SIMUPOR

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SIMULATION OF MICROSCALE BIOGEOCHEMICAL PROCESSES IN POROUS MEDIA USING ADVANCED COMPUTER VISION METHODOLOGIES

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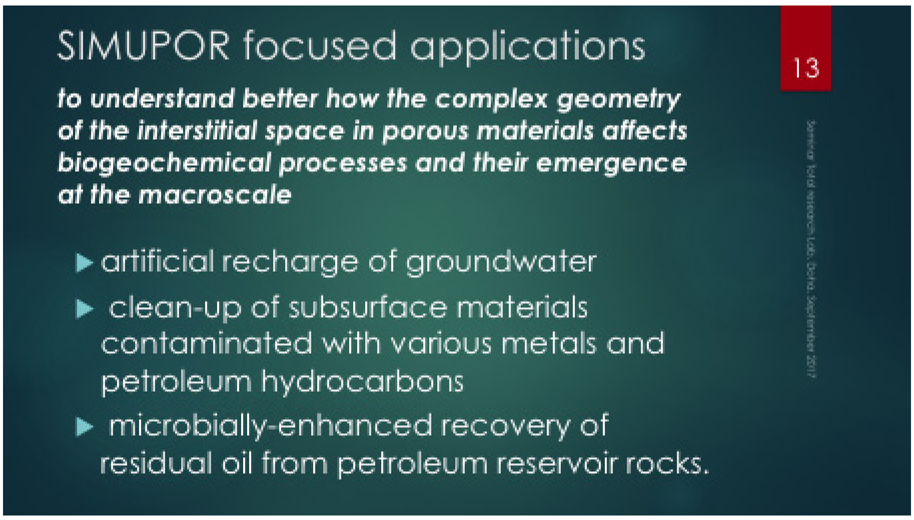
CONTEXT AND OBJECTIVE

Researchers in several institutions are currently attempting to understand how the microscale heterogeneity of soils influences the activity of microorganisms and the fate of organic matter, whose mineralization could have a significant effect on climate change. In Qatar, similar preoccupations arise about the microscale heterogeneity of porous media, but for reasons that are very different. Indeed, here, the need to understand better how the complex geometry of the interstitial space in porous materials affects biogeochemical processes and their emergence at the macroscale is especially important in relation to the artificial recharge of groundwater, to the clean-up of subsurface materials contaminated with various metals and petroleum hydrocarbons, and to the microbially-enhanced recovery of residual oil from petroleum reservoir rocks.

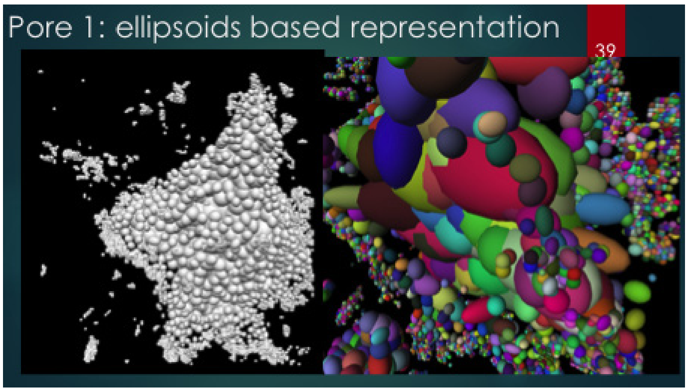
Progress in this general area has been significant over the last 5 years, in large part due to remarkable technological advances in X-ray scanners, improvements in the mathematical description of porous media, as well as the prediction of microbial processes. Nevertheless, many questions still remain unanswered, and various practical limitations have to be overcome. In particular, both the computer vision tools that are currently available, and the techniques used to simulate biogeochemical processes in porous media need to be far more computationally efficient than they are at the moment, to enable us to handle samples of porous media that are of sufficient size to be representative of the systems from which they emanate. In addition, methods need to be developed to upscale process descriptions from the level of small samples to that of entire porous formations and reservoir rocks, so that, eventually, useful predictive tools can be made available to stakeholders.

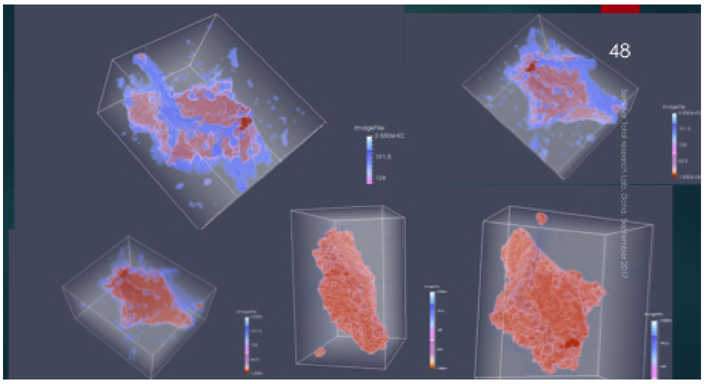
In that general context, the objective of the proposed research is to cause a quantum leap forward in the geometric description and modeling of porous media, to enable researchers to simulate efficiently the various biogeochemical processes involved in groundwater recharge, aquifer decontamination, and microbially-enhanced oil recovery. A second objective of the research is to devise ways to speed computations significantly, to make it feasible to upscale modeling efforts from the microscale to spatial scales of practical interest in Qatar.
Earth monitoring project develop.

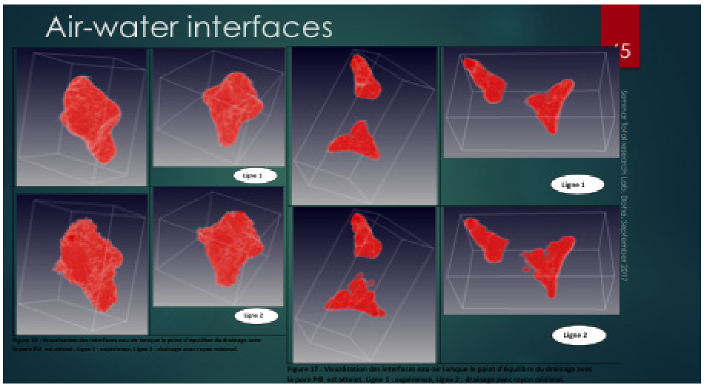


ACTIVITIES

A first step toward these objectives will consist of setting up a number of small laboratory microcosms, using natural porous media from representative areas of the country, and replicating conditions relevant to the three different targeted contexts. Before they get inoculated with microorganisms and injected with contaminants or oil, and experiments are initiated, these microcosms will be imaged via micro-X-ray computed tomography (µCT), to obtain high-resolution images of the solid phase. While these microcosms are being set up and scanned, work will be devoted to the elaboration of a new strategy, based on previous research by one of the project PIs on genetic algorithms, to segment the 3-dimensional grey scale µCT images, i.e., to to transform them into binary, black-and-white representations, which will be needed later to simulate biogeochemical processes. Two algorithms have been developed in the last few years to achieve this without the need for operator intervention, but improvements are still desirable in terms of both efficiency and speed. In the next stage of the research, a 3D shape modelling method, designed to simplify the description of the pore geometry in porous media, will be extended greatly to take into account more complex geometric primitives than the simple spheres that it can handle at the moment. Specifically, ellipsoids and super ellipsoids will be implemented, with the result that computations will be much faster. At the same time, we shall research various options to also speed up another computational approach used to model dynamical processes in porous media, the Lattice-Boltzmann method, which several of us have already used extensively in previous projects, in part as a reality check for the simulations based on geometrical primitives. At present, LB schemes can handle only small 3D images. It is crucial to speed computations up and enable them to deal with larger spatial domains. This will be achieved by parallelizing our LB code to allow it to run on a cluster of Graphic Processing Units







(GPU), and by using advanced domain decomposition techniques that have been proposed recently. With these drastically improved computational tools, we shall simulate the outcomes of the different microcosm experiments, and assess how closely the simulation results are to experimental observations, as well as where further research is needed.

An important component of the research will consist in analyzing in detail different avenues by which the descriptions obtained with the computer models can be scaled up from the microscopic level to the macroscopic scale, suitable for the development of practical strategies that stakeholders will be able to implement. To that end, we shall simulate multiple scenarios, involving different microscale configurations of the systems being described, and statistical correlations will be investigated between simulation outputs and various macroscale descriptors of microscale heterogeneity (for example the tortuosity and connectivity of the porous media, or the average spreading out of microorganisms in the pore space). We anticipate these correlations to lead us to a thorough understanding of what ingredients are needed in a robust, fully macroscopic description of biogeochemical processes in porous media. Ultimately, this will drive the research to the production of predictive tools that stakeholders will be able to use in their every day practice. To facilitate this transition, every effort will be made throughout the project to involve Qatari stakeholders and keep them abreast of our progress.