Porous Media, Small and Large: From Atomistic Modeling of Nano-porous Membranes to Simulation of Flow and Transport in Geological Formations

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Flow, transport, reaction, adsorption and deformation (FTRAD) constitute a fascinating set of phenomena that occur in a wide variety of porous media and materials over widely disparate length scales, from molecular, to pore, core, and field scales. In this presentation four classes of fundamental problems are described and the approaches to their modeling are discussed. We first describe a process-based modeling of fabrication of a nano-porous membrane based on quantum mechanical calculations and molecular dynamics simulations. The goal is to be able to mimic the laboratory process by which such a membrane is fabricated, so that by developing an accurate model of the process the performance of the membranes is optimized. This is shown schematically Figure 1 for a SiC nanoporous membranes.

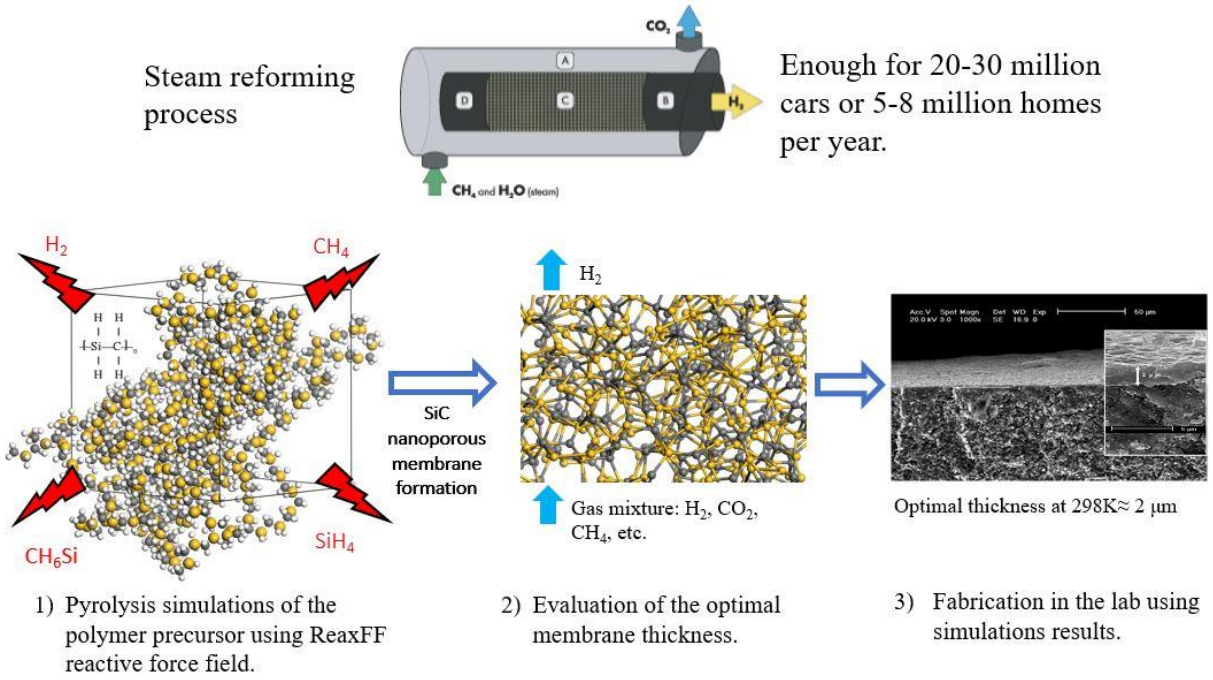

Figure 1

Next, we outline a general approach to modeling of adsorption and swelling of several types of core-scale porous materials, ranging from coal and sandstones, to metal-organic frameworks that have wide applications. This is shown schematically in Figure 2.

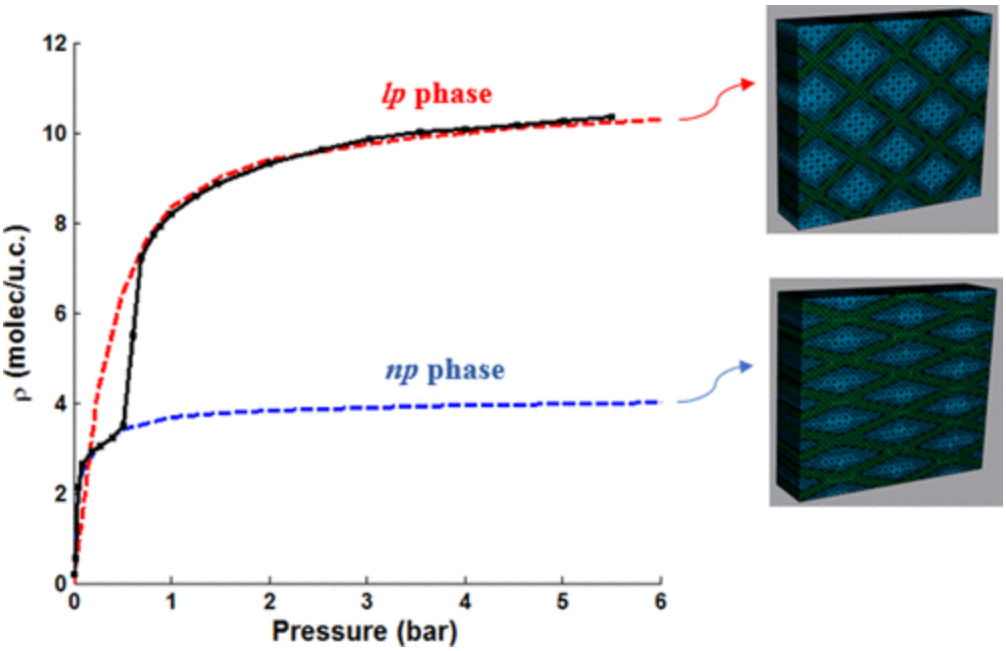

Figure 2

The problem of reconstruction of porous materials and media based on limited data, such as their two- or three-dimensional images, is described next, and a new method based on curvelet transforms for speeding up simulation of the FTRAD in such images is discussed. Here, the goal is to not only generate accurate realizations of a heterogeneous material or a porous medium based on very limited amount of data, but also because image-based simulation of FTRAD is gaining increasing popularity, to speed up such simulation. This is shown schematically in Figure 3.

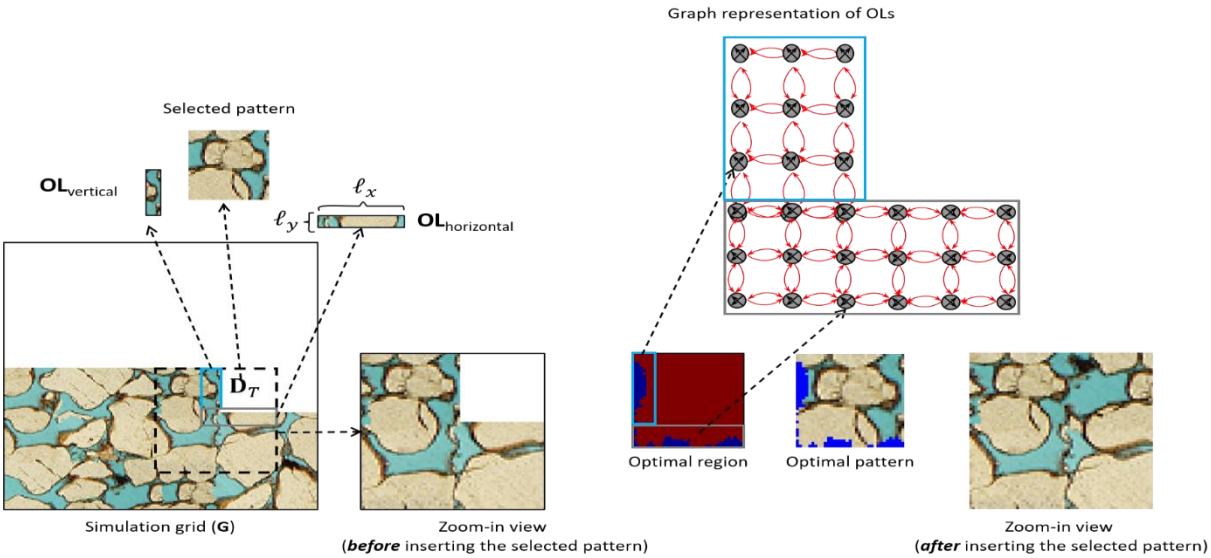

Figure 3

Finally, we describe the problem of upscaling of models of porous media, from the high-resolution “geological model” to a coarse scale model at field scale. We describe an upscaling approach based on multiresolution wavelet transformations. In particular, we show that the approach can be applied to upscale not only models that are based on computational grids with regular grid blocks, but also to those in which the grid is completely unstructured. This is shown schematically in Figure 4.

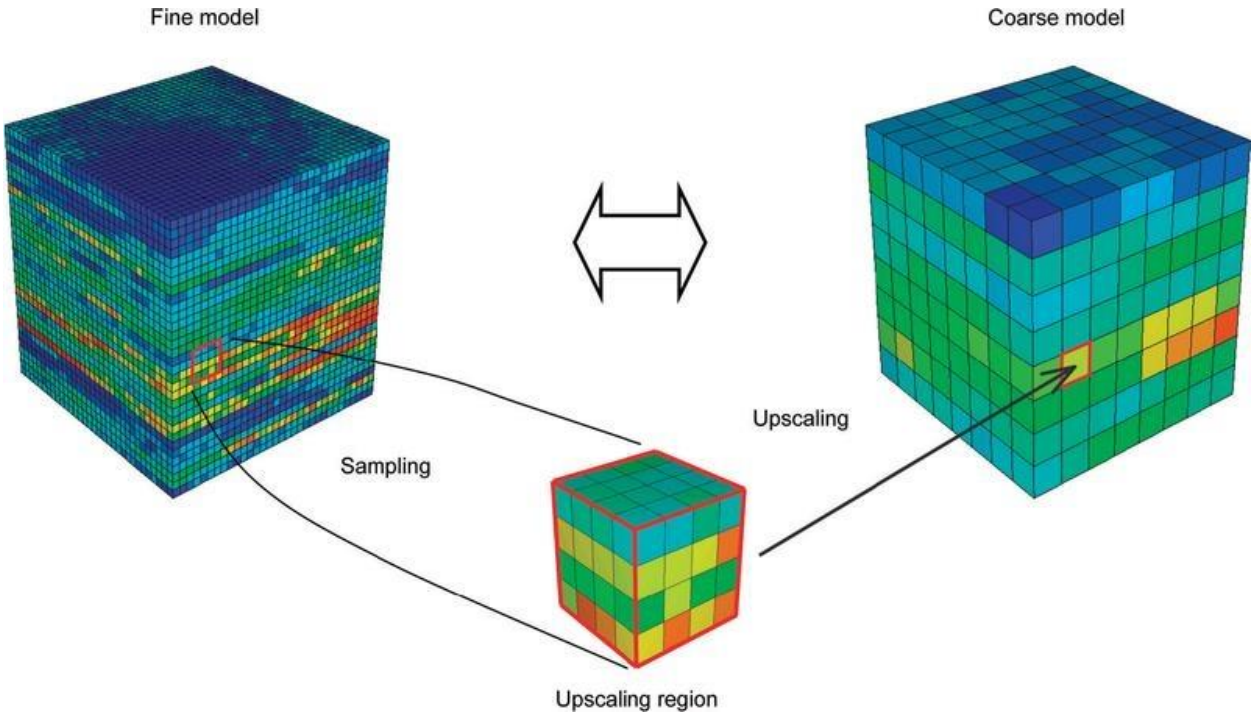

Figure 4