GPU-accelerated Lattice Boltzmann Method (LBM) for Fluid Flow and Solute Transport in Porous Media — Applications in Geoenvironment

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Background: Computational Geosciences, Physics, Mathematics, Fluid Mechanics (CFD)
Available projects: 2
Preferred project period: 01.04.2024 – 30.06.2024

Project Outline:

The constitutive relationships for fluid flow and solute transport in porous media, such as capillary pressure-saturation curves, relative permeability-saturation curves, dispersivity-saturation, and mass transfer rates, form the cornerstones of continuum-scale Darcy-scale flow and transport. These relationships link the porous medium characteristics to the macroscopic proxies and parameters. The complex nature of geological samples representing heterogeneous complex layered porous media in pore-scale controls the macroscopic two-phase flow and solute transport. One ubiquitous heterogeneity in natural rocks is the pore size spatial distribution and correlation that can be inferred and characterized using pore-scale imaging techniques such as x-ray computed tomography.

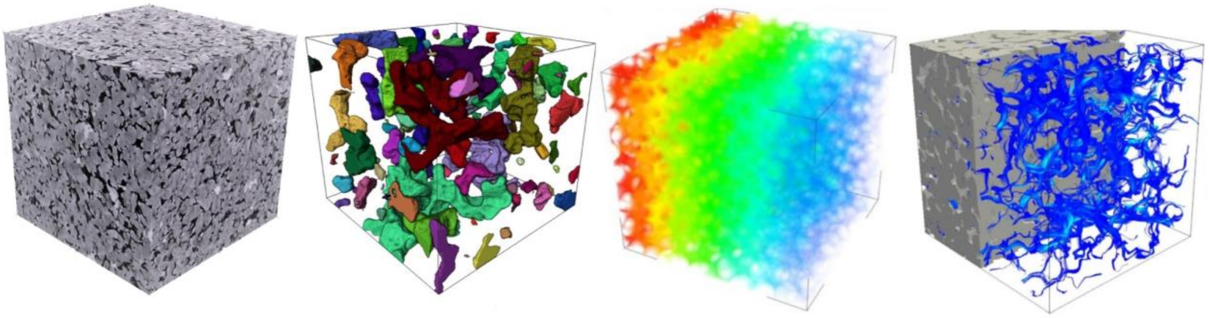

Figure 1. Solving advection-diffusion-reaction equations on real porous media geometry of geological media after acquiring high-resolution x-ray tomography and digital image analysis for segmenting tomograms.

The Lattice Boltzmann Method (LBM) is widely used for diverse geoenvironmental and geoenergy applications to simulate fluid flow and solute transport in porous media. Numerical modeling of advection-diffusion-reaction (ADR) processes pose a formidable computational challenge due to the complex geometry of the porous media and the multiscale multicomponent nature of the flow, transport, and reactions. Computational fluid dynamics (CFD) based on the Navier-Stokes equations is now widely used in industry, often run on high performance computer clusters of CPU nodes. Direct Numerical Simulation of pore-scale processes can delineate moments of interest (in space and time) and elucidate underlying mechanisms and governing factors in ADR studies.

The LBM is based on the Boltzmann equation and kinetic theory as opposed to the conventional CFD that directly solves the NS equations. A promising advantage of LBM over NS solvers is the inherent capabilities for parallelism owing to the local data access pattern. In LBM, the computation on each node is independent, and the data transmission only happens between two adjacent nodes. This localized data communication mode and inherent additivity of its numerical implementation make LBM ideal for GPU parallel computation. GPU parallel computation becomes increasingly more desired because of the high performance and efficiency than the traditional computation on CPUs. The computation capacity of GPUs is order(s) of magnitude greater than the mainstream CPUs in terms of memory bandwidth and peak performance. Therefore, CUDA-enabled GPU parallel computation will shape the future of demanding computational tasks such as those in porous media research.

Research Objectives:

The primary goal of this project is to construct an advanced numerical framework tailored for pore- and meso-scale reactive transport studies in porous media, all while substantially reducing computational costs. Our innovative approach centers around the integration of an optimized Lattice Boltzmann Method (LBM) solver executed on Graphics Processing Units (GPUs) using CUDA (Compute Unified Device Architecture). Additionally, we explore the option of coupling this GPU-based LBM solver with a Navier-Stokes (NS) solver executed on central processing units (CPUs), strategically balancing computational resources for enhanced efficiency.

Research Scope:

The exploration of advection-diffusion-reaction (ADR) equations for pore-scale porous media flows, grounded in the real geometry (static/dynamic) derived from x-ray tomography imaging data, has emerged as a pivotal pursuit in Computational Geosciences. This trajectory is driven by the diverse applications and adaptability of such simulations. Addressing this challenge necessitates a multidisciplinary approach, encompassing image processing, computational fluid modeling, and high-performance computing.

We propose the implementation of Volumetric Lattice Boltzmann Method (VLBM) for velocity field simulation as an advanced technique, meticulously designed to accurately track the solid to fluid ratio on the smooth solid boundary lattices. This innovative methodology involves coupling the direct flow simulator with a multicomponent solute transport system. Furthermore, we advocate for the incorporation of a geochemical module, such as Phreeqc or Reaktoro, if needed, to facilitate voxel-based local equilibrium and kinetic reactions. This comprehensive strategy aims to elevate the precision and applicability of our research endeavors in understanding complex fluid dynamics within porous media.

Opportunities for Candidates:

Candidates will receive training and responsibilities, engaging in curiosity-driven research under supervisor guidance. They will be part of disseminating project outcomes through conference proceedings and peer-reviewed articles. The project offers exposure to fluid flow and reactive transport processes relevant to various applications, from CO2 storage to geothermal energy. Additionally, candidates will master programming skills (CUDA, C++, and Python), enhancing their career prospects.

This comprehensive project aims to advance understanding in geoenvironmental applications, leveraging cutting-edge technologies for efficient and accurate simulations in porous media research.