Generalized multiscale finite element methods for a class of nonlinear flow problems

Eric Chung
Department of Mathematics
Chinese University of Hong Kong

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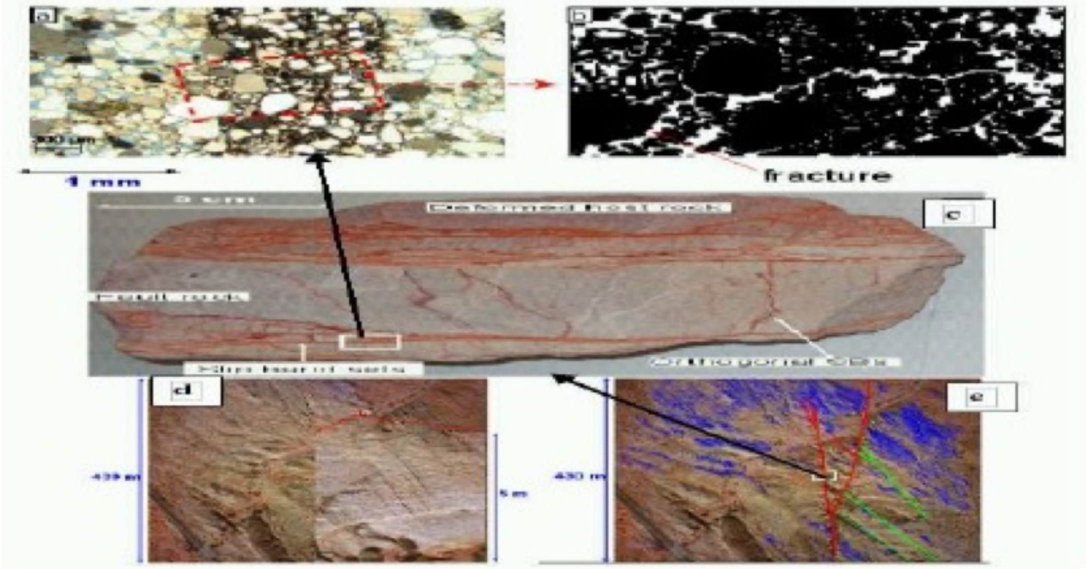
Multiscale problems

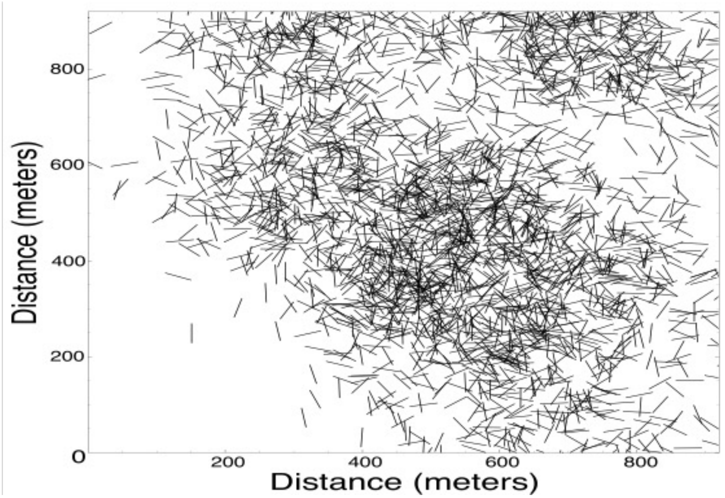
- Physical parameters (e.g. permeability, fractures, …) with multiple scales & high contrast
- Simulations need fine grid to resolve heterogeneities, which is computationally expensive
- Accurate coarse-grid models are necessary

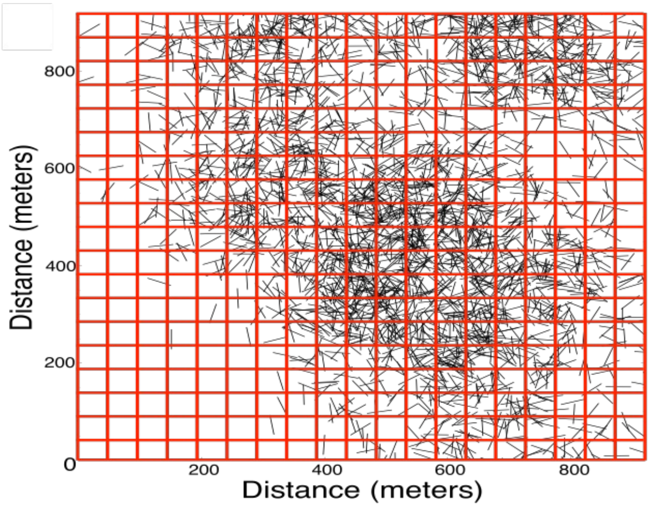


Acknowledgements: K. Sternlof, A. Ahmadov,

Model coarsening

- Use a coarse grid, which does not resolve scales and contrasts
- Coarse-grid computational model is constructed by local simulations
- Coarse grid size is fixed, and is chosen according to computational concerns
- Model enhancements can be done by offline or online model updates





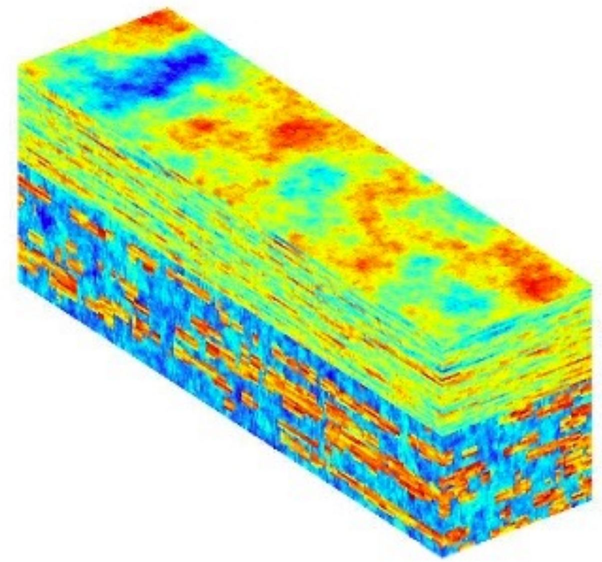
A model problem

- Consider the multiscale problem

$$-\nabla \cdot (\kappa \nabla u) = f \quad \text{in} \quad \Omega$$
$$u = 0 \quad \text{on} \quad \partial\Omega$$

where $\kappa(x)$ is a high contrast multiscale coefficient, and $f(x)$ is a given source function

- Develop coarse-grid model based on rigorous mathematical analysis
- Challenges:
  - How to add more degrees of freedom per coarse element
  - How to identify channels and localize their effects



Local multiscale basis functions

- Auxiliary multiscale functions: spectral problem on each coarse cell K (coarse d.o.f)

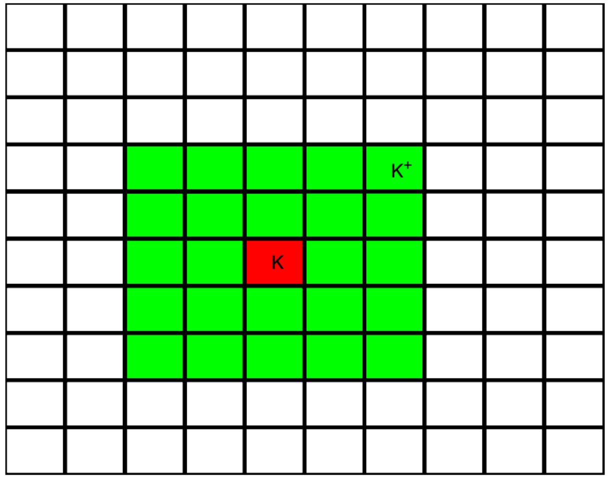
$$a_K(\phi, w) = \lambda s_K(\phi, w)$$

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

- Each auxiliary function $\phi_i^{(K)}$ will give a multiscale basis function $\psi_{i,\text{ms}}^{(K)}$
- Perform constraint energy minimization on oversampled region

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

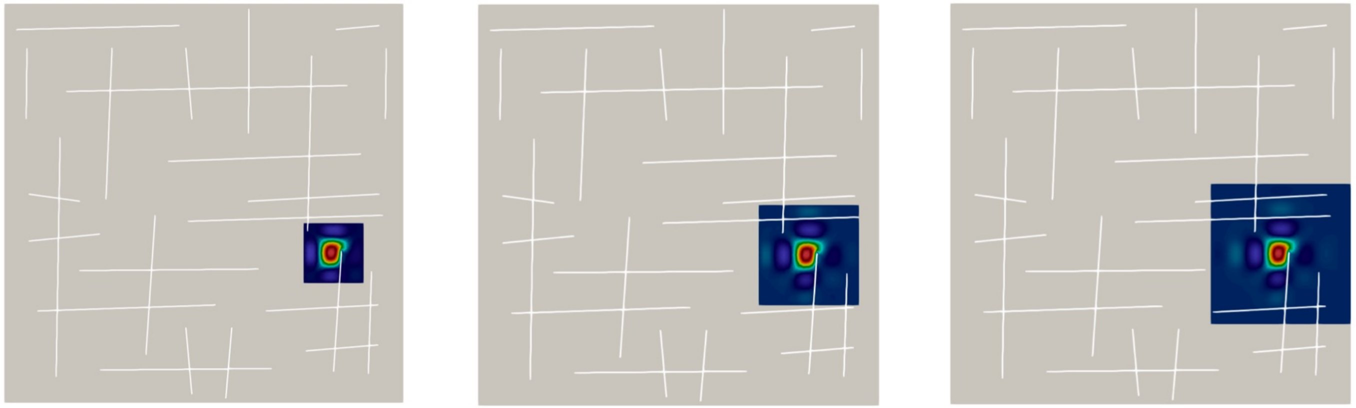
with constraints $s_K(\psi, \phi_\ell^{(K)}) = \delta_{\ell i}$ and $s_J(\psi, \phi_\ell^{(J)}) = 0$



Chung, Efendiev and Leung, 2018

Decay of basis functions and error bound

- Basis functions have exponential decay property for high contrast media



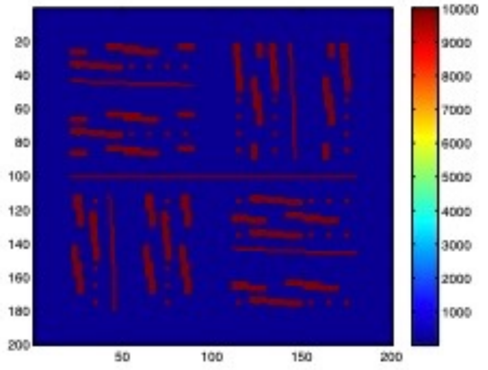
- This gives the size of the oversampled region, which is $O\ (\ \log(\kappa_c/H)\ )$
- Error bound independent of scales and contrasts of the media

$$\|u - u_H\|_V \lesssim H\Lambda^{-\frac{1}{2}}\|f\|_2 \qquad \text{where} \qquad \Lambda = \min_K \lambda_{l_K+1}^{(K)}$$

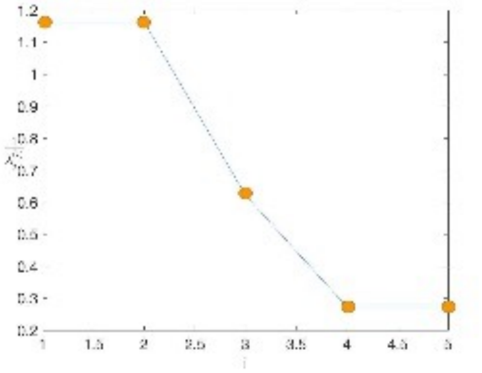
assuming l_K basis functions are constructed for the coarse cell K

Eigenvalues and channels

- Number of small eigenvalues is related to high contrast channels

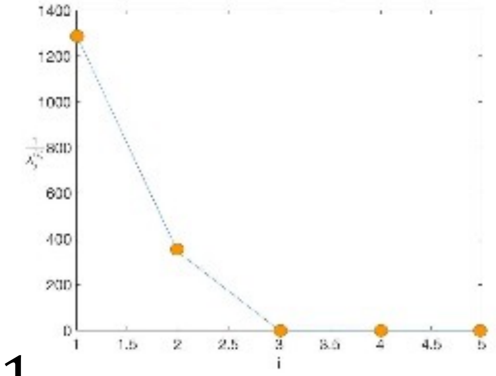


$$a_K(\phi, w) = \lambda s_K(\phi, w)$$

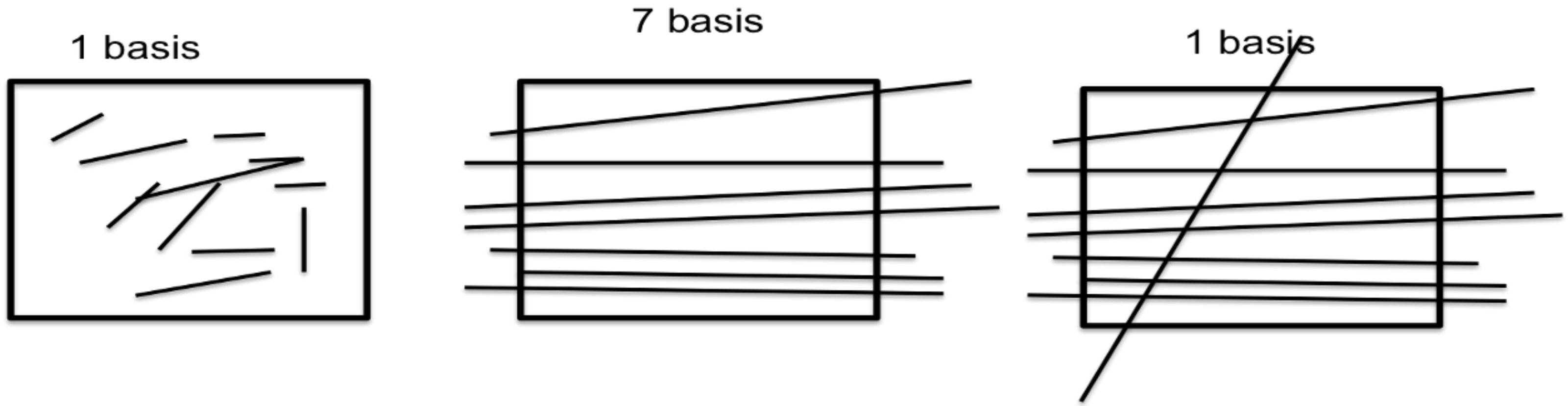


Contrast = 10

$\frac{1}{\lambda}$

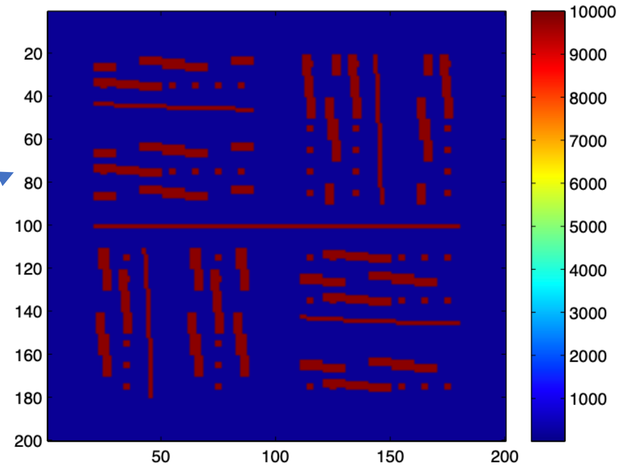


Contrast = 1000



Example

- Consider a high contrast heterogeneous coefficient κ
- Error for different choices of coarse grid sizes



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%

- Error for different numbers of basis functions

Number basis per element	H	# oversampling coarse layers	L_2error	energy error
1	1/10	4	77.30%	87.07%
2	1/10	4	30.21%	49.66%
3	1/10	4	24.27%	44.46%
4	1/10	4	0.11%	1.50%
5	1/10	4	0.08%	1.26%

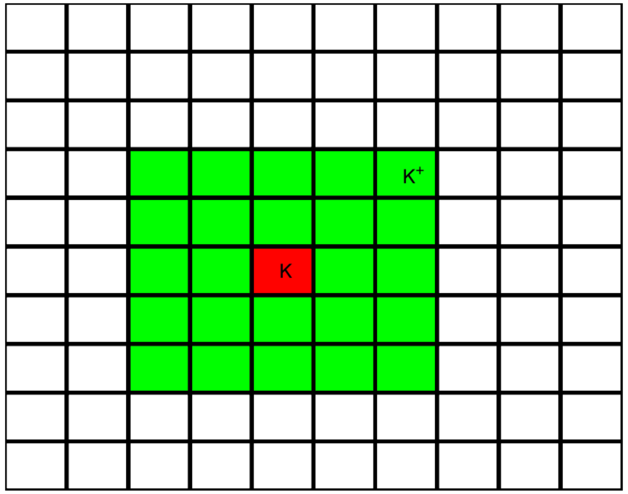
Online model enrichment

- Online basis functions* β by solving local problems using local residuals

$$a(\beta, v) + s(\pi\beta, \pi v) = r_{K^+}(v)$$

(Solve in oversampled region)

- Adaptive enrichment: fixed $0 < \theta < 1$, start with offline basis functions
- Compute a solution $u_H^{(m)} \in V_H^{(m)}$
- Compute local residuals δ_i
- Choose k coarse cells using the condition $\sum_{i=k+1}^{N} \delta_i^2 < \theta \sum_{i=1}^{N} \delta_i^2$
- Compute basis, and repeat



Convergence theory:

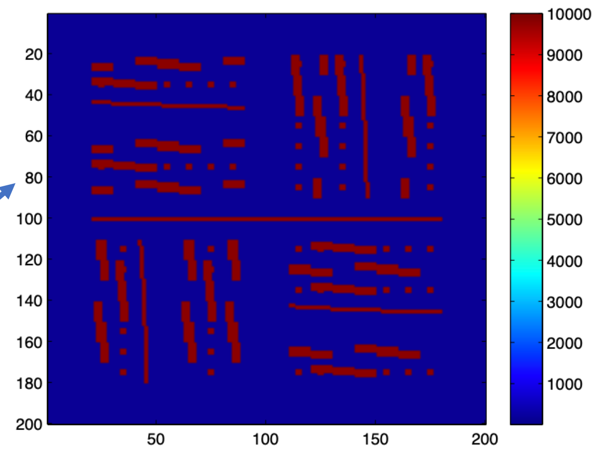
$$\|u - u_H^{(m+1)}\|_a^2 \lesssim (E + \theta)\|u - u_H^{(m)}\|_a^2$$

(where $E \to 0$ exponentially when oversampling size increases)

*Chung, Efendiev and Leung, 2018

Example

- Consider a high contrast heterogeneous coefficient κ



- Error for uniform enrichment ($\theta = 0$)

Number of offline basis	online iteration	oversampling layers	L_2 error	energy error
3	0	2	30.01%	82.57%
3	1	2	0.0066%	0.0030%
3	2	2	4.45e-07%	1.22e-07%

- Error for adaptive enrichment ($\theta = 0.1$)

Number of offline basis	DOF	oversampling layers	L_2 error	energy error
3	300	2	30.01%	82.57%
3	356	2	8.68%	22.06%
3	378	2	4.87%	5.41%
3	392	2	4.46%	1.50%

Upscaling: motivated by multiscale ideas

- Define local basis functions such that coarse degrees of freedoms have physical meaning, e.g. average solutions in each continua
- In general

$$u_H = \sum_K \sum_\ell u_\ell^{(K)} \psi_{\ell,\text{ms}}^{(K)}$$

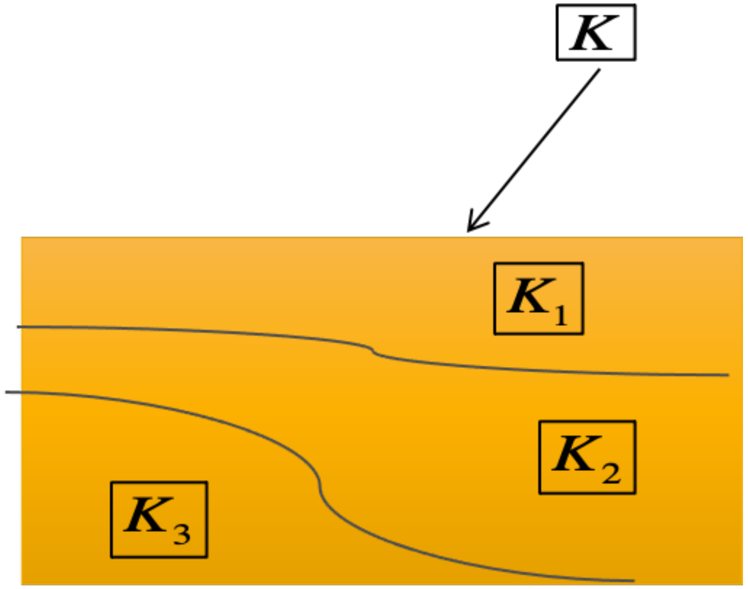
- If we define the basis functions such that

$$\int_{K_m} \psi_{\ell,\text{ms}}^{(K)} = \delta_{m\ell}$$

- Then we have

$$\int_{K_m} u_H = u_m^{(K)}$$

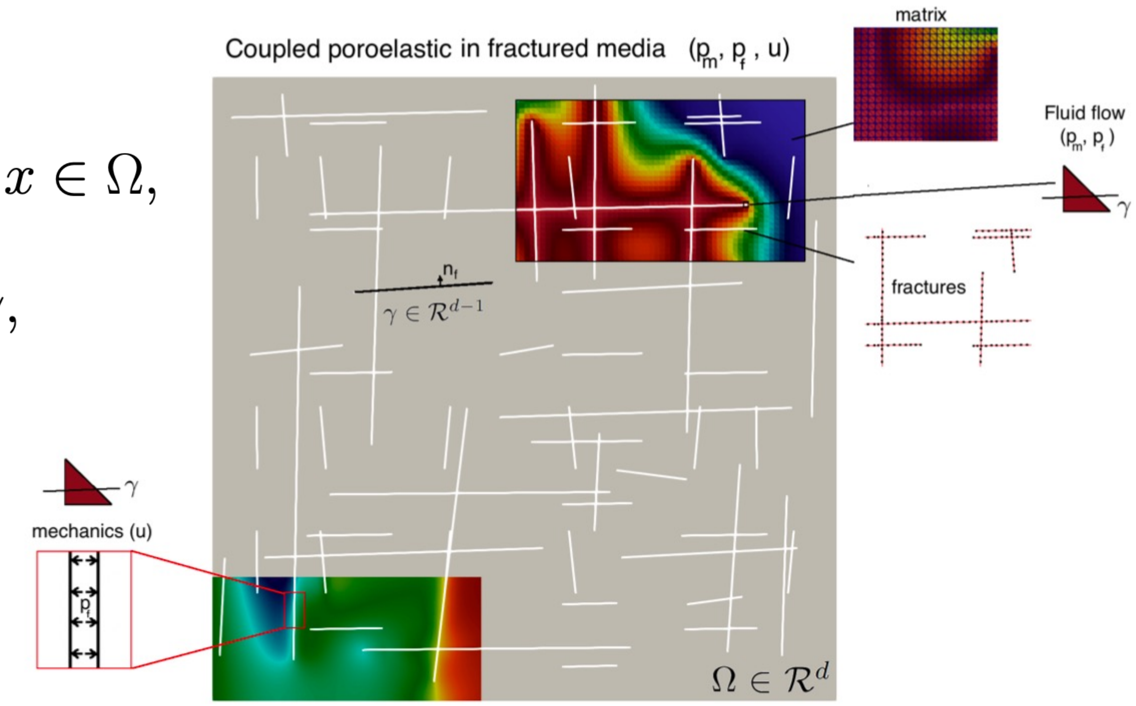
- This motivates the constraint energy minimization for basis construction



Example 1

- Consider a poroelastic problem in fracture porous media

$$a_m \frac{\partial p_m}{\partial t} + \alpha \frac{\partial \varepsilon^v}{\partial t} - \operatorname{div}(b_m \operatorname{grad} p_m) + \eta_m \beta(p_m - p_f) = f_m, \quad x \in \Omega,$$
$$a_f \frac{\partial p_f}{\partial t} + \frac{\partial b}{\partial t} - \operatorname{div}(b_f \operatorname{grad} p_f) + \eta_f \beta(p_f - p_m) = f_f. \quad x \in \gamma,$$
$$-\operatorname{div}\left(\sigma(u) - \alpha p_m \mathcal{I}\right) + r_f p_f = 0, \quad x \in \Omega.$$



- where p_m and p_f are matrix and fracture pressures
- u is the displacement field

Vasilyeva, Chung, Efendiev and Kim, 2019

Constraints

- Pressure basis functions (matrix)

$$\int_{K_j} \psi_0^i \, dx = \delta_{i,j}, \quad \int_{\gamma_j^{(l)}} \psi_0^i \, ds = 0, \quad l = \overline{1, L_j},$$

- Pressure basis functions (fracture)

$$\int_{K_j} \psi_l^i \, dx = 0, \quad \int_{\gamma_j^{(l)}} \psi_l^i \, ds = \delta_{i,j}\delta_{m,l}, \;\; m = \overline{1, L_j},$$ where $$\gamma_j^{(l)} = K_j \cap \gamma^{(l)}$$

- Displacement

(1) X-component, $\psi^{X,i}$:

$$\int_{K_j} \psi_x^{X,i} \, dx = \delta_{i,j}, \quad \int_{K_j} \psi_y^{X,i} \, dx = 0,$$

(2) Y-component, $\psi^{Y,i}$:

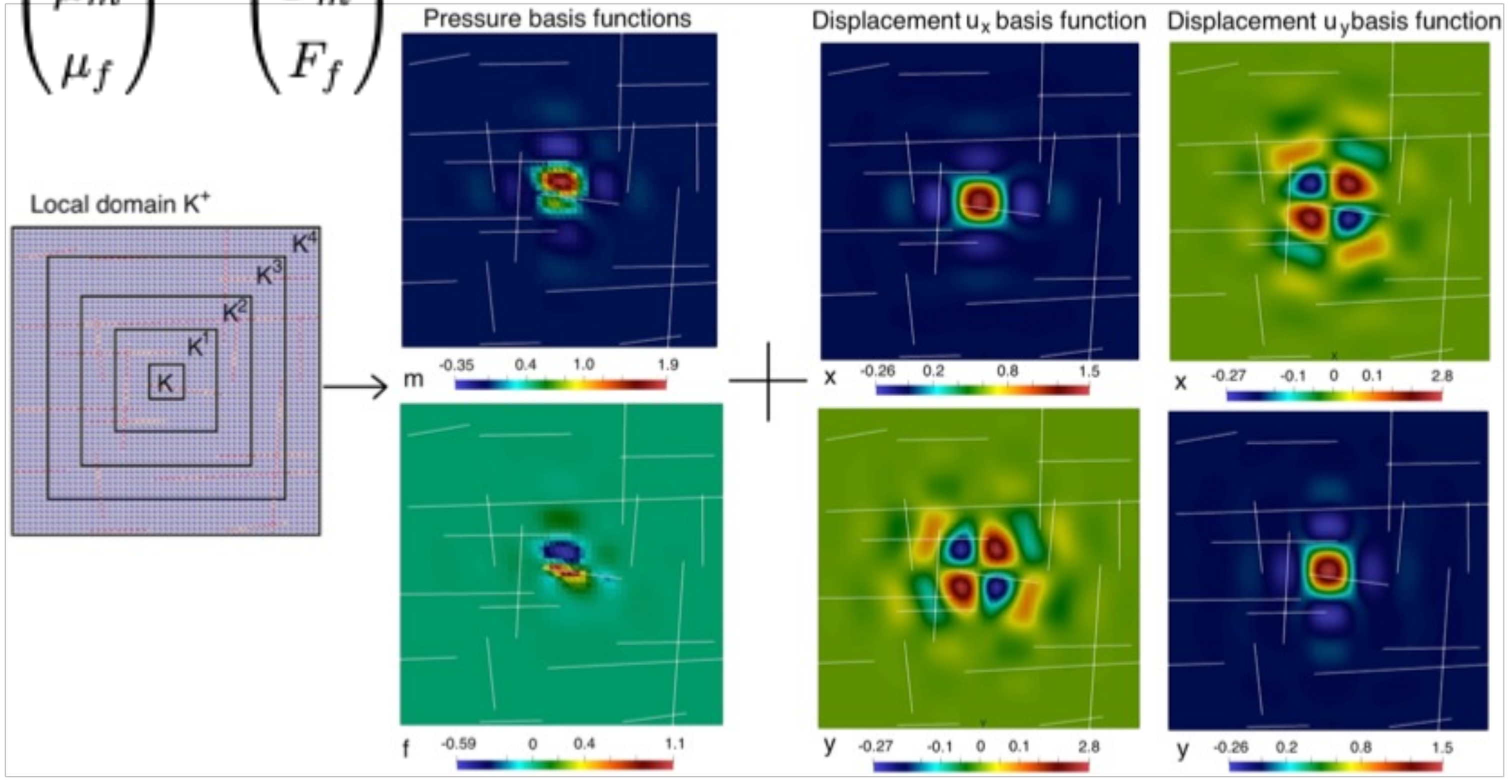
$$\int_{K_j} \psi_x^{Y,i} \, dx = 0, \quad \int_{K_j} \psi_y^{Y,i} \, dx = \delta_{i,j}.$$

Basis function: local problems with constraints

$$\begin{pmatrix} A_m^{K_i^+} + Q^{K_i^+} & -Q^{K_i^+} & C_m^T & 0 \\ -Q^{K_i^+} & A_f^{K_i^+} + Q^{K_i^+} & 0 & C_f^T \\ C_m & 0 & 0 & 0 \\ 0 & C_f & 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_m \\ \psi_f \\ \mu_m \\ \mu_f \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ F_m \\ F_f \end{pmatrix}$$

Local problem for pressure basis

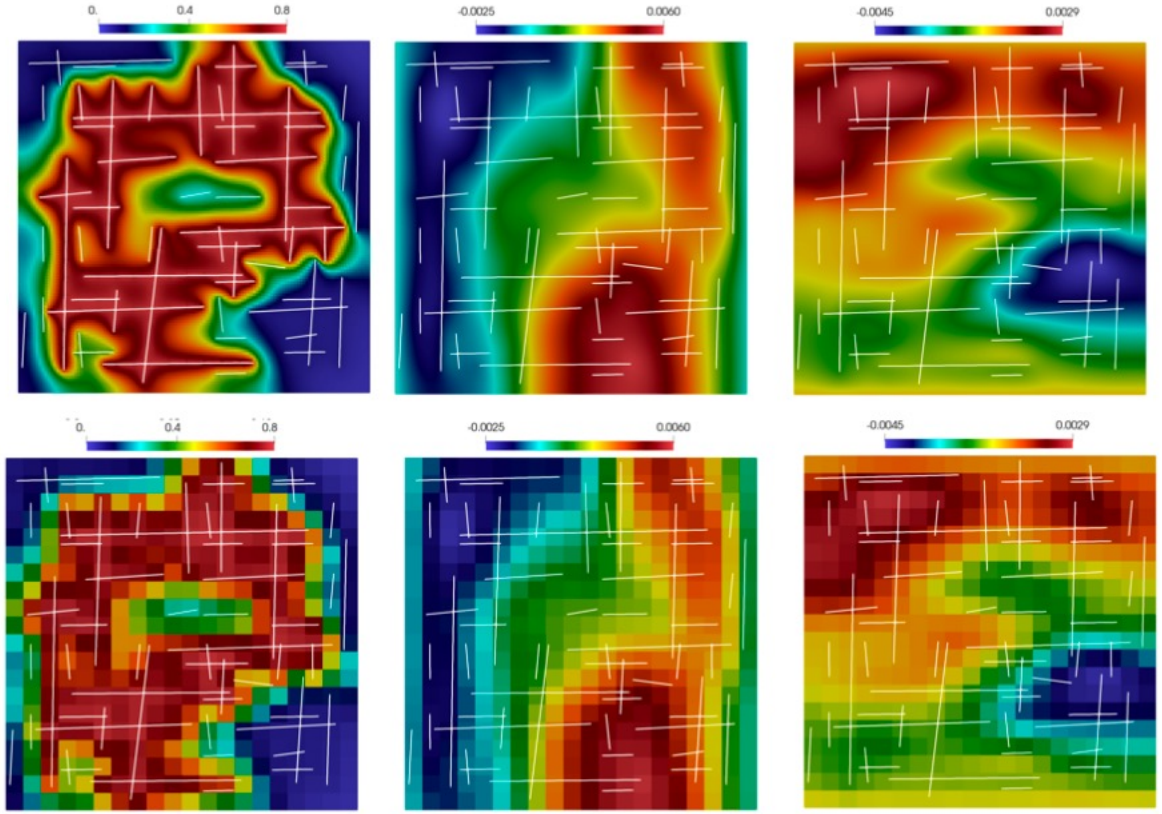
The matrices C_m and C_f define the constraints



Results

Fine

Coarse



K^s	e_p	e_{u_x}	e_{u_y}
Coarse grid 20×20			
1	4.740	86.865	82.598
2	0.723	43.721	37.034
3	0.369	6.716	4.668
4	0.359	2.718	2.854
Coarse grid 40×40			
1	1.986	96.667	95.454
2	0.191	78.718	74.957
3	0.174	30.550	25.220
4	0.158	4.1302	3.321
6	0.157	1.127	1.233

Fine problem size: 59394

Coarse problem size: 1393 (20x20), 5165 (40x40)

Example 2

- Consider geothermal systems

Flow terms

(i) r_{mf} and r_{fm}

(ii) $-\,\mathrm{div}(k_m\,\mathrm{grad}p_m)$

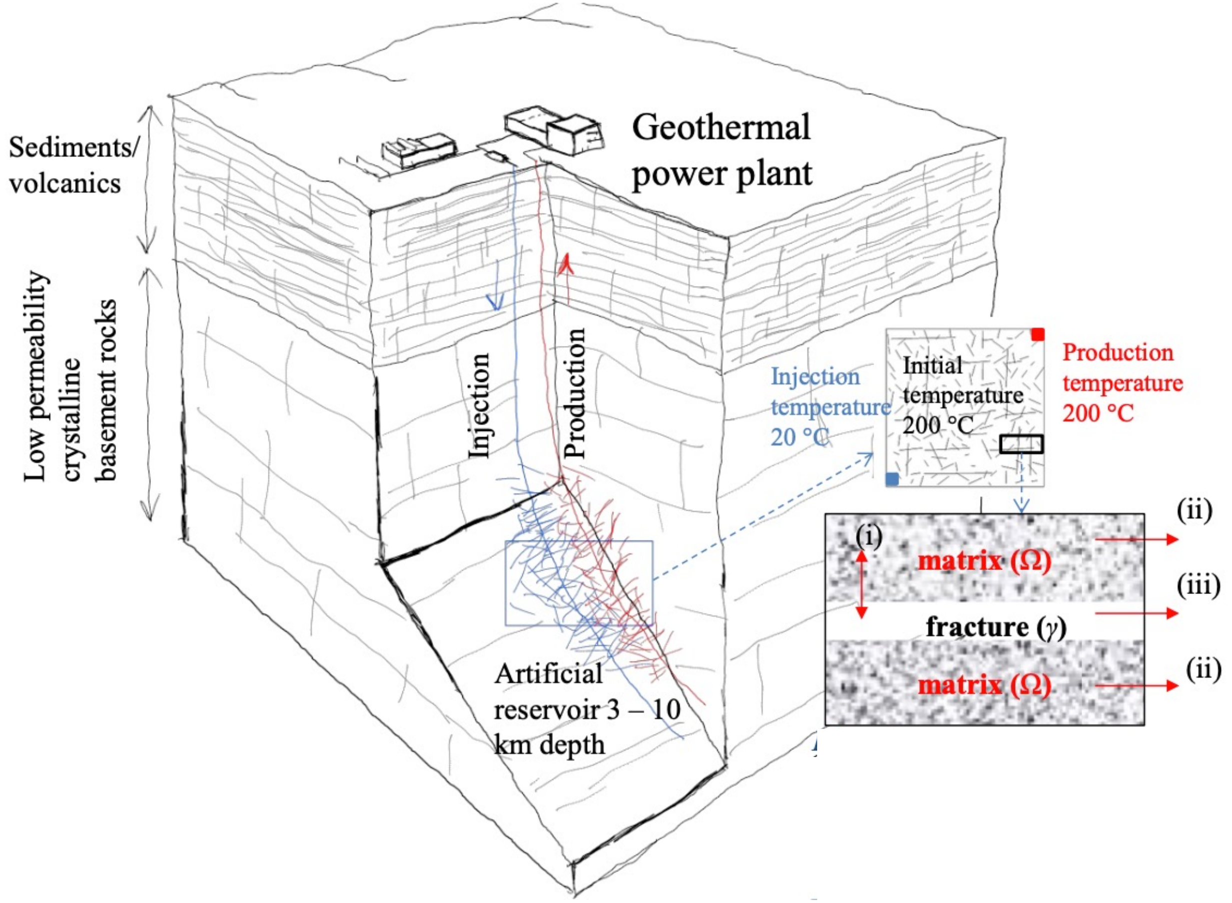
(iii) $-\,\mathrm{div}(k_f\,\mathrm{grad}p_f)$

Heat transfer terms

(i) L_{mf} and L_{fm}

(ii) $(c\rho)_m\mathrm{div}(q_m T_m) - \mathrm{div}(\lambda_m\,\mathrm{grad}p_m)$

(iii) $(c\rho)_f\mathrm{div}(q_f T_f) - \mathrm{div}(\lambda_f\,\mathrm{grad}p_f)$



Vasilyeva, Babaei, Chung, Alekseev, 2019

- Flow equations

$$a_m \frac{\partial p_m}{\partial t} - s_m \frac{\partial T_m}{\partial t} - \operatorname{div}\left(k_m \operatorname{grad} p_m\right) + r_{mf} = g_m^p, \quad x \in \Omega,$$

$$a_f \frac{\partial p_f}{\partial t} - s_f \frac{\partial T_f}{\partial t} - \operatorname{div}\left(k_f \operatorname{grad} p_f\right) - r_{fm} = g_f^p, \quad x \in \gamma,$$

- Heat transfer equations

$$(c\rho)_m \frac{\partial T_m}{\partial t} + (c\rho)_w \operatorname{div}(q_m T_m)$$

$$- \operatorname{div}\left(\lambda_m \operatorname{grad} T_m\right) + L_{mf} = (c\rho)_w g_m^T, \quad x \in \Omega,$$

$$(c\rho)_f \frac{\partial T_f}{\partial t} + (c\rho)_w \operatorname{div}(q_f T_f)$$

$$- \operatorname{div}\left(\lambda_f \operatorname{grad} T_f\right) - L_{fm} = (c\rho)_w g_f^T, \quad x \in \gamma,$$

Results

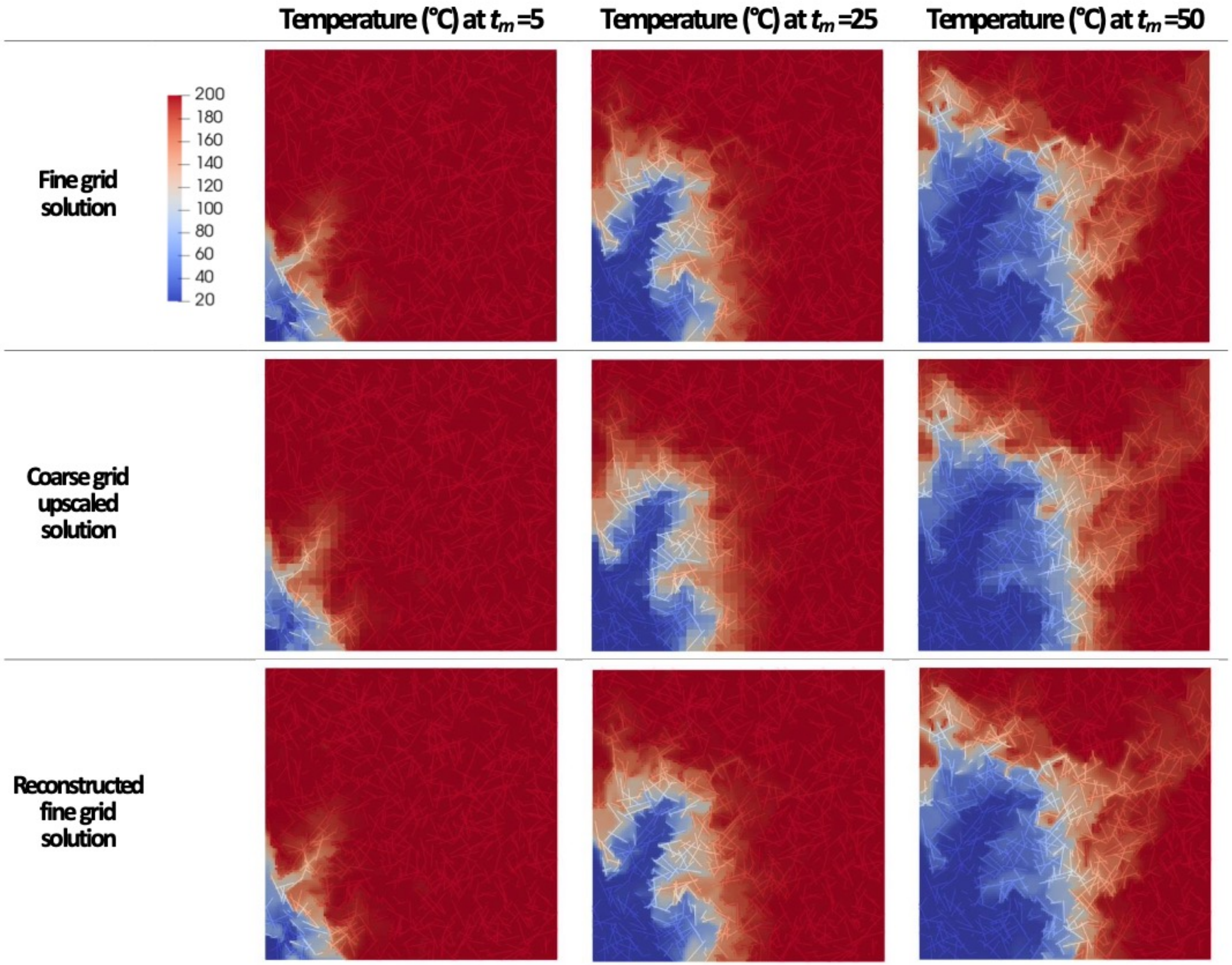
- Consider a domain with 1000 fracture lines
- Fine grid has 26,935 DOFs and coarse grid has 5,104 DOFs

Geometry 2

Error at the final time

K^M	e^C_{heat}	e^F_{heat}
Geometry 2		
1	-	-
2	43.955	60.192
3	22.208	33.411
4	1.257	1.717
6	0.088	0.113

K^M	e^C_{flow}	e^F_{flow}
Geometry 2		
1	-	-
2	0.134	2.066
3	0.034	0.206
4	0.031	0.041
5	0.031	0.031



Temperature (°C) at t_m =5
Temperature (°C) at t_m =25
Temperature (°C) at t_m =50
Fine grid solution
Coarse grid upscaled solution
Reconstructed fine grid solution
200
180
160
140
120
100
80
60
40
20

Nonlinear upscaling

- Local nonlinear maps instead of basis functions
- Consider a nonlinear multiscale problem

$$U_t + G(x, U, \nabla U) = g$$

where G is a nonlinear multiscale operator

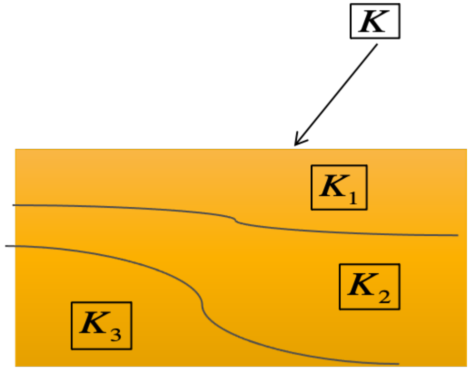
- (1) Identify macroscopic variables
- (2) Instead of basis function, we solve local problem, with constraints related to the macroscopic variables, to obtain downscaling maps

$$\phi_t + G(x, \phi, \nabla \phi) = \mu$$

Map: $U \mapsto \phi$

- (3) Obtain the coarse grid model

Choosing macroscopic variables



- These are typically average solutions on continua
- The variables $\{U_j^{n,i}\}$, for the i-th coarse element, j-th continua within the element and n-th time step
- Our goal is to find a coarse-scale equation for these variables. The equation has the following general form

$$U_j^{n+1,i} - U_j^{n,i} - \overline{G}_j^i(\overline{U}^L) = 0$$

- where $\overline{G}_j^i$ is an average operator determined for the i-th coarse element and j-th continua within the element
- $L = n$ or $n + 1$

Local downscaling maps

- Computation of the average operator $\overline{G}_j^i$ needs local solutions
- Let $c = \{c_m^{(l)}\}$ be a set of values defined on continua: l-th element, m-th continua
- The local problem is defined as: find $N_{\omega_i}(x; c)$ such that

$$G(x, N_{\omega_i}(x; c), \nabla N_{\omega_i}(x; c)) = \sum_{m,l} \mu_{i.m}^{(l)}(c) I_{K_m^{(l)}} \text{ in } \omega_i^+$$

subject to the constraints

$$\int_{\omega^+} N_{\omega_i}(x; c) I_{K_m^{(l)}}(x) = c_m^{(l)}$$

- The above problem is solved on an oversampled region (using a fine mesh numerically)

Coarse-grid model

- The global downscaling function is defined using the macroscopic values

$$\mathcal{F}(\overline{U}) = \sum_i N_{\omega_i} \chi_{\omega_i}$$

- To define the coarse-grid model, we approximate the solution as $U \approx \mathcal{F}(\overline{U})$ in

$$U_t + G(x, U, \nabla U) = g$$

and use the following variational form

$$(\frac{\partial}{\partial t}\mathcal{F}(\overline{U}), V_H) + (G(x, \mathcal{F}(\overline{U}), \nabla \mathcal{F}(\overline{U})), V_H) = (g, V_H)$$

(V_H = test function)

- Applying time discretization

$$(\mathcal{F}(\overline{U}^{n+1}), V_H) - (\mathcal{F}(\overline{U}^{n}), V_H) + \Delta t(G(x, \mathcal{F}(\overline{U}^{L}), \nabla \mathcal{F}(\overline{U}^{L})), V_H) = \Delta t(g, V_H)$$

Example

- Consider two-phase flow equations

$$-div(\lambda(S)\kappa\nabla p) = q_p$$
$$\partial_t S + \nabla\cdot(uf(S)) = q,\ \ u = -\lambda(S)\kappa\nabla p$$

- This can be written in the general form as

$$\partial_t(MU) + \nabla\cdot G(x,t,U,\nabla U) = g$$

- We define $U = (S, P)$
- The nonlinear operator $G(x,U,\nabla U) = (G_1(x,U,\nabla U)), G_2(x,U,\nabla U))$ where

$$G_1(x,U,\nabla U) \ = (\kappa(x)F(S)\nabla P) \qquad G_2(x,U,\nabla U) \ = (\kappa(x)\lambda(S)\nabla P)$$

- Also, we take $\mathrm{MU} = (S, 0)$

Vasilyeva, Leung, Chung, Efendiev and Wheeler, 2019, 2020

- We will solve the following local problem to obtain downscaling function
- The oversampled domain ω_E is defined for each coarse edge E
- Given macroscopic values for pressure $\bar{P} = \{\bar{P}_i^j\}$, for saturation $\bar{S} = \{\bar{S}_i^j\}$, we find the local downscaling functions $(N_{p,E}, u_{ms,E}, N_{s,E})$ by

$$\int_{\omega_E} \lambda^{-1}(\bar{S}) u_{ms}(\bar{S},\bar{P}) \cdot v - \int_{\omega_E} N_{p,E}(\bar{S},\bar{P}) \nabla \cdot v = 0 \; \forall v$$

$$\int_{\omega_E} \nabla \cdot (u_{ms}(\bar{S},\bar{P})) w + \int_{\omega_E} \mu_p w = 0$$

$$\int_{\omega_E} N_{p,E}(\bar{S},\bar{P}) I_{K_i^{(j)}} = \bar{P}_i^j$$

$$-div(\lambda(S)\kappa\nabla p) = q_p$$

$$u = -\lambda(S)\kappa\nabla p$$

Constraint for pressure

$$\int_{\omega_E} \nabla \cdot (u_{ms}(\bar{S},\bar{P}) \tilde{f}(N_{s,E}(\bar{S},\bar{P}))) w + \int_{\omega_E} \mu_s w = 0$$

$$\int_{\omega_E} N_{s,E}(\bar{S},\bar{P}) I_{K_i^{(j)}} = \bar{S}_i^j$$

$$\partial_t S + \nabla \cdot (u f(S)) = q$$

Constraint for saturation

- We next find the coarse-scale equation by finite volume scheme
- Recall the equations

$$-div(\lambda(S)\kappa\nabla p) = q_p$$
$$\partial_t S + \nabla\cdot(uf(S)) = q,\ \ u = -\lambda(S)\kappa\nabla p.$$

- Applying finite volume scheme, and using the downscaling functions

$$\sum_{m,l} T_{i,l}^{j,m}(\overline{P}_i^{n+1,j} - \overline{P}_n^{n+1,m}) = \overline{Q}_i^{n+1,j}$$
$$\overline{S}_i^{n+1,j} - \overline{S}_i^{n,j} - \sum_{E\cap\partial K_i^{(j)}} (n_{\partial K_i^{(j)}}\cdot n_E)\overline{F}_E^n = \overline{Q}_{i,w}^{n+1,j}.$$

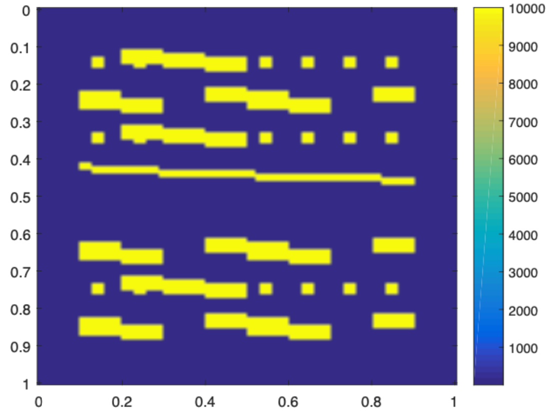
where

$$T_{i,l}^{j,m} = -\sum_{E\cap\partial K_i^{(j)}} \int_E u_{ms}(\overline{S}^n, \vec{e}_i^{\,j}))\cdot n_{\partial K_i^{(j)}}$$
$$\overline{F}_E^n = \Delta t \int_E \tilde{f}(N_{s,E}(\overline{S}^n, \overline{P}^{n+1}))\, u_{ms,E}(\overline{S}^n, \overline{P}^{n+1})\cdot n_E$$
$$\overline{Q}_i^{n+1,j} = \int_{K_i^{(j)}} q(t_{n+1},\cdot),\ \ \overline{Q}_{i,w}^{n+1,j} = \Delta t \int_{K_i^{(j)}} q_w(t_{n+1},\cdot)$$

$$[\vec{e}_i^{\,j}]_l^m = \delta_{jm}\delta_{il}$$

- Note that the ”fluxes” are nonlinear functions of saturations and pressures in neighboring cells.

$$\lambda_w(S) = S^2,$$
$$\lambda_o(S) = (1-S)^2$$



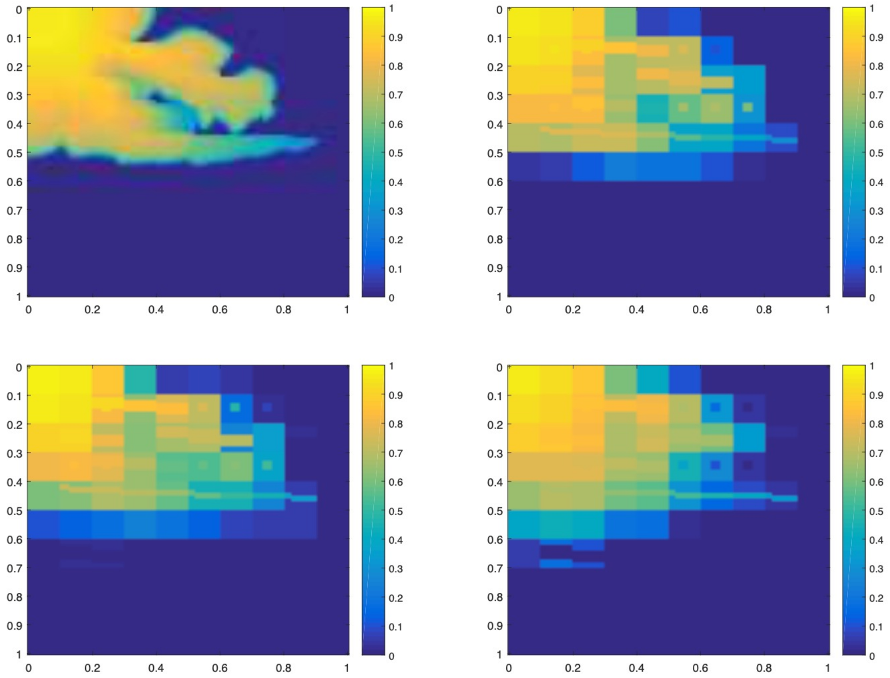
κ

T	$\frac{\lVert \bar{S}_{ms} - \bar{S} \rVert_{L^2}}{\lVert \bar{S} \rVert_{L^2}}$	$\frac{\lVert \bar{S}_{FVM} - \bar{S} \rVert_{L^2}}{\lVert \bar{S} \rVert_{L^2}}$
2.5	10.64%	20.79%
5	8.60%	23.71%

Relative errors

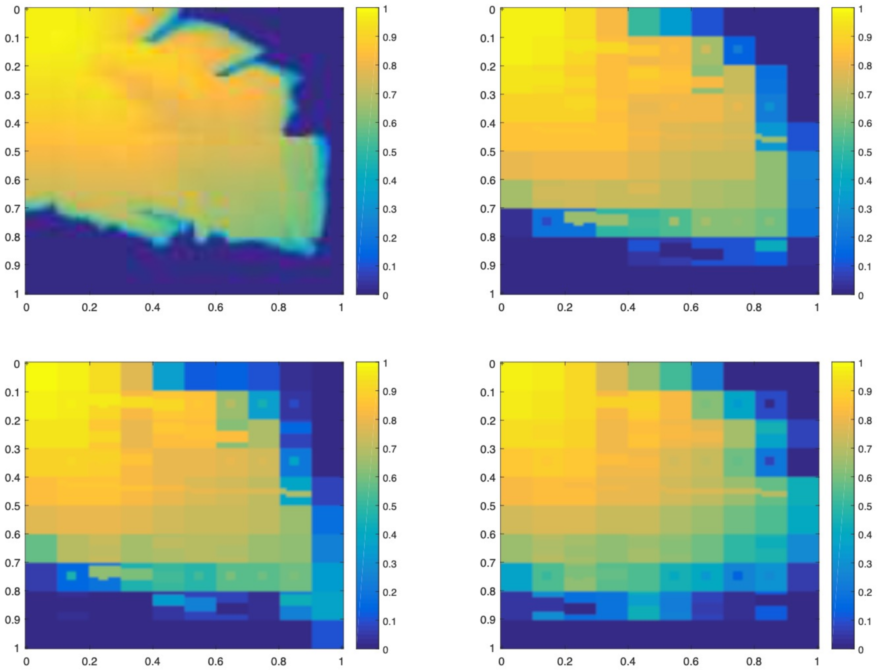
Saturation

S $\bar{S}$



$\bar{S}_{ms}$ $\bar{S}_{FVM}$

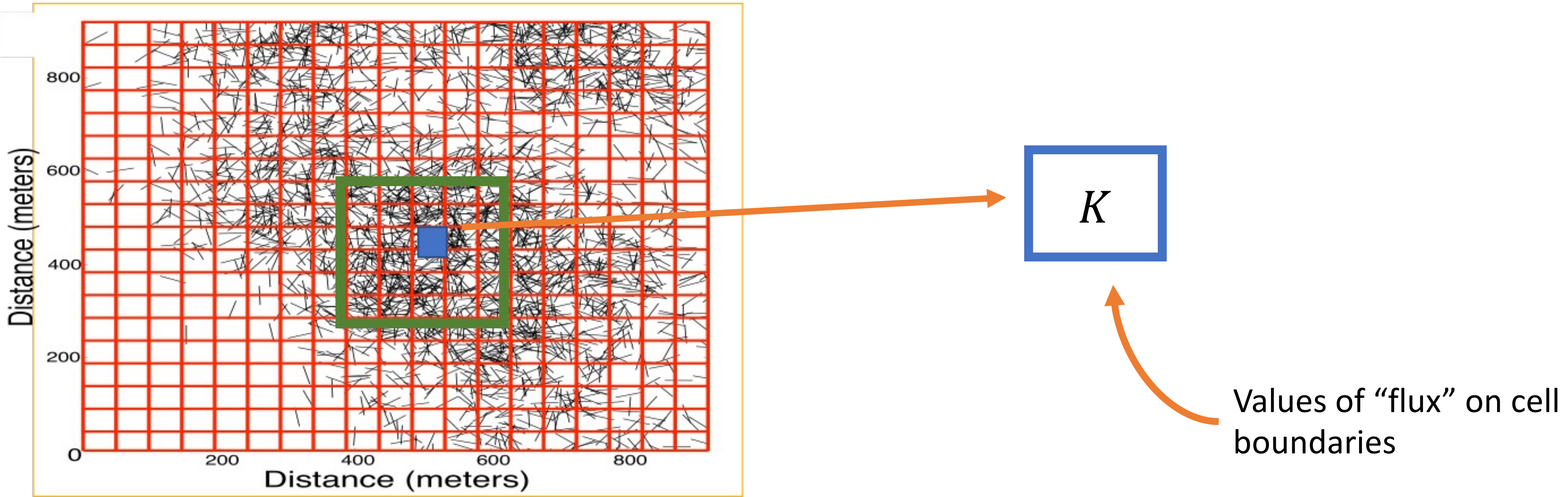
T=2.5



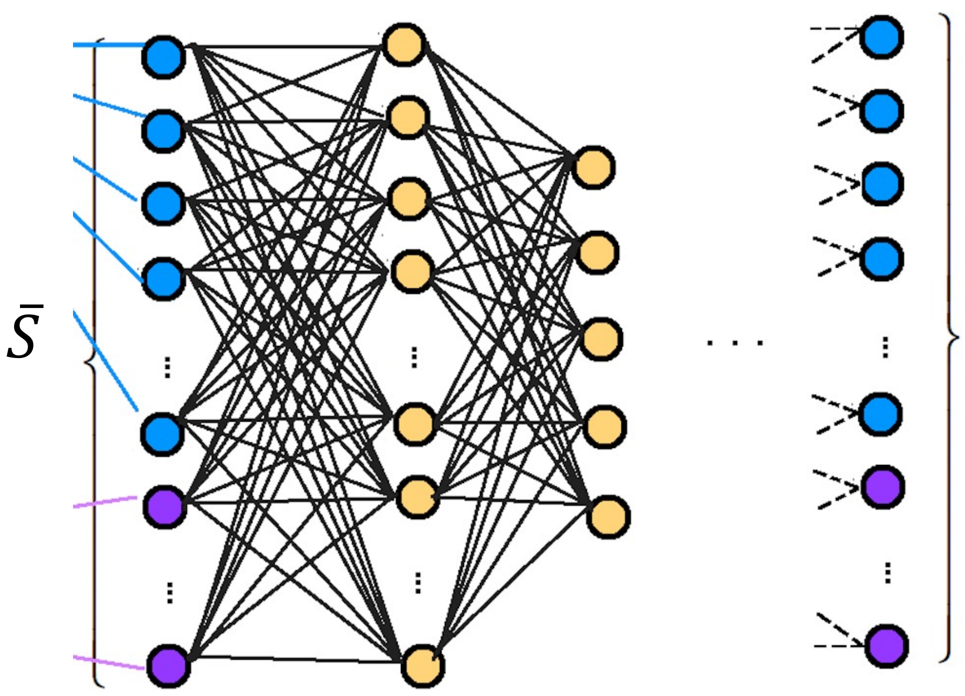
T=5

Learning coarse-scale models

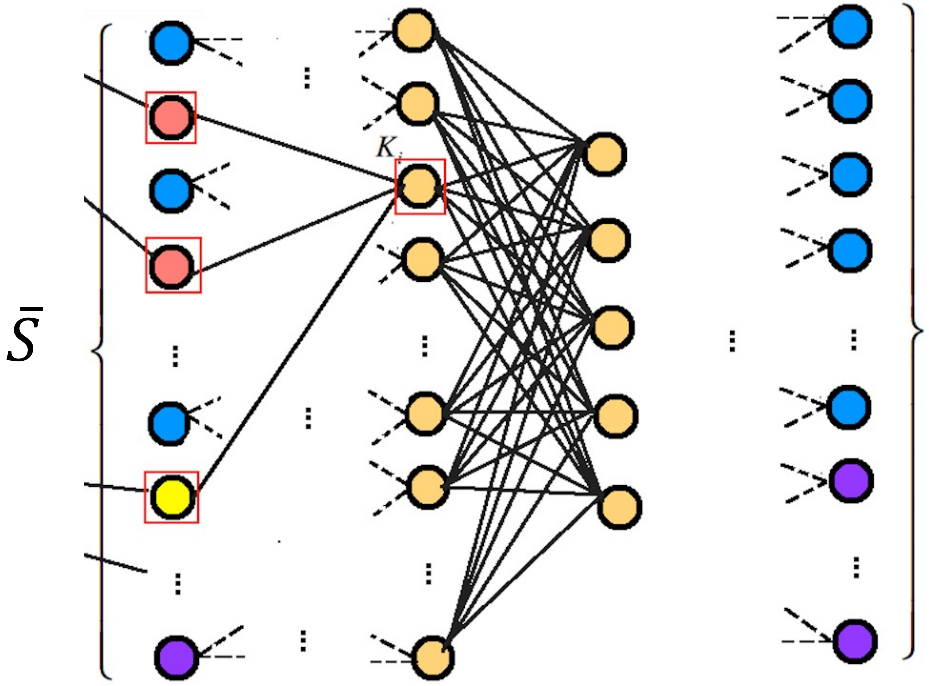
- The coarse-scale models require solutions of local nonlinear problems
- These problems need to be solved on-the-fly
- Coarse edge values of the downscaling function are needed
- We can build a map between macroscopic values and the edge values of downscaling functions, this map can be used to form the coarse-scale equation



- Machine learning is helpful in building such map
- Training data can be obtained from simulations or measurements, lead to a data-driven computational model
- We use ideas from deep neural networks, localized upscaling concepts lead to localized network models

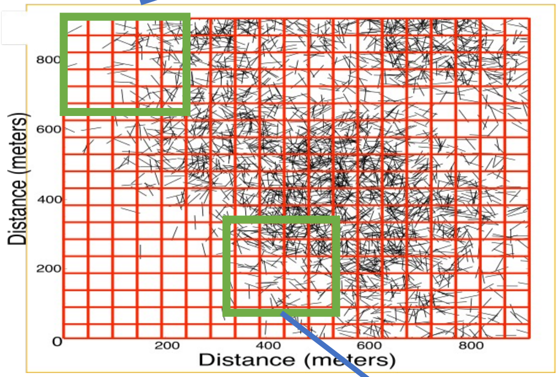


Fully connected



Locally connected

Training concepts

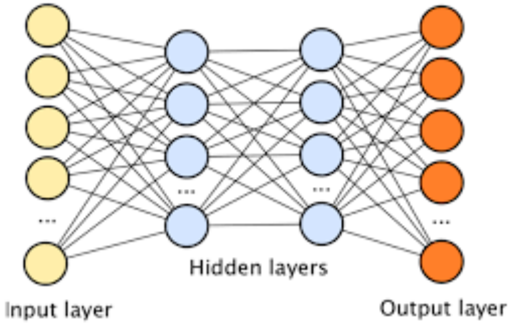


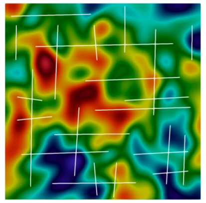
K_1^+

K_i^+

K_j^+

CNN





Oversampled domains

A CNN layer
if needed

A local network

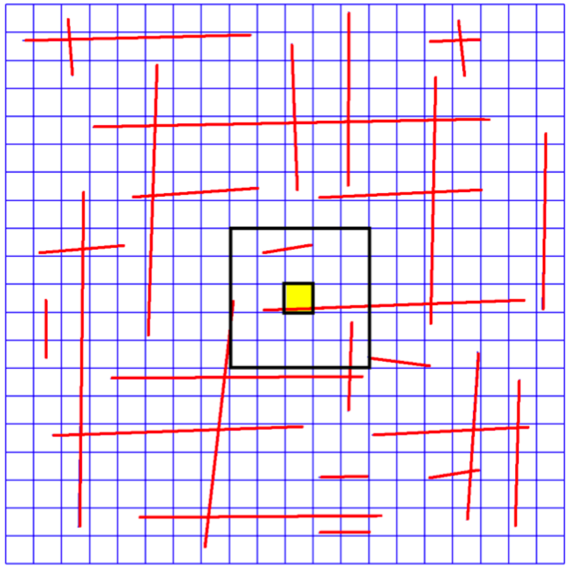
Downscaling
function

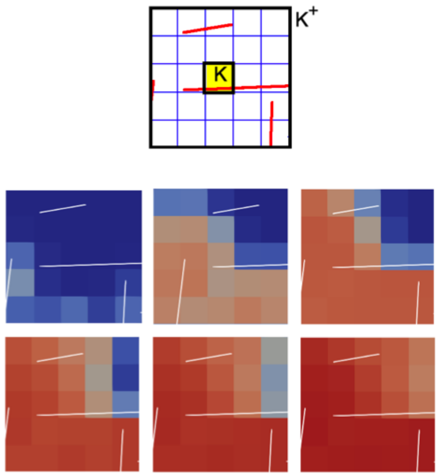
Example

- Consider the two-phase flow problem in fracture media

$$-div(\lambda(S)\kappa\nabla p) = q_p$$
$$\partial_t S + \nabla\cdot(uf(S)) = q, \quad u = -\lambda(S)\kappa\nabla p.$$

- Compute the relative permeabilities by deep neural networks





Error	Nonlocal, ML	
	MAE (%)	RMSE (%)
Training		
$f_{w,1}$	1.167	0.752
$f_{w,2}$	1.479	1.252
$f_{w,3}$	2.000	2.031
$f_{w,4}$	2.121	1.934
$f_{w,5}$	1.161	1.067
Testing		
$f_{w,1}$	1.163	0.827
$f_{w,2}$	1.417	1.099
$f_{w,3}$	1.814	1.662
$f_{w,4}$	2.149	1.958
$f_{w,5}$	1.093	0.939

Thank you