Computational Issues in Oil Field Applications:

Methodologies and Robust Algorithms for Subsurface Simulators

Workshop I:
Multiphysics, Multiscale, and Coupled Problems in Subsurface Physics

Mary F. Wheeler
## Acknowledge

### Collaborators

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<thead>
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</thead>
<tbody>
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</tr>
</tbody>
</table>
Research Initiative: Closed-loop Workflow

I. FLUID-DRIVEN FRACTURE PROPAGATION

II. PHASE & CHEMICAL EQUILIBRIUM

- Gas Phase: CO₂, 4C₄H₁₀, & H₂O
- Oleic Phase: CO₂, 4C₄H₁₀, & H₂O
- Aqueous Phase: CO₂, CO₃²⁻, HCO₃⁻, Cl⁻, CaCO₃, H⁺, OH⁻, & H₂O
- Solid Phase: CaCO₃

III. SIMULATOR DEVELOPMENT

IV. UNCERTAINTY QUANTIFICATION

- Geomechanical Tools for Secure CO₂ Storage
  - Interfacial I/O Visualization
  - Solvers
  - Geomechanical Reaction
  - Mobility Control
  - Geomechanics
  - Compositional Kn/Ps
  - Hydrogen Kn/Ps
  - Parameter Estimation
  - Uncertainty Quantification

- History matching and Prediction
- Wall bottom-hole pressure (kPa)

- Time (days): 0, 200, 400, 600, 800, 1000, 1200
V. BIG DATA: Cross-cutting Initiative
I. FLUID-DRIVEN FRACTURE PROPAGATION

Objectives

Develop a fracture propagation method (phase field) driven by multiphysics, multiphase fluid flow

Three dimensional computations using mesh adaptivity with coupling displacements, phase field, and pressure system

In the phase field fracture propagation model, primal-dual active set & fixed-stress iteration is coupled to solve the whole system

Demonstrate the potential of the phase field for treating practical engineering applications by providing numerical examples

Joining and branching of non-planar hydraulic fractures in 3D heterogeneous media.
Advantage of Phase Field Model

- Classical theory of crack propagation [Griffith 1921]
- Diffusive crack zones for free discontinuity problems
- \(\Gamma\)-Convergent approximation [Ambrosio-Tortorelli 1992]
- Variational methods based on energy minimization
  [Francfort-Marigo 2003], [Miehe et al. 2010]

Variation methods based energy minimization

[Real fractures] [Interface approach] [Diffusive approach using Phase field]
Advantage of Phase Field Model

- Fixed-topology approach avoiding re-meshing
- Determine crack nucleation, propagation, and the path automatically
- Simple to handle joining and branching of (multiple) cracks
- Promising findings for future ideas as an indicator function based on theory and numerical simulations
# Governing System: Biot’s System

## Biot’s system

<table>
<thead>
<tr>
<th>Fracture with maximum pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>- The pressure starts to decrease when the fracture starts to propagate.</td>
</tr>
</tbody>
</table>

### Pressure Diffraction System

\[
\rho_R \partial_t \left( \frac{1}{M} p_R + \alpha \nabla \cdot u \right) - \nabla \cdot \frac{K_R \rho_R}{\eta_R} (\nabla p_R - \rho_R g) = q_R \quad \text{in} \quad \Omega_R(t) \times (0,T) \\
\rho_F \partial_t \left( \frac{c_F}{\eta_F} p_F \right) - \nabla \cdot \frac{K_F \rho_F}{\eta_F} (\nabla p_F - \rho_F g) = q_F - q_L \quad \text{in} \quad \Omega_F(t) \times (0,T) \\
[p_j] = 0 \quad \text{on} \quad \Gamma(t) \times (0,T) \\
[K_j (\nabla p_j - \rho_j g)] \cdot n = 0 \quad \text{on} \quad \Gamma(t) \times (0,T)
\]

### Mechanics and Phase Field

\[
E_e(u, p, \phi) = \int_\Lambda \frac{1}{2}((1 - k)\phi^2 + k) G e(u) : e(u) \, dx - \int_{\partial\Lambda} \tau \cdot u \, dS \\
- \int_\Lambda (\alpha - 1)\phi^2 \text{div} \, u \, dx + \int_\Lambda (\phi^2 \nabla p) u \, dx + G_c \int_\Lambda \left( \frac{1}{2\varepsilon^2} (1 - \phi^2) + \frac{\varepsilon}{2} |\nabla \phi|^2 \right) \, dx
\]

### Linear Elasticity

### Newton Iteration

### Primal-dual Active Set Method

---

[Heister-W.Wick 2015 CMAME]

[Lee-W.-Wick 2016 CMAME]
Numerical Examples of Phase Field

Multiple fractures propagating near wellbore [Lee-W.-Wick 2016]

- Fracture propagation
- Pressure distribution
Three parallel fractures in 3D domain [Lee-W.-Wick 2016]

- Not all fractures are growing due to stress-shadowed effects.
Numerical Examples of Phase Field

Multiple fractures in a 3D heterogeneous medium [Lee-W.-Wick 2015]

II. GEOCHEMICAL REACTIONS

Objectives

- Model geochemical reactions of injected CO$_2$ in carbonate reservoirs during EOR or CO$_2$ sequestration
- In situ brines with reactive ionic species
- Study the effect of reactive species on CO$_2$ concentration
- Quantify the effect using changes in miscibility conditions during CO$_2$ EOR

[Phase & Chemical Equilibrium of CO$_2$]
Coupled phase and chemical equilibrium

- Gibbs Free Energy Minimization
- Equation of State (EOS)

\[
\frac{\partial}{\partial t} \left( \sum_{j} S_{j} p_{j} x_{ij} \right) + \nabla \cdot \sum_{j} \left( \rho_{j} x_{ij} u_{j} - S_{j} D_{ij} \cdot \nabla \left( \rho_{j} x_{ij} \right) \right) = \sum_{j} \left( q_{ij} + r_{ij} \right)
\]

\[
u_{j} = -K \frac{k_{r,j}}{\mu_{j}} \left( \nabla p_{j} - \rho_{m,j} g \right)
\]

where \( r_{ij} \): rate of change of component \( i \) in phase \( j \) due to chemical equilibrium

\( (r_{ij} = 0 \) if no reaction)
Example: Effect of Reactions on CO₂ Concentration

Concentration profiles at $P_{\text{avg}} = 2,200$ psi after 0.12 hours of CO₂ injection

- Red curve ( ): concentration profiles with equilibrium reactions
- Black curve ( ): concentration profiles without equilibrium reactions
- Reactions in aqueous phase consume CO₂ altering phase equilibrium and hence miscibility conditions.
- Higher in situ water saturation results in lower CO₂ concentrations.
Locally Conservative Flow and Transport- Enhanced Galerkin

Transport Equation

\[ \partial_t (\rho \phi c) + \nabla \cdot (\rho \mathbf{u} c - \mathbf{D}(\mathbf{u}) \nabla c) = c^* q^* \]

- Inflow and outflow boundary conditions.
- Initial condition: \( c(x, 0) = c_0(x) \ \forall x \in \Omega \).

\[ \rho(p) = \rho_0 (1 + c_F p), \text{ and } \varepsilon \equiv 0 \]

\( c^+, q^+ \): source term, \( c^-, q^- \): sink term.

Locally Conservative Flux : Weighted Interior Penalty (Ern et al., 2007)

\[
\begin{align*}
\mathbf{U}^n |_T &= -\kappa \nabla P^n, \quad \forall T \in \mathcal{T}_h \\
\mathbf{U}^n \cdot \mathbf{n} |_e &= -\kappa_e \{\nabla P^n\} \cdot \mathbf{n} + \alpha(k) h_e^{-1} \kappa_e [P^n], \quad \forall e \in \mathcal{E}_h^0, \\
\mathbf{U}^n \cdot \mathbf{n} |_e &= g_N, \quad \forall e \in \mathcal{E}_h^{N,\partial}, \\
\mathbf{U}^n \cdot \mathbf{n} |_e &= -\kappa \nabla P^n \cdot \mathbf{n} + \alpha(k) h_e^{-1} \kappa (P^n - g_D), \quad \forall e \in \mathcal{E}_h^{D,\partial},
\end{align*}
\]

\[ \kappa_e \{\nabla v\} = \beta_e (\kappa^+ (\nabla v)^+ + (1 - \beta_e) (\kappa^- (\nabla v)^-)) \]

\[ \beta_e := \frac{\kappa^-}{\kappa^+ + \kappa^-} \quad \kappa_e := \frac{2 \kappa^+ \kappa^-}{\kappa^+ + \kappa^-} \]

- \( \kappa = \frac{K}{\mu}, \kappa_e \): Harmonic mean on the edge
- \( \alpha, k \): coefficients for the penalty term
Locally Conservative Flow and Transport - Enhanced Galerkin

- EG Transport – Entropy residual stabilization [Guermond et al. 08, 11]

Concentration values over the time steps (observe spurious oscillations)

(a) n=50  (b) n=100  (c) n=150  (d) n=200

(e) n=50  (f) n=100  (g) n=150  (h) n=200
Hele-Shaw cell: viscous fingering in a homogeneous channel [Lee-W. 2016]

Figure: Concentration values for each time steps with corresponding adaptive mesh refinement at the right column.
III. SIMULATOR DEVELOPMENT

Objectives

Complete simulator development with numerical schemes for coupled processes

- Develop computational methods for coupled processes based on multiscale discretization for flow, geomechanics & geochemistry

- Development of efficient solvers & pre-conditioners

- Model CO₂ storage field sites & perform compositional simulations

CO₂ Sequestration Site at Cranfield, Mississippi, USA
Framework of IPARS

- **IPARS** (Integrated Parallel Accurate Reservoir Simulator)

  Development of integrated flow, geochemistry, and geomechanics framework

- Interface I/O Visualization
- Solvers
- Multiphase Flow & Physics
- Advanced Grids
- Well Management

- 3 Phase EOS Flash
- Geochemical Reaction
- Mobility Control
- Geomechanics
- Compositional Kr-Pc
- Hysteresis Kr-Pc

- Parameter Estimation
- Uncertainty Quantification
Compositional Model

3-Phases: \( \alpha \in \{o, w, g\} \) \( N_c \)-Components: \( i \in \{w, 2, \ldots, N_c\} \)

Mass Conservation of component \( i \):

\[
\frac{\partial}{\partial t} \left( \sum_{\alpha} \phi S_\alpha \rho_\alpha \xi_{i\alpha} \right) + \nabla \cdot \sum_{\alpha} \left( \rho_\alpha \xi_{i\alpha} u_\alpha - \phi S_\alpha D_{i\alpha} \cdot \nabla (\rho_\alpha \xi_{i\alpha}) \right) = \sum_{\alpha} q_{i\alpha}, \text{ in } \Omega \times (0, T].
\]

Darcy’s Law for phase \( \alpha \) flux:

\[
u_\alpha = -K \frac{k_{r\alpha}}{\mu_\alpha} (\nabla \rho_\alpha - \rho_{m,\alpha} g).
\]

\( S_\alpha \) saturation \( \xi_{i\alpha} \) mole fraction \( \mu_\alpha \) viscosity
\( \phi \) porosity \( K \) absolute permeability \( \rho_{m,\alpha} \) mass density
\( q_{i\alpha} \) source/sink \( k_{r\alpha} \) relative permeability \( g \) gravity
\( u_\alpha \) Darcy flux \( D_{i\alpha} \) diffusion-dispersion
Concise Form of Equations

Concentration of component $i$

$$N_i = \sum_\alpha \rho_\alpha S_\alpha \xi_{i\alpha},$$

Source of component $i$

$$q_i = \sum_\alpha q_{i\alpha},$$

Advective flux of component $i$

$$F_i = -K \sum_\alpha \rho_\alpha \xi_{i\alpha} \frac{k_{r\alpha}}{\mu_\alpha} \left( \nabla p_\alpha - \rho_{m,\alpha} g \right),$$

Diffusive flux of component $i$

$$J_i = - \left( \sum_\alpha \phi S_\alpha D_{i\alpha} \left( \nabla \rho_\alpha \xi_{i\alpha} \right) \right).$$

Concise form of component concentration equation:

$$\frac{\partial}{\partial t} \left( \phi N_i \right) + \nabla \cdot (F_i + J_i) = q_i, \quad \text{in } \Omega \times (0, T].$$
Constraints, Initial, and Boundary Conditions

**Primary model unknowns** \( p_{\text{ref}}, N_1, \ldots, N_{N_c} \)

- **Saturation constraint**
  \[ \sum_{\alpha} S_\alpha = 1 \quad \Rightarrow \quad \frac{N_w}{\rho_w} + \left( \frac{1 - \nu}{\rho_o} + \frac{\nu}{\rho_g} \right) \sum_{i=2}^{N_c} N_i = 1 \]

- **Capillary pressure**
  \[ p_{c\alpha}(S_{\text{ref}}) = p_\alpha - p_{\text{ref}} \quad \Rightarrow \quad p_{c\alpha}(p_{\text{ref}}, \tilde{N}) = p_{c\alpha}(S_{\text{ref}}) \]

- **Slightly compressible for water phase**
  \[ \rho_w(p_{\text{ref}}) = \rho_{w,0} \exp \left[ C_w(p_{\text{ref}} + p_{cw} - p_{\text{ref},0}) \right] \]

- **Cubic EOS for hydrocarbon phases**
  \[ \rho_\alpha(p_{\text{ref}}, \tilde{N}_{HC}) = \frac{p_\alpha}{Z_\alpha RT}, \alpha \neq w \]

- **No-flow boundary conditions**
  \[ (F_i + J_i) \cdot n = 0, \quad \text{on } \partial \Omega \times [0, T] \]

- **Initial conditions**
  \[ p_{\text{ref}} = p^0, \quad N_i = N_i^0, \quad \text{on } \Omega \times \{ t = 0 \} \]
Hydrocarbon Phase Behavior Model

Peng-Robinson Equation of State
(for compressibility $Z$-factor; coefficients determined by pressure, temperature, composition)

\[ Z_\alpha = \bar{Z}_\alpha - C_\alpha \]
\[ \bar{Z}_\alpha^3 + h_1 \bar{Z}_\alpha^2 + h_2 \bar{Z}_\alpha + h_3 = 0 \]  \hspace{1cm} (1)

Rachford-Rice Equation
(for vapor fraction $v$)

\[ \mathcal{R}_g = \sum_i \frac{(k_i - 1)z_i}{1 + (k_i - 1)v} = 0 \]  \hspace{1cm} (2)

“Mixing Rule”
(for mass balance)

\[ \xi_i^v = \frac{z_i}{1 + (k_i - 1)v}, \quad \xi_i^g = k_i \xi_i^g \] \hspace{1cm} (3)

Fugacity Coefficient Equation
\[ f_i^\alpha = \text{fugacity} \quad \Phi_i^\alpha = f_i^\alpha / (\xi_i^\alpha \ p) = \text{fugacity coefficient} \]

\[ f_i^g = f_i^g \]
\[ \mathcal{R}_i = \ln(\Phi_i^\alpha) - \ln(\Phi_i^g) - \ln(k_i) = 0 \] \hspace{1cm} (4)

Flash Algorithm (Solved with Newton iteration)
1. Solve (2) for $v$.
2. Evaluate $\xi_i^\alpha$ using (3).
3. Solve (1) for $Z_\alpha$.
4. Evaluate $\Phi_i^\alpha$, check (4) for convergence. Update $\delta(ln \ k_i)$, goto 1.
Multipoint Flux Mixed Finite Elements

- Multipoint Flux Mixed Finite Element Spaces
  - 2D quadrilaterals
    - Pressure
    - Velocity
    - 2 fluxes/edge
  - 3D hexahedra
    - 4 fluxes/face
- Special Quadrature Rules
  \[ K^{-1}(\hat{x}) = \frac{1}{J_E} D F_E^T K^{-1}(F_E(\hat{x})) D F_E. \]
  \[ (K^{-1}q,v)_Q,E = (K^{-1}\hat{q},\hat{v})_{\hat{Q},\hat{E}} \equiv \frac{|\hat{E}|}{n_v} \sum_{i=1}^{n_v} K^{-1}(\hat{r}_i)\hat{q}(\hat{r}_i) \cdot \hat{v}(\hat{r}_i), \]
  - At every vertex, 12 flux DOFs eliminated in terms of 8 pressure DOFs.
- Logically structured distorted hexahedral grids
- No saddle point system with a mixed method.
  - 27-point stencil
  - Positive definite linear system
  - Symmetric or non-symmetric
- Other capabilities:
  - Can handle full tensor permeability.
  - Finite element convergence theory.
  - Two-point flux schemes are not convergent on distorted hexahedra.
Fully Discrete Formulation

Component Flux:

\[
\left\langle \frac{1}{\Lambda_{i,h}} \left( K^{-1} F_{i,h}^{k+1}, v_h \right) \right\rangle_{Q,E} - \left( p_{\text{ref},h}^{k+1}, \nabla \cdot v_h \right)_E = - \int_{\partial E \cap \partial \Omega} p_{\text{ref},h} \cdot n \, dS - \left( \frac{1}{\Lambda_{i,h}} \sum_{\alpha \neq \text{ref}} \rho_{\alpha,h}^{k} \xi \lambda_{\alpha,h}^{k} \nabla \phi_{\alpha,h}^{k} P_{\alpha,h}, v_h \right)_E + \left( \frac{1}{\Lambda_{i,h}} \sum_{\alpha} \rho_{\alpha,h}^{2} \phi_{\alpha,h}^{k} \xi_{i,h}^{k} g, v_h \right)_E,
\]

Component Conservation Equation:

\[
\left( \frac{\phi_{h}^{k+1} N_{i,h}^{k}}{\Delta t}, w_h \right)_E + \left( \nabla \cdot F_{i,h}^{k+1}, w_h \right)_E - \left( \nabla \cdot \sum_{\alpha} \left\{ \phi_{h}^{k+1} S_{\alpha,h}^{k} D_{i,h} \cdot \nabla \left( \rho_{\alpha,h}^{k} \xi_{i,h}^{k} \right) \right\}, w_h \right)_E = \left( q_{i,h}, w_h \right)_E + \left( \frac{\phi_{h}^{n} N_{i}^{n}}{\Delta t}, w_h \right)_E.
\]

- Solved with IMPEC scheme, iterative coupling
- Enhanced BDDF$_1$ mixed finite element space
- Symmetric and non-symmetric quadrature rules (Q)
- $\Lambda_i$’s are positive quantities
Ex: Strong Scaling, Hard Phase Behavior

- Initial reservoir composition: \{C3=0.1, C6=0.3, C10=0.1, C15=0.1, C20=0.4\}
- Gas injection well composition: \{C1=0.99, C3=0.01\}
Ex: Runtimes and Speedup

Strong Scaling, Hard Phase Behavior

- Both coefficient assembly and updates scale optimally. Coefficient time twice as large as previous cases.
- Flash calculations order of magnitude more expensive, but still small fraction of total time. Scales better because not merely located by wells.
- Linear solver scales to 256 procs, and again decreases at 1024 procs.

<table>
<thead>
<tr>
<th>Procs</th>
<th>Coeff.</th>
<th>Flash</th>
<th>Solve</th>
<th>Update</th>
<th>Total*</th>
</tr>
</thead>
<tbody>
<tr>
<td>64</td>
<td>7510</td>
<td>404</td>
<td>3208</td>
<td>470</td>
<td>11530</td>
</tr>
<tr>
<td>128</td>
<td>3845</td>
<td>317</td>
<td>1993</td>
<td>262</td>
<td>6426</td>
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<tr>
<td>256</td>
<td>1956</td>
<td>105</td>
<td>1405</td>
<td>138</td>
<td>3616</td>
</tr>
<tr>
<td>512</td>
<td>1064</td>
<td>72</td>
<td>3404</td>
<td>68</td>
<td>4750</td>
</tr>
<tr>
<td>1024</td>
<td>592</td>
<td>36</td>
<td>1598</td>
<td>34</td>
<td>2460</td>
</tr>
</tbody>
</table>

Speedup normalized to 64 procs.
Ex: Weak Scaling, Simple Phase Behavior

- Same simple phase behavior as Example 2, but with **weak scaling**. Need to keep problem characteristics the same on different levels.
  - Each processor owns 10,000 elements. Domain size increases with number of processors.
  - Grid blocks remain 5x10x10 [ft$^3$], in order to keep same time steps.
  - Well locations are center of domain, and center of four quadrants.

<table>
<thead>
<tr>
<th>Procs.</th>
<th>Elements</th>
<th>Coeff.</th>
<th>Flash</th>
<th>Solve</th>
<th>Update</th>
<th>Total*</th>
</tr>
</thead>
<tbody>
<tr>
<td>64</td>
<td>640,000</td>
<td>295</td>
<td>14</td>
<td>255</td>
<td>17</td>
<td>576</td>
</tr>
<tr>
<td>256</td>
<td>2,560,000</td>
<td>176</td>
<td>9</td>
<td>342</td>
<td>10</td>
<td>550</td>
</tr>
<tr>
<td>1024</td>
<td>10,240,000</td>
<td>172</td>
<td>8</td>
<td>440</td>
<td>9</td>
<td>732</td>
</tr>
</tbody>
</table>

- Coeff, flash, and update improved from 64 to 256 procs, then remained const.
- Linear solver time increased slightly (note the problem is changing).
- Total time remains roughly constant, giving a positive weak scaling result.
Low-Tension Gas Flood Case Study: ColInj, WAG, SAG

### Gas mobility control methods

- **Water Alternating Gas (WAG)**
- **Surfactant-alternate-gas (SAG)**
  - The 1\textsuperscript{st} surfactant lowers $S_o$: reducing IFT
  - The 2\textsuperscript{nd} surfactant controls gas mobility: generating foam
- **Simultaneous Water and Gas (ColInj)**

#### WAG

- Inject the 1\textsuperscript{st} surfactant. Then, alternate water & gas

#### SAG

- Inject the 1\textsuperscript{st} surfactant. Then, alternate 2\textsuperscript{nd} surfactant foam & gas

#### CoInj

- SI: IFT-reduction surfactant; SF: Foam agent

**Total fluid injection = 5 PV (960 + 30 days)**

**Surfactant-Assisted Water-Alternate-Gas (1:1)**

- Water + Residual Oil to Water
Low-Tension Gas Flood Case Study: CoInj, WAG, SAG

Model description

- $\Phi = 0.2; \frac{k_v}{k_h} = 0.1; S_o^{initial} = S_{orw} = 0.35$
- Initial pore volume = 53.4 MSTB
- $T^{initial} = 90^\circ F; p^{initial} = 1,500 psia$
- Initial oil composition:
  - $C_{10}=30\%; C_{15}=40\%; C_{20}=30\%$
- Oil composition effect on ME phase behavior (2 set of parameters vs. EACN)

Simulation results

- Investigate hysteresis effects at gridblock M
- Oil Saturation at the end of injection
- Case 1: WAG
  - Higher residual oil saturation at lower layers after WAG
- Case 2: SAG
  - Lower residual oil saturation than WAG in the high permeability streak
- Case 3: CoInj
  - Lower residual oil saturation than SAG in the high permeability streak

Injector

Producer

High permeability streak in a low permeability matrix
Low-Tension Gas Flood Case Study: $K_{rg}$ and $S_{gt}$ at the Gridblock M

Cycle-dependent relative permeability in multi-cycle WAG processes

- As the cycle number increases from the 1\textsuperscript{st} to the 8\textsuperscript{th},
  - Gas relative permeability decreases in time.
  - Gas normalized trapped saturation increases monotonically.
    
    \textit{due to hysteresis!}

![Diagram showing cycle-dependent relative permeability and trapped saturation over time](image-url)
Effect of Water Alternating Gas (WAG) and Foam on CO₂ Sequestration

Introduction

- Three-phase relative permeability and hysteresis models are essential to accurately model CO₂ sequestration in aquifers.
- Once non-wetting phase saturation (here CO₂) decreases in porous media it traps by capillary forces (relative perm hysteresis, Beygi, 2016).
- Foam exhibits multiple steady-state behaviors at the same injection conditions (foam generation hysteresis, Lotfollahi et al., 2016).
- Three-phase relative permeability and hysteresis models have been implemented and coupled with foam models in IPARS.
Effect of Water Alternating Gas (WAG) and Foam on CO₂ Sequestration

Findings

- Missing relative permeability hysteresis during WAG process underestimate WAG performance significantly.
- In surfactant alternating gas (Foam) process, strong foam is generated in the high permeability streak and divert the flow into low permeability matrix.
## Poro-plasticity

- **Geomechanical Effects of CO₂ Injection with a Poro-plasticity Model**

<table>
<thead>
<tr>
<th>Fluid Flow</th>
<th>( \frac{\partial (\rho (\phi_0 + \alpha \varepsilon_r + \frac{1}{M} (p - p_0)))}{\partial t} + \nabla \cdot \left( \frac{K}{\mu} (\nabla p - \rho g \nabla h) \right) - q = 0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stress Equilibrium</td>
<td>( \nabla \cdot (\sigma'' + \sigma_o - \alpha (p - p_0) I) + f = 0 )</td>
</tr>
<tr>
<td>Hooke’s Law</td>
<td>( \sigma'' = D^e : (\varepsilon - \varepsilon^p) )</td>
</tr>
<tr>
<td>Druker-Prager Yield Surface</td>
<td></td>
</tr>
<tr>
<td>Strain-Displacement Relation</td>
<td>( \varepsilon = \frac{1}{2} (\nabla u + \nabla^T u) )</td>
</tr>
<tr>
<td>Plastic Strain Evolution</td>
<td>( \varepsilon^p = \lambda \frac{\partial F(\sigma'')}{\partial \sigma''}, \text{ at } Y(\sigma'') = 0 )  ( \varepsilon^p = 0, \text{ at } Y(\sigma'') &lt; 0 )</td>
</tr>
<tr>
<td>Yield and Flow Functions</td>
<td>( Y = q + \theta \sigma_m - \tau_0 )  ( F = q + \gamma \sigma_m - \tau_0 )</td>
</tr>
</tbody>
</table>
Model Field Sites

Objectives

- Measure mechanical properties in laboratory
- Collect other existing data (seismic, well logs, etc.)
- Measure impact of geochemical alteration on mechanical properties
- Study rock dissolution and its effect on weakening the rocks and creating leakage pathways
- Enhanced simulation for studying and quantifying parameters, e.g. reservoir over pressure, chemical and thermal loading

Site 1: Cranfield, MS, USA

Site 2: Frio, TX, USA

Modeling, simulation & uncertainty analysis with application to CO₂ storage sites (Cranfield, MS & Frio, TX)
Example 2: Large-Scale Parallel Cranfield CO₂ Sequestration Case

CO₂ concentration on distorted grid
IV. UNCERTAINTY QUANTIFICATION

- Calibration process of rock and fluid properties in subsurface models

**A Priori Model**
- Multi-modal (permeability, md)

**History Matching**
- Parameterization
- Forward Modeling
- Inverse Modeling
- Gaussian

**A Posteriori Model**
- Multi-modal (permeability, md)
Parallel Multi-objective Optimization for CCS at Cranfield

Reservoir Characterization & Optimization

<table>
<thead>
<tr>
<th>OS</th>
<th>Algorithm</th>
<th>Simulator</th>
<th>Run</th>
<th>Storage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scientific Linux</td>
<td>• Global-objective genetic algorithm</td>
<td>GA.exe</td>
<td>• Parallel</td>
<td>• Supercomputer</td>
</tr>
<tr>
<td>Windows 8</td>
<td>• Global-objective evolution strategy</td>
<td>ES.exe</td>
<td>Evaluate model</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Multi-objective genetic algorithm</td>
<td>NSGA-II.exe</td>
<td>Evaluate model</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Multi-objective evolution strategy</td>
<td>ε-MOES.exe</td>
<td>Evaluate model</td>
<td></td>
</tr>
</tbody>
</table>

Builder.exe

ECL

IPARS

CMG COMPUTER MODELLING GROUP LTD

The University of Texas at Austin

WHAT STARTS HERE CHANGES THE WORLD
Objective: validate pulse testing as an active monitoring tool for potential CO$_2$ leakage detection at geological carbon sequestration sites

(Lu et al., 2013)
Three wells in the DAS (Detailed Area of Study) of Cranfield sector model

200 ft

100 ft

(http://www.beg.utexas.edu/gccc/cranfield.php)
Subsurface Modeling of Cranfield Sector Model

Grid top of Cranfield sector model

- 661,760 = 20x188x176 grid cells
- Grid size: 4 ft x 50 ft x 50 ft
- Side View

Aerial View

- Dip ≈ 2°
- Grid Top (ft)
- Injector
- Producer
- Monitor

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Bottomhole pressure at the CO$_2$ injection well 31F-1

Before update    After update    Observed

(Delshad et al. 2013)    (Min et al. SPE-182641)
Compositional Simulations of Pulse Testing in the DAS

150-minute baseline experiment at the monitoring well 31F-2

- Observed pressure
- Simulated pressure
- Pressure anomalies obtained from observed & simulated pressure
150-minute Baseline and Leak Experiments at Well 31F-2

Observation results

Simulation results
V. BIGDATA

**Characterization**
- Computation of seismic wave propagation in fractured media
- Statistical (pattern recognition) schemes for identification of fracture characteristics from dynamic data

**Simulation**
- Large scale reservoir simulation of coupled compositional flow model and fracture propagation using Dataspaces
- Modeling of proppant filled fractures using Enhanced Galerkin

**Optimization**
- Optimized well spacing for hydraulic fracturing
- Multi-objective optimization process to choose geologic models based on observed flow and geomechanical responses
BIGDATA: Collaborative Research for Fractured Subsurface Characterization Using High Performance Computing and Guided by Big Data

- Data staging As-a-Service
  Data staging enables coupling of multi-physics with big data

Seismic  Microseismic  Flow  Fracture  InSAR

- Geophysics
- Reservoir Engineering
- Big Data Analytics

- Wave propagation in fractured porous medium
- Fracture propagation
- Data assimilation
- Production forecasts

- Pattern recognition
- Deep neural network

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Enriched Galerkin and Wave Propagation

- Phase Field and Seismic Wave Propagation in Fractured Media (Sen et al., 2017)

Wavefield using discrete fractures 540,384 Fractures – DG.

Orthogonal fracture planes.

(a) Parallel to fracture
(b) Normal to fracture.

- Locally Conservative Finite Element Method
  - Enriched Galerkin approximations for flow & transport
  - Chemical reactions and viscous fingering
  - Extended for seismic wave propagation

Viscous fingering in a two homogeneous channel.

Dynamic mesh adaptivity.
Subsurface Fracture Characterization

Pattern Recognition for Fractured Reservoir Characterization Using Subsurface Big Data (led by Dr. Sanjay Srinivasan in Pennsylvania State University)

- **Objective**
  - Identify fracture location & orientation in low signal-to-noise ratio seismic data

- **Input training images**
  - Seismic amplitude slices
  - Fracture and non-fracture window examples

- **Validation data**
  - Ku-Maloob-Zaap fields (Gulf of Mexico)
  - 3D seismic
  - Number of traces: 6,476,056
  - Number of fractures: 1,000,000+
Toolbox for Subsurface Big Data Analytics

- Framework of a Computer-Assisted Optimization Toolbox: UT-OPT

- Input builder
  - Choose reservoir simulator
  - Choose optimization algorithm
  - Simulate & optimize multiple runs

- Model order reduction
  - Level set
  - Feature selection
  - Non-Gaussian

- Data science
  - Data assimilation
  - Global-objective optimization
  - Multi-objective optimization

- Framework of UT-OPT.

- Model Update

- CSM IPARS
- CSM Phase-field
- Schlumberger ECLIPSE
- CMG-GEM
- CMG-IMEX
- CMG-STARS

- Experiment 1
- Experiment 2
- ...
Workflow for Multiphysics Coupling of IPARS and deal.II using Dataspaces
Key Features of Service-Oriented Staging (led by Dr. Manish Parashar at Rutgers University)

- **Dynamic**: coupled applications can join and leave staging areas without affecting other applications.
- **Persistent**: The staging service and the staged data remains persistent across instances of the component applications. Applications can join and leave the staging service whenever they need access to it.
- **Efficient**: Optimizes the write performance by routing data from requesting client applications to the closest staging servers.
- **Resilient**: The staging service can be backed up and restarted as needed.

Adaptive Data I/O System (ADIOS) that are to be coupled with forward models and assimilation/optimization algorithms.
Coupled Compositional Flow Simulations with Fracture Propagation

Fluid Pressure

Water Saturation

C6 Component Concentration
Conclusions

- Ongoing works: multidisciplinary collaboration with multi-universities, industry, government laboratories
  - Part of training graduate students for future work force

- Big data: service-oriented data staging for coupling geophysics and flow with data
  - Key features of data staging: dynamic, persistent, efficient, and resilient

- Development of high-fidelity algorithms: EG, Phase Field, Multipoint Flux, etc.
  - Flow, transport, and mechanics in fractured porous media
  - Wave propagation
  - Data assimilation & multiobjective optimization
  - Machine learning & pattern recognition