# Maximization of Permanent Trapping of CO<sub>2</sub> in the Highest-Porosity Formations of the Rock Springs Uplift Project Number: FE0004832

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Developing the Technologies and Building the
Infrastructure for CO<sub>2</sub> Storage
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#### Presentation Outline

- Benefit to the Program
- Project Overview
- Technical Status
  - Experimentation and Modeling: Pore and Core Scales
  - Modeling and Simulation: Core and Field Scales
- Accomplishments to Date
- Summary

### Benefit to the Program

#### Program goal:

'Develop technologies that will support industries' ability to predict
 CO<sub>2</sub> storage capacity in geologic formations to within ±30 percent.'

#### Benefits statement:

The research project is focused on performing reservoir conditions experiments to measure steady-state relative permeabilities, residual saturations, interfacial tensions, and contact angles to inform models at pore, core, and reservoir scales. These can then be used to develop improved understanding of displacement mechanisms leading to design of strategies to maximize trapping.

# **Project Overview:**Goals and Objectives

#### Goal:

 The overall goal of this project is to provide information that will assist in maximizing the permanent trapping of supercritical CO<sub>2</sub> (scCO<sub>2</sub>), and co-contaminants (referred to as 'mixed scCO<sub>2</sub>') in deep saline aquifers.

#### Objectives:

- Measurement of reservoir conditions drainage and imbibition relative permeabilities, irreducible brine and residual mixed scCO<sub>2</sub> saturations and relative permeability scanning curves (hysteresis).
- Characterization of wettability through measurements of contact angles and interfacial tensions under reservoir conditions.
- Development of physically-based dynamic core-scale pore network model.
- Development of new, improved high-performance modules for the UW-team simulator to provide new capabilities to the existing model in order to include hysteresis in the relative permeability functions, geomechanical deformation and an equilibrium calculation (for mixed scCO<sub>2</sub>).
- Validation of the compositional reservoir model against well-characterized unsteady-state coreflooding experiments.
- Numerical study of long term permanent trapping of mixed scCO<sub>2</sub>, through high-resolution numerical experiments taking into account reservoir heterogeneity, saturation history, dissolution, capillary trapping and geomechanical deformation.

#### **Technical Status**

Project includes two major groups of tasks (6 UW faculty members):

#### 1. Experimentation and Modeling: Pore and Core Scales

- Task 2: Relative permeability measurements at reservoir conditions
- Task 3: IFT and CA measurements at reservoir conditions
- Task 4: Dynamic pore-scale modeling to predict k<sub>r</sub> and P<sub>c</sub> functions

#### 2. Modeling and Simulation: Core and Field Scales

- Task 5: Reservoir modeling activities
- Task 6: Development of the UW-team compositional simulator
- Task 7: Geomechanics model development
- Task 8: Field-scale numerical experiment

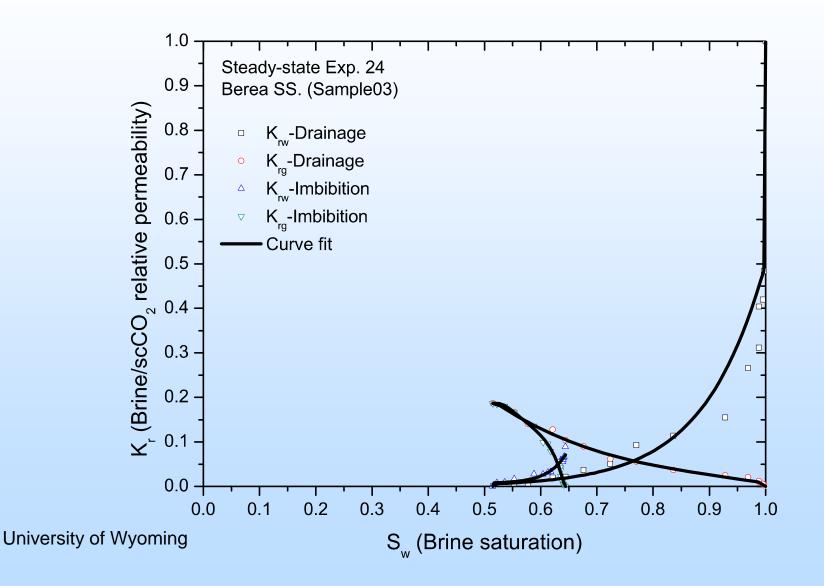
# Experimentation and Modeling Pore and Core Scales

- Measurement of relative permeability functions
- Development pore-scale network models

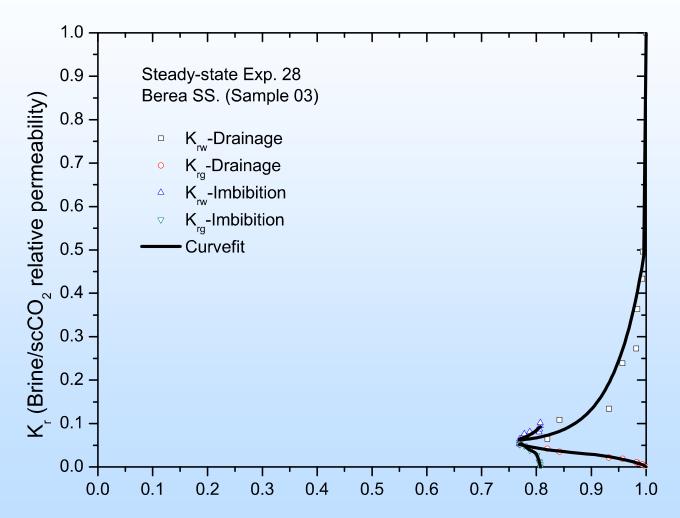




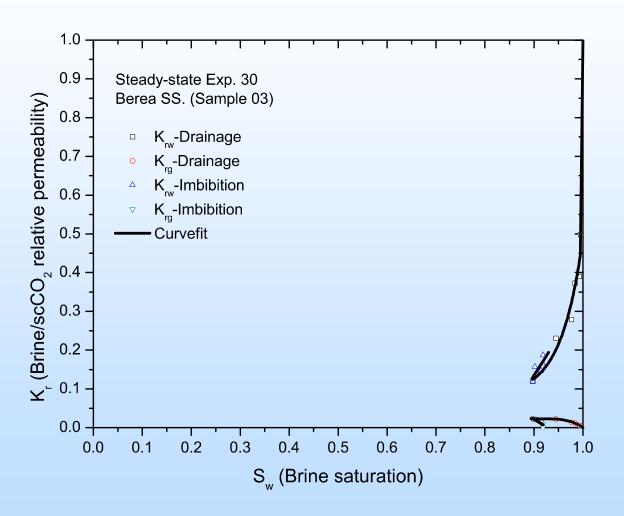
Vertical positioning system

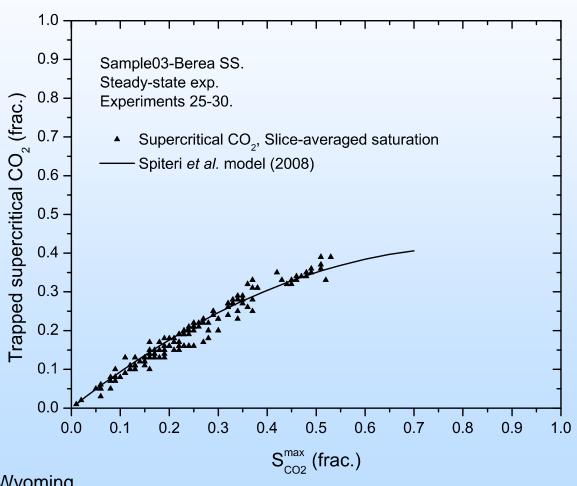


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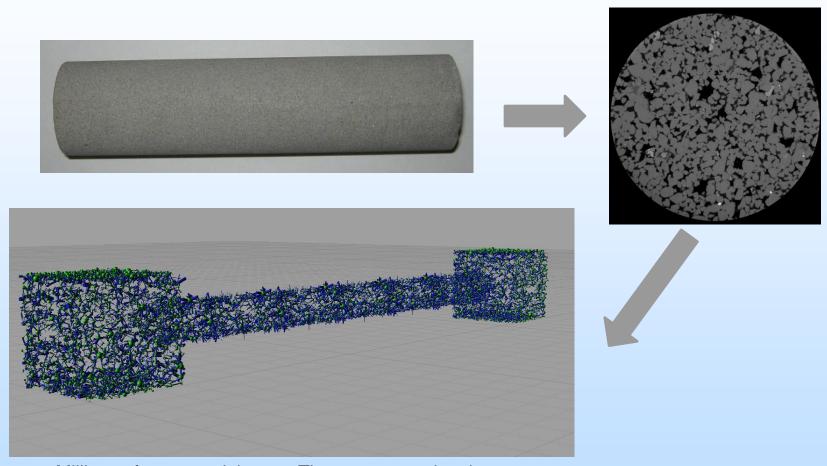
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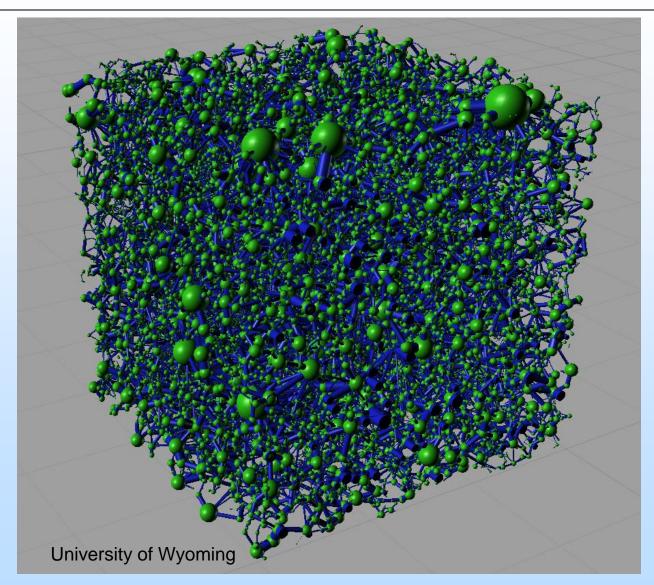
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# Development of physically-based dynamic pore-scale network model (Task 4)



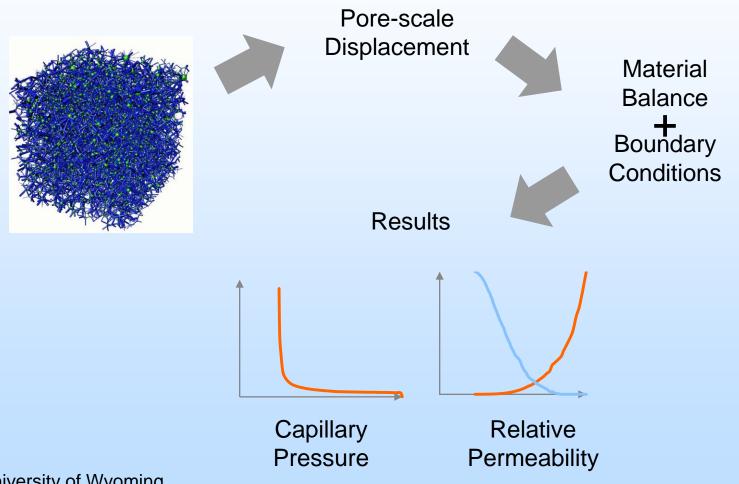
Millions of pores and throats. They represent the size, distribution and connectivity of micro pores.

# Development of physically-based dynamic pore-scale network model (Task 4)



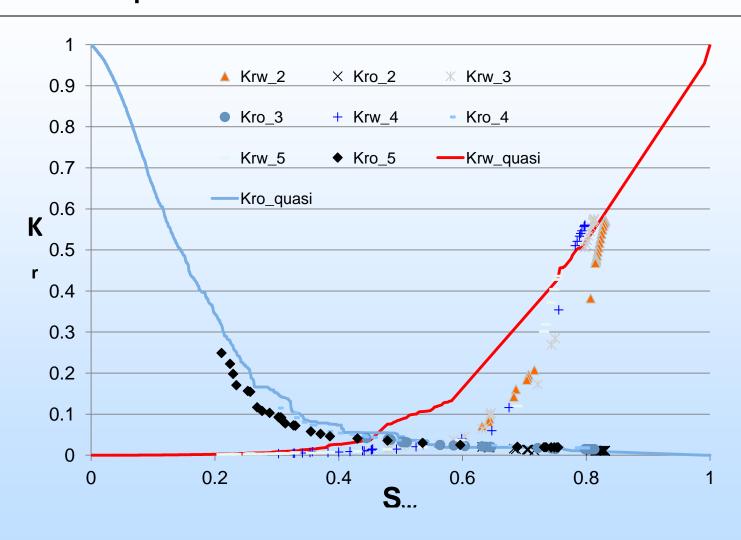
Equivalent pore network constructed for Bentheimer Sandstone using high-resolution microtomography images.

#### Development of physically-based dynamic pore-scale network model (Task 4)



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# Development of physically-based dynamic pore-scale network model (Task 4)



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# Modeling and Simulation Core and Field Scales

- Reservoir Modeling Activities
- Development of the UW-team Simulator

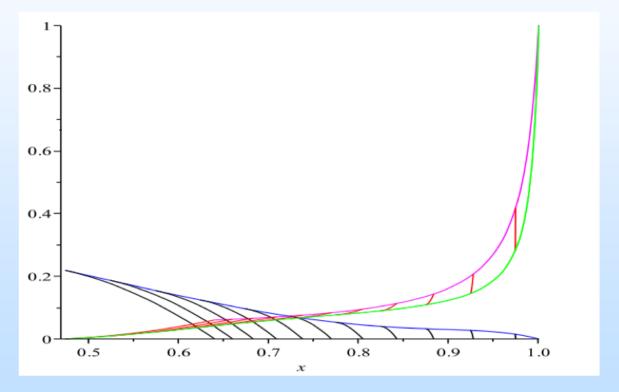
#### Reservoir Modeling Activities (Task 5)

#### Relative permeability hysteresis

- Construction of a mathematical model of two-phase relative permeability hysteresis measured experimentally at deep reservoir conditions
- Analysis of its wave structure, by solving the associated Riemann problem, and development of an appropriate numerical procedure for its simulation
- Code verification

### Reservoir Modeling Activities Relative Permeability Hysteresis

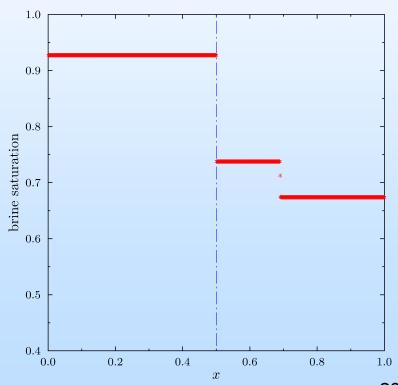
Two-phase relative permeability functions constructed to fit the experimental data



Brine saturation (x) vs. permeabilities (y).

### Reservoir Modeling Activities Relative Permeability Hysteresis

- Mathematical analysis (Riemann solutions) vs. numerical solutions
- Fully nonlinear system describing mass conservation and hysteresis effects
- Example:
- Gravity points to the left
- Solution: Stationary discontinuity and a right-propagating shock
- Naive numerical schemes: incorrect answer



### Development of the UW-team simulator

(Tasks 6 and 7)

- Multi-phase, multi-component, compositional model for CO<sub>2</sub> injection development
- To be used both at the core scale (model validation) and field scale (prediction of injected CO<sub>2</sub> location)
- Educational tool: code development (graduate course developed and taught), HPC

### Development of the UW-team simulator Strategy for discretization

- Operator splitting:
- The problem is decomposed into components representing relatively simple physics
- Accuracy: adequate numerical methods for distinct PDEs
- Computational efficiency: distinct time steps for distinct physical processes

Example: 2-phase flows

Example: 2-phase flows
$$(p_n, v_n)$$

$$(p_{n-1}, v_{n-1}, S_{n-1})$$

$$(S_{n-1}, v_n) \xrightarrow{\text{Transport}} S_n \xrightarrow{\text{new values}} (p_n, v_n)$$
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#### Development of the UW-team simulator Numerical methods

- Locally conservative procedures:
- Hyperbolic systems: Explicit, high-resolution Central Schemes
  - Riemann solvers not needed
  - Naturally parallelizable in CPU-GPU machines
  - Correct solutions: hysteresis
- Elliptic and parabolic problems: Mixed finite elements
  - Accurate velocity fields in the presence of rapidly varying coefficients
  - Parallelization through multiscale mixed methods in CPU-GPU machines

# Development of the UW-team simulator Model validation: Bayesian framework

#### Context

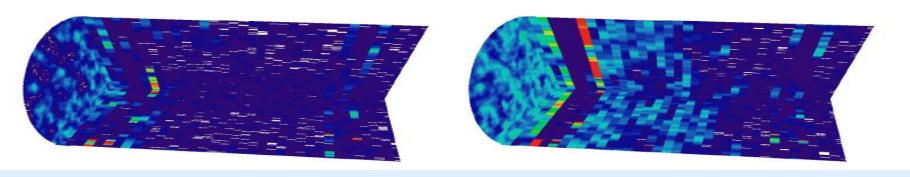
- Characterization at the mm scale
- Prediction at the core scale
- Goal: validation of the compositional model at the Darcy scale against experimental data

#### The framework for UQ: MCMC/MC

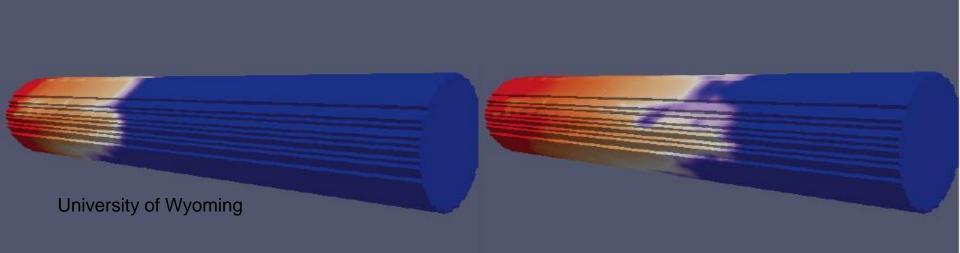
- Static data: porosity field at the mm scale (perm. field unknown)
- Dynamic data: saturation fields at the mm scale, pressure drop, production curve

# Development of the UW-team simulator Model validation: Bayesian framework

Reservoir-conditions drainage experiment



#### Simulation results



### Accomplishments to Date

- 1. Milestones 1-4 were completed:
  - Update Project Management Plan Hold kickoff meeting of Pls with govt. partners
  - Acquisition of rock samples and micro-CT images for pore-level network model
  - Measurement of unsteady-state core-flooding experimental data required for code validation
  - Measurement of steady-state relative permeabilities for code validation
- 2. A new state-of-the-art IFT and contact angle apparatus was built from scratch and validated
- 3. Development of fully parallel dynamic pore-scale network model is nearing completion
- 4. Development of hysteresis model was completed
- 5. Development of phase equilibrium calculation module for scCO<sub>2</sub>, SO<sub>2</sub>, and brine is nearing completion
- 6. Development of compositional simulator was completed
- 7. Code validation for the UW-Team simulator (Milestones 5) is on track for completion in September
- 8. Active dissemination of findings through publications and presentations in scientific meetings

### Summary

#### Key findings

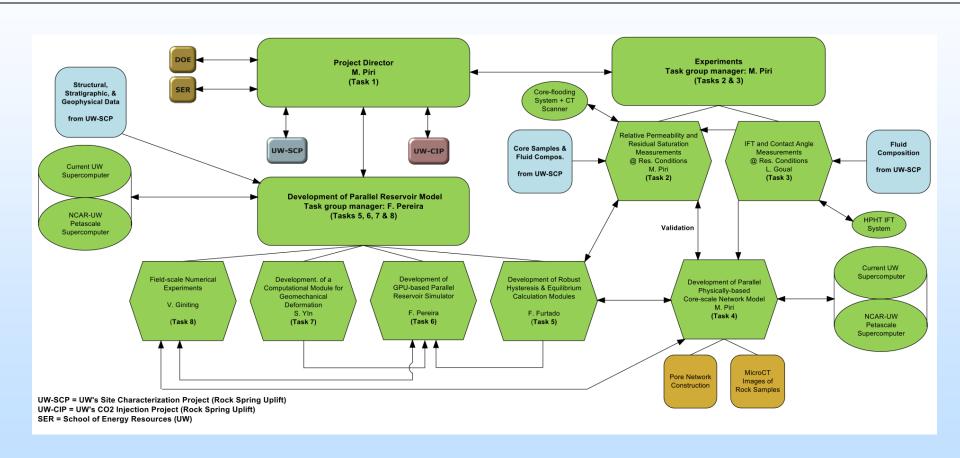
- Significant fractions of initial CO<sub>2</sub> in place can be stored through residual trapping
- Lower initial CO<sub>2</sub> saturation leads to higher trapping efficiency (R=S<sub>CO2r</sub>/S<sub>CO2</sub><sup>max</sup>)
- Trapping efficiency between 49 to 83% of CO<sub>2</sub> in place
- Accurate numerical approximation of transport problems with hysteresis

#### Future Plans

- Perform additional relative permeability and residual saturation measurement experiments at reservoir conditions
- Develop a fully parallel version of the phase equilibrium module
- Dynamic pore-scale modeling of imbibition in large networks
- Completion of geomechanics module
- Compositional reservoir simulations on large computer clusters, UQ studies

## Thank you

## Appendix-Organization Chart



### Appendix - Gantt Chart

Task	Description	BP1 - Year 1				BP2 - Year 2				BP3 – Year 3			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1	Project Management and Planning	8	17	25	33	42	50	58					
2	Measurement of mixed scCO <sub>2</sub> /brine steady-state drainage and imbibition relative permeabilities in samples from RSU at reservoir conditions	15	25	38	50	60	65	70					
3	Measurement of mixed scCO <sub>2</sub> /brine interfacial tension and contact angles at reservoir conditions	5	8	12	20	33	57	67					
4	Development of physically-based dynamic parallel corescale pore network model for samples from RSU	15	26	32	38	45	51	60					
5	Reservoir modeling activities	17	34	40	52	63	70	85					
6	Development of the UW-team simulator	5	10	25	33	50	65	75					
7	Development of a computational module for geomechanical deformation	0	0	0	10	18	30	60					
8	Field-scale numerical experiments	5	10	17	25	30	40	50					

# List peer reviewed publications generated from project per the format of the examples below

#### Journal, one author:

 Ginting, V., 2012, Time integration techniques for Richards equation. Procedia Computer Science, v. 5, p. 670-678, available at <a href="http://www.sciencedirect.com/science/article/pii/S1877050912001937">http://www.sciencedirect.com/science/article/pii/S1877050912001937</a>.

#### Journal, multiple authors:

- Akbarabadi, M., and Piri, M., 2011. Relative permeability hysteresis and permanent capillary trapping characteristics of supercritical CO<sub>2</sub>/brine systems: an experimental study at reservoir conditions, Advances in Water Resources, in press.
- Aquino, J., Francisco, A., Pereira F., and Souto H., 2011. A hybrid method for the simulation of radionuclide contaminant plumes in heterogeneous unsaturated formations. Progress in Nuclear Energy, v. 53, issue 8, p. 1159-1166, available at: <a href="http://www.sciencedirect.com/science/article/pii/S0149197011001600">http://www.sciencedirect.com/science/article/pii/S0149197011001600</a>

- Bi, C., and Ginting, V., 2011. Two-grid discontinuous Galerkin method for quasi-linear elliptic problems. Journal of Scientific Computing, v. 49, no. 3, p. 311-331, DOI: 10.1007/s10915-011-9463-9, available at: <a href="http://www.springerlink.com/content/r306035x11288485/">http://www.springerlink.com/content/r306035x11288485/</a>
- Douglas, C., Efendiev, Y., Ewing, R., Ginting, V., Lazarov, R., Cole, M.J., and Jones, G., 2011, Least-squares approach for data recovery in dynamic data-driven applications simulations. Journal of Computing and Visualization in Science, v. 13, no. 8, p. 365-375, available at: <a href="http://www.springerlink.com/content/f462x17j71543p22/">http://www.springerlink.com/content/f462x17j71543p22/</a>
- Estep, D., Ginting, V., and Tavener, S., 2012. A posteriori analysis of a multirate numerical method for ordinary differential equations. Computer Methods in Applied Mechanics and Engineering, v. 223, p. 10-27, available at:
   <a href="http://www.sciencedirect.com/science/article/pii/S0045782512000631">http://www.sciencedirect.com/science/article/pii/S0045782512000631</a>
- Furtado, F., Ginting, V., Pereira, F., and Presho M., 2011. Operator splitting multiscale finite volume element method for two-phase flow with capillary pressure. Transport in Porous Media, v. 90, no. 3, p. 927-947, DOI: 10.1007/s11242-011-9824-8, available at: <a href="http://www.springerlink.com/content/d432ph13736k211m/">http://www.springerlink.com/content/d432ph13736k211m/</a>

- Ginting, V., Pereira, F., Presho, M., and Wo. S., 2011, Application of the two-stage Markov chain Monte Carlo method for characterization of fractured reservoirs using a surrogate flow model. Computational Geosciences, v. 15, no. 4, p. 691-707, DOI: 10.1007/s10596-011-9236-4, available at: <a href="http://www.springerlink.com/content/l83x28477g67l418/">http://www.springerlink.com/content/l83x28477g67l418/</a>
- Ginting, V., and Presho, M., 2011. Model reduction techniques for characterization of fractured subsurfaces. Procedia Computer Science, v. 4, p. 938-947, available at: <a href="http://www.sciencedirect.com/science/article/pii/S1877050911001578">http://www.sciencedirect.com/science/article/pii/S1877050911001578</a>
- Ginting, V., Pereira, F. and Rahunanthan, A., 2012. Multiple Markov Chains Monte Carlo approach for flow forecasting in porous media, Procedia Computer Science, v. 9, p. 707-716, available at: <a href="http://www.sciencedirect.com/science/article/pii/S1877050912001974">http://www.sciencedirect.com/science/article/pii/S1877050912001974</a>
- Mendes, M., Murad, M., and Pereira F., 2011. A new computational strategy for solving two-phase flow in strongly heterogeneous poroelastic media of evolving scales. International Journal for Numerical and Analytical Methods in Geomechanics, DOI: 10.1002/nag.1067, available at: <a href="http://onlinelibrary.wiley.com/doi/10.1002/nag.1067/abstract">http://onlinelibrary.wiley.com/doi/10.1002/nag.1067/abstract</a>

- Pereira, F., and Rahunanthan, A., 2011, A semi-discrete central scheme for the approximation of two-phase flows in three space dimensions. Mathematics and Computers in Simulation, v. 81, issue 10, p. 2296-2306, available at: <a href="http://www.sciencedirect.com/science/article/pii/S0378475411000528">http://www.sciencedirect.com/science/article/pii/S0378475411000528</a>.
- Presho, M., Wo, S., and Ginting, V., 2011. Calibrated dual porosity, dual permeability modeling of fractured reservoirs. Journal of Petroleum Science and Engineering, v. 77, no. 3-4, p. 326-337, available at:
  - http://www.sciencedirect.com/science/article/pii/S0920410511000878

#### Publication:

- Francisco, A., Ginting, V., Pereira, F., and Rigelo, J., 2011. A multiscale mixed method for porous media flows. Proceedings of MAMERN11: 4th International Conference on Approximation Methods and Numerical Modeling in Environmental and Natural Resources, Saidia, Morocco, May 23-26.
- Barber, J., Ginting, V., Pereira F., and Rahunanthan, A., 2011. Dynamic data integration for characterization of fractured subsurface. Proceedings of MAMERN11: 4th International Conference on Approximation Methods and Numerical Modeling in Environmental and Natural Resources, Saidia, Morocco, May 22-26.
- Ginting, V., Pereira, F., Rahunaathan, A., 2012. Forecasting Production in an Oil Reservoir Simulation and Its Challenges, Proceedings of ENUMATH: 9th European Conference on Numerical Mathematics and Advanced Applications, Leicester, United Kingdom, September 5-9.
- Akbarabadi, M., and Piri M., 2011. Geologic storage of carbon dioxide: an experimental study of permanent capillary trapping and relative permeability.
   SCA2011-04: International Symposium of the Society of Core Analysts held in Austin, Texas, USA, September 18-21.