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PORE-SCALE SIMULATION OF MULTIPHASE FLOW IN POROUS MEDIA WITH APPLICATIONS TO GEOLOGICAL SEQUESTRATION OF CARBON DIOXIDE

Allocation: Illinois/250 Knh
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EXECUTIVE SUMMARY

Advances in noninvasive imaging of rock along with continued developments in computing power open up the exciting possibility of direct numerical simulation of pore-scale physics that are relevant to a variety of subsurface energy processes. In particular, we can investigate the fundamental pore-scale flow processes that control migration and trapping of supercritical carbon dioxide during carbon capture and storage, which is a key technology to mitigate emission of greenhouse gasses into the atmosphere. Direct numerical simulation of pore-scale multiphase flow physics is a grand computational challenge since a fine spatial grid is required to capture the complex pore geometry, while a large spatial domain must be included for a statistically representative sample. Although the lattice Boltzmann method (LBM) is generally known to be an effective numerical scheme, we did considerable work to develop a flexible code that is optimized for manycore processors. We used our code in conjunction with unique microfluidics experiments to investigate the role of inertial effects during rapid pore-scale displacements.

RESEARCH CHALLENGE

Understanding the migration of multiple fluids within pore spaces in subsurface geological formations is critical for addressing important problems such as enhanced oil recovery, groundwater pollution from leaking tanks or pipelines, geothermal energy production, and geological sequestration of carbon dioxide (CO_2). The last application, capture and geological storage of CO_2, provides a means of reducing CO_2 emissions into the atmosphere, by capturing CO_2 from major stationary sources and injecting it into suitable deep rock formations. Fingering and fluid displacement patterns at the pore scale can have a profound impact on large-scale phenomena such as the relative permeability relationship and residual trapping of fluids. Therefore, it is of great importance to study the detailed pore-scale displacement patterns of CO_2 injection in porous media under reservoir conditions.

Laboratory rock core flooding experiments are a major tool for investigating multiphase flow in CO_2 storage and petroleum reservoir applications. However, these experiments are limited since they are difficult, time-consuming, and expensive, and it is challenging to visualize the dynamic displacement process within the rock with sufficient time and space resolution. Pore-scale direct numerical simulation (DNS) in porous media reconstructed from micro-CT (computed tomography) scanned images of real rock has become increasingly popular. In addition to visualizing fluid displacement in porous media with high resolution, DNS also provides full-flow field information and has the flexibility to independently adjust fluid parameters for parametric study. Despite the rapid development of modern processors, the computation cost for such DNS is still very high. Fine spatial grid resolution is required to represent the pore space, yet a relatively large volume of rock must be modeled in order to have a representative volume element. Achieving this requires further development of high-performance codes to utilize GPU computing power as well as to improve parallel efficiency.

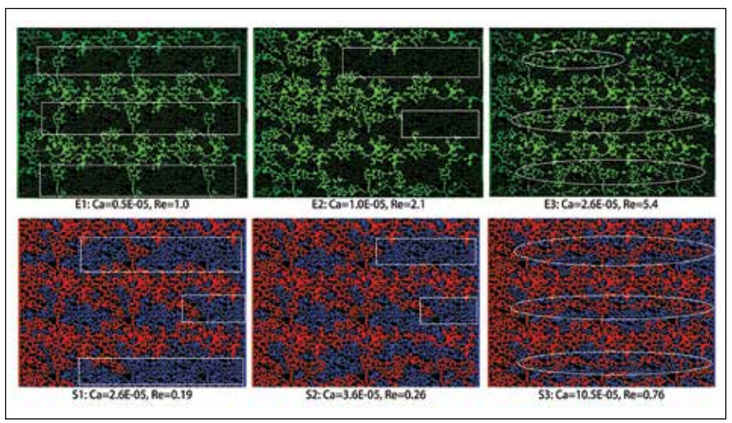

Figure 1: Comparison of CO_2 invasion patterns at approximately steady state between the simulations and experiments at different Ca. Red fluid represents liquid CO_2, blue fluid represents water, and solid grains are in black. E0, E1, E2, E3, and E4 denote the experimental results. S1, S2, and S3 denote the simulation results.

METHODS & CODES

The LBM [1] is particularly suited for numerical simulation of complex fluid flow with complex geometries. The LB color fluid multiphase model ensures a relatively sharp interface and completely immiscible fluids; therefore, it has been widely adopted for multiphase flow in porous media. We developed and optimized a portable and scalable LB code based on a variant of the multiple relaxation time (MRT) color-fluid multiphase LB model [2]. The code employs a MPI-OpenMP/OpenACC hybrid programing model so that it can run on CPUs, GPUs, and MIC processors. Preprocessors are employed to compile the code for different platforms. The code achieves two times speedup on Blue Waters' GPU node and scales almost ideally up to 512 GPU nodes thanks to the implementation of overlapped communication and computation. A typical simulation (on a 500X500X500 grid for 5 million iterations) takes 40 GPU nodes 43 hours to complete (1,736 node-hours).

RESULTS & IMPACT

During the BW project period, we further developed our existing code and successfully ported our code to GPUs and other manycore processors. We plan to make the code open source, which enables users to easily utilize computing power from manycore processors. The development of the code and its applications to pore-scale simulation of multiphase flow in porous media will be reported in a future publication.

LBM simulations and experiments of liquid CO_2 displacing water in a 2D heterogeneous micromodel at reservoir pressure conditions were performed and compared for the first time to evaluate the capability of LBM to capture detailed fluid invasion patterns. Our research collaborators at University of Notre Dame conducted the state-of-the-art experiments. The simulations reproduce qualitatively similar trends as the experiments for changes in invasion patterns as Ca (Capillary Number—ratio of viscous to capillary forces) increases, as shown in Fig. 1. The major discrepancy between experiments and simulations is the development of secondary CO_2 pathways (demarcated by ellipses in Fig. 1), which occur at a much higher Ca in the simulations. The inertial effects are ignored in most pore-scale studies due to the small bulk Re (Reynolds Number—ratio of inertial to viscous forces). However, recent studies show that local Re could be much higher than the bulk Re and hence the inertial effects may not be ignored. Due to computational cost and numerical stability issues, the LBM simulation uses proxy fluids with a much larger viscosity compared to the experiment. Our further studies of the effects of Re shows that the significantly reduced inertial effects in the simulation alter the preferential multiphase flow pathways and are responsible for the discrepancy between the simulations and experiments. The above work has been submitted to the *Journal of Contaminant Hydrology* and is currently under review. Further investigation on the impact of inertial effects in real rocks will be performed in the future. We will demonstrate, for example, how the inertial effects alter the preferential flow pathways in a Bentheimer sandstone for different Ca, as shown in Fig. 2.

WHY BLUE WATERS

Due to the complex geometry and complex interfacial dynamics, the computational cost of DNS is very high. Blue Waters offers a large number of CPU and GPU nodes, which is essential to our research. Our code was initially designed for CPU platforms and was later ported to GPU platforms. The availability of both CPU and GPU nodes enabled us to perform required simulations while at the same time developing faster GPU code.

A single iteration step in LB simulation can be completed in a very short time, but a typical simulation requires millions of iterations. Therefore, LB simulation requires very low latency on message passing, which cloud resources cannot provide.

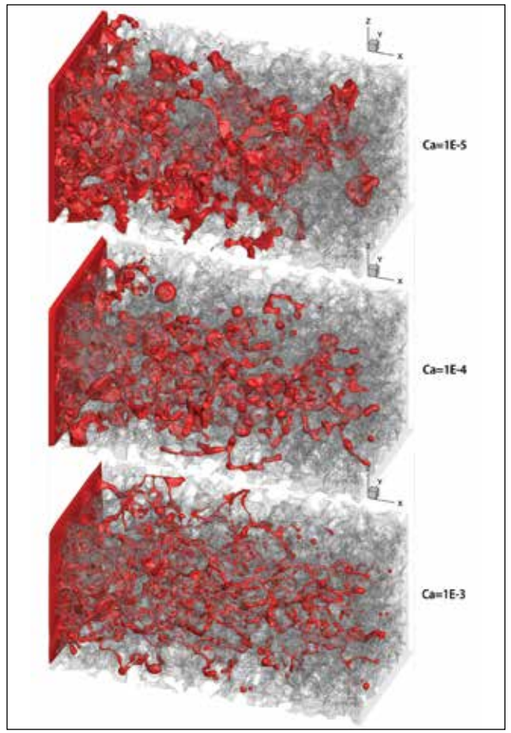

Figure 2: Invasion patterns of liquid CO_2 at different Ca on a Bentheimer sandstone. Brine is transparent and the solid surfaces are shown in grey.