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Title: Coupling lattice Boltzmann and continuum equations for flow and reactive transport in porous media.

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Coupling lattice Boltzmann and continuum equations for flow and reactive transport in porous media.

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Rough Heuristics

Continuum grid size:

- pore throats $4-8$ unknowns $\rightarrow$ 30 unknowns per grain + throat
- ~ 10 "grains" to form REV

$\hookrightarrow$ $\sim \mathbf{300^2}$ **unknowns**, per continuum REV (in 2D)

Time constraints:

- LB requires $^{v}/_{c} \ll 1 \approx 10^{-1}$

$\hookrightarrow$ $\sim \mathbf{3 \times 10^3}$ timesteps to cross a single continuum cell.

Basic continuum problem: 100^2 continuum cells

$\hookrightarrow$ $\sim \mathbf{3 \times 10^5}$ timesteps to cross continuum domain

$\hookrightarrow$ $\sim \mathbf{3000^2}$ unknowns in domain

For a 10 μm grid size, our domain is ~ 30 cm, and (assuming water) ran for ~ 50 s.

$\sim$ **1 hour on 512 CPU cores.**

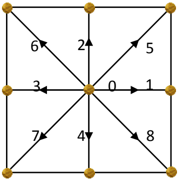
Pore-scale methodology: the Lattice Boltzmann Method

- Why the LB method?
  - Fully parallel algorithm
  - Easy to implement in complex geometries
  - Interfacial dynamics are automatic (no interface tracking)
- Single phase LB method:
  - Solves the discrete Boltzmann eq. for a distribution of particles $f_i(\mathbf{x}, t)$

$$\underbrace{f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t)}_{\text{Streaming}} = \underbrace{\Lambda \left[f_i^{eq}(\mathbf{x}, t) - f_i(\mathbf{x}, t) \right]}_{\text{Collision}}$$

  - $\mathbf{e}_i$ is the discretized velocity
  - f_i^{eq} is the equilibrium distribution function
  - Λ is the relaxation operator

$$\rho = \sum_i f_i \qquad \rho\mathbf{u} = \sum_i f_i \mathbf{e}_i \qquad p = c_s^2 \rho \qquad \nu = c_s^2 (\tau - 0.5)\Delta t$$



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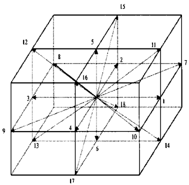
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- Navier-Stokes:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

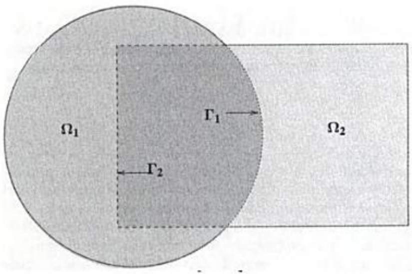
$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right]$$

Taxila LBM

https://software.lanl.gov/taxila/trac

- Brings together many advances in the LBM from LANL into a single software framework.
- Released as open source software to further enhance collaboration and engage the LB community.
- *Taxila*:
  - solves both single-, multi-phase and multicomponent flow in complex geometries for in 2D and 3D.
  - demonstrates strong scaling to hundreds of thousands of cores.
  - leverages the Portable, Extensible Toolkit for Scientific Computation (PETSc) for data structures, communication, and parallel I/O.
- Coupled to `PFloTran`, which allows for micro-scale reactive transport modeling and hybrid, multi-scale modeling.

Overlapping domain decomposition (Schwarz 1870)

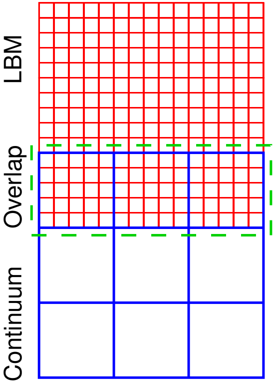


Schwarz

- Initially applied to identical equations in each domain as a method of solving complex domains.
- Can apply to different physical equations, assuming the physics are equivalent in the overlap region.

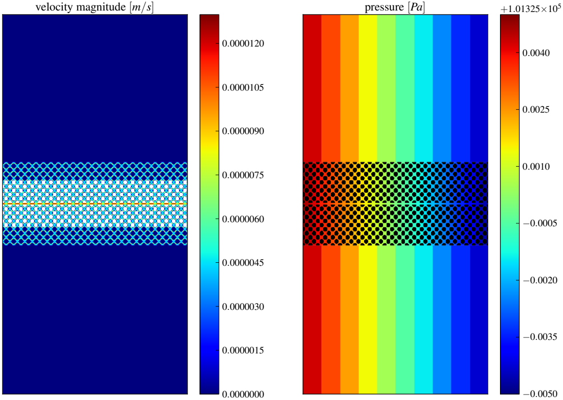
Hybrid solution process

Idea: use overlapping domain decomposition with an overlap where the pore-scale Navier-Stokes system upscales to the continuum Darcy system.



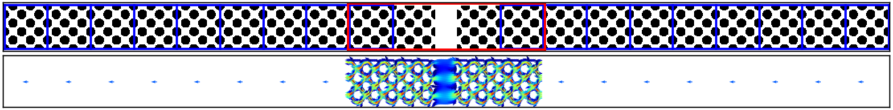
- Calculate consistent properties within the overlap (ϕ, K)
- Initialize pressure, flow everywhere, setting boundary conditions from the initial condition.
- do $t = 0 ... t_{final}$:
  - Advance each subdomain by Δt using BCs
  - Interpolate continuum domain pressure to form BC for LBM.
  - Integrate LBM mass flux (or pressure) to form BC for Continuum.

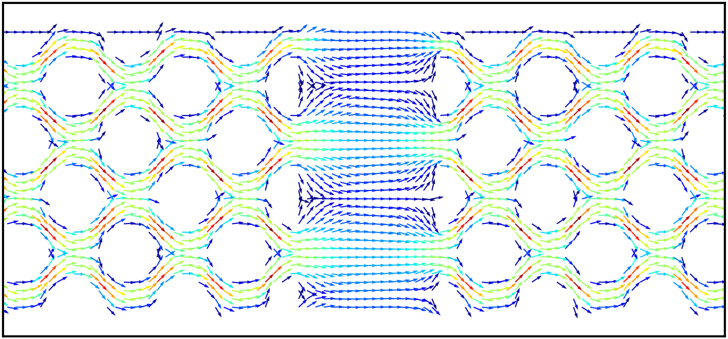
Verification: Flow along a fracture



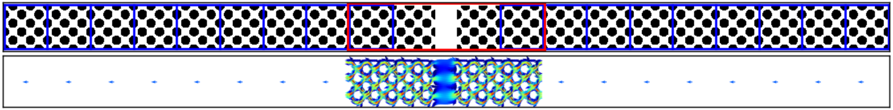
- LB domain of resolution 1000x400, continuum domains with resolution 10x10
- Mean velocity in the LBM domain (including zero velocity in the wall nodes) are equal to the Darcy velocity in the overlap region.
- Verification: Total flux of the hybrid calculation is equal (to tolerance) to the total flux of a LB simulation on the full domain.

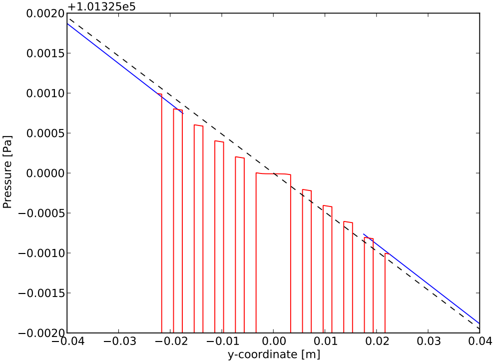
Flow across a fracture





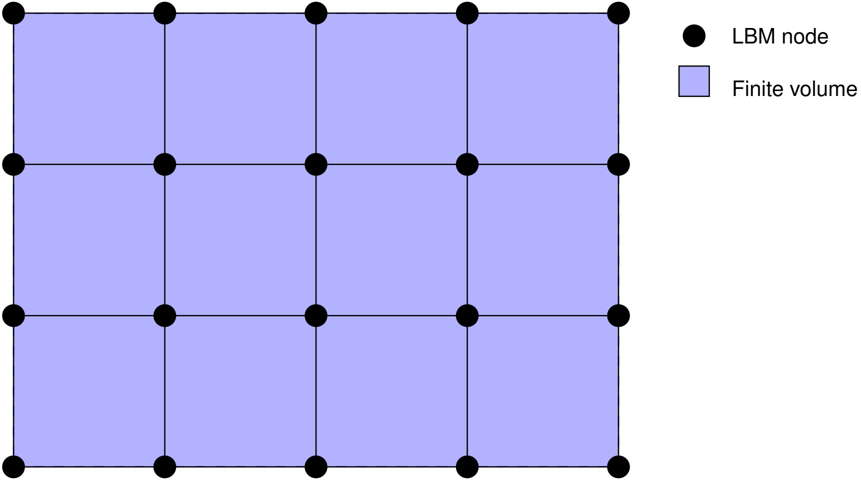
Flow across a fracture (left to right)





Pressure field across the fracture in the continuum region (blue) and pore-scale region (red).

Porescale chemistry: Coupling LBM (flow) to PFLOTRAN (reactive transport)



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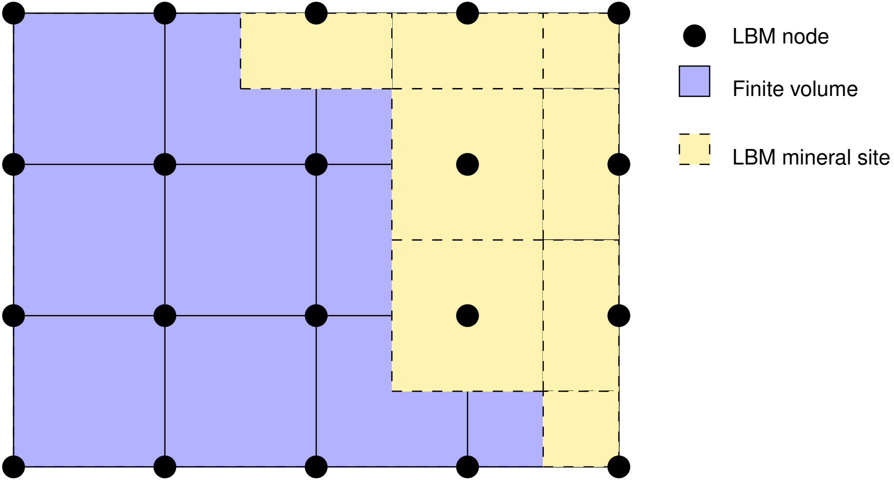

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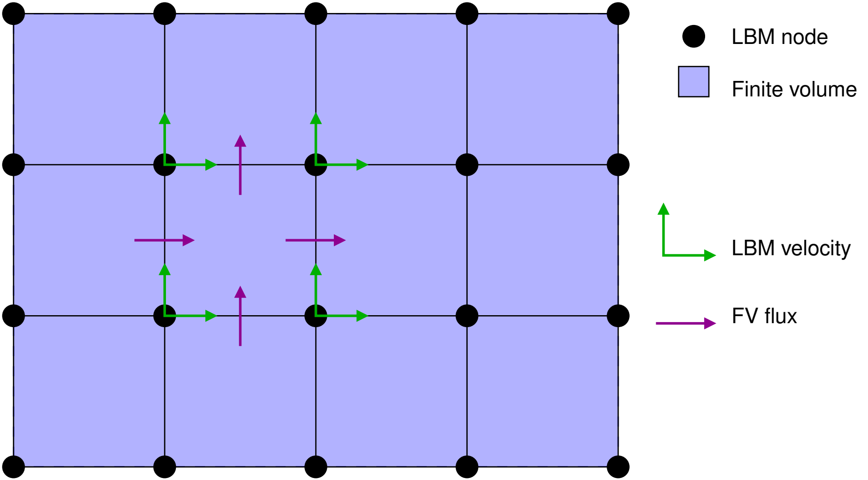

Hybrid Extension to Reactive Transport

Conclusions

Introduction and Motivation

- In spatially and temporally localized instances, capturing sub-reservoir scale information is necessary.
- Capturing sub-reservoir scale information everywhere is neither necessary, nor computationally possible.

The lattice Boltzmann Method for solving pore-scale systems.

- At the pore-scale, LBM provides an extremely scalable, efficient way of solving Navier-Stokes equations on complex geometries.

Coupling pore-scale and continuum scale systems via domain decomposition.

- By leveraging the interpolations implied by pore-scale and continuum scale discretizations, overlapping Schwartz domain decomposition is used to ensure continuity of pressure and flux.
- This approach is demonstrated on a fractured medium, in which Navier-Stokes equations are solved within the fracture while Darcy's equation is solved away from the fracture
- Coupling reactive transport to pore-scale flow simulators allows hybrid approaches to be extended to solve multi-scale reactive transport.