Optimization and Reduced-Order Modeling of Geological Carbon Storage Operations

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Key Collaborators on Work Presented

- **David Cameron** (optimization of carbon storage operations)
- **Z. Larry Jin** (ROM for CO$_2$ injection, building on work by Jincong He)
- **Sumeet Trehan** (ROM for oil/water)
Carbon Capture and Storage

Capture / compress → Transport → Inject → Monitor / remediate

https://energy.gov/fe/science-innovation/carbon-capture-and-storage-research/overview-carbon-storage-research
CO₂ Trapping Mechanisms

https://data.geus.dk/nordiccs/terminology.xhtml

http://www.bigskyco2.org/node/127
Optimization Problem Statement

• Minimize measure of aggregate mobility of CO$_2$ in target region (e.g., just below cap rock) over $T$ years:

$$\min_{y,u} J(y, u) = \frac{1}{T} \int_{t=0}^{T} \sum_{i \in \text{top layer}} \left( \frac{\rho_g k_{rg}}{\mu_g} \right)_i dt$$

$y$: well placement variables, $u$: injection rate variables

• With uncertainty,  $\min E[J(y, u)] \approx (1/N_k) \sum_{1}^{N_k} J_k(y, u, m_k)$

• Could define $J$ in terms of pressure buildup, well costs, …

• Related work: Shamshiri & Jafarpour (2012), Petvipusit et al. (2014), Babaei et al. (2015, 2016)
Basic Pattern Search

- Local search
- Naturally parallelizable
- Convergence theory based on stencil reduction
- Mesh adaptive direct search (MADS) uses oriented stencil

Optimization in $\mathbb{R}^2$

(Kolda et al., 2003; slide from Obi Isebor)
Particle Swarm Optimization (PSO)

- Global stochastic search
- Solutions are particles in a swarm
- Solution update given by:

\[
\begin{align*}
x_i(k + 1) &= x_i(k) + v_i(k + 1) \cdot \Delta t \\
v_i(k + 1) &= \omega \cdot v_i(k) \\
&\quad + c_1 \cdot D_1(k) \cdot (x_{i_{pbest}}^k - x_i(k)) \quad \text{(cognitive)} \\
&\quad + c_2 \cdot D_2(k) \cdot (x_{i_{nbest}}^k - x_i(k)) \quad \text{(social)}
\end{align*}
\]

PSO parameters: \( \omega, c_1, c_2; \ D_1(k), D_2(k) \sim U(0,1) \)

Can globally explore solution space; no guarantees of convergence (Eberhart and Kennedy, 1995)
PSO-MADS Hybrid Algorithm*

*Isebor, Echeverría Ciaurri, Durlofsky (2014a,b)
Aquifer Simulation Model

- Grid: 39x39x8
- Large boundary volume to provide pressure support
- Relative permeability hysteresis included; no mineralization or $p_c(x)$
Simulation & Optimization Variables

- \((i, j)\) locations of 4 horizontal injection wells (prescribed to be in the bottom layer)

- Rates in each well in 6 control periods (inject \(5 \times 10^6\) tonnes \(\text{CO}_2\) per year for 30 years)

- Corresponds to 2.5% of storage aquifer PV

- \(N_v = 30\) optimization variables (no brine cycling), \(~22–30\) PSO particles
Minimize CO$_2$ Mobility (PSO)

![Graph showing the decrease in CO$_2$ mobility over the number of function evaluations.](image_url)
Well Locations and CO\textsubscript{2} Mobility

Injection wells – bottom layer; CO\textsubscript{2} – top layer
Optimal Injection Rates

- W4 injects for 15 years; W1 injects more at late times
Mobile CO$_2$ in Top Layer
Brine Cycling Strategies in CCS

- Related strategies proposed by Leonenko & Keith (2008), Nghiem et al. (2009, 2010), Anchliya (2012)
Brine Cycling Process (illustration)
Brine Cycling Process

CO₂ injector

Mobile CO₂
Brine Cycling Process

CO₂ injector
Mobile CO₂
Brine Cycling Process

$CO_2$ injector

Mobile $CO_2$

$t = 30$ yrs
Brine Cycling Process

$t = 60$ yrs

CO$_2$ injector

Mobile CO$_2$
Brine Cycling Process

Brine injector
Brine producer
CO₂ injector
Mobile CO₂
Brine Cycling Process

CO₂ injector

Mobile CO₂
Brine Cycling Process
Brine Cycling Process

CO₂ injector

Mobile CO₂
Brine Cycling Optimization

• Minimize measure of aggregate mobility of CO$_2$ in top or target layer over $T$ years:

$$
\min_{y,u_1,u_2} J(y, u_1, u_2) = \frac{1}{T} \int_{t=0}^{T} \sum_{i \in \text{top layer}} \left( \frac{\rho_g k_{rg}}{\mu_g} \right)_i \, dt
$$

$y$: well placement variables

$u_1$: injection rate variables

$u_2$: times and volumes for 3 brine cycling events, subject to specified total brine PV cycled

• Determine total of $N_v = 47$ optimization variables
Brine Cycling Optimization Results

Pore volume as fraction of 15x15x8 core region
(0.03 PV of core region
~0.01 PV of storage aquifer)
Optimization under Geological Uncertainty

- Minimize expected value of time-averaged mobility over $N_k$ prior realizations $m_k$:

$$E[J(y, u)] \approx \frac{1}{N_k} \sum_{k=1}^{N_k} J_k(y, u, m_k)$$

$$J_k(y, u, m_k) = \frac{1}{T} \int_0^T \sum_{i \in t_k} \left( \frac{\rho_g k_{rg}}{\mu_g} \right)_i \, dt$$

$t_k$: target layer in model $m_k$

- No brine cycling in these examples
Optimization under Geological Uncertainty

• Expected value of time-averaged mobility over $N_k = 10$ prior (Gaussian) realizations

Default (6900)  
Optimized (5300)
Optimization under Geological Uncertainty (5 new true models)

<table>
<thead>
<tr>
<th>Model</th>
<th>Default</th>
<th>A priori opt. rates &amp; locs</th>
</tr>
</thead>
<tbody>
<tr>
<td>True 1</td>
<td>6080</td>
<td>4890</td>
</tr>
<tr>
<td>True 2</td>
<td>6150</td>
<td>5370</td>
</tr>
<tr>
<td>True 3</td>
<td>6380</td>
<td>4660</td>
</tr>
<tr>
<td>True 4</td>
<td>9020</td>
<td>7670</td>
</tr>
<tr>
<td>True 5</td>
<td>7760</td>
<td>5710</td>
</tr>
<tr>
<td>Average</td>
<td>7080</td>
<td>5660</td>
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Improvement from a priori optimization ~20%
## Optimization under Geological Uncertainty (5 new true models)

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<td>4660</td>
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<tr>
<td>True 4</td>
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<td>4940</td>
</tr>
<tr>
<td>Average</td>
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<td>5660</td>
<td>5250</td>
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Maximum additional improvement from closed-loop, ~7%
## Optimization under Geological Uncertainty
(5 new true models)

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<th>Deterministic optimization</th>
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<tr>
<td>Average</td>
<td>7080</td>
<td>5660</td>
<td>5250</td>
<td>4340</td>
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Additional improvement from knowledge of $m$, ~23%
POD-based Reduced-Order Models for Reservoir Simulation (partial list)

- **POD only**: van Doren, Markovinovic, Jansen (2006); Cardoso et al. (2009)

- **POD-DEIM**: Ghasemi, Yang, Gildin, Efendiev, Calo (2015); Yang, Gildin, Efendiev, Calo (2017); Yoon, Alghareeb, Williams (2016)

- **POD-TPWL**: Cardoso & Durlofsky (2010); He et al. (2011,2014,2015); Fragoso, Horowitz, Rodrigues (2015)

- **POD-TPWQ**: Trehan & Durlofsky (2016)

- **ROMs for optimization**: Jansen & Durlofsky (2017)
Proper Orthogonal Decomposition and Trajectory Piecewise Linearization (POD-TPWL)

Basic idea
Use states and derivative matrices generated and saved during training run(s) to represent new solutions

Approach

• Run training simulations \( g(x, u) = 0 \)
• Record states, Jacobian matrices, etc. \( (x^i, \frac{\partial g^i}{\partial x^i}) \)
• Represent new solutions \( x^{n+1} \) as expansions around saved states \( (x^i, x^{i+1}) \)
• Map into low-dim reduced space \( \xi \) using POD \( x = \Phi \xi \)

TPWL: Rewienski & White (2003); Vasilyev et al. (2003); Qu & Chapman (2006), …
Gas – Water Flow Equations

• Mass balance equations for \( j = \text{gas, water} \)

\[
\phi \frac{\partial S_j}{\partial t} - \nabla \cdot (\lambda_j k \cdot \nabla p) + q_j = 0
\]

\( S_j \) - phase saturation, \( p \) - pressure
\( \lambda_j(S_j) \) - phase mobility, \( k \) - permeability tensor, \( q_j \) - source

• Discretize: \( x \) - states \((p, S_w)\), \( u \) - controls \((p_{\text{well}})\), \( O(10^4 - 10^6) \) grid blocks \((n_b)\)

\[
g(x^{n+1}, x^n, u^{n+1}) = A(x^{n+1}, x^n) + F(x^{n+1}) + Q(x^{n+1}, u^{n+1}) = 0
\]

• Newton’s method: \( J\delta = -g, \ J = \partial g/\partial x \)
TPWL for Reservoir Flow Equations

Discretized flow equations:

\[ g^{n+1} = A^{n+1} + F^{n+1} + Q^{n+1} = 0 \]

Linearized representation for new state \( x^{n+1} \):

\[ g^{n+1} = 0 \approx g^{i+1} + \frac{\partial g^{i+1}}{\partial x^{i+1}} (x^{n+1} - x^{i+1}) + \frac{\partial g^{i+1}}{\partial x^i} (x^n - x^i) + \frac{\partial g^{i+1}}{\partial u^{i+1}} (u^{n+1} - u^{i+1}) \]

<table>
<thead>
<tr>
<th>x: states (p, S)</th>
<th>u: controls (BHPs)</th>
</tr>
</thead>
</table>

training run: (i, i + 1)  test run: (n, n + 1)
Expansion around Saved States + POD

• Linearized representation (note $J^{i+1} = \partial g^{i+1} / \partial x^{i+1}$):

$$J^{i+1}(x^{n+1} - x^{i+1}) = - \left[ \frac{\partial g^{i+1}}{\partial x^i} (x^n - x^i) + \frac{\partial g^{i+1}}{\partial u^{i+1}} (u^{n+1} - u^{i+1}) \right]$$

• Introduce POD basis ($x = \Phi \xi$, with $\Phi \in \mathbb{R}^{2n_b \times l}$ from SVDs of training-run snapshots):

$$J^{i+1} \Phi (\xi^{n+1} - \xi^{i+1}) = - \left[ \frac{\partial g^{i+1}}{\partial x^i} \Phi (\xi^n - \xi^i) + \frac{\partial g^{i+1}}{\partial u^{i+1}} (u^{n+1} - u^{i+1}) \right]$$

• Now have over-determined system of $2n_b$ equations in $l$ unknowns ($l \ll 2n_b$)
Constraint Reduction for Low-Order System

• Petrov-Galerkin approach: \( \Psi^{i+1} = J^{i+1} \Phi \in \mathcal{R}^{2n_b \times l} \)

\[
(\Psi^{i+1})^T J^{i+1} \Phi (\xi^{n+1} - \xi^{i+1}) \\
= - (\Psi^{i+1})^T \left[ \frac{\partial g^{i+1}}{\partial x^i} \Phi (\xi^n - \xi^i) + \frac{\partial g^{i+1}}{\partial u^{i+1}} (u^{n+1} - u^{i+1}) \right]
\]

• Solving for \( \xi^{n+1} \) (linear, \( l \)-dimensional system):

\[
\xi^{n+1} = \xi^{i+1} - (J_r^{i+1})^{-1} \left[ \left( \frac{\partial g^{i+1}}{\partial x^i} \right)_r (\xi^n - \xi^i) + \left( \frac{\partial g^{i+1}}{\partial u^{i+1}} \right)_r (u^{n+1} - u^{i+1}) \right]
\]

\[
J_r^{i+1} = (\Psi^{i+1})^T J^{i+1} \Phi \\
\left( \frac{\partial g^{i+1}}{\partial x^i} \right)_r = (\Psi^{i+1})^T \frac{\partial g^{i+1}}{\partial x^i} \Phi \\
\left( \frac{\partial g^{i+1}}{\partial u^{i+1}} \right)_r = (\Psi^{i+1})^T \frac{\partial g^{i+1}}{\partial u^{i+1}}
\]
**POD-TPWL with Multiple Derivatives**

- All trainings provide derivatives and snapshots
- More general ‘point selection’ criteria required
POD-TPWL Flowchart

Online Process

- Test controls
- POD-TPWL
  - Reduced derivatives: \( \{J_r^i\}_1, \{J_r^i\}_2, \ldots, \{J_r^i\}_5 \)
  - Training states for POD: \( \{x^i\}_1, \{x^i\}_2, \ldots, \{x^i\}_5 \)

Multiple Derivatives

Offline Process

- Training controls
- AD-GPRS (HFS)

Post Processing

- Primary Output
  - Flash
  - Secondary Output
Problem Setup

- Gaussian log-permeability, low-perm at layer 7
- Full model: 43 km x 43 km x 150 m
- Storage aquifer: 2.8 km x 2.8 km x 150 m
- Storage aquifer model: 35 x 35 x 15 blocks
Training and Test Injection Rates

- Field injection rate: 0.3 million tonnes of CO$_2$ per year
Test Case: BHPs for Well 2

- Single derivative uses snapshots from 5 trainings
- POD-TPWL speed up $\approx 100-150x$
CO$_2$ Molar Fractions at Target Layer (after 20 years)

Training (HFS)  

Test (HFS)
POD-TPWL Accuracy for Test Run

Single derivative

Multiple derivatives

$|\text{TPWL} - \text{HFS}|$

$|\text{TPWL} - \text{HFS}|$
Optimization Methodology

- Minimize aggregate CO$_2$ at target layer
  - Combine MADS (NOMAD) with POD-TPWL
  - Use of multiple derivatives avoids re-training
Optimization Setup

- Channelized aquifer derived from Stanford VI
- Fixed field injection rate, inject for 20 years (2.8% of total PV), 4 control periods, 12 opt. variables
- 5 training runs (multiple derivatives) for POD-TPWL
Optimization Results

- Full-order: 0.98
- Best POD-TPWL: 0.96
**CO₂ Plume Locations (Cross Sections)**

Initial guess, Well 3

Optimized solution, Well 3

Initial guess, Well 1

Optimized solution, Well 1
Accuracy of POD-TPWL Solution

$|\text{TPWL} - \text{HFS}|$, Well 3

$|\text{TPWL} - \text{HFS}|$, Well 1
Second-Order Treatment for Oil-Water Systems

- Quadratic representation for new state $\mathbf{x}^{n+1}$ now includes Hessian-type terms

$$
\mathbf{g}^{n+1} = 0 \approx \mathbf{g}^{i+1} + \frac{\partial \mathbf{g}^{i+1}}{\partial \mathbf{x}^{i+1}} (\mathbf{x}^{n+1} - \mathbf{x}^{i+1}) + \frac{\partial \mathbf{g}^{i+1}}{\partial \mathbf{x}^{i}} (\mathbf{x}^{n} - \mathbf{x}^{i}) + \\
\frac{\partial \mathbf{g}^{i+1}}{\partial \mathbf{u}^{i+1}} (\mathbf{u}^{n+1} - \mathbf{u}^{i+1}) + \frac{1}{2} \frac{\partial}{\partial \mathbf{x}^{i+1}} (\frac{\partial \mathbf{g}^{i+1}}{\partial \mathbf{x}^{i+1}}) (\mathbf{x}^{n+1} - \mathbf{x}^{i+1})(\mathbf{x}^{n+1} - \mathbf{x}^{i+1}) + \ldots
$$

- Introduce POD basis: $\mathbf{x} = \Phi \xi$

- Apply constraint reduction: pre-multiply by $(\Psi^{i+1})^T$

- Resulting ROM is low-dimensional but nonlinear; solve using Newton’s method
Simulation Results using POD-TPWQ

- 2D oil-water simulation
- 3 injectors, 3 producers
- Consider large BHP perturbation relative to training run
P1 Oil & Water Rates – Larger BHP Perturbations

Oil rate (bbl/d) vs. Time [days]

- High-fidelity test solution
- Training solution
- POD-TPWL
- POD-TPWQ

Water rate (bbl/d) vs. Time [days]

- High-fidelity test solution
- Training solution
- POD-TPWL
- POD-TPWQ
Multifidelity ROM-based Optimization

- Perform preprocessing HFS (training) runs
- Construct POD-TPWL & POD-TPWQ models
- Optimize using POD-TPWL model
- Validate optimized solution via HFS

- Use POD-TPWQ as error estimator; retrain with HFS as required
- HFS: expensive
- POD-TPWL, POD-TPWQ – inexpensive ROMs
- POD-TPWQ as error estimator
Optimization Problem Setup

- 2D oil-water simulation, maximize NPV
- 2 injectors, 3 producers
- 8 control steps per well → 40 optimization variables
- Numerical gradients from ROM
- Economic parameters – oil: $80/bbl, water cost: $6/bbl
- \(~13,000\) POD-TPWL runs, 37 POD-TPWQ runs
- Elapsed time, 12 processors: \(~20\times T_{HFS}\) (~50\times speedup)

Optimization with HFS gives nearly identical NPV, requires \(~940\times T_{HFS}\)
Summary

- Applied computational optimization to minimize risk in carbon storage problems
  - Well locations and time-varying injection rates
  - Brine cycling to further reduce risk
  - Optimization under uncertainty
  - *Leak detection with PCA representation of geology*

- Developed ROM for CO$_2$ problems (injection stage)
  - Showed benefit of multiple-derivative treatment
  - Employed POD-TPWL in MADS-based optimization
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- Jincong He (now at Chevron)
- Stanford Center for Computational Earth & Environmental Sciences (CEES)
Main References


- Zin, Z.L., Durlofsky, L.J. Reduced-order modeling of CO₂ storage operations, in review.
