Nonlocal models of transport in multiscale porous media:
something old and something new, something borrowed ...
Outline

1. Introduction and motivation
   - Flow and transport in subsurface, nomenclature
   - Multiscale flow and transport in subsurface, experimental results

2. Something old: double porosity models
   - Literature review
   - Double porosity models, diffusion+advection

3. Something new: building a new model
   - Ideas and steps
   - Computational experiments
   - Construct affine approximations
   - Model calculations
   - Computational experiments with elements of upscaled model

NSF 0511190 “Model adaptivity in porous media”, DOE 98089 “Modeling, Analysis, and Simulation of Multiscale Preferential Flow”.
Also, see presentations at NSF-CMBS Nevada 5/20-25, DOE Multiscale workshop Tacoma, 5/25-30 (links from my webpage)
Flow coupled to transport $\mathcal{F}(\Theta) = 0$ with $\Theta = (u, p, c)$

**Flow**

$$u = -K \nabla p, \quad \nabla \cdot u = 0$$

**Diffusive-dispersive transport**

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

**Definitions**

$$D(u) := \text{diffusion} + \text{dispersion}$$

$$:= d_{mol} I + |u| (d_{long} E(u) + d_{transv} (I - E(u)))$$

$$E(u) = \frac{1}{|u|^2} u_i u_j$$

$$D(u) \approx d_{mol} I + d_{long} |u| E(u)$$
Model $\mathcal{F}(\Theta) = 0$ with $\Theta = (\rho, \mathbf{u}, c)$

$$\mathbf{u} = -K \nabla \rho, \quad \nabla \cdot \mathbf{u} = 0$$

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

$K_{\text{fast}}$, $K_{\text{slow}}$ give $\mathbf{u}_{\text{fast}}$, $\mathbf{u}_{\text{slow}}$ give $D_{\text{fast}}$, $D_{\text{slow}}$
Introduction and motivation
Something old: double porosity models
Something new: building a new model

Flow and transport in subsurface, nomenclature
Multiscale flow and transport in subsurface, experimental results

Advection+diffusion in multiscale media: tailing

Breakthrough curves = total concentration at outlet

MOVIE
Advection+diffusion in multiscale media: tailing

Breakthrough curves = total concentration at outlet

![Breakthrough curves graph]

- Pure advection
- Advection + diffusion

![Breakthrough curves graph with additional models]
Experimental visualization by Haggerty et al

Presentation at SIAM Annual 2004 by Haggerty

[BZH+04] Brendan Zinn, Lucy C. Meigs, Charles F. Harvey, Roy Haggerty, Williams J. Peplinski, and Claudius Freiherr von Schwerin,

Experimental breakthrough curves

Results from \[\text{ZMH}^+ 04]\]
Challenge in view of the experimental results

- Not-well separated scales:
  - *double porosity* diffusion model does not fit in low/intermediate contrast regime
  - $\epsilon_0 > 0$ is fixed (perhaps the homogenized model not good enough? need a corrector?)
  - $\frac{K_{fast}}{K_{slow}}$ small, moderate, intermediate, or large

- Evidence of advection-diffusion-dispersion in $\Omega_{slow}$ and advection-dispersion in $\Omega_{fast}$

- Related project (Wood, Haggerty, Waymire, Thomann, Ramirez, OSU) on Taylor-Aris dispersion/skew diffusion models

- Other results on tailing \([HG95, HMM00, HFMM01]\)

Formidable challenge: find an upscaled model similar to double-porosity which can capture all of the above


Introduction and motivation

Something old: double porosity models

Something new: building a new model

Literature review

Double porosity models, diffusion+advection


\[ \Omega = \bigcup_i \hat{\Omega}_i, \quad \Omega_{\text{slow}} = \bigcup_{i=1} \Omega_i, \]
\[ \partial \Omega_{\text{slow}} \cap \partial \Omega_{\text{fast}} \equiv \bigcup_i \Gamma_i \]
\[ \Omega = \Omega_{\text{slow}} \cup \Omega_{\text{fast}} \cup \bigcup_i \Gamma_i \]
\[ |\hat{\Omega}_i| \approx \varepsilon_0 \]
Averaged (single porosity) model

Exact model at microscale

\[ D = D_{\text{slow}}, D_{\text{fast}} \]

replaced by homogenized model

Compute homogenized coefficients \( \tilde{D} \)

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

\[
\begin{cases}
- \nabla \cdot D \nabla \omega_j(y) = \nabla \cdot (D e_j), & y \in \Omega_0 \\
\omega_j & \Omega_0 - \text{periodic}
\end{cases}
\]
Averaged (single porosity) model

**Exact model at microscale**

\[
\mathbf{D} = \mathbf{D}_\text{slow}, \mathbf{D}_\text{fast}
\]

**replaced by homogenized model**

Compute homogenized coefficients \( \mathbf{\tilde{D}} \)

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

\[
\begin{cases}
- \nabla \cdot \mathbf{D} \nabla \omega_j(\mathbf{y}) = \nabla \cdot (\mathbf{D} e_j), & \mathbf{y} \in \Omega_0 \\
\omega_j & \Omega_0 \text{ - periodic}
\end{cases}
\]

But this doesn’t work very well for time-dependent problems with large contrast \( D_{\text{fast}}/D_{\text{slow}} \)
Double porosity model: main idea I

Exact model at microscale

\[ D = D_{\text{slow}}, D_{\text{fast}} \]

replaced by homogenized model with two sheets

\[ \tilde{D} \]

with \( \tilde{D} \) plus cell model

Compute homogenized coefficients \( \tilde{D} \)

\[
\begin{align*}
\tilde{D}_{jk} &= \frac{1}{|\Omega_0|} \int_{\Omega_0} D_{jk}(y)(\delta_{jk} + \partial_k \omega_j(y))dA \\
- \nabla \cdot D \nabla \omega_j(y) &= \nabla \cdot (D e_j), \quad y \in \Omega_{0,\text{fas}} \\
\omega_j &\Omega_0 - \text{periodic}
\end{align*}
\]
Double porosity model: main idea I

**Exact model at microscale**

\[ D = D_{slow}, D_{fast} \]

**replaced by homogenized model with two sheets**

**Compute homogenized coefficients \( \tilde{D} \)**

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

\[
\begin{cases}
- \nabla \cdot D \nabla \omega_j(y) = \nabla \cdot (D_{\text{ef}}), & y \in \Omega_0, \text{fas} \\
\omega_j & \Omega_0 \text{ periodic}
\end{cases}
\]

This formulation introduces nonlocal effects and works very well for time-dependent problems with large contrast \( D_{fast}/D_{slow} \)
Double porosity model: main idea II

**Exact model at microscale**

\[
D = D_{\text{slow}}, D_{\text{fast}}
\]

**Global equation, \( x \in \Omega \)**

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

\[
q_i(t) = \Pi_{0,i}^* (\Pi_{0,i}(\tilde{c}))
\]

**Cell problem, \( x \in \Omega_i \)**

\[
\phi_{\text{slow}} \frac{\partial c_i}{\partial t} - \nabla \cdot D_{\text{slow}} \nabla c_i = 0
\]

\[
c_i|_{\Gamma_i} = \Pi_{0,i}(\tilde{c})
\]

This formulation works well for single & multi-phase multicomponent problems and has been implemented in commercial reservoir simulators.
Recall double porosity models for diffusion

**Exact $\epsilon_0$ model** $\mathcal{F}_{\epsilon_0}(\Theta_{\epsilon_0}) = 0$

\[
\phi_\alpha \frac{\partial c_\alpha}{\partial t} - \nabla \cdot D_\alpha \nabla c_\alpha = 0, \quad x \in \Omega_\alpha, \quad \alpha = \text{fast, slow}
\]

plus interface conditions on $\partial \Omega_{\text{slow}} \cap \partial \Omega_{\text{fast}}$:

\[
c_{\text{fast}} = c_{\text{slow}}, \quad D_{\text{fast}} \nabla c_{\text{fast}} \cdot \nu = D_{\text{slow}} \nabla c_{\text{slow}} \cdot \nu
\]

**Approximate microstructure model**

[Arb89a, Arb97] $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

\[
\phi \frac{\partial \tilde{c}}{\partial t} + \sum_{i} \chi_i q_i(t) - \nabla \cdot \tilde{D} \nabla \tilde{c} = 0
\]

\[
q_i(t) = \Pi_{0,i}^* (\Pi_{0,i}(\tilde{c}))
\]

- also for multiphase problems [DA90]

**Homogenized model**

[ADH90, HS90, Pes92] $\mathcal{F}_\epsilon(\epsilon_0) \rightarrow \mathcal{F}_0(\Theta_0) = 0$

\[
\phi \frac{\partial \tilde{c}}{\partial t} + \tau * \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot \tilde{D} \nabla \tilde{c} = 0,
\]

- analysis and convergence
- computational approach [Pes95, Pes96, DPS97]

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Local (cell) problem and averages $\Pi_0, \Pi^*_0$

Local averages $\Pi_{0,i}, \Pi^*_{0,i}$

\[
\Pi_{0,i} \xi := \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \xi(x) dA
\]

\[
\Pi^*_{0,i} \gamma := \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} \mathbf{D}_{\text{slow}} \nabla c_i(\gamma)(x, t) \cdot \nu ds = \Pi_{0,i}(\phi_{\text{slow}} \frac{\partial c_i(\gamma)}{\partial t})
\]

where $c_i = c_i(\gamma)$ solves the local (cell) problem

\[
\phi_{\text{slow}} \frac{\partial c_i}{\partial t} - \nabla \cdot \mathbf{D}_{\text{slow}} \nabla c_i = 0, \quad x \in \Omega_i,
\]

\[
c_i = \gamma(x, t), \quad x \in \partial \Omega_i
\]
Double porosity models for diffusion-advection

**Exact $\epsilon_0$ model** $F_{\epsilon_0}(\Theta_{\epsilon_0}) = 0$

\[
\phi \frac{\partial c_\alpha}{\partial t} - \nabla \cdot (D_\alpha \nabla c_\alpha - u_\alpha c_\alpha) = 0, \quad x \in \Omega_\alpha, \; \alpha = \text{fast, slow}
\]

plus interface conditions on $\partial \Omega_{\text{slow}} \cap \partial \Omega_{\text{fast}}$

**Approximate microstructure model**

[Arb89b] $\tilde{F}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

\[
\tilde{\phi} \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i - \nabla \cdot (\tilde{D} \nabla \tilde{c} - \tilde{u} \tilde{c}) = 0,
\]

\[q_i(t) = \Pi_{1,i}^*, (\Pi_{1,i}(\tilde{c}))\]

$\Pi_1 =$ local $L_2$ projections onto linears, $\Pi_1^*$ its dual.

Numerical model only.

**Limit $\epsilon \to 0$ model** [DS01] $F_0(\Theta_0) = 0$

\[
\tilde{\phi} \frac{\partial \tilde{c}}{\partial t} + \phi_{\text{slow}} \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot (\tilde{D} \nabla \tilde{c} - \tilde{u} \tilde{c}) = 0
\]

\[\phi_{\text{slow}} \frac{\partial \tilde{c}}{\partial t} \approx \Pi_0^*, (\Pi_{1,i}(\tilde{c}))\]

$\Pi_1 =$ local Taylor. Cell problem:

$u_{\text{slow}} \approx 0$, symmetry exploited.
Why these are not enough ... and other related results

Approximate microstructure model

\[ \mathcal{F}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0 \]

Numerical model only.

Limit \( \epsilon \to 0 \) model

\[ \mathcal{F}_0(\Theta_0) = 0 \]

Cell problem: \( u_{\text{slow}} \approx 0 \). Use \( \Pi_0^* \) for flux.

Want to have \( \tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0 \)

constructed with “global” (upscaled) flavor (akin diffusion model

\[ \phi \frac{\partial \tilde{c}}{\partial t} + \tau \ast \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot (\tilde{D} \nabla \tilde{c} - \tilde{u} \tilde{c}) = 0, \]

or secondary diffusion as in [CS95]

- account for (lack of) separation of scales \( \epsilon_0 > 0 \) and advection-dispersion
- track transition between different regimes of phenomena

Other models known in hydrology/applied math and geosciences

- Gerke van Genuchten 1993 (for Richards’ equation)
- nonlocal models of dispersion (Cushman et al)
- stochastic models, method of moments

[Arb89b] [DS01] [CS95] [XC04] [GR87]
Why these are not enough ... and other related results

Approximate microstructure model

\[ \mathcal{F}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0 \]

Numerical model only.

Limit \( \epsilon \to 0 \) model

\[ \mathcal{F}_0(\Theta_0) = 0 \]

Cell problem: \( \mathbf{u}_{\text{slow}} \approx 0 \). Use \( \Pi^* \) for flux.

Want to have \( \tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0 \)

constructed with “global” (upscaled) flavor (akin diffusion model

\[ \phi \frac{\partial \tilde{c}}{\partial t} + \tau * \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot (\tilde{D} \nabla \tilde{c} - \tilde{u} \tilde{c}) = 0, \]

or secondary diffusion as in

\[ \text{[CS95]} \]

- account for (lack of) separation of scales \( \epsilon_0 > 0 \) and advection-dispersion
- track transition between different regimes of phenomena

Other models known in hydrology/ applied math and geosciences

- Gerke van Genuchten 1993 (for Richards’ equation)
- nonlocal models of dispersion (Cushman et al)
Building the upscaled model $\tilde{F}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

Want to have $\tilde{F}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$
constructed with “global” flavor.

- Computational experiments on microscale
- Building the model
  - use the model \textit{á la} [Arb89b] but with different $\Pi_1, \Pi_1^*$,
  - construct convolution approximations of all terms \textit{á la} [Pes92] with a family of kernels
- simulate the upscaled nonlocal model for a continuum of regimes of phenomena
  - kernels reflect the regimes
Introduction and motivation

Something old: double porosity models

Something new: building a new model

Ideas and steps

Computational experiments
Construct affine approximations
Model calculations
Computational experiments with elements of upscaled model

Computational experiments at microscale

GOAL: reproduce qualitatively experimental results, understand significance of different regimes of flow and transport

Row-20-3-5 breakthrough curves

MOVIES
Choice of fine approximations $\Pi_1$

Recall $\Pi_0 f := \frac{1}{|\Omega_0|} \int_{\Omega_0} f(\mathbf{x}) dA$, assume here $|\Omega_0| = 1$. 

Denote $\mathbf{x}^C$ - center of mass of $\Omega_0$. 

General affine approximation $f(\mathbf{x}) \approx \Pi_1 f := m + n \cdot \mathbf{x}$, $\mathbf{x} \in \Omega_0$

Choice of $m, n$

- **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: $(f, \nu)_{\Omega_0} = (m + n \cdot \mathbf{x}, \nu)_{\Omega_0}$, $\forall$ affine $\nu$

- **$H^1(\Omega_0)$** projection: $f(\mathbf{x}) \approx \Pi_1 f := \Pi_0 f + \Pi_0 \nabla f \cdot (\mathbf{x} - \mathbf{x}^C)$

Basis functions not necessarily orthogonal.
Dual affine approximations $\Pi_i^*$ to $\Pi_1$

- $L_2(\Omega_0)$-projection onto affines, use an orthonormal basis $(\phi_0, \phi_1, \phi_2)$

$$\Pi_1 f(x) = \sum_k f_k \phi_k(x)$$

Flux calculations

$$\Pi_i^* q = \sum_k q_k \phi_k(x), \quad q_k = \Pi_0(q\phi_k)$$

- $H^1(\Omega_0)$ projection:

$$f(x) \approx \Pi_0 f + \Pi_0 \nabla f \cdot (x - x^C)$$

Note $(1, (x - x^C)_1, (x - x^C)_2)$ are not necessarily orthogonal!

$$\Pi_i^* q = q_0 \xi_0(x) + q_1 \xi_1(x) + q_2 \xi_2(x)$$

We use $H^1(\Omega_i)$-projection denoted $\Pi_{1,i} \equiv \Pi_i$ and $P_i^* \equiv \Pi_i^*$
Calculate $\Pi_i$ and $\Pi_i^*$

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

$$
\Pi_i(w)(x) \equiv \frac{1}{|\hat{\Omega}_i|} \left( \int_{\hat{\Omega}_i} w(y) \, dA + \sum_{k=1}^2 \left[ \int_{\hat{\Omega}_i} \partial_k w(y) \, dA \right] (x_k - (\hat{x}_i^C)_k) \right)
$$

Dual $\Pi_i^*: (H^1(\hat{\Omega}_i))^* \mapsto (H^1(\Omega))^*$ affine approximation of flux $q \in H^{-1/2}(\Gamma_i)$

$$
\langle \Pi^*_i(q), w \rangle = \langle q, \Pi_i(w) \rangle, \forall w \in C_0^\infty(\Omega)
$$

with $\langle q, v \rangle := \sum_i \int_{\Gamma_i} q(s)v(s)ds$ uses moments $M^0_i, M^1_i$

$$
\langle q, \Pi_i(w) \rangle = \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} q(s) \left[ \int_{\hat{\Omega}_i} wdA + (s - x_i^C) \int_{\hat{\Omega}_i} \nabla wds \right]
$$

$$
= \int_{\Omega} \bar{\chi}_i(x) \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} q(s)ds w(x) dA + \int_{\Omega} \bar{\chi}_i(x) \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} q(s)(s - x_i^C)ds \cdot \nabla w(x) dA
$$

$$
= \int_{\Omega} \bar{\chi}_i(x) M^0_i(q) w(x) dA - \int_{\Omega} \nabla \cdot (\bar{\chi}_i(x) M^1_i(q)) w(x) dA = \langle \Pi^*_i(q), w \rangle
$$
Calculations $\Pi_i$ and $\Pi_i^*$ summary

Affine approximation $\Pi_i : H^1(\Omega) \hookrightarrow H^1(\hat{\Omega}_i)$

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

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

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

Note the last term is a scaled line source!
Application of Green’s theorem to moments

For any smooth region $D$, smooth $\mathbf{v} = (v_1, v_2)$ and $\hat{\mathbf{x}}^C \in D$,

$$
\int_D (\nabla \cdot \mathbf{v})(x_k - (\hat{\mathbf{x}}^C)_k) dA = \int_{\partial D} \mathbf{v} \cdot \nu (x_k - (\hat{\mathbf{x}}^C)_k) ds - \int_D v_k dA
$$

hence for the flux from the cell $q(s) = (D_i \nabla c_i(s) - \mathbf{v}_i c_i(s)) \cdot \nu$

$$
M^1_i(q) = \int_{\Omega_i} \left( \nabla \cdot (D_i \nabla c_i(y, t) - \mathbf{v}_i c_i(y, t)) (y - \hat{\mathbf{x}}^C_i) + D_i \nabla c_i(y, t) - \mathbf{v}_i c_i(y, t) \right) dA.
$$

$$
= - \sum_i \bar{\chi}_i(x) \int_{\Omega_i} \left( \phi_i \frac{\partial c_i}{\partial t}(y, t)(y - \hat{\mathbf{x}}^C_i) + D_i \nabla c_i(y, t) - \mathbf{v}_i c_i(y, t) \right) dA
$$
Cell problem: elementary solutions

Cell problem solved for $u^j_i, j = 0, 1, 2$

$$\phi_{\text{slow}} \frac{\partial u^j_i}{\partial t} - \nabla \cdot (D_{\text{slow}} \nabla u^j_i - u_{\text{slow}} u^j_i) = 0, \mathbf{x} \in \Omega_i,$$

$$u^j_i(\mathbf{x}, 0) = 0, \mathbf{x} \in \Omega_i$$

$$\begin{cases}
u^0_i|_{\Gamma_i} = 1, \\
u^1_i|_{\Gamma_i} = (\mathbf{x} - \mathbf{x}_i^C)_1, \\
u^2_i|_{\Gamma_i} = (\mathbf{x} - \mathbf{x}_i^C)_2
\end{cases}$$

Represent the solution to the cell problem

$$\phi_{\text{slow}} \frac{\partial c_i}{\partial t} - \nabla \cdot (D_{\text{slow}} \nabla c_i - u_{\text{slow}} c_i) = 0, \mathbf{x} \in \Omega_i,$$

$$c_i(\mathbf{x}, 0) = 0, \mathbf{x} \in \Omega_i$$

$$c_i|_{\Gamma_i} = \Pi_{1,i}(c_*)(\mathbf{x}, t)$$

$$\equiv A^0_i(t) + (A^1_i, A^2_i) \cdot (\mathbf{x} - \mathbf{x}_i^C),$$

By linearity $c_i(\mathbf{x}, t) = \int_0^t \sum_{j=0}^2 \frac{\partial u^j_i}{\partial t}(\mathbf{x}, t - s) A^j_i(s) ds = \sum_{j=0}^2 \frac{\partial u^j_i(\mathbf{x}, \cdot)}{\partial t} \ast A^j_i$
Putting it together

Solution to the cell problem $c_i(x, t) = \sum_{j=0}^{2} \frac{\partial u_j^i(x, \cdot)}{\partial t} \ast A^j_i$

$$\phi_{\text{slow}} \frac{\partial c_i}{\partial t} - \nabla \cdot (D_{\text{slow}} \nabla c_i - u_{\text{slow}} c_i) = 0, \ x \in \Omega_i,$$

$$c_i(x, 0) = 0, \ x \in \Omega_i$$

$$c_i|_{\Gamma_i} = \Pi_{1, i}(c_*)(x, t) \equiv A^0_i(t) + (A^1_i, A^2_i) \cdot (x - \hat{x}^C_i), \ x \in \Gamma_i$$

Use $u^i_j$ and $A_j$ so that $\Pi_{1, i}(c_*)(x, t) \equiv A^0_i(t) + (A^1_i, A^2_i) \cdot (x - \hat{x}^C_i)$

Compute the normal flux

$$q(s) \equiv (D_{\text{slow}} \nabla c_i - u_{\text{slow}} c_i) \cdot \eta, \ s \in \Gamma_i$$

... and its affine approximations $\Pi^*_1, i q$ using $A_j, u^i_j$

... and the moments $M^0_i(q), M^1_i(q)$. 

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Write the moments $M_i^0(q), M_i^1(q)$ in terms of $A_k$ and $u_i^j$

Define the kernels for each $i$ and each function $u_i^j, j = 0, 1, 2$ by

$$S_i^{j0}(t) \equiv \int_{\Omega_i} \phi_i \frac{\partial u_i^j}{\partial t}(x, t) \, dA, \quad 0 \leq j \leq 2.$$ 

$$S_i^{jk}(t) \equiv \int_{\Omega_i} \phi_i \frac{\partial u_i^j}{\partial t}(x, t)(x_k - (\hat{x}_i^C)_k) \, dA, \quad 1 \leq k \leq 2.$$ 

$$T_i^j(t) \equiv (T_i^{j1}, T_i^{j2}) \equiv \int_{\Omega_i} (D_i \nabla - \mathbf{v}_i) \frac{\partial u_i^j}{\partial t}(x, t) \, dA.$$ 

Together we have 15 scalar kernels, some of which will be zero due to symmetry/lack of thereof.
Introduction and motivation
Something old: double porosity models
Something new: building a new model

Computational experiments

Model summary (suppress $i$, $\bar{\chi}_i$ etc.)

$$\frac{\partial}{\partial t} \left\{ \phi \ast c + S^{00} \ast c + (S^{01}, S^{02}) \ast \nabla c - \nabla \cdot (S^{10} \ast c + (S^{11}, S^{12}) \ast \nabla c) \right\}$$
$$- \nabla \cdot \left\{ D \ast \nabla c - v \ast c + T^0 \ast c + (T^1, T^2) \ast \nabla c \right\} = 0$$

- Convolution kernels for different regimes of diffusion vs advection
  - no advection
  - with advection
  - with significant advection

- Upscaled problem with nonlocal terms

- Comparison between exact model and upscaled model with nonlocal terms and computed kernels
Convolution kernels: regimes of $Pe = \frac{\text{advection}}{\text{diffusion}}$

Solution $u^j$ and the associated kernels $S^{j0}$, $S^{j1}$, $T^{j1}$

$j = 0$

- No advection
- With advection
- Large advection

$j = 1$

- No advection, boundary condition = 1
- With advection, boundary condition = 1
- Large advection, boundary condition = 1
**Upscaled model: numerical treatment**

- Nonlocal diffusion (FE+time-stepping on $c_t$) \cite{Pes95} stable, convergence $O(\triangle t + h^2)$, singular kernels
- Nonlocal diffusion with secondary diffusion terms (as in viscoelasticity) \cite{Thomee,Lin,Ewing'91-'01} with nonsingular kernels
- Nonlocal advection (FD+time-stepping): stable, convergent $O(\triangle t + h)$ \cite{P06}, singular kernels
- Nonlocal advection+diffusion+secondary diffusion+secondary advection:
  - Issues of memory storage, need adaptive treatment
  - Relative importance of the terms $\nabla c_*$, $\nabla^2 c_*$: adaptivity a must

**pore-scale modeling (with K. Augustson)**

**unsaturated flow models**

**use experimental results by Wildenschild et al.**
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Connection to mortar upscaling

[PWY02, Pes05]
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Małgorzata S. Peszyńska, Ralph E. Showalter
Nonlocal models of transport in multiscale porous media: something old and something new...
Summary: the upscaled model

\[
\begin{align*}
\frac{\partial}{\partial t} \left( \phi_* c_*(x, t) + \sum_{i=1}^{N} \chi_i(x) \int_0^t S_{i0}^0(t - \tau) \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} c_*(y, \tau) \, dA \, d\tau \right) \\
+ \sum_{i=1}^{N} \chi_i(x) \int_0^t \sum_{j=1}^2 S_{i0}^j(t - \tau) \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \partial_j c_*(y, \tau) \, dA \, d\tau \\
- \nabla \cdot \sum_{i=1}^{N} \chi_i(x) \int_0^t \sum_{j=0}^2 (S_{i1}^j(t - \tau), S_{i2}^j(t - \tau)) \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \partial_j c_*(y, \tau) \, dA \, d\tau \\
- \nabla \cdot (D_* \nabla c_*(x, t) - v_* c_*(x, t)) \\
+ \sum_{i=1}^{N} \chi_i(x) \int_0^t \sum_{j=0}^2 (T_{i1}^j(t - \tau), T_{i2}^j(t - \tau)) \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \partial_j c_*(y, \tau) \, dA \, d\tau \\
= 0, \quad x \in \Omega, \quad t > 0.
\end{align*}
\]
Introduction and motivation
Something old: double porosity models
Something new: building a new model

Ideas and steps
Computational experiments
Construct affine approximations
Model calculations
Computational experiments with elements of upscaled model