Homogenization and Multiscale Modeling

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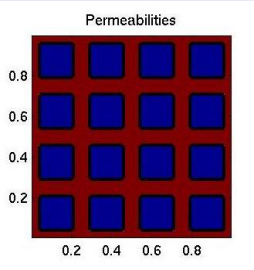
Origins

Homogenization is a collection of methods to approximate a heterogeneous problem by a homogeneous one.

Example (Elliptic)

$\mathcal{A}^\epsilon(u^\epsilon) = f : \quad -\sum(a^\epsilon_{ij}(x)u^\epsilon_{x_i})_{x_j} = f$, where $a^\epsilon_{ij}(x) = a_{ij}(x/\epsilon)$, and $a_{ij}(\cdot)$ are 1-*periodic* in $\Re^n$.

Exact model at microscale



$a_{ij}(x/\epsilon)$

replaced by homogenized model

with constant $\tilde{a}_{ij}$

First Issues

Question

Can we find a limiting problem, $\mathcal{A}u = f$, whose solution u characterizes the limit, $\lim_{\epsilon \to 0} u^\epsilon = u$?

Example (Elliptic)

$\mathcal{A}(u) = f : \quad -\sum(\tilde{a}_{ij} u_{x_i})_{x_j} = f$, where $\tilde{a}_{ij}$ are constant.

This is the *homogenized equation* with *effective* coefficients.

Question

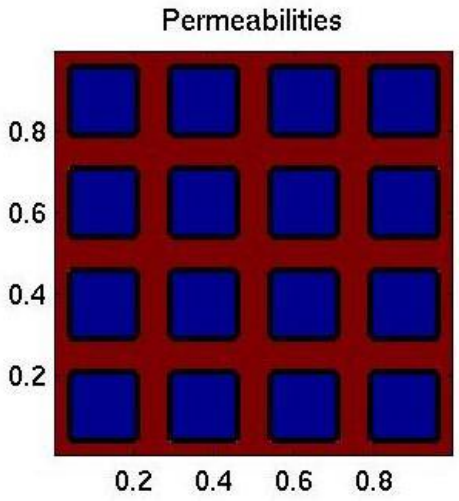
Is $\mathcal{A}$ of the same type as A^ϵ?

The answer is frequently 'No!'.

An Elliptic Problem

Let Y be the unit cube in $\Re^N$. Assume $a(\cdot)$ is Y-periodic. We want to approximate the solution to the *singular problem*

$$u^\epsilon \in H_0^1(\Omega):$$
$$\int_\Omega a(x/\epsilon)\nabla u^\epsilon(x)\cdot\nabla\varphi(x)\,dx = \int_\Omega F(x)\varphi(x)\,dx \text{ for all } \varphi \in H_0^1(\Omega). \tag{1}$$

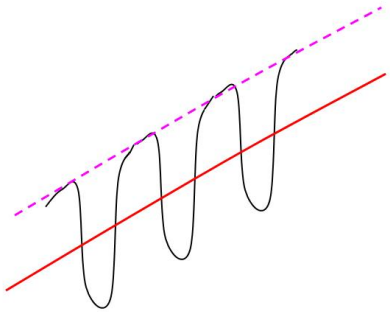


The approximation

We seek an approximation

$$u^\epsilon(x) = u(x, x/\epsilon) + \epsilon U(x, x/\epsilon) + \mathcal{O}(\epsilon^2), \quad x \in \Omega,$$

in which each $u(x, y)$ and $U(x, y)$ is Y-periodic.



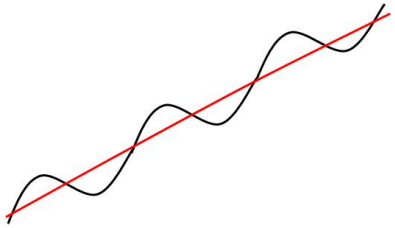
The gradient is given (formally) by

$$\nabla u^\epsilon(x) = \nabla_x u(x, x/\epsilon) + \frac{1}{\epsilon}\nabla_y u(x, x/\epsilon) + \nabla_y U(x, x/\epsilon) + \mathcal{O}(\epsilon).$$

The solution u^ϵ has a bounded gradient, so $\nabla_y u(x,y) = 0$ and

$$u^\epsilon(x) = u(x) + \epsilon U(x, x/\epsilon) + \mathcal{O}(\epsilon^2) \tag{2a}$$

$$\nabla u^\epsilon(x) = \nabla u(x) + \nabla_y U(x, x/\epsilon) + \mathcal{O}(\epsilon) \tag{2b}$$



Substitute (2) into (1) with a test function of the same form

$$\varphi(x) + \epsilon\Phi(x, x/\epsilon)$$

where $\Phi(x,y)$ is Y-periodic for each $x \in \Omega$.

The variational form

Two-scale limits $\epsilon \to 0$ give the system

$$u \in H_0^1(\Omega), \quad U \in L^2(\Omega, H_\#^1(Y)) :$$
$$\int_\Omega \int_Y a(y)(\nabla u(x) + \nabla_y U(x,y)) \cdot (\nabla \varphi(x) + \nabla_y \Phi(x,y))\, dy\, dx$$
$$= \int_\Omega F(x)\varphi(x)\, dx \text{ for all } \varphi \in H_0^1(\Omega), \quad \Phi \in L^2(\Omega, H_\#^1(Y)). \quad (3)$$

The homogenized system

Decouple the system:

$$U \in L^2(\Omega, H^1_\#(Y)) :$$

$$\int_\Omega \int_Y a(y)(\nabla_y U(x,y) + \nabla u(x)) \cdot \nabla_y \Phi(x,y)\, dy\, dx = 0$$

$$\text{for all } \Phi \in L^2(\Omega, H^1_\#(Y)). \quad (4a)$$

$$u \in H^1_0(\Omega) :$$

$$\int_\Omega \int_Y a(y)(\nabla u(x) + \nabla_y U(x,y))\, dy \cdot \nabla \varphi(x)\, dx = \int_\Omega F(x)\varphi(x)\, dx$$

$$\text{for all } \varphi \in H^1_0(\Omega). \quad (4b)$$

The Cell problem

The local problem (4a) is equivalent to requiring

$$U(x,\cdot) \in H^1_\#(Y):$$
$$\int_Y a(y)(\nabla_y U(x,y) + \nabla u(x)) \cdot \nabla_y \Phi(y)\, dy = 0 \text{ for all } \Phi \in H^1_\#(Y).$$

Define $\omega_i(y)$ for each $1 \le i \le N$ to be the solution of the cell problem

$$\omega_i \in H^1_\#(Y): \int_Y a(y)(\nabla_y \omega_i(y) + \mathbf{e}_i) \cdot \nabla_y \Phi(y)\, dy = 0 \text{ for all } \Phi \in H^1_\#(Y). \tag{5}$$

where $\mathbf{e}_i$ is the indicated coordinate vector in $\Re^N$.

The Homogenized problem

By linearity the solution is given by

$$U(x,y) = \sum_{i=1}^{i=N} \partial_i u(x)\omega_i(y)$$

This is substituted into (4b) to obtain

$$u \in H_0^1(\Omega) :$$

$$\int_\Omega \tilde{a}_{ij}\partial_i u(x) \cdot \partial_j \varphi(x)\, dx = \int_\Omega F(x)\varphi(x)\, dx \qquad \text{for all } \varphi \in H_0^1(\Omega). \quad (6)$$

where the *constant* coefficients are given by

$$\tilde{a}_{ij} = \int_Y a(y)\left(\delta_{ij} + \partial_j \omega_i(y)\right)\, dy\,. \quad (7)$$

The approximate solution

$$u^\epsilon(x) = u(x) + \epsilon\, \nabla u(x) \cdot (\omega_1(x/\epsilon), \omega_2(x/\epsilon), \ldots, \omega_N(x/\epsilon)) + \mathcal{O}(\epsilon^2)\,,$$

$$\nabla u^\epsilon(x) = \\ \nabla u(x) + \nabla u(x) \cdot (\nabla\omega_1(x/\epsilon), \nabla\omega_2(x/\epsilon), \ldots, \nabla\omega_N(x/\epsilon)) + \mathcal{O}(\epsilon)$$

of the singular elliptic problem.

Homogenization

Alain Bensoussan, Jacques-Louis Lions, and George Papanicolaou.
Asymptotic analysis for periodic structures, volume 5 of *Studies in Mathematics and its Applications*.
North-Holland Publishing Co., Amsterdam, 1978.

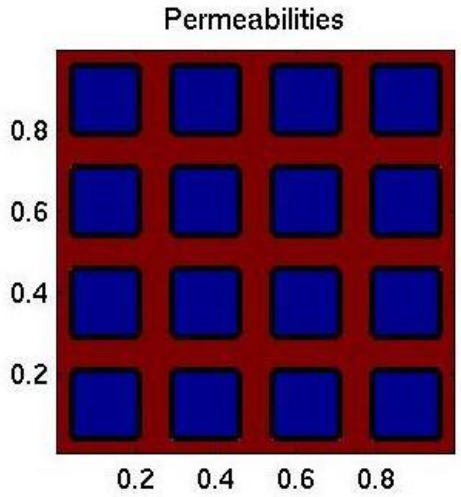
Enrique Sánchez-Palencia.
Nonhomogeneous media and vibration theory, volume 127 of *Lecture Notes in Physics*.
Springer-Verlag, Berlin, 1980.

V. V. Jikov, S. M. Kozlov, and O. A. Oleinik.
Homogenization of differential operators and integral functionals.
Springer-Verlag, Berlin, 1994.

Multiscale Flow and Transport ... the model

$$\begin{aligned} \mathbf{u}(x) = -\mathbf{K}(x)\nabla p(x), \quad \nabla \cdot \mathbf{u}(x) &= 0 \\ \phi \frac{\partial c(x,t)}{\partial t} + \nabla \cdot (\mathbf{u}(x)c(x,t) - \mathbf{D}(\mathbf{u}(x))\nabla c(x,t)) &= 0 \end{aligned}$$

K_{fast}, K_{slow} $\longrightarrow$ $\mathbf{u}_{fast}$, $\mathbf{u}_{slow}$ $\longrightarrow$ $\mathbf{D}_{fast}$, $\mathbf{D}_{slow}$



The Parabolic Equation

The Exact Model ... with fine-scale coefficients

$$\phi(x)\frac{\partial c}{\partial t} - \nabla \cdot \mathbf{D}(x)\nabla c = 0, \quad x \in \Omega,$$

with $\mathbf{D}(x) = \mathbf{D}_{slow}$ on Ω_{slow} and $= \mathbf{D}_{fast}$ on Ω_{fast} .

... or in transmission form

$$\phi_\alpha \frac{\partial c_\alpha}{\partial t} - \nabla \cdot \mathbf{D}_\alpha \nabla c_\alpha = 0, \quad x \in \Omega_\alpha, \ \alpha = fast, slow$$

with the interface conditions on $\partial\Omega_{slow} \cap \partial\Omega_{fast}$:

$$c_{fast} = c_{slow}, \quad \mathbf{D}_{fast}\nabla c_{fast} \cdot \nu = \mathbf{D}_{slow}\nabla c_{slow} \cdot \nu$$

The Classical Case

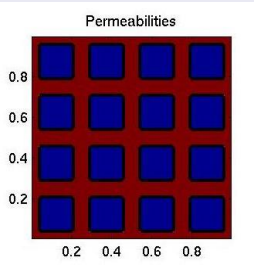
The coefficients are $D = [D_{fast}, D_{slow}]$:

$$\tilde{\phi}\frac{\partial \tilde{c}}{\partial t} - \nabla \cdot \tilde{\mathbf{D}} \nabla \tilde{c} = 0$$

- The fine-scale geometry is eliminated . . .
  . . . replaced by the constant effective coefficient $\tilde{\mathbf{D}}$.
- The upscaled limit is of the same type . . . a single equation.
- The fast and slow regions are coupled by gradients of the solution (flux) .
- Accurate only in this low contrast case.

... the algorithm

Exact model at microscale

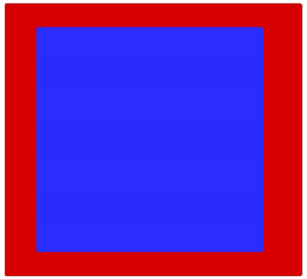


$\mathbf{D}(x) = \mathbf{D}_{slow}, \mathbf{D}_{fast}$

replaced by homogenized model

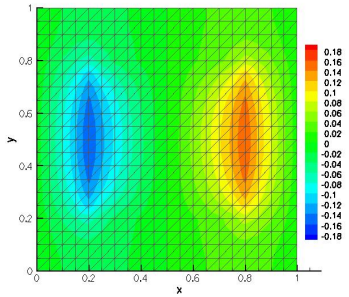
with constant $\tilde{\mathbf{D}}$

Compute homogenized coefficient $\tilde{\mathbf{D}} = \tilde{\mathbf{D}}(\mathbf{D}_{fast}, \mathbf{D}_{slow})$



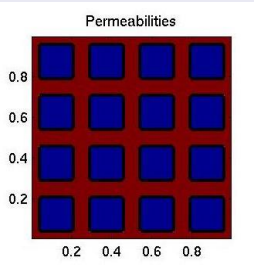
$$\tilde{D}_{jk} = \frac{1}{|\Omega_0|} \int_{\Omega_0} D_{jk}(\mathbf{y})(\delta_{jk} + \partial_k \omega_j(\mathbf{y}))dA$$

$$\begin{cases} -\nabla \cdot \mathbf{D}(\mathbf{y}) \nabla \omega_j(\mathbf{y}) & = \nabla \cdot (\mathbf{D}(\mathbf{y})\mathbf{e}_j), \\ \omega_j(\mathbf{y}) \text{ is} & \Omega_0 - \text{ periodic.} \end{cases}$$



... the algorithm

Exact model at microscale



$\mathbf{D}(x) = \mathbf{D}_{slow}, \mathbf{D}_{fast}$

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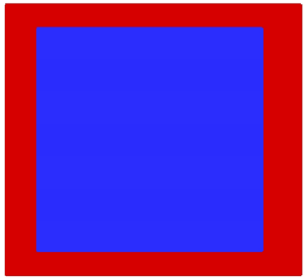
Compute homogenized coefficient $\tilde{\mathbf{D}} = \tilde{\mathbf{D}}(\mathbf{D}_{fast}, \mathbf{D}_{slow})$



$$\tilde{D}_{jk} = \frac{1}{|\Omega_0|} \int_{\Omega_0} D_{jk}(\mathbf{y})(\delta_{jk} + \partial_k \omega_j(\mathbf{y}))dA$$

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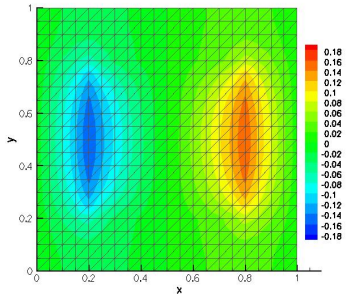


It works well for problems with low contrast $\mathbf{D}_{fast}/\mathbf{D}_{slow}$

The Obstacle Problem . . . a special case

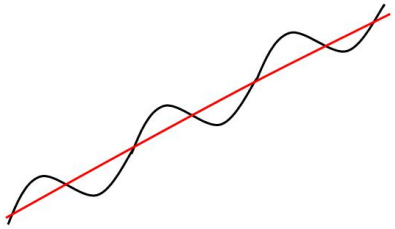
The coefficients are $D = [D_{fast}, 0]$:

$$\tilde{\phi}^0 \frac{\partial \tilde{c}^0}{\partial t} - \nabla \cdot \tilde{\mathbf{D}}^0 \nabla \tilde{c}^0 = 0$$

- The slow region Ω_{slow} is impervious.

Classical homogenization is not adequate for time-dependent problems with large contrast $\mathbf{D}_{fast}/\mathbf{D}_{slow}$

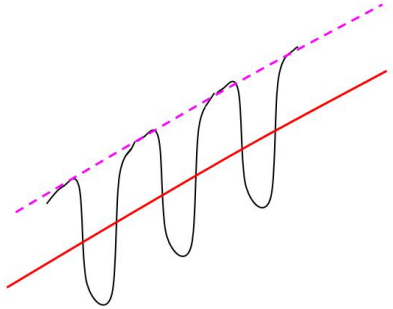
Low contrast: classical homogenization



$\| u_\epsilon \|_0 + \| \nabla u_\epsilon \|_0 \leq C$

local averages

High contrast: double porosity models



$\| u_\epsilon \|_0 + \epsilon \| \nabla u_\epsilon \| \leq C$

local averages versus special averages

The Double-porosity model

The coefficients are $D = [D_{fast}, \epsilon_0^2 D_{slow}]$:

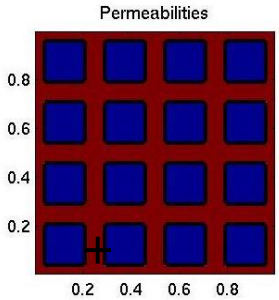
$$\tilde{\phi}^0 \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{\mathbf{D}}^0 \nabla \tilde{c} = 0, \quad q_i(t) = \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} \mathbf{D}_{slow} \nabla c_i \cdot \nu ds,$$

$$\phi_{slow} \frac{\partial c_i}{\partial t} - \nabla \cdot \mathbf{D}_{slow} \nabla c_i = 0, \quad c_i|_{\Gamma_i} = \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \tilde{c}(\mathbf{x}) dA.$$

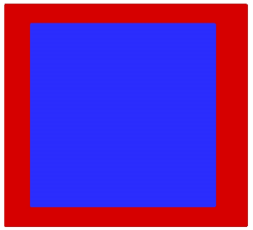
- The upscaled model is a system, highly parallel.
- The coupling from the cell to global equation is via gradients.
- The coupling from the global equation to the cell is via the values.
- The contribution of the cells is a secondary storage.
- Accurate only in this high contrast case.
- It will not couple any advective effects to the local cell.

Double-porosity Micro-structure Model

Exact model



replaced by two layers



Global equation, $x \in \Omega$

$$\tilde{\phi}^0 \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{\mathbf{D}}^0 \nabla \tilde{c} = 0$$

$$q_i(t) = \Pi^*_{0,i}(\mathbf{D}_{slow} \nabla c_i(\cdot, t) \cdot \nu)$$

Cell problem at each $x \in \Omega_i$

$$\begin{aligned} \phi_{slow} \frac{\partial c_i}{\partial t} \quad - \quad & \nabla \cdot \mathbf{D}_{slow} \nabla c_i = 0 \\ c_i|_{\Gamma_i} \quad = \quad & \Pi_{0,i}(\tilde{c})(t) \end{aligned}$$

Notes

- The coefficients in the global equation are precisely those of the obstacle problem.
- The cell input to the global equation is

$$q_i(t) = \frac{1}{|\hat{\Omega}_i|} \frac{\partial}{\partial t} \int_{\Omega_i} \phi_{slow} c_i(\mathbf{x}, t)\, d\mathbf{x}$$

  ...the rate of secondary storage.
- The spatially-constant input to the cell problem will *not* transmit any advective transport.

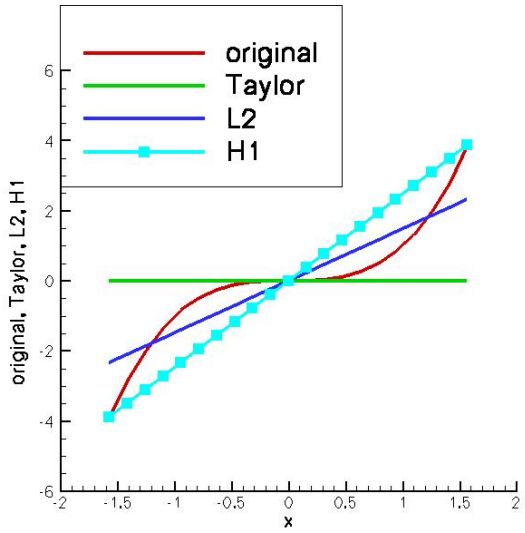
We shall more tightly couple the cell by replacing the constant coupling with an affine coupling to the surrounding fast medium. This will provide a gradient coupling.

Affine approximations Π_1

AVERAGE: $\Pi_0 f = \frac{1}{|\Omega_0|}\int_{\Omega_0} f(\mathbf{x})dA$; assume here $|\Omega_0| = 1$.
Denote $\mathbf{x}^C$ - center of mass of Ω_0.
General affine approximation $f(\mathbf{x}) \approx \Pi_1 f := m + \mathbf{n}\cdot\mathbf{x}, \quad \mathbf{x} \in \Omega_0$

Choice of $m, \mathbf{n}$

- Taylor ($f \in C^1(\Omega_0)$) about midpoint
  $f(\mathbf{x}) \approx f(\mathbf{x}^C) + \nabla f(\mathbf{x}^C)(\mathbf{x} - \mathbf{x}^C)$
- $L_2(\Omega_0)$-projection onto affines that is:
  $(f, v)_{\Omega_0} = (m + \mathbf{n}\cdot\mathbf{x}, v)_{\Omega_0}, \forall$ affine v
- $H^1(\Omega_0)$ projection:
  $f(\mathbf{x}) \approx \Pi_1 f := \Pi_0 f + \Pi_0 \nabla f \cdot (\mathbf{x} - \mathbf{x}^C)$



Summary: the affine coupling Π_i and its dual Π_i^*

Affine coupling $\Pi_i : H^1(\Omega) \mapsto H^1(\hat{\Omega}_i)$

$$\Pi_i(w)(x) \equiv \Pi_0 w + \Pi_0(\nabla w) \cdot (\mathbf{x} - \mathbf{x}^C)$$

Its dual $\Pi_i^* : H^1(\hat{\Omega}_i)^* \mapsto H^1(\Omega)^*$ pointwise

$$\Pi_i^*(q)(\mathbf{x}) = \bar{\chi}_i(\mathbf{x}) M_i^0(q) - \nabla \cdot \bar{\chi}_i(\mathbf{x}) \mathbf{M}_i^1(q)$$

Double-porosity Model with secondary flux

$$\tilde{\phi}^0 \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{\mathbf{D}}^0 \nabla \tilde{c} = 0,$$

$$\phi_{slow} \frac{\partial c_i}{\partial t} - \nabla \cdot \mathbf{D}_{slow} \nabla c_i = 0,$$

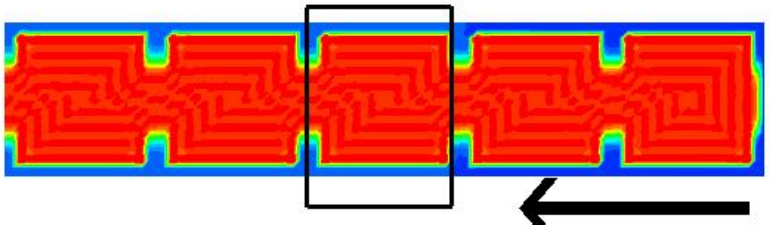
$$c_i|_{\Gamma_i} = \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \tilde{c} dA + \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \nabla \tilde{c}\, dA \cdot (\mathbf{x} - \mathbf{x}^C).$$

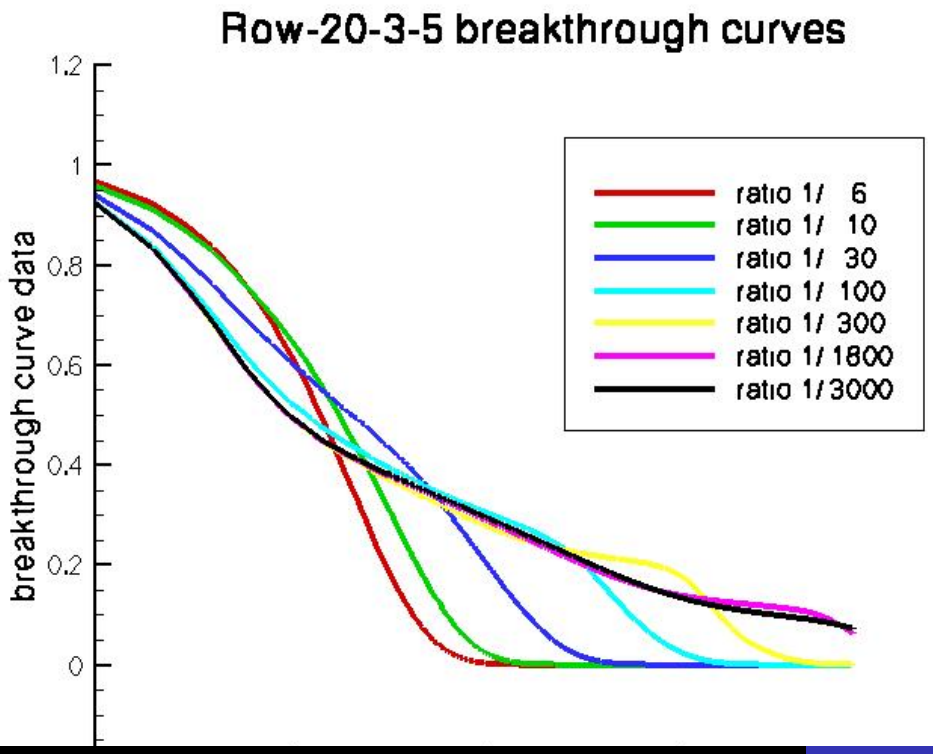
$$q_i(t) = \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} \mathbf{D}_{slow} \nabla c_i \cdot \nu ds - \nabla \cdot \frac{\bar{\chi}_i(\mathbf{x})}{|\hat{\Omega}_i|} \int_{\Gamma_i} \mathbf{D}_{slow} \nabla c_i \cdot \nu\, (\mathbf{x} - \mathbf{x}^C) dS$$

This is $\frac{\partial}{\partial t}$ (secondary storage) $-\nabla\cdot$ (secondary flux) from the local cells.

Computational experiments at microscale

GOAL: reproduce qualitatively experimental results





Porous Media

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