984. Multicontinuum modeling for heterogeneous porous media processes

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Congratulations to Prof. Jun Yao!
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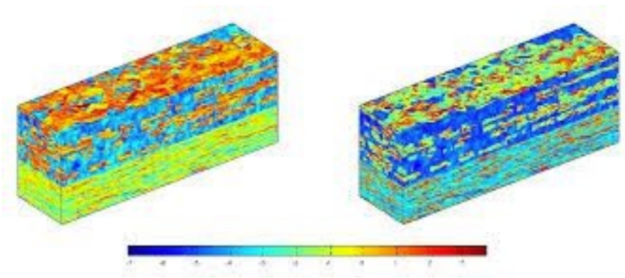
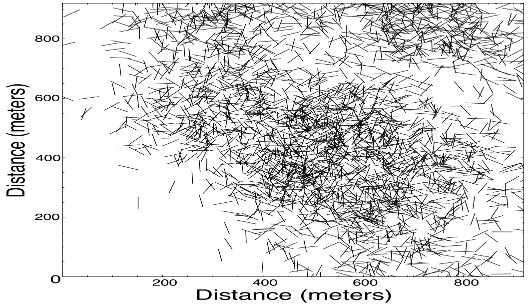
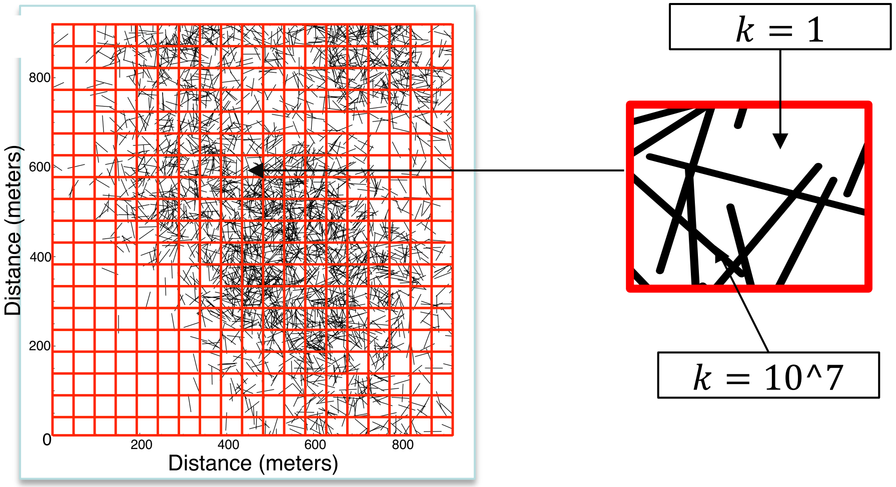
Multiscale problems

- Scales, complex heterogeneities, high contrast (H vs. contrast), e.g.,

e.g., $-\mathrm{div}(k(x)\nabla u)=f.$



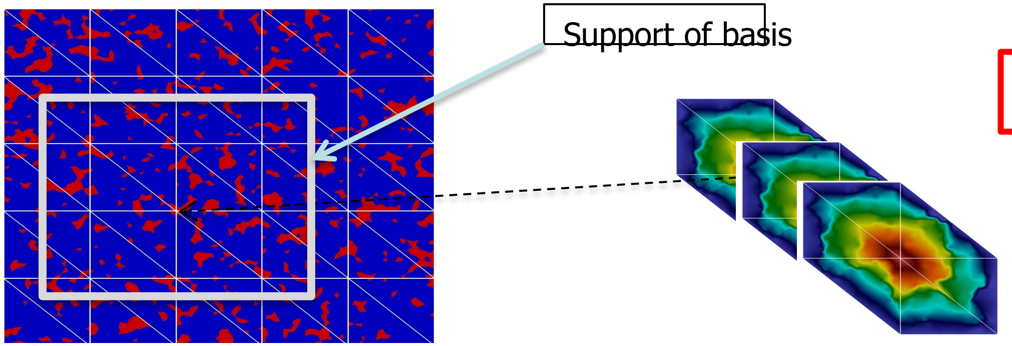




- Fine-grid (grid that resolves fine-scale features) simulations are not practical.
- Coarse grid does not resolve the physical scales
- Coarse grid does not resolve the contrast (w.r.t. to H)

Multiscale vs multicontinuum

Consider $\nabla \cdot (\kappa(x)\nabla u) = f(x)$.



Multiscale methods: Seek u $= \sum_i u_i^j \phi_i^j$

ϕ_i^j are basis for macroscopic location j, i is basis number.

Result: Discretization "A u =b"

Goal: To solve the equation on a coarse grid.

Multicontinuum method: Seek u $= \sum_i \phi_i U_i + \phi_i^m \nabla_m U_i$.

. ϕ_i are local cell problems for continua i.

Result: Macroscopic PDE $\nabla\left(\alpha_{ij}\nabla U_j\right) + \beta_{ij}\nabla U_j + \gamma_{ij}U_j = g_i$

Goal: To derive macroscopic models (PDEs).

Goal of this talk is to derive macroscopic models for two-phase flow and transport

Constraint Energy Minimizing GMsFEM*.GMsFEM identifying multicontinua.

- The idea is to construct a local space that “solution operator doesn’t see”.

For each coarse element K, we define the local spectral problem by

$$a_K(\phi, w) = \lambda s_K(\phi, w)$$

where

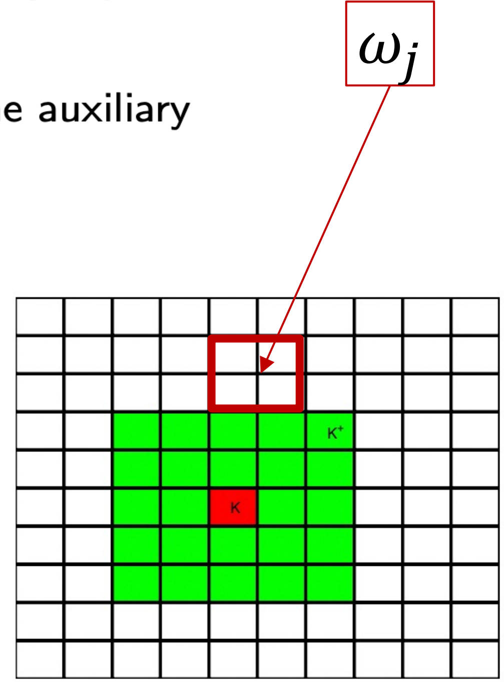
$$a_K(\phi, w) = \int_K \kappa \nabla\phi \cdot \nabla w, \quad s_K(\phi, w) = \int_K \widetilde{\kappa}\phi w$$

and $\widetilde{\kappa} = \kappa \sum |\nabla\chi_j|^2$, where we define $\{\chi_j\}$ as partition of unity functions with respect to the coarse grid.

We take the first l_K eigenfunctions with small eigenvalues, we define the auxiliary space as

$$V_{\text{aux}}^{(K)} := \text{span}\{\phi_i^{(K)} \, : \, 1 \le i \le l_K\} \quad \text{and} \quad V_{\text{aux}} := \oplus_K V_{\text{aux}}^{(K)}$$

It identifies number of high contrast channelized networks in a cell.



$$\phi_i^{\omega_j}\chi_j \; - \text{GMsFEM basis}$$

- Efendiev, Galvis, Efendiev, MMS 2009, JCP 2010
- Chung, Efendiev, Leung, 2017;

Oversampled constraint problems

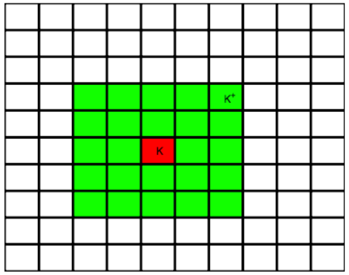
We construct the multiscale basis functions. For a given $\phi_i^{(K)}$ and an oversampled region $K^+ \supset K$

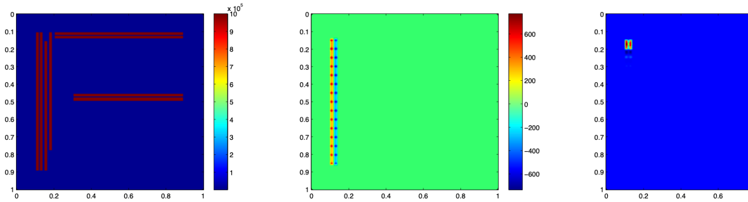
$$\min_{\psi \in H_0^1(K^+)} \int_{K^+} \kappa |\nabla \psi|^2$$

subject to the constraints

$$s_J(\psi, \phi) = 0, \quad \forall \phi \in V_{\text{aux}}^{(J)}, \quad \forall J \subset K^+, \ J \neq K$$
$$s_K(\psi, \phi_\ell^{(K)}) = \delta_{\ell i}$$

Solving the above, we obtain the multiscale basis functions $\{\psi_{i,\text{ms}}^{(K)}\}$ The multiscale space V_H is the span of all these $\{\psi_{i,\text{ms}}^{(K)}\}$, for all K.





Convergence of CEM-GMsFEM

The scheme: find $u_H \in V_H$ such that

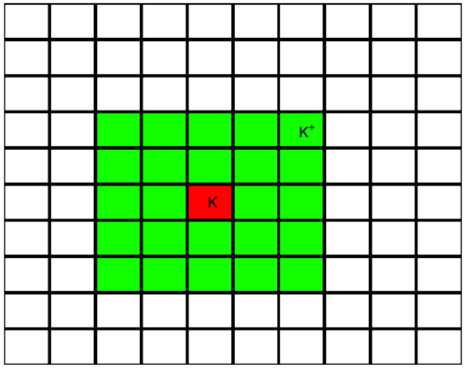
$$a(u_H, v) = (f, v), \quad \forall v \in V_H$$

We prove the convergence bound:

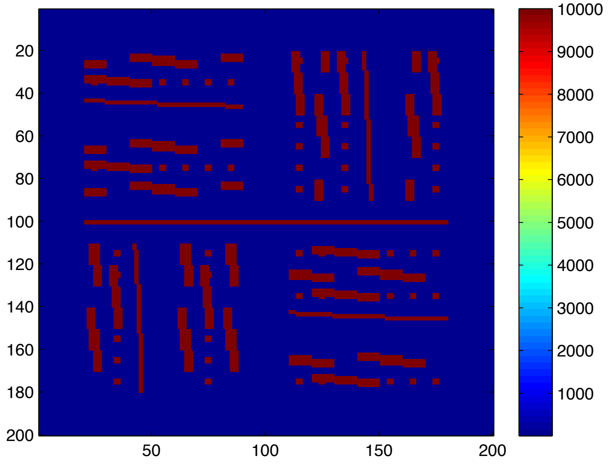
$$\|u - u_H\|_V \lesssim H\Lambda^{-\frac{1}{2}} \|f\|_2 \quad \text{provided} \quad k = O(\log(\kappa_c / H))$$

where k is the number of oversampling layers, and

$$\Lambda = \min_K \lambda^{(K)}_{l_K+1}$$



Numerical results



Layer \ Contrast	1e+4	1e+6	1e+8	1e+10
3	3.73%	3.89%	11.99%	65.19%
4	3.72%	3.72%	3.73%	5.14%
5	3.72%	3.72%	3.73%	3.72%

Number basis per K	H	# oversampling coarse layers	L_2error	energy error
3	1/10	3	0.33%	3.73%
3	1/20	4 (log(1/20)/log(1/10)*3=3.9031)	0.047%	1.17%
3	1/40	5 (log(1/40)/log(1/10)*3=4.8062)	0.010%	0.47%
3	1/80	6 (log(1/40)/log(1/10)*3=5.7093)	0.0015%	0.15%

Can be used (1) Online methods/solvers (2) temporal splitting…

*Chung, Efendiev, Leung, CEM-GMsFEM, 2017

Multicontinua GMsFEM method. Motivation.

$u = \sum_i \phi_i^j u_i^j$. ϕ_i^j −basis for coarse location j

$\phi_i^j = G_i^j \chi^j$, where G_i^j are local eigenvectors, and χ^j - MsFEM basis functions

$\chi^j = \phi_0^j + Z_i^j \cdot \nabla \phi_0^j$, where ϕ_0^j − standard “hat” basis

$$\phi_i^j = G_i^j \phi^j = G_i^j \phi_0^j + (G_i^j Z_i^j) \cdot \nabla \phi_0^j = N_i \phi_0^j + M_i \cdot \nabla \phi_0^j$$

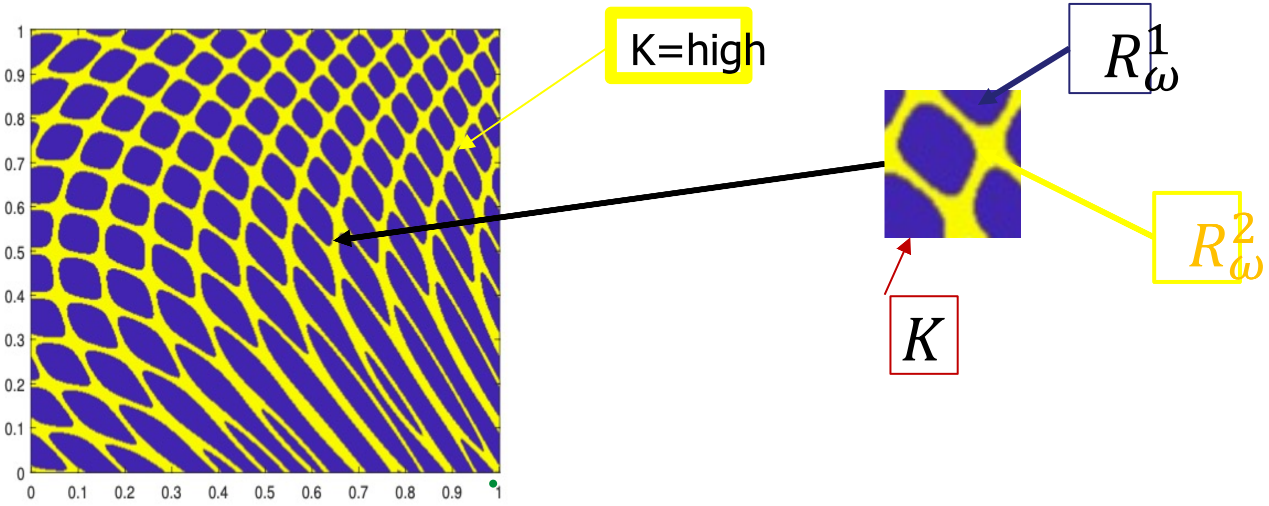
$G_i^j \approx N_i$ (independent of j)
are smoothly varying if properly indexed

Multicontinua GMsFEM method

- Define $\psi_i, \psi_i = 1$ in continua i and 0 otherwise

- Solve the extended-local problems $N_i, such\ that$

$$L(N_i) = g_i, \int_K N_i\psi_j = \delta_{ij}\int_K \psi_j$$



Multicontinua GMsFEM method

- Define $\psi_i, \psi_i = 1$ in continua i and 0 otherwise

- Construct multiscale basis functions ϕ_i^j *as*

$\phi_i^j = N_i\phi_0^j +$ ”$M_i \cdot \nabla\phi_0^j$”, where ϕ_i^j solves local problems and M_i vanishes on the boundary of coarse cells

- Then, $u_H =$ $\sum_{i,j}\phi_i^j u_i^j = \sum_i N_i(\sum_j \phi_0^j u_i^j) + M_i(\sum_j \phi_0^j u_i^j) = \sum_i N_i U_i + M_i \cdot \nabla U_i$

$$U_i = \sum_j u_i^j \phi_0^j \; - \text{smooth function w.r.t. } x$$

Elliptic equation

$$a(u_H, v_H) = \int_\Omega \kappa \nabla u_H \cdot \nabla v_H, \qquad f(v_H) = \int_\Omega f v_H.$$

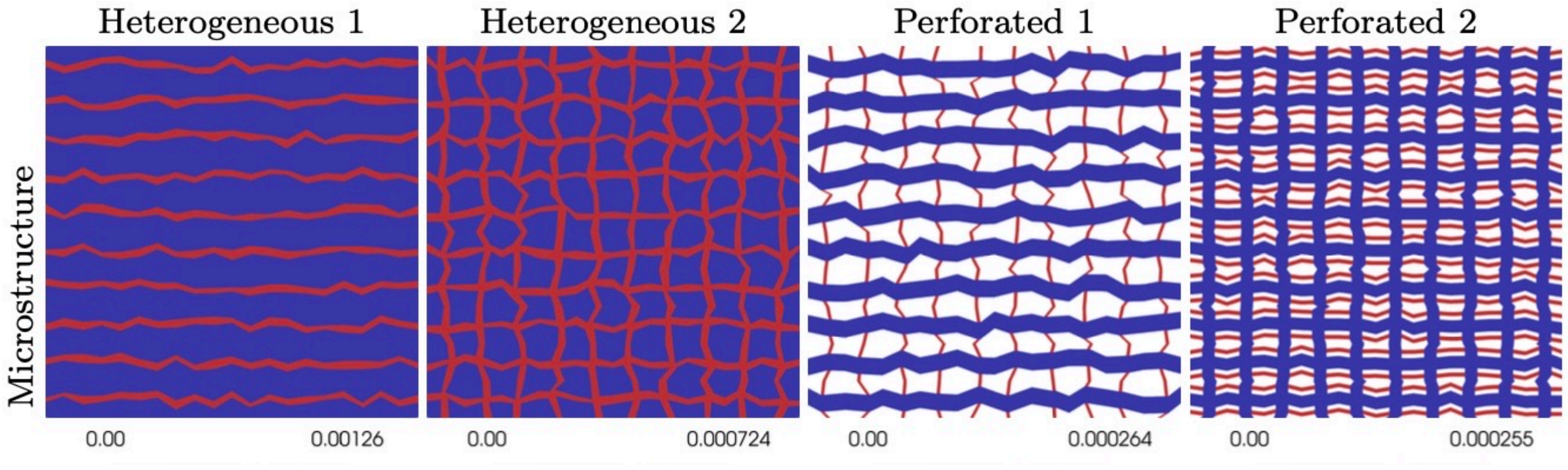
$$u_H = \sum_i N_i U_i + \sum_i M_i \cdot \nabla U_i, \quad v_H = \sum_j N_j V_j + \sum_j M_j \cdot \nabla V_j.$$

$$\begin{aligned} a(u_H, v_H) = \sum_K \sum_{i,j} \int_K \kappa \Big[& (\nabla N_i \cdot \nabla N_j) U_i V_j + (\nabla N_i \cdot B_j) U_i \nabla V_j \\ & + (B_i \nabla U_i \cdot \nabla N_j) V_j + (B_i \nabla U_i) \cdot (B_j \nabla V_j) \Big], \end{aligned}$$

$$\int_\Omega (\alpha_{ij} U_i V_j + \beta_{ij} U_i \nabla V_j + \gamma_{ij} \nabla U_i V_j + \theta_{ij} \nabla U_i \cdot \nabla V_j) = \int_\Omega (F_j V_j + G_j \cdot \nabla V_j).$$

$$\alpha_{ji} U_i - \nabla \cdot (\theta_{ji} \nabla U_i) - \nabla \cdot (\beta_{ji} U_i) + \gamma_{ji} \cdot \nabla U_i = F_j - \nabla \cdot G_j.$$

Numerical result



Microstructure	$e_2^{(1)}$	$e_2^{(2)}$
Heterogeneous 1	7.67 %	6.23 %
Heterogeneous 2	6.11 %	15.24 %
Perforated 1	5.19 %	7.31 %
Perforated 2	3.50 %	2.95 %

Two-phase flow

- Two-phase flow at pore scale

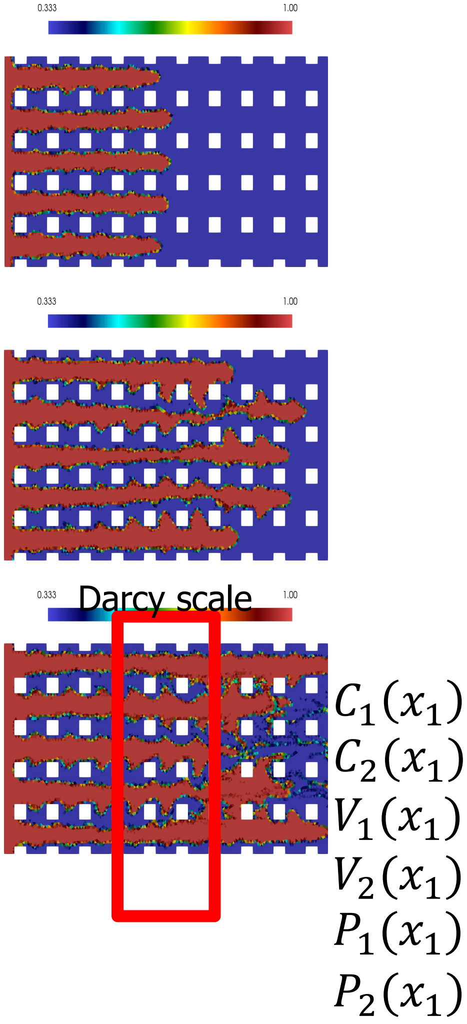
$$-\nabla p + \nabla\cdot(\mu(\phi)\nabla u) = f + \nabla\phi,$$

$$\nabla\cdot u = 0, \phi_t + u\cdot\nabla\phi = \Delta\mu(\phi)$$

$$\phi = 1\ (water), \phi = 0\ (oil)$$

We define the continua based on $\phi, i.e.,$

$$\psi_1 = 1-\phi, \psi_2 = \phi.$$



$C_1(x_1)$
$C_2(x_1)$
$V_1(x_1)$
$V_2(x_1)$
$P_1(x_1)$
$P_2(x_1)$

Multicontinuum two-phase flow

One pressure continua and 2 velocity continua

$$\phi_i^j = N_i\phi_0^j + M_i \cdot \nabla\phi_0^j \; - \mathit{velocity\ basis}$$

$$v(x) = N_i(x)V_i(x) + M_i(x) \cdot \nabla V_i(x),$$

Variational formulation

$$\int_{\Omega_f} 2\mu\, \varepsilon(v) : \varepsilon(w)\, dx + \int_{\Gamma_s} \beta\, v_\tau \cdot w_\tau\, ds - \int_{\Omega_f} p_0(x)\, \nabla \cdot w\, dx = \int_{\Omega_f} f \cdot w\, dx$$

$$\begin{aligned}
&\int_{\Omega_f} 2\mu\, \varepsilon\left(N_iV_i + M_i \cdot \nabla V_i\right) : \varepsilon\left(N_jW_j + M_j \cdot \nabla W_j\right) dx \\
&+ \int_{\Gamma_s} \beta\left(N_iV_i + M_i \cdot \nabla V_i\right)_\tau \cdot \left(N_jW_j + M_j \cdot \nabla W_j\right)_\tau ds \\
&- \int_{\Omega_f} \nabla p_0(x)\, \left(N_jW_j + M_j \cdot \nabla W_j\right) dx = \int_{\Omega_f} f \cdot \left(N_jW_j + M_j \cdot \nabla W_j\right) dx.
\end{aligned}$$

Multicontinuum model

Variational macroscopic formulation

$$\int_{\Omega_f} \alpha_{ij} V_i W_j \, dx + \int_{\Omega_f} \gamma_{ij} \nabla V_i \, W_j \, dx + \int_{\Omega_f} \gamma_{ji} V_i \, \nabla W_j \, dx + \int_{\Omega_f} \theta_{ij} \nabla V_i \cdot \nabla W_j \, dx$$
$$- \int_{\Omega_f} \rho_j \nabla p_0(x) W_j dx = \int_{\Omega_f} \eta_j W_j \, dx + \int_{\Omega_f} \zeta_j \cdot \nabla W_j \, dx.$$

Strong-form macroscopic formulation

$$\alpha_{ij} V_i - \nabla \cdot (\theta_{ij} \nabla V_i) + \gamma_{ij} \nabla V_i + \gamma_{ji}^T \nabla V_i + \rho_j \nabla p_0 = \eta_j - \nabla \cdot \zeta_j$$

If $\mathrm{v} = N_i^v V_i$, then $\alpha_{ij} V_{\mathrm{i}} + \rho_j \nabla p_0 = 0, div(\zeta_{ij} V_i) = 0$

For concentration, we use $c = N_i^c C_i$

$$(C_i)_t + \nabla \cdot (\xi_{ij} C_j) = 0 \rightarrow (C_i)_t + \nabla \cdot (\xi_{ij} V_j) = \cdots$$

Two-Phase Flow Simulations

Test A

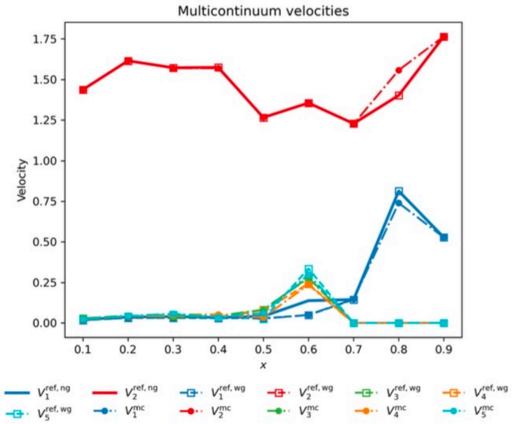
Test B

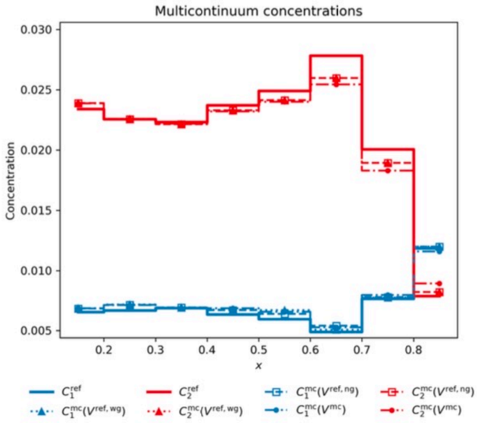
Test C

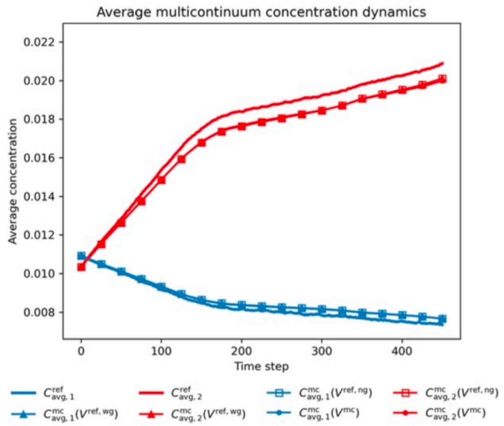
Test D

Test E

Numerical results







Numerical results

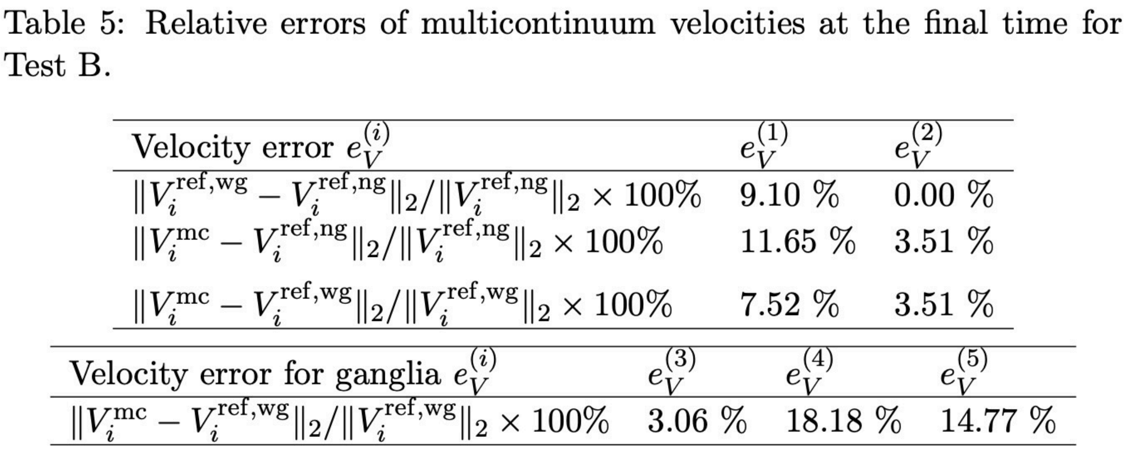


Table 5: Relative errors of multicontinuum velocities at the final time for Test B.

Velocity error $e_V^{(i)}$	$e_V^{(1)}$	$e_V^{(2)}$
$\|V_i^{\text{ref,wg}} - V_i^{\text{ref,ng}}\|_2/\|V_i^{\text{ref,ng}}\|_2 \times 100\%$	9.10 %	0.00 %
$\|V_i^{\text{mc}} - V_i^{\text{ref,ng}}\|_2/\|V_i^{\text{ref,ng}}\|_2 \times 100\%$	11.65 %	3.51 %
$\|V_i^{\text{mc}} - V_i^{\text{ref,wg}}\|_2/\|V_i^{\text{ref,wg}}\|_2 \times 100\%$	7.52 %	3.51 %

Velocity error for ganglia $e_V^{(i)}$	$e_V^{(3)}$	$e_V^{(4)}$	$e_V^{(5)}$
$\|V_i^{\text{mc}} - V_i^{\text{ref,wg}}\|_2/\|V_i^{\text{ref,wg}}\|_2 \times 100\%$	3.06 %	18.18 %	14.77 %

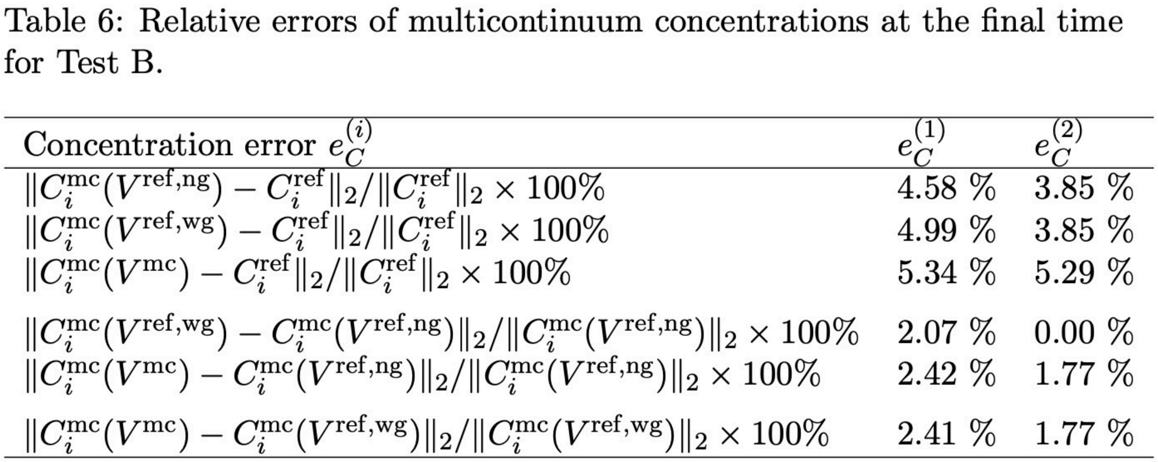


Table 6: Relative errors of multicontinuum concentrations at the final time for Test B.

Concentration error $e_C^{(i)}$	$e_C^{(1)}$	$e_C^{(2)}$
$\|C_i^{\text{mc}}(V^{\text{ref,ng}}) - C_i^{\text{ref}}\|_2/\|C_i^{\text{ref}}\|_2 \times 100\%$	4.58 %	3.85 %
$\|C_i^{\text{mc}}(V^{\text{ref,wg}}) - C_i^{\text{ref}}\|_2/\|C_i^{\text{ref}}\|_2 \times 100\%$	4.99 %	3.85 %
$\|C_i^{\text{mc}}(V^{\text{mc}}) - C_i^{\text{ref}}\|_2/\|C_i^{\text{ref}}\|_2 \times 100\%$	5.34 %	5.29 %
$\|C_i^{\text{mc}}(V^{\text{ref,wg}}) - C_i^{\text{mc}}(V^{\text{ref,ng}})\|_2/\|C_i^{\text{mc}}(V^{\text{ref,ng}})\|_2 \times 100\%$	2.07 %	0.00 %
$\|C_i^{\text{mc}}(V^{\text{mc}}) - C_i^{\text{mc}}(V^{\text{ref,ng}})\|_2/\|C_i^{\text{mc}}(V^{\text{ref,ng}})\|_2 \times 100\%$	2.42 %	1.77 %
$\|C_i^{\text{mc}}(V^{\text{mc}}) - C_i^{\text{mc}}(V^{\text{ref,wg}})\|_2/\|C_i^{\text{mc}}(V^{\text{ref,wg}})\|_2 \times 100\%$	2.41 %	1.77 %

“Brinkman” or Darcy

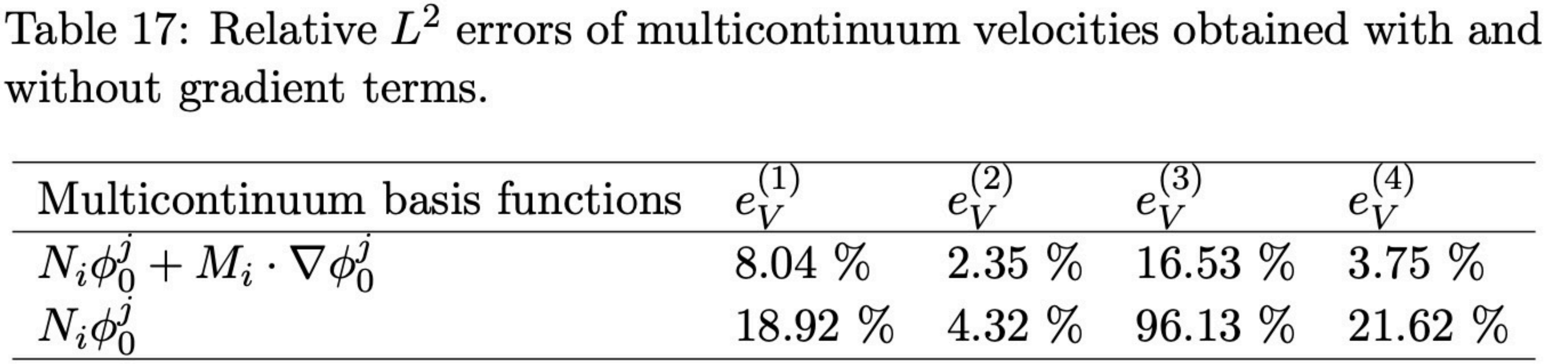


Table 17: Relative L^2 errors of multicontinuum velocities obtained with and without gradient terms.

Multicontinuum basis functions	$e_V^{(1)}$	$e_V^{(2)}$	$e_V^{(3)}$	$e_V^{(4)}$
$N_i\phi_0^j + M_i \cdot \nabla\phi_0^j$	8.04 %	2.35 %	16.53 %	3.75 %
$N_i\phi_0^j$	18.92 %	4.32 %	96.13 %	21.62 %

*Accuracy of proposed macroscopic model can be improved by adding continua

* These results show that new model (Brinkman-type) are more accurate

Conclusions

- MC-GMsFEM provides accurate upscaling and macroscopic modeling for two-phase flow
- Continua for velocity defined based on concentrations can be improved
- Effective for various multicontinuum applications

Thank You !

Congratulations Prof. Jun Yao!