Embracing heterogeneous simulation of complex fluid flows

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Motivation

• Scientific opportunities and challenges associated with new data sources
  • *Digital Rock Physics*: experimental data + simulation to understand geologic materials

• Challenges associated with exascale
  • Theoretical performance gains due to accelerators
  • Massive parallelism, massive data
Complementary Processors

GPU
- Slow clock speed
- Massive parallelism

CPU
- Fast clock speed
- Modest parallelism
Simulation as Data Analysis
Multiphase flow in the subsurface

- Oil and gas recovery
- Carbon sequestration
- Contaminant transport
X-ray tomography based on synchrotron light sources can be used to obtain three-dimensional images of complex microscopic systems.

- Observe fluid configurations within geologic materials such as rock (sub-micron resolution).

- Projected rate of data generation from light sources could reach 1 petabyte per hour by 2020.

- Light source intensity outpacing Moore’s law.
• Complex 3D microstructure of rocks directly observed (nanometer to micrometer length scale)

• Fluid movement within these spaces determines transport at larger scales (meter to kilometer)

• Physics-based modeling to predict movement of fluids within microstructure
Application Parallelism

- Large 3D images ($1000^3 - 2000^3$ voxels)
  - 5 minutes of scan time required to produce image
  - Hundreds to thousands of compute nodes per image
- Large number of simulations to deliver scientific value
  - Time sequences from synchrotron (many images)
  - Multiple cases per image
Lattice Boltzmann Methods

- Lattice Boltzmann methods (LBMs) have been devised to model a wide range of transport phenomena
  - Single phase flow, transport of multiple species
  - Two and three-phase flow
  - Complex boundaries can be accommodated easily
- Calculations of the LBM are typically local
  - Scale very well in distributed memory
  - Can be implemented efficiently on GPU and other architectures that rely on SIMD
Multiphase Simulation

- Lattice Boltzmann method: order of magnitude speedup using GPU
- Domain decomposition to distribute across nodes
- One MPI task per node

McClure et al. (2014) doi: 10.1109/IPDPS.2014.67

Parallel performance in million-lattice updates per second (MLUPS) for multiphase lattice Boltzmann simulator on Titan (90% parallel efficiency on 4,096 compute nodes)
Workflow

Data Acquisition → Pre-processing → Simulation → Data Analysis & Post-processing

Data Exploration

Raw data fields from simulation saved to disk

www.arc.vt.edu
Workflow Summary

Data Acquisition

Pre-processing (inverse modeling)

Physics Modeling

Multiscale Analysis

Simulator

Reduced Representation of Simulation Data
Order of magnitude smaller than raw data fields

www.arc.vt.edu
Workflow Summary

• Homogenization theory: develop multiscale relationships for partial differential equations that describe transport phenomena

• Integral geometry approaches to statistically characterize the geometry / topology

• Percolation theory: understand the role of connectivity for transport in complex systems

Connected components analysis applied to identify connected portions of a phase within simulation
Intranode Task Management

- Every task performed within a dedicated MPI communicator
- Data movement between CPU and GPU controlled explicitly
- C++11 threads used to spawn analysis tasks
- Task dependencies are incorporated into threadpool class
Intranode Parallelism

**Multiphase simulation**
- Lattice Boltzmann

**Analysis**
- Connected components
- Extract interfaces
- Topological analysis
- Solve \( \frac{\partial \phi}{\partial t} = \text{sign}(\phi) (1 - |\nabla \phi|) \)

**Data reduction**
- Average quantities

Titan Compute Node

Multiphase simulation

- Lattice Boltzmann

Analysis

- Connected components
- Extract interfaces
- Topological analysis
- Solve \( \frac{\partial \phi}{\partial t} = \text{sign}(\phi) (1 - |\nabla \phi|) \)

Data reduction

- Average quantities
Conclusions

• Analyzing the simulation state *in situ* allows us to extract an order of magnitude more information tracking the system behavior.

• Heterogeneous compute node is advantageous for our complex workload which can be decomposed using task parallelism.

• Even data-driven workloads can be compute bound! It depends on the questions we ask and how smart we are with the data.
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