



Multiscale Discretizations for Flow, Transport, and Mechanics in Porous Media

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Outline

- Motivation
- Mortar mixed finite element (MMFE) methods for multiphase flow problem
- Time splitting for MMFE for multiphase flow and mixed/Godunov methods for diffusion-dispersion and reactive transport
- Numerical experiments
- Extensions to DG and DG-MMFE for flow and Galerkin for elasticity
- Conclusions
- Current and Future Work

Motivation



- Goal is to solve heterogeneous subsurface flow problems: multiphase flow, coupled with reactive transport and geomechanics in a multiscale setting.
- Applications: NAPL remediation, monitoring of nuclear wastes, C02 sequestration saline aquifers.
- Traditional method uniform grid everywhere, too expensive. Mortars lead to attractive dynamic meshing strategies and multiphysics couplings.
- Cannot avoid if physical domain is irregular! No single smooth map to a regular computational grid exists.



Societal Needs in Relation to Geological Systems

Resources Recovery

- Petroleum and natural gas recovery from conventional/unconventional reservoirs
- In situ mining
- Hot dry rock/enhanced geothermal systems
- Potable water supply
- Mining hydrology

Waste Containment/Disposal

- Deep waste injection
- Nuclear waste disposal
- CO₂ sequestration
- Cryogenic storage/petroleum/gas

Underground Construction

- Civil infrastructure
- Underground space
- Secure structures

Site Restoration

- Aquifer remediation
- Acid-rock drainage









StratigraphicSolubilityHydrodynamicMineralTrappingTrappingTrappingTrapping

Celia et al, 2002

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Diffusion-Dispersion



Solved fully-implicitly using Expanded MFEM with full-tensor

Introduce $\tilde{\mathbf{z}} = -\nabla c$, $\mathbf{z} = \mathbf{D}_i^* \tilde{\mathbf{z}}$ Find $\tilde{\mathbf{z}}_{h,iw}^{m+1}|_{\Omega_j} \in \tilde{\mathbf{V}}_{h,j}$, $\mathbf{z}_{h,iw}^{m+1}|_{\Omega_j} \in \mathbf{V}_{h,j}$, $c_{h,iw}^{m+1}|_{\Omega_j} \in W_{h,j}$ such that:

$$\left(\frac{\varphi_i^{*,m+1}c_{h,iw}^{m+1} - \widehat{T}_i}{\Delta \tau^{m+1}}, w\right)_{\Omega_j} + \left(\nabla \cdot \mathbf{z}_{h,iw}^{m+1}, w\right)_{\Omega_j} = 0, w \in W_{h,j}$$
$$(\widetilde{\mathbf{z}}_{h,iw}^{m+1}, \mathbf{v})_{\Omega_j} = (c_{h,iw}^{m+1}, \nabla \cdot \mathbf{v})_{\Omega_j} - \left\langle \mathcal{P}_j c_{h,iw}, \mathbf{v} \cdot \mathbf{n}_j \right\rangle_{\Gamma_j}, \mathbf{v} \in \mathbf{V}_{h,j}$$

$$(\mathbf{z}_{h,iw}^{m+1}, \mathbf{\tilde{v}})_{\Omega_j} = (\mathbf{D}_i^{*,m+1} \mathbf{\tilde{z}}_{h,iw}^{m+1}, \mathbf{\tilde{v}})_{\Omega_j}, \mathbf{\tilde{v}} \in \mathbf{\tilde{V}}_{h,iw}$$





- Flow is independent of transport.
- Inter-phase distribution of species assumed to be ``locally equilibrium" controlled, instantaneously.
- Ignore adsorption.



Preliminaries



 $\bar{\Omega} = \bigcup_{i=1}^{n_b} \bar{\Omega}_i$: computational domain is decomposed into non-overlapping subdomain blocks

$$\Gamma_{ij} = \partial \Omega_i \cap \partial \Omega_j, \quad \Gamma = \bigcup_{i,j=1}^{n_b} \Gamma_{ij}, \quad \Gamma_i = \partial \Omega_i \cap \Gamma = \partial \Omega_i \setminus \partial \Omega$$

On each block $\Omega_i : \mathcal{T}_{h,i}$ - finite element partition
 $\mathbf{V}_{h,i} \times W_{h,i} \subset H(\operatorname{div}; \Omega_i) \times L^2(\Omega_i) - \operatorname{MFE}$ spaces on $\mathcal{T}_{h,i}$

On each interface $\Gamma_{i,j}$: $\mathcal{T}_{H,i,j}$ – interface finite element grid $M_{H,i,j} \subset L^2(\Gamma_{i,j})$ – mortar space on $\mathcal{T}_{H,i,j}$

$$\mathbf{V}_{h} = \bigoplus_{i=1}^{n_{b}} \mathbf{V}_{h,i}, \qquad W_{h} = \bigoplus_{i=1}^{n_{b}} W_{h,i} \qquad M_{H} = \bigoplus_{1 \le i < j \le n_{b}} M_{H,i,j}$$

Mortar Domain Decomposition

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$$\begin{split} \left(\frac{\Delta(\varphi\rho_{\alpha,h}S_{\alpha,h})^{n}}{\Delta t^{n}},w\right)_{\Omega_{i}} + \left(\nabla\cdot\rho_{\alpha,h}^{n}\mathbf{u}_{\alpha,h}^{n},w\right)_{\Omega_{i}} &= (q_{\alpha}^{n},w)_{\Omega_{i}}, w\in W_{h,i}\\ \left(\left(\frac{K}{\mu_{\alpha,h}}\right)^{-1}\tilde{\mathbf{u}}_{\alpha,h}^{n},\mathbf{v}\right)_{\Omega_{i}} &= (p_{\alpha,h}^{n},\nabla\cdot\mathbf{v})_{\Omega_{i}} - \left\langle p_{\alpha,H}^{n},\mathbf{v}\cdot\mathbf{n}_{i}\right\rangle_{\Gamma_{i}}\\ &+ (\rho_{\alpha,h}^{n}g\nabla D,\mathbf{v})_{\Omega_{i}}, \quad \mathbf{v}\in\mathbf{V}_{h,i}\\ (\mathbf{u}_{\alpha,h}^{n},\tilde{\mathbf{v}})_{\Omega_{i}} &= (k_{r\alpha,h}^{n}\tilde{\mathbf{u}}_{\alpha,h}^{n},\tilde{\mathbf{v}})_{\Omega_{i}}, \quad \tilde{\mathbf{v}}\in\tilde{\mathbf{V}}_{h,i}\\ \left\langle \begin{bmatrix} \mathbf{u}_{\alpha,h}^{n}\cdot\mathbf{n} \end{bmatrix}_{i,j}, \zeta \right\rangle_{\Gamma_{i,j}} &= 0, \quad \zeta\in M_{H,i,j} \end{split}$$



Let
$$\mathbf{M}_{H} = M_{H} \times M_{H}$$
. Define
 $b^{n}(\psi, \eta) = \sum_{1 \leq i < j \leq n_{b}} \sum_{\alpha} \int_{\Gamma_{i,j}} \left[\rho_{\alpha,h}^{n} \mathbf{u}_{\alpha,h}^{n}(\psi) \cdot \mathbf{n} \right]_{ij} \eta_{\alpha} ds$
where $\psi = (p_{w,H}^{n}, S_{w,H}^{n}) \in \mathbf{M}_{H}, \ \eta = (\eta_{w}, \eta_{w}) \in \mathbf{M}_{H}$

Define the non-linear interface operator $\mathcal{B}^n : \mathbf{M}_H \to \mathbf{M}_H$ by

$$\left\langle \mathcal{B}^{n}\psi,\eta\right\rangle =b^{n}(\psi,\eta),\quad\forall\eta\in\mathbf{M}_{H}$$

Then $(\psi, p_{\alpha,h}^n(\psi), S_{\alpha,h}^n(\psi), \mathbf{u}_{\alpha,h}^n(\psi))$ solves the multiphase flow equations when $\mathcal{B}^n(\psi) = 0$

Interface problem is solved by "inexact Newton-GMRES" scheme





Mass balance of species *i* in phase α : $\frac{\partial(\varphi c_{i\alpha}S_{\alpha})}{\partial t} + \nabla \cdot (c_{i\alpha}\mathbf{u}_{\alpha} - \varphi S_{\alpha}\mathbf{D}_{i\alpha}\nabla c_{i\alpha}) = r(c_{i\alpha})$ $\mathbf{D}_{i\alpha}\nabla c_{i\alpha} \cdot \mathbf{n} = 0$

- Diffusion-Dispersion tensor $\mathbf{D}_{i\alpha} = \mathbf{D}_{i\alpha}^{\text{diff}} + \mathbf{D}_{i\alpha}^{\text{hyd}}$:
- Molecular diffusion: $\mathbf{D}_{i\alpha}^{\text{mol}} = \tau_{\alpha} d_{\text{m},i\alpha} \mathcal{I}$ Physical dispersion: $\varphi S_{\alpha} \mathbf{D}_{i\alpha}^{\text{hyd}} = d_{t,\alpha} |\mathbf{u}_{\alpha}| \mathcal{I} + (d_{l,\alpha} - d_{t,\alpha}) \frac{\mathbf{u}_{\alpha} \mathbf{u}_{\alpha}^{T}}{|\mathbf{u}_{\alpha}|}$
- Source term: $r(c_{i\alpha}) = r_{i\alpha}^{I} + \varphi S_{\alpha} r_{i\alpha}^{C} + q_{i\alpha}$, where $r_{i\alpha}^{I}$ is influx/efflux from other phases, $r_{i\alpha}^{C}$ is chemical rate of decay $q_{i\alpha}$ is a source (or sink) term



Assume an equilibrium partitioning of species between phases:

$$c_{ilpha} = heta_{ilpha} c_{ilpha_0}$$

Sum over all phases for a given species:

$$\frac{\partial(\varphi_i^* c_{iw})}{\partial t} + \nabla \cdot (c_{iw} \mathbf{u}_i^* - \mathbf{D}_i^* \nabla c_{iw}) = r_i^*(\mathbf{c}_w)$$
$$\mathbf{D}_{iw} \nabla c_{iw} \cdot \mathbf{n} = 0$$
$$\mathbf{u}_i^* = \varphi \sum_{\alpha} \theta_{i\alpha} S_{\alpha} \qquad \mathbf{u}_i^* = \sum_{\alpha} \theta_{i\alpha} \mathbf{u}_{\alpha}$$
$$\mathbf{v}_i^* = \varphi \sum_{\alpha} S_{\alpha} \theta_{i\alpha} \mathbf{D}_{i\alpha} \qquad r_i^*(\mathbf{c}_w) = \varphi \sum_{\alpha} r_{i\alpha}^C - r_{iR} + \sum_{\alpha} q_{i\alpha}$$

Note: $\sum_{\alpha} r_{i\alpha}^{I} + r_{iR} = 0$, where r_{iR} is the influx/efflux of species *i* into the stationary phase





$$\left(\frac{\partial \varphi_i^* c_{iw}}{\partial t}, w\right)_{\Omega_j} + (\nabla \cdot (c_{iw} \mathbf{u}_i^*), w)_{\Omega_j} = \left(\sum_{\alpha} q_{i\alpha}, w\right)_{\Omega_j}, w \in W_j$$

Solved using a Godunov scheme

First order Godunov scheme

Let
$$T_i^m = \varphi_i^{*,m} c_{h,iw}^m$$
, solve for \overline{T}_i from

$$\left(\frac{\overline{T}_i - T_i^m}{\Delta \tau^{m+1}}, w\right)_{\Omega_j} + \sum_{E \in \mathcal{T}_{h,j}} \left\langle c_{h,iw}^{m,\text{upw}} \mathbf{u}_{h,i}^{*,m+1/2} \cdot \mathbf{n}_E, w \right\rangle_{\partial E} = \left(\sum_{\alpha} q_{i\alpha}, w\right)_{\Omega_j}$$



Define
$$\Phi(t) \equiv \text{diag}\{\varphi_i^*(t)\}, \quad \mathbf{T} = \mathbf{T}(t) \equiv \Phi(t)\mathbf{c}_w$$
, and
 $r_i^{*,C}(\mathbf{T}) \equiv \varphi \sum_{\alpha} r_{i\alpha}^C(\Phi^{-1}(t)\mathbf{T}) \quad \text{Then} \quad \frac{\partial \mathbf{T}_i}{\partial t} = r_i^{*,C}(\mathbf{T})$

Solved by explict ODE integration using Runge-Kutta

Second order Runge-Kutta scheme

$$k_{1,i} = \Delta \tau^{m+1} r_i^{*,C}(\overline{\mathbf{T}})$$
$$k_{2,i} = \Delta \tau^{m+1} r_i^{*,C} \left(\overline{\mathbf{T}} + \frac{1}{2} \mathbf{k}_1\right)$$
$$\widehat{T}_i = \overline{T} + k_{2,i}$$



$$\mathcal{P}_j: L^2(\Gamma_j) \to L^2(\Gamma_k) \text{ is an } L^2\text{-orthogonal proj. s.t. } \forall \phi \in L^2(\Gamma_j)$$
$$\langle \phi - \mathcal{P}_j \phi, \mathbf{v} \cdot \mathbf{n}_j \rangle_{\Gamma_{k,j}} = 0, \ \forall \mathbf{v} \in \mathbf{V}_{h,i}, \forall k \text{ such that } \overline{\Omega}_k \cap \overline{\Omega}_j \neq \emptyset$$





Algorithm





NAPL Remediation



- Bio-remediation of NAPL using microbes
- Advection-Diffusion-Reaction
- Discontinuous permeability field with barriers
- Two flowing phases quarterfive spot
- External BC: no-flow and zero diffusive flux
- IC: NAPL, microbes occupy 0 < y < 40 ft and O₂, N₂ occupy 40 < y < 400 ft.
- Domain: 20 ft x 400 ft x 400 ft
- Reference case: NX=20, NY=40, NZ=40





Flow Pattern in Multi-block





Reference Solution



Concentrations of tracer, NAPL, microbes and bio-degraded product at 100 days





Comparison to Mortar Scheme

Tracer & NAPL concentrations at 5, 50, 100 days





Microbe & product concentrations at 5, 50, 100 days







- DG and Mixed FEM can be combined for treating flow using mortar spaces
- DG is applicable for both flow and transport on non-matching grids
- Examples for single-phase slightly compressible flow follow



DG-MFEM, 3 blocks with a fault



- 250 x 100 x 100 ft
- 2 ft wide fault: 10000 mD, φ=0.01
- 4 geological layers: 10, 100, 300, 10 mD, φ=0.2
- BC:
 500 psi at x=0
 400 psi at x=250,
 noflow o.w.
- r=2, k=0 (RT0), m=0



DG-DG, **Oxbow problem**

- 4 blocks with 6 wells
- 900 x 500 x 24 ft
- 1 production, 5 injection wells
- K_{xx} = K_{yy}={200,30,40}, K_{zz}={25,5,3}, φ={0.22,0.08,0.09}
- BC: P_{inj} = 700 psi,
 P_{prod} = 500 psi, noflow on the outer bdry
- nonmatching grids, r=2, m=1

Unstructured Mesh

Top view, 4 blocks

Magnified grid around well

Linear Elasticity Problem

Find $u \in H^1(\Omega)$ s.t.

$$-\nabla \cdot \boldsymbol{\sigma}(u) = f \quad \text{in } \Omega \\ u = u_D \qquad \text{on } \Gamma_D \\ \boldsymbol{\sigma}(u)\mathbf{n} = t_N \qquad \text{on } \Gamma_N$$

$$\boldsymbol{\sigma}(u) = \lambda \nabla \cdot uI + 2\mu \boldsymbol{\varepsilon}(u)$$
$$\boldsymbol{\varepsilon}(u) = \frac{1}{2} \left(\nabla u + \nabla u^T \right)$$

- anisotropic Hooke's law
- kinematic equation
- $$\begin{split} &u: \text{displacement}\\ &\pmb{\varepsilon}: \text{linearized strain tensor}\\ &\pmb{\sigma}: \text{Cauchy stress}\\ &\lambda>0, \mu>0: \text{Lamé parameters} \end{split}$$

Domain Decomposition

 $\Omega = \Omega_1 \cup \Omega_2 \cup \Gamma_{12}$ Find u with $u|_{\Omega_i} \in H^1(\Omega_i)$ s.t.

On each block Ω_i :

 $-\nabla \cdot \boldsymbol{\sigma}(u) = f \quad \text{in } \Omega_i$ $u = u_D \qquad \text{on } \Gamma_{D_i} = \partial \Omega_i \cap \Gamma_D$ $\boldsymbol{\sigma}(u)\mathbf{n} = t_N \qquad \text{on } \Gamma_{N_i} = \partial \Omega_i \cap \Gamma_N$

On the interface Γ_{12} : $[u] = 0, \quad [\boldsymbol{\sigma}(u)] n_1 = 0, \quad \text{on } \Gamma_{12} \quad : \text{ transmission conditions}$

 $\mathcal{T}_h(\Omega_i)$ – a conforming partition of $\Omega_i, i = 1, 2$ \mathcal{E}_H – mortar finite element partition on Γ_{12} , independent of interior meshes

 $X_{h,i} = \{ \boldsymbol{v}_{h,i} \in L^2(\Omega_i) : \boldsymbol{v}_{h,i}|_{\widetilde{\Omega}_i} \in H^1(\widetilde{\Omega}_i), \forall E \in \mathcal{T}_{h,i}, \boldsymbol{v}_{h,i}|_E \in I\!\!P_k(E) \}$ $\Lambda_H = \{ \boldsymbol{\lambda}_H \in L^2(\Gamma_{12}) : \forall \tau \in \mathcal{E}_H, \boldsymbol{\lambda}_H |_{\tau} \in I\!\!P_l(E) \}$ $\forall \boldsymbol{v}_h \in X_h, \ |\boldsymbol{v}_h|_{X_h} = \left(\sum |\boldsymbol{v}_{h,i}|_{h,i}^2\right)^{1/2}$ $egin{aligned} egin{aligned} egin{aligne} egin{aligned} egin{aligned} egin{aligned} egin$ $+ 2 \mu \left(\|\varepsilon(\boldsymbol{v}_{h,i})\|_{L^2(\widetilde{\Omega}_i)}^2 + \sum \|\varepsilon(\boldsymbol{v}_{h,i})\|_{L^2(E)}^2 \right)$

Error Estimates

$$\begin{aligned} \boldsymbol{u}_{h} - \boldsymbol{u}|_{X_{h}} + \left((\lambda + 2\,\mu) \sum_{i=1}^{2} \left(\sum_{\gamma \in \Gamma_{h,i}} \frac{\sigma_{\gamma}}{h_{\gamma}} \| \boldsymbol{u}_{h,i} - \boldsymbol{u}_{D} \|_{L^{2}(\gamma)}^{2} \right. \\ \left. + \sum_{\gamma \in S_{h,i}} \frac{\sigma_{\gamma}}{h_{\gamma}} \| [\boldsymbol{u}_{h,i}]_{\gamma} \|_{L^{2}(\gamma)}^{2} + \sum_{\tau \in \mathcal{E}_{H}} \frac{\sigma_{\tau}}{H_{\tau}} \| \boldsymbol{u}_{h,i} - \boldsymbol{\lambda}_{H} \|_{L^{2}(\tau)}^{2} \right) \right)^{1/2} \\ \left. \leq C \left(h^{r-1} \left(\left(\frac{h}{H} \right)^{1/2} + \left(\frac{H}{h} \right)^{1/2} \right) + H^{\bar{r}-1/2} Z \right), \end{aligned}$$

where $r = \min(k + 1, s)$ and $\bar{r} = \min(\ell + 1, s - 1/2)$

$$Z = 1$$
, if DG strips are used
 $Z = \left(\frac{H}{h}\right)^{1/2}$, if CG everywhere

Elastic Beam

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)}$$

$$\boldsymbol{u} = \begin{pmatrix} -3\alpha x^2 y\\ \alpha x^3 + \frac{3\alpha\lambda}{\lambda + 2\mu} x(y^2 - c^2) \end{pmatrix}$$

$$\boldsymbol{f} = \begin{pmatrix} 6\alpha\mu\frac{3\lambda+4\mu}{\lambda+2\mu}y\\0 \end{pmatrix}$$

 $E = 2.0E + 5 \text{ N m}^{-2}$ $\nu = 0.3$ L = 10 mc = 0.5m $\alpha = -1.0\text{E-3 m}^{-2}$

Displacement in y-direction

Convergence Rates

	Rectangular mesh				Triangular mesh				
	l = 1		l = 2		l = 1		l = 2		
1/h	Iter.	Error	Iter.	Error	Iter.	Error	Iter.	Error	
4	45	3.98E + 0	65	4.46E + 0	44	$1.10E{+1}$	65	1.16E+1	
8	60	1.53E + 0	69	2.04E + 0	59	3.87E + 0	67	4.81E + 0	
16	78	6.52E-1	83	8.11E-1	79	1.40E+0	81	1.79E + 0	
32	106	3.05E-1	96	3.55E-1	107	6.46E-1	93	7.99E-1	
64	146	1.48E-1	106	1.65E-1	148	3.24E-1	103	4.11E-1	
128	205	7.33E-2	121	7.88E-2	207	1.57E-1	119	1.88E-1	
OR		$O(h^{1.14})$		$O(h^{1.18})$		$O(h^{1.21})$		$O(h^{1.19})$	
ER		$O(h^{1.0})$		$O(h^{0.7})$		$O(h^{1.0})$		$O(h^{0.7})$	

Linear Subdomain Approx. (k=1)

		Rectange	ılar mes	sh	Triangular mesh			
	l = 1		l = 2		l = 1		l = 2	
1/h	Iter.	Error	Iter.	Error	Iter.	Error	Iter.	Error
4	47	4.78E-1	73	1.44E-2	47	9.78E-1	72	1.05E-1
- 8	62	1.71E-1	101	3.10E-3	61	2.27E-1	96	1.14E-2
16	78	6.07E-2	136	6.83E-4	81	7.77E-2	132	2.40E-3
32	106	2.15E-2	189	1.60E-4	107	2.37E-2	185	5.35E-4
64	155	7.60E-3	264	3.85E-5	149	6.90E-3	260	1.26E-4
OR		$O(h^{1.49})$		$O(h^{2.14})$		$O(h^{1.76})$		$O(h^{2.38})$
ER		$O(h^{1.5})$		$O(h^{2.0})$		$O(h^{1.5})$		$O(h^{2.0})$

Quadratic Subdomain Approx. (k=2)

Conclusions

- Mortar methods defined and implemented for
 - Fully implicit multiscale method (MMFE) for multiphase flow coupled to a mixed/Godunov method for advection-diffusionreaction problems on non-matching grids.
 - Elasticity
- Variably refined sub-domains results in significant savings in computational time (1 domain with fine grid takes twice the time as 3 domains) for multphase flow coupled to reactive transport
 - Multiblock domain solution agrees very well with single-domain fine-everywhere
- Mortar approach allows for legacy code reuse and
 - Cheaper way to handle irregular geometries
 - Ideally suited for handling geological faults, fractures, etc.

- Explore dynamic load balancing for treating reactions in parallel computations
- Apply error estimates for flow & transport to make suitable choice of sub-domain grids and mortar degrees of freedom
- Ading sharper a posteriori error estimators for adaptive mesh refinement (with M. Vohralík)
- Geomechanics model extensions to include permeability dependence on stress and coupling to nonisothermal EOS compositional flow model

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