Property & Transport Modeling

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Bulk properties, transport properties, material/solute transport

Idealized structures, structural models, explicit structures.

Air flow lines in polar firn (Freitag et al)
Outline for today

Bulk properties, transport properties, material/solute transport

Macroscopic/homogenization:
  means, bounds and 'mixing models'

Percolation theory

Structural models
  Schön, rocks
  sea ice

Pore scale modeling
  Network models
  Lattice Boltzmann

Most idealized structure

Most faithful structure
Modeling Approaches

1. Bounds and means
   Simplest results, useful

2. Kozeny-Carman
   Porosity, structure, percolation thresholds

3. Applied structural models
   Specific materials, composition/cementation/anisotropy
   Self-consistent effective medium (see Berryman, AGU)

4. Pore scale modeling
   Image structures, LB simulations, network models
   Pore-scale effects + critical processes, hydrogeology, remediation, resource development
Flow velocity prediction?
Femlab (finite element matlab)

Abdullah Cihan, University of Tennessee, Knoxville
Solute Transport

0 seconds after slug/pulse injection

Bulk Concentrations v.s t
Means and bounds

\[ J_Q = k_{\text{eff}} \nabla T \]

(a) Parallel

\[ k_p = \sum_i \phi_i k_i \]

Arithmetic mean;

(b) Series

\[ k_s = \left( \sum_i \frac{\phi_i}{k_i} \right)^{-1} \]

harmonic mean;

\[ k = \prod_i k_i \phi_i \]

geometric mean

No physical picture, but it works!
Maxwell & Hashin-Shtrikman

Rigorous bounds if only have statistical homogeneity and isotropy.

\[ k = k_1 \frac{2k_1 + k_2 - 2\phi_2(k_1 - k_2)}{2k_1 + k_2 + \phi_2(k_1 - k_2)} \]

Originally for electric permittivity

+ also thermal conductivity, electrical conductivity

Originally for magnetic susceptibility

\[ K_u = k_2 + \frac{c_1}{\left[1/(k_1 - k_2)\right] + \left[c_2/(3k_2)\right]} \quad c \leftrightarrow \phi \]

\[ K_l = k_1 + \frac{c_2}{\left[1/(k_2 - k_1)\right] + \left[c_1/(3k_1)\right]} \]

Either lower or upper limit applies exactly for Maxwell spheres (when matrix phase has lower or higher conductivity)
Means and bounds

![Graph showing thermal conductivity as a function of fraction low conductivity phase]

- Parallel (Voigt) Bound
- Series (Reuss) Bound
- Geometric Mean
- HS Upper Bound
- HS Lower bound
Structural Model: Sea Ice

Salinity, Temperature, density

\[ s = \frac{g(\text{salt})}{g(\text{water})} \]

Temperature \[\text{°C}\]

\( V_{\text{ice}}, V_{\text{brine}}, V_{\text{air}} \)

Volume fractions

Component properties

Simplified geometric models

Effective medium property

*Weeks & Ackley, 1986*
Structural Models: Schön, Rocks

Effect of cementation/bonding, and anisotropy.

1. Calculate property in micro-system
2. Transform to the macro-system
   eg. Tensorial elastic properties

Schön, Physical Properties of Rocks, p 268.
Structural Models: Schön, Rocks

\[ \phi = \left( \frac{b}{a} \right)^3 \left( 2 \frac{a}{b} - 1 \right) \left( \frac{\alpha_{\text{grain}}}{\alpha_{\text{pore}}} \right) \]

Density

Elastic wave velocities, dry porous rock

\[ V = \left\{ \left[ \frac{M_s}{d_s} \right] \cdot \left[ \frac{2}{1 + M_s / M_c} \right] \cdot \left[ \frac{G(a, b, \alpha_g, \alpha_p)}{1 - \phi} \right] \cdot \left[ s_{mn}(\alpha, f) \right] \right\}^{1/2} \]

Solid velocity  Cementation  Pore geometry  Structural anisotropy

\( M \) – plane wave modulus; \( G \) – geometric factor; \( s_{mn} \) – tensorial transfer matrix
\( d \) – density;
Pore scale Modeling

Obtain 3D internal structure from X-ray Computed Tomography

Characterize pore space

Apply pore scale modelling to calculate flow, permeability, solute transport etc. (eg. LBM, computational fluid dynamics codes)

Imaged, generated, ‘reconstructed’

e.g. Fontainebleau sandstone, Martys and Hagedorn, 2002

Sea ice ‘dynamic’: porosity and permeability depend on S,T
Lattice Boltzmann Modeling

Simulate fluids from a microscopic perspective.
Fluid ‘particles’ stream + collide in a ‘lattice-land’.

Fully recover Navier-Stokes equation

Amenable to complex boundaries.

Highly suitable for parallelization.

Casey Miller, UNC Chapel Hill (www, ppt)
**Lattice Boltzmann Modeling**

\[
f_i - \text{‘particle distribution function’}
\]

(Probability of a) particle moving in this direction

\[
f_i(x + v_i \Delta t, t + \Delta t) = f_i(x, t) + \frac{1}{\tau} \left( f_i^{eq}(x, t) - f_i(x, t) \right)
\]

Streaming + colliding

\[
\rho = \sum_i f_i
\]

\[
\rho \bar{u} = \sum_i f_i \bar{v}_i
\]

density

momentum
Lattice Boltzmann Recipe

Matlab Central file exchange
Google: matlab lattice Boltzmann

Read obstacle file
Initialize density distribution
Loop for time steps / iterations
{
  Stream fluid ‘particles’
  Check for obstacles (bounce back)
  Calc. $\rho$ and $v_\alpha$ components, and $f_\alpha^{eq}$
  Collide: ie. calculate relaxation
  check convergence
}
Output momentum and density distributions.
Take care with obstacle handling and imaging!
Validate against pipe flow and sphere pack geometries.
LB more powerful than this though.. (and in 3D)

Multi-component (eg. water, oil in sandstone)

Multi-phase (gas and liquid)

Solute transport (advection and diffusion)
  - breakthrough curves

Percolation-like models
  – ‘probabilistic boundaries’

Turbulent flows

www.fiu.edu/~thorned/LB/
Lattice Boltzmann Summary

‘Lattice-land’ kinetics lead (quite amazingly!) to Navier-Stokes behavior

(explicit, $O(\Delta t)$, $O(\Delta x^2)$, finite difference approx to incompressible N/S)

Ingredients:
1. lattice
2. Collision operator ($f_{eq}$)
3. Obstacle handling conditions

Pros: Complex geometries, highly parallelizable, multi-phase multi-component flow, suspension/tracer transport

Care: needed with implementation:
lattice choice, boundary handling, collision operator, validation
Modeling Survey Summary

1. Bounds and means
   Simplest results, useful

2. Kozeny-Carman
   Porosity, structure, percolation thresholds

   *Seek simplest picture that captures behavior, but no simpler!*

3. Applied structural models
   Specific materials, composition/cementation/anisotropy

   *Self-consistent effective medium (see Berryman, AGU)*

4. Pore scale modeling
   Image structures, LB simulations, network models

*What are relevant/dominant length scales for processes?*
A Real System: Vuggy Carbonate Aquifer

Pipe Creek, Texas

River basin Area

Limestone matrix with caprinid fossils

4-6 cm diameter Cretaceous caprinid fossil
Flow and Transport Modeling

Provide link between structure and experiment.
Can system be understood in terms of an effective permeability?
What controls tracer (solute) transport?

Matrix (no vugs) \( k = 10 \) mDarcy
Sub-sample (~10 cm)\(^3\) \( k = 100 \) Darcy

Computer tomography slices (0.5 x 0.5 x 1.5 mm)
Flow and Transport: Approaches

1. Medial axis and statistics
   - Simple pipe flow
   - Simple pipe networks
   - Medial-axis pipe networks

2. CT output structures
   - ‘Darcy code’: modeling
   - 2D Lattice Boltzmann

3. Dual porosity model fitting
Insights from Poiseuille Flow

\[ \bar{u} = -\frac{k}{\mu} \nabla p \]

\[ k_{pipe} = \frac{r_0^2}{8} \quad 1 \text{ Darcy (D)} \sim 10^{-12} \text{ m}^2 \]

Parallel
\[ k_{eff} = \sum k_i \frac{a_i}{l_i} \]
Large \( k \) dominate

Series
\[ \frac{1}{k_{eff}} = \sum \left( k_i \frac{a_i}{l_i} \right)^{-1} \]
Small \( k \) dominate
Insights from Poiseuille Flow

\[ \bar{u} = -\frac{k}{\mu} \nabla p \]

\[ k_{pipe} = \frac{r_0^2}{8} \]

1 Darcy (D) ~ $10^{-12}$ m$^2$

d = 10 cm

\[ k_{mx} = 10 \text{ mD}, \quad k_{pipe} = 45 \text{ D} \]

\[ n=2: \quad k_{eff} = 90 \text{ Darcy} \]

Small constrictions can strongly control $k_{eff}$
Pipe Network Model

INPUT: Medial axis path network

NB: more usual to use pore/throat network, but we had medial axis data available first!
Pipe Network Formulation

Poiseuille flow

\[ q_i = -\frac{\pi r^4}{8 \mu L_i} (P_i - P_r) \]

Mass balance

\[ \sum q_{in} = \sum q_{out} \]

Conjugate gradient method on normal equations:

\[ A^T A x = A^T b \]
### Medial Axis Network

**Simulated Permeability**

![Medial Axis Network Diagram]

<table>
<thead>
<tr>
<th></th>
<th>$K_{xu}$</th>
<th>$K_{xd}$</th>
<th>$K_{yu}$</th>
<th>$K_{yd}$</th>
<th>$K_{zu}$</th>
<th>$K_{zd}$</th>
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<tbody>
<tr>
<td>50×50×50$^a$</td>
<td>1 $\times$ 10$^6$</td>
<td>2 $\times$ 10$^6$</td>
<td>8 $\times$ 10$^6$</td>
<td>1 $\times$ 10$^6$</td>
<td>1$\times$10$^6$</td>
<td>1 $\times$ 10$^6$</td>
</tr>
<tr>
<td>100×100×100</td>
<td>10500</td>
<td>30200</td>
<td>152</td>
<td>439</td>
<td>9630</td>
<td>839</td>
</tr>
<tr>
<td>300×300×300</td>
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<td>1110</td>
<td>985</td>
<td>1400</td>
<td>3080</td>
<td>606</td>
</tr>
</tbody>
</table>

$^a$ Image resolutions. Medial axis flow paths are used for simulation.

$^b$ Flow directions.

**Upscaling dependence and Variability**

- **2-scale problem**!
- Voxel-sized restrictions to flow
- Vug scale ~ sample size
**Image coarsening**

- cut central 300x300x100 subset of the segmented image
- original z-direction slices multiplied 3 times to match resolution in x- & y-directions $\rightarrow 300^3$
- the image coarsened by using majority rule in the boxes of appropriate size

**Results:**

<table>
<thead>
<tr>
<th>Size</th>
<th>Porosity</th>
<th>Connectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$300^3$</td>
<td>17.8%</td>
<td>83.3%</td>
</tr>
<tr>
<td>$100^3$</td>
<td>17.2%</td>
<td>83.0%</td>
</tr>
<tr>
<td>$50^3$</td>
<td>16.9%</td>
<td>84.7%</td>
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</table>

Connectivity = percentage of pore space in the largest connected component
References


