Pore-Scale Physics and Large-Scale Flow Simulation

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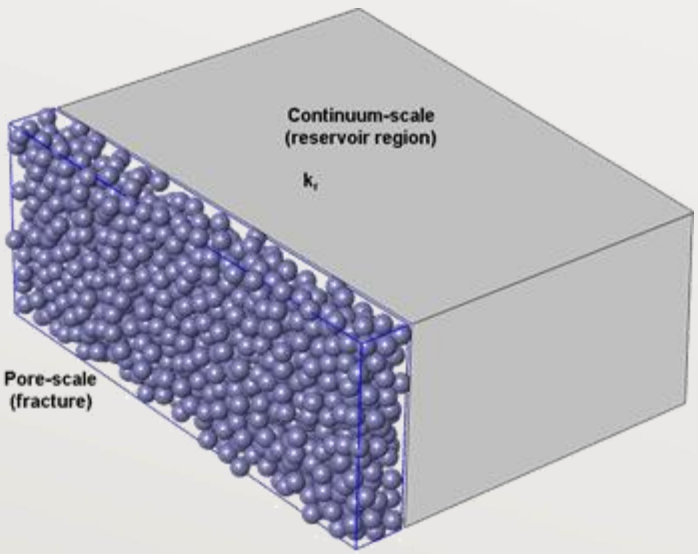
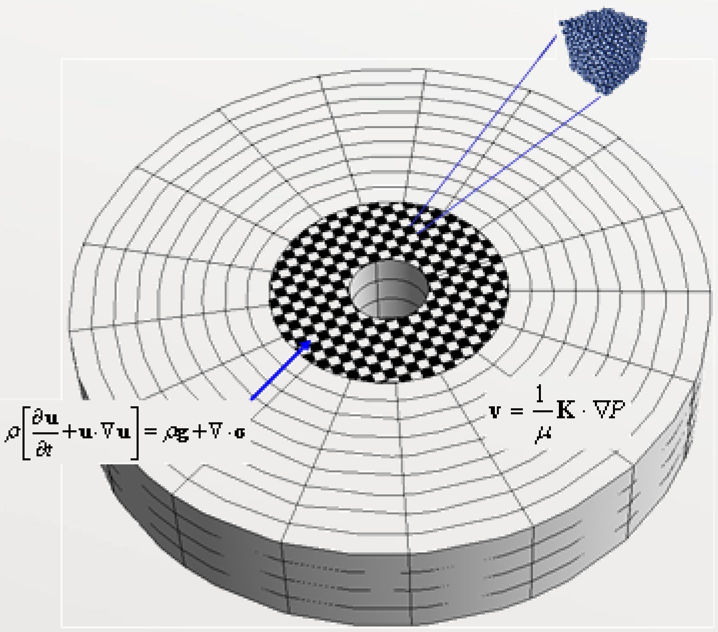
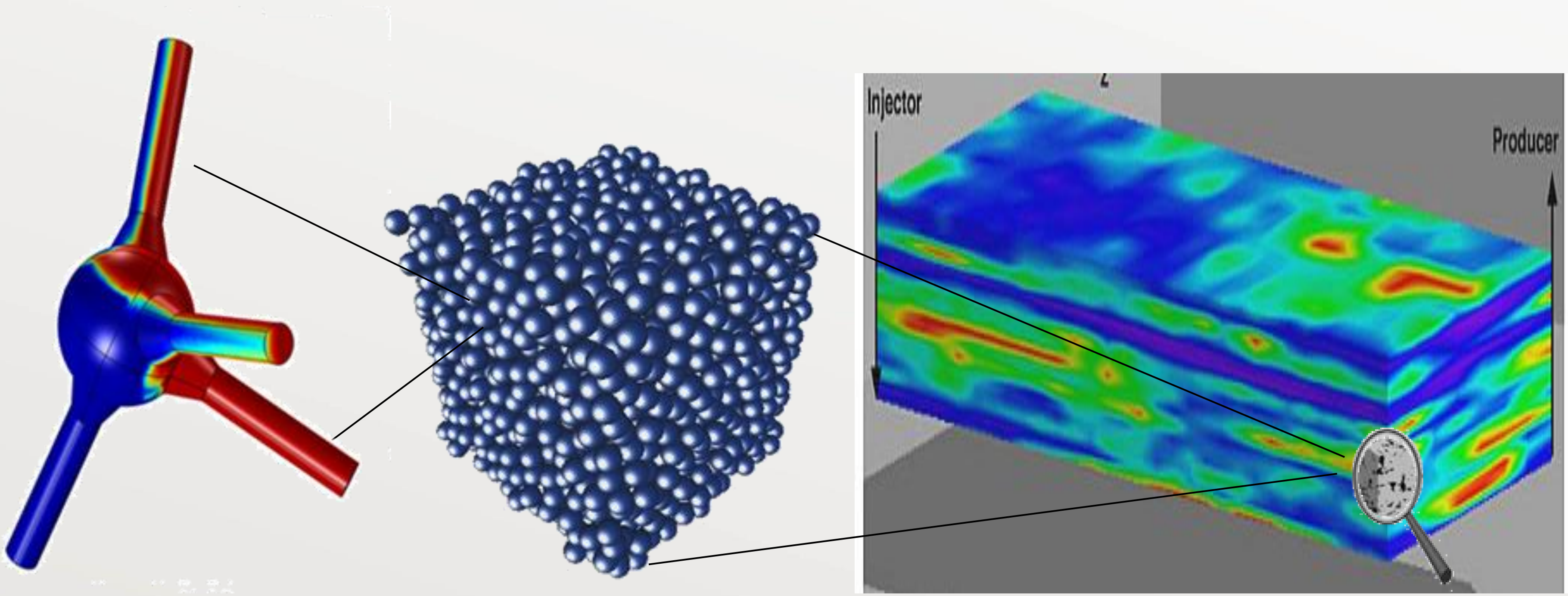
Computational Issues in Oil Field Applications Tutorials

March 22, 2017





10^{-9} m	10^{-5} m	10^{-1} m	10^{2} m
streamline scale	**pore scale**	**continuum scale**	**macroscopic scale**



Adapted from Karsten Thompson, LSU

10^{-9} m	10^{-5} m	10^{-1} m	10^{2} m
streamline scale	**pore scale**	**continuum scale**	**macroscopic scale**

Fundamental, but impractical for "engineering-scale" modeling

$$\upsilon \nabla^2 u - \nabla p = 0 \qquad \nabla \cdot u = 0$$

$$u = 0 |_{\partial B}$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D \nabla c + uc) = 0$$

$$-n \cdot D \nabla c = k(c^n - c_0^n)$$

Upscaling →

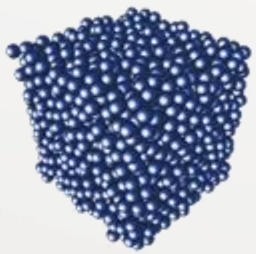
Practical for "engineering-scale" problems. Parameters mostly based on modeling or empiricism

$$\nabla \cdot ({}^{K}\!/\!_{\mu} \nabla P) = 0$$

$$\frac{\partial C}{\partial t} + \nabla \cdot (-\overline{D} \nabla C + \overline{u} C) + R(C) = 0$$

Adapted from Karsten Thompson, LSU

Petrophysical Experimental Measurements

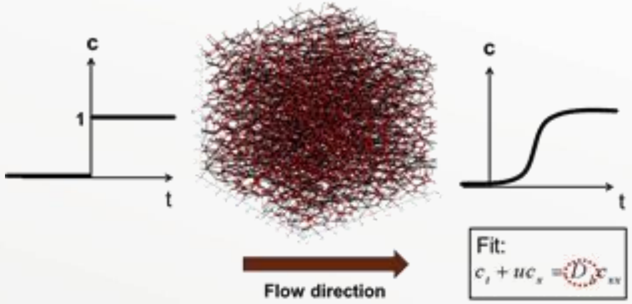


Porosity

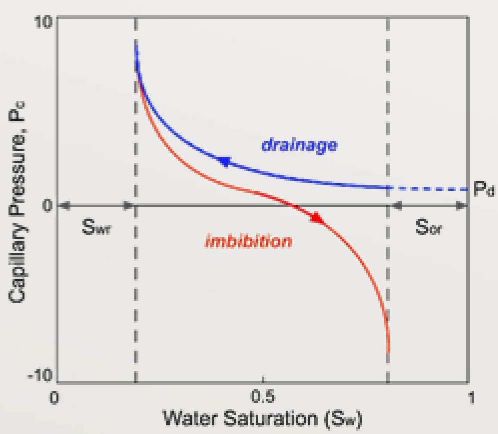
$$\phi = \frac{V_{void}}{V_{bulk}}$$

Permeability

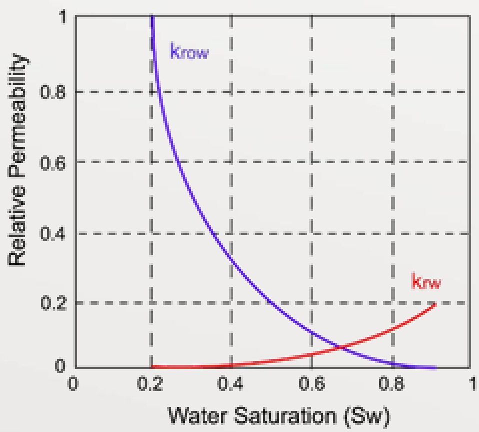
$$k = \frac{q\mu L}{A\Delta P}$$



Dispersion

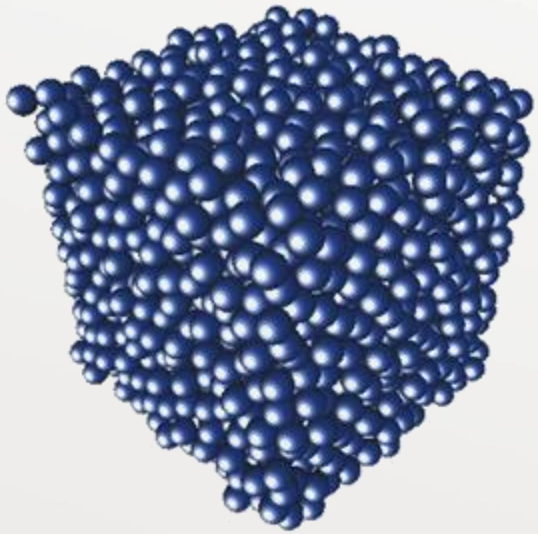


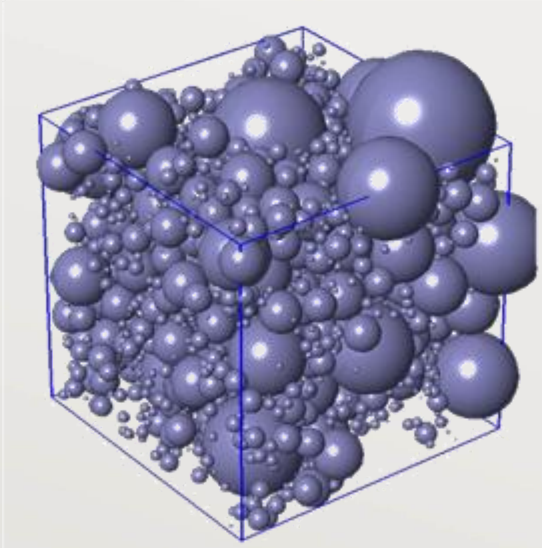
Capillary Pressure $P_c\left(S_w\right) = P_{nw} - P_w$



Relative Permeability $k_{r\alpha} = \frac{q_\alpha \mu L}{kA\Delta P}$

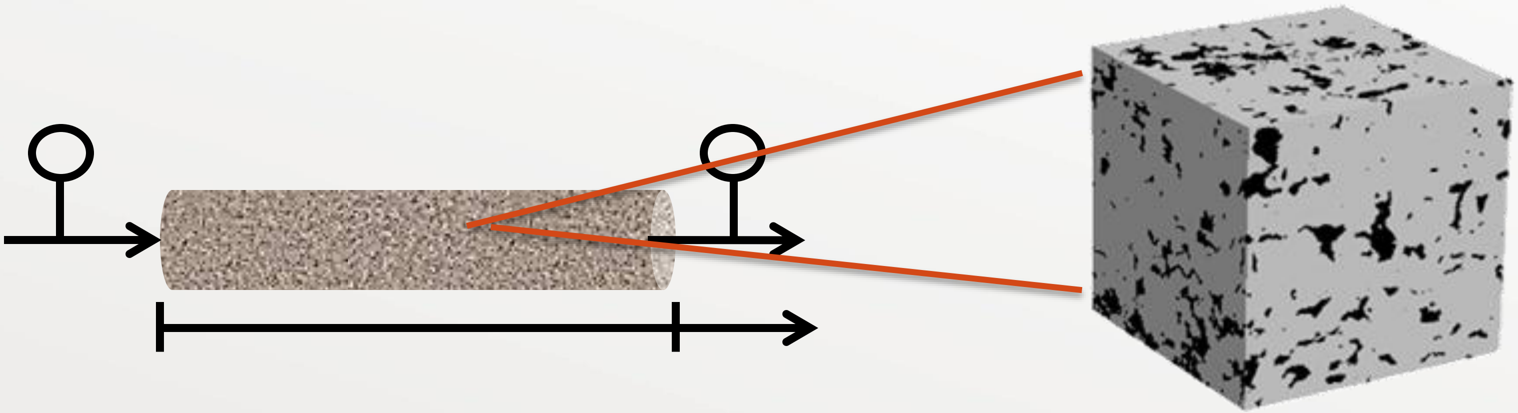
Computer-Generated Materials





- Digitally create porous medium
- Place particles
  - Provide location (spatially correlated)
  - Size distribution
  - Ensure no overlap, gravitationally stable
- Attempt to create synthetic, real rocks
  - Change grain shape
  - Diagenesis, cementation, etc.

3D Imaging and Image Processing



- X-ray micro-CT (XMT) used to image the rock sample (~ mm^3) and collect slices
- Voxels used to discretize the medium
- Grey-scale (e.g. 0 to 255) used to distinguish rock from void space/fluids
- Segmentation and filtering often required

Digital Rocks Portal: *Preserving, visualization and upscaling based on porous media images*

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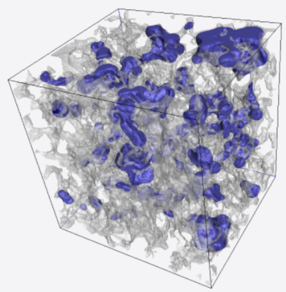

Direct simulation of residual phase (disconnected blobs in blue) in Berea Sandstone (imaged based pore grain surface shown in transparent gray).

Digital Rocks Portal

Digital Rocks is a data portal for fast storage and retrieval, sharing, organization and analysis of images of varied porous micro-structures. It has the purpose of enhancing research resources for modeling/prediction of porous material properties in the fields of Petroleum, Civil and Environmental Engineering as well as Geology.

This platform allows managing, preserving, visualization and basic analysis of available images of porous materials and experiments performed on them, and any accompanying measurements (porosity, capillary pressure, permeability, electrical, NMR and elastic properties, etc.) required for both validation on modeling approaches and the upscaling and building of larger (hydro)geological models.

Browse Published Projects

Research public datasets that are hosted on Digital Rocks. You can view, search, and download metadata, raw and derived data, and find publications related to datasets that Digital Rocks users have uploaded and published.

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- **Upload and document** large datasets
- **Publish and reference** data in papers (DOI)
- **Visualize data remotely** on parallel cluster (Texas Advanced Computing Center)

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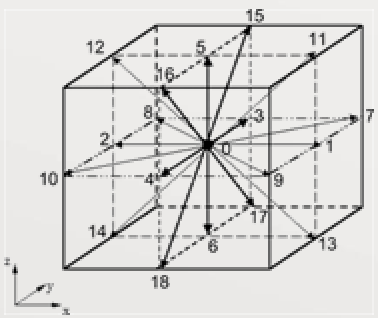
TACC CENTER FOR PETROLEUM & CPGE GEOSYSTEMS ENGINEERING NSF

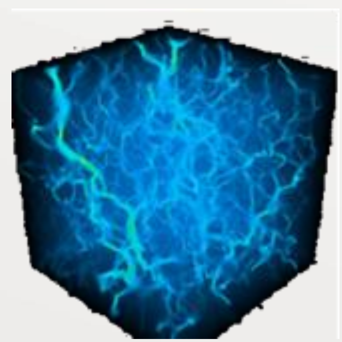
Direct Numerical Simulation

- **Computational Fluid Dynamics** (e.g. FEM)

- **Lattice Boltzmann Method**. Fluid described by moving particles. Particles have finite number of discrete velocity values.
  - Collective behavior of particles represented by “particle distribution function” (PDF): $f(\boldsymbol{X}, \boldsymbol{V}, t)$
  - Equation of motion for the PDF is known as the Boltzmann equation:

$$\frac{\partial}{\partial t} f(\boldsymbol{X}, \boldsymbol{V}, t) + V \cdot \nabla f(\boldsymbol{X}, \boldsymbol{V}, t) = \Omega(f(\boldsymbol{X}, \boldsymbol{V}, t))$$

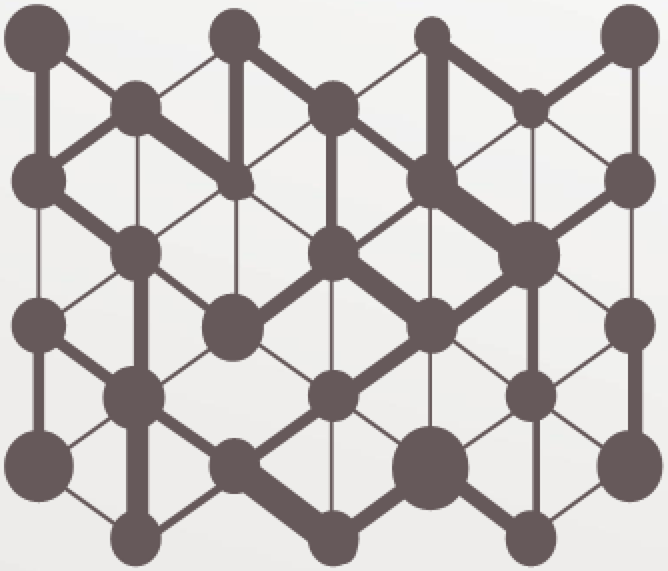




Flow velocity in pore space
(Aaltosalmi, 2005)

- **Smoothed Particle Hydrodynamics (SPH)** divides fluid into a set of discrete element (particles) and trace the movement of each particle. Lagrangian formulation of the Navier-Stokes equation

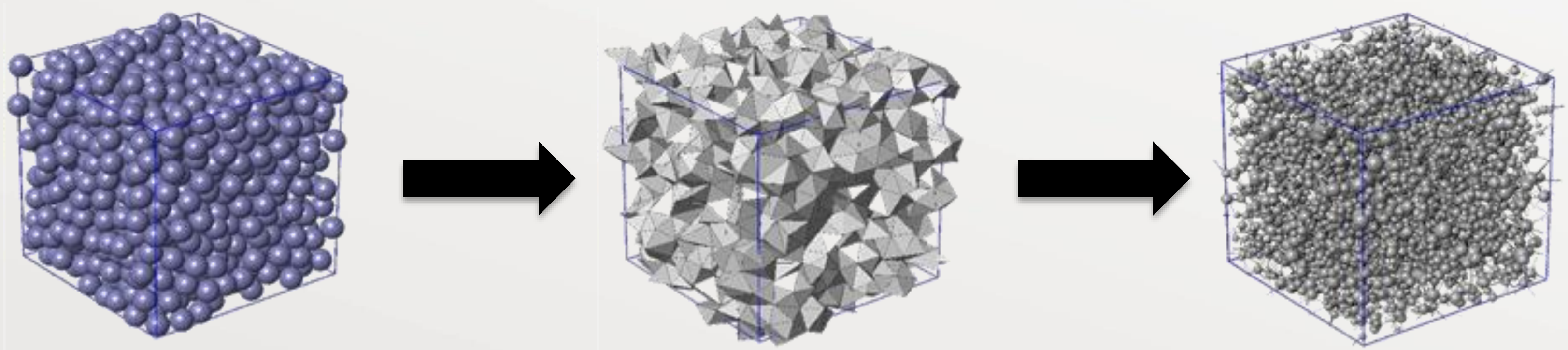
Pore-Scale Network Modeling



Network Generation Techniques

- **Statistical methods** create a network of pores and throats that mimic the statistics of properties of the original medium

- **Grain-based methods** are usually tied to approaches that represent grain positions in porous media

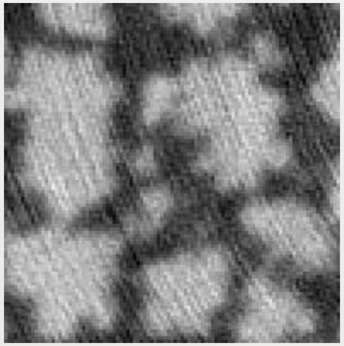


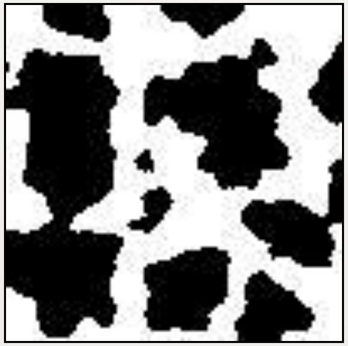
- **Medial Axis** can be used to thin the void space, from which one can map out the pores and throats in the network (skeleton is formed)

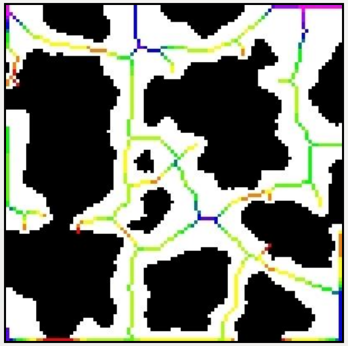
Example Image Analysis Workflow

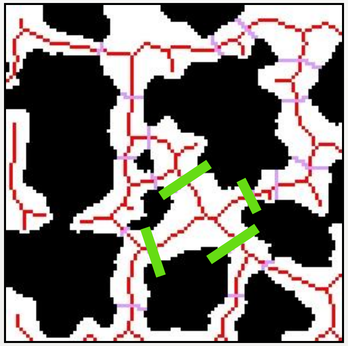
Rock models/grain network.
formation resistivity factor,

direct fluid flow simulation…









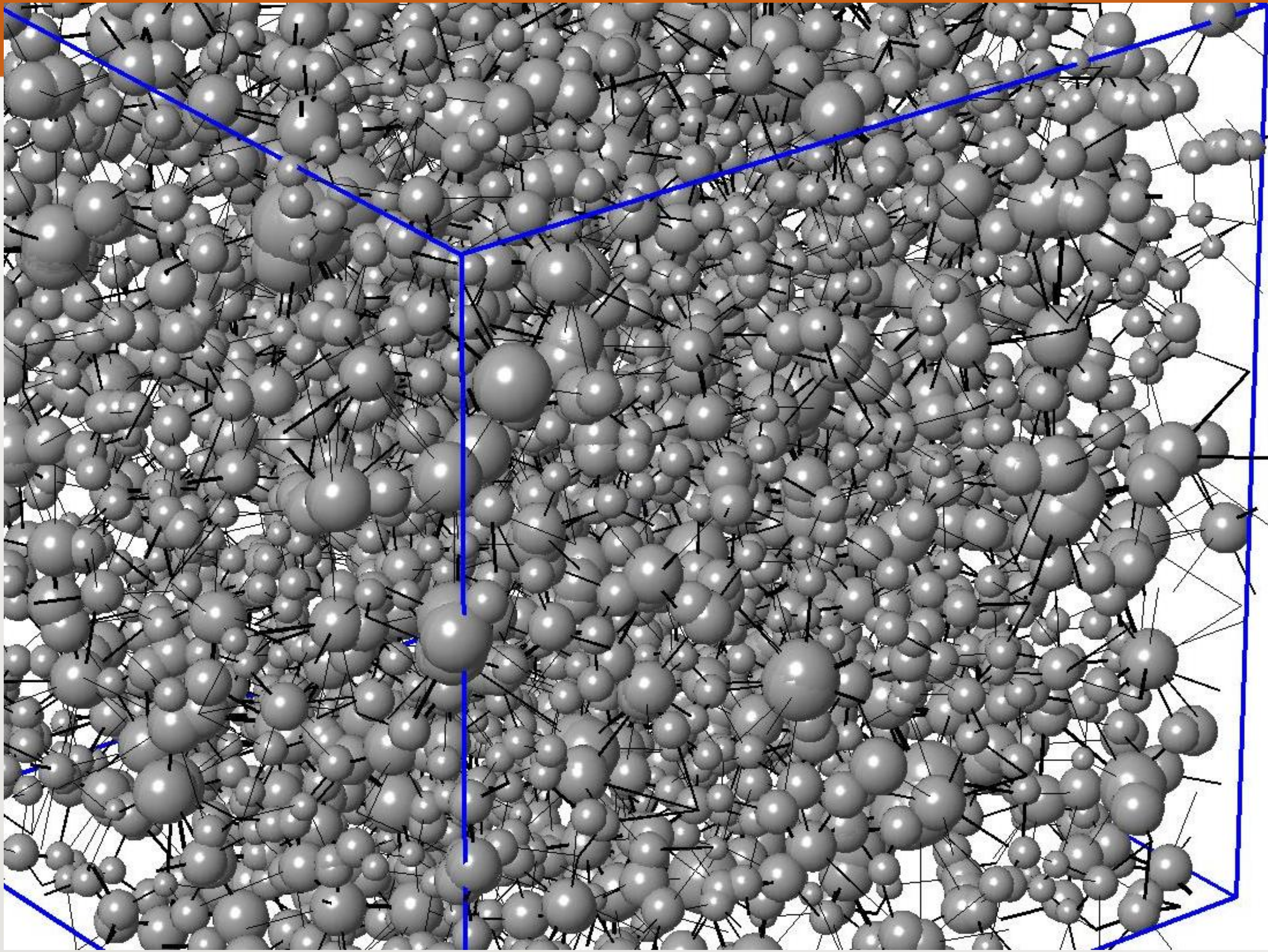
Segmentation

Medial Axis (MA) extraction

Throat finding +
pore partitioning

Pore/throat
characterization
Semi-upscaled simulation

From 3DMA-Rock software webpage
B. Lindquist & M. Prodanovic

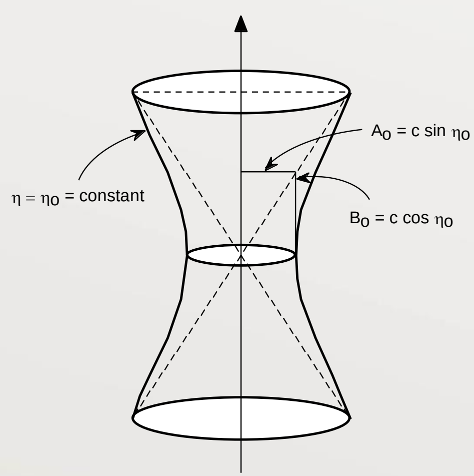


Network Parameters and Statistics

Variable Association	Variable Name	Variable Type	Dimension
Network	Domain dimensions	vector	length
Pore	Location	vector	length
	Void volume	scalar	length^3
	Maximum inscribed radius	scalar	length
Throat	Interconnectivity:periodicity	scalar:vector	
	Cross-sectional area	scalar	length^2
	Maximum inscribed radius	scalar	length
	Surface area	scalar	length^2
	Hydraulic conductivity	scalar	length^3

Hydraulic Conductivity

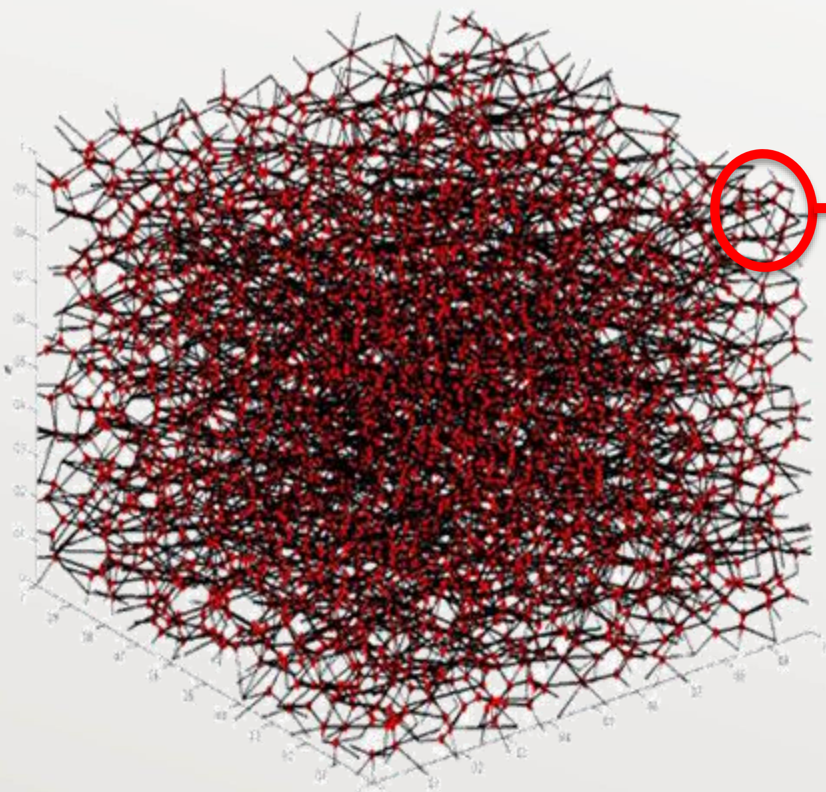
$$g_{ij} = \frac{\pi R_{eff,ij}}{8L_{ij}}; R_{eff,ij} = \frac{2A}{P}$$

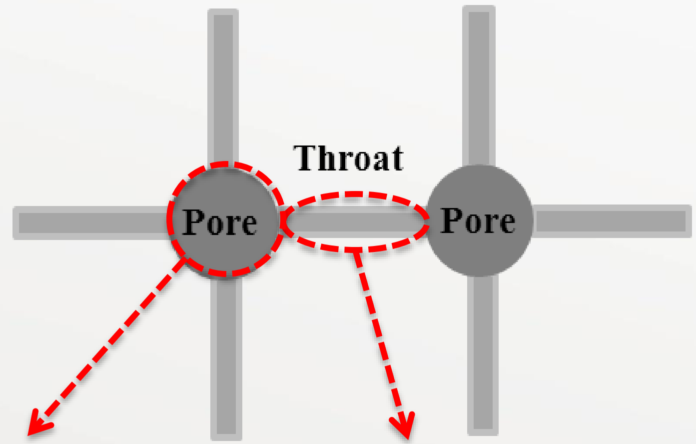


$$\frac{g_{venturi}}{g_{tube}} = \frac{4L(1+2\zeta_o)(1-\zeta_o)^2}{3r_{eff}(\sin \eta_o)^3\left(\frac{\lambda_R}{\lambda_R^2+1} + \tan^{-1}\lambda_R\right)}$$

Happel and Brenner (1973);
Thompson and Fogler (1997)

Mass and Momentum Balance Equations

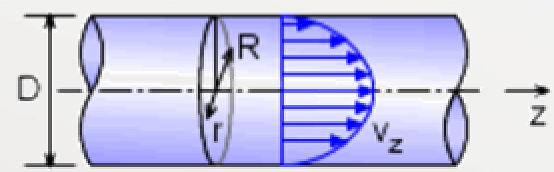




Mass Balance:

$$\sum_{j=1}^{n} \dot{m}_{ij} = 0$$

$$\left(\nabla \cdot u = 0\right)$$



$$\dot{m}_{ij} = \frac{\rho \pi R^4}{8 \mu L}(p_j - p_i) = \frac{g_{ij}}{\mu}(p_j - p_i)$$

$$\left(\upsilon \nabla^2 u - \nabla p = 0\right)$$

Matrix Equations and Solution Methods

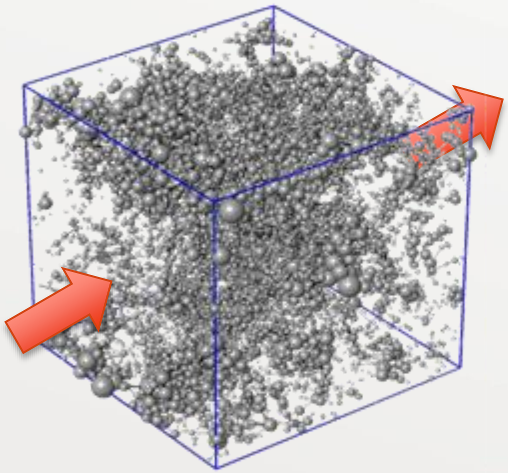
$$
\frac{1}{\mu}\underbrace{\begin{pmatrix}
\sum_j g_{1j} & -g_{12} & 0 & \cdots & -g_{1N} \\
-g_{21} & \sum_j g_{2j} & -g_{23} & & 0 \\
0 & -g_{32} & \sum_j g_{3j} & & \\
 & & & \ddots & \\
-g_{N1} & 0 & 0 & & \sum_j g_{Nj}
\end{pmatrix}}_{N\times N}
\underbrace{\begin{pmatrix} P_1 \\ P_2 \\ P_3 \\ \vdots \\ P_N \end{pmatrix}}_{N\times 1}
=
\underbrace{\begin{pmatrix} \frac{g_{in}}{\mu} P_{Bin} \\ 0 \\ 0 \\ \vdots \\ \frac{g_{out}}{\mu} P_{Bout} \end{pmatrix}}_{N\times 1}
$$

- *N×N* Matrix is square, sparse and diagonally-dominate
- *Not banded* in general
- System can be solved using indirect solvers (e.g. Conjugate Gradients)

Permeability Calculation

$$q = \frac{kA}{\mu}\frac{\Delta P}{L}$$

Darcy's Law



$$k = \frac{\mu L_{network} \sum_{j=1}^{N_{edges}} \frac{g_{ij}}{\mu}\left(P_j - P_i\right)}{A\left(P_{in} - P_{out}\right)}$$

- Calculate both faces to confirm mass balance
- Periodic or no-flow BCs on other four faces
- Measure anisotropy by changing flow direction
- Matches experimental data well in many cases

Non-Darcy Flow in Porous Media

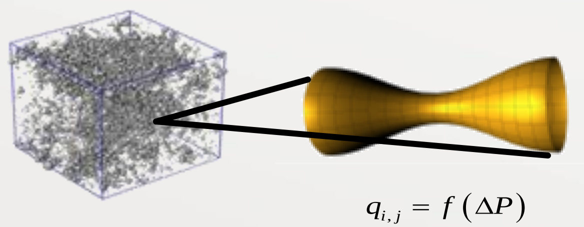
Navier-Stokes Equations

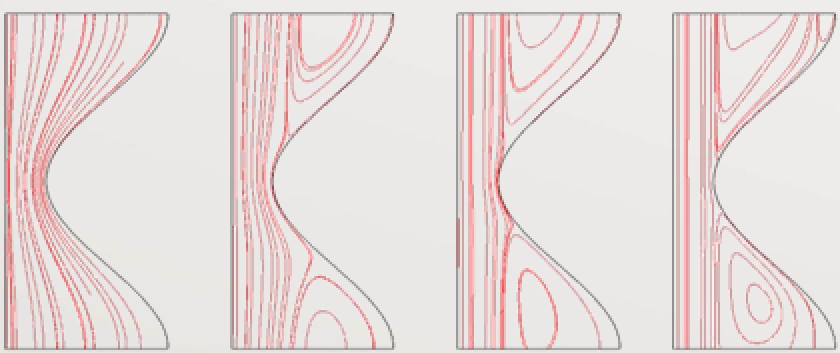
$$\rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla \mathbf{P} + \mu \nabla^2 \mathbf{v}, \nabla \cdot \mathbf{v} = 0$$

Forchheimer Equation

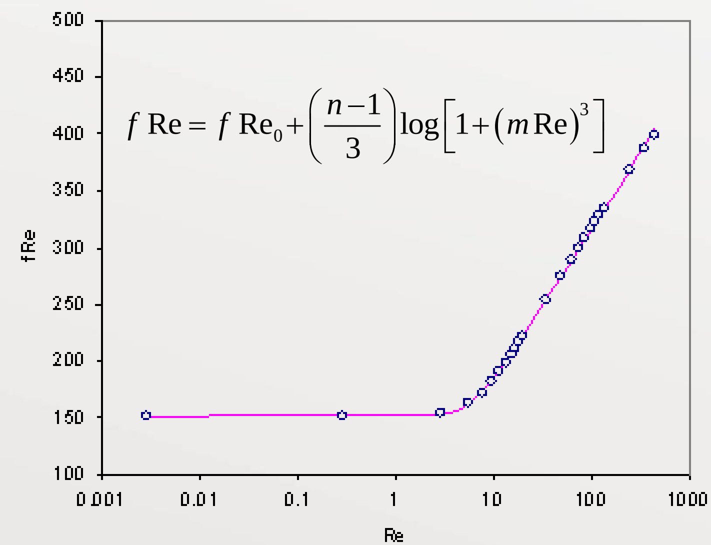
$$\frac{\partial P}{\partial z} = -\frac{\mu}{K} v + \rho \beta v^n; n = 2$$

FEM simulations in throats to develop pore level equations

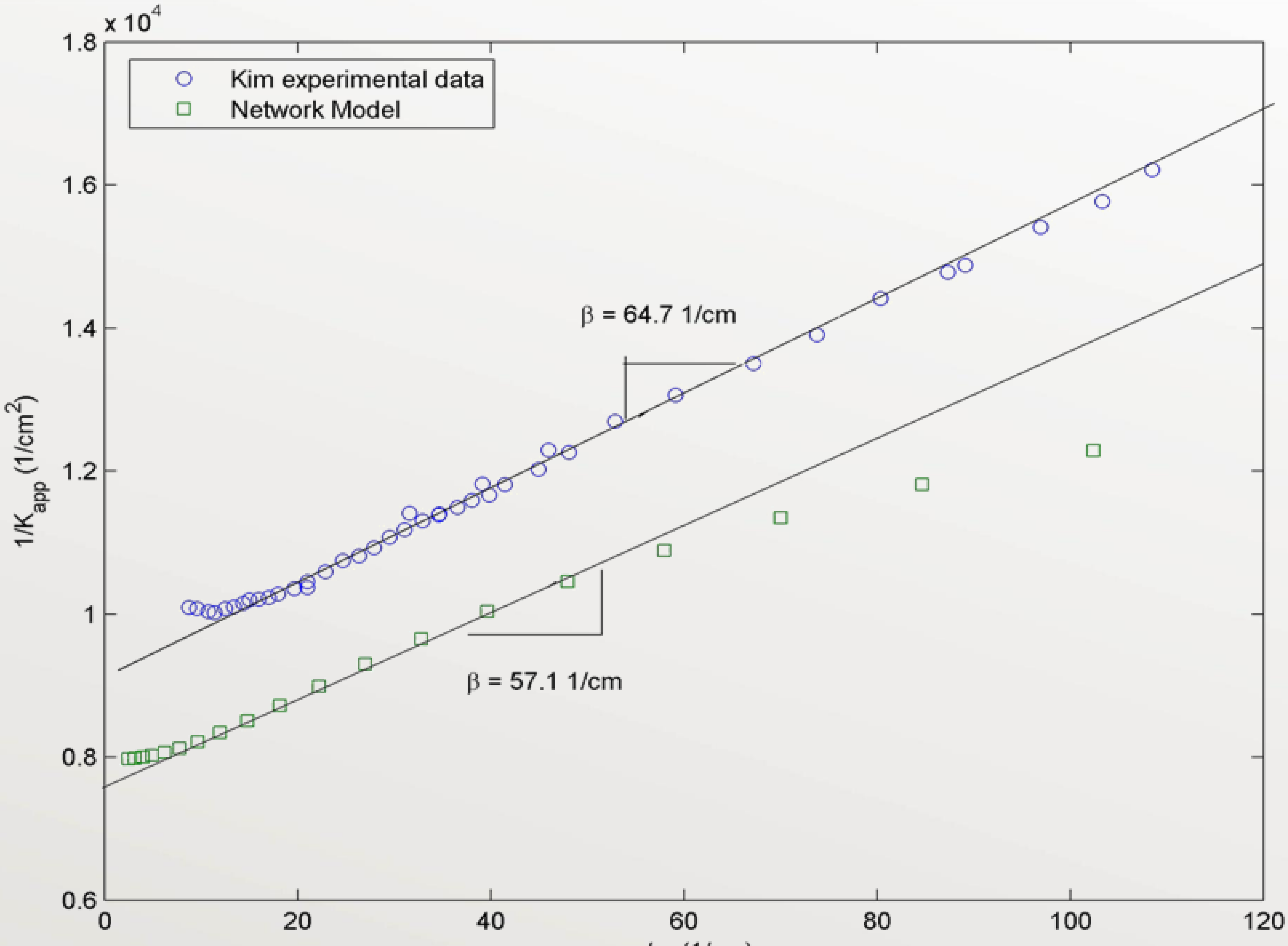




(a) Re = 0 (b) Re = 25 (c) Re = 150 (d) Re = 600



Comparison with Experimental Data



Shear-Thinning Flows in Porous Media

- Non-Newtonian fluids have a shear-dependent viscosity
- Relationship between flowrate and pressure is nonlinear, so system of non-linear equations arises

$$\sum_{j=1}^{n} q_{ij} = 0$$

$$q_{ij} = \frac{n\pi R^{3+1/n}}{(3n+1)(2\mu_0 l)^{1/n}} \left(P_i - P_j\right)^{1/n}$$

Power-law

$$q_{ij} = \frac{\pi R^4}{8\eta_0 l} \Delta P \left[1 + \frac{4}{\alpha+3} \left(\frac{\Delta P_{ij} R}{2\tau_{1/2} l} \right)^{\alpha-1} \right]$$

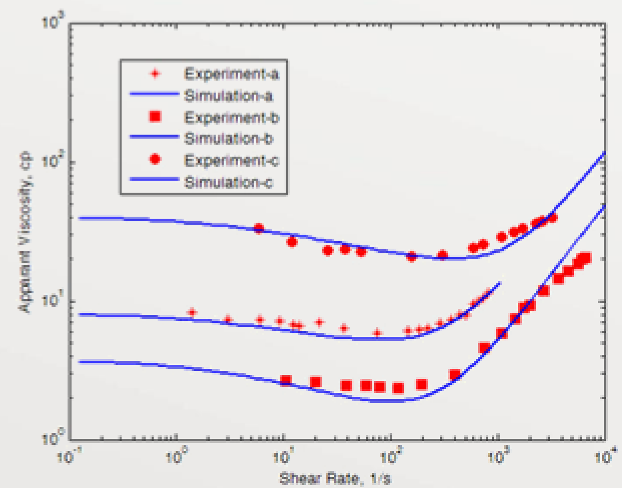
Ellis

- Performed FEM simulations in throats to correct for irregular geometry

- Modified "Darcy's Law" plotted as apparent viscosity

$$u = -\frac{k}{\mu_{app}} \frac{\partial p}{\partial x}$$

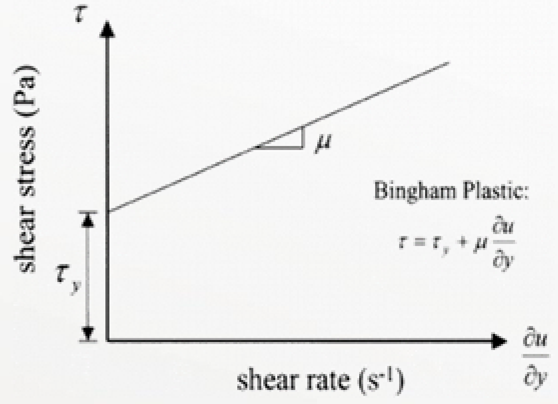
$$\mu_{app} = \mu_\infty + \left(\mu_p^0 - \mu_\infty\right)\left[1 + \left(\lambda \dot{\gamma}_{eff}\right)^{\alpha}\right]^{(n-1)/\alpha} + \mu_{\max}\left[1 - \exp\left(\lambda_2 \tau_r \dot{\gamma}_{eff}\right)^{n_2 - 1}\right]$$



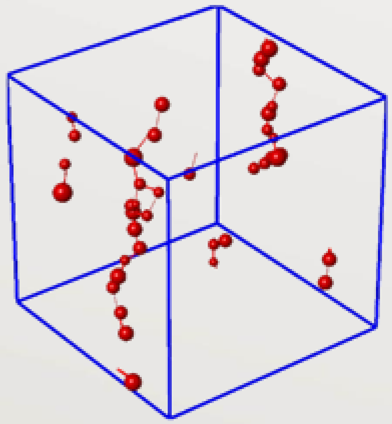
Yield Stress Flow in Porous Media

- Fluids with a yield stress require minimum stress to flow

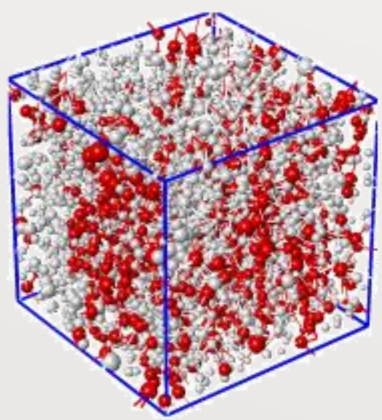
- Equation for flowrate is nonlinear and complicated because of yield stress



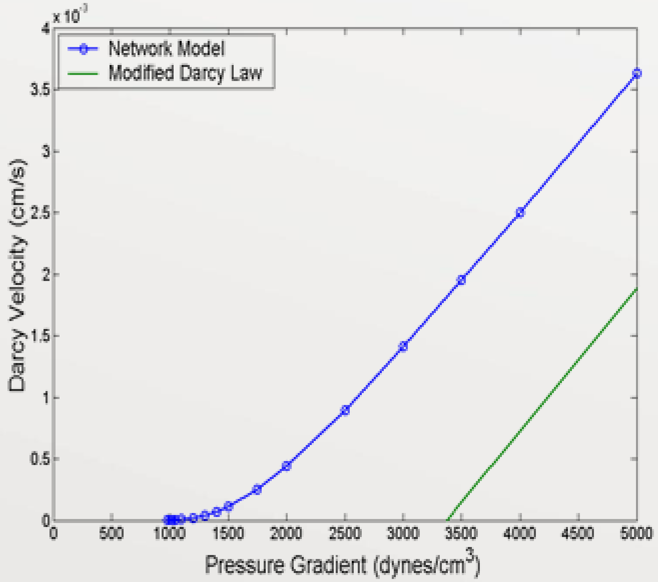
$$q_{ij} = \begin{cases} \dfrac{\pi R_{ij}^4}{8\mu_0 l}\Delta P\left[1 - \dfrac{4}{3}\left\{\dfrac{2\tau_0 l}{\Delta P R_{ij}}\right\} + \dfrac{1}{3}\left\{\dfrac{2\tau_0 l}{\Delta P R_{ij}}\right\}^4\right] & if \quad \Delta P > \Delta P_c \\ 0 & \text{otherwise} \end{cases}$$



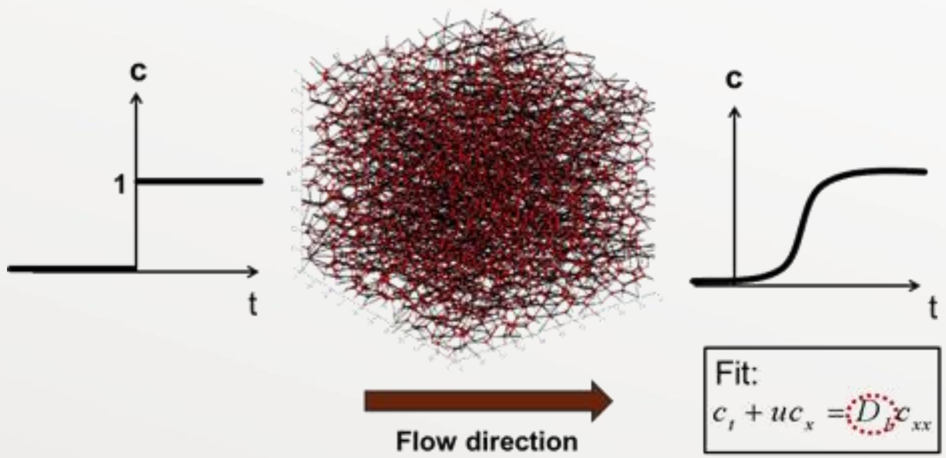
Threshold gradient

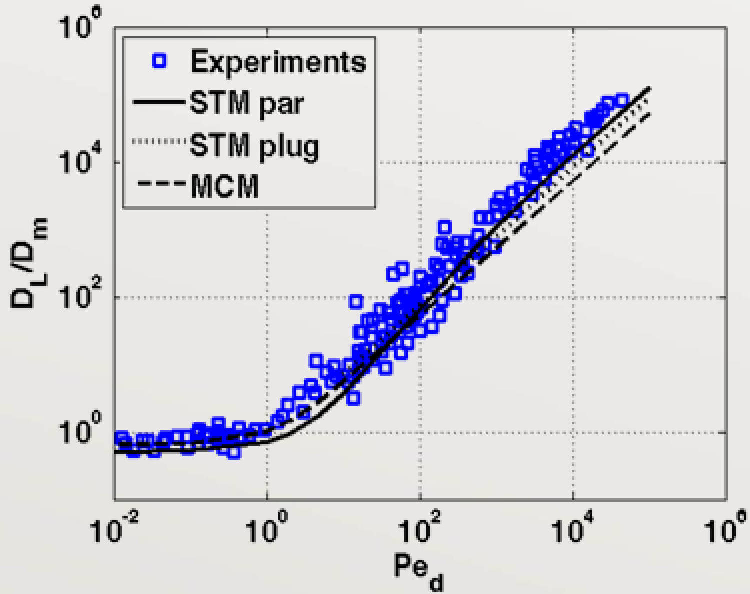


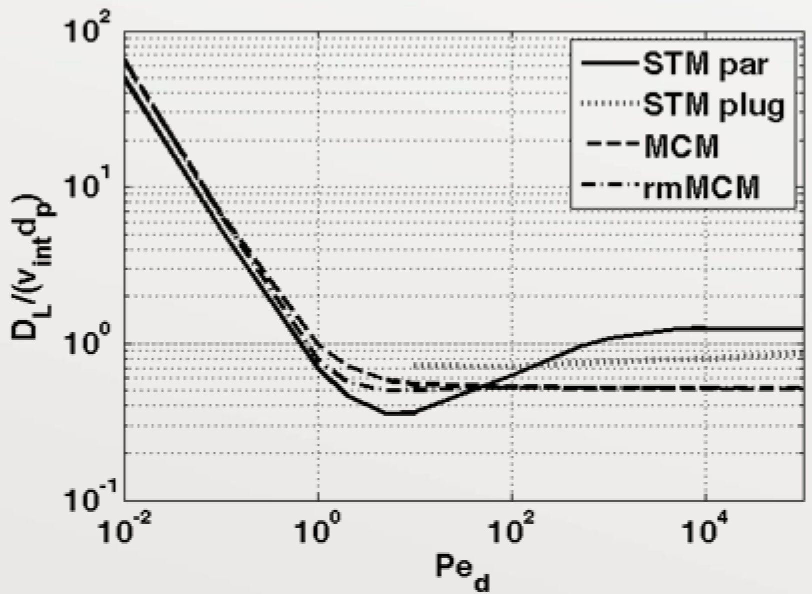
20% above threshold



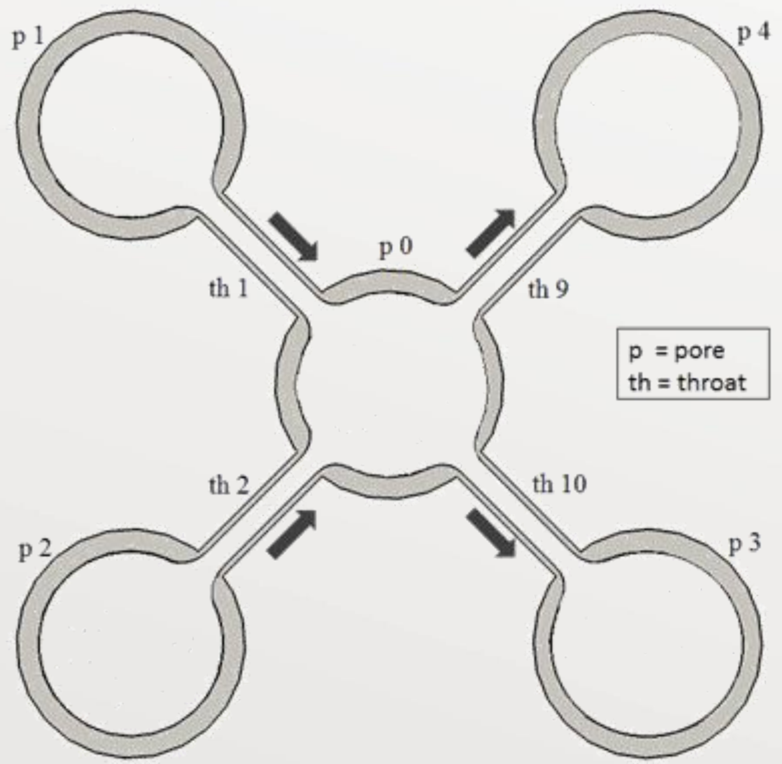
Solute Transport in Porous Media







The Mixed Cell Method (old):



Solute Balance:

$$V_{p0}\frac{dc_0}{dt} =$$ (accumulation)

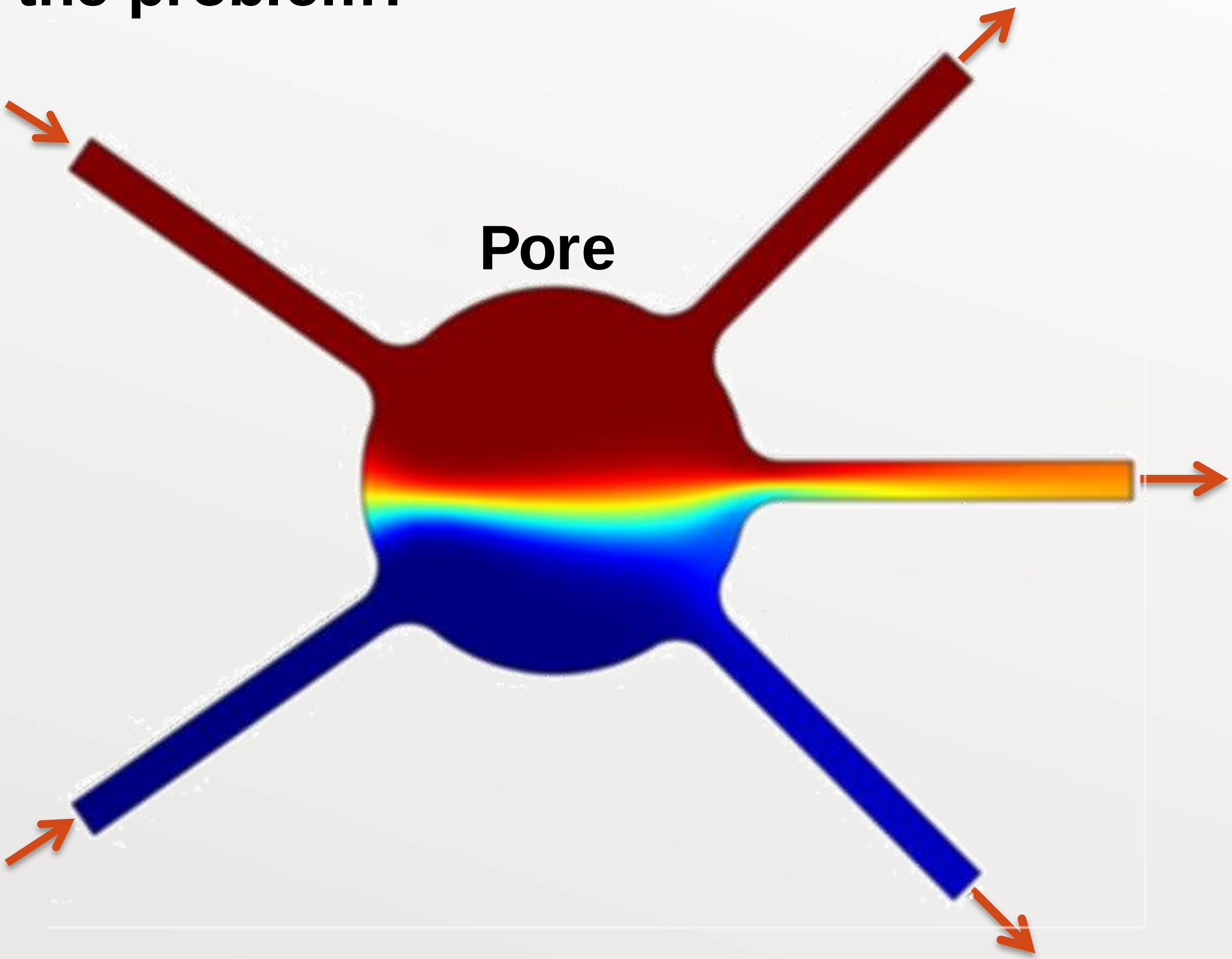
$$\sum_{j=1}^{N_{th}} c_j^{up} q_{0j} +$$ (convection)

$$\sum_{j=1}^{N_{th}} D_m a_{0j} \frac{\Delta c_{0j}}{l_{0j}} +$$ (diffusion)

$$R(c_0)$$ (reaction)

"perfect mixing" implicitly assumed!

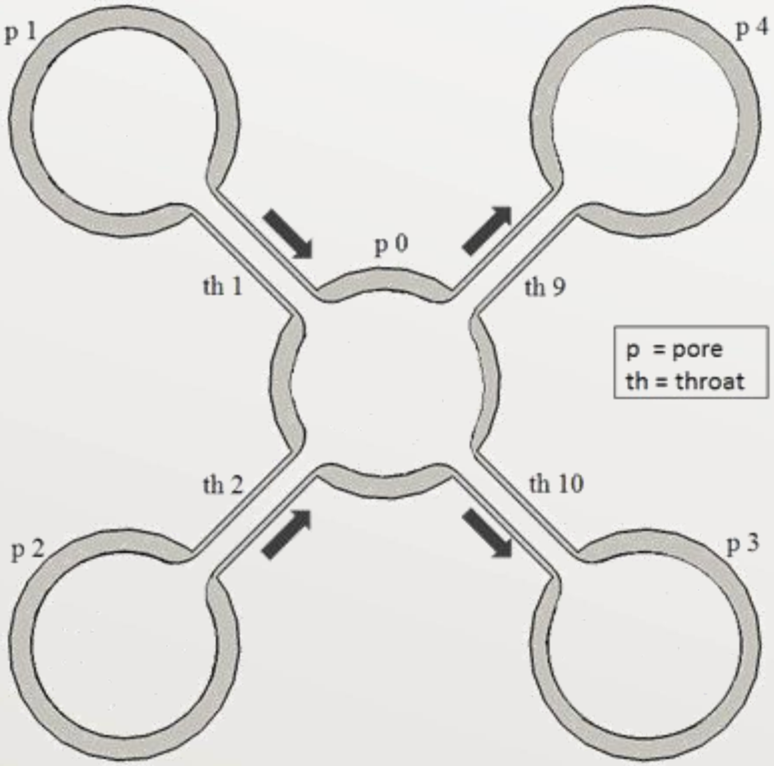
What is the problem?



1) How do streamlines split?
2) How much mixing is there?

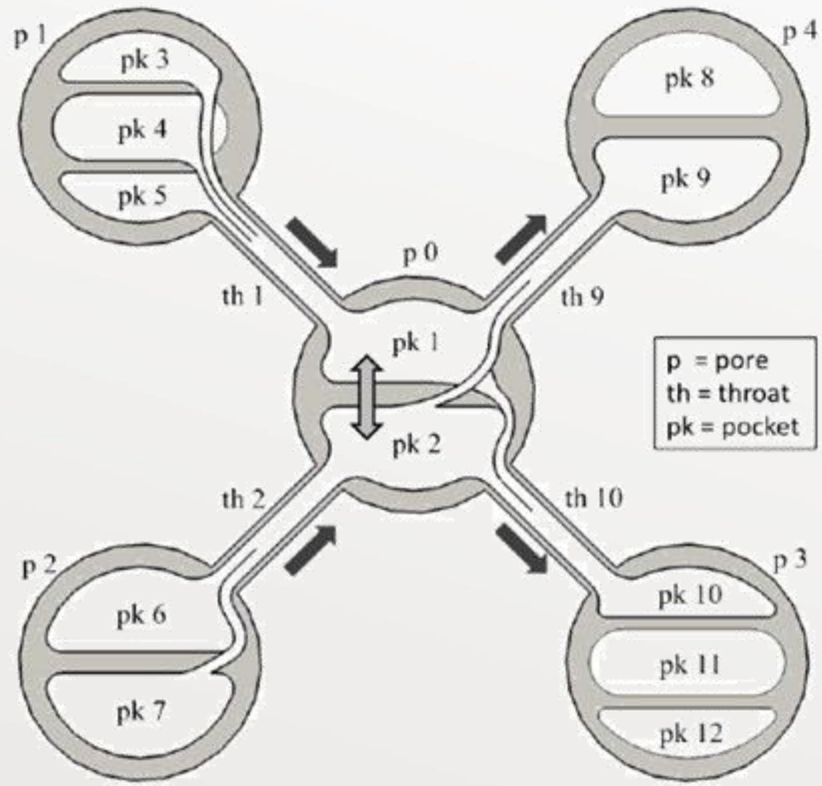
What we propose:

MCM (old)

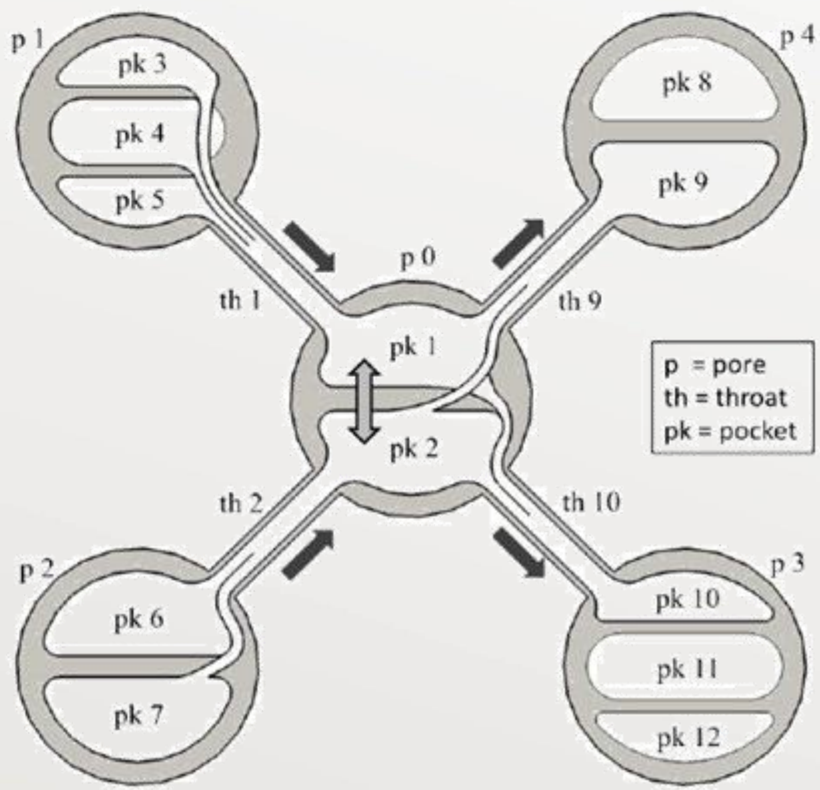


“perfect mixing” implicitly assumed!

SSM (new)



The Streamline Splitting Method (new):



Solute Balance:

$$V_1 \frac{dc_1}{dt} = \qquad \text{(accumulation)}$$

$$\sum_{j=1}^{N_{th}} q_j x_{1j}^{up} c_j^{up} + \qquad \text{(convection)}$$

$$\sum_{j=1}^{N_{th}} D_m a_{1j} x_{1j}^{up} \frac{c_j - c_1}{l_{1j}} + \qquad \text{(diffusion)}$$

$$R(c_1) + \qquad \text{(reaction)}$$

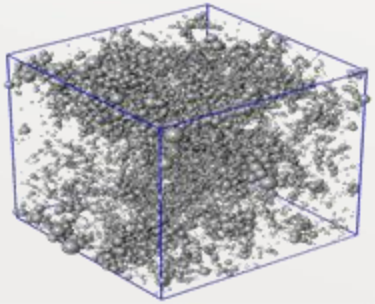
$$\Psi_{21}(c_2, c_1) \qquad \text{(intra-pore diffusion)}$$

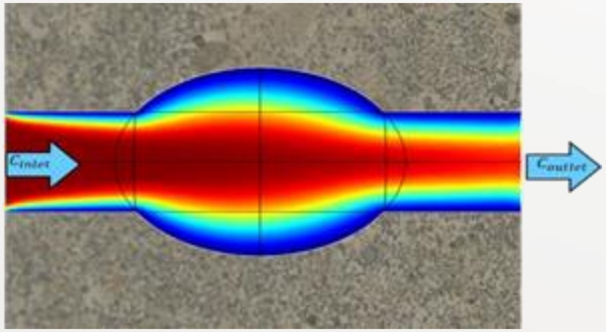
X: Accounts for **splitting streamlines**

Ψ: Accounts for **Intra-pore diffusion**

Reactive Flow and Transport

Microscopic inputs

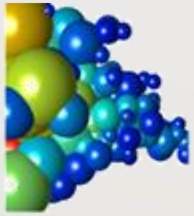


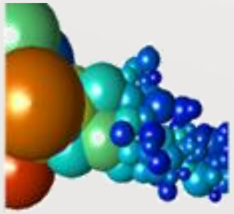


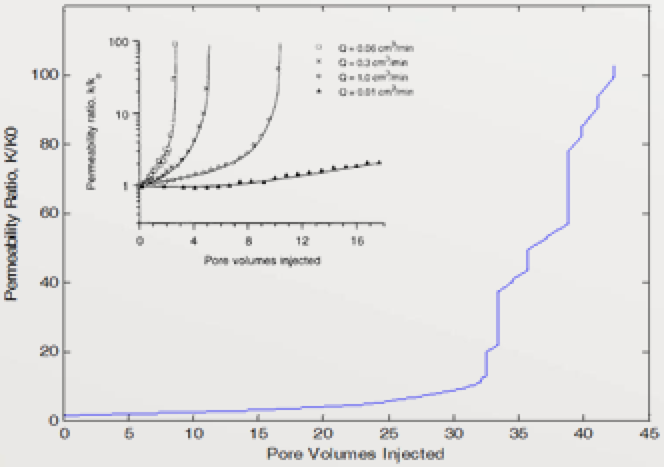
$$Sh = A\log(B\ Re + 1)$$

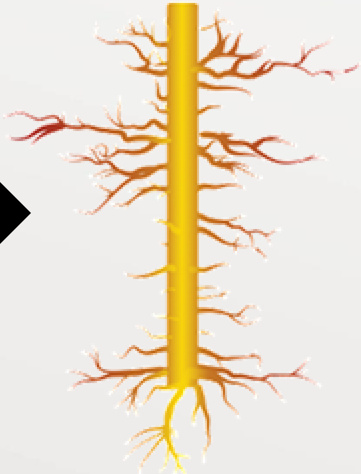
$$V_{Dissolved} = \frac{K_{mt}}{2} A\Delta C\Delta t \frac{M}{\rho}$$

Macroscopic Outputs:

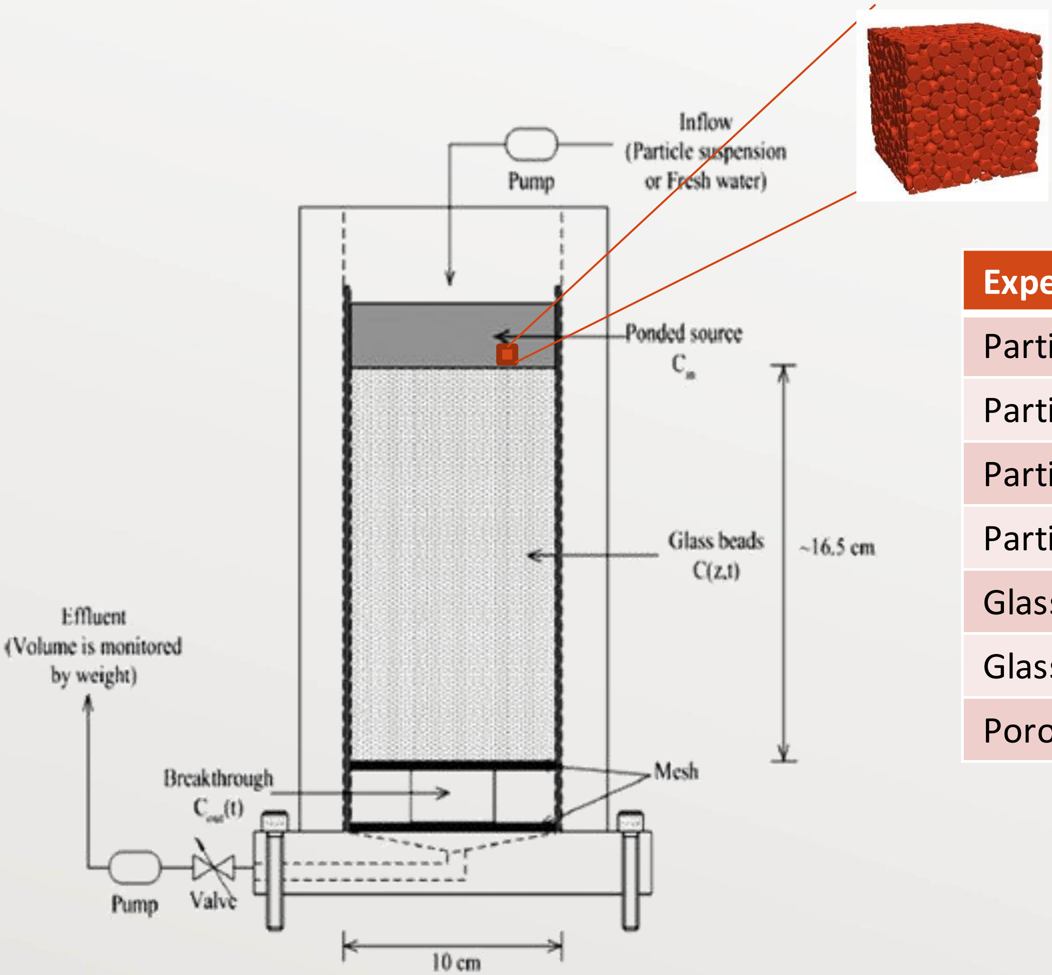








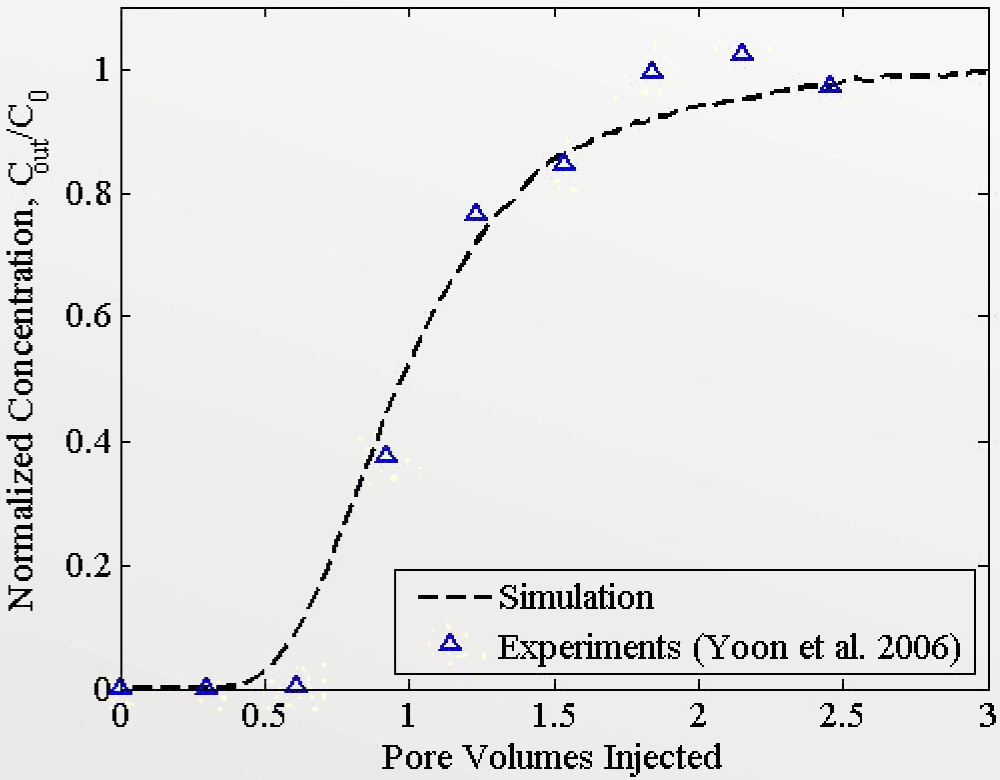
Model validation with published data



Experiment Parameter	
Particle Concentration	50 mg/L
Particle Zeta Potential	-110 mV
Particle Diameter	0.1~15 um
Particle Specific Gravity	1.1
Glass Beads Zeta Potential	-50 mV
Glass Beads Diameter	4 mm
Porosity	0.37

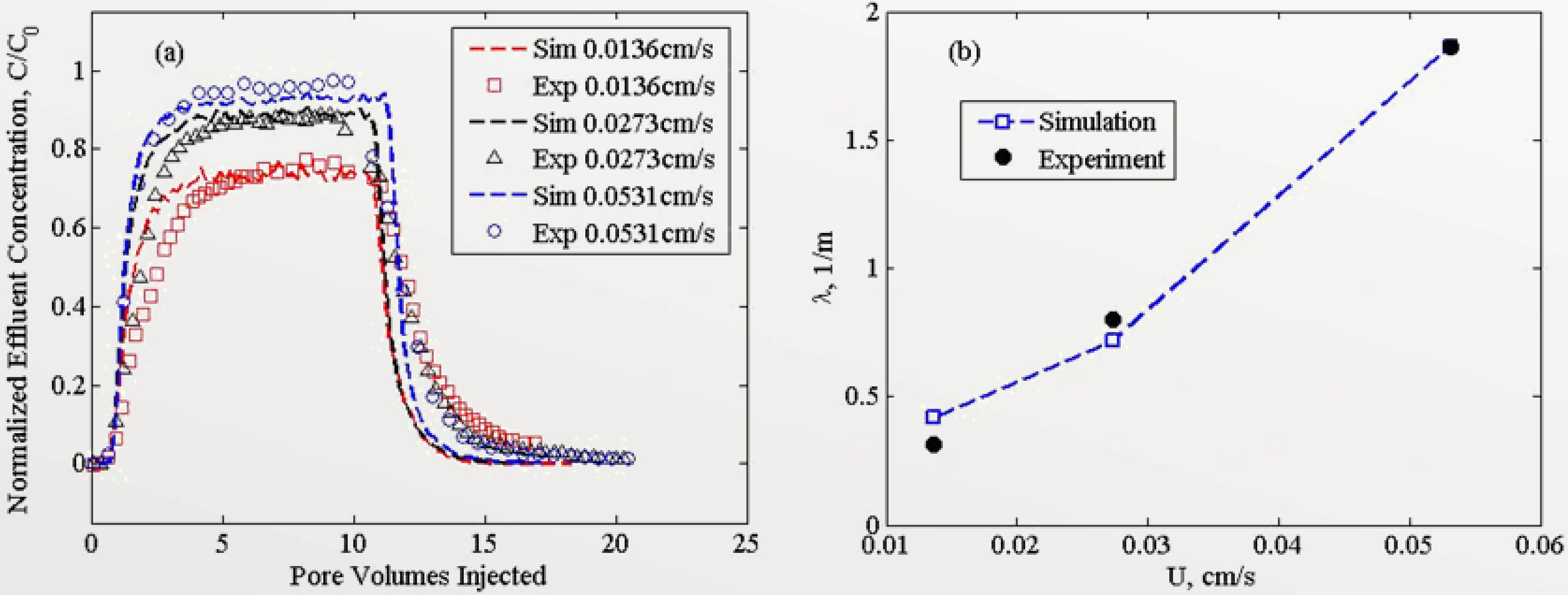
(Yoon et al. 2006)

Model validation---tracer test



- No particle retention (No body force and surface force)
- U = 0.0462 cm/s

Model validation---effluent concentration



❑Well predict filtration coefficients at different flow velocities.

(Yoon et al. 2006)

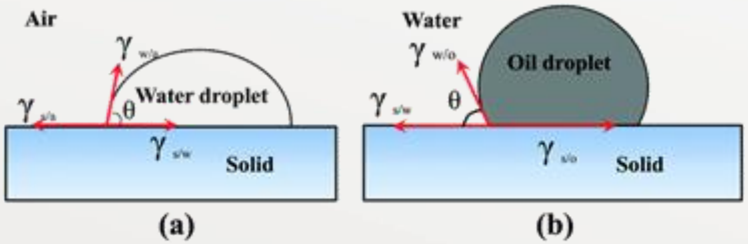
Multiphase Flow

Key References:

- V. Joekar-Niasar & S. M. Hassanizadeh (2012)
- Al-Gharbi and Blunt (2005)
- Oren et al. (1998)

Terms and Definitions

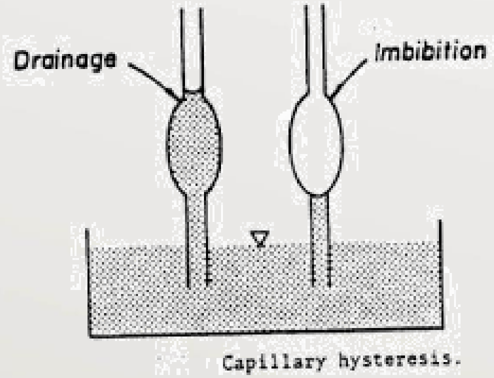
Wettability is the affinity of a fluid to a surface in the presence of another immiscible fluid



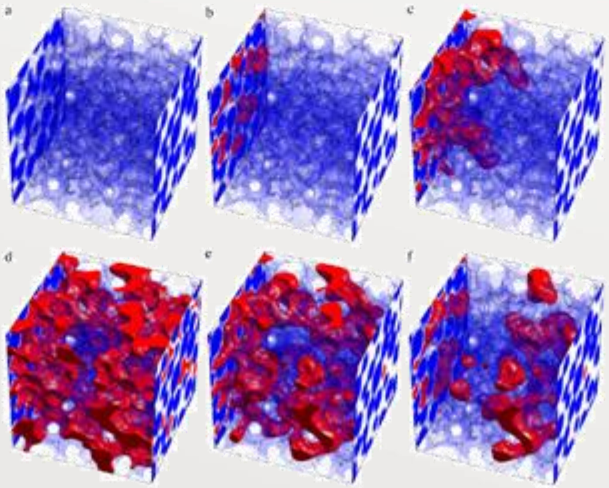
http://pubs.rsc.org

$$P_c = \gamma\left(\frac{1}{R_1} + \frac{1}{R_2}\right) \Rightarrow \frac{2\gamma\cos\theta}{r}\left(\text{capillary tube}\right)$$

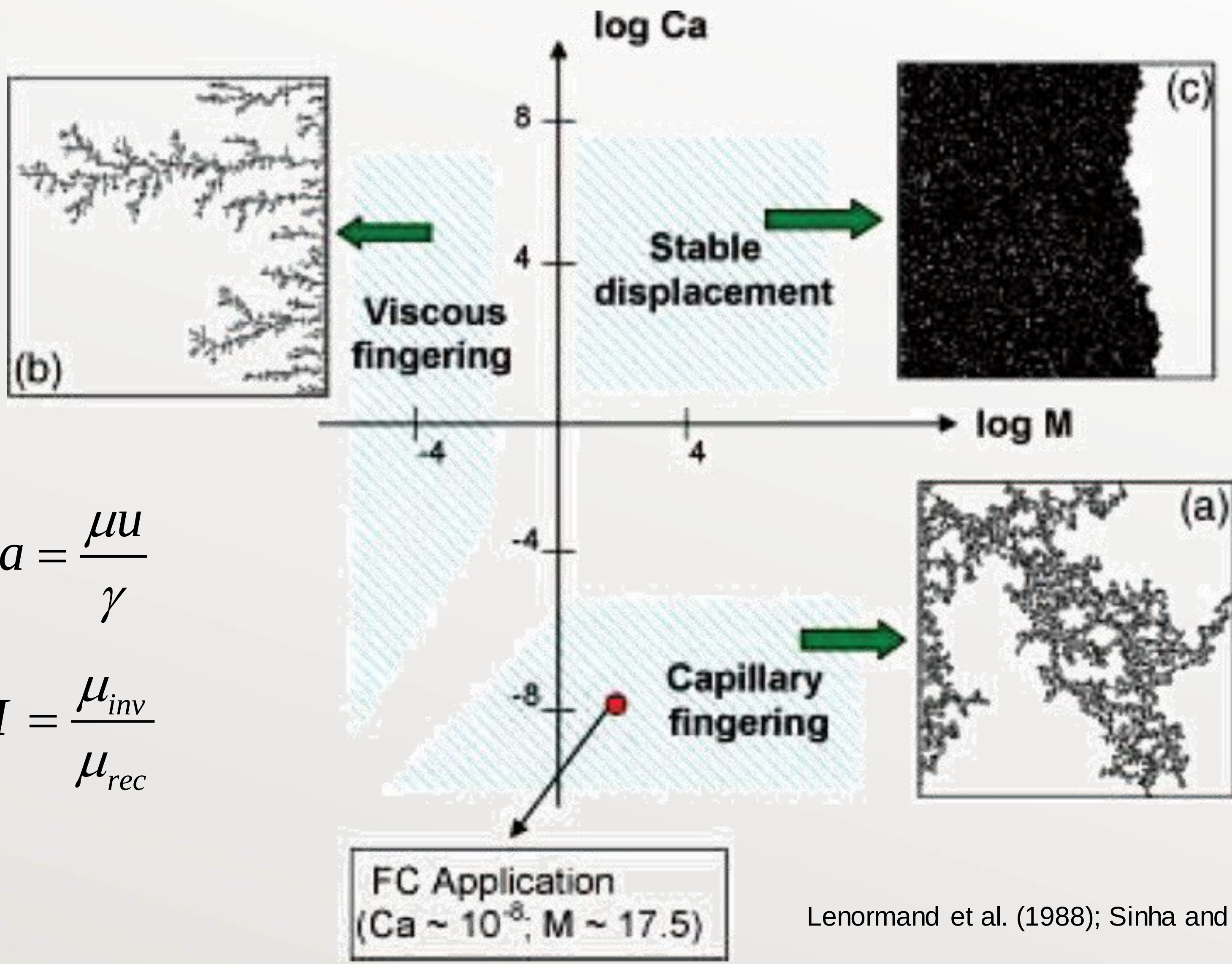
Drainage is the displacement of a wetting fluid by non-wetting fluid; **Imbibition** is the reverse process



web.mst.edu



Capillary Number and Mobility

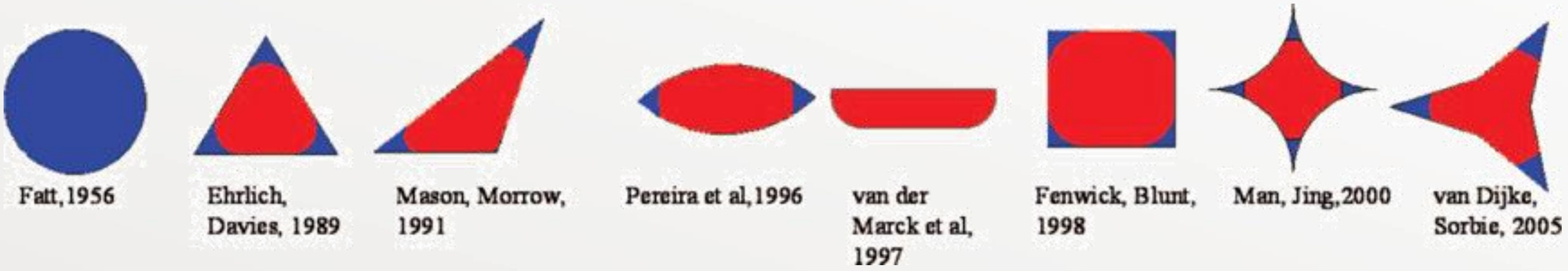


$$Ca = \frac{\mu u}{\gamma}$$

$$M = \frac{\mu_{inv}}{\mu_{rec}}$$

Lenormand et al. (1988); Sinha and Wang (2007)

Pore Geometry and Cross Sections

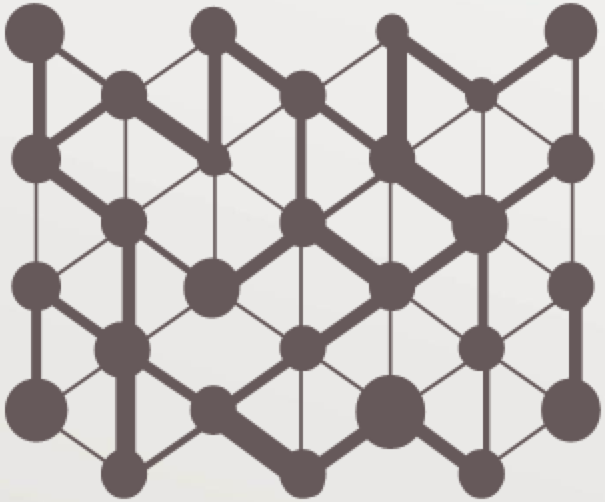


Joekar-Niasar and Hassanizadeh (2012)

- Important to capture irregular cross sections of pores and throats
- Wetting fluid "wets" the surface and remains connected through crevices
- Use idealized shapes (e.g. traingles) with shape factors $G=A/P^2$
- Finite Element simulations used to compute phase conductivities

Quasi-Static Immiscible Discplacement

- Capillary dominated (Ca ~ 0) common in real applications
- No flow/dynamics
- Displacement is "rule-based" (invasion percolation). Fluid fills a pore if pressure drop exceeds threshold (capillary entry) pressure



Capillary Pressure Calculation

1. Impose a pressure boundary condition (reservoir of fluid)

2. Use “rule-based” algorithm to compute equilibrium saturation

3. Increase pressure and repeat steps 1 and 2 to develop curve

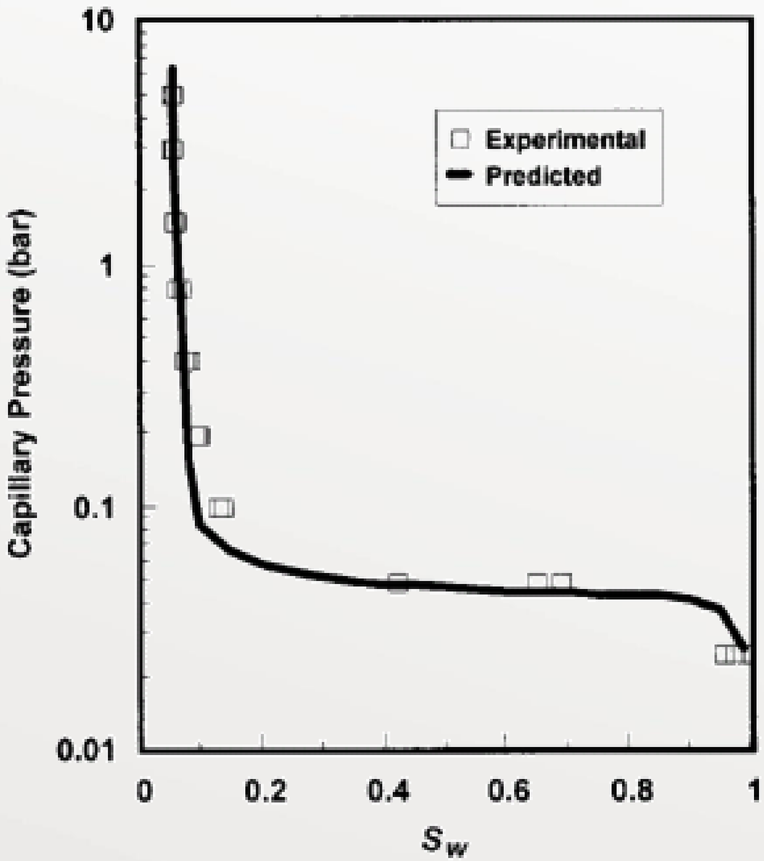


Fig. 13—Comparison between predicted and measured primary drainage capillary pressure for the water-wet Bentheimer sandstone.

Oren et al. (1998)

Quasi-Static Relative Permeability Calculation

1. At a given equilibrium saturation impose a pressure gradient
2. Solve fluid flow (system of equations)
3. Compute pressure field and steady-state flowrates for each phase
4. Back-calculate relative permeability at S_w
5. Repeat steps 1-4 at different saturation

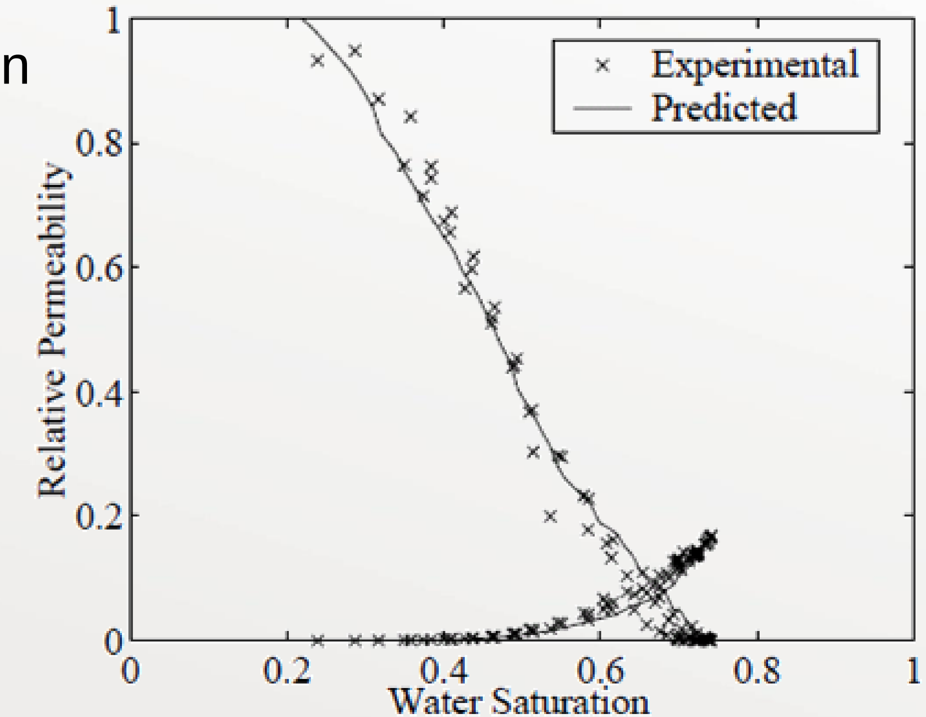


Figure 8: Predicted waterflooding relative permeability for water-wet Berea sandstone (lines) compared to experimental data by Oak (crosses)[31].

Valvatne and Blunt, 2003

Multiphase Viscous Flows (Dynamic Network Models)

Single pressure

$$V_i \frac{\partial S_i^w}{\partial t} + \sum_{j=1}^{N} q_{ij} S_{ij}^w = 0$$

$$q_{ij} = \frac{g_{ij}}{\mu} \Delta_{ij}$$

$$S_i^w + S_i^{nw} = 1$$

$$P_c^{ij} = f\left(geometry\right)$$

Two-pressure

$$V_i \frac{\partial S_i^\alpha}{\partial t} + \sum_{j=1}^{N} q_{ij}^\alpha = 0$$

$$q_{ij}^\alpha = \frac{g_{ij}^\alpha}{\mu^\alpha} \left(P_i^\alpha - P_j^\alpha\right)$$

$$S_i^w + S_i^{nw} = 1$$

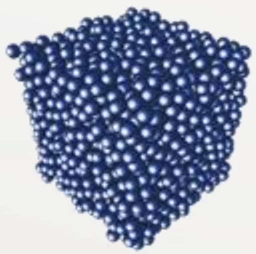
$$P_c^{ij} = f\left(geometry\right)$$

Pore-Network Modeling vs. Reservoir Simulation

	Network Model	Reservoir Simulation
Nodes	"pores"	"cells/grids/elements"
Flow coefficient	conductivity	transmissibility
Scale	10^{-5} to 10^{-2} m	10^{0} to 10^{5} m
Gridding	Unstructured	(un)Structured
Discretization	Fixed	User determined
Flow Regime	Capillary Dominated	Viscous Dominated
Compressibility	Negligible	Important

Hybrid Modeling and Upscaling Techniques

Petrophysical Experimental Measurements

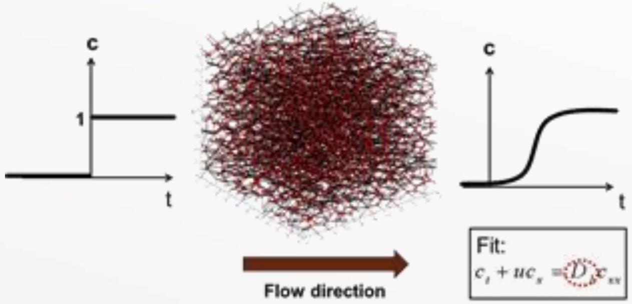


Porosity

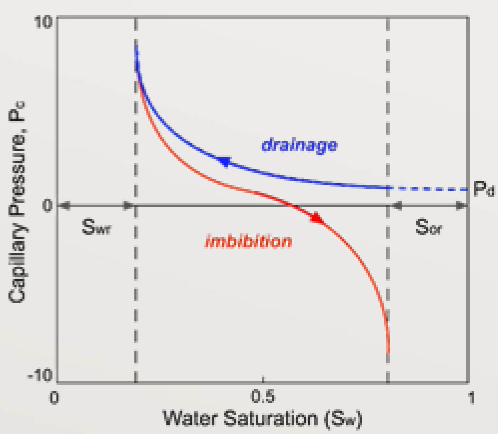
$$\phi = \frac{V_{void}}{V_{bulk}}$$

Permeability

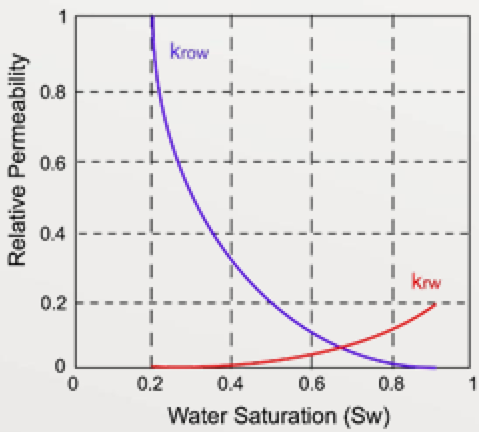
$$k = \frac{q\mu L}{A\Delta P}$$



Dispersion



Capillary Pressure $P_c(S_w) = P_{nw} - P_w$



Relative Permeability

$$k_{r\alpha} = \frac{q_\alpha \mu L}{kA\Delta P}$$

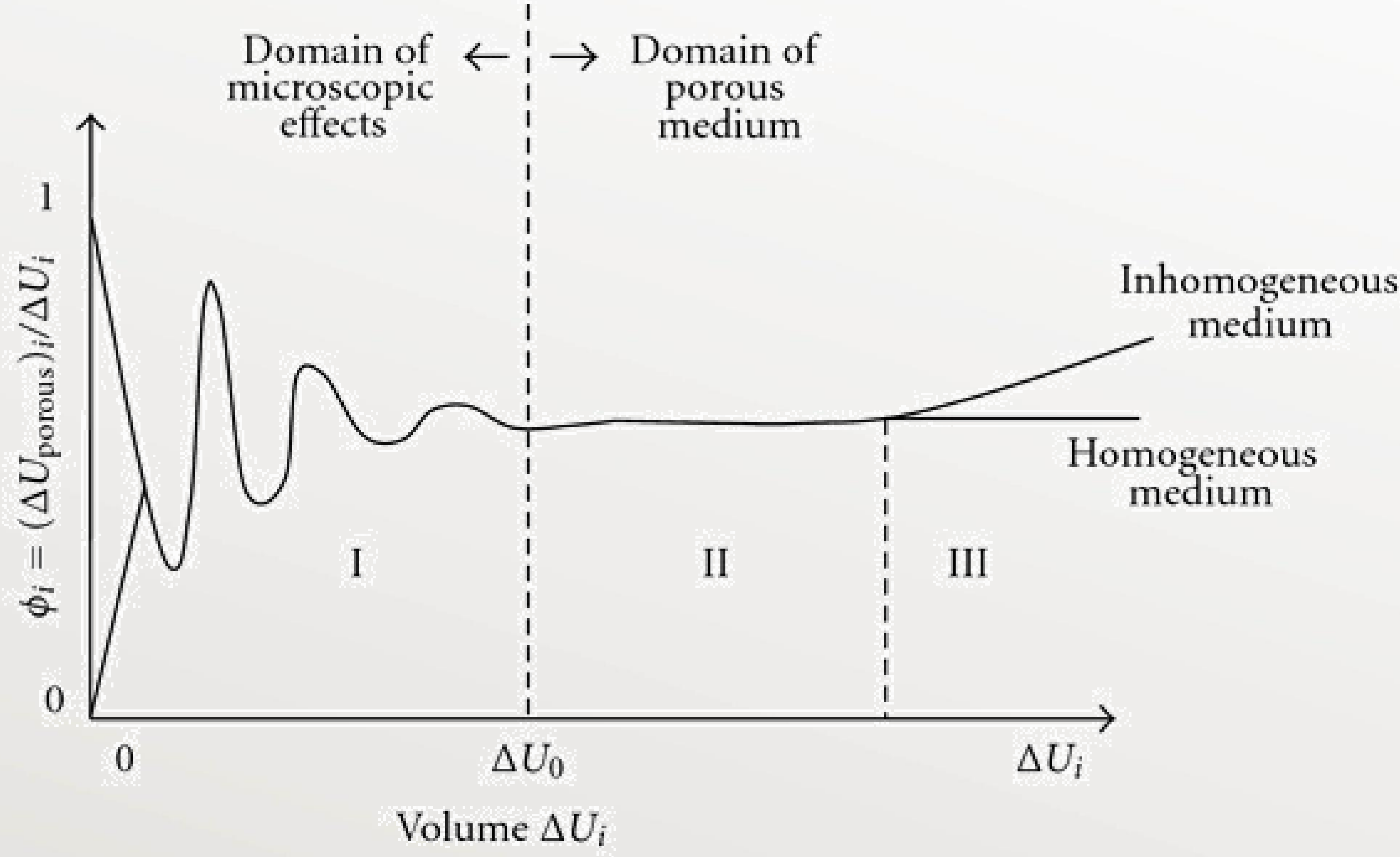
Pore-Scale Models as Stand-Alone Tools

- Predictive network models can be used to obtain macroscopic properties for substitution into continuum simulators
  - Permeability (Bryant et al., 1993)
  - Relative permeability curves (Baake and Oren, 1997)
  - Capillary pressure curves (Dillard and Blunt, 2000)
  - Effective viscosity for non-Newtonian fluids (Lopez et al., 2003; Balhoff and Thompson, 2004)
  - Dispersion coefficients (Bijeljic et al., 2004; Acharya et al., 2007)

- Models can be used as a complement for experimental tests

- But…
  - Is direct upscaling sufficient?
  - Shouldn’t the boundary conditions depend on flow behavior upstream?
  - How can we include pore-scale models in a multiscale setting?

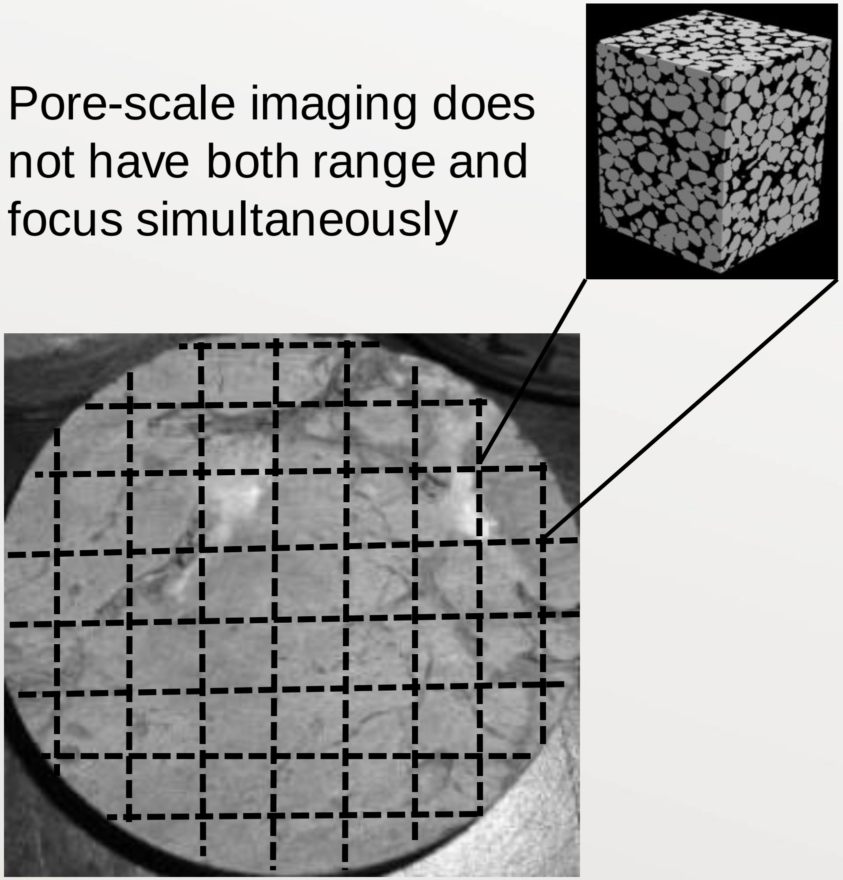
Representative Elementary Volume



Adapted from Bear (1972)

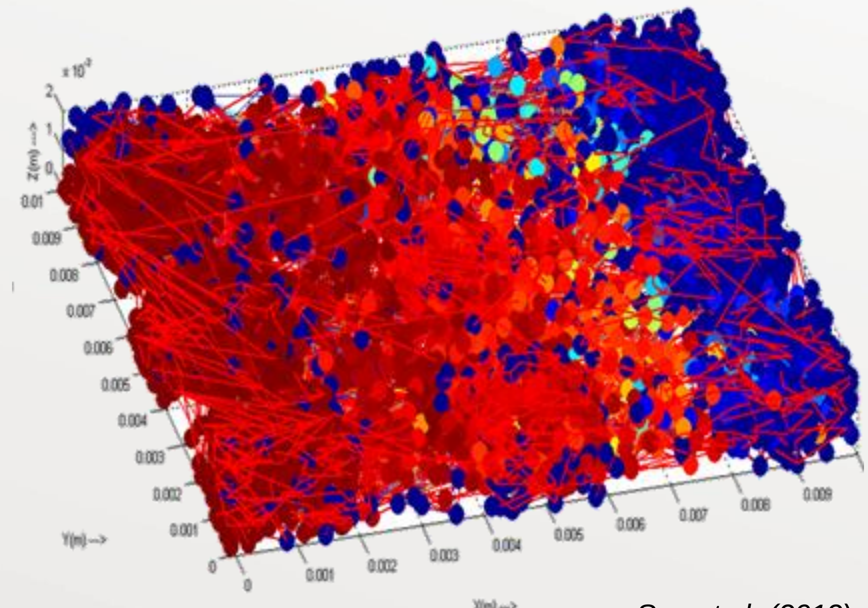
Related problems:

Pore-scale imaging does not have both range and focus simultaneously



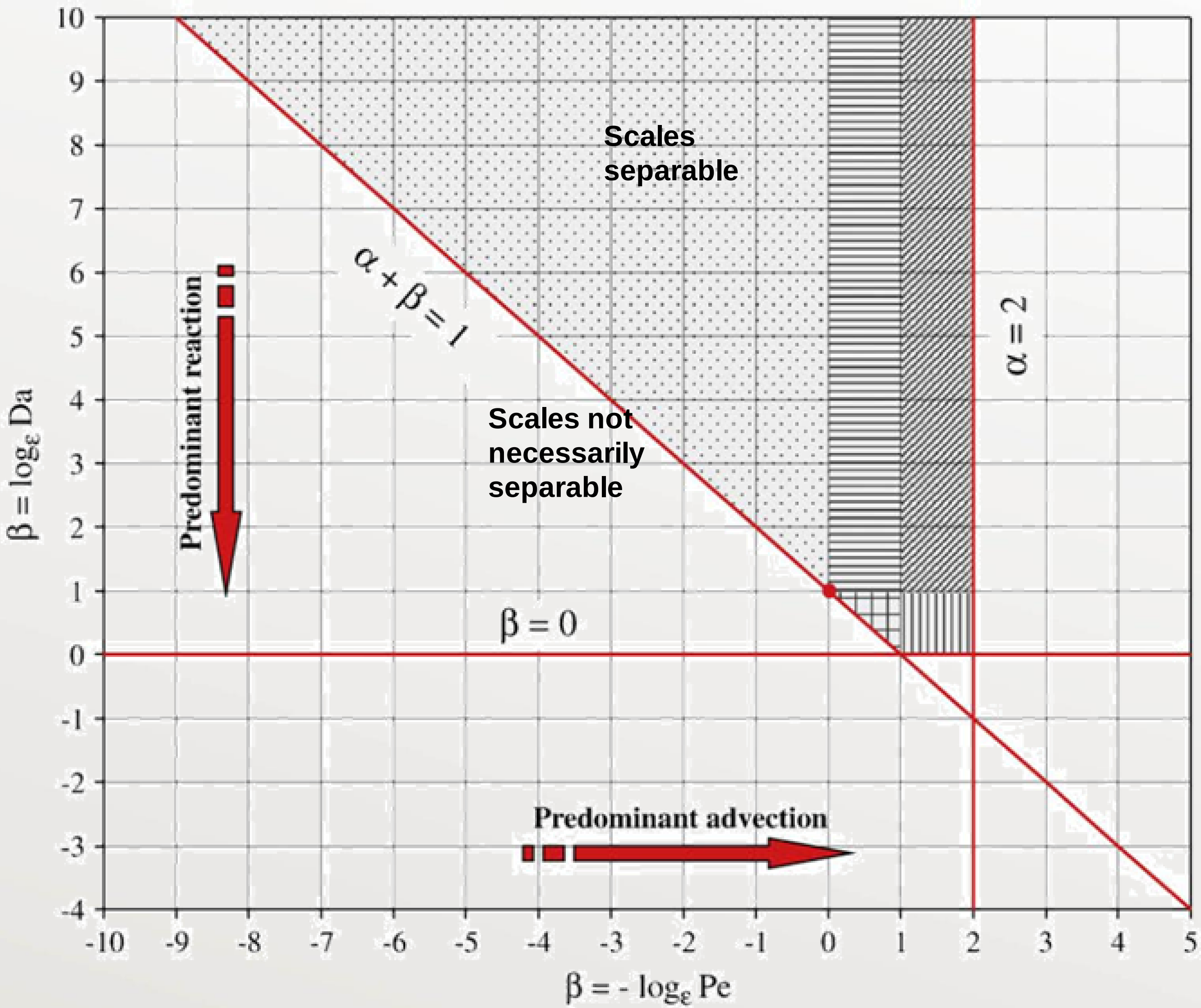
Svec and Grigg (2001)

Bigger samples required for ascertaining the REV size



Sun et al. (2012)

Validity of continuum description:

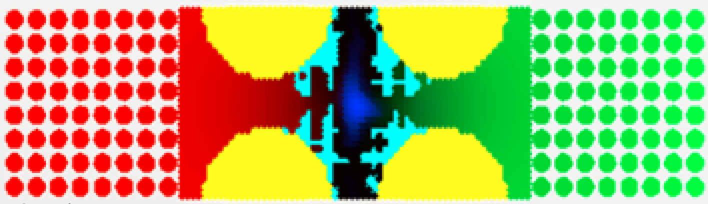


Battiato and Tartakovsky (2011), Battiato et al. (2009)

1) Intrusive methods, Handshake methods, SPH-based methods:

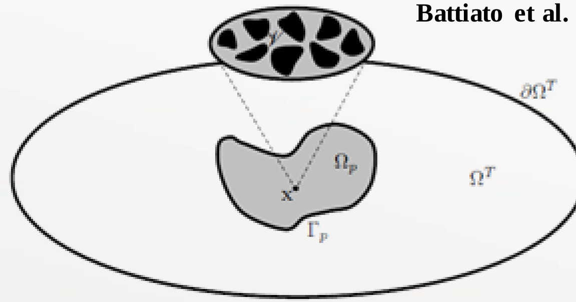
Tartakovsky et al. (2006), Scheibe et al. (2007), Tartakovsky et al. (2008) , Battiato et al. (2011), etc.

Scheibe et al. (2007)



Continuum **Pore-scale (Mixing zone)** **Continuum**

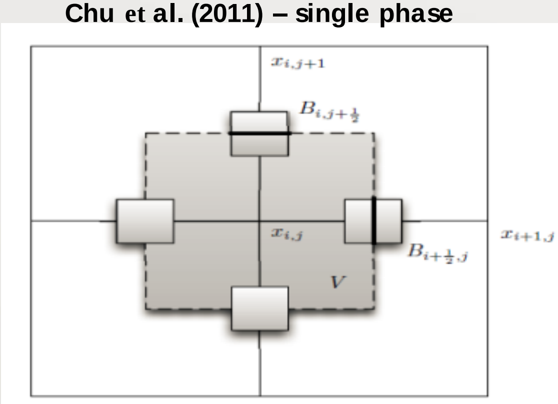
Battiato et al. (2011)



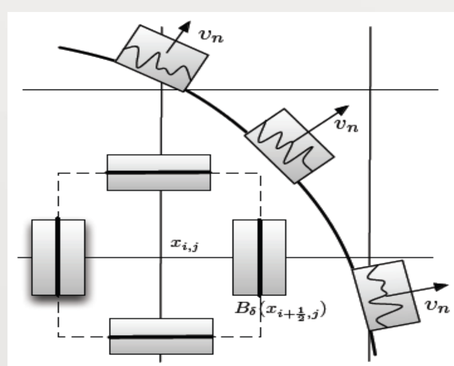
2) Heterogeneous multiscale based method (HMM), etc.:

Weinan et al. (2003), Weiqing & Weinan (2004), Chu et al. (2011a, 2011b), Sheng and Thompson (2013)

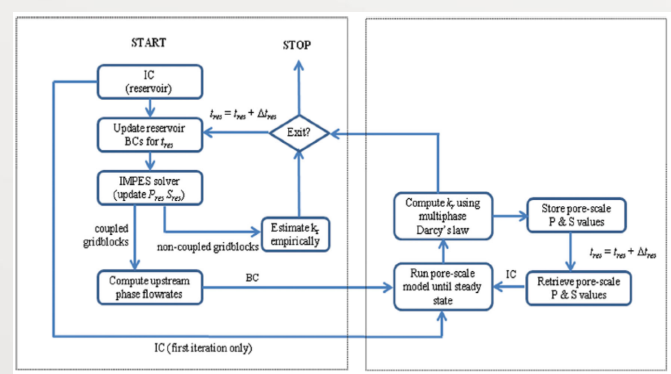
Chu et al. (2011) – single phase



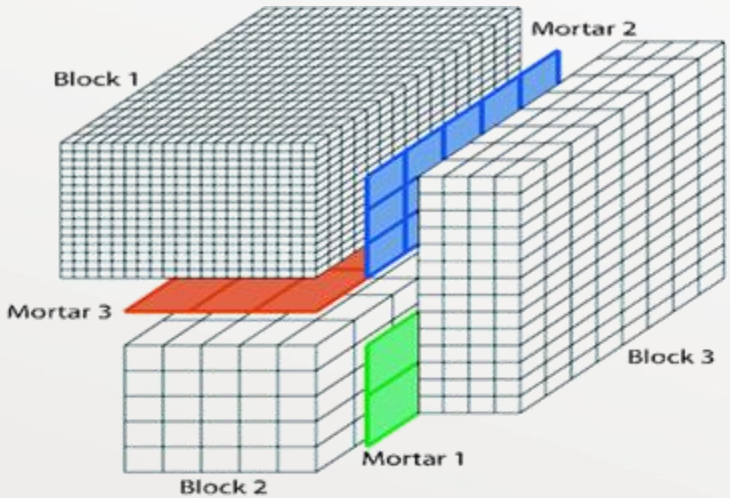
Chu et al. (2011) – two phase



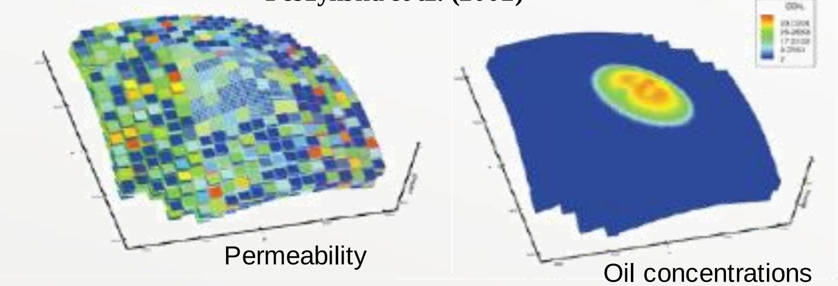
Sheng and Thompson (2011) – two phase



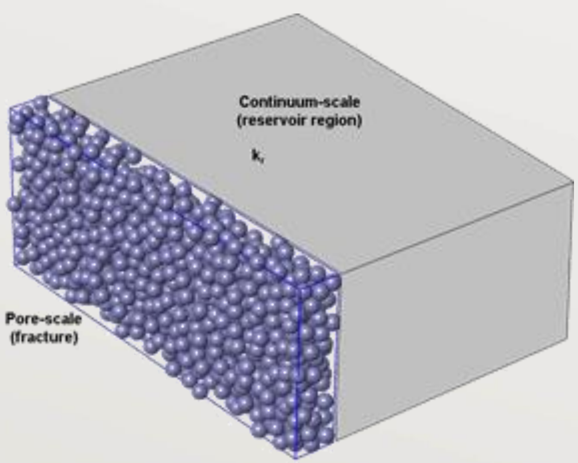
3) Multiblock/Multidomain Mortar Approach:



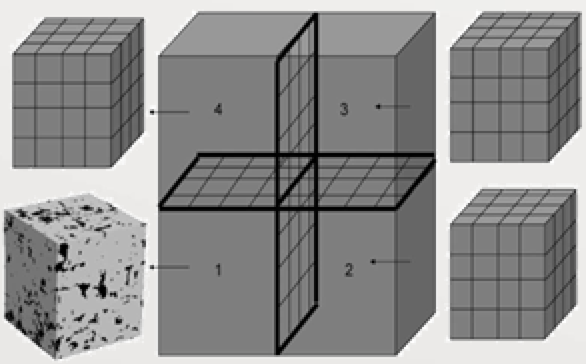
Peszynska et al. (2002)



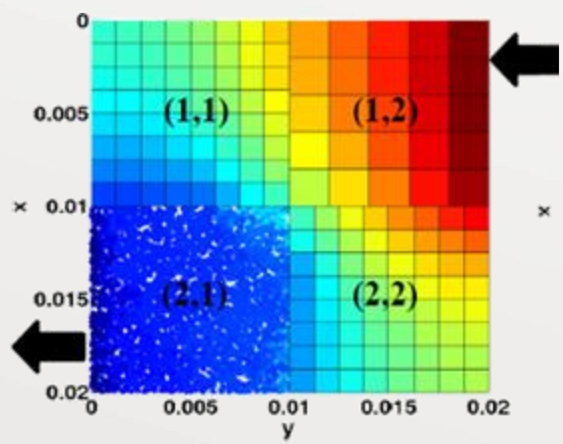
Balhoff et al. (2007)



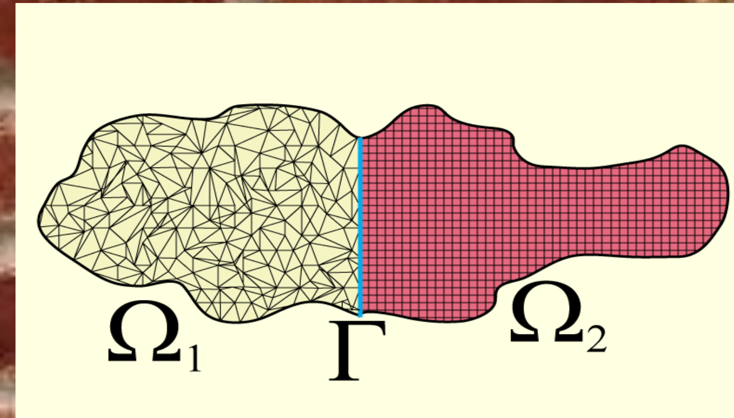
Balhoff et al. (2008)



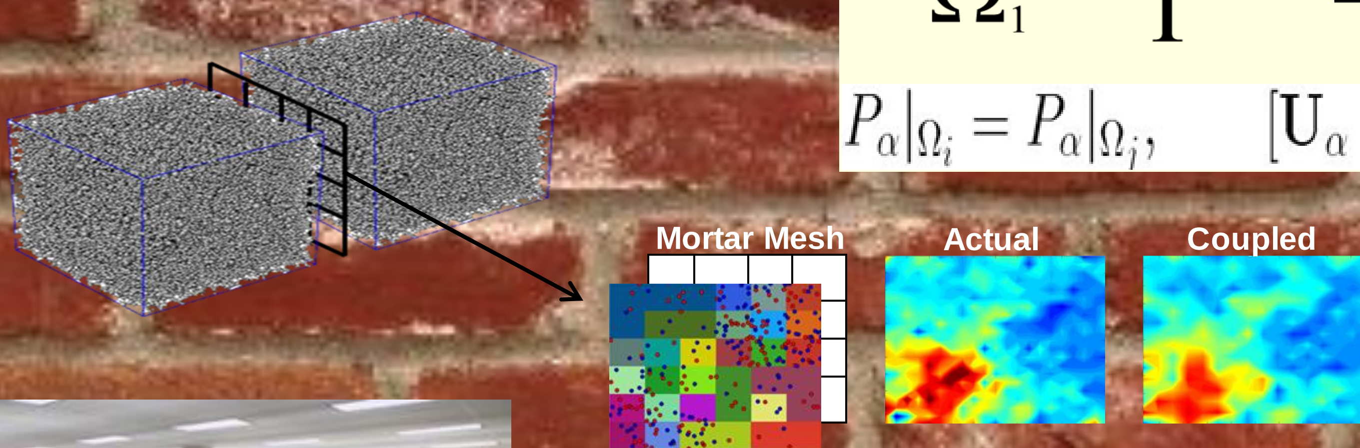
Mehmani and Balhoff (2014)



Mortars are finite element based function spaces forming the interface conditions between subdomains.

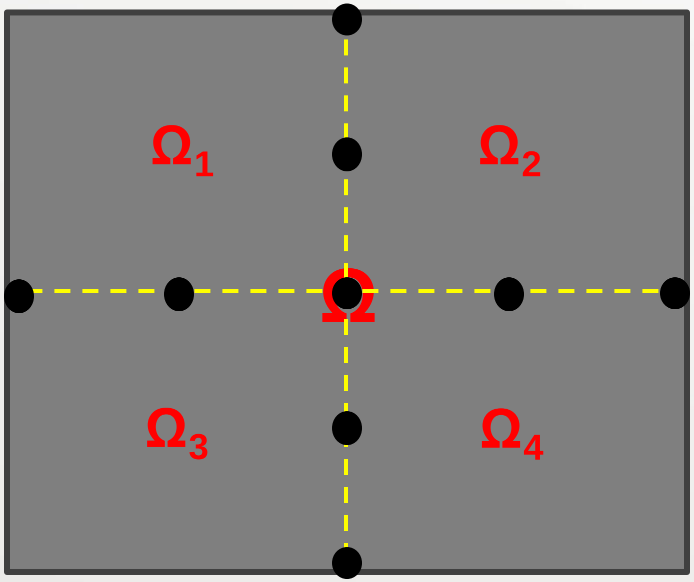


$$P_\alpha|_{\Omega_i} = P_\alpha|_{\Omega_j}, \qquad [\mathrm{U}_\alpha \cdot \nu]_{ij} = 0$$



- Subdomains are independent and can be solved in parallel
- Subdomains can be different in: physics, numerical method, discretization, and scale

How Do Mortars Work?



Objective:

Find subdomain solutions such that flux is continuous between them

Algorithm 1 (FD):

1) Guess interface unknowns

$$P|_{\Gamma_{ij}} = \sum_k \alpha_k \psi_k (x, y)$$

2) Solve subdomains
3) Compute "jump in flux" at interfaces

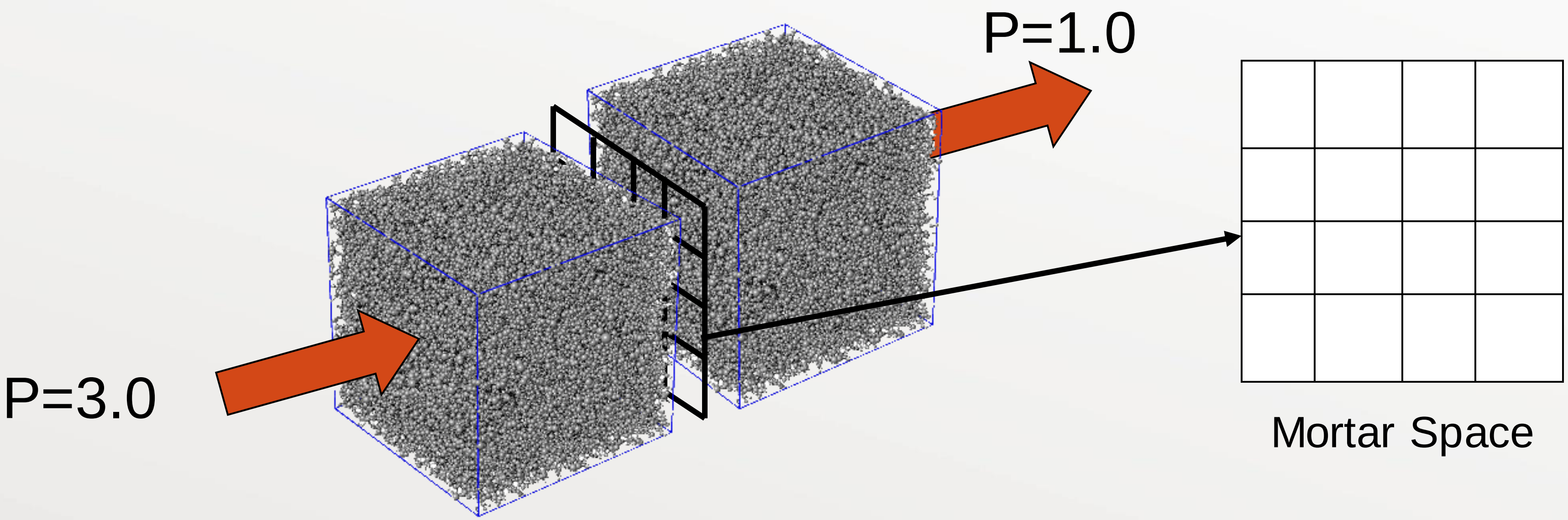
$$F_k(\vec{\alpha}) = \int_{\Gamma_{ij}} [\![\vec{n}.\vec{q}]\!] . \psi_k = 0 \quad \forall \psi_k \in M_{h_{ij}}$$

4) Iterate

Pros:
1) Easy to implement
2) Subdomains are "black boxes"

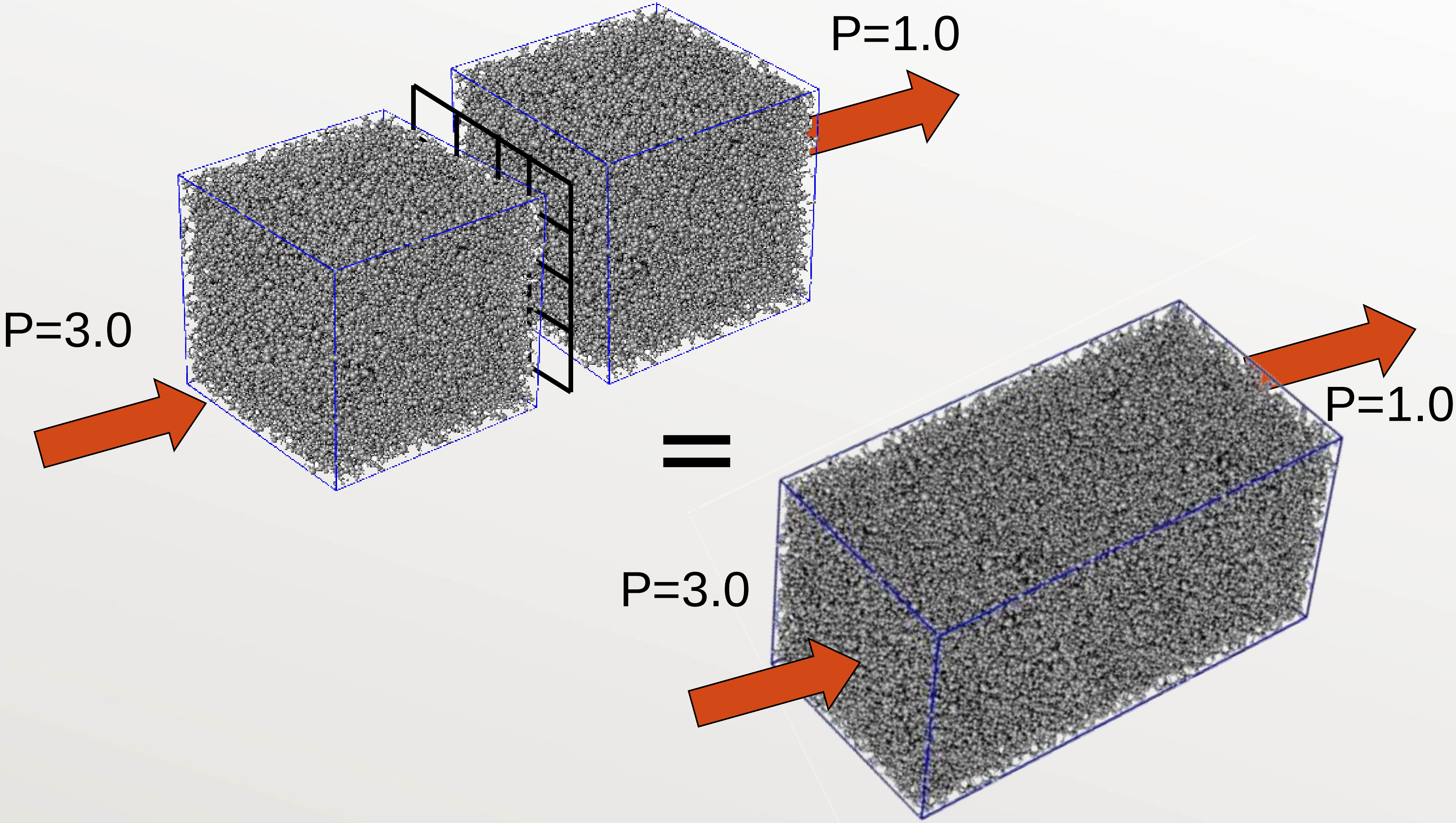
Con:
Potentially inefficient (esp. when nonlinear)

Model Validation Problem

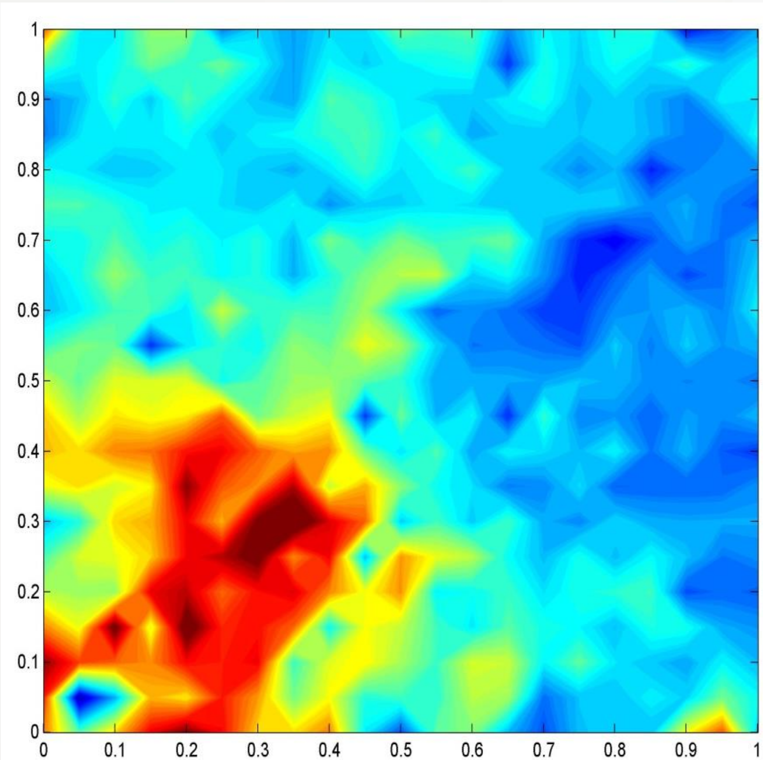


- Periodic network model coupled to its replica
- Still want to solve as stand-alone tools
- What pressure field P(x,y) at the interface will result in weakly matched fluxes? P = 2.0?

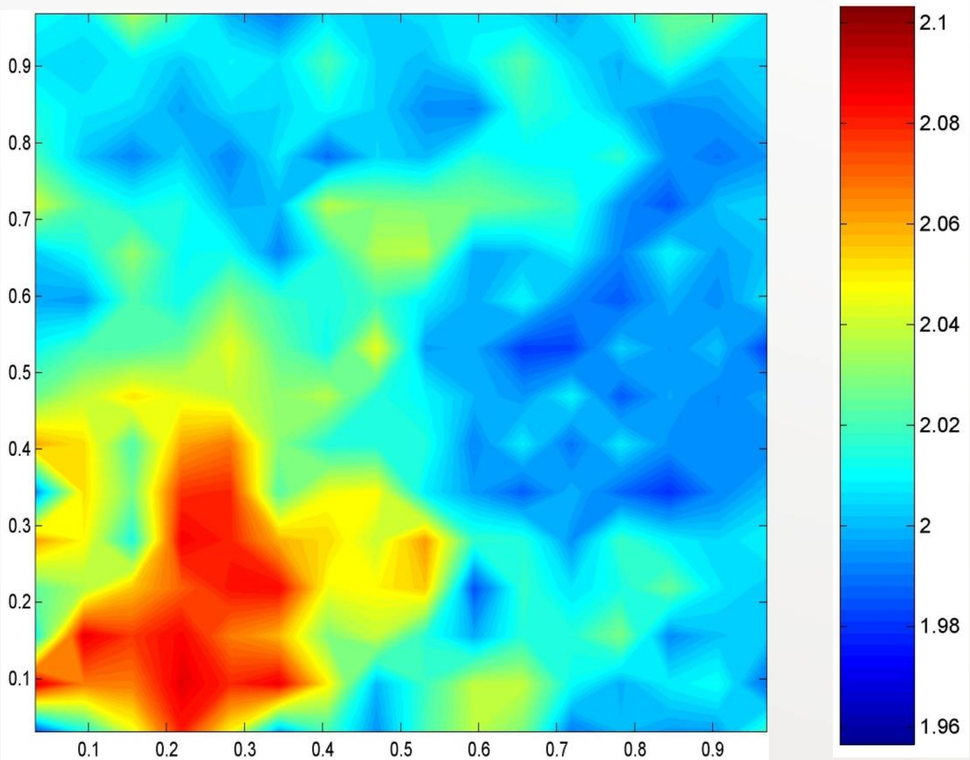
Model Validation Problem



Actual Versus Mortar Approximation



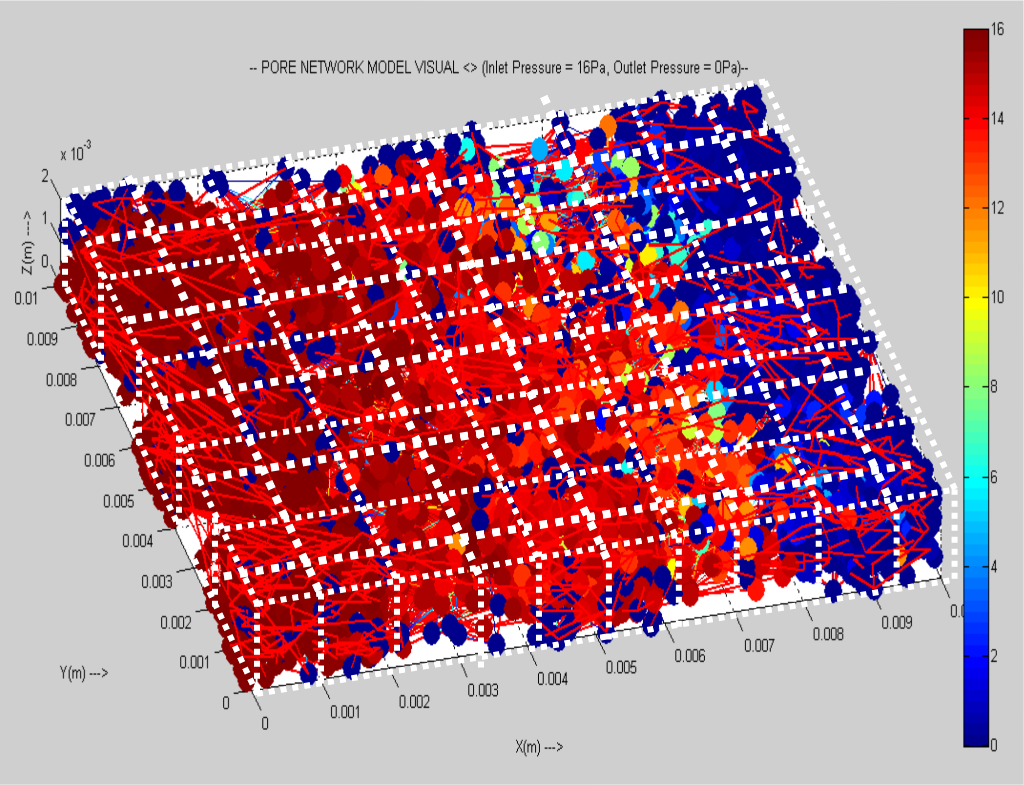
Actual



8x8 Quadratic Mortars

Upscaling - Single Phase Flow

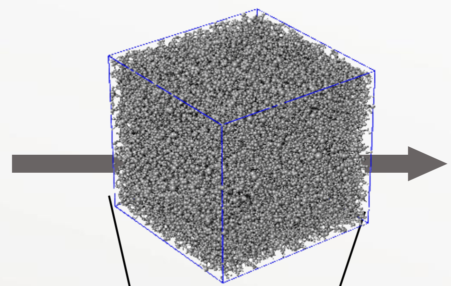
- Create large (million pore) network models
  - Very heterogeneous
  - Abrupt changes in pore structure
- Solve pressures, flows in the network
- Back-calculate permeability using Darcy's law (K_{TRUE})



Straightforward Upscaling Approach

- Split the network into several smaller networks and solve
- Back-calculate each sub-network permeability
- Upscale to get K_{FD} for entire domain using a traditional finite difference upscaling

$K_{FD} \neq K_{TRUE}$



No-Flow BC

Pin = 16 Pa (left) — Pout = 0 Pa (right)

750.5	1515.7	394.1	867.5	722.9	488.9	1331.8	1110.1	535.7	387.5
24.7	17.0	13.0	103.6	9.8	35.0	17.0	127.3	21.9	453.2
14.4	2761.9	6.3	618.4	1190.9	54.1	2920.9	12.0	1984.0	16.4
4.5	16.3	13.3	33.8	34.5	1980.1	27.3	94.2	6.3	374.3
7.5	10.8	2218.1	2160.3	6.8	10.6	14.9	16.9	5.8	13.4
12.0	10.5	18.7	14.6	30.7	3225.1	24.2	1330.0	17.7	3315.3
14.0	921.7	155.6	2743.2	7.1	27.2	8.5	1825.9	9.9	82.9
22.5	15.1	18.6	9.6	305.4	7.1	11.2	7.4	11.8	11.8
10.2	32.0	14.4	1456.9	16.2	6.4	1784.4	15.4	106.3	2279.3
18.2	19.8	103.5	18.9	6.3	61.5	12.5	108.2	14.0	7.4

No-Flow BC

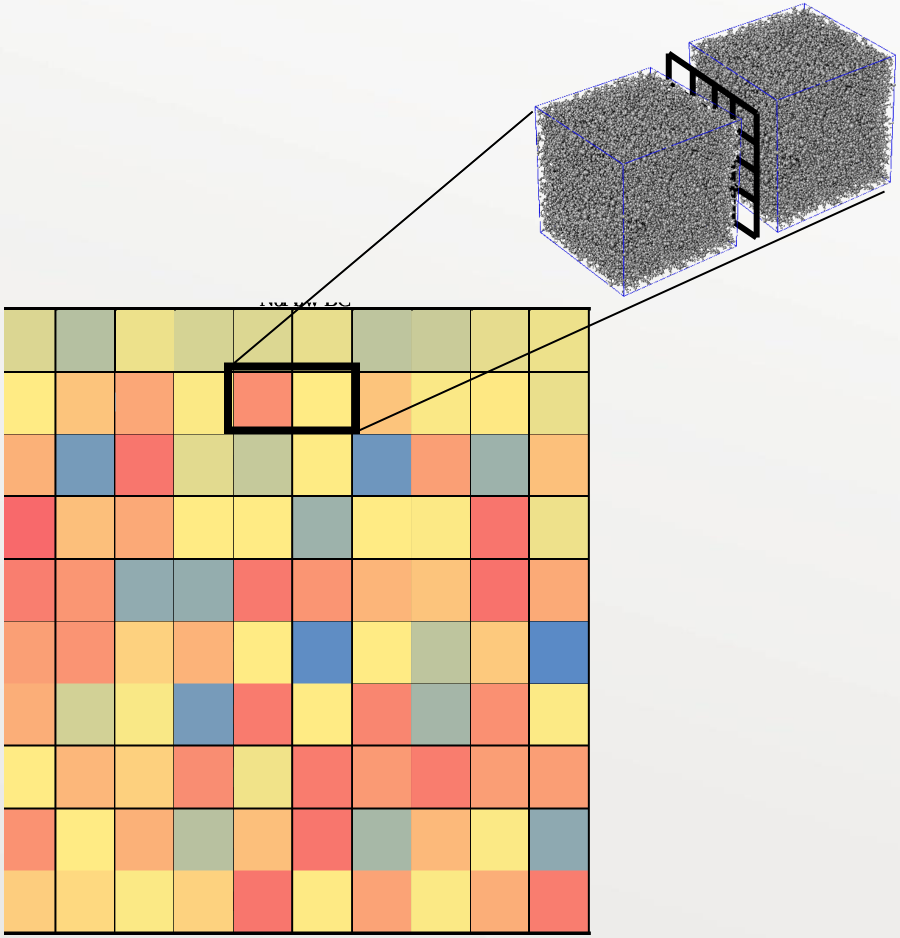
K
3315
2947
2580
2212
1844
1476
1108
740
372
5

$$\nabla \cdot \left(\mathbf{K} \nabla P \right) = 0$$

Upscaling…a Mortar Approach

- Split networks at natural boundaries
- Couple all networks using FEM mortars
- Calculate upscaled K_{MORTAR}

$$K_{MORTAR} \cong K_{TRUE}$$



Upscaling Results

- K_{MORTAR} better match to K_{TRUE} (0.255,0.234) than K_{FD} (0.191,0.175) for higher-order mortars and smaller grids

	Linear				Quadratics			
Order	K_{xx}	K_{yy}	% Error K_{xx}	% Error_K_{yy}	K_{xx}	K_{yy}	% Error_K_{xx}	% Error_K_{yy}
1	1.02	0.49	298.88	107.70	0.86	0.42	238.56	78.72
2	0.86	0.42	237.23	80.96	0.61	0.35	137.12	51.00
4	0.60	0.36	133.12	52.88	0.31	0.27	22.26	16.51
6	0.44	0.31	72.22	32.61	0.27	0.24	7.05	4.24
8	0.31	0.28	22.32	18.39	0.264	0.237	3.19	0.95

Global Jacobian Schur (GJS) Method

Formulate the problem into one global system

$$0 = F_i^f(\vec{p}_i, \vec{\alpha})|_{\Omega_i}, \quad \forall i = 1, \ldots, n_\Omega$$

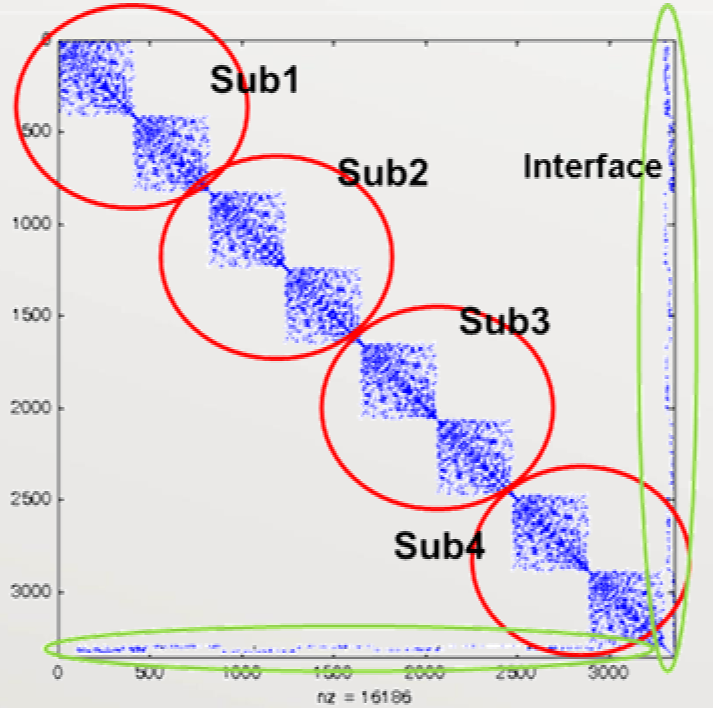
$$0 = G^f(\vec{p}_i, \vec{\alpha})|_{\Gamma}, \qquad \Gamma = \bigcup \Gamma_{ij}$$

$$F_i^f := \nabla.(K\nabla)|_h$$

$$G_k^f(\vec{p}, \vec{\alpha}) = \int_{\Gamma_{ij}} \left[\!\left[\vec{n} . \vec{q} \right]\!\right] . \varphi_k$$

$$\vec{q} := -K\nabla p \qquad K = \frac{k}{\mu}$$

Flow



$$J_g \delta\vec{x} = \begin{pmatrix} J_{F^{fl}/p} & J_{F^{fl}/\alpha} \\ J_{G^{fl}/p} & J_{G^{fl}/\alpha} \end{pmatrix} \begin{pmatrix} \delta\vec{p} \\ \delta\vec{\alpha} \end{pmatrix} = -\begin{pmatrix} \vec{F}^{fl} \\ \vec{G}^{fl} \end{pmatrix} = -\vec{F}_g$$

<u>Schur Complement</u>

$$S\delta\vec{\alpha} = \vec{R}$$

$$S = J_{G^{fl}/\alpha} - J_{G^{fl}/p} J_{F^{fl}/p}^{-1} J_{F^{fl}/\alpha}$$

$$\vec{R} = -(\vec{G}^{fl} - J_{G^{fl}/p} J_{F^{fl}/p}^{-1} \vec{F}^{fl})$$

Global Jacobian Schur (GJS) with Transport

Formulate both flow and transport into one global system

$$0 = F_i^f(\vec{p}_i, \vec{\alpha})|_{\Omega_i}, \quad \forall i = 1, \ldots, n_\Omega$$
$$0 = G^f(\vec{p}_i, \vec{\alpha})|_{\Gamma}, \quad \Gamma = \bigcup \Gamma_{ij}$$

$$F_i^f := \nabla.(K\nabla)|_h$$
$$G_k^f(\vec{p}, \vec{\alpha}) = \int_{\Gamma_{ij}} \left[\!\left[\vec{n}.\vec{q} \right]\!\right] . \varphi_k$$
$$\vec{q} := -K\nabla p \qquad K = \frac{k}{\mu}$$

Flow

$$\frac{\partial \vec{c}_i}{\partial t} = F_i^{tr}(\vec{c}_i, \vec{\beta}, t)|_{\Omega_i}, \quad \forall i = 1, \ldots, n_\Omega$$
$$0 = G^{tr}(\vec{c}_i, \vec{\beta}, t)|_{\Gamma}, \quad \Gamma = \bigcup \Gamma_{ij}$$

$$F_i^{tr} := -v_i.\nabla + \nabla.(D\nabla) + R|_h$$
$$G_k^{tr}(\vec{c}, \vec{\beta}, t) = \int_{\Gamma_{ij}} \left[\!\left[\vec{n}.\vec{q}_c \right]\!\right] . \varphi_k$$
$$\vec{q}_c := vc - D\nabla c$$

Transport

F_i^f = *space discretized flow operator*

G_k^f = *flow interface condition*

α = *Lagrange – multiplier for pressure*

k = *permeability / conductivity*

μ = *viscosity*

p = *pressure*

F_i^{tr} = *space discretized transport operator*

G_k^{tr} = *transport interface condition*

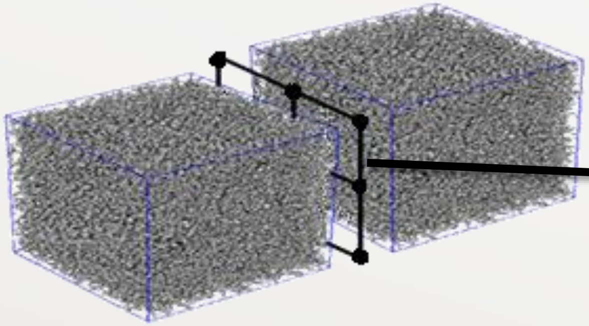
β = *Lagrange – multiplier for concentration*

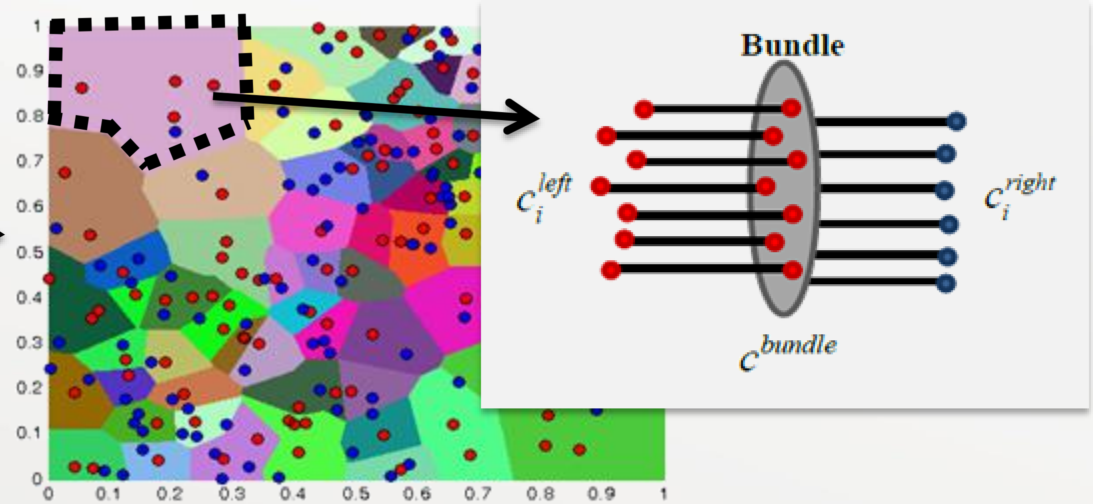
v = *fluid velocity*

D = *diffusion / dispersion coefficient*

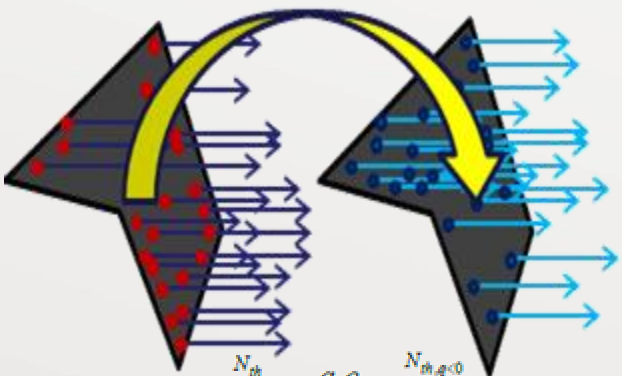
φ_k = *mortar basis functions*

Option b: Explicit Coupling of Transport:





$$\mathrm{P}: C_{outlet} \rightarrow C_{Inlet}$$



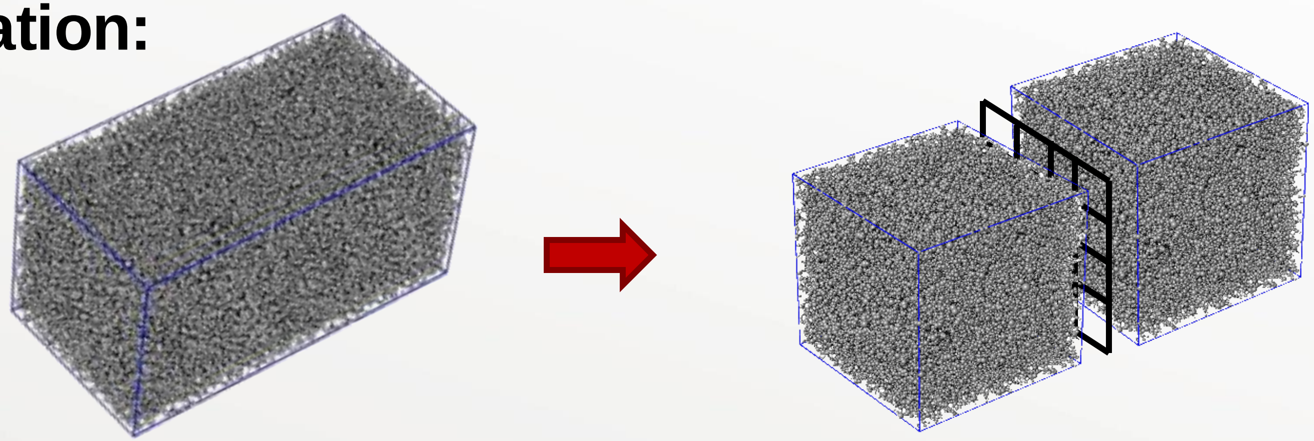
$$G_k^{fl}(\vec{p},\vec{\alpha}) = \int_{\Gamma\cap bundle} \left[\!\left[\vec{n}\cdot\vec{v}\right]\!\right]\varphi_k = \sum_{i=1}^{N_{left}} q_i^{left} + \sum_{i=1}^{N_{right}} q_i^{right} = 0$$

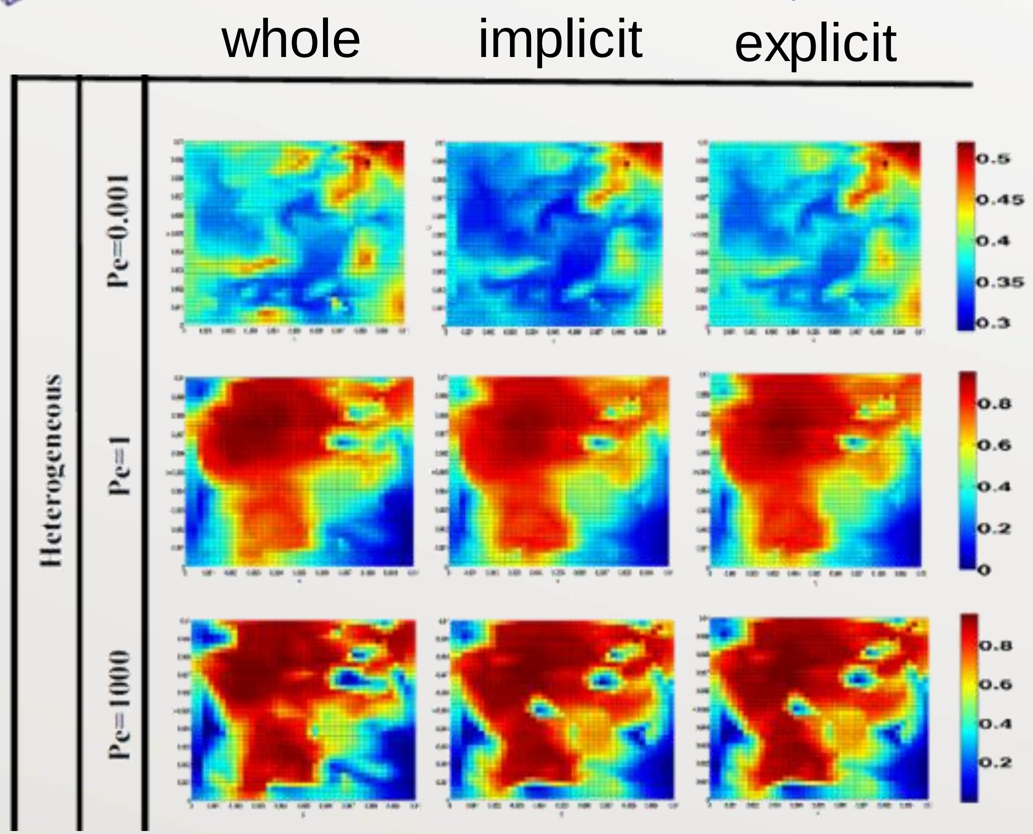
$$G_k^{tr}(\vec{c},\vec{\beta},t) = \int_{\Gamma\cap bundle} \left[\!\left[\vec{n}\cdot\vec{v}_c\right]\!\right]\varphi_k = \sum_{i=1}^{N_{left}} q_{c_i}^{left} + \sum_{i=1}^{N_{right}} q_{c_i}^{right} = 0$$

$$q_{c_i} = q_i c\,|_{upwinded} - Da_i \frac{c_i - c_{bundle}}{l_i}$$

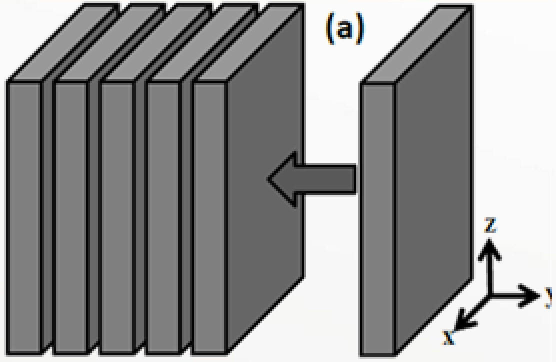
$$\beta_{bundle} = \frac{\sum_{i=1}^{N_{th}} D_i \frac{a_i c_i}{l_i} - \sum_{i=1}^{N_{th,q<0}} q_i c_i}{\sum_{i=1}^{N_{th}} D_i \frac{a_i}{l_i} + \sum_{i=1}^{N_{th,q>0}} q_i}$$

Verification:

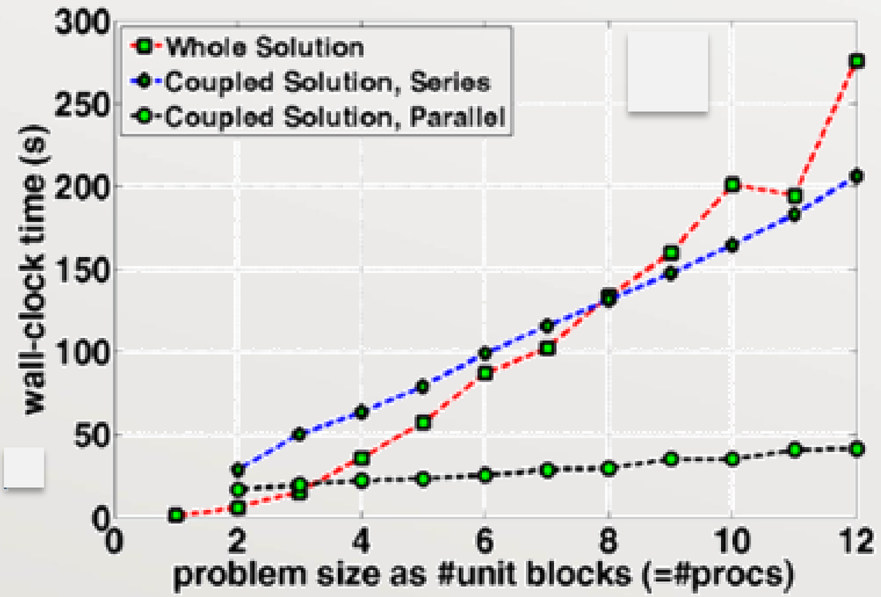




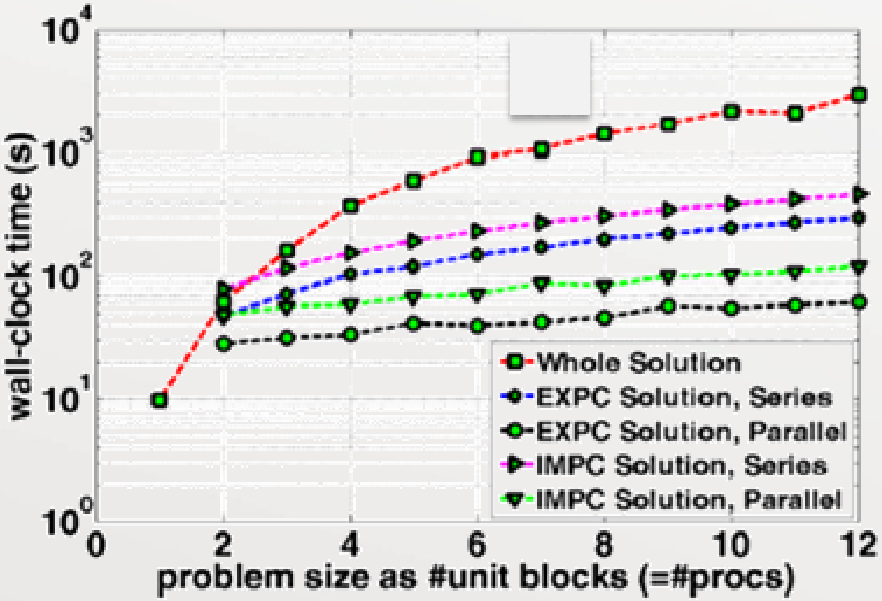
Computational Performance:



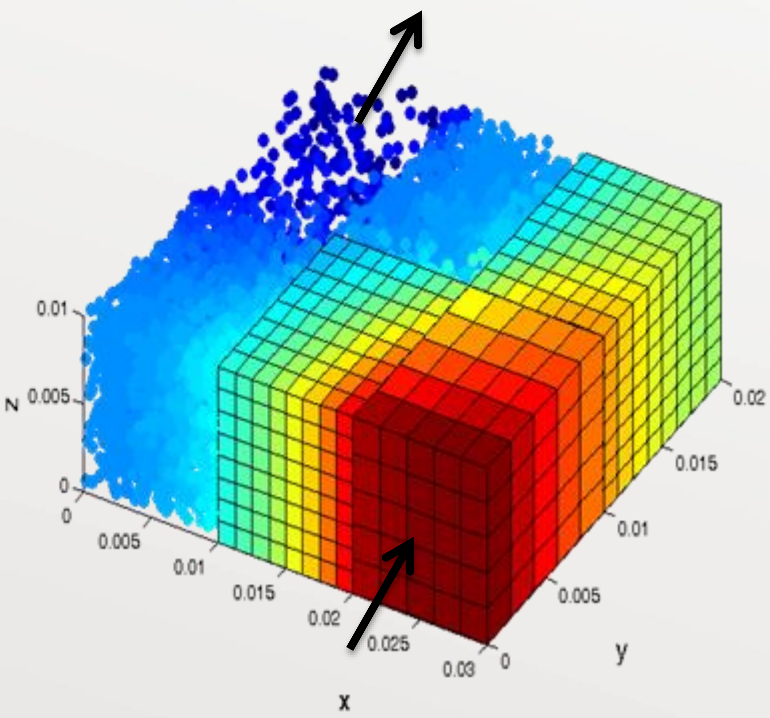
Flow



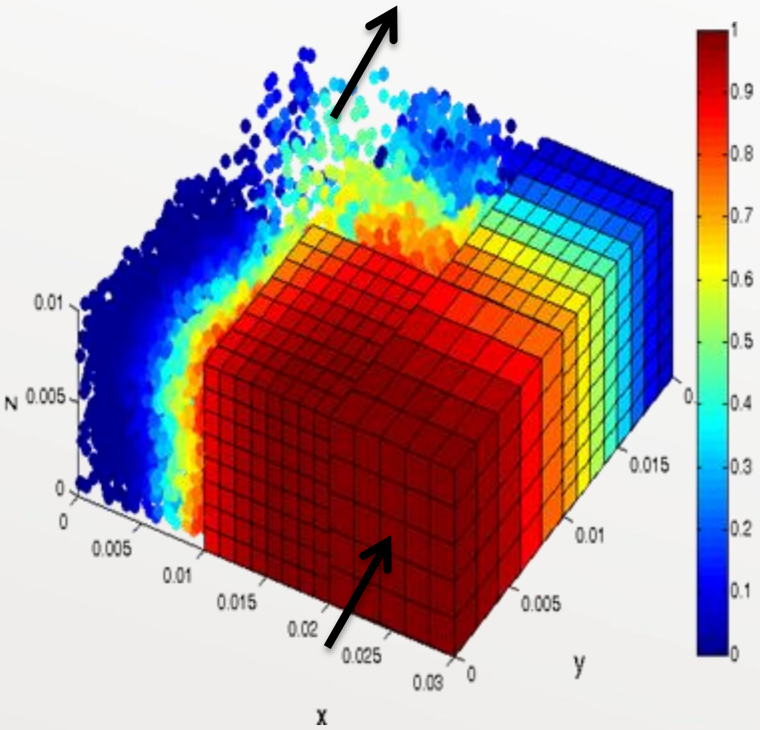
Transport



Hybrid Modeling



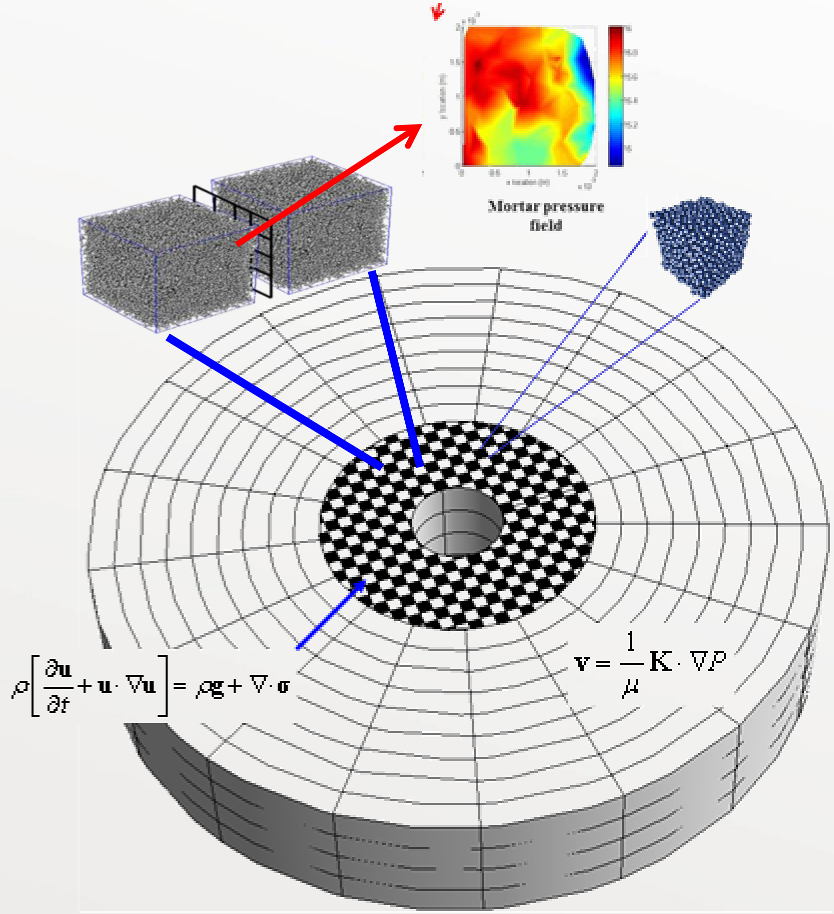
Pressure



Concentration

Multiscale, Hybrid Near-Well Reservoir Simulator

- 7500, 3D pore-network models near wellbore in “pore-scale region”
- ~30-75 million total pores
- 10000 grid blocks in outer “Darcy region”
- Models coupled using mortars
- Solve on multiple processors in parallel

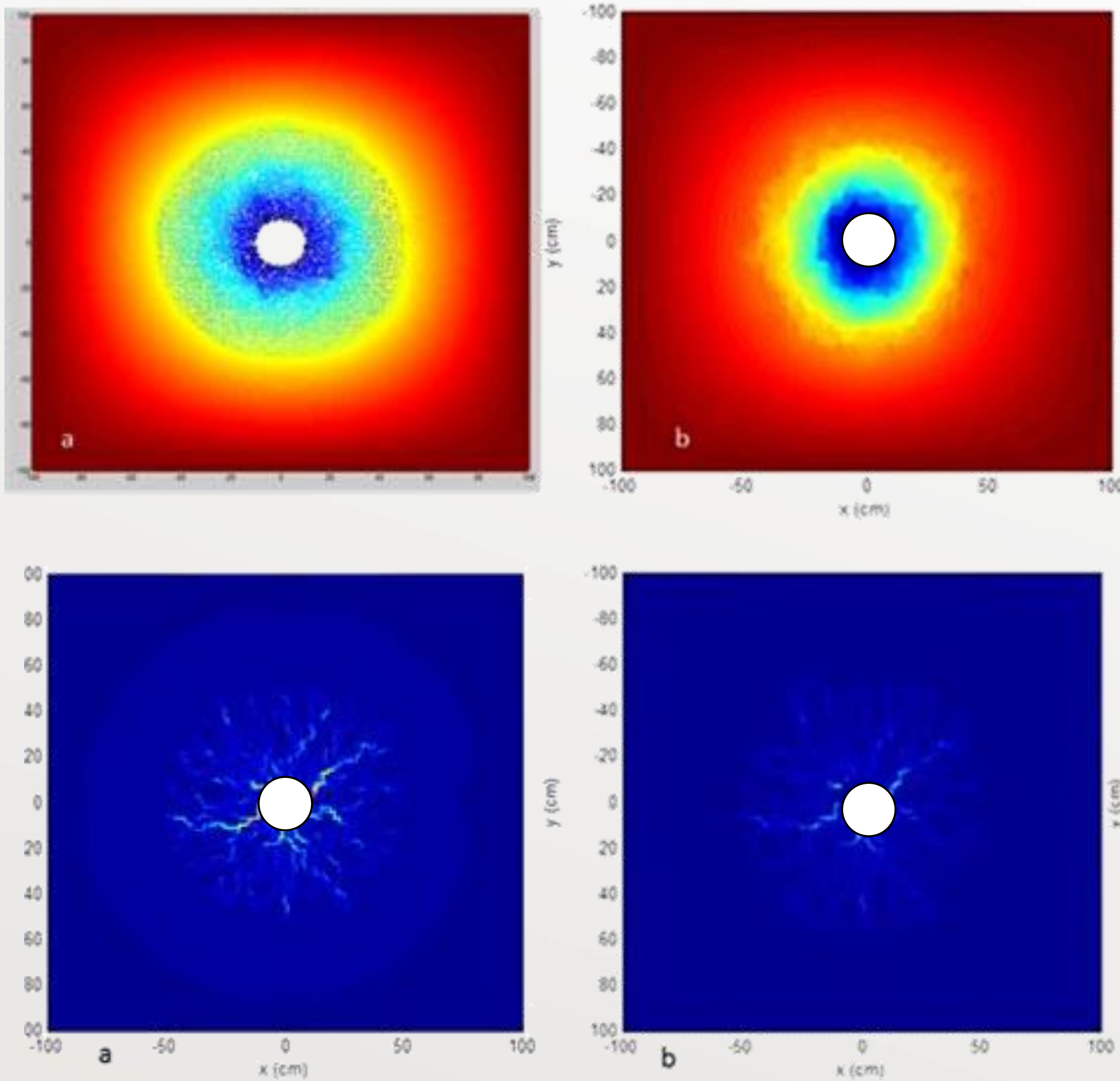


Sun et al., Energy and Fuels (2012)

Direct Upscaling Insufficient!

Pressure Field

Flux Field



Hybrid, Multiscale Mortar | **A Priori Direct Upscaling**

Discussion:

- Pore-scale modeling can be predictive only if:
    1. Topology is honored
    2. Streamline-scale equations reflect fundamental physics

- Even then, direct upscaling may be insufficient

- Mortar methods provide several advantages
    - Modeling larger pore-scale domains
    - Ease of hybrid modeling
    - Good computational scale up
    - Parallel computing