Mortar Coupling of Multiphase Flow and Reactive Transport on Non-Matching Grids

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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
- Conclusions
- Current and Future Work

Societal Needs in Relation to Geological Systems

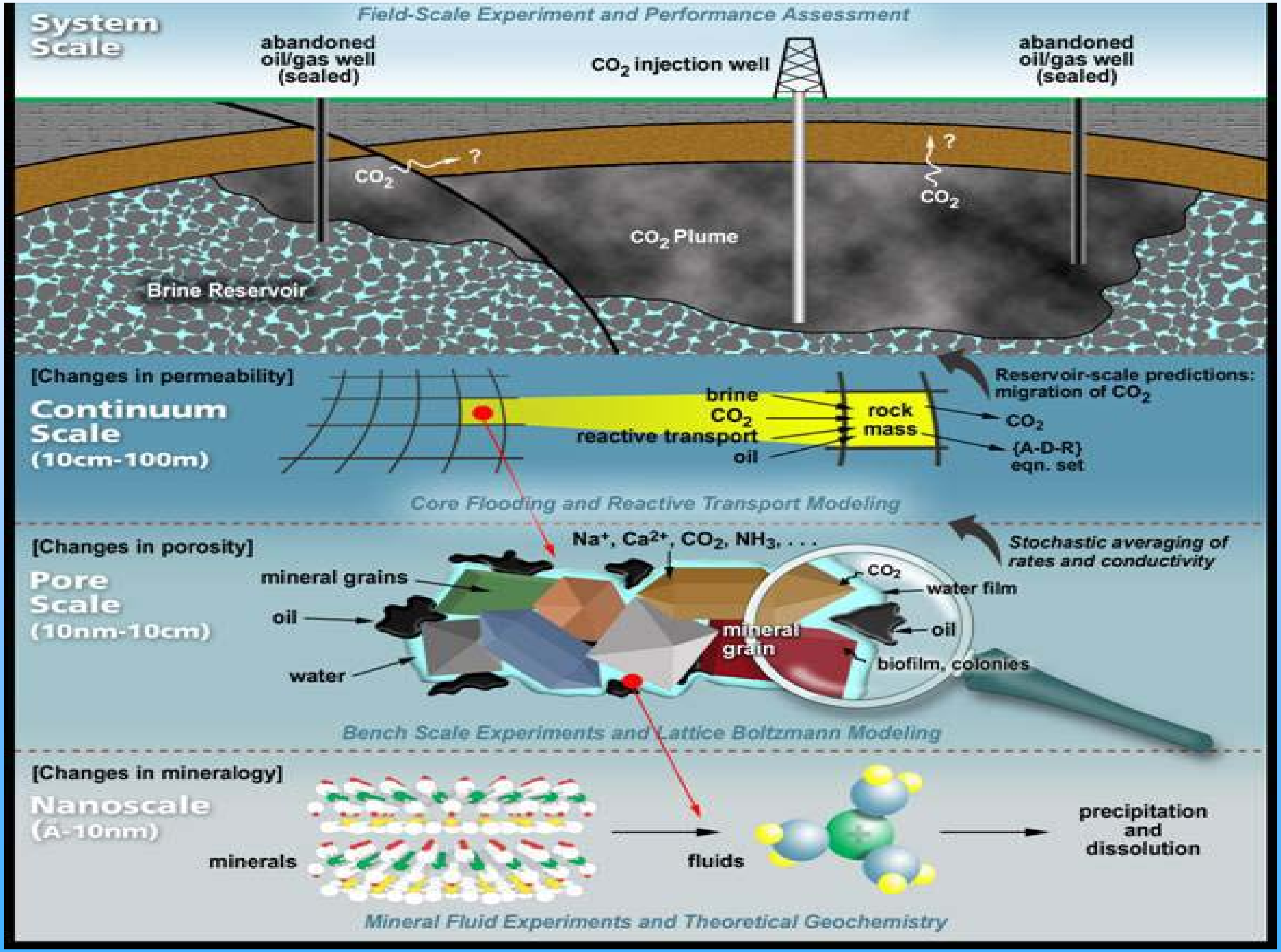
Resources Recovery
- Petroleum and natural gas recovery from conventional/unconventional reservoirs
- *In situ* mining
- Hot dry rock/enhanced geothermal systems
- Potable water supply
- Mining hydrology

Waste Containment/Disposal
- Deep waste injection
- Nuclear waste disposal
- CO_2 sequestration
- Cryogenic storage/petroleum/gas

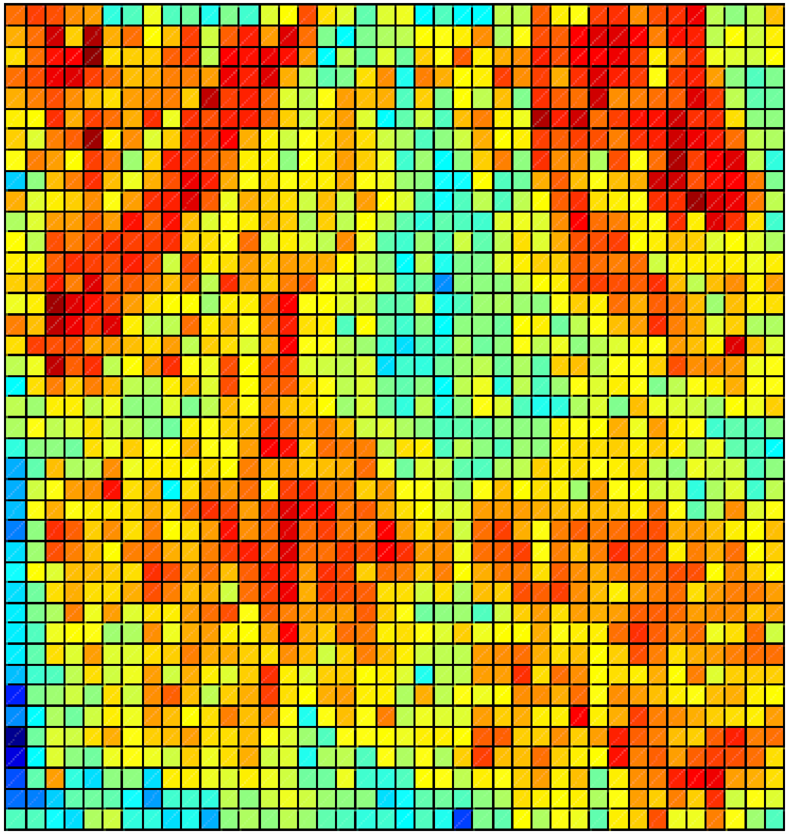
Underground Construction
- Civil infrastructure
- Underground space
- Secure structures

Site Restoration
- Aquifer remediation
- Acid-rock drainage

CO_2 Sequestration

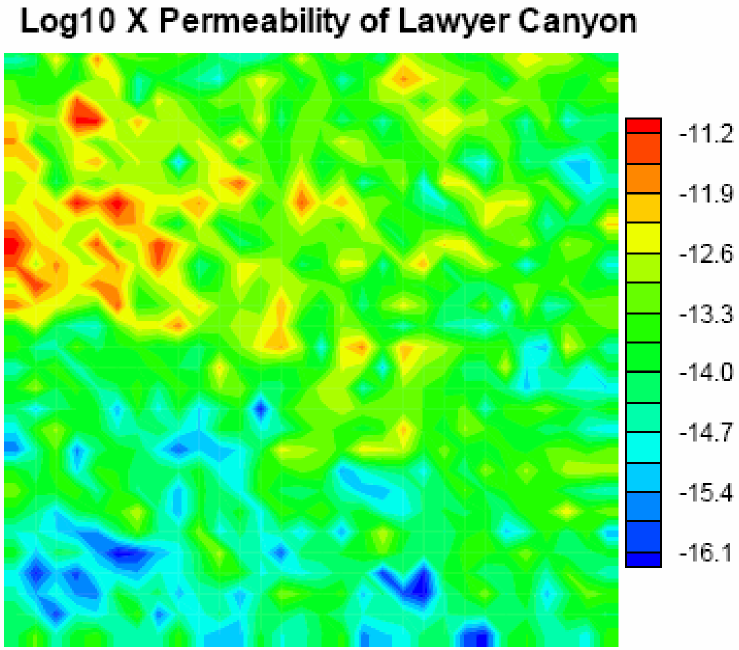


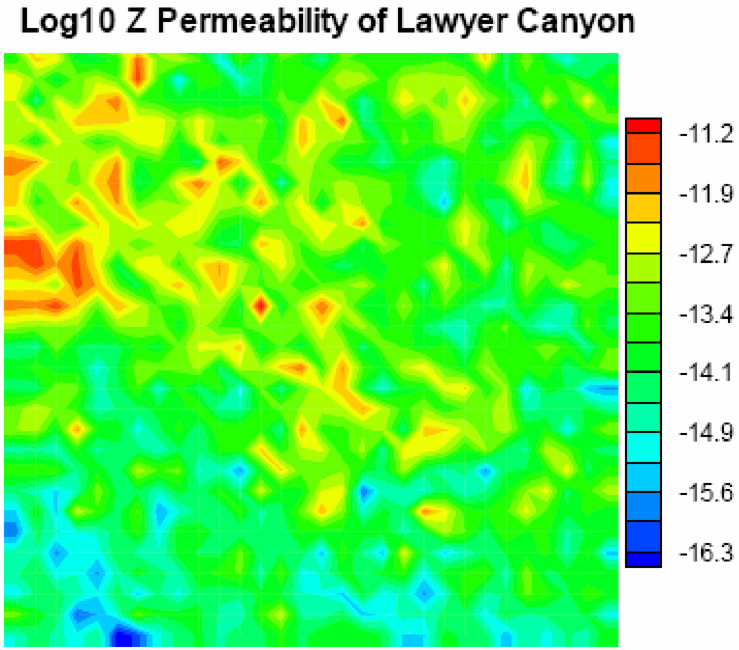
Millimeter-Scale Natural Heterogeneity in Perm *K*



Arco thin slice data, mm scale
(ranges by a factor of 4)

Meter-Scale Natural Heterogeneity in Permeability K





Lawyer Canyon data, meter scale
(ranges by a factor of 10^6)

Difficulty. Fine-scale variation in the permeability K leads to fine-scale variation in the solution $(\mathbf{u}, p)$.

Motivation

- Goal is to solve flow coupled with transport in a multiscale setting.
- Applications: NAPL remediation, monitoring of nuclear wastes, modeling angiogenesis
- Traditional method - uniform grid everywhere, may be too expensive. Mortar scheme leads to attractive dynamic meshing strategies.
- Cannot avoid if physical domain is irregular! No single smooth map to a regular computational grid exists.

Simplifying Assumptions

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

Preliminaries

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

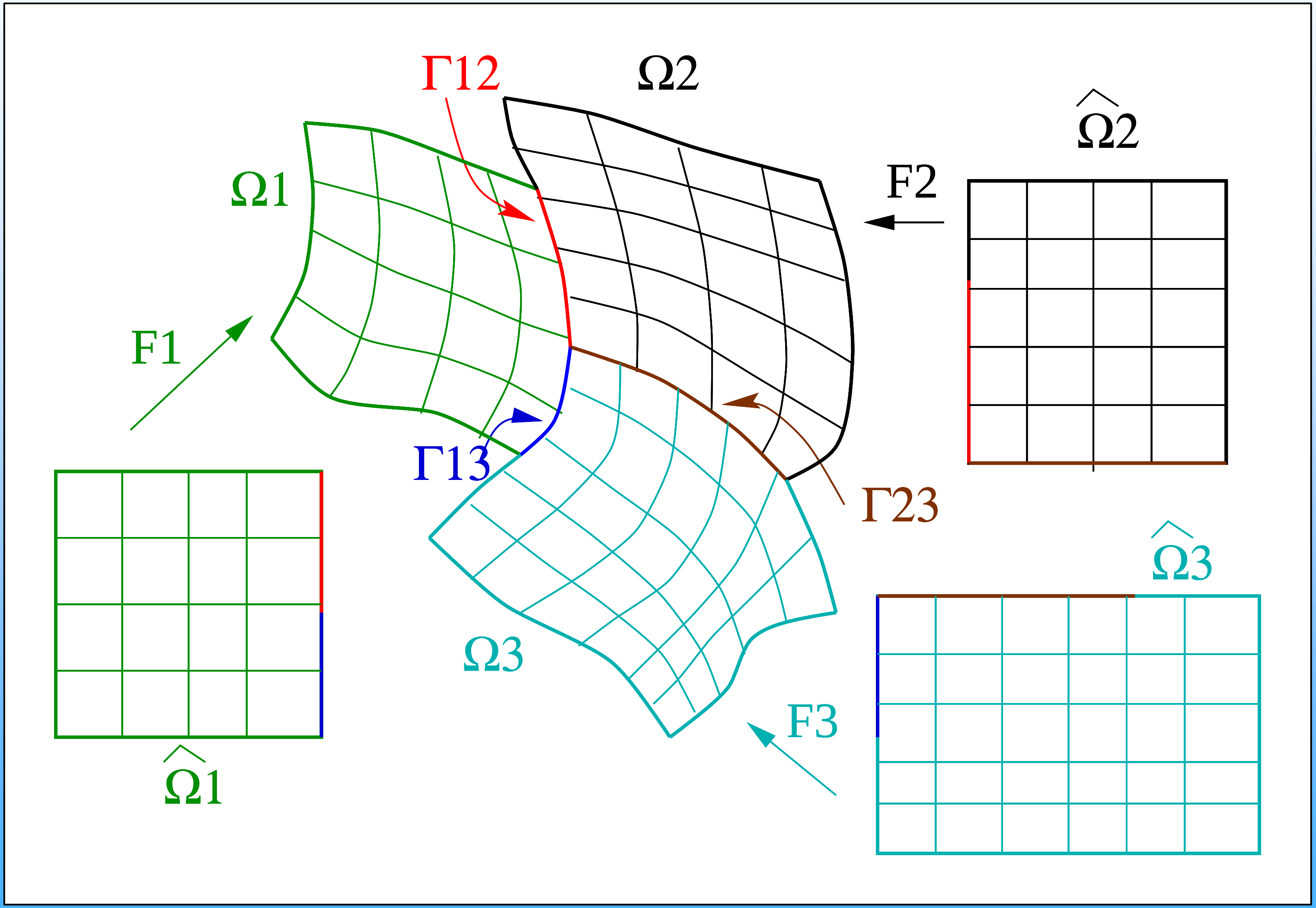
$$\Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j, \quad \Gamma = \cup_{i,j=1}^{n_b} \Gamma_{ij}, \quad \Gamma_i = \partial\Omega_i \cap \Gamma = \partial\Omega_i \backslash \partial\Omega$$

On each block Ω_i : $\mathcal{T}_{h,i}$ – finite element partition
$\mathbf{V}_{h,i} \times W_{h,i} \subset H(\mathrm{div};\Omega_i) \times L^2(\Omega_i)$ – 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



Equations for Multiphase Flow

Mass balance in each sub-domain: $\dfrac{\partial(\varphi\rho_\alpha S_\alpha)}{\partial t}+\nabla\cdot(\rho_\alpha \mathbf{u}_\alpha) = q_\alpha$

Darcy's law (constitutive equation): $\mathbf{u}_\alpha = -\dfrac{k_{r\alpha}(S_\alpha)K}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g \nabla D)$

Saturation constraint: $\sum_\alpha S_\alpha = 1$

Capillary pressure relation: $p_c(S_w) = p_n - p_w$

Continuity: On each interface $\Gamma_{i,j}$ physically meaningful BC applied:

$$p_\alpha|_{\Omega_i} = p_\alpha|_{\Omega_j} \quad [\mathbf{u}_\alpha\cdot\mathbf{n}]_{i,j} \equiv \mathbf{u}_\alpha|_{\Omega_i}\cdot\mathbf{n}_i + \mathbf{u}_\alpha|_{\Omega_j}\cdot\mathbf{n}_j = 0$$

Expanded MMFE Method for Flow

Introduce a pressure gradient term to avoid inverting $k_{r\alpha}$:

$$\tilde{\mathbf{u}}_\alpha = -K/\mu_\alpha(\nabla p_\alpha - \rho_\alpha g \nabla D), \quad \mathbf{u}_\alpha = k_{r\alpha}(S_\alpha)\tilde{\mathbf{u}}_\alpha$$

In a backward Euler multi-block, we seek $\mathbf{u}^n_{\alpha,h}|_{\Omega_i} \in \mathbf{V}_{h,i}$, $\tilde{\mathbf{u}}^n_{\alpha,h}|_{\Omega_i} \in \tilde{\mathbf{V}}_{h,i}$, $p^n_h|_{\Omega_i} \in W_{h,i}$, $S^n_h|_{\Omega_i} \in W_{h,i}$, $p^n_H|_{\Gamma_{i,j}} \in M_{H,i,j}$, $S^n_H|_{\Gamma_{i,j}} \in M_{H,i,j}$ for $1 \le i < j \le n_b$, such that:

$$\left(\frac{\Delta(\varphi\rho_{\alpha,h}S_{\alpha,h})^n}{\Delta t^n}, w\right)_{\Omega_i} + \left(\nabla \cdot \rho^n_{\alpha,h}\mathbf{u}^n_{\alpha,h}, w\right)_{\Omega_i} = (q^n_\alpha, w)_{\Omega_i}, w \in W_{h,i}$$

$$\left(\left(\frac{K}{\mu_{\alpha,h}}\right)^{-1}\tilde{\mathbf{u}}^n_{\alpha,h}, \mathbf{v}\right)_{\Omega_i} = (p^n_{\alpha,h}, \nabla \cdot \mathbf{v})_{\Omega_i} - \left\langle p^n_{\alpha,H}, \mathbf{v}\cdot\mathbf{n}_i\right\rangle_{\Gamma_i} + (\rho^n_{\alpha,h} g \nabla D, \mathbf{v})_{\Omega_i}, \quad \mathbf{v} \in \mathbf{V}_{h,i}$$

$$(\mathbf{u}^n_{\alpha,h}, \tilde{\mathbf{v}})_{\Omega_i} = (k^n_{r\alpha,h}\tilde{\mathbf{u}}^n_{\alpha,h}, \tilde{\mathbf{v}})_{\Omega_i}, \quad \tilde{\mathbf{v}} \in \tilde{\mathbf{V}}_{h,i}$$

$$\left\langle \left[\mathbf{u}^n_{\alpha,h}\cdot\mathbf{n}\right]_{i,j}, \zeta\right\rangle_{\Gamma_{i,j}} = 0, \quad \zeta \in M_{H,i,j}$$

Reduction to an Interface Problem

Let $\mathbf{M}_H = M_H \times M_H$. Define

$$b^n(\psi,\eta) = \sum_{1\le i<j\le n_b} \sum_\alpha \int_{\Gamma_{i,j}} \left[\rho^n_{\alpha,h}\mathbf{u}^n_{\alpha,h}(\psi)\cdot\mathbf{n}\right]_{ij} \eta_\alpha \, ds,$$

where $\psi = (p^n_{w,H}, S^n_{w,H}) \in \mathbf{M}_H$, $\eta = (\eta_w, \eta_w) \in \mathbf{M}_H$

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

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

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

Interface problem is solved by “inexact Newton-GMRES” scheme

Reactive Species Transport

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

Phase-Summed Equations

Assume an equilibrium partitioning of species between phases:

$$c_{i\alpha} = \theta_{i\alpha} c_{i\alpha_0}$$

Sum over all phases for a given species:

$$\frac{\partial(\varphi_i^* c_{iw})}{\partial t} + \nabla \cdot (c_{iw}\mathbf{u}_i^* - \mathbf{D}_i^* \nabla c_{iw}) = r_i^*(\mathbf{c}_w)$$

$$\mathbf{D}_{iw} \nabla c_{iw} \cdot \mathbf{n} = 0$$

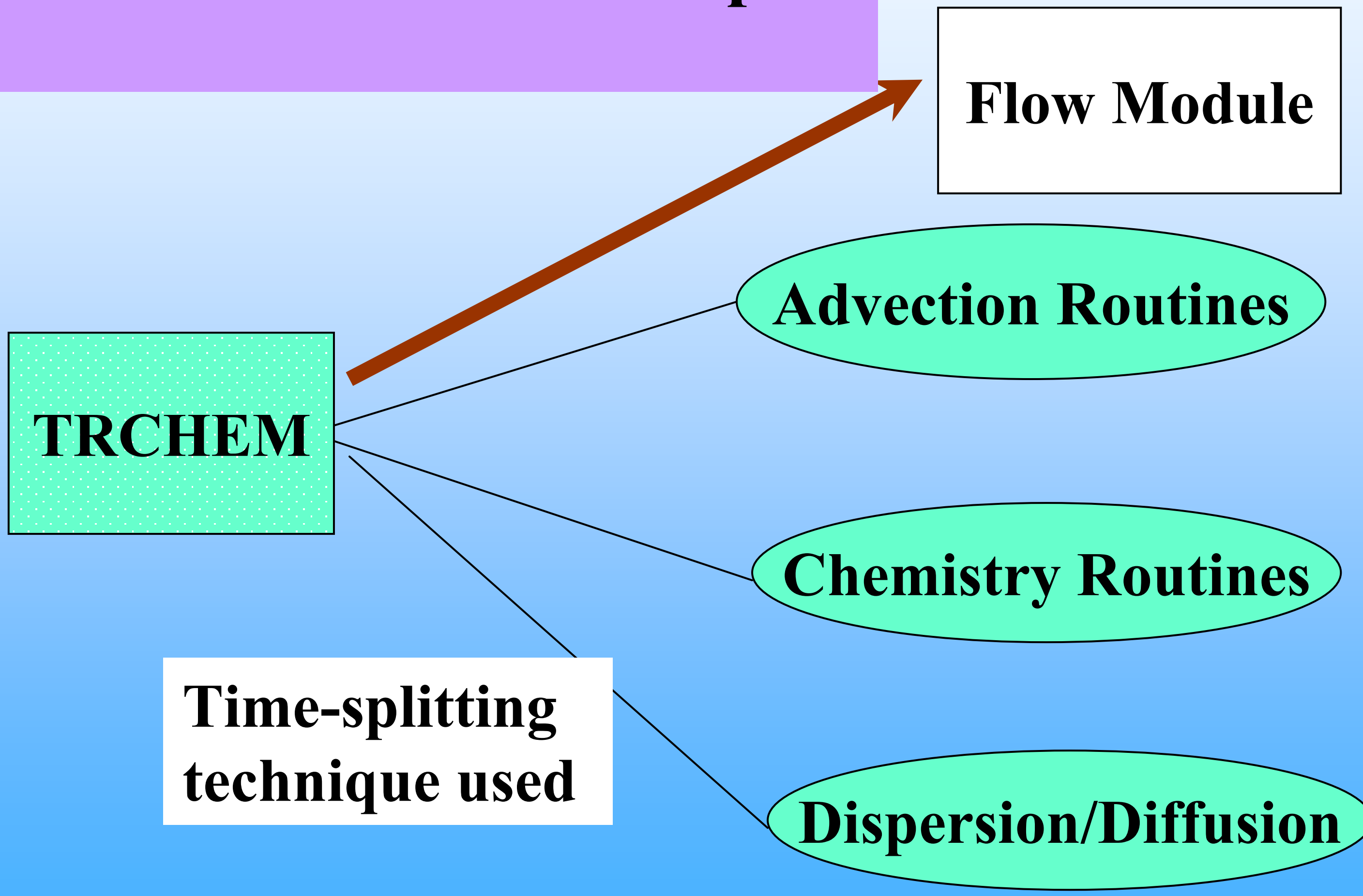
$$\varphi_i^* = \varphi \sum\nolimits_\alpha \theta_{i\alpha} S_\alpha \qquad u_i^* = \sum\nolimits_\alpha \theta_{i\alpha} \mathbf{u}_\alpha$$

$$\mathbf{D}_i^* = \varphi \sum\nolimits_\alpha S_\alpha \theta_{i\alpha} \mathbf{D}_{i\alpha} \qquad r_i^*(\mathbf{c}_w) = \varphi \sum\nolimits_\alpha r_{i\alpha}^C - r_{iR} + \sum\nolimits_\alpha q_{i\alpha}$$

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

IPARS-TRCHEM Structure

IPARS TRCHEM =
Flow and Reactive Transport



Advection

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

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

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

Chemical Reaction

Define $\Phi(t) \equiv \mathrm{diag}\{\varphi_i^*(t)\}, \quad \mathbf{T} = \mathbf{T}(t) \equiv \Phi(t)\mathbf{c}_w,$ 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

$$k_{1,i} = \Delta\tau^{m+1}\, r_i^{*,C}(\overline{\mathbf{T}})$$

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

$$\widehat{T}_i = \overline{T} + k_{2,i}$$

Diffusion-Dispersion

$$\frac{\partial(\varphi_i^* c_{iw})}{\partial t} - \nabla \cdot \mathbf{D}_i^* \nabla c_{iw} = 0$$

Solved fully-implicitly using Expanded MFEM with full-tensor

Introduce $\tilde{\mathbf{z}} = -\nabla c, \quad \mathbf{z} = \mathbf{D}_i^* \tilde{\mathbf{z}}$

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:

$$\left(\frac{\varphi_i^{*,m+1} c_{h,iw}^{m+1} - \widehat{T}_i}{\Delta\tau^{m+1}}, w \right)_{\Omega_j} + \left(\nabla \cdot \mathbf{z}_{h,iw}^{m+1}, w \right)_{\Omega_j} = 0, w \in W_{h,j}$$

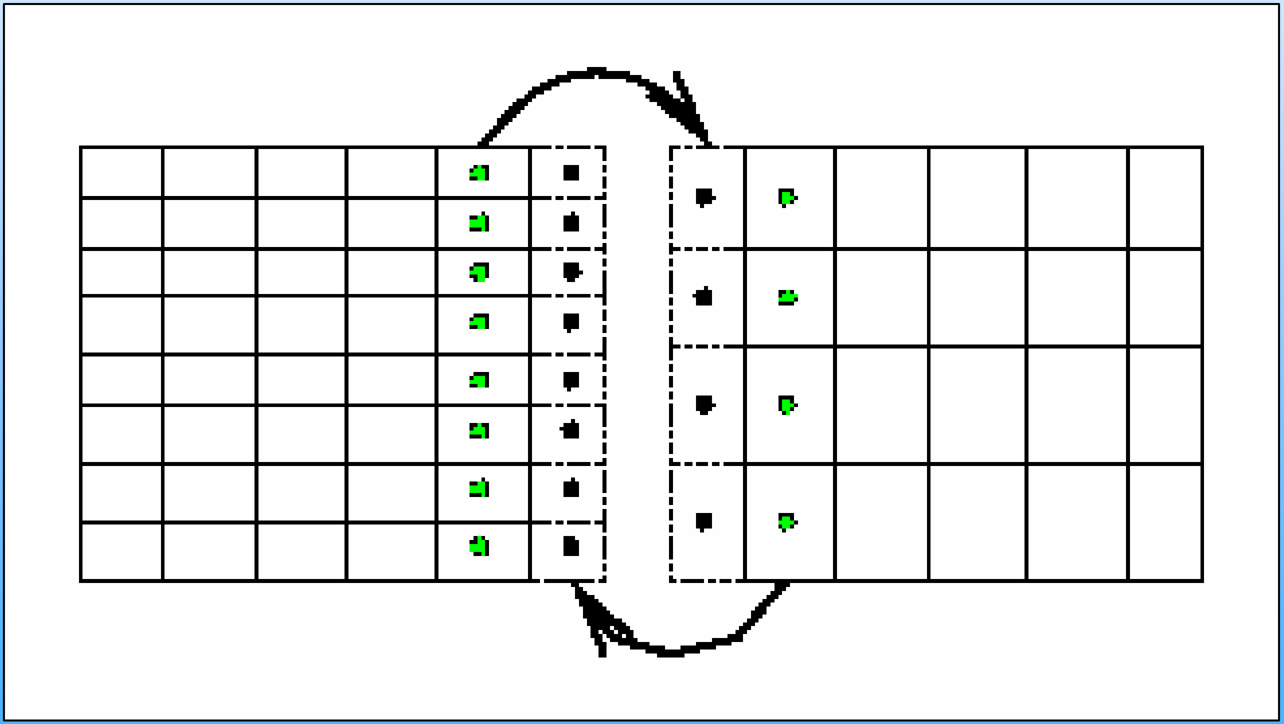
$$(\tilde{\mathbf{z}}_{h,iw}^{m+1}, \mathbf{v})_{\Omega_j} = (c_{h,iw}^{m+1}, \nabla \cdot \mathbf{v})_{\Omega_j} - \left\langle \mathcal{P}_j c_{h,iw}, \mathbf{v} \cdot \mathbf{n}_j \right\rangle_{\Gamma_j}, \mathbf{v} \in \mathbf{V}_{h,j}$$

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

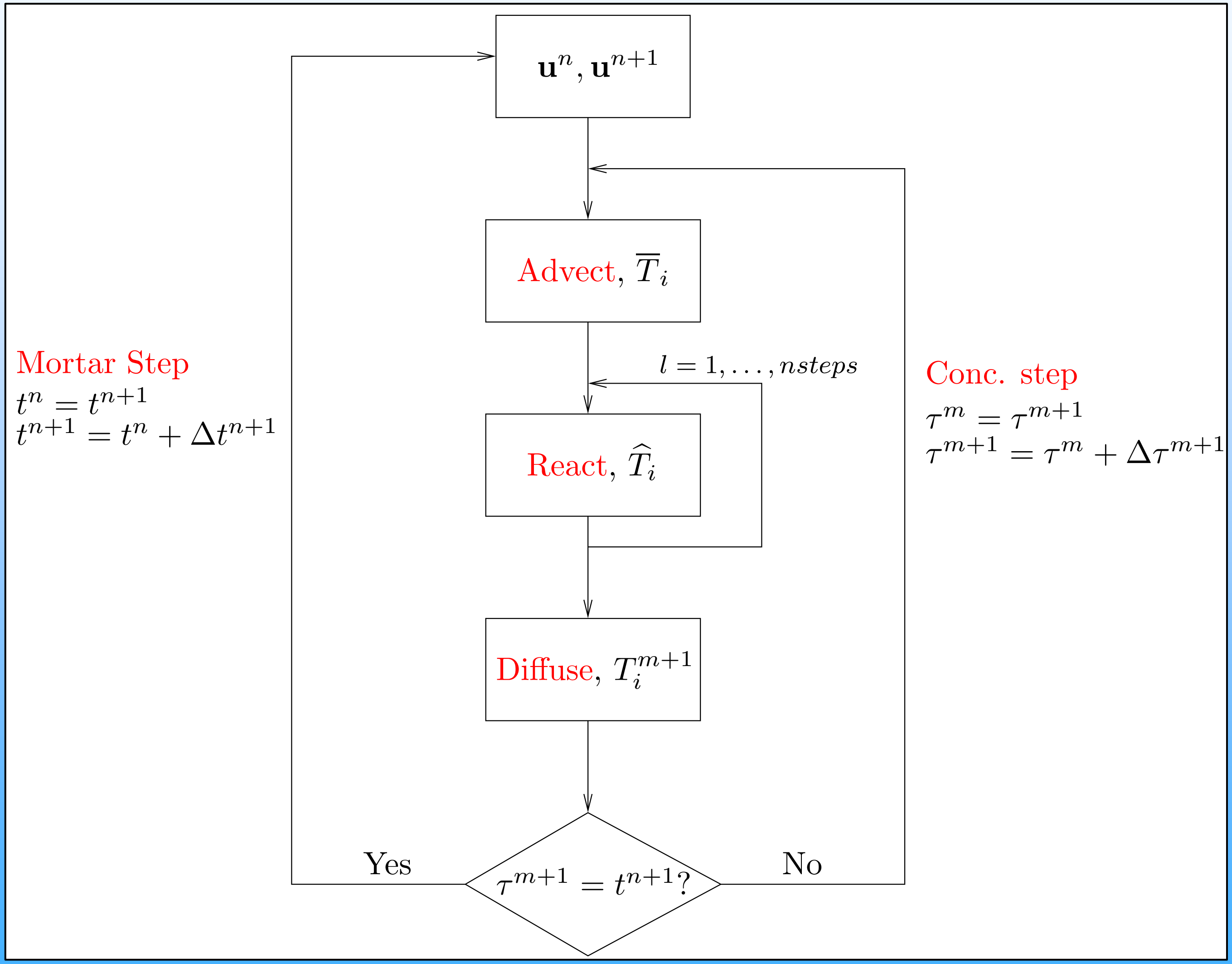
Accounting for Non-matching grids in Transport Problem

$\mathcal{P}_j : L^2(\Gamma_j) \to L^2(\Gamma_k)$ is an L^2-orthogonal proj. s.t. $\forall \phi \in L^2(\Gamma_j)$

$$\langle \phi - \mathcal{P}_j \phi, \mathbf{v} \cdot \mathbf{n}_j \rangle_{\Gamma_{k,j}} = 0, \ \forall \mathbf{v} \in \mathbf{V}_{h,i}, \forall k \text{ such that } \overline{\Omega}_k \cap \overline{\Omega}_j \neq \emptyset$$



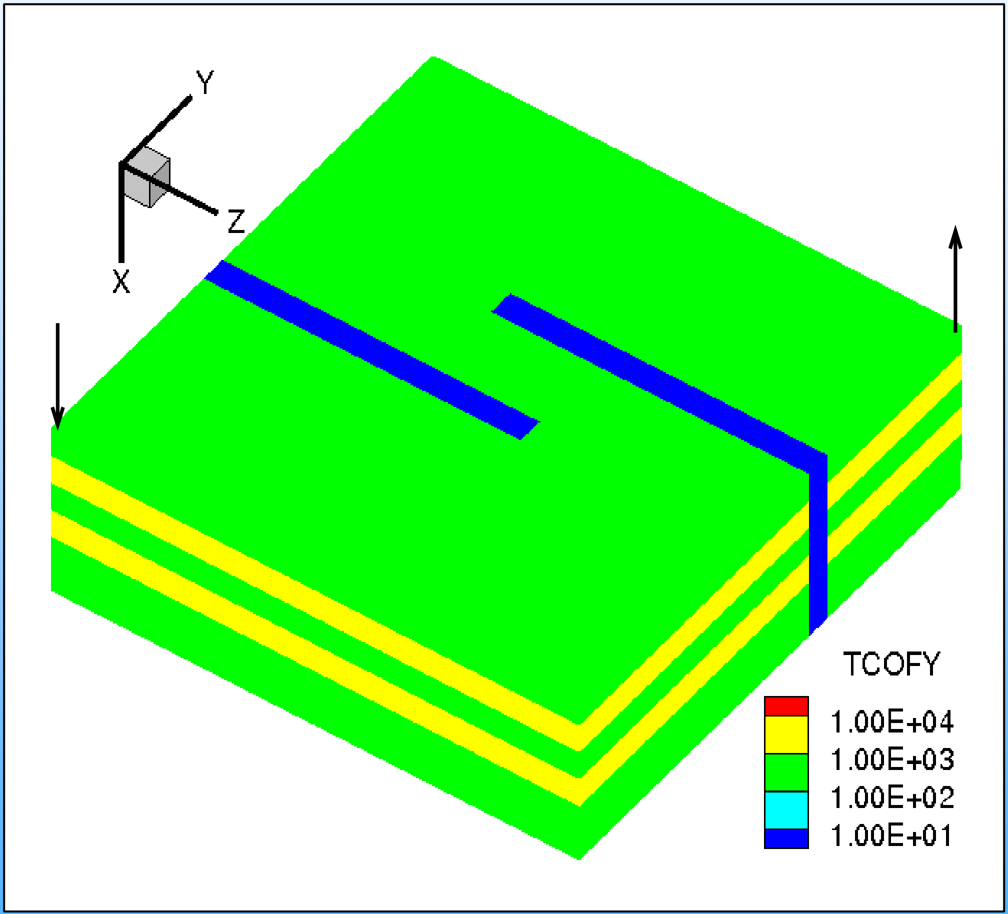
Algorithm



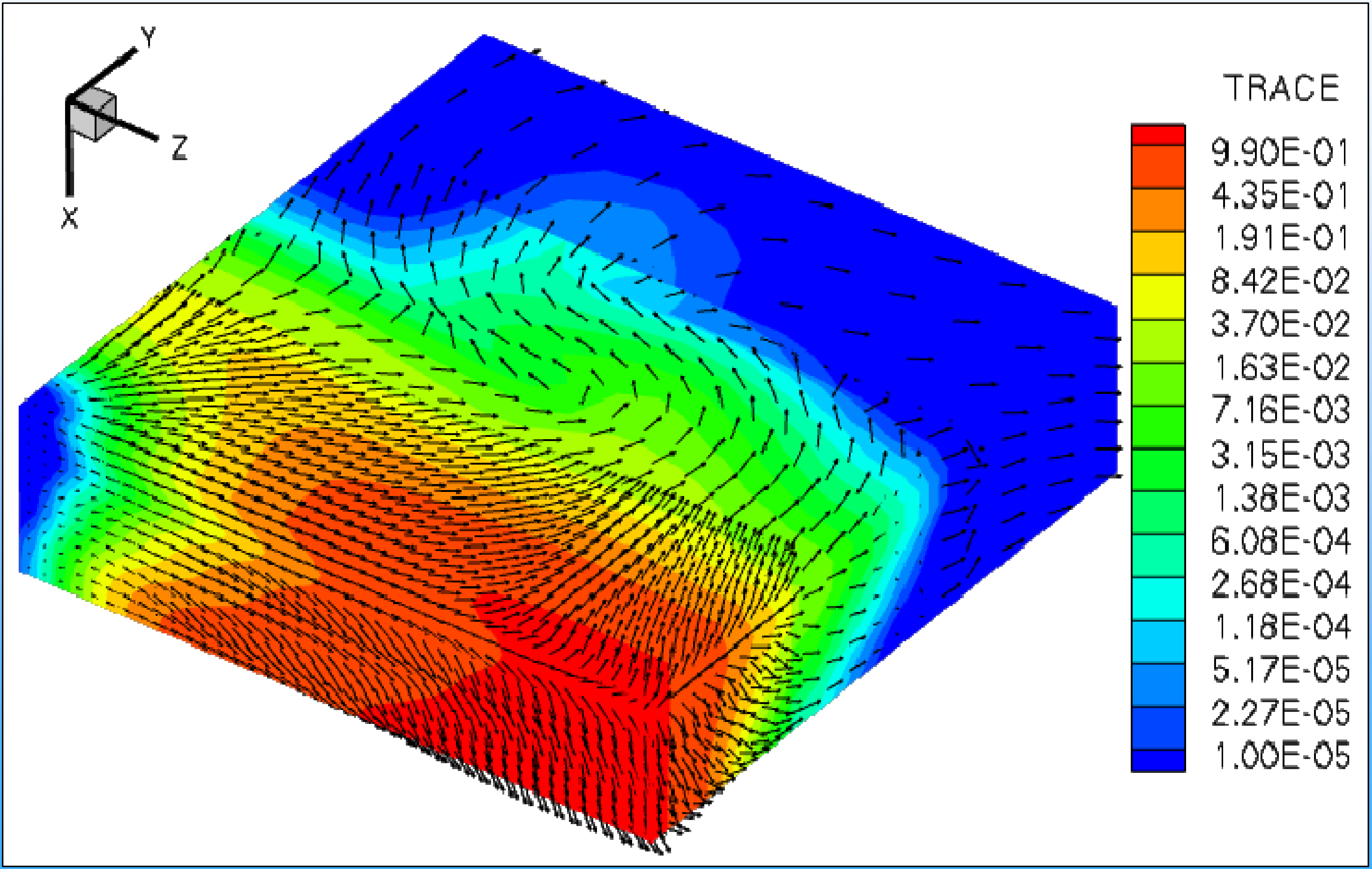
$\mathbf{u}^n, \mathbf{u}^{n+1}$
Advect, $\overline{T}_i$
$l = 1, \ldots, nsteps$
React, $\widehat{T}_i$
Diffuse, T_i^{m+1}
$\tau^{m+1} = t^{n+1}?$
Yes
No
Mortar Step
$t^n = t^{n+1}$
$t^{n+1} = t^n + \Delta t^{n+1}$
Conc. step
$\tau^m = \tau^{m+1}$
$\tau^{m+1} = \tau^m + \Delta \tau^{m+1}$

NAPL Remediation

- Bio-remediation of NAPL using microbes
- Advection-Diffusion-Reaction
- Discontinuous permeability field with barriers
- Two flowing phases - quarter-five spot
- External BC: no-flow and zero diffusive flux
- IC: NAPL, microbes occupy $0 < y < 40$ ft and O_2, N_2 occupy $40 < y < 400$ ft.
- Domain: 20 ft x 400 ft x 400 ft
- Reference case: NX=20, NY=40, NZ=40

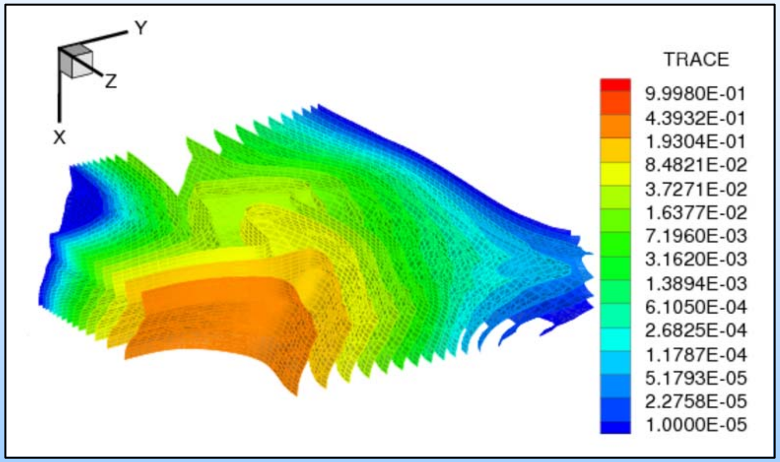


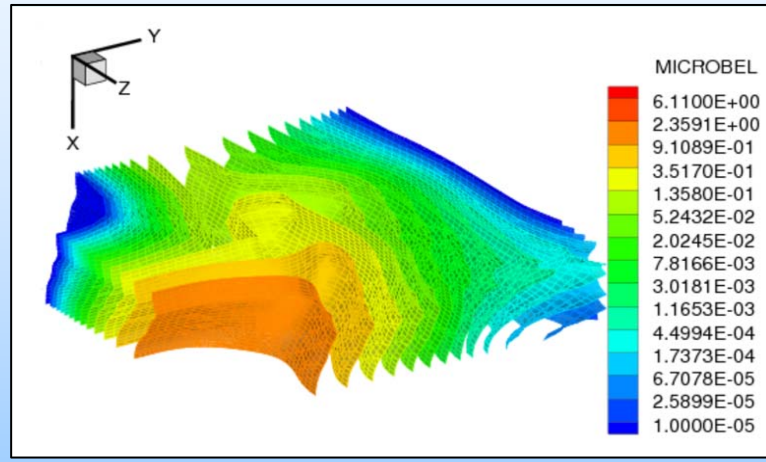
Flow Pattern in Multi-block

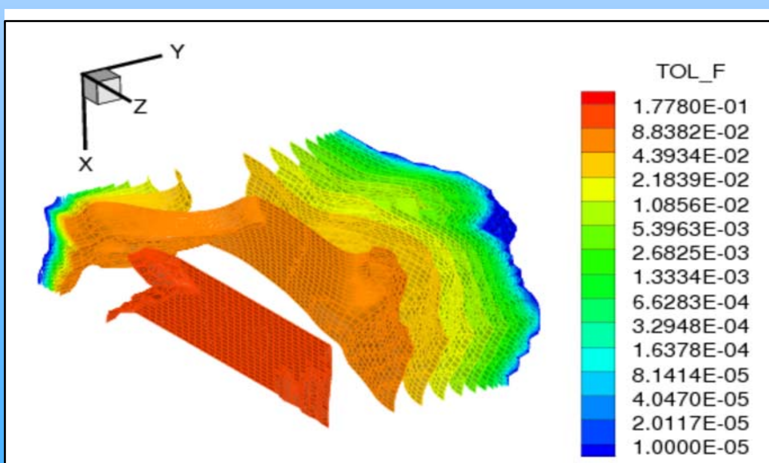


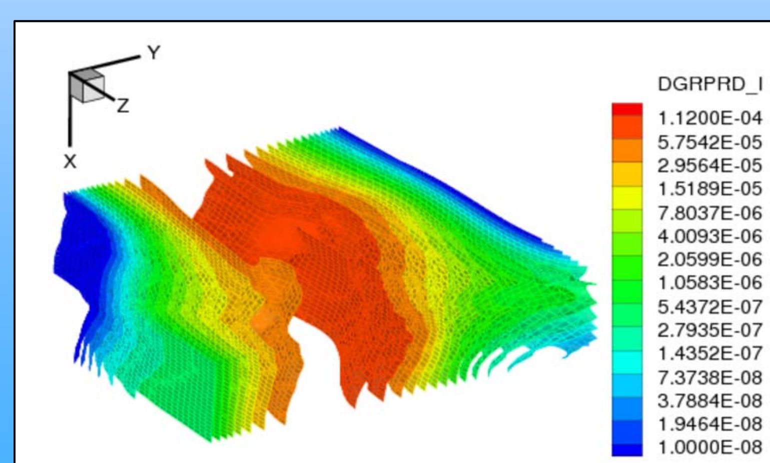
Reference Solution

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



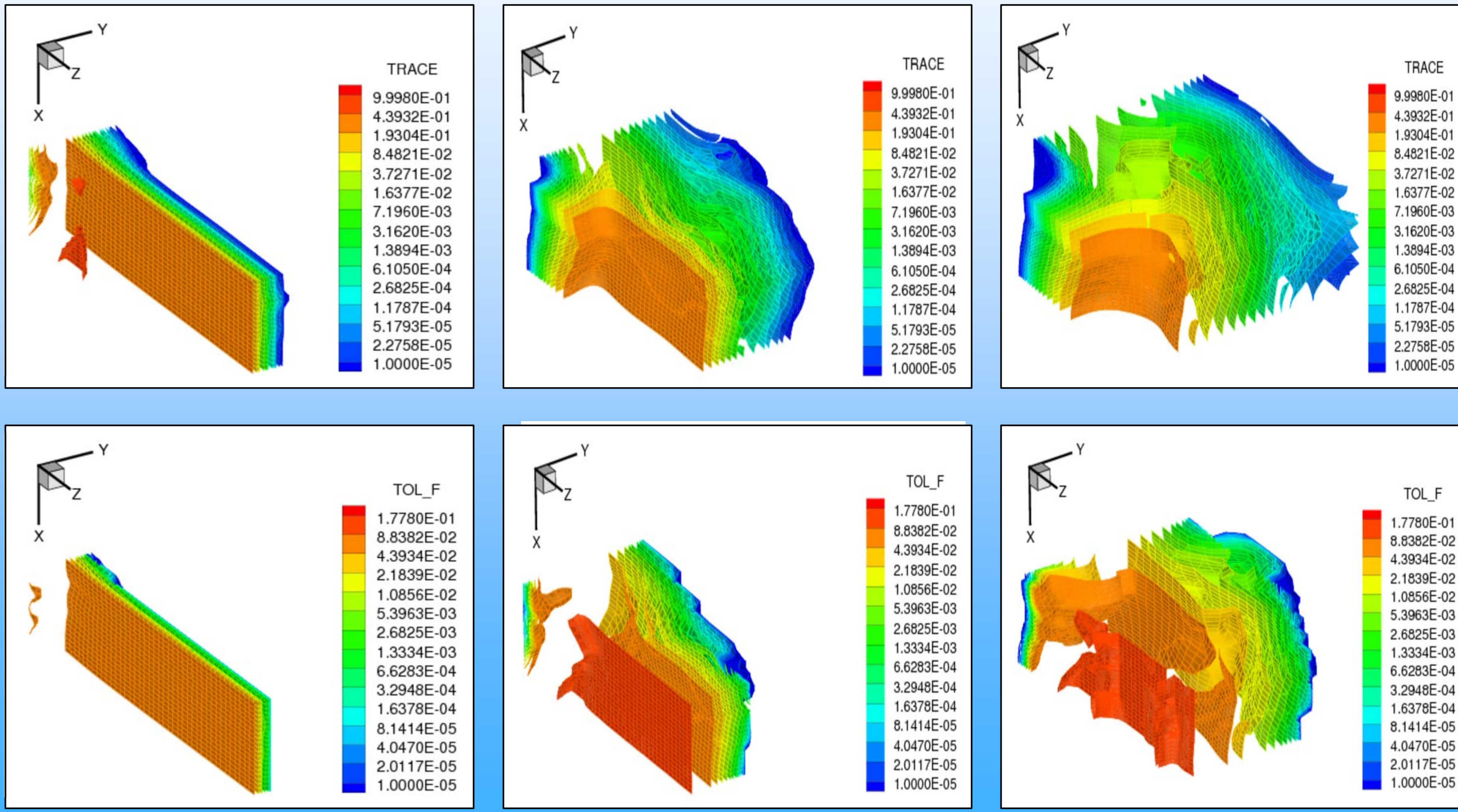






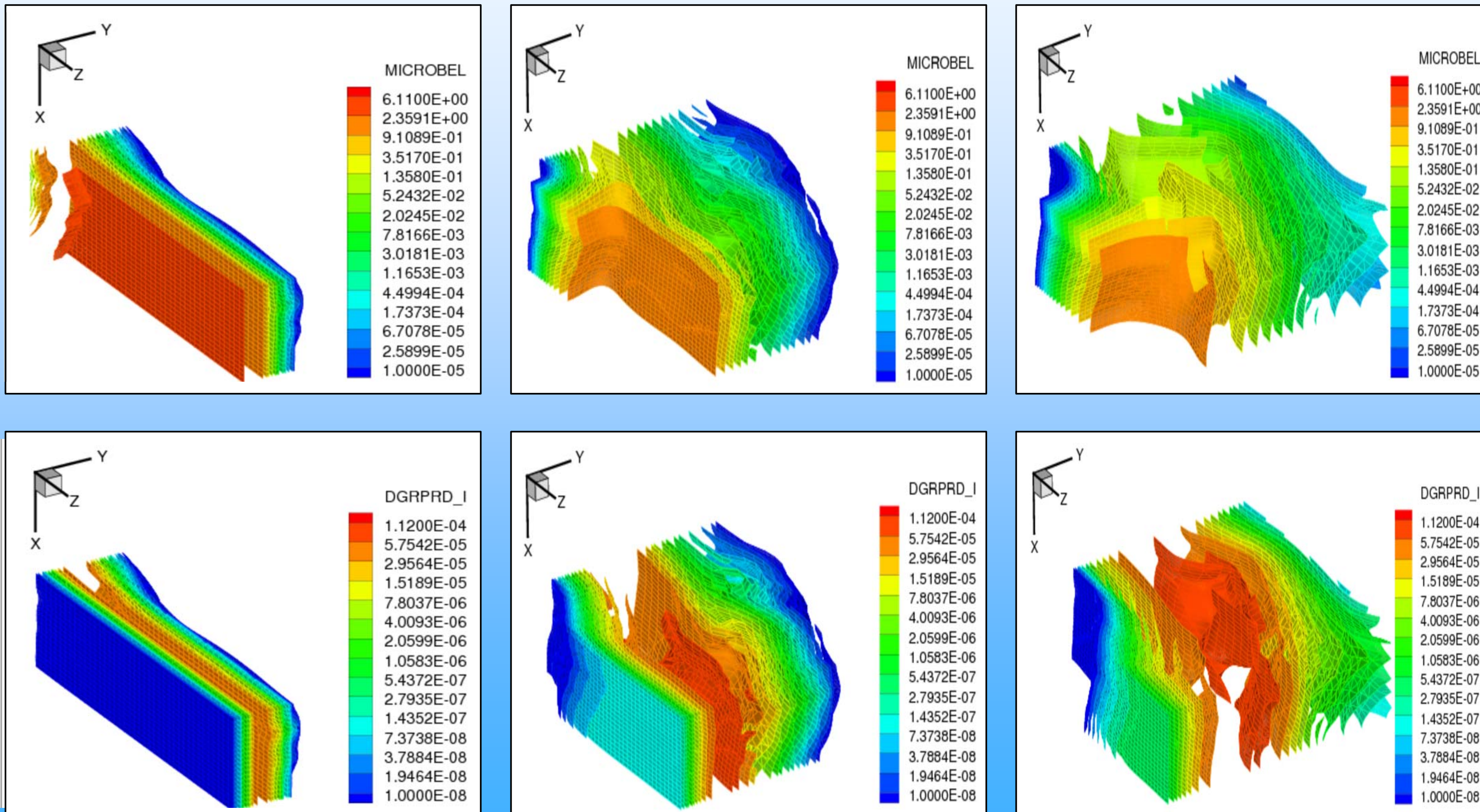
Comparison to Mortar Scheme

Tracer & NAPL concentrations at 5, 50, 100 days



Comparison to Mortar Scheme, cont'd

Microbe & product concentrations at 5, 50, 100 days



HOG for Species Advection

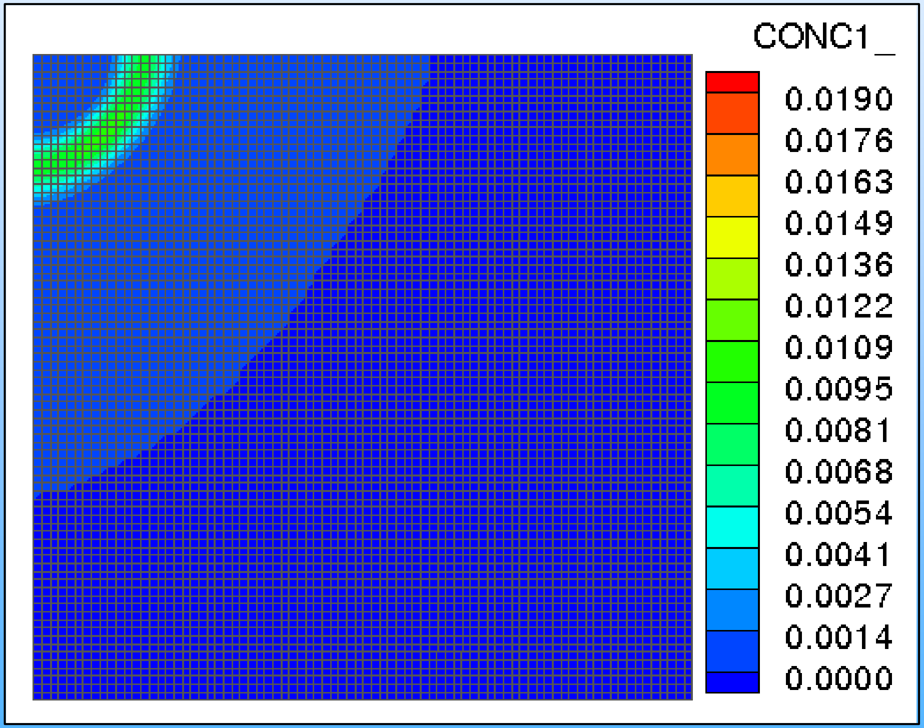
- Consider a single species advection in single phase flow.

- Problem Description:
  - Grid: 3d, 80 x 80 x 4 (elements: 5ft cubes)
  - Initial concentration of species = 1 lbM/cu-ft at location (1,1,1)
  - Two wells in a quarter-five spot pattern, (pressure specified), causing a radial flow for species.

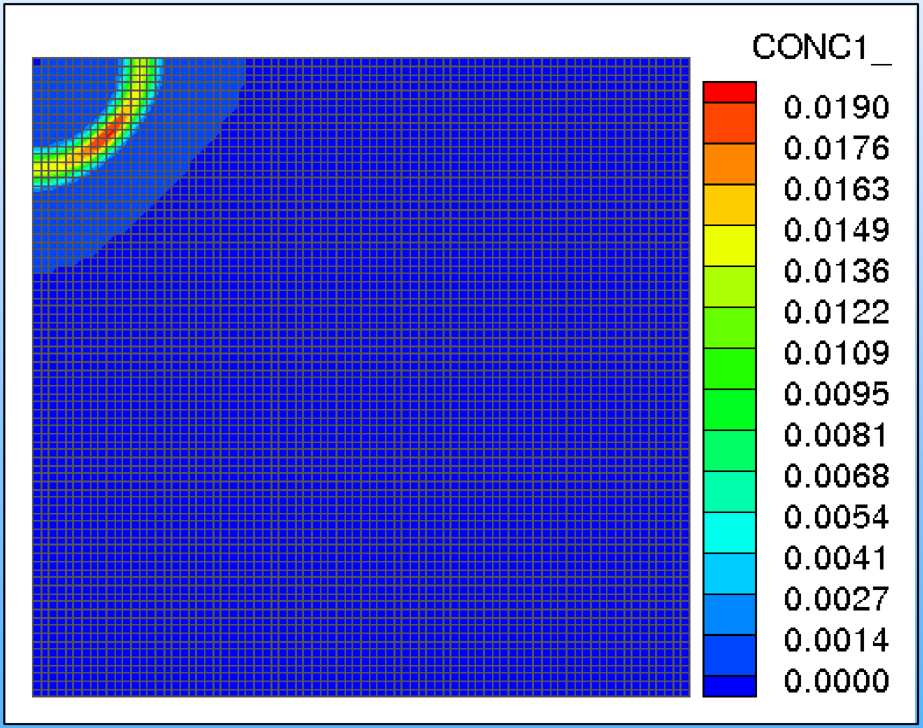
HOG for Species Advection

Solution shows species concentration at 15 days

First Order Godunov



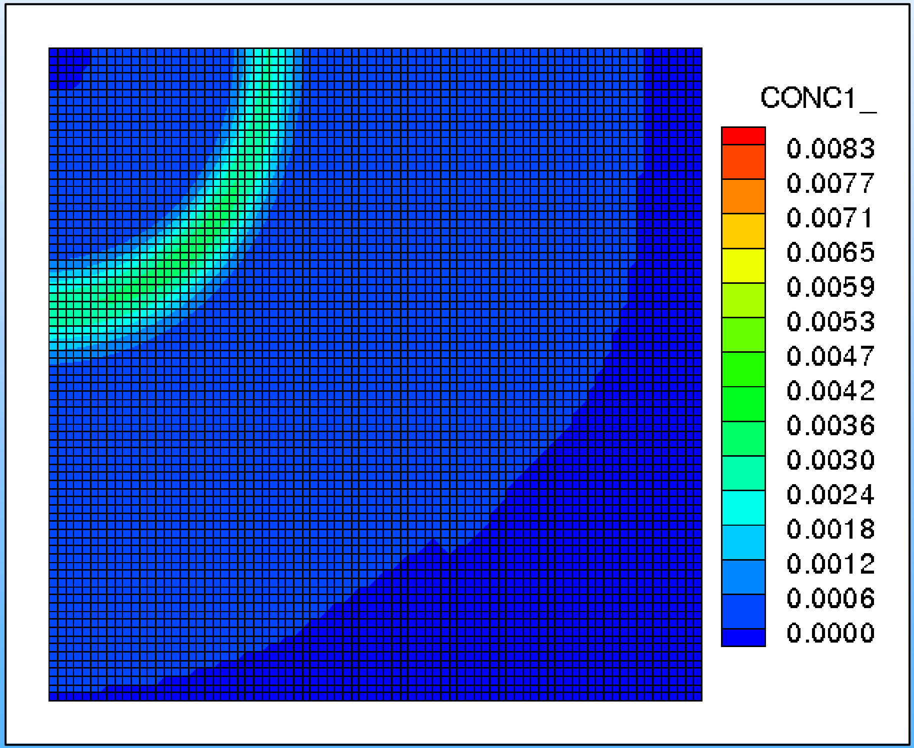
Higher Order Godunov



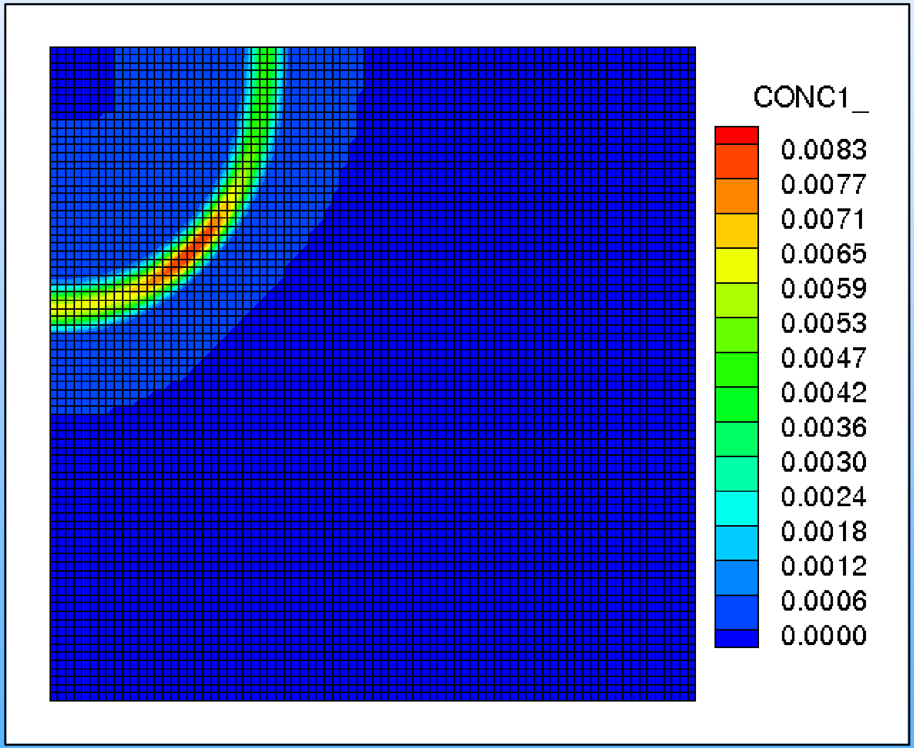
HOG for Species Advection

Solution shows species concentration at 40 days

First Order Godunov



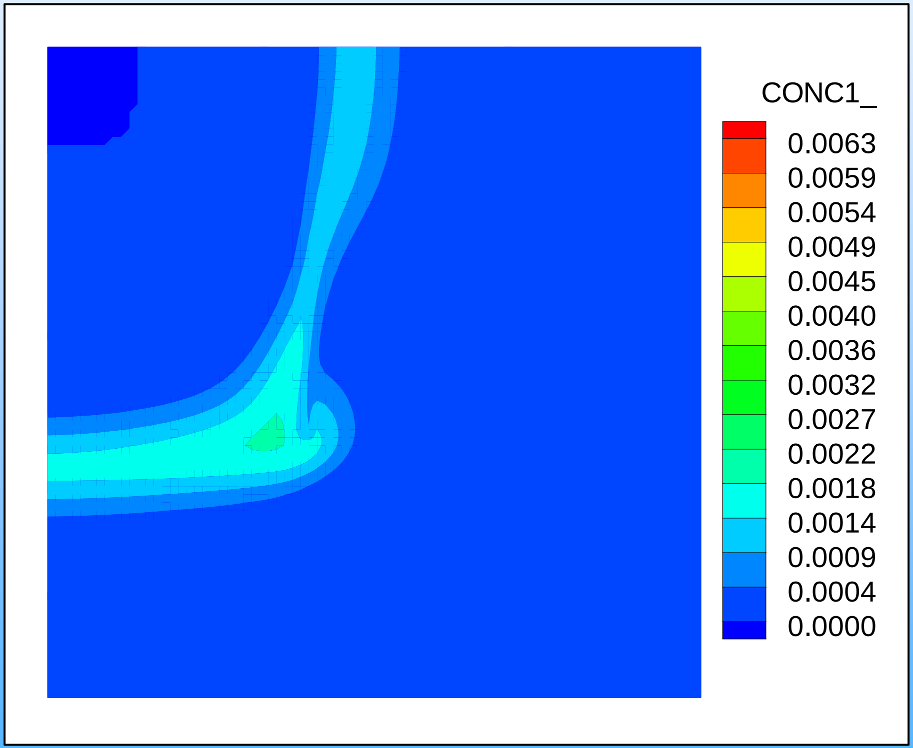
Higher Order Godunov



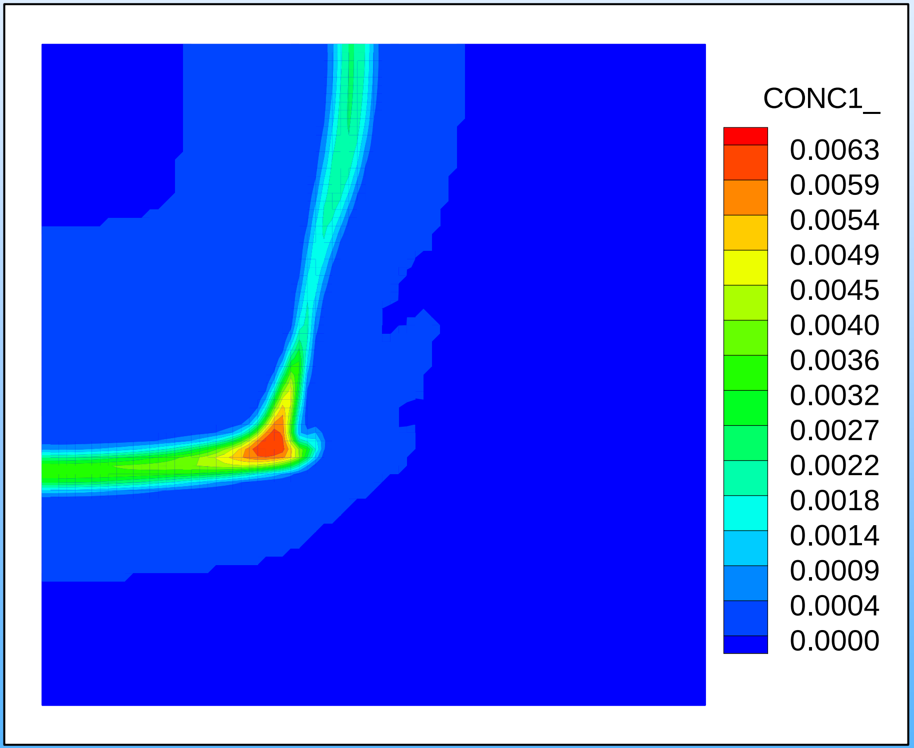
HOG for Species Advection

Solution shows species concentration at 80 days

First Order Godunov



Higher Order Godunov



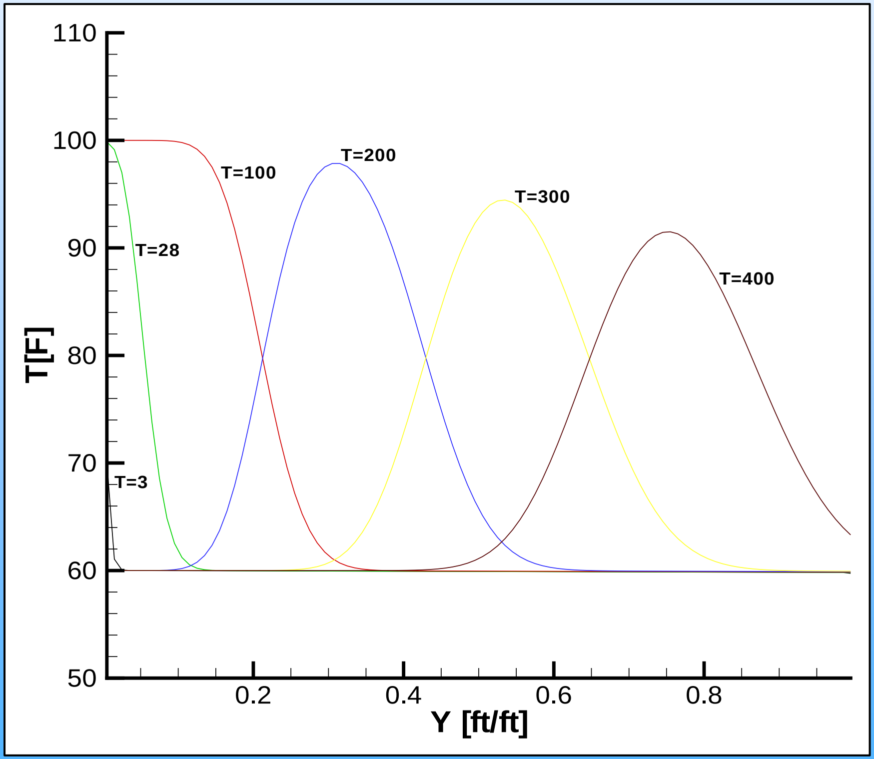
Higher Order Godunov (HOG)

- Consider a 1-d thermal advection in single phase flow to validate the implementation of the HOG scheme.
- Problem Description:
  - Initial reservoir temperature, 60^{o} F
  - Hot water injected at 100^{o} F for 100 days
  - After 100 days, water injected at 60 F (original temperature of reservoir)
  - Simulation time: 400 days
  - Purely hyperbolic problem (pulse solution).

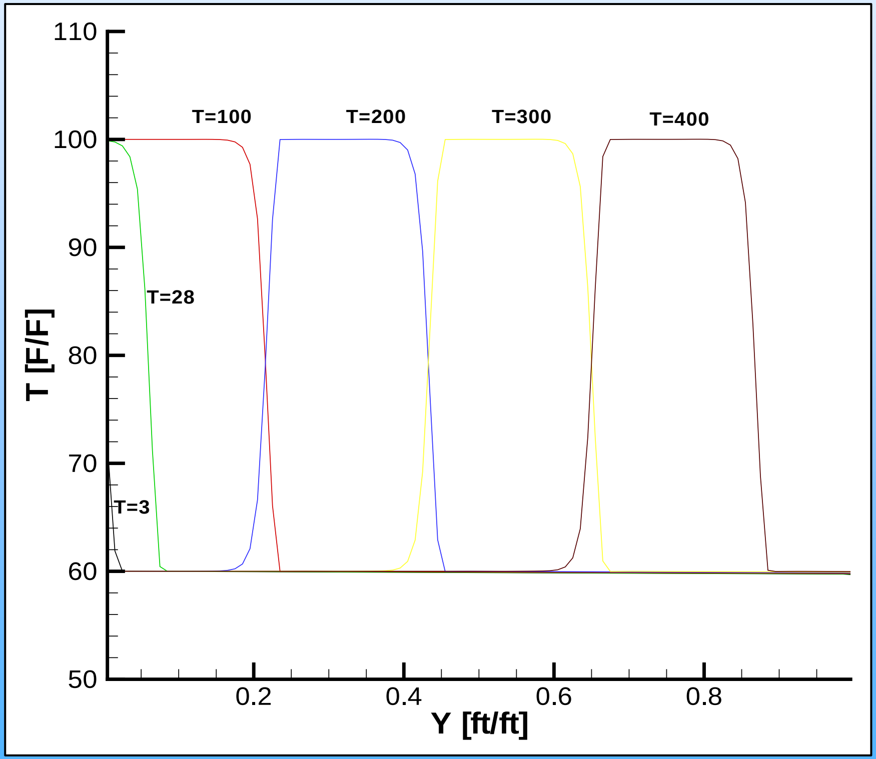
HOG for Thermal Advection

Snapshots at t = 3, 28, 100, 200, 300 and 400 days

First Order Godunov



Higher Order Godunov



Multinumeric Extensions

- 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

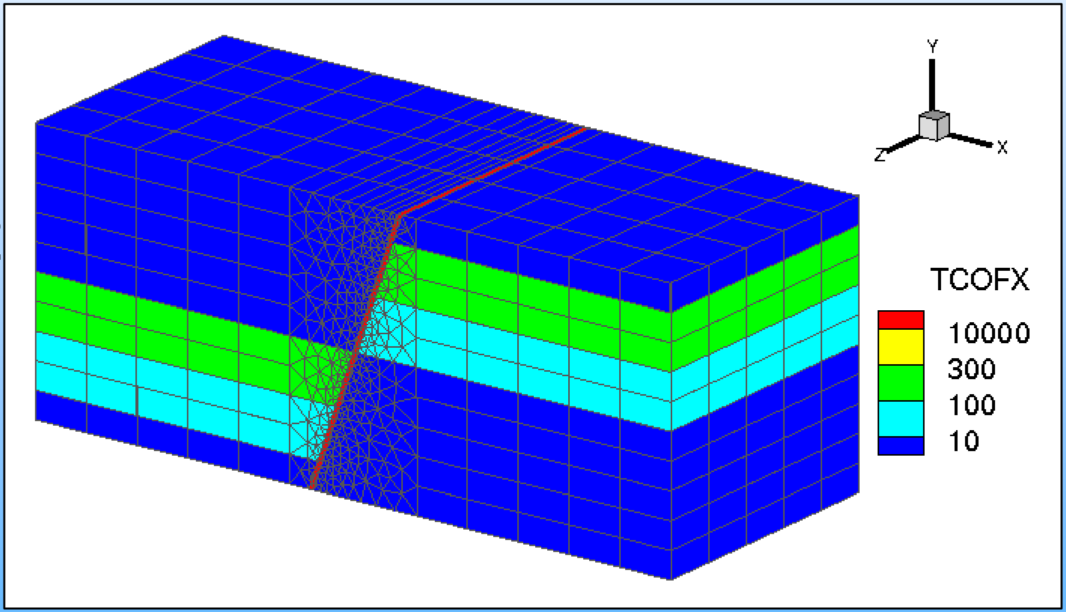
DG-MFEM, 3 blocks with a fault

- 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:

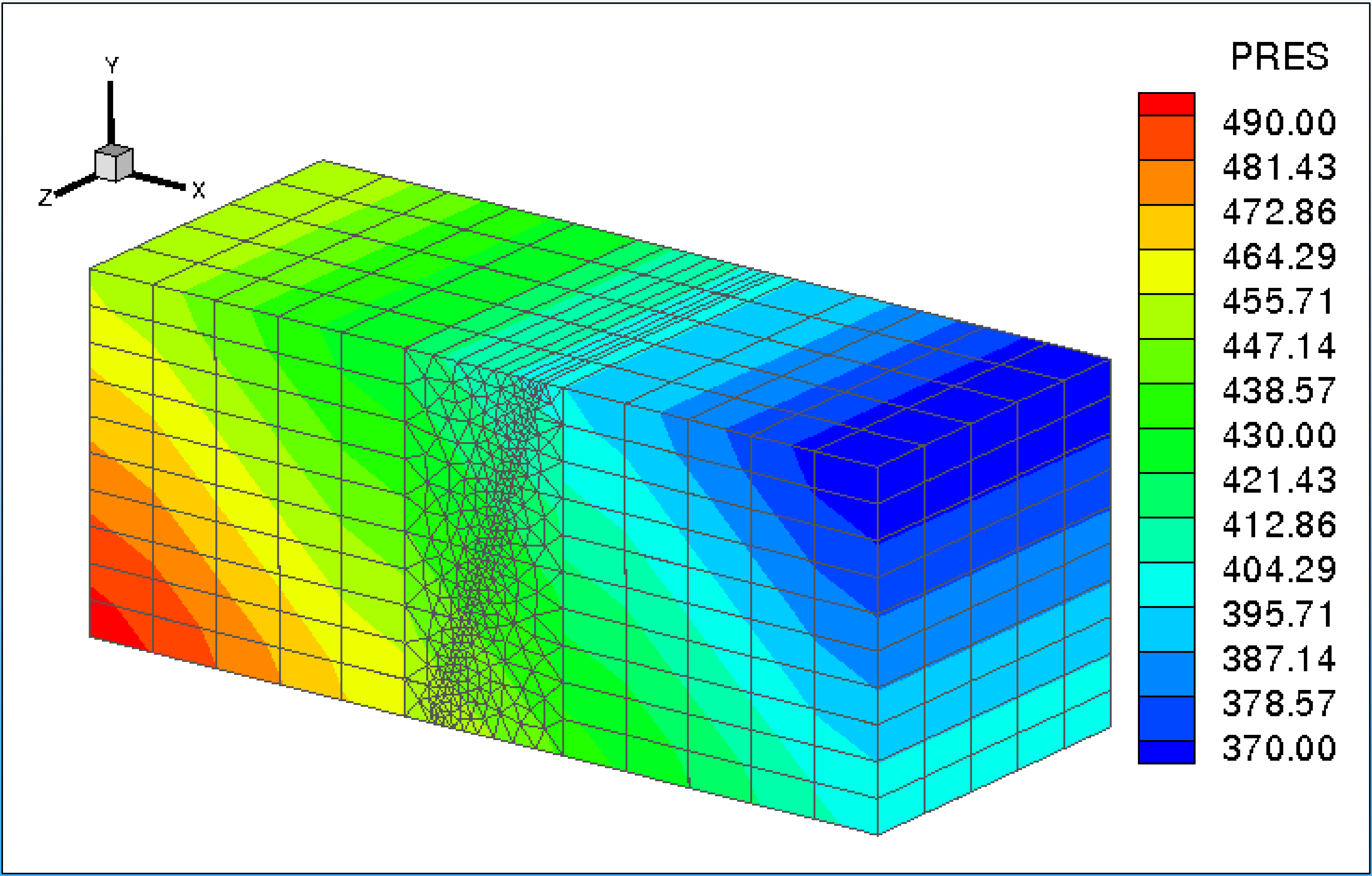
  500 psi at x=0

  400 psi at x=250,

  noflow o.w.
- r=2, k=0 (RT0), m=0

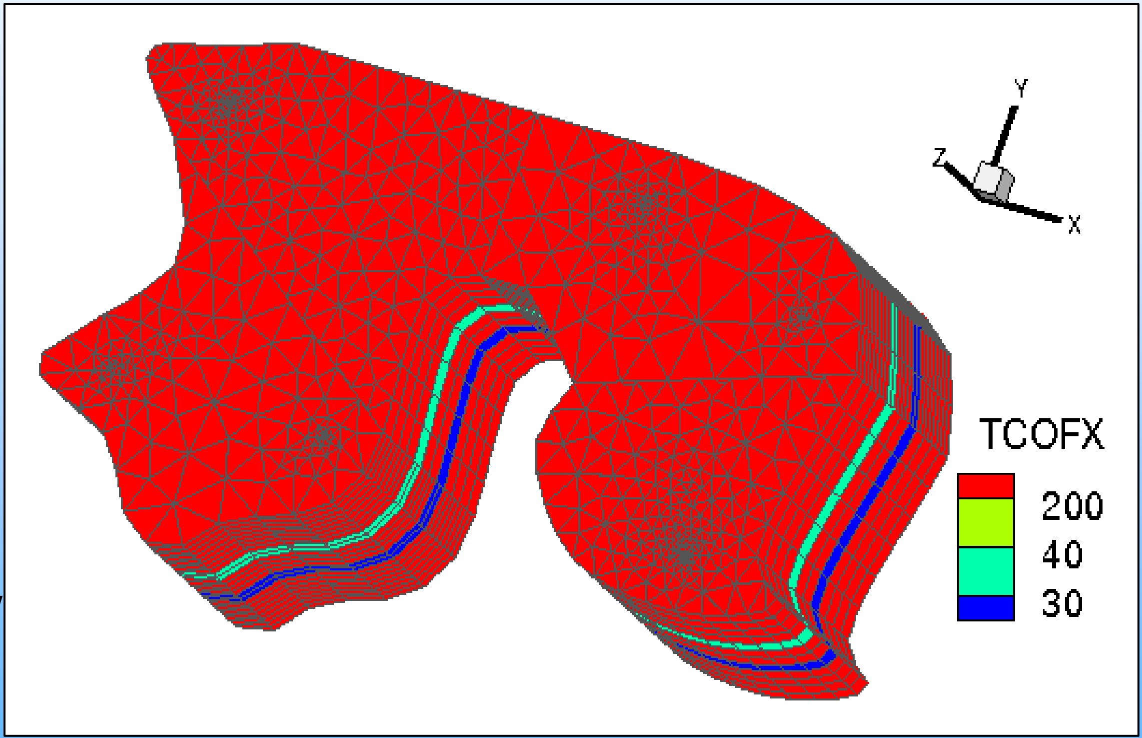


3 blocks with a fault : Solution

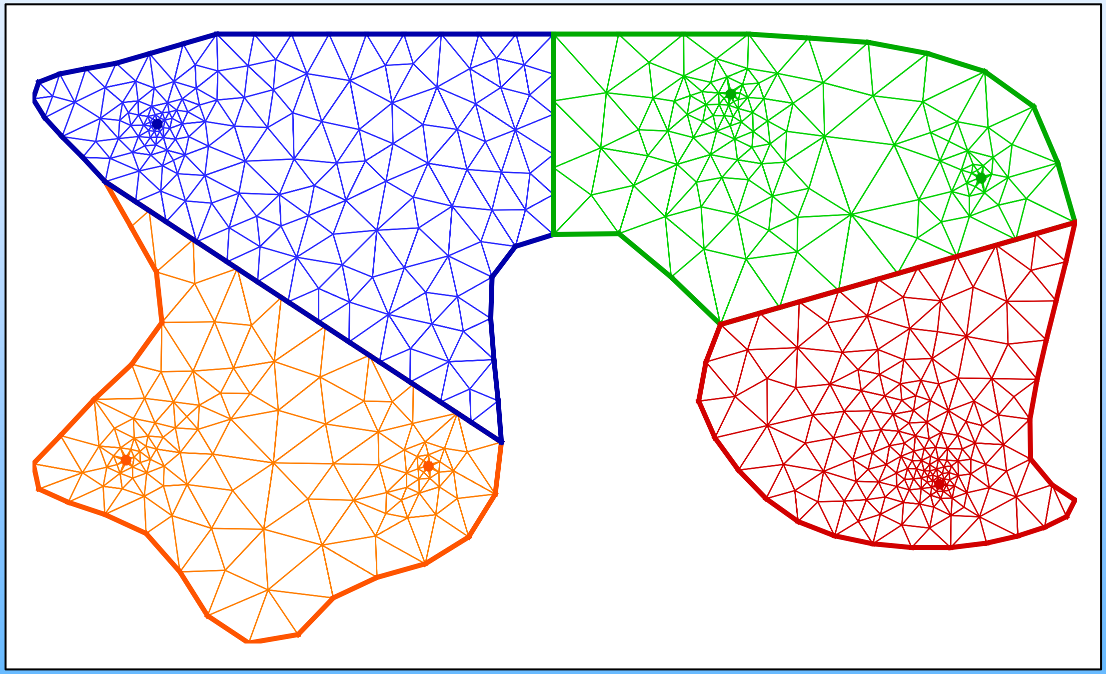


DG-DG, Oxbow problem

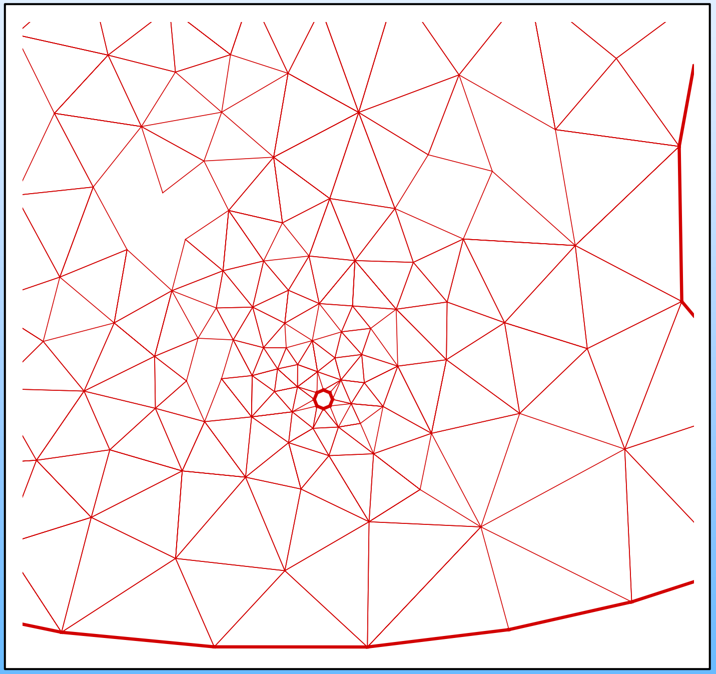
- 4 blocks with 6 wells
- 900 x 500 x 24 ft
- 1 production, 5 injection wells
- K_{xx} = K_{yy}={200,30,40}, K_{zz}={25,5,3}, ϕ={0.22,0.08,0.09}
- BC: P_{inj} = 700 psi, P_{prod} = 500 psi, noflow on the outer bdry
- nonmatching grids, r=2, m=1



Unstructured Mesh

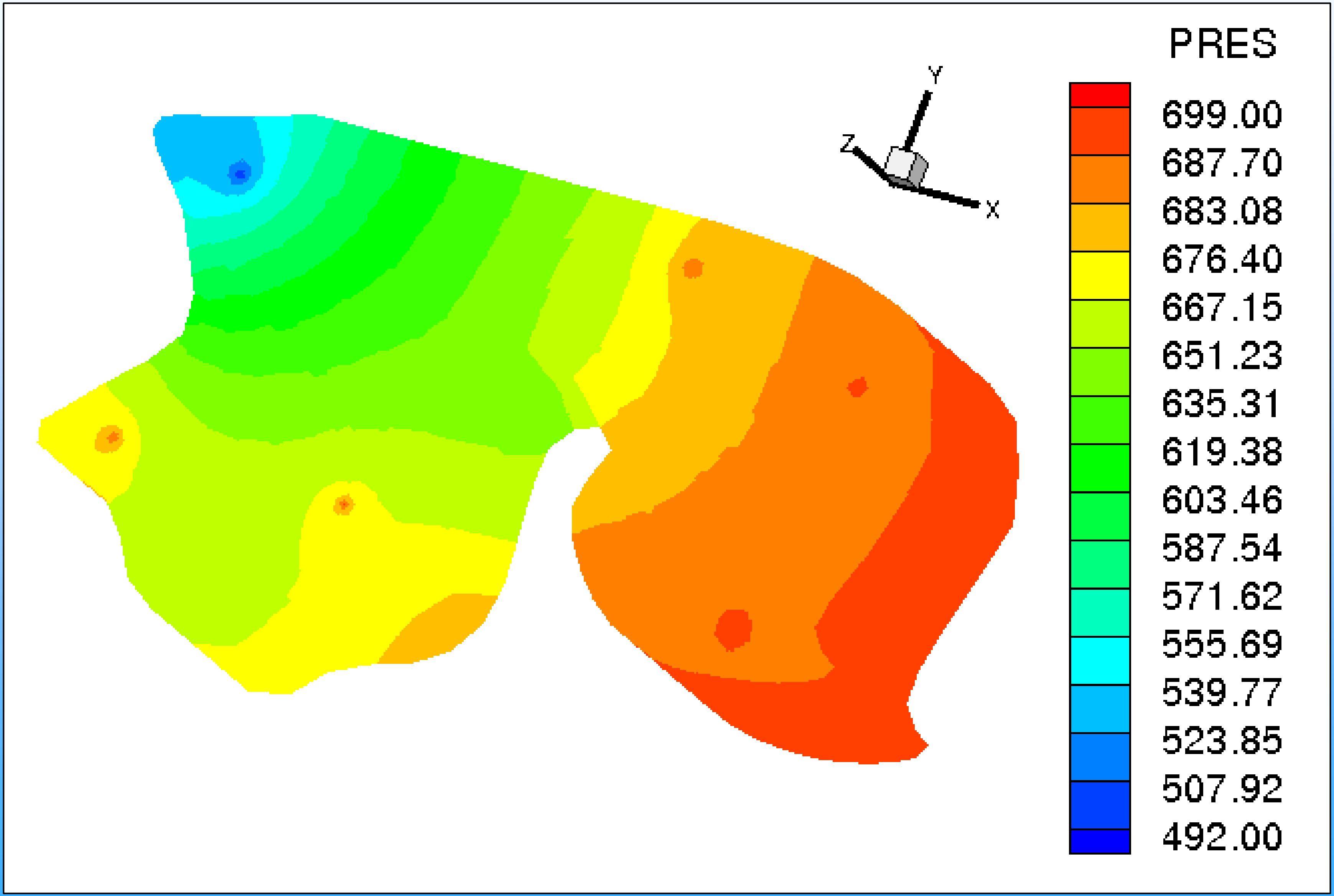


Top view, 4 blocks



Magnified grid around well

Oxbow problem: Solution



Conclusions

- Fully implicit multiscale method (MMFE) for multiphase flow that is coupled to a mixed/Godunov method for advection-diffusion-reaction problems on non-matching grids, has been defined
- Variably refined sub-domains results in significant savings in computational time (1 domain with fine grid takes twice the time as 3 domains)
- Multiblock domain solution agrees very well with single-domain fine-everywhere

Current and Future Work

- Explore enhanced ``velocity'' method for diffusion-dispersion and dynamic load balancing for treating reactions in parallel computations
- Theoretical extensions of the Dawson & Wheeler paper on operator-splitting methods for advection-diffusion-reaction are being investigated for these problems
- 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)