then our method will be used for the simulation of drainage in a 2D pore network and compared to similar studies. We will discuss more particularly the impact of drying and kelvin effect on gas drainage patterns.

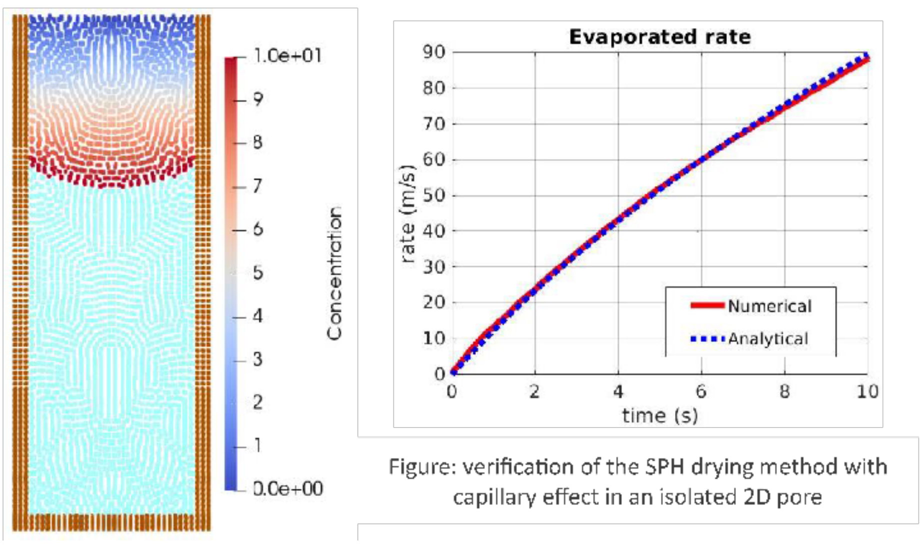


Figure: verification of the SPH drying method with capillary effect in an isolated 2D pore

S2013. A coupled numerical simulation model of heat and flow for the dynamic process of porphyry magma intruding-cooling based on phase transformation

Kaiqi Wang (Sun Yat-sen University)
Room: auditorium 2022-09-01 16:40

In recent years, many researchers have proposed that the formation of porphyry copper deposits depends on the pre-enrichment of key metals caused by the saturation of sulfide in silicate magma, and the sulfide saturation is a key step to heterogeneous melt in the middle and shallow crust. Cannibalization process of sulphide-riched domians may be related to the injection of more primitive mafic melts into crustal chamber. Such processes are found in many porphyry series, but their role in mineralization remains a mystery. Those intrusions and the release of their volatiles may trigger sudden local sulfide undesaturation in the chamber, resulting in the generation of large amounts of metal-rich, sulfur-containing volatiles and the emplacement of porphyry intrusions.

A coupled numerical simulation model of heat and flow for the dynamic process of porphyry magma intruding-cooling (degassing and crystallization separation) based on phase transformation is established. By setting the boundary conditions, initial conditions, physical parameters of intrusion-hostrock body and phase conversion relationship of the model, the finite element numerical modeling software is used to construct the numerical simulation of cooling phase separation dynamics of porphyry intrusions, and the simulation results are outputed under different initial conditions and physical parameters of geologic body.

S21 Landscape evolution models: tectonics, relief, climate

Sebastien Carretier (IRD, GET),
Jean Braun (GFZ)

Landscape evolution models simulate the dynamics of the continental surface by erosion and sedimentation on geological time scales (1ka-100Ma). The development of these models has accompanied the very significant progress in geomorphology since the 1980s. Despite the uncertainties in the erosion laws, these models provide a better understanding of the coupling between tectonic and climatic phenomena and surface processes. One of the major challenges of these models is using them in inversion procedures in order to reconstruct the evolution of topography, climate and tectonics, particularly from sedimentological data. This requires reducing their calculation time and defining the appropriate spatial and temporal scale for their parameterisation. Another challenge concerns the analysis and understanding of the internal dynamics of geomorphological systems at different scales, from that of a river to that of an alluvial plain, but accounting for all the couplings at different scales between hillslopes and rivers. The acceleration in the availability of very high resolution topographic data allows for an increasingly detailed analysis of the topography in 3D, both on the hillslopes of mountains and on alluvial plains. But these new scales of observation challenge models to develop new algorithms capable of accounting for processes at these fine scales while integrating them at the landscape scale over large time scales. Finally, there is a need to develop the modelling of submarine landform dynamics and the continent-ocean interface over long time scales, as well as wind erosion-sedimentation dynamics. This session welcomes contributions on the development of new algorithms to address these issues.

S2101. Data science for complex earth systems: A hybrid approach

Hui Tang (Deutsches GeoForschungsZentrum GFZ)
Room: 101 2022-09-01 09:50

For many challenging research problems in earth science, a purely theory-based approach will be extremely difficult since these problems are usually characterized by complex, multi-scale, and multi-physics that can only be represented partly by equation systems. Meanwhile, data science methods have been demonstrated to be effective for studying complex nonlinear systems, but they rely on large amounts of high-resolution labels for training, which are usually unavailable in the surface-process modeling community. Achieving a complete understanding of the earth system requires a synergistic combination of data-driven and physics-based models, as well as a critical need to quantify model uncertainties and understand complex system behavior. In this talk, I will highlight how physics-based and equation-based models can be combined with machine learning methods to achieve this. I will also present several examples from various earth surface processes to demonstrate the importance of embedding physical constraints within data science models and highlight the benefits of this hybrid approach to reduce training data requirements compared to other machine learning applications.

S2102. Recent advances in dune physics using a real-space cellular automaton laboratory

Clement Narteau (Institut de Physique du Globe de Paris)
Room: 101 2022-09-01 10:15

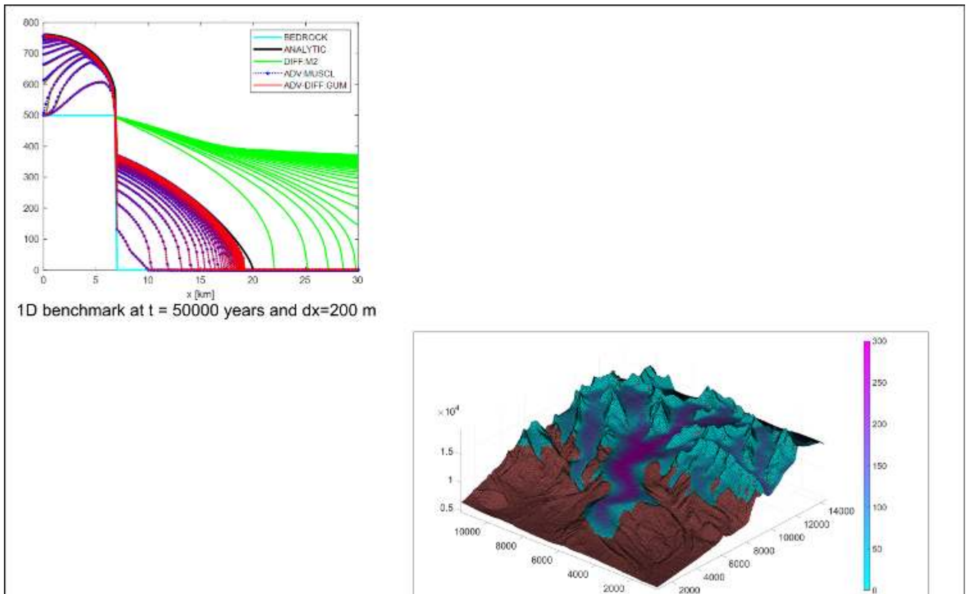
We present the Real-Space Cellular Automaton Laboratory (ReSCAL), a powerful and versatile generator of 3D stochastic models. The objective of this software suite is to investigate the dynamics of complex geophysical systems from collective behaviors emerging from short-range interactions. Models in ReSCAL are constructed from a limited number of discrete states distributed on a cellular grid. An elementary cell is a real-space representation of the physical environment and pairs of nearest-neighbor cells are called doublets. Each individual physical process is associated with a set of doublet transitions and a transition rate, which injects the relevant characteristic time scale into the model. Thanks to a modular approach, we can simulate and combine a wide range of physical processes.

We describe different ingredients of ReSCAL using the dune model. We show that, depending on the wind regime and sand availability, we can reproduce of large variety of dune patterns. As in sand seas, bedform dynamics in the model cover a wide range of length scales, from the elementary wavelength that perturbs the initial sand beds to the size of the giant dune that scales with the depth of the flow. On these giant dunes, superimposed dunes are likely to develop, favoring dune-dune interactions and the growth of a hierarchy of dune features. Most importantly, we propose also a strategy to determine the elementary length and time scales of the model from direct comparisons between the mechanisms of emergence in the simulations and in nature. Using this scaling, we show how the model can be used to provide original information about complex dune fields on Earth and other planetary bodies from a set of well-defined physical quantities. To conclude, we discuss how ReSCAL can be applied and developed across many geoscience disciplines to complement continuous numerical models and improve forecasting accuracy.

S2103. A Schaerfetter-Gummel based model for glacier modeling

Mustapha Zakari (CNRS-OTELO),
Jérôme Lavé (CRPG - Centre de Recherches Pétrographiques et Géochimiques)
Room: 101 2022-09-01 10:40

To explore paleoclimatic issues based on past glacial landforms, or to implement the role of glacier erosion in landscape evolution models, it is essential to have simplified but fast ice flow codes to be able to explore multiple scenarios of glacial advances or to follow relief evolution over millions of years. Efficient numerical models for ice-flow simulations are commonly based on the shallow ice approximation (SIA) where ice is considered as a viscous shallow fluid and where a 2D continuity equation is solved to get ice surface elevations. Most SIA models solve a non-linear diffusion formulation (including internal deformation and basal sliding) of the continuity equation which generally produces negative values and mass conservation issues in steep mountains glaciers. Recently a non-linear advection formulation was proposed with an explicit in time and MUSCL (Monotonic Upstream-centered Scheme for Conservation Laws) in space numerical scheme and with TVD (Total Variation Diminishing) tests to avoid negative values (Jarosch et al, Restoring mass conservation to shallow ice flow models over complex terrain. The Cryosphere, 2013). We have implemented this scheme and verified indeed better mass conservation, but the explicit time step limitation can become too restrictive for long time simulations. To overcome this limitation, we propose an advection diffusion formulation of the continuity equation and solve it with the Schaerfetter Gummel Method (SGM). Initially developed for drift diffusion density models arising in semi-conductor and plasma discharges modeling, SGM allows to automatically switch from a centered scheme to an upwind one by considering advection-to-diffusion ratio. We develop 1D, 2D in space with explicit, semi-implicit and implicit in time formulations for all 3 continuity equation formulations. We compare them on a 1D benchmark and on a 2D glacier. First results show a better computational efficiency (by an order of magnitude or more) for the implicit SGM.



1D benchmark at t = 50000 years and dx=200 m

Schaerfetter Gummel Method: Ice thickness (m) at t = 500 years (dx = 50 m)

S2104. Unified landslide hazard assessment using hurdle models: a case study in the Island of Dominica

Erin Bryce (University of Glasgow),
Luigi Lombardo (Department of Earth System Analysis, University of Twente),
Cees J van Westen (Department of Earth System Analysis, University of Twente),
Hakan Tanyas (Department of Earth System Analysis, University of Twente),
Daniela Castro-Camilo (University of Glasgow)
Room: 101 2022-09-01 11:05

Climatically-induced natural hazards are a threat to communities. They can cause life losses

and heavy damage to infrastructure, and due to climate change, they have become increasingly frequent. This is especially the case in tropical regions, where major hurricanes have consistently appeared in recent history. Such events induce damage due to the high wind speed they carry, and the high intensity/duration of rainfall they discharge can further induce a chain of hydro-morphological hazards in the form of widespread debris slides/flows. The way the scientific community has developed preparatory steps to mitigate the potential damage of these hydro-morphological threats includes assessing where they are likely to manifest across a given landscape. This concept is referred to as susceptibility, and it is commonly achieved by implementing binary classifiers to estimate probabilities of landslide occurrences. However,

predicting where landslides can occur may not be sufficient, for it fails to convey

how large landslides may be. This work proposes using a flexible Bernoulli-log-Gaussian hurdle model to simultaneously model landslide occurrence and size per areal unit. Covariate and spatial information are

introduced using a generalised additive modelling framework. To cope with the high spatial resolution of the data, our model uses a Markovian representation of the Matérn covariance function based on the stochastic partial differential equation (SPDE) approach. Assuming Gaussian priors, our model can be integrated into the class of latent Gaussian models, for which inference is conveniently performed based on the integrated nested Laplace approximation method. We use our modelling approach in Dominica, where hurricane Maria (September 2017) induced thousands of shallow flow-like landslides passing over the island. Our results show that we can not only estimate where landslides may occur and how large they may be, but we can also combine this information in a new unified landslide hazard model.

S2105. Inverting two-dimensional landscapes for uplift histories

Alex Lipp (Imperial College London),
Conor O'Malley (Imperial College London),
Gareth G Roberts (Imperial College London)
Room: 101 2022-09-01 11:30

Fluvial landscapes record histories of tectonic uplift modulated by erosional processes including river incision. Inverse modeling of one-dimensional river profiles for spatio-temporal uplift rate histories has been widely used to extract these tectonic signals from landscapes. However, underlying this approach is the restrictive assumption of fixed drainage planforms through time. In many circumstances such an assumption is invalid. Therefore an inverse model of landscape evolution that does not contain this restriction is desirable. Here we describe such a model, by inverting two-dimensional landscapes for spatio-temporally variable uplift. Using synthetic examples we will discuss how an appropriate choice of objective function is required to obtain a smooth, convex misfit space suitable for optimisation. Misfit spaces are investigated for a range of objective functions for relevant model parameters (uplift location, time and magnitude). Using a two-dimensional landscape evolution model based on the the widely-used stream power law we can hence recover uplift signals from synthetic landscapes. This approach provides potential for better understanding interplay between tectonics, drainage migration and erosion.

S22 Mathematical Geodynamics

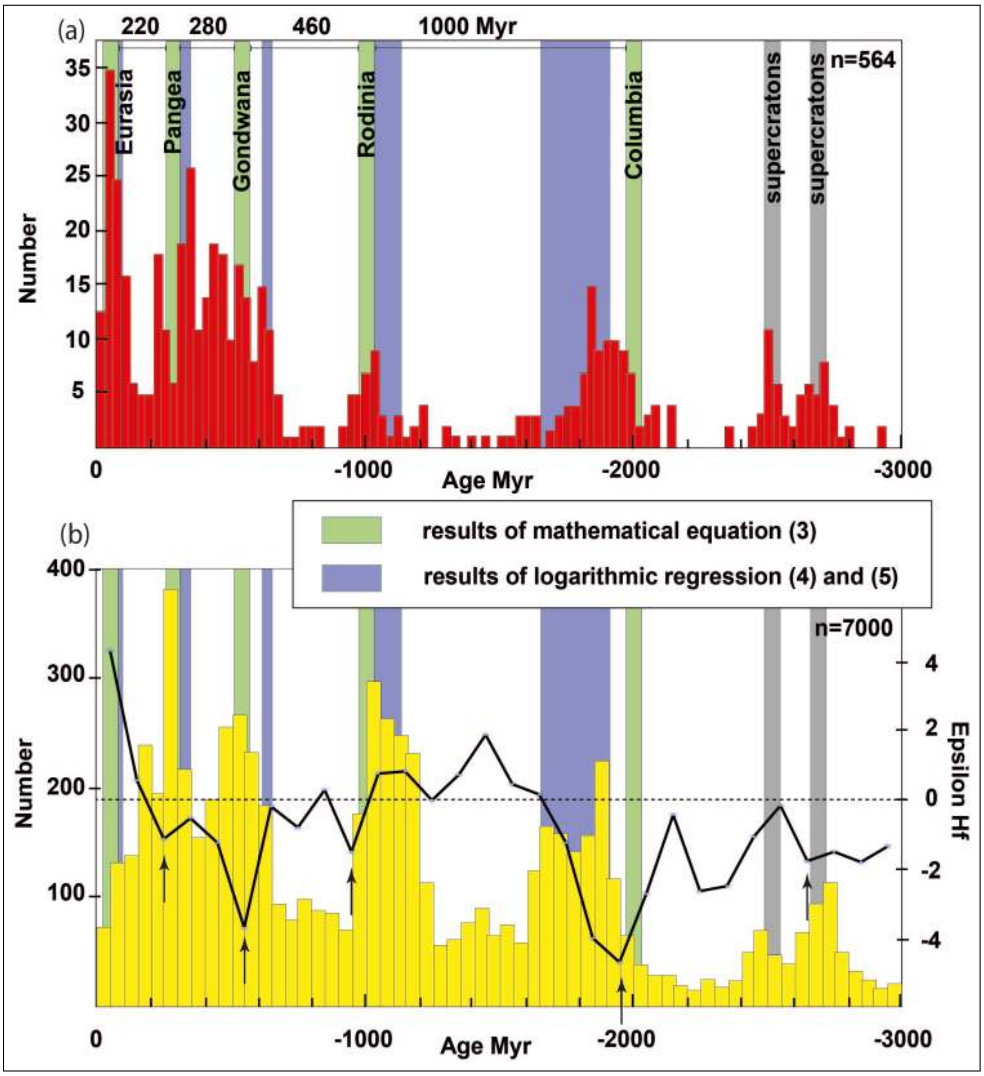
Paul Cupillard (Univ. Lorraine),
Florian Wellmann (RWTH Aachen)

This session welcomes new mathematical developments for infering large-scale features and processes.

S2201. Mathematical equation recovers acceleration of the Supercontinent cycle

Arnaud Broussolle (Chinese Academy of Geological Sciences)
Room: 102 2022-08-30 14:35

The supercontinent cycle has been the focus of researchers for many years, but the parameters of its cyclicity remain a central debate; thus, prediction of the occurrence of the next supercontinent remains elusive. In this research, a mathematical point of view is adopted, based on the assumption that the supercontinent Columbia assembled at -2,000 Myr (X(-2)) and the supercontinent Rodinia assembled at -1,000 Myr (X(-1)). The younger supercontinents are calculated following this mathematical equation: X(n)=2*X(n-1)-X(n-2)-(540/3 n), where X(n) represents the assembly and n the position of the supercontinent in the sequence. Therefore, Gondwana (X(0)) amalgamated at -540 Myr, Pangea (X(1)) at -260 Myr, Eurasia (X(2)) at -40 Myr and Pangea Proxima (X(3)) might form at +160 Myr. Moreover, two logarithmic regressions give fairly similar results, confirming that a constant acceleration of the supercontinent cycle is probable. The detrital zircon, the metamorphic and the epsilon hafnium records support the assemblies' hypotheses that produce the mathematical equation. But, a recent supercontinent or "megacontinent" called Eurasia lacks strong geological evidences in the three datasets. These findings might reconcile the paradox brought by the closer ages in time for the Earth's more recent supercontinental assemblies and the assumed constant cyclicity of the cycle.



(a)
220
280
460
1000 Myr
n=564
Eurasia
Pangea
Gondwana
Rodinia
Columbia
supercratons
supercratons
Number
Age Myr
(b)
results of mathematical equation (3)
results of logarithmic regression (4) and (5)
n=7000
Number
Epsilon Hf
Age Myr

S2202. Automatic tools for quantitative analysis of multi - scale spatial slip variabilities from DEM and DOM

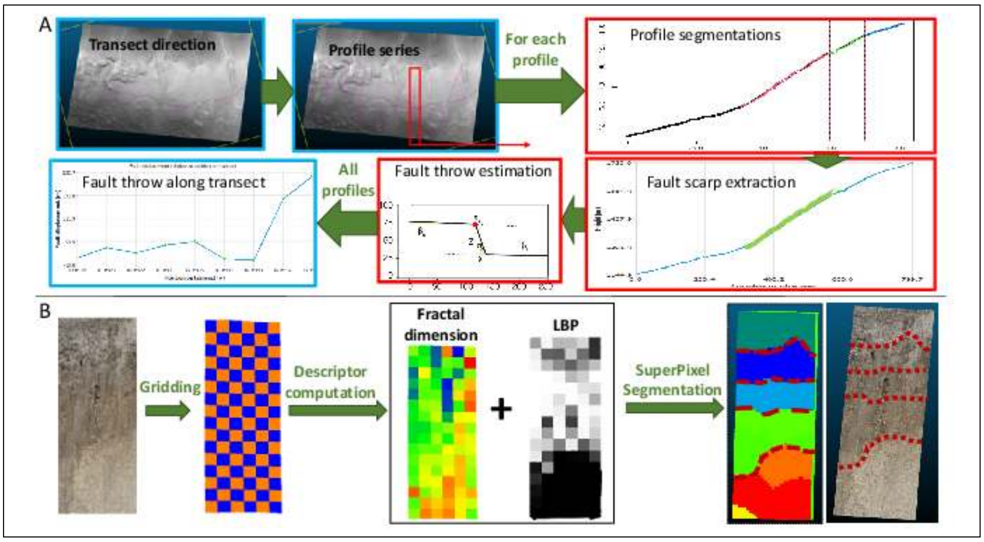
Sophie Viseur (CEREGE, Aix-Marseille Université),
T. Lamara,
G. Parel,
L Benedetti
Room: 102 2022-08-30 15:00

Quantitative geomorphology is proven very valuable to better understand the slippage of segmented faults and the earthquake occurrence cyclicity, hence to significantly improve seismic hazard anticipation. Lidar and photogrammetry are key techniques for quantitative geomorphology by providing Digital Elevation Models (DEM) at regional scales and Digital Outcrop Model (DOM) at decametre to kilometre outcrop scales

At the regional scale, topographic profiles are the common support for studying the cumulative displacement associated with successive palaeo-seismic events. Indeed, the slope changes in topographic profiles show the fault displacements. A semi-automatic approach (SPARTA) has been proposed recently to facilitate these successive computations but still requires manual steps. In this work, an automatic tool is proposed for: firstly, automatically extracting from DEM a regular series of topographic profiles along a user-defined transect; secondly, dividing each profile into successive segments depending on slope changes, extracting the fault scarps and computing the fault throw.

At the outcrop scale, a challenge is to unravel the successive portions exhumed by palaeo-seismic events using surface roughness and texture analysis along exposed fault scarps. Some authors proposed to delimit seismic events from DOMs using fractal dimension computation on surface roughness. To our knowledge, no work relies on texture changes. In computer graphics, textural descriptors such as LBP are used to exhibit texture changes in pictures. In this work, an approach combining fractal dimension and LBP descriptors is proposed to delimit palaeoearthquake events from DOMs. Compared to existing approaches, the delimitation is not simply performed on vertical profiles of descriptor averages, but directly on 2D descriptor maps using SuperPixel approaches.

Both approaches have been developed as CloudCompare plugins and applied on active faults located in the Apennines range in Italy and responsible of recent earthquakes (2016 seismic sequence). The different results are discussed and compared with previous works.


A
Transect direction
Profile series
For each profile
Profile segmentations
Fault scarp extraction
Fault throw estimation
All profiles
Fault throw along transect
B
Gridding
Descriptor computation
Fractal dimension
LBP
SuperPixel Segmentation

S2203. Absolute and relative motion of three tectonic plates assuming two fixed Euler poles: I. Rotation of plates with quaternions

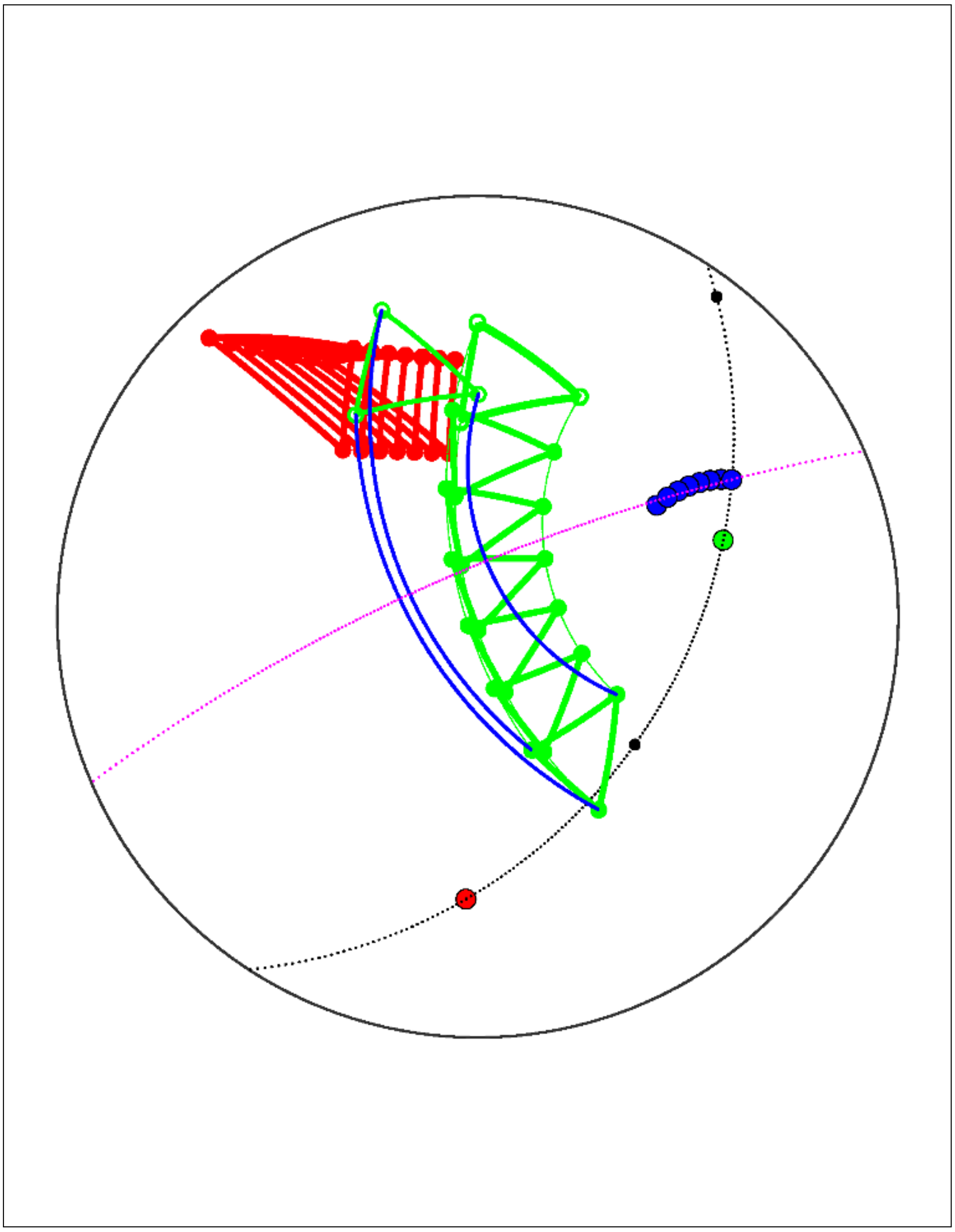
Helmut Schaeben (TU Bergakademie Freiberg),
Uwe Kroner (TU Bergakademie Freiberg),
Tobias Stephan (University of Calgary)
Room: 102 2022-08-30 15:25

In treatises on 'Plate Tectonics' infinitesimal, instantaneous or finite rotations are applied to model the absolute or relative motion of plates. Infinitesimal and finite rotations with small angles must not be confused. Infinitesimal rotations refer to a mathematical limit, when the angle of rotation tends to zero.

Concatenation of infinitesimal rotations simplifies to summation of their axes of rotation, the angle of the resulting rotation is infinitesimal. Finite rotations do not commute, no matter how small the angles are. Concatenation of two different finite rotations with different small angles of rotation generally yields a resulting rotation with an axis far off the normalized sum of the two initial axes of rotation.

Only infinitesimal rotations give rise to the geologically paradigmatic 'global plate circuit closure' stating that the axis of the rotation resulting from concatenating two different infinitesimal rotations linearly depends on the two initial axes of rotation. The 'plate circuit constraint' is a mathematical property of infinitesimal rotations, it is not a geological property of tectonic plates.

To model how the locations of plates have changed over geological times of hundreds of millions of years, successive concatenation of finite rotations applies. For two finite rotations and their concatenation the three axes of rotation are not generally linearly dependent. As will be derived applying real unit quaternions, for a set of stationary (absolute) 'Euler poles', geologists' term for axes of rotation, the resulting relative Euler poles of their successive concatenation migrate in a complex manner with time. If the angles of rotations, i.e. if the rates are equal, the resulting Euler pole migrates along a great circle. Dropping the assumption of stationary absolute Euler poles the complexity of the plates' motion increases further and requires more involved models than presented here.



S2204. Absolute and relative motion of three tectonic plates: II. Applications

Uwe Kroner (TU Bergakademie Freiberg),
Tobias Stephan (University of Calgary),
Helmut Schaeben (TU Bergakademie Freiberg)
Room: 102 2022-08-30 15:27

For the analysis of plate motions different reference systems can be applied. Absolute plate motions reflect the movement of plates with respect to a global quasi-stationary reference system. This can be either the mantle beneath the lithosphere or external extragalactic sources, i.e., quasars. In contrast, relative plate motions describe the kinematics of a pair of plates, one assumed to be moving and the other one assumed to be fixed. Then the fixed plate constitutes the reference system. Here we investigate the behavior of two moving plates with fixed rotational axes relative to a third plate representing the reference system. Our two examples are

i) the current motion of Somalia and India relative to Eurasia, and

ii) the early Paleozoic motion of the lithospheric plates of Gondwana and Laurentia relative to an arbitrarily fixed East-European plate which were modeled for the Paleozoic assembly of the supercontinent Pangea.

We visualize the migration pattern of the resultant third rotational axis of Somalia relative to India and Gondwana relative to Laurentia of example (i) and (ii) respectively. For these axes we show the complex migration pattern as theoretically derived in part I of our contribution "Absolute and relative motion of three tectonic plates". Our results underline that the migrating axis does not generally follow the great circle spanned by the two stationary Euler poles as traditionally assumed.

S23 Digital Outcrops

Pauline Collon (Université de Lorraine, CNRS, GeoRessources),
Sophie Viseur (CEREGE, Aix-Marseille Université),
Andrea Bistacchi (Università degli Studi di Milano-Bicocca)

This session is dedicated to the processing and computer-based interpretation of digital outcrop models.

S2301. A semi-automatic workflow for fracture network characterization on large Digital Outcrop Models

Stefano Casiraghi (University of Milan - Bicocca),
Andrea Bistacchi (Università degli Studi di Milano-Bicocca),
Federico Agliardi (Università degli Studi di Milano-Bicocca),
Bruno Monopoli (LTS - Land Technology & Services SRL, Treviso),
Gloria Arienti (University of Milano-Bicocca),
Giovanni Dal Piaz (LTS - Land Technology & Services SRL, Treviso),
Davide Bertolo (Regione Autonoma Valle d'Aosta),
Gabriele Benedetti (Università degli Studi di Milano-Bicocca)
Room: auditorium 2022-09-02 14:40

Characterization of fracture networks in large continuously exposed outcrops is essential for the analysis and modelling of mechanical and hydraulic properties of the rock mass (i.e. rock plus fractures). Our methodology is based on a combination of field surveys and analysis of Digital Outcrop Models (DOMs) obtained from ground-based and/or UAS photogrammetric or laser scanning surveys. Field surveys allow characterizing kinematics, relative chronology, and mineralization of fractures, that are fundamental to define their evolution and to separate fracture sets.

Whatever the survey technique was, its output is a point cloud DOM (PC-DOM), colorized with RGB values, that should have a density (points/area) sufficient to characterize the smallest relevant structural features. Additionally, a textured surface DOM (TS-DOM) can be generated.

The first step of DOM analysis is carried out "manually", selecting facets (PC-DOM) and traces (TS-DOM) with suitable software tools (e.g. Compass plugin in CloudCompare). This allows selecting different sets of structures, characterizing their orientation statistics, and assigning them to sets defined in the field (with kinematics, chronology, etc.). This step also allows understanding how well the structural features recognized in the field are represented in the DOM.

The second step of DOM analysis consists in an automatic segmentation or tracing with algorithms calibrated with results of the manual interpretation. Overall, this results in a supervised semi-automatic workflow, allowing to extract huge structural datasets in a reasonable time, maintaining the connection with kinematic and chronological observations carried out in the field.

The fracture datasets can be eventually characterized with tools allowing to estimate statistical distributions of different parameters of the fracture sets using virtual scanlines and/or scanareas, and these distributions can be used to model different properties of the fracture networks or generate stochastic DFN models.

S2302. Applying Image Analysis and Segmentation on Outcrop Data

Athanasios Nathanail (Heriot-Watt University),
Daniel Arnold (Heriot Watt University),
Vasily Demyanov (Heriot-Watt University),
Andy Gardiner (Heriot-Watt University)
Room: auditorium 2022-09-02 15:05

Our work focuses on developing Instance Segmentation and Object Detection algorithms that can assist in locating and identifying objects and features crucial to the geological interpretation of an outcrop. This is accomplished by pointing out and labeling the spots on the outcrops that provide useful clues for the depositional environment interpretation. In geology, it is important to have enough visual data of geological features/structures, as the formation of geological concepts and depositional interpretations is heavily based on the visual input. The input data used for both models are 2D images taken from outcrops. We use image analysis and segmentation to change the representation of an image into colorful segments, helping us distinguish in seconds the important parts of an outcrop, leading to a quicker formation of geological concepts and depositional environment interpretations.

Building our segmentation and object detection models requires two different Convolutional Neural Network (CNN) models. 1) Our object detection model uses an algorithm to predict the class and bounding box location of each instance in our image to locate sedimentary structures and fossils if present. 2) The instance segmentation model we developed is using bounding boxes and masks to segment layers, in order to estimate lithology and structural features. The combination of both models' results will provide us with geological observations including lithology and grain size estimation, sedimentary structures, structural features, and fossils that will lead us to form depositional environment interpretation for the examined outcrop.

S2303. Automated structural characterization and DFN modelling of a fracture network from an outcrop LiDaR dataset

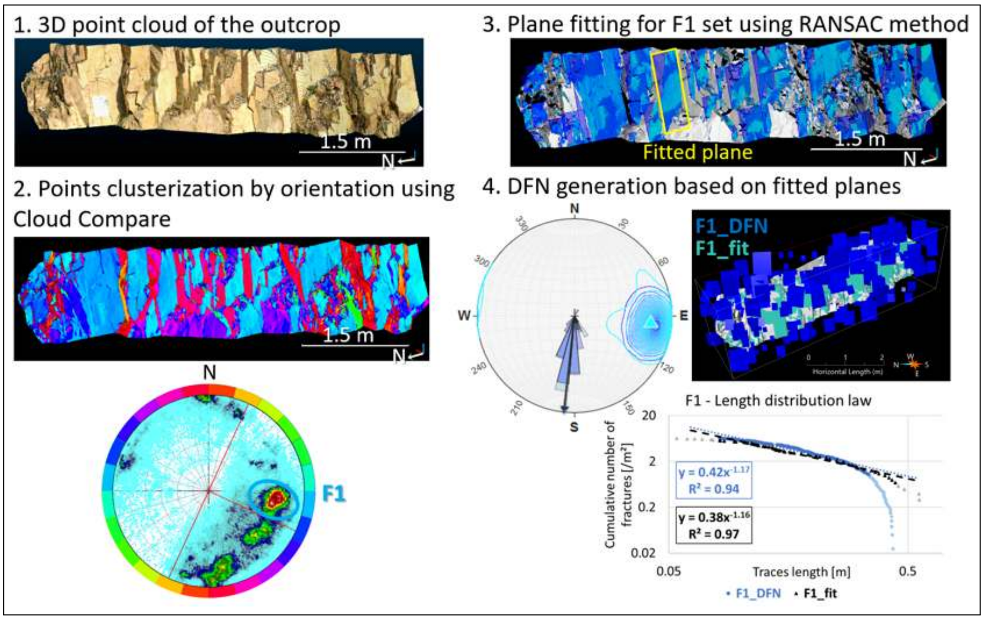
Sylvain Favier (Université de Lorraine, CNRS, CREGU, GeoRessources),
Lionel Bertrand (ENEREX Sas),
Claire Bossennec (TU Darmstadt),
Yoram Teitler (Université de Lorraine, CNRS, GeoRessources),
Julie Jeanpert (SGNC, DIMENC, New Caledonia),
Yves Géraud (GeoRessources Laboratory, University of Lorraine),
Michel Cathelineau (Université de Lorraine, CNRS, GeoRessources),
Fabrice Golfier (Université de Lorraine, CNRS, GeoRessources)
Room: auditorium 2022-09-02 15:30

Quantification of fracture network properties is crucial for many subsurface applications, from reservoir modelling to water management. The LiDAR technology offers great opportunities to provide safe access and finer description of remote outcrops with a relatively fast and efficient data acquisition. Yet, the provided datasets remain underexploited in terms of structural fracture network characterization and properties quantification.

Many automated approaches develop 2D methods to extract and characterize traces with occasional applications to 2D DFN generation. Full extension to 3D point cloud remains challenging due to difficulties in characterizing the 3D spatial and geometrical organization. To overcome such difficulties, some 3D semi-automatic workflows extract geometrical and spatial properties from map data or manually on the point cloud. However, very few of the previously published research shows a fully integrated process that includes an automated extraction of the fracture network properties and application to DFN model generation.

This study proposes a semi-automated workflow integrating both LiDAR 3D point cloud and classical structural scanline, to extract the necessary properties to build a DFN model. The workflow is fully detailed on a case study located in the Limagne Basin where a digital scanline is compared with classical scanline acquired on the field. The contribution of each method is discussed. An application to a photogrammetric dataset of an outcrop located in the Goro Mine (New Caledonia) is presented (estimated permeabilities compared to field data) to outline the potentialities for water management.

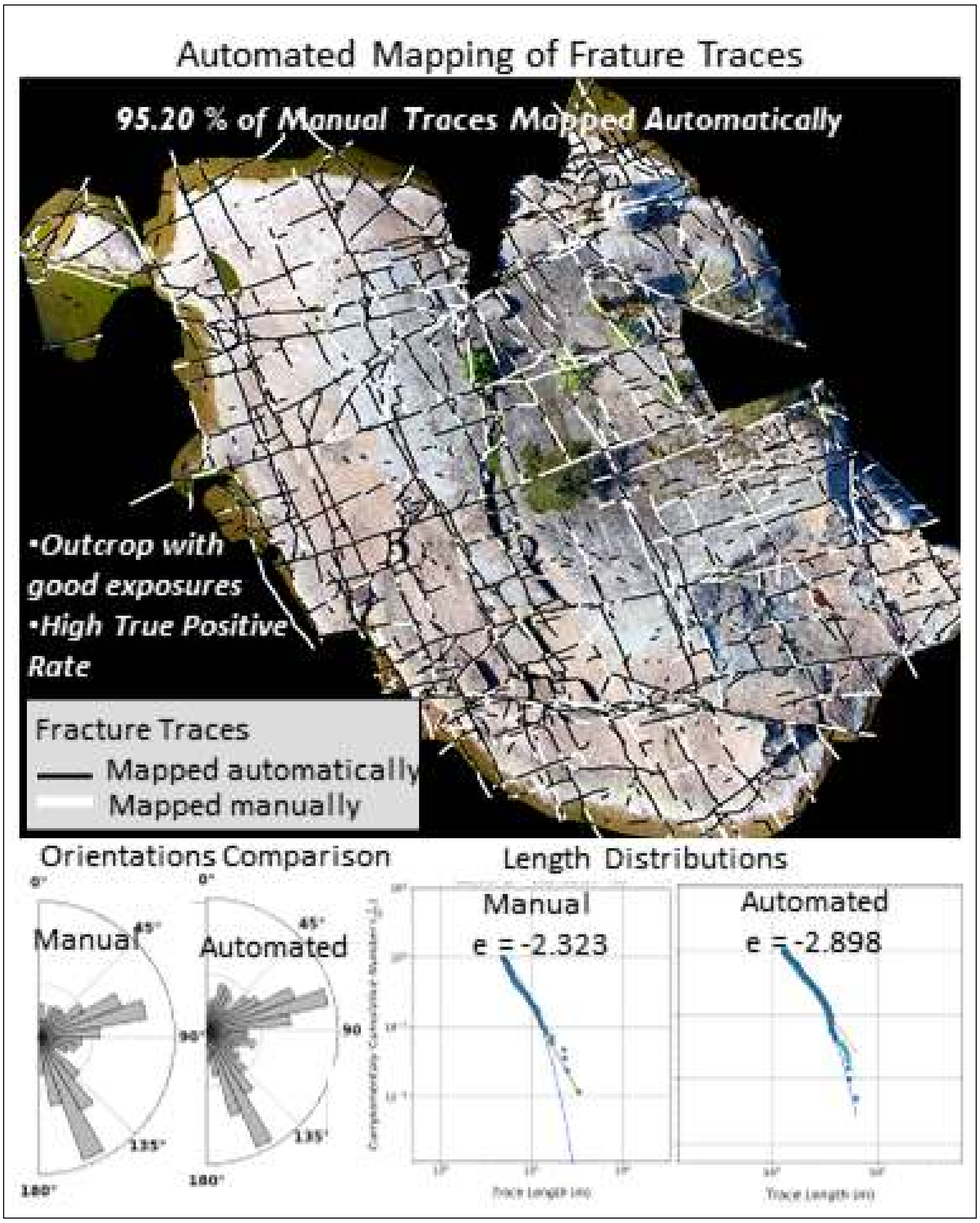
The modelled results show a good fit with the field data for the orientation distribution. However, some differences in the length distribution law coefficients are identified. They are explained by the lack of quantitative field data, and the approximations made for the fracture length on the digital scanline. Both examples highlight the great potentialities of such workflow for structural, fluid flow and transport modelling.


1. 3D point cloud of the outcrop
1.5 m
N
2. Points clusterization by orientation using Cloud Compare
1.5 m
N
F1
3. Plane fitting for F1 set using RANSAC method
Fitted plane
1.5 m
N
4. DFN generation based on fitted planes
N
W
E
S
F1_DFN
F1_fit
F1 - Length distribution law
y = 0.42x-1.17
R² = 0.94
y = 0.38x-1.16
R² = 0.97
Cumulative number of fractures [/m²]
Traces length [m]
F1_DFN
F1_fit

S2304. Convolutional neural networks for automated mapping of bedrock fracture traces from UAV-acquired images.

Bijal Chudasama (Geological Survey of Finland),
Nikolas Ovaskainen (Geological Survey of Finland),
Jonne Tamminen
Room: auditorium 2022-09-02 15:55

Deep learning methods have found applications in several fields of natural resources and geoscientific research. In this study we present the use of deep learning for automated mapping of bedrock fracture traces. A U-Net convolutional neural network was used for semantic segmentation and mapping of the fracture traces from high resolution aerial photographs acquired by unmanned aerial vehicles (UAV). This study was implemented on the islands around Loviisa in southern Finland. The spatial resolution of the aerial photographs was 6mm, hence facilitating accurate digitization of fracture traces of exposed bedrock for creation of training data. The trained model has an overall accuracy of 0.986 and the true positive rate of 70%. Islands with well-exposed bedrock surfaces show true positive rates up to 98 % (using 5 cm buffer for accuracy assessments). The fractures were also validated topologically, and the trace networks were analysed for the size-frequency and orientation distributions. The results of the automatically mapped fracture traces are comparable to the manually digitized traces. This study hence successfully demonstrates the application of modern machine learning method for fast and efficient mapping of bedrock fracture traces from UAV-acquired images that is important for mapping natural resources such as groundwater resources or hydrocarbon resources. An example of results is presented in the graphical abstract.


Automated Mapping of Frature Traces
95.20 % of Manual Traces Mapped Automatically
•Outcrop with good exposures
•High True Positive Rate
Fracture Traces
Mapped automatically
Mapped manually
Orientations Comparison
Manual
Automated
0°
45°
90°
135°
180°
Length Distributions
Manual
e = -2.323
Automated
e = -2.898

S24 Climate and Land Use

Gregoire Mariethoz (University of Lausanne),
Jerome Lave (CRPG - CNRS)

S2401. Plantations and ecosystem transition in the Santchou landscape of Cameroon: A hybrid remote sensing analysis

Jude N. Kimengsi (The University of Bamenda),
Reeves M. Fokeng (The University of Bamenda)
Room: 102 2022-09-02 11:05

Protected area landscapes continue to witness significant transition and transformation – this is driven, amongst others, by the rapid expansion of agro-plantations. While scientific and policy emphasis has significantly explored the drivers of forest landscape transition, an issue which seem to have eluded geographical literature rests, in part, on the limited geospatial evidence linked to plantations and the dynamics of forest ecosystems. To stem this knowledge gap, this paper maps the spatial extent of oil palm and cocoa cultivars in the Santchou Wildlife Reserve using high resolution Earth Observation Data. We employ high-resolution images (30cm) and Sentinel-2 MSI (10m), buttressed by Object-based Image Segmentation Classification in the spatial distinctive mapping of these crops vis-à-vis other land cover/use in the reserve. The geospatial analysis point to the fact that in the northeastern mountainous section of the reserve, the south and southwestern low-lying portion was highly encroached by these crops with dominancy of oil palm plantations. The unauthorized expansion of commercial agriculture constitutes a crucial landscape management challenge, especially of vertebrate species, most of which (e.g Dwarf Elephants). Habitat degradation and forest loss was shown to be highly driven by commercial cropping of oil palm and cocoa within the reserve. Future landscape management approaches need to strongly consider the regulation of plantation expansion, against the backdrop of rising interest to leverage ecotourism.
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S2402. Statistical Investigation of surface urban heat island inequality within a city

Bakul Budhiraja (Postdoctoral Fellow, QUB Belfast),
Jennifer McKinley (Queen's University Belfast),
Karmeshu Karmeshu (Shiv Nadar University)
Room: 102 2022-09-02 11:30

The anthropogenic climate change increases the risk and frequency of heat waves especially for cities with their increasing urban heat island (UHI) effect. The urban disparity in our cities further exacerbates the heat risk for the vulnerable population residing in the high urban density neighbourhoods. The paper aims to understand the underlying cause of surface urban heat island inequality as a result of the urban density and the lack of natural infrastructure. A case study of Delhi with its four sub-cities based on different planning designs has been performed. The surface urban heat island intensity is measured using an agricultural reference. The urban heat variation in neighbourhoods is analysed using the probability distribution of land surface temperature (LST). The MODIS LST data for a decade has been analysed using Google Earth Engine. The Kullback–Leibler divergence statistics are determined for the distance between the distribution of data. The UHI intensity difference between the sub-cities is 2 to 6.5 C. It was interesting to know that the region with highest urban density yielded the maximum value of distance measure, high UHI intensity, dense urban form Local Climate Zone (LCZ 2 or 3) and less pervious land cover. The neighbourhoods on the lowest end of urban density spectra enjoy minimum value of distance measure, low UHI intensity (0 to 2 C), open urban form (LCZ 5 or 6) and more pervious infrastructure. This is indicative of the fact the population living in high urban density neighbourhoods not only suffers from environmental heat stress but also lack of access to natural infrastructure leading to double jeopardy. Similar work is carried out in Belfast, a coastal city with Industrial past and low population density. The nature-based solutions (NBS) and policy guidelines have been suggested for the vulnerable neighbourhoods to cope with increasing risk of heat waves.

S2403. Timing of Global Change

Bjorn Birnir (University of California, Santa Barbara),
Alethea B. T. Barbaro (Delft University of Technology),
Samuel Subbey (Institute of Marine Research, Bergen)
Room: 102 2022-09-02 11:55

Because of its responsiveness to changes in the marine environment, it has been suggested by Rose in 2005 that the capelin, a small pelagic fish that is key to the ecology and fisheries of the North Atlantic, could be seen as a “canary in the coalmine” to detect signals of changes in the Arctic Ocean.

We will describe the historical data that make possible a quantitative assessment of the geographical shift capelin migration-paths and spawning grounds undergo with increasing temperature, and the time it takes to make these shifts long-lasting. Then we introduce recent data that make these quantitative measurements more accurate and predictive. The Copernicus database of the European Union is used to examine the evolution of the returning Atlantic water (from Svalbard) that is forming a warmer and saltier boundary current under the colder and fresher East Greenland polar current. The returning Atlantic water has a temperature range (-1 to 3 degrees Centigrade) suitable for feeding migrations

of the capelin. This current is reaching further north along the coast of North East Greenland and we use Copernicus to simulate this evolution. We then validate the Copernicus data with measurements made in the fall expeditions of the Marine and Freshwater Research Institute, in Iceland, along the East Coast of Greenland. We identify trends in Copernicus data showing that the returning Atlantic water boundary current may reach the major glacier streams draining a large portion of the Greenland Glacier, in the relatively near future, and use the capelin data to predict when this may happen.

Contributions by topic

NEW792.1 Statistics

S0305, S0603, S0715, S0804, S1016, S1105, S1806

M010 Two Point Geostatistics

S0901, S1002, S1011, S1015, S1017, S1018, S1506, S1606, S1704, S1705, S1809

M020 Multi Point Geostatistics

S0101, S0104, S0105, S0106, S0112, S0114, S0116, S0409, S0905, S1003, S1423

M030 Model-Based Geostatistics

S0113, S1001, S2301

M040 Point Processes

S0301, S0305, S0310, S0311, S0313, S0603, S0607, S1802

M050 Time Series Analysis

S1501, S1504

M060 Space-Time Processes

S0504, S1002, S1104, S1701, S1707, S1709

M070 Fractal and Multi-Fractal Modelling

S0005, S0805, S1009, S1423, S1615

M080 Image Analysis

S0714, S0715, S1023, S1601, S1702, S1906, S2302, S2401

M090 Stochastic Geometry and Stereology

S0313, S0606, S1008, S1105, S1602, S1803

M100 Other Spatial and Space-Time Statistical Methods

S1202, S1706, S2104

M110 Spectral and Hyperspectral Data

S0716, S1019, S1023

M120 Compositional Data Analysis

S0701, S0702, S0716, S0721, S0801, S0802, S0804, S0805, S0807, S0808, S1009, S1017, S1021, S1502

M130 Spherical Mathematics, Probablity and Statistics

S2203, S2204

M140 Multivariate Statistics

S0701, S0805, S0808, S1011, S1012, S1710

M150 Bayesian Statistics

S0314, S0402, S0406, S0716, S1104, S1418, S1602, S1604, S2104

M160 Machine Learning

S0108, S0109, S0202, S0203, S0205, S0207, S0209, S0211, S0212, S0213, S0214, S0305, S0312, S0402, S0406, S0606, S0708, S0714, S0802, S0803, S0804, S0808, S1003, S1006, S1009, S1017, S1023, S1024, S1301, S1402, S1404, S1409, S1410, S1411, S1414, S1416, S1420, S1422, S1423, S1601, S1611, S1612, S1614, S1801, S1806, S2101, S2302

M170 Optimisation and Operations Research

S0415, S0416, S0606, S0704, S1005, S1303, S1614

M190 Numerical modelling and numerical simulation

S0108, S0415, S0603, S0605, S0710, S1013, S1101, S1105, S1106, S1407, S1421, S1607, S1614, S1902, S1903, S1905, S1906, S2001, S2002, S2003, S2005, S2006, S2009, S2010, S2012, S2013, S2103

M200 Data Assimilation and data Integration

S0404, S0503, S1104, S1205, S1407, S1409, S1412, S1503, S1603, S1604, S1611

M210 Inverse Problems

S0202, S0401, S0402, S0404, S0406, S0407, S0410, S0415, S0416, S0906, S1604, S1605, S1906, S2105

M220 3D geodata and modeling of 3D objects

S0601, S1101, S1102, S1106, S1301, S1305, S1307, S1308, S1312, S1407, S1601, S1610, S1611, S2008, S2010

M230 Geographic and Geoscience Information Systems

S0803, S1201, S1204, S2008, S2402

M240 space/space-time geo-databases

S1101, S1203

M250 e-Geosciences and geoscience information exchange standards

S0110, S0501

M260 other computer sciences methods

S0108, S0110, S0502, S0712, S0802, S1005, S1304, S2102

M270 other mathematical methods

S0110, S0201, S0602, S1022, S1307, S1904, S2202

A010 Geomorphology and Quaternary geology

S0105, S0203, S0404, S0901, S2101, S2102, S2103, S2105

A020 Stratigraphy and Sedimentology

S0108, S0110, S0404, S1101, S1104, S1602, S2302

A030 Tectonics, Stress, Strain, and Fractures

S0605, S1303, S1304, S1305, S1803, S2203, S2204, S2301

A040 Petrology, Mineralogy and Crystallography

S0205, S0701, S0704, S0708, S0710, S0712, S0715, S0801, S0804, S0905, S1019, S1305, S1412

A050 Natural hazard and geological risk assessment

S0415, S0802, S0805, S1409, S1504, S2002, S2104

A060 Oil and Hydrocarbon Energy Resources

S0108, S0201, S0415, S0601, S0606, S0607, S1102, S1104, S1601, S1603, S1604, S1605, S1607, S1611, S1612, S1613, S1614, S1615, S1802, S1902, S1905, S2005, S2012

A070 Mineral Resources, Mining and Geometallurgy

S0114, S0116, S0209, S0412, S0416, S0502, S0714, S0716, S0719, S0808, S1001, S1002, S1003, S1006, S1008, S1009, S1010, S1011, S1012, S1013, S1015, S1016, S1017, S1021, S1022, S1023, S1024, S1308, S1312, S1402, S1403, S1410, S1411, S1416, S1418, S1420, S1421, S1422, S1423, S1424, S1704, S1809, S2013, S2303

A080 Soil mechanics and geotechnics

S0802, S0803, S1414, S1906, S2303

A090 Water: Sea, Surface and Subsurface

S0108, S0113, S0202, S0211, S0407, S0606, S0711, S0906, S1105, S1503, S1611, S1806, S1903, S1905, S2012, S2403

A100 Climatology, Meteorology, Cryology, Atmosphere

S1501, S1707, S1906, S2103

A120 Soil Science: pedology and edafology

S0803

A130 Geochemistry

S0205, S0701, S0702, S0713, S0721, S0805, S0807, S0808, S1009, S1204, S1423

A140 Isotope Geochemistry

S0713

A150 Chemical Analytics in the geosciences

S0314, S0702

A160 Geophysics and Geodesy

S0003, S0104, S0210, S0401, S0402, S0406, S0410, S0413, S0414, S0415, S1605

A170 Remote Sensing

S0105, S0214, S0312, S0802, S1202, S1605, S1702, S1706, S2401, S2402

A180 Geography

S0213, S1201, S2402

A190 Other topics in the geosciences

S0101, S0207, S0308, S0310, S0402, S0504, S0602, S0719, S1009, S1106, S1203, S1709, S1801, S1902, S2003, S2008, S2009, S2202, S2402

A200 Other topics outside the geosciences

S0005, S0311, S0313, S0501

A210 Geothermal engineering

S1506, S2303

A220 Hydrocarbons and CO2 sequestration

S0409, S0606, S0713, S1611, S2001, S2005, S2010, S2011, S2012

A230 Urban Geology

S0112, S1205

A240 Environmental Geo-engineering

S1104, S1610, S1701, S1806, S1905, S1906

Author Index