Advancing Models for Multiphase Flow in Porous Medium Systems

J.E. McClure[1] M.A. Berrill[2] C.P Fower[3] C.T. Miller[3]

[1]Advanced Research Computing, Virginia Tech

[2]Scientific Computing Group, Oak Ridge National Lab

[3]Department of Env. Sci. & Eng., University of North Carolina at Chapel Hill

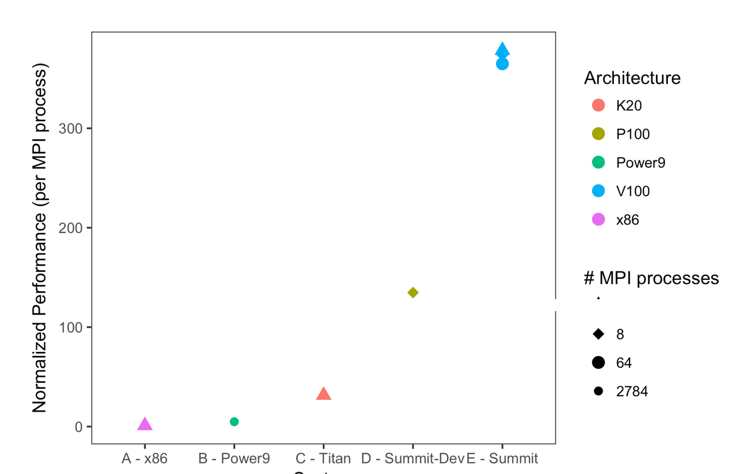
Abstract

Multiphase flow processes in the subsurface are fundamentally important for many applications including a wide range of hydrologic processes, geological carbon sequestration and emerging energy recovery technologies such as hydraulic fracturing. Mathematical models that describe these complex processes have long relied on empirical approaches that neglect important aspects of the system behavior. New data sources now make it possible to directly measure previously inaccessible information and access the true geometry of geologic materials. This information can be exploited to support a new generation of theoretical models that are constructed based on multiscale principles for thermodynamics and continuum mechanics. We show how information from synchrotron-based X-ray micro-tomography (micro-CT) can be used to inform models that can account for interfacial dynamics and other aspects of multiphase flow in porous medium systems. We also explore how this approach can be applied to address long-standing challenges related to subsurface heterogeneity, including geometric effects associated with spatial hetereogeneity and surface heterogeneity associated with the chemical composition of geologic materials.

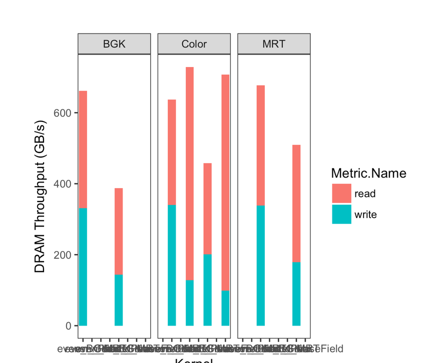
Computational Methods

Our lattice Boltzmann simulators are capable of using either CPU or GPU with excellent parallel efficiency. Early access to *summit* and *summit-dev* allowed our project to tune performance implement new features based on the architecture. Key

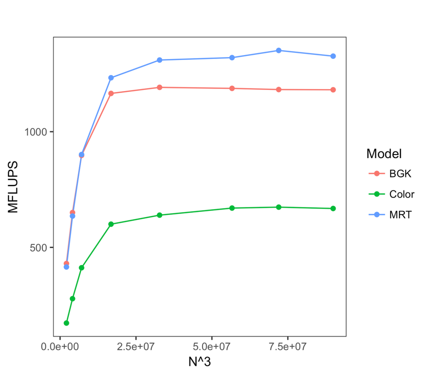
- Code refactoring to better use common computational elements between different physical models
- Updated data structures for the lattice Boltzmann method to make more efficient use of memory for digital rock images
- New algorithms to increase GPU memory bandwidth efficiency
- Reduction in CPU-GPU data movement
- Increased overlap between MPI communication with GPU kernels
- New LBM models for non-Newtonian fluids and three-fluid flow



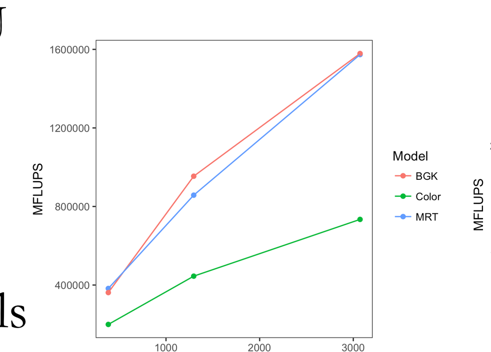
a. performance comparison for different architectures



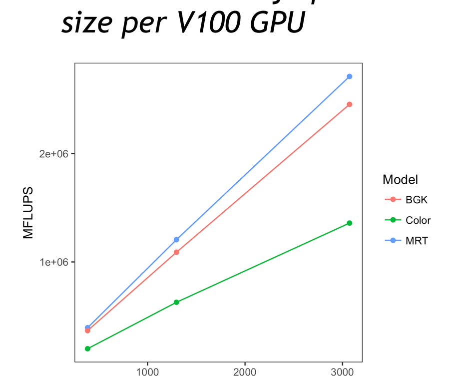
b. bandwidth utilization for CUDA kernels on V100 GPU



c. performance as determined by problem size per V100 GPU



d. strong scaling



e. weak scaling

Figure 1. Performance of lattice Boltzmann simulators on summit.

As a result of code optimizations and advantages of the Summit architecture, the performance of LBMs will increase dramatically. Figure 1a shows a comparison between various archiectures, including both Titan and Summit. Figure 2b shows that CUDA kernels without our simulator achieve between 50%-80% of the theoretical peak bandwidth for the V100 GPU. Compared to previous GPU architectures, more work is needed to get the full performance of the GPU. Strong and weak scaling results are reported in Figure 1d and 1e, respectively.

Further, we have developed sophisticated *in situ* data analysis routines to extract multiscale averages throughout the course of a simulation:

- Simulation completely occupies GPU
- CPU cores used to analyze simulation state in real-time based on task parallelism
- Wide range of analysis tasks are performed
  - execute in distributed memory
  - respect data locality
  - manage dependencies between tasks
- Analysis costs completely hidden behind simulation
- I/O performed in the background within own task
- Leverage heterogeneous node architecture

Scientific Impact

The relationship between microscopic processes and macroscopic transport phenomena has always been a topic of speculation for those who model flow in porous media. Computational methods and experimental micro-CT together provide a mechanism to access quantitative information at the microscale. Traditional models for two-fluid flow in porous media were developed based on an approximate view that flow occurred within static fluid regions that form connected pathways through the porous medium. By simulating two-fluid flow in digital rocks, we are able to reveal the true reality. As shown in Fig. 3, some flow conditions can lead to ganglion dynamics. In this regime, non-wetting phase flow paths undergo constant rearrangement as fluid regions snap-off to form new ganglia and then coalesce as ganglia migrate through the porespace. As the flow rate increases, the phase geometry evolves to create more efficient conduits for flow. These conduits are evident from Fig. 4, which shows how the non-wetting phase topology changes as the flow rates increase. These effects can be parameterized based on the capillary number *Ca*, which is the non-dimensional ratio of interfacial to viscous forces. As the capillary number increases, the flow is able to overcome interfacial forces, leading to new topological arrangements that are not accessible when interfacial forces dominate. We have been able to characterize these topological changes at the macroscale by considering the changes in interfacial area and Euler characteristic, which are the relevant topological invariants[5].

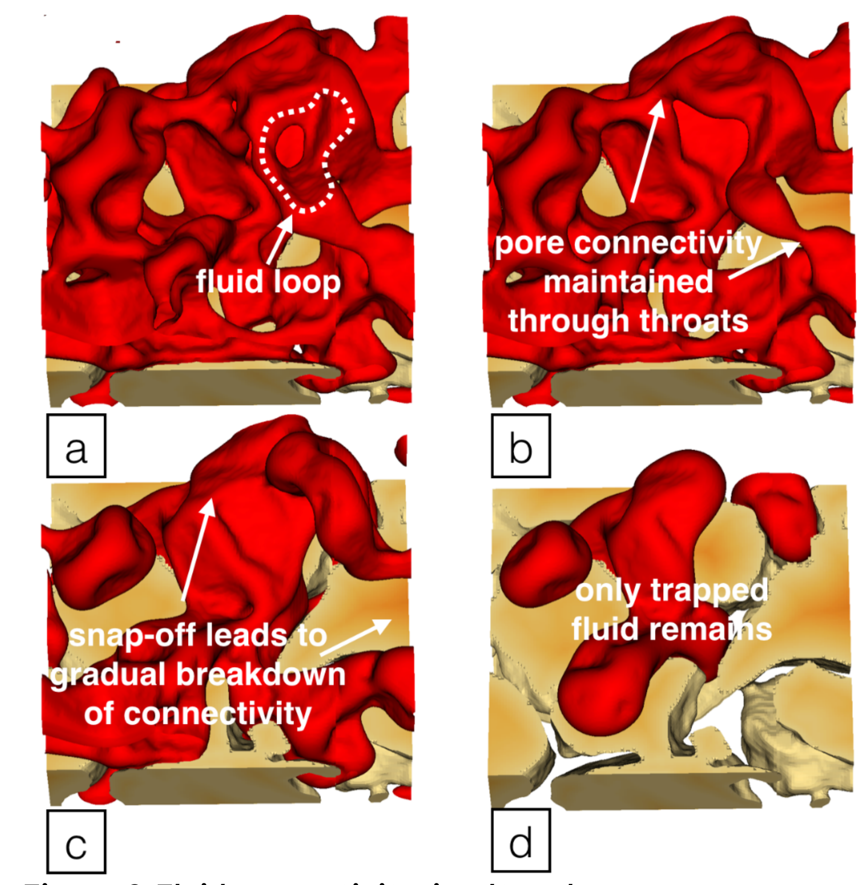


Figure 3.Fluid connectivity is altered as a consequence of snap-off and coalescence events that occur at the porescale. These can be captured by direct simulation

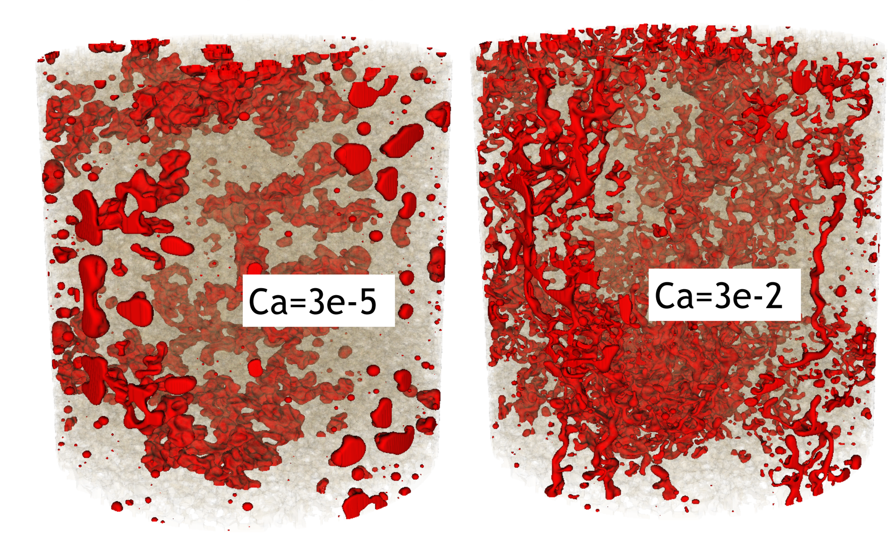


Figure 4. Non-wetting phase fluid configurations simulated at different capillary numbers based on synchrotron-based fast micro-CT experiments of steady state flow in a sandstone. Topological changes in the phase distribution result in more efficient larger-scale transport.

Future Work

Summit will enable relastic direct numerical simulations of fluid flow at scales that approach the laboratory scale. This is significant because traditional constitutive relationships are determined at this scale, and simulation will become a viable alternative to these methods.

Our current and future work includes

- simulation of core-scale constitutive relationships
- assessment of the representative elementary volume (REV)
- generalized descriptions of the geometric state that hold under a wider rnage of conditions
- Effort to characterize length scale heterogeneity in geologic systems based on digital rock physics
- Simulations that account for surface heterogeneities due to mineral composition

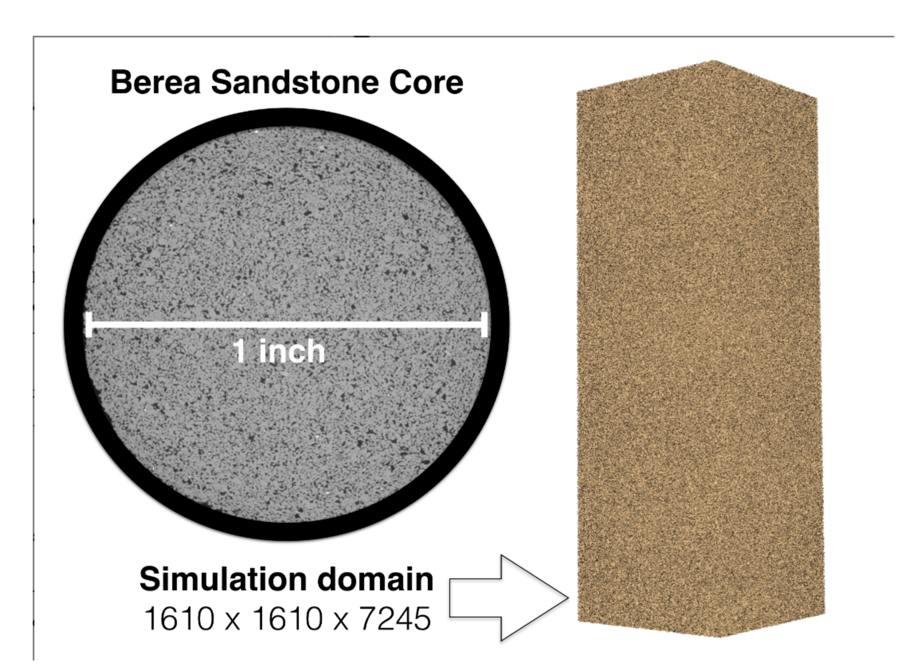


Figure 4. The summit supercomputer will enable pore-scale simulation of flow processes at the laboratory scale, making computation a viable means to predict clousre information.

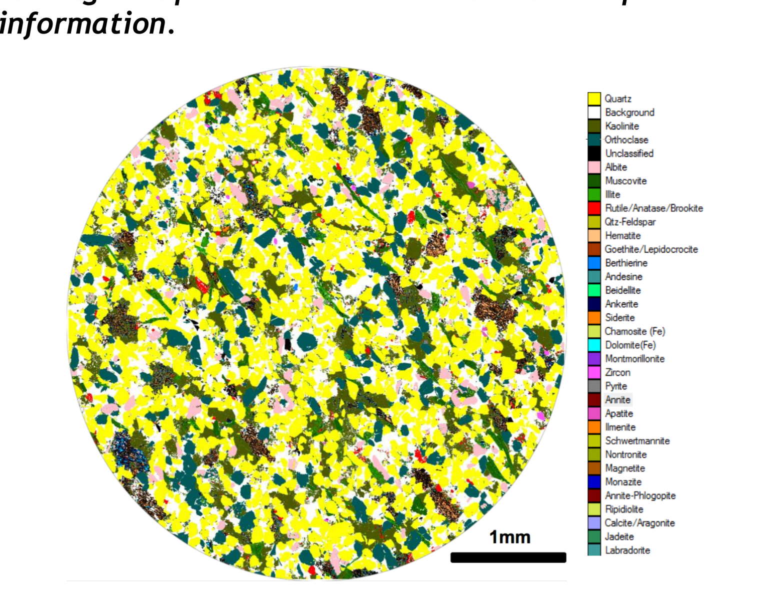


Figure 5.1: A 2D slice of reservoir sandstones SEM-EDS mineral map with 2 μm resolution embedded in the resin

References

1 W.G. Gray and C.T. Miller (2014) *Introduction to the Thermodynamically Constrained Averaging Theory for Porous Medium Systems*. Springer.

2 J.E. McClure, H. Wang, J.F. Prins, C.T. Miller and W. Feng (2014) Petascale Application of a Coupled CPU-GPU Algorithm for Simulation and Analysis of Multiphase Flow Solutions in Porous Medium Systems. *28th Annual IEEE International Parallel & Distributed Processing Symposium (IPDPS)*

3 W.G. Gray, A.L. Dye, J.E. McClure, L. Pyrak-Nolte and C.T. Miller (2015) On the dynamics and kinematics of two-fluid-phase flow in porous media. *Water Resources Research*, Vol. 51, pp. 5365-5381.

4 J.E. McClure, M.A. Berrill, W.G. Gray and C.T. Miller (2016) Tracking interface and common curve dynamics for two-fluid flow in porous media. *Journal of Fluid Mechanics*, Vol. 796 pp. 211-232.

5 R.T. Armstrong, J.E. McClure, M.A. Berrill, M. Rucker, S. Schlueter, and S. Berg (2016) Beyond Darcy's law: the role of phase topology and ganglion dynamics for two fluid flow. Physical Review E. 94 (4), 043113

6 J.E. McClure, M.A. Berrill, W.G. Gray and C.T. Miller (2016) Influence of phase connectivity on the relationship among capillary pressure, fluid saturation, and interfacial area in two-fluid-phase porous medium systems. Physical Review E. 94 (3), 033102

This work was supported in part by National Science Foundation grant 0941235, Department of Energy grant DE-SC0002163, grant W911NF-14-1-0287 from the Army Research Office. An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

VirginiaTech Invent the Future

Advanced Research Computing

Contact: James E. McClure (email: mcclurej@vt.edu)