Article, Published Version

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# Uncertainty quantification across scales in the subsurface world

Hydrolink

# UNCERTAINTY QUANTIFICATION ACROSS SCALES IN THE SUBSURFACE WORLD

BY ALBERTO GUADAGNINI, GIOVANNI PORTA & MONICA RIVA

The research team at Politecnico di Milano (Italy) tackles conceptual, theoretical and numerical approaches to study flow, transport and chemical/biological reactions in natural subsurface porous and fractured media under uncertainty. Our approach is to recognize the importance of tracking and quantifying the impact of uncertainty across scales to ultimately identify uncertainty controls to constrain predictions. This article discusses some key aspects of our research approach and vision on current challenges associated with groundwater quality and quantity.

The Earth's subsurface hosts key resources for the development of society. Aquifers provide invaluable freshwater reserves across several regions worldwide, water demand being largely satisfied by renewable or non-renewable resources hosted by subsurface reservoirs. Similar to all natural systems, geological media exhibit an intrinsic variability of properties, which is the result of a variety of processes that have shaped their formation and current internal make-up. Sedimentary systems, for instance, are the result of the sedimentation of various materials deposited over millions of years. The properties of such geological bodies display remarkable variability across a variety of (space and/or time) scales, associated with physical, chemical or biological heterogeneities (see Figure 1).

Proper and sustainable management of these systems in the complex and ever changing modern environment requires solid scientific understanding and handling of uncertainty to address system functioning and feedbacks amongst its multiple components. Acquiring this knowledge often benefits from comprehensive and scientifically sound conceptual and theoretical frameworks, which are then translated in mathematical and numerical models. The need for modeling is especially compelling when dealing with the Earth's subsurface because of limited direct access to it. Therefore, efforts aimed at managing subsurface resources ubiquitously rely on a (model or) representation of reality. The hydraulic conductivity, a key parameter for the characterization of subsurface materials, is arguably the most heterogeneous parameter in Earth sciences, with laboratory data spanning more than ten orders of magnitude. Paucity of observations and the documented marked spatial heterogeneity in the properties of natural subsurface systems require devising strategies and tools that take into account uncertainty in management and engineering studies and decisions. In this context, stochastic approaches have been developed, motivated by recognizing both the importance of spatial variability and the impossibility of describing in an exhaustive manner the spatial distribution of variables of interest. As such, a non-deterministic framework of analysis is required. In the following we briefly review some of the main elements that we faced in our research concerning the characterization of subsurface systems under uncertainty.

Our research group is based in the Metropolitan area of Milano (Italy), residing in the Po river Valley where the vast majority of drinking water supply is associated with groundwater resources. Yet, the quality and the quantity of this invaluable resource are threatened by anthropogenic activities, including pollution resulting from industrial or agriculture activities, as well as by geogenic sources of hazardous substances (e.g., arsenic or chromium [1], [2]). Improved scientific understanding of the flow and transport processes and accounting for the uncertainty in the description of the system may be the only realistic approach to handling (qualitatively and quantitatively) integrated hydrological problems with sparse data. Original results in this sense have been recently attained through scientific outputs of the project

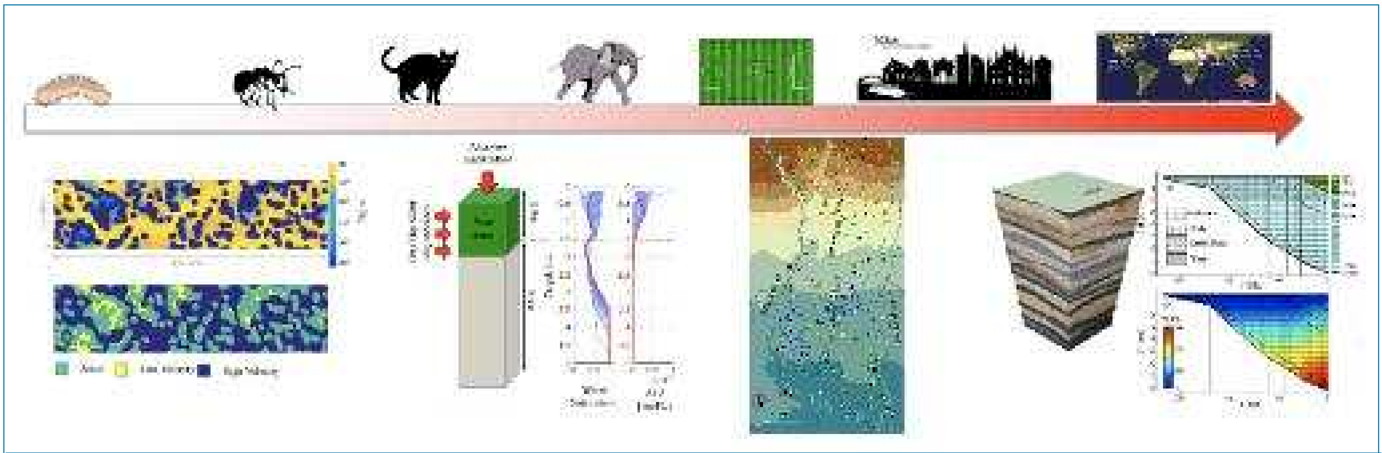


Figure 1. Flow and transport processes in subsurface porous media across scales (images modified from [7], [5], [4], [11])

WE-NEED (Water Needs, Availability, Quality and Sustainability; http://www.we-need.polimi.it [3]), funded by the European Union and the Italian Ministry for Education, University and Research under the 2015 Joint Activities developed by the Water Challenges for a Changing World Joint Programme Initiative (Water JPI). This major project was recently completed under the coordination of Prof. M. Riva and with participation of international partners from Israel (Weizmann Institute of Science), Portugal (University of Aveiro), and Spain (Polytechnical University of Catalunya). A significant challenge underpinning the set-up of a model of an aquifer system is how to address optimal data acquisition, system monitoring, and use of the ensuing information content. This important issue is addressed in detail by WE-NEED upon considering two major aquifer systems in Italy, associated with the areas of Bologna and Cremona, respectively. While the former is a key source of water for the metropolitan area of Bologna (the lower aquifer provides 80% of all groundwater used for drinking and industrial purposes), the strategic importance of the latter is related to the presence of a high number of natural high-quality water springs constituting the main supply to agriculture and key environmental drivers, with significant social, historical and touristic value. As an example, Figure 2 depicts the location of the study area and some aspects of the available dataset, which constitutes a unique source of information for the characterization of the system functioning. These data have enabled us to assess the effect on groundwater flow simulations of alternative conceptual models used to represent the spatial arrangement of geomaterials characterizing the internal architecture of the aquifer [4], a result which constitutes one of the major outputs of WE-NEED and is available to local water companies.

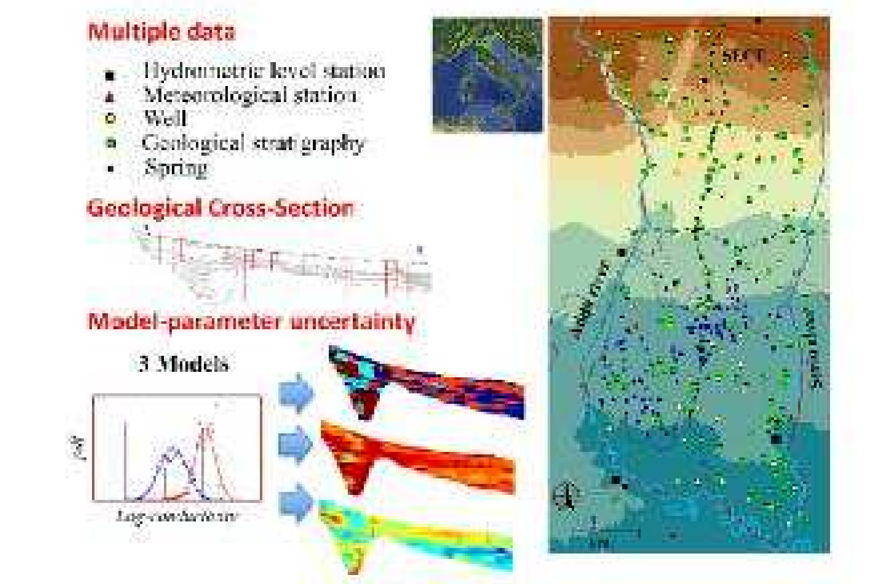



Figure 2. Integration of multiple sources of information and modeling approaches for field scale numerical simulation of groundwater flow in the Cremona area (Italy) (modified from [4])

Assessing quality of groundwater resources requires joint analysis of fluid flow and transport of chemicals dissolved in the water phase. The complexity of the problem is exacerbated by the observation that chemically- and biologically-driven reactive processes typically affect transport in subsurface environments due to a variety of processes, including, e.g., mineral-water interactions or processes such as sorption-desorption or microbial activity. As the ability to fully describe these processes in the natural environment is still very limited, there is a need for approaches that can assist to improve the understanding of system behavior and quantify the implications of the uncertainty associated with model structure and the ensuing parameters. Some of our recent work shows that relying on appropriate sensitivity analysis tools is critical to enhance the knowledge of these complex processes. As an example, the geochemical response of groundwater to environmental factors, such as temperature or redox conditions, may display a strongly nonlinear behavior (see Figure 3). In such cases the sensitivity of the model can be only measured by combining local sensitivity analysis (that can detect local nonlinearities) with global sensitivity analysis approaches (enabling us to measure the overall impact of uncertain model parameters on key statistics of modeling goals). When considering a simplified geochemical model of hexavalent chromium (Cr(IV)) geogenic release [2], we show that combining various techniques is key to obtain a proper assessment of parameter uncertainty and the way it propagates to modeling targets as well as to identify which model inputs should be further subject to improved observation to enhance the ability to meet given modeling goals.

An increase of the complexity of the modeled processes may yield more pronounced

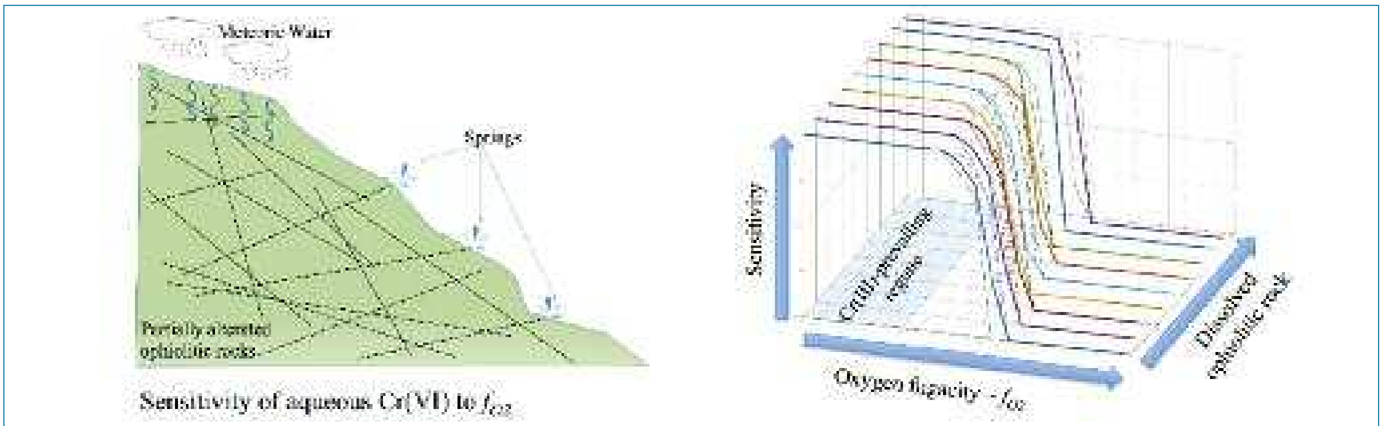



Figure 3. Groundwater quality under uncertain environmental conditions: conceptual and geochemical modeling of hexavalent chromium (Cr(VI)) at hillslope scale. Sensitivity of Cr(VI) to oxygen fugacity exhibits highly nonlinear patterns (modified from [2])

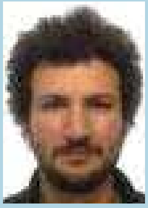
couplings and nonlinearities, as suggested by our recent analysis of atrazine biodegradation in agricultural soils [5]. This issue was considered through the implementation of a coupled reaction network of biogeochemical processes, including aerobic and anaerobic processes activated by various functional microbial groups. The model requires specifying 74 biochemical parameters to describe the kinetic response of the system. The results show that uncertainty propagation across these processes taking place in natural soils and under transient conditions yields multimodal distributions for prescribed modeling goals. This implies that diverse and mutually exclusive final system states are likely to occur. Available prior information may not be strongly informative to allow discriminating amongst such states. In this context, sensitivity analysis tools such as those developed in [6] can be used to improve process understanding through model diagnosis, as well as guide environmental monitoring investments, enabling one to prioritize the acquisition of data that can potentially assist to identify parameters that are actually informative on the system response.

While characterizing state-of-the-art models under uncertainty is of utmost importance, existing models and tools need to be improved to resolve the limitations that hamper state-of-the-art modeling strategies. A key research question in this context concerns the ability to transfer information and uncertainties across scales. Even seemingly homogeneous porous media may display a relatively complex geometry and structure at the microscale. This implies, for instance, that fluid velocity at the scale of the pore space is characterized by relevant spatial variability, with spatial distributions entailing preferential flow regions (fast channels) and stagnant areas. These features are well known and explored in the recent literature which documents pore-scale data sets and modeling efforts. In this context, there is still the need for approaches that are capable to transfer such richness of pore-scale information to larger scales, where it could be used to strengthen the interpretation of laboratory or field scale observations. Local fluctuations and gradients, due to pore-scale features such as channeling or segregated stagnant regions [7], [8], may heavily impact nonlinear reaction rates. In general, these features may be critically important for the parameterization of processes that take place unevenly in space (e.g., surface reactions such as adsorption-desorption). Our work in this context provides original operational frameworks and quantitative tools to transfer and upscale available information.
With reference to scaling aspects, our research team has developed and applied a theoretical framework and model enabling us to transfer information on statistics of system parameters across diverse spatial scales in real scenarios, and to quantify the way they impact the statistics of the system states (e.g., fluxes and concentrations).

Relying on the mounting evidence that many spatially varying quantities exhibit non-Gaussian behavior over a multiplicity of scales, we have developed a theoretical model that captures documented scalable non-Gaussian geostatistics of Earth and environmental variables [9], [10]. Such a model allows blending observations of hydraulic parameter distributions into a new framework and is adaptable to diverse spatial/temporal scales. In this context, a key innovative aspect is the development of methodologies and algorithms to generate random fields, exploiting available data to be employed in computational analyses of groundwater flow and transport, with the aim of quantifying risk in realistic (non-Gaussian) environments.

In summary, the core activity of the team is focused on a variety of scientific/application-oriented objectives with the aim of providing quantitative understanding and process-based models of hydrogeological systems and the geochemical behavior of reactive chemical species in environmentally and industrially relevant subsurface settings under model and parametric uncertainty. Our studies aim at identifying and developing methods to incorporate uncertainty quantification and its propagation across observation scales, as grounded on direct observations at diverse scales of interest. The research emphasizes the consequences of human actions on groundwater resources by coupling field and laboratory evidence with original theoretical and modeling concepts. This can support the evaluation of the sustainability of current and future plans for aquifer development with the aim of providing an effective governance perspective while maximizing ecosystem preservation. ■

**Alberto Guadagnini** is Professor of Hydraulic Engineering and Head of the Department of Civil and Environmental Engineering at Politecnico di Milano (Italy). Chair of the Communication Committee of the International Society for Porous Media (Interpore). Vice Chair of the Committee on Groundwater Hydraulics and Management (IAHR). Executive Editor of Hydrology and Earth System Sciences. Main research interests include statistical scaling of hydrological quantities, stochastic groundwater hydrology, multiscale flow and transport in porous media, multiphase flows, enhanced oil recovery and environmental footprint of shale gas development.



**Giovanni Porta** is currently associate professor at Politecnico di Milano (Italy). The core of his recent and ongoing research is focused on developing models and methods to improve the current understanding of reactive transport processes in porous media. Target applications span across a wide range of disciplines, processes and scales from micron/seconds scales to geological settings involving km-scale domains evolving across millions of years. He is 2019 Junior Marchi Lecturer (award by the Italian Hydraulic Engineering Society (GII)).

**Monica Riva** is Professor of Groundwater and Fluid Mechanics at Politecnico di Milano (Italy). She has managed several research projects focusing on groundwater resources and stochastic approaches. She is currently the coordinator of the Water JPI project WE-NEED. Chair of the EGU Groundwater Division and Vice-chair of the Interpore Council (International Society for Porous Media). Her key areas of expertise include data assimilation, stochastic inverse modeling, uncertainty quantification, and multiphase flows.

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