Simulating Three Dimensional Flow in Porous Media

An immersed boundary method approach

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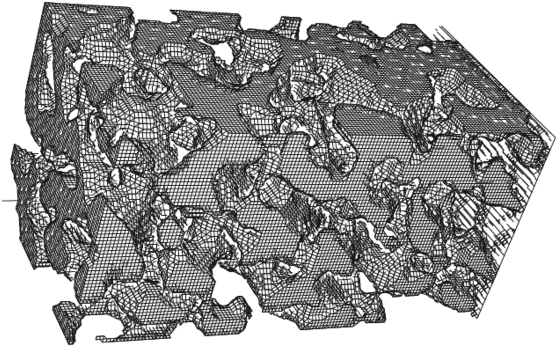
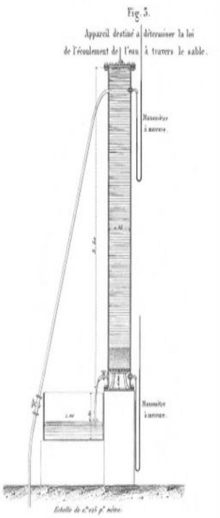
An immersed boundary method is applied within EULAG to resolve flow through three dimensional porous media.



Darcy's Experiment

Darcy's Law

$$\frac{Q}{A} = -k\frac{\nu}{g}\frac{\Delta H}{L}$$



Methods for Simulating Flow Through Porous Media

The Lattice-Boltzmann method approximates the Navier-Stokes equations using the Boltzmann equations on a discrete lattice and can be applied to either single or multiphase flow in arbitrary geometries [Succi(2001)] [Chen and Doolen(1998)].

Smooth particle hydrodynamics simulates flow in a Lagrangian setting to reduce computational needs [Tartakovsky and Meakin(2005a)], [Tartakovsky and Meakin(2005b)].

Generating an unstructured mesh within the pore-space and finite element or finite volumes method to numerically solve the Navier-Stokes equations on that mesh [Zaretskiy et al.(2010)Zaretskiy, Geiger, Sorbie, and Förster].

Imposing Internal Boundary Conditions

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} &= -\nabla \pi' + \mathbf{g}' + \mu \triangle \mathbf{v} - \alpha \mathbf{v} \\ \nabla \cdot \mathbf{v} &= 0 \end{aligned}$$

- $\alpha(\mathbf{x}) = 0$ within the fluid admits Navier-Stokes flows away from the solid boundaries, while requiring $\alpha(\mathbf{x}) \gg 1$ within the solid assures $\mathbf{v} \to 0$ there.
- An Immersed boundary method that imposes boundary conditions within the governing equations, [Peskin(1972)] [Mittal and Iaccarino(2005)]
- Stands upon MPDATA and the preconditioned nonsymmetric Krylov-subspace solver with in EULAG.

Initial work in *Pores resolving simulation of Darcy flows* [Smolarkiewicz and Winter(2010)]

A little about α

- The IMB allows the simulations to remain on uniform Cartesian grid and avoids complex mesh generation.
- Each run takes about $\approx$ 10 minutes of wall clock time using 64 processors while other numerical methods such as lattice Boltzmann and smooth particle hydrodynamics take $\approx$10 hours to converge on thousands of processors.
- In [Smolarkiewicz et al.(2007)], the authors used this IMB to reproduce wind tunnel experiments of flow around solid bodies.

Design of Experiments

Study the effect that variations in pore-space geometry and topology have on properties in the fluid velocity field inside of synthetic data and tuff and glass beads.

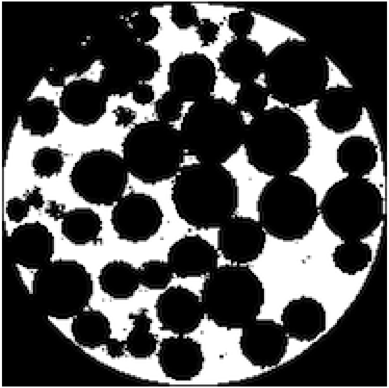
- Cartesian Domain
  $L_x \times L_y \times L_z = 1.27 \times 10^{-2} \times 1.27 \times 10^{-2} \times 2.55 \times 10^{-2}$ m^3
- Resolved with $N_x \times N_y \times N_z = 128 \times 128 \times 256$
- $\Delta x = \Delta y = \Delta z = 10^{-4}$ m
- $\Delta t = 5 \cdot 10^{-5}$ s
- Courant Number ≈ 0.2
- Periodic domain in the vertical direction with no flow on the lateral boundaries.
- Run the simulation past steady state then evaluate the flow field.

Porous Media

1. Use real pore spaces from high resolution imaging using X-Rays and MRI or carefully slicing a pore-space.
2. Stochastically generated synthetic porous media using level set percolation.

Real Porous Media

Glass Beads



1 pixel = 17.1 micron

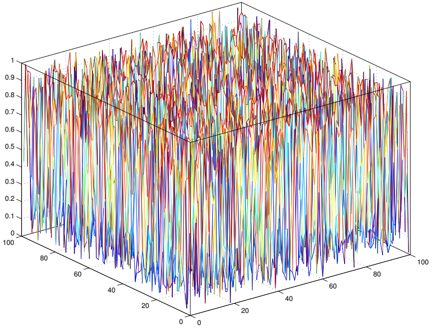
Crushed Dry Tuff

1 pixel = 16.8 micron

ref : Wildenschild et al., 2004 and Culligan et al., 2004

Stochastic Generation of Synthetic Porous Media

1. Generate independent identically distributed random variables uniformly on a lattice.
2. Numerical convolution of the random field to create a correlated random surface.
3. Apply a threshold the surface to determine void space and solid space.
4. The result is a complex network of interconnected pores.



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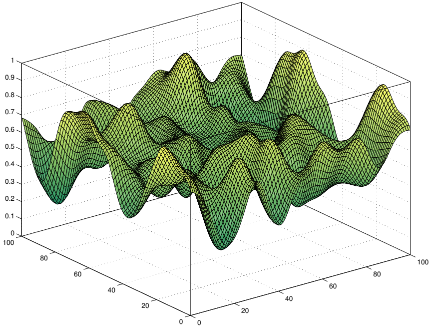

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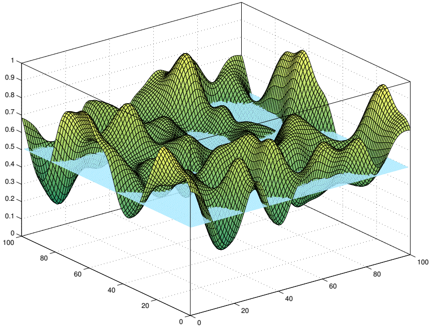

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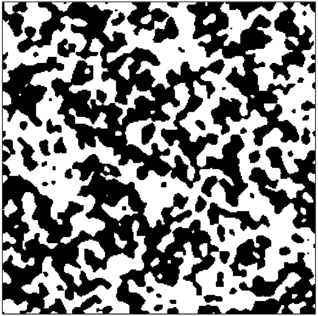
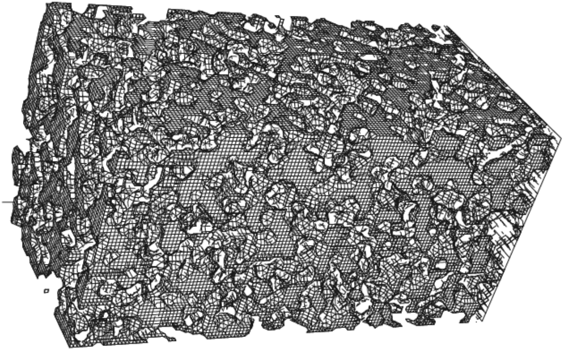


Synthetic Porous Media



Shown as 1/8th of actual domain

ref: *Pores resolving simulation of Darcy flows* [Smolarkiewicz and Winter(2010)]

Bulk Properties

Porosity,

$$n = V_P/V,$$

measures the relative capacity of a porous medium to hold water while mean hydraulic radius,

$$R = V_P/A,$$

indicates the average level of connectivity in the network. A is the total interstitial area between the pore space and the solid matrix.

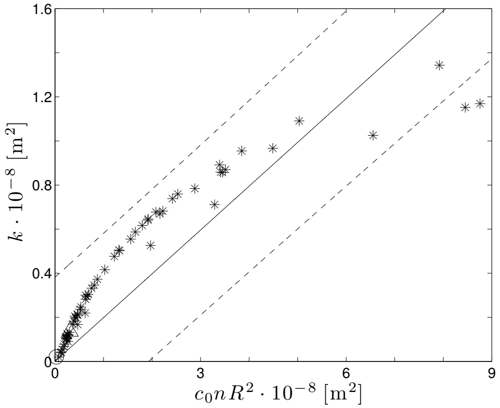
Kozeny Equation

Kozeny equation

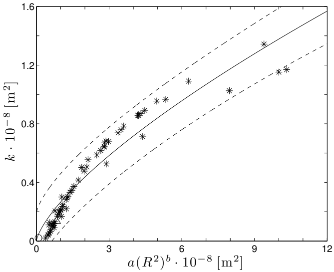
$$k = c_0 n R^2$$

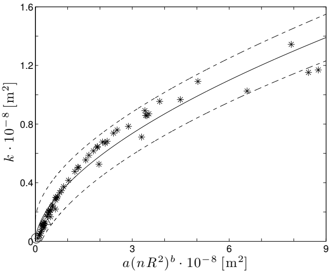
$$c_0 = 1/5$$

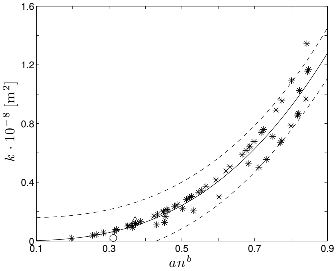
(Predicted value [Bear(1988)])



Power-Law Alternatives







$$
\begin{aligned}
(a) \quad k &= \quad a(R^2)^b \\
(b) \quad k &= \quad a(n)^b \\
(c) \quad k &= \quad a(nR^2)^b
\end{aligned}
$$

Comparison of Models

Table: Accuracy of the four fitted models.

Model Form	Fit	s_d^2
$k(nR^2) = c_0 nR^2$	$\hat{k} = 0.19nR^2$	$2.26 \cdot 10^{-16}$
$k(nR^2) = a(nR^2)^b$	$\hat{k} = 1.68 \cdot 10^{-4}(nR^2)^{0.58}$	$3.12 \cdot 10^{-17}$
$k(n) = an^b$	$\hat{k} = 1.72 \cdot 10^{-8}(n)^{2.83}$	$3.72 \cdot 10^{-17}$
$k(R^2) = aR^{2b}$	$\hat{k} = 1.37 \cdot 10^{-3}(R^2)^{0.71}$	$5.61 \cdot 10^{-17}$

The sum of squared departures of the simulated data from the model estimates, $s_d^2 = \sum_{i=1}^{N}(\hat{k}_i - k_i)^2$.

Comparison of Models

Table: Analysis of Variance

Model	P	s_M^2/P	$N-P$	$s_d^2/(N-P)$	F
Kozeny eq.	1	$1.74 \cdot 10^{-15}$	62	$3.65 \cdot 10^{-18}$	475.77
power law $k(nR^2)$	2	$9.65 \cdot 10^{-16}$	61	$5.16 \cdot 10^{-19}$	1866.17
power law $k(n)$	2	$9.62 \cdot 10^{-16}$	61	$6.11 \cdot 10^{-19}$	1574.55
power law $k(R^2)$	2	$9.52 \cdot 10^{-16}$	61	$9.20 \cdot 10^{-19}$	1034.89

The model sum of squares, $s_M^2 = \sum_{i=1}^{N} (\hat{k}_i - \langle k \rangle)^2$, reflects the ability of the model to capture the structure of the data as departures from the sample mean, $\langle k \rangle$. The ratio,

$$F = \frac{s_M^2/P}{s_d^2/(N-P)}$$

can be used to compare models.

Restricted Domain

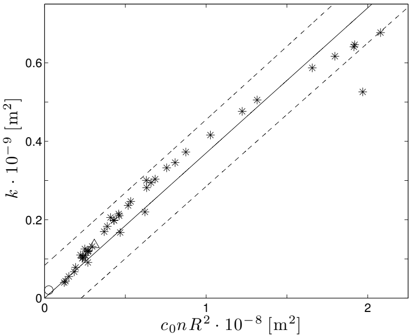
We also consider a restricted porosity domain $n \in (0.2, 0.7)$ as defined by [Xu and Yu(2008)]

Kozeny equation

$$k = 0.37nR^2$$

$$F = 1132.82$$

The computed Kozeny coefficient, $c_0 = 0.37$, is within the range $1/6 < c_0 < 1/2$ reported by Carman [Carman(1956)].



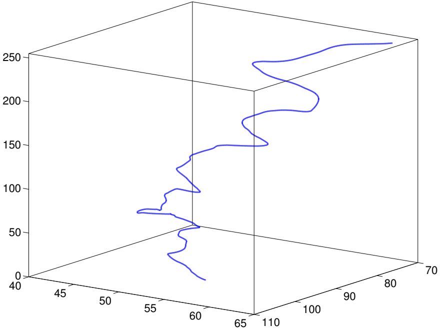
Particle Trajectories

Using an explicit fourth order Runga-Kutta scheme the equation for the motion of a particle starting at the point $\mathbf{x}_0$,

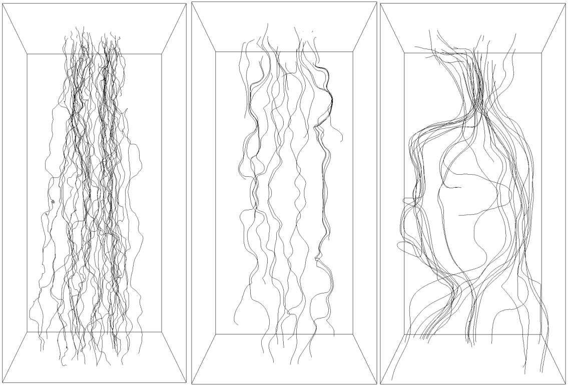
$$\frac{d\mathbf{x}(t,\mathbf{x}_0)}{dt} = \mathbf{v}(\mathbf{x}(t,\mathbf{x}_0))$$

is numerically integrated forward in time.

Trilinear interpolation is used to compute the particle velocity at locations between computational nodes.



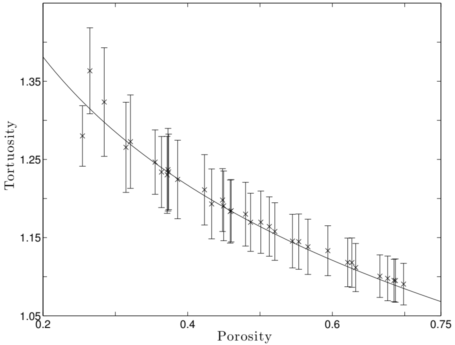
Particle Trajectories



Particle Trajectories in a synthetics media (left), glass bead (center), and tuff (right);

Particle Trajectories : Tortuosity and Porosity

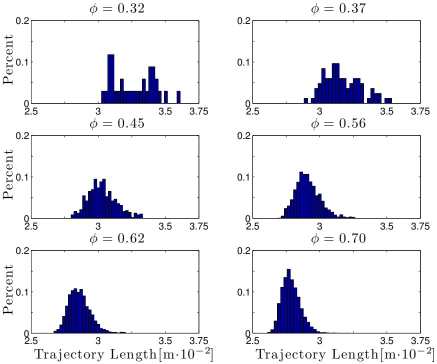
- Tortuosity, $\tau(a,b) = l_S/l$, of a trajectory connecting two points a and b is the dimensionless ratio of total length of the trajectory, l_S, over the Euclidean distance between a and b, $l = \|a-b\|_2$.
- Porosity $n = V_p/V$ is the dimensionless ratio of the volume of void space over the bulk volume of a porous medium.



$$\tau(n) = 1 - a\log(n)$$

Particle Trajectories : Trajectory Length

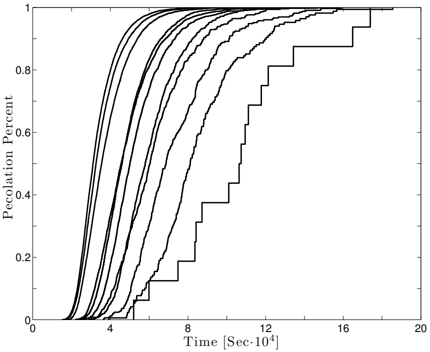
As the porosity of the synthetic medium increases the variance of the distributions of trajectory lengths decrease indicating that the trajectories are becoming more uniform.



Particle Trajectories : Breakthrough Curves

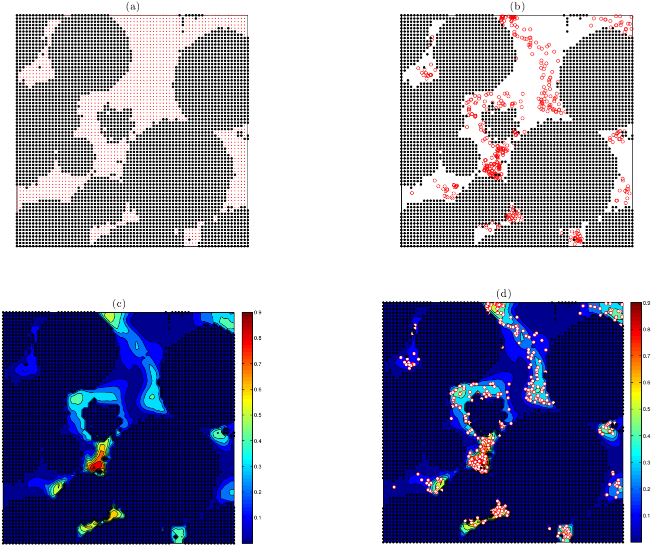
The empirical distribution function of particle travel time through the domain is similar to the classically defined breakthrough curve for an advection dispersion equation.

As the porosity of the synthetic medium increases the breakthrough curves sharpen indicating the velocity becomes more homogenous.



Particle Trajectories : Channeling

Observational domain size : $1.15 \cdot 10^{-7}\text{m} \times 1.15 \cdot 10^{-7}\text{m} \times 2.3 \cdot 10^{-7}\text{m}$



Particle Trajectories : Channeling

Additional Applications

1. Chemical transport and reaction within a porous medium.
2. Spatially varying α to represent permeability on the continuum scale as an alternative to solving the flow equations.
3. Further investigation of which physical characteristics lead to channeling.

Thank you

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