Upscaling of Brinkman Equations with the Lattice Boltzmann method

and reduced order modelling

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Introduction: Multiscale Modeling

- Full scale simulations often not feasible
- General Goal: Reducing model complexity
  - Rigorous Homogenization/Effective Medium via. Asymptotics
  - Model Reduction Techniques, Eg. POD/DMD.
  - Local Model Reduction $\rightarrow$ Multiscale Finite Elements
  - Upscaling/Upgridding Effective properties

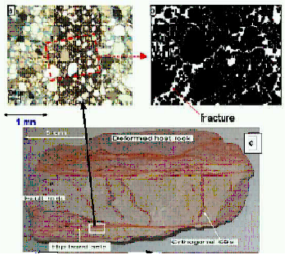


Figure : Pore Scale, Fracture Scale, and Darcy Scale.

Introduction: Multiscale Modeling

- Goals:
  - Develop and test different solvers and techniques
  - Upscaling Algorithms to coarse grid from fine grid
  - POD model reduction techniques to expedite computation
  - Done in an Lattice Boltzmann Method (LBM) framework.

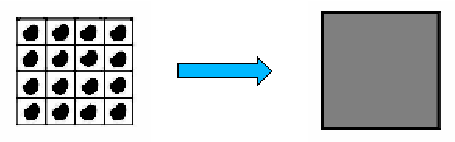
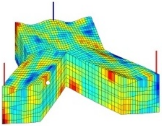


Figure : Averaging Fine-Scale Features

Discretization Methods

- Wide array of solution techniques
- Finite Volume and Finite elements etc.
- And of course Multiscale-FVM/FEM
- LBM based of Boltzmann equations from Kinetic Theory
- Hydrodynamic Limit yields Navier-Stokes (Golse et al)
- Various advantages (disadvantages) to each approach



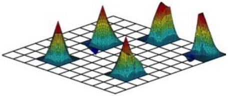


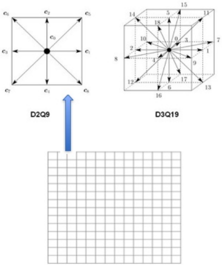
Figure : Discretization Methods (Sintef, Krogstad et al. and Y. Efendiev)

Lattice Boltzmann Method: Navier-Stokes

Discretize space and time into $\Delta x, \Delta t$, and $c = \Delta x/\Delta t$, and velocity over a discrete lattice of unit vectors $\{e_\alpha\}_{\alpha=0}^{8}$, the evolution of the distribution f_α is given by

$$f_\alpha(x + e_\alpha \Delta t, t + \Delta t) = f_\alpha(x,t) + \frac{1}{\tau}(f_\alpha^{(eq)}(x,t) - f_\alpha(x,t))$$

Here we use the BGK approximation for the collision integral and the dynamics of the system are governed by $f_\alpha^{(eq)}(x,t)$.



Lattice Boltzmann Method: Navier-Stokes

We may relate the distribution function to physical quantities by taking moments

$$\rho(x,t) = \sum_{\alpha=0}^{8} f_\alpha(x,t)\ ,\ (\rho u)(x,t) = \sum_{\alpha=0}^{8} f_\alpha(x,t),$$

and the equilibrium function is, for suitable weights ω_α,

$$f_\alpha^{(eq)}(x,t) = \omega_\alpha \rho \left(1 + \frac{3e_\alpha u}{c^2} + \frac{9(e_\alpha u)^2}{2c^4} - \frac{3(u)^2}{2c^2}\right)$$

In (certain) hydrodynamic limits, the above density and momentum satisfy the Navier-Stokes equations.

Lattice Boltzmann Method: Navier-Stokes

Applying the Chapman-Enskog Expansions with respect to the Knudsen number K, then taking moments

$$f_\alpha = f_\alpha^{(1)} + K f_\alpha^{(2)}$$
$$\frac{\partial}{\partial t} \to K \frac{\partial}{\partial t_1} + K^2 \frac{\partial}{\partial t_2}$$

In certain hydrodynamic limits, density and momentum approximate the (in)compressible Navier-Stokes equations.

$$\frac{\partial u}{\partial t} + \nabla p - \Delta u + u \nabla u = f \text{ in } \Omega,$$
$$\text{div}(u) = 0 \text{ in } \Omega \text{ , } u = 0 \text{ on } \partial\Omega.$$

Add pore-structure $\varepsilon \to \Omega \to \Omega_\varepsilon$ via contraint boundary conditions.

The Brinkman Model

- Want to input pore-structure via penalization
- High flow and low flow regions
- Large contrast in flow properties
- Applications: Carbonates/ Filtration Devices
- Fissures and large fractures/vuggs in rock matrices (cf. Popov et al, 2009, Ligaarden Ingeborg et al 2010)

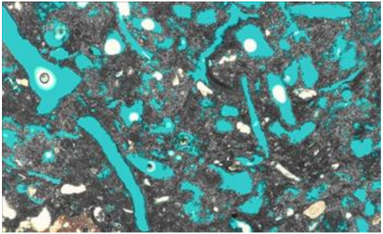


Figure : Carbonate Reservoir Pore Geometry (CIPR, Jakobsen et al.)

The Brinkman model

The Brinkman equations

$$\nabla p - \Delta u + \boxed{k_\varepsilon^{-1} u(x)} = f \text{ in } \Omega,$$
$$\text{div}(u) = 0 \text{ in } \Omega \text{ , } u = 0 \text{ on } \partial\Omega.$$

- Add global linear forcing term to Stokes (or NS)
- Permeability has small scales features ε
- Brinkman Coefficient related to permeability $\alpha_\varepsilon = k_\varepsilon^{-1}$
- If $\alpha_\varepsilon \to 0$, free-flow Stokesian regime
- If $\alpha_\varepsilon \to$ "Large", Darcy regime as the resistive term dominates
- **Want LBM method to approximate Brinkman model**

LBMs for Brinkman Equation

Use a forcing model based on (Guo Z., and Zhao T. 2002),

$$f_\alpha(x+\Delta t e_\alpha, t+\Delta t) = f_\alpha(x,t) + \frac{f_\alpha^{(eq)}(x,t) - f_\alpha(x,t)}{\tau} + \Delta t F_\alpha(x,t)$$

$$F_\alpha = \omega_\alpha \rho \left(1 - \frac{1}{2\tau}\right) e_\alpha \cdot \left(-\frac{\phi\nu}{k_\varepsilon} u + \phi G, \right) / c_s^2$$

$$f_\alpha^{(eq)} = \omega_\alpha \rho \left(1 + \frac{e_\alpha \cdot u^{(eq)}}{c_s^2}\right) \text{(Truncated Linearized)}$$

$$u^{(eq)} = \frac{\sum_{\alpha=0}^{8} e_\alpha f_\alpha + \frac{1}{2}\Delta t \rho \left(-\frac{\phi\nu}{k_\varepsilon} u + \phi G, \right)}{\rho},$$

τ so that $\nu_{\text{eff}} = c_s^2(\tau - 0.5)\Delta t$, $c_s = c/\sqrt{3}$ is the sound speed.
ϕ is porosity, ν physical viscosity, G external forcing.

Equating u and $u^{(eq)}$ we have

$$u = \frac{\sum_{\alpha=0}^{8} \vec{e}_\alpha f_\alpha + \frac{\Delta t}{2}\phi\rho G}{\rho(1 + \frac{\phi \Delta t \nu}{2k_\varepsilon})}.$$

In the incompressible limit $|u| \ll c_{\mathrm{s}}$, with the Chapman-Enskog expansion the pressure $p = c_{\mathrm{s}}^2\rho$ and u converge to

$$\begin{aligned} \frac{\partial u}{\partial t} &= -\frac{1}{\rho_0}\nabla p + \nu_{\mathrm{eff}}\Delta u - \frac{\phi\nu}{k_\varepsilon}u + \phi G, \\ \nabla \cdot \vec{u} &= 0. \end{aligned} \tag{1}$$

Note with $\tau \to 1/2(!)$, then $\nu_{\mathrm{eff}} \to 0$. Steady state yields Darcy.

LBMs Upscaling Algorithm

Idea:

- Given k_ε, $(\Delta x, \Delta t)$ discretize fine grid
- Generate (in this case) nested course grid $(\Delta X, \Delta t$ or ΔT
- Solve local periodic (easy BC) in each coarse grid via LBM
- Solve above problems to steady state
- Using the conservation of average fluxes compute k^*

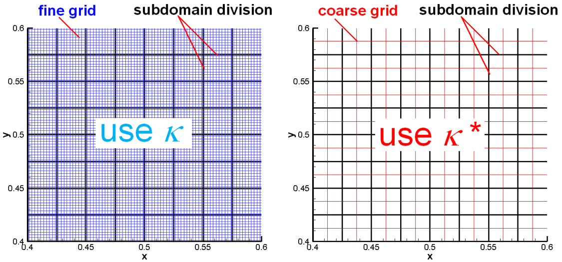


Figure : Schematic models of the fine and coarse grids.

LBMs Upscaling Algorithm

Conservation of average fluxes to compute k^*.

- On each coarse grid K, we suppose

$$\langle u_{per}(k_\varepsilon, G)\rangle_K = \langle u_{per}(k^*, G)\rangle_K$$

- k^* and G are constant on K, with periodic BC we have

$$f_\alpha(k^*)(x + \Delta t e_\alpha, t + \Delta t) = f_\alpha(k^*)(x, t), \text{ as } t \to \infty$$

- We obtain after some manipulation the analytic formula

$$f_\alpha(k^*) = \omega_\alpha \rho_0 (1 + \frac{e_\alpha}{c_s^2} \cdot \frac{k^* \cdot G}{\nu})$$

  and thus,

$$u_{per}(k^*, G) = \frac{k^* \cdot G}{\nu}$$

- Using the equivalence of average fluxes we obtain

$$\boxed{\langle u_{per}(k_\varepsilon, G)\rangle_K = \frac{k^* \cdot G}{\nu}}$$

LBM Upscaling: Examples

Layered Media Test Case:

- 10 Layers, $k_1 = 10^{-12} m^2$ in odd layers and $k_2 = c * k_1$ in even
- For k^*_{xx}, $G = (2,0) ms^{-2}$, Take $\tau = .53 \rightarrow v_{eff} = .01 m^2 s^{-1}$
- For k^*_{yy}, $G = (0,2) ms^{-2}$, Take $\tau = .5 \rightarrow v_{eff} = 0 m^2 s^{-1}$

Table : Computed κ^*_{xx}, $\kappa_1 = 10^{-12}$ m^2 and $\nu_{\text{eff}} = 0.01$ m^2 s^{-1}

$\frac{\kappa_2}{\kappa_1}$	$[\frac{1}{2}(\frac{1}{\kappa_1} + \frac{1}{\kappa_2})]^{-1}$	κ^*_{xx} by LBM
2	1.33333×10^{-12}	1.33333×10^{-12}
10	1.81818×10^{-12}	1.81818×10^{-12}
50	1.96078×10^{-12}	1.96078×10^{-12}

LBM Upscaling: Examples

Checkerboard Media Test Case:

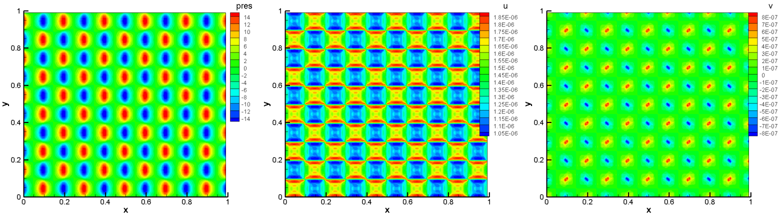


Figure : Distributions of p, u_x and u_y, $\nu_{\mathrm{eff}} = 0$ m^2 s^{-1}, $G_{\mathrm{const}} = (2, 0)$ m s^{-2}, $\kappa_1 = 10^{-12}$ m^2 and $\dfrac{\kappa_2}{\kappa_1} = 2$.

LBM Upscaling: Examples

Checkerboard Media Test Case:

Table : Verification of computed κ^*_{xx}, $\kappa_1 = 10^{-12}$ m^2 and $\nu_{\text{eff}} = 0$ m^2 s^{-1}

$\frac{\kappa_2}{\kappa_1}$	$\sqrt{\kappa_1 \kappa_2}$	κ^*_{xx} by LBM
2	1.41421×10^{-12}	1.41418×10^{-12}
10	3.16227×10^{-12}	3.14081×10^{-12}
50	7.07106×10^{-12}	6.45938×10^{-12}

LBM Upscaling: Examples

More complicated media

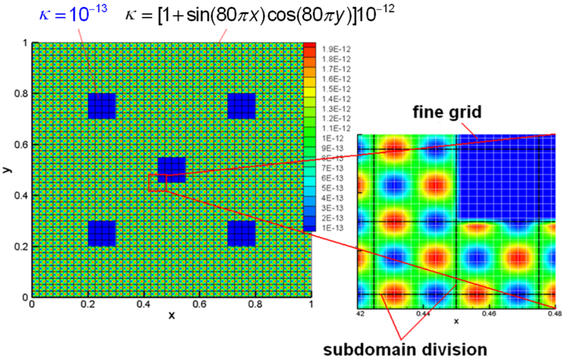


Figure : Distribution of the permeability $\kappa(\vec{x})$, $\kappa_{\text{const}} = 10^{-13}$.

LBM Upscaling: Examples

More complicated media

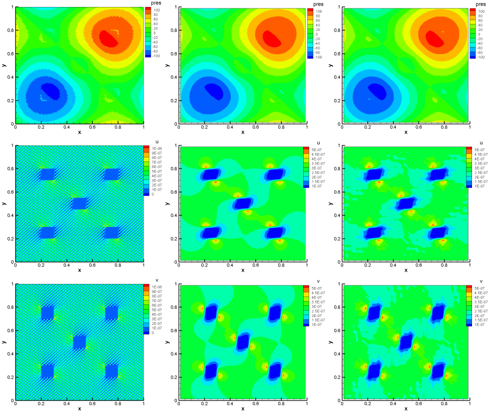


Figure : Comparisons of p, u_x and u_y between the fine-grid results (left), fine-grid averaged results (middle) and coarse-grid results using κ^* (right), $\nu_{\text{eff}} = 0$ m^2 s^{-1}, $\vec{G} = (\sin \pi x, \sin \pi y)$ m s^{-2}, $\kappa_{\text{const}} = 10^{-13}$ m^2.

Model Reduction

- LBMs are fast, but must be solved to steady state
- Can be computationally expensive for complex RVEs
- Can use model reduction to expedite the solves
- LBMs must be reformulated into Mat-Vec

Proper Orthogonal Decomposition

Suppose we have large system $N \times N$ evolution operator A, for $n = 0, 1, \cdots$ we have unknown F^{n+1}, $N \times 1$ satisfies the fine resolution equation

$$F^{n+1} = AF^n$$

Take M Snapshots of the solution in the initial stages form S $N \times M$,

$$S = [F_1, F_2, \ldots, F_M]$$

Form matrix $R = S^T S$, $M \times M$ (Generally $M << N$).
Note could form SS^T but would be $N \times N$.

Proper Orthogonal Decomposition

Solve the eigenvalue problem

$$R\psi_i = \lambda_i \psi_i$$

Take the POD basis to be the first $r =$(Reduced dimension) vectors of the form

$$\phi_i = \frac{1}{\sqrt{\lambda_i}} S\psi_i$$

Form the $N \times r$ matrix $\Psi = [\phi_1, \cdots, \phi_r]$
We can now set $F^{(n)} = \Psi F_r^{(n)}$ and have the reduced system

$$\Psi^T \Psi F_r^{(n+1)} = \Psi A \Psi F_r^{(n)}$$

$$\boxed{F_r^{(n+1)} = A_r F_r^{(n)}}$$

here $r << N$.

LBM reformulated for POD

We may write the equilibrium function as

$$f_\alpha^{eq}(\vec{x},t) = \omega_\alpha[(1+\frac{3\tau\Delta t\phi}{2c^2c_\varepsilon}e_\alpha\cdot G)\sum_\beta f_\beta(x,t) + \frac{3}{c^2}(1+\frac{\tau}{c_\varepsilon}-2\tau)e_\alpha\cdot\sum_\beta e_\beta f_\beta(x,t)]$$

where $c_\varepsilon = \frac{1}{2}+\frac{\Delta t\phi\nu}{4k_\varepsilon}$. We assume k is scaler. Denote

$$G_{\alpha\beta}(x) = \omega_\alpha[(1+\frac{3\tau\Delta t\phi}{2c^2c_\varepsilon}e_\alpha\cdot G)+\frac{3}{c^2}(1+\frac{\tau}{c_\varepsilon}-2\tau)e_\alpha\cdot e_\beta]$$

LBM reformulated for POD

We may write using the Einstein summation convection

$$f_\alpha^{eq}(x,t) = G_{\alpha\beta}(x) f_\beta(x,t)$$

We may rewrite the scheme

$$\begin{aligned} f_\alpha(x+\Delta t e_\alpha, t+\Delta t) &= \left(\left(1-\frac{1}{\tau}\right)\delta_{\alpha\beta} + \frac{1}{\tau} G_{\alpha\beta}(x)\right) f_\beta(x,t) \\ &= A_{\alpha\beta}(x) f_\beta(x,t). \end{aligned}$$

In 2-Dimensions let us denote the grid $x^{i,j}$, then we have

$$f_\alpha(x^{i,j}+\Delta t e_\alpha, t+\Delta t) = A_{\alpha\beta}(x^{i,j}) f_\beta(x^{i,j},t)$$

The evolution operator can be reformulated.

LBM reformulated for POD

Assuming that $x^{i,j}$ is not on the boundary, from the shifting rules of the LBM model $D2Q9$ we may write

$$f_\alpha(x^{i,j}, t + \Delta t) = A_{\alpha\beta}(x^{\sigma(\alpha;i,j)}) f_\beta(x^{\sigma(\alpha;i,j)}, t).$$

Here σ is the shift operator which is a function given by the reverse shift rules

$$\sigma(\alpha; i, j) = \begin{cases} (i,j) & \alpha = 0 \\ (i-1,j) & \alpha = 1 \\ (i,j-1) & \alpha = 2 \\ (i+1,j) & \alpha = 3 \\ (i,j+1) & \alpha = 4 \\ (i-1,j-1) & \alpha = 5 \\ (i+1,j-1) & \alpha = 6 \\ (i+1,j+1) & \alpha = 7 \\ (i-1,j+1) & \alpha = 8 \end{cases}$$

If $x^{i,j}$ is on the boundary must be adapted.

For notational simplicity it what follows let

$$F_{\alpha}^{i,j}(t) = f_{\alpha}(x^{i,j}, t) \ , \ A_{\alpha\beta}^{i,j} = A_{\alpha\beta}(x^{i,j})$$

Rewriting the evolution in this notation

$$\begin{aligned} F_{\alpha}^{i,j}(t+\Delta t) &= \sum_{\beta} A_{\alpha\beta}^{\sigma(\alpha;i,j)} F_{\beta}^{\sigma(\alpha;i,j)}(t) \\ &= \sum_{kl} \sum_{\beta} \left(I_{ijkl}^{\alpha} A_{\alpha\beta}^{kl} \right) F_{\beta}^{kl}(t) \\ &= \sum_{kl} \sum_{\beta} B_{ijkl}^{\alpha\beta} F_{\beta}^{kl}(t) \end{aligned} \quad (2)$$

Here the 5-tensor I_{ijkl}^{α} is like a generalized Kronecher delta that respects the shift operator σ. More specifically,

$$I_{ijkl}^{\alpha} = \begin{cases} 1 & \text{if } \sigma(\alpha; k, l) = \sigma(\alpha; i, j) \\ 0 & \text{otherwise} \end{cases}$$

LBM reformulated for POD

For $j, i = 1, 2, \cdots, N$ and $\alpha = 0, 1, \cdots 8$ we flatten the data to a new index as

$$m(\alpha, i, j) = i + (j-1)N + \alpha N^2,$$

for $m = 1, 2, \cdots, M$ and here $M = N + (N-1)N + 8N^2,$.
We flatten

$$\mathbb{F}_m = \mathcal{F}\left(F_\alpha^{ij}\right),$$

and the flattening of the 6-tensor as

$$\mathbb{B}_{mq} = \mathcal{F}\left(B_{ijkl}^{\alpha\beta}\right).$$

Thus, we may rewrite the evolution as

$$\boxed{\mathbb{F}_m(t + \Delta t) = \mathbb{B}_{mq}\mathbb{F}_q(t)}$$

LBM POD Examples: Test Case

Using Fortran test code...

- $\Omega = [0,1]^2$, Periodic Boundaries, $\Delta x = \frac{1}{30}$,$\Delta t = \frac{1}{30000}$
- $[0,2]$ time interval, $G = (1,0), \rho_0 = 10, \tau = .95, \phi = .8$
- $k = .001$ in two inclusions, $k = 1$ else.
- Offline Snapshot IC: $f_\alpha^{i,j} = 10 + sin(x)$
- Online IC: $f_\alpha^{i,j} = 10$
- 200 Snapshots, every 10 time steps.
- Post process from $f_\alpha \to u_x$, L^2 Rel Errors at $t = 1$.

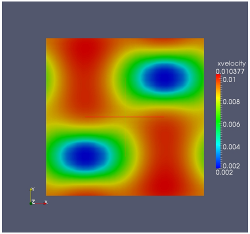


Figure : x-Velocity : Fine-Solve

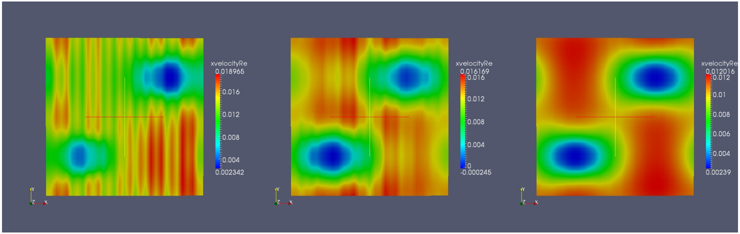


Figure : x-Velocity :5 Modes (67%), 10 Modes (40%), 15 Modes (15%)

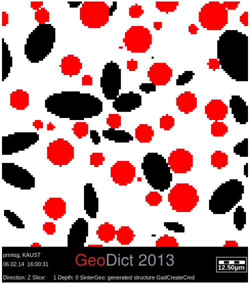


Figure : Geodict Geometry

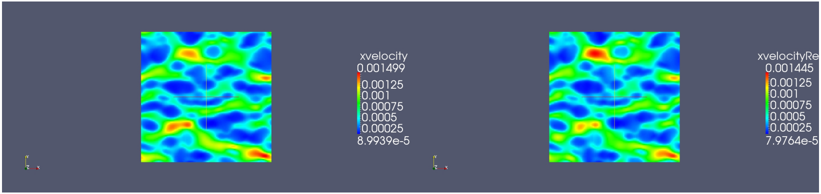


Figure : x-Velocity : Full vs Reduced

LBM POD: Few Casual Observations

In the process of data collection and interpretation...

- Must take snapshot windows bigger than 1 time step
- Due to slow evolution Δt small for stability explicit scheme
- Works well for u, however $p \approx \rho$ does not work well
- Model gives small pressure variations not picked up by POD
- POD highlights high flow regions, usually diffusive

Future works

- Test Robustness of the Modes w.r.t perturbations in k_ε
- Explicit Schemes of LBM-Brinkman (for stability)
- Comparison/Utilization of DMD
- Nonlinear regimes no truncation, nonlinear forcings
- DEIM methods for nonlinear ROM
- Upscaling/POD on more complicated geometries

Questions

Thank you for your time.