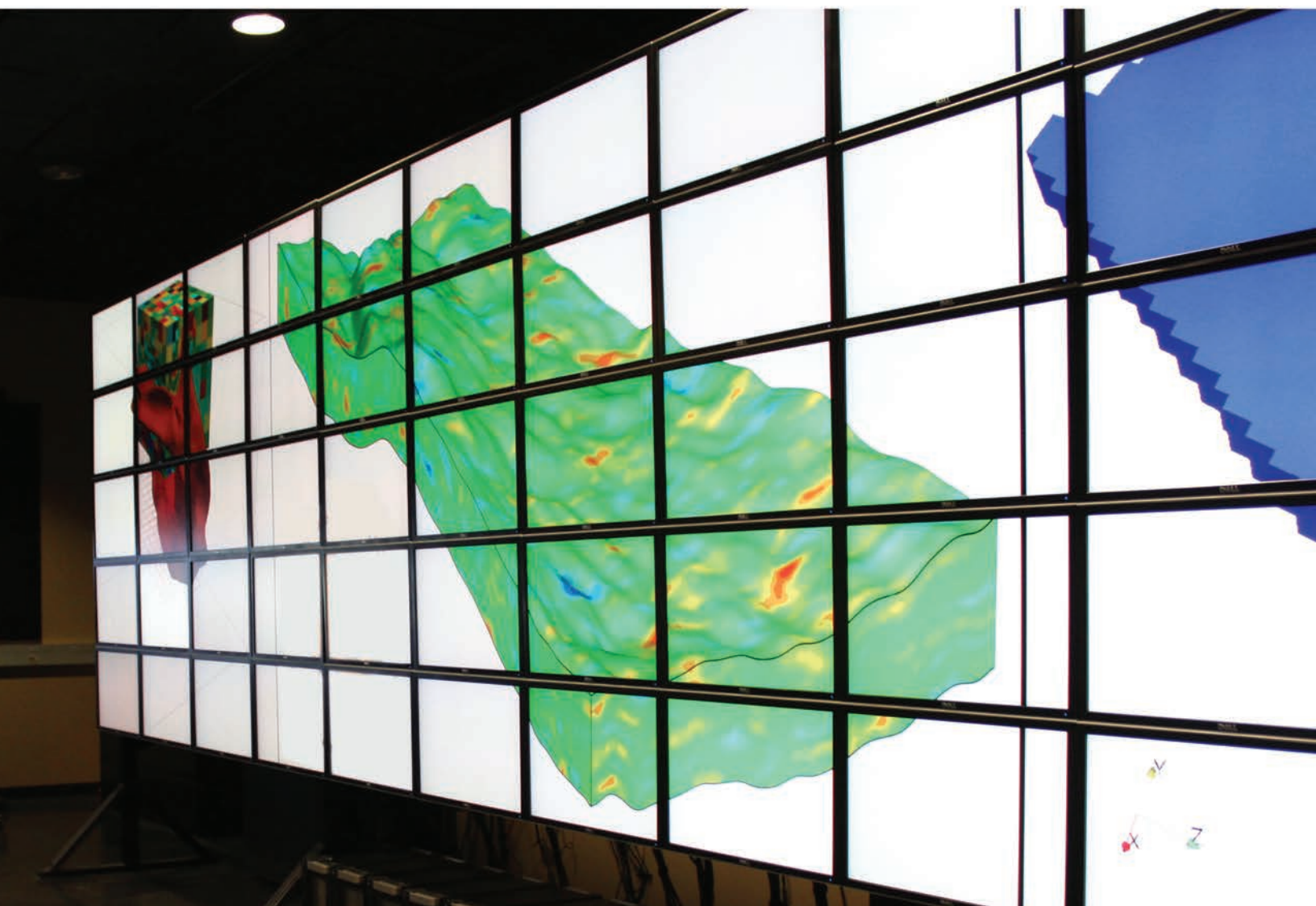




CENTER FOR SUBSURFACE MODELING

Institute for Computational Engineering and Sciences

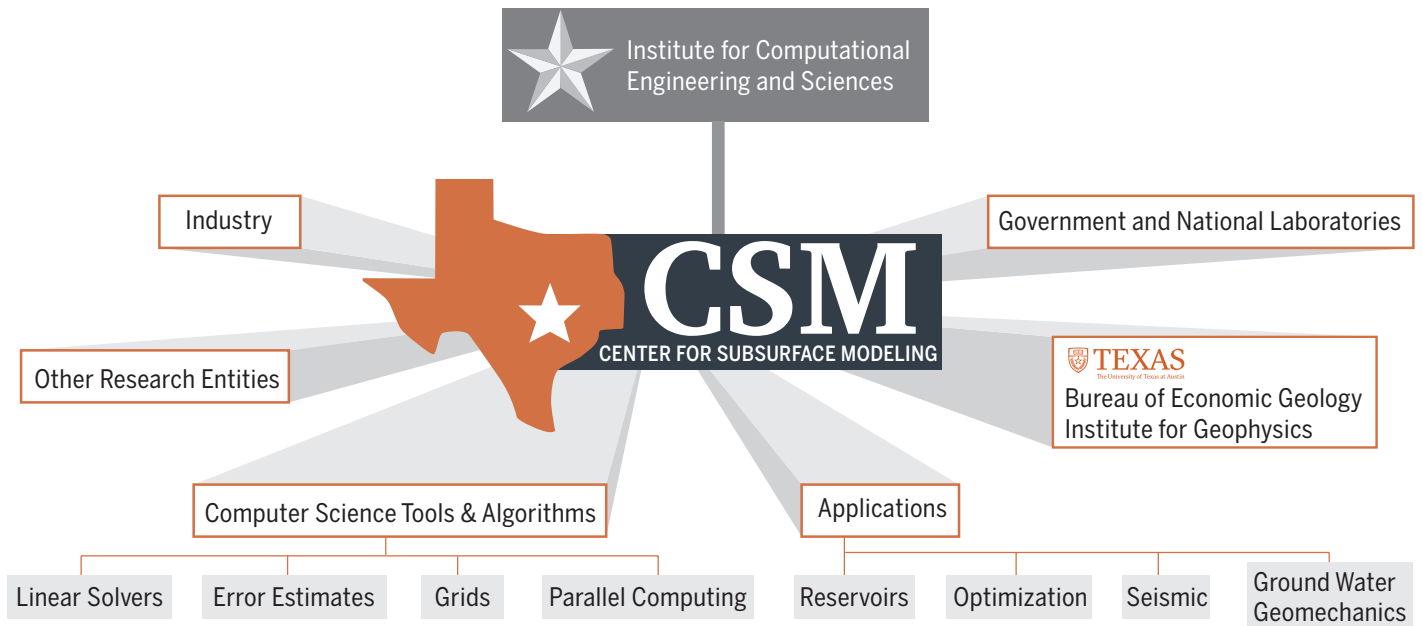
2016-2017



At the Center for Subsurface Modeling, we strive to meet today's numerical modeling challenges by bringing together mathematicians, engineers, geoscientists, and computational scientists in a cooperative environment. We believe that a multidisciplinary approach is the best way to obtain accurate, reliable, and efficient solutions to real-world problems.

We actively work with academic and industrial collaborators throughout the world to deliver cutting edge scientific advancements in the form of toolsets for subsurface applications. Our research continually seeks to improve our physical understanding of subsurface phenomena using consistent mathematical modeling and advanced numerical solution techniques. We use high performance computing to reduce computational costs associated with complex models. Funds from our Industrial Affiliates program and federal agencies have helped us to develop our own parallel computing environment, which enables us to test and prove new concepts in advanced modeling and simulation.

In a rapidly changing world, the Center for Subsurface Modeling is dedicated to developing solutions to tomorrow's modeling challenges - *today*.



2016 Highlight: Professor Mary F. Wheeler Receives Grand Challenge Award

Four faculty received ICES' 2016 W.A. "Tex" Moncrief Grand Challenge Awards, based on their highly compelling research proposals related to the Grand Challenges in computational engineering and sciences that affect the competitiveness and international standing of the nation.

Wheeler's project will develop a simulation to identify the likelihood of sinkholes developing from injection of wastewater and carbon sequestration in the subsurface. Research has already established that the formation of sinkholes requires three conditions: (1) presence of a thick dissolvable rock formation (like salt caverns); (2) large, higher temperature, fluid flow rates of unsaturated fluid, and (3) conditions for mechanical destabilization and rock failure. Wheeler's group will conduct computational studies of the microscopic degree to which each of these conditions must exist for the sinkhole to occur. This includes taking into account common rock and cavern environments, paired with the components of the wastewater or rate of carbon sequestration.

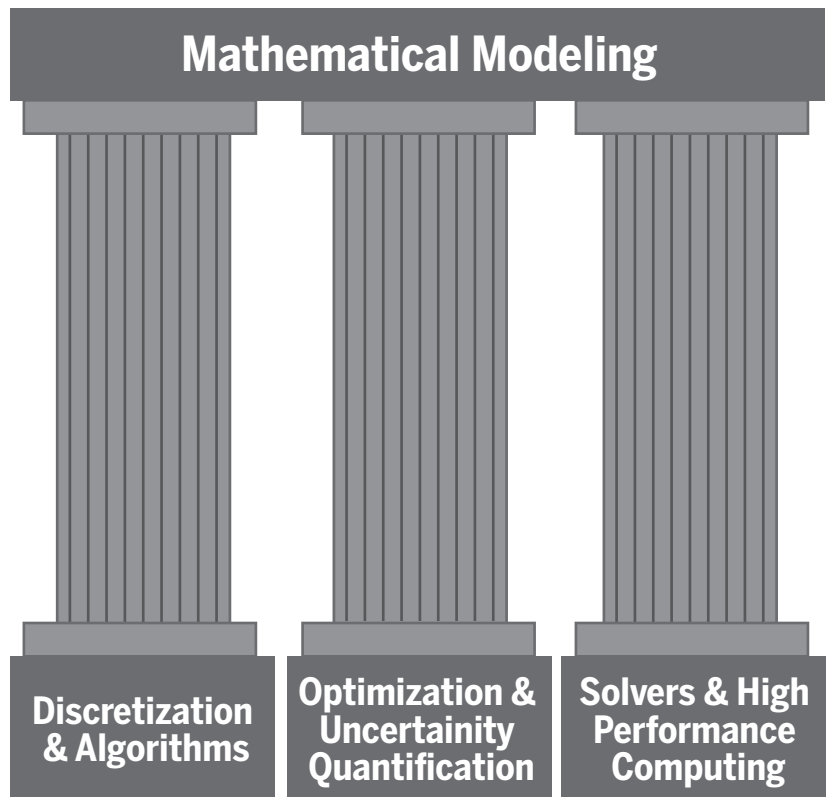


ICES' 2016 Moncrief Grand Challenge Awardees: Thomas Hughes, professor of aerospace engineering and engineering mechanics; Chandrajit Bajaj, professor of computer science; Mary Wheeler, professor of aerospace engineering and engineering mechanics, and of petroleum and geosystems engineering; and Ofodike "DK" Ezekoye, professor of mechanical engineering.

Research

An accurate description of complex subsurface phenomena warrants understanding of the underlying physical processes using consistent mathematical modeling and robust numerical solution techniques. Such models require parameter estimation using novel history matching approaches to quantify the uncertainties associated with subsurface heterogeneities. CSM researchers collaborate with experts spanning across various disciplines to model flow and transport of fluids in reservoirs of varying complexities (heterogeneous media; fractured and vuggy) accounting for fluid phase behavior, geochemical reactions and geomechanical deformations (subsidence).

These modeling advancements are implemented in our in house reservoir simulator (IPARS – Integrated Parallel Accurate Reservoir Simulator) or available as stand alone toolsets for specific applications. Our model developments assist industrial affiliates in their field deployment efforts.



Research Projects

Modeling and Applications

- CO₂ Sequestration Modeling
 - Long term storage evaluation in saline aquifers
 - Geochemical and physical (hysteretic capillarity and relative permeability) trapping
 - Case studies: CO₂ injection into Cranfield and Bravo Dome fields
- Enhanced Oil Recovery Modeling
 - Chemical enhanced oil recovery: alkali, surfactant, polymer
 - Gas flooding: CO₂, N₂ + flue gases
 - Foam flooding
 - Phase behavior models: chemical and gas flooding
 - Field scale studies using parallel simulations
- Fractured Reservoir Modeling
 - Phase-field modeling for hydraulic fracture propagation
 - Coupled flow and geomechanics modeling for fractured reservoirs
 - Integrated toolset for fractured reservoir management
- Melt Migration
 - Multiphase Darcy-Stokes flow
 - Robust numerical algorithms

Discretization and Error Estimation

- Eulerian-Lagrangian schemes for transport and fluid-structure interaction
- Discontinuous Galerkin method for two phase flow with capillary pressure
- Mimetic finite difference method on polyhedral elements
- Multipoint flux method on distorted hexahedra, including full tensor permeability, iteratively coupled poroelasticity, and equation of state compositional flow

- Robust a posteriori error estimation with multiphase flow using temporal, nonlinear, linear, and spatial error indicators
- Representation of non-planar fractures and interfaces
- Enhanced velocity method with nonmatching hexahedral grids
- Convergence and stability analysis of iterative flow & geomechanics coupling algorithms

Optimization, Data Assimilation, and Uncertainty Quantification

- Multidimensional scaling, clustering, model selection, and parameterization
- Stochastic collocation and Monte Carlo methods
- Bayesian model comparison and model averaging
- Production optimization and control
- Reservoir history matching with parameter estimation using parallel ensemble-based workflow
- Integration of time-lapse (4D) seismic and geomechanical data into reservoir models

Solvers and High Performance Computing

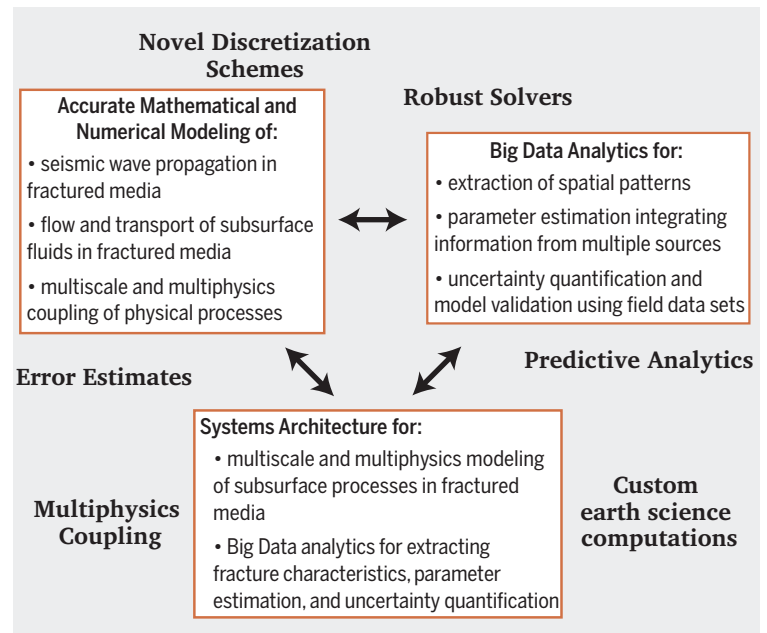
- Multiscale, multiphysics, and multinumerics coupling (flow, mechanics, energy balance, and chemistry)
- Domain decomposition and mortar method
- Multilevel, multigrid, and other specialized preconditioners
- Unconstrained optimization algorithms for nonlinear flow solvers

BIGDATA: Collaborative Research: IA: F: Fractured Subsurface Characterization Using High Performance Computing and Guided by Big Data *(funded by NSF)*

Natural fractures act as major heterogeneity in the subsurface that control flow and transport of subsurface fluids and chemical species. Their importance cannot be underestimated, because their transmissivity may result in undesired migration during geologic sequestration of CO₂, they strongly control heat recovery from geothermal reservoirs, and they may lead to induced seismicity due to fluid injection into the subsurface. Advanced computational methods are critical to design subsurface processes in fractured media for successful environmental and energy applications.

This research emphasizes high performance computation (HPC) approaches for characterizing fractures using large subsurface seismic data sets, BIG data analytics for extraction of fracture related information from seismic inversion results and long-duration dynamic data, and advanced computational approaches for modeling flow, transport, and geomechanics in fractured subsurface systems.

Successful completion will enable design of technologies for addressing key societal issues such as safe energy extraction from the surface, long-term sequestration of large volumes of greenhouse gases and safe storage of nuclear waste in the subsurface.



Overview of the three-tiered research plan for fractured subsurface characterization

Computational Models for Evaluating Long Term CO₂ Storage in Saline Aquifers

(funded by NSF and KAUST through the Academic Excellence Alliance Program)

Geologic sequestration is a proven means of permanent CO₂ greenhouse gas storage, but it is difficult to design and manage such efforts. Predictive computational simulation may be the only means to account for the lack of complete characterization of the subsurface environment, the multiple scales of the various interacting processes, the large areal extent of saline aquifers, and the need for long time predictions. This project investigates high fidelity multiscale and multiphysics algorithms necessary for simula-

tion of multiphase flow and transport coupled with geochemical reactions and related mineralogy, and geomechanical deformation in porous media to predict changes in rock properties during sequestration. The work will result in a prototypical computational framework with advanced numerical algorithms and underlying technology for research in CO₂ applications, which has been validated and verified against field-scale experimental tests.

Center for Frontiers of Subsurface Energy Security *(funded by DOE)*

Currently mankind extracts most of the fuel for the global economy from underground. The byproducts of consuming this fuel enter the atmosphere or remain on the surface. This situation is no longer tenable. A critical step toward future energy systems will be the ability to cycle fuel byproducts back to their original home: the Earth's subsurface. Applications of this concept include storing CO₂ in deep geologic formations and securing radioactive materials in appropriately engineered repositories. Our goal is to fill gaps in the knowledge base so that subsurface storage schemes are reliable from the moment they open. Two scientific Grand Challenges, which will be investigated in this project, contribute to the gap between forecast and outcome in geologic systems. First, byproduct storage schemes will

operate in a far-from-equilibrium state. Second, it is difficult to explain the emergence of patterns and other manifestations of correlated phenomena across length and time scales.



Collaborative Research: Error Estimation, Data Assimilation and Uncertainty Quantification for Multiphysics and Multiscale Processes in Geological Media *(funded by NSF)*

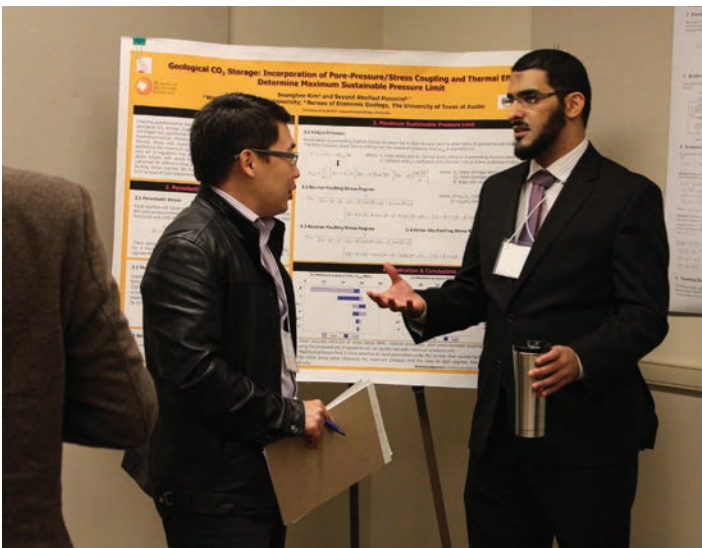
The application of high performance computing to model subsurface processes occurring over multiple spatial and temporal scales is a science grand challenge that has important implications to society at large. Research on this grand challenge is at the confluence of advanced mathematics, computer science, fluid and solid mechanics and applied probability and statistics. We are engaging in a fresh new perspective by investigating and formulating rigorous error estimators for the numerical schemes employed to model multiphysics, multiscale processes in subsurface media. These error estimators, when coupled with advanced computational methods, can significantly speed up the task of uncertainty assessment and feedback control of subsurface processes.

We are also developing a uncertainty quantification scheme that will utilize the error estimators and rigorous quantification of prior geologic uncertainty. Underlying the computational and uncertainty quantification schemes will be a computer framework that rigorously takes into account the dynamic and complex communication and coordination patterns resulting from multiphysics, multinumetrics, multiscale and multidomain couplings. In addition, we will investigate realistic physical models such a carbon sequestration in saline aquifers with real field data from the Cranfield Mississippi demonstration site. The ultimate transformative goal is to achieve predictive and decisional simulations, in which engineers reliably predict, control, and manage human interaction with geosystems.

Multiscale Modeling and Simulation of Multiphase Flow Coupled with Geomechanics *(funded by DOE)*

This project develops algorithms that will enable scientists and engineers to readily model complex flow processes in porous media taking into account the accompanying deformations of the porous solids. Fluid motion and solid deformation are inherently coupled, but current major commercial packages for multiphase flow in porous media only model porous flow while solid deformation is normally integrated into a study in an ad hoc manner or must be included through complex iterations between one software package that models fluid flow and a separate package that models solid deformations. There are numerous field applications that would benefit from a better understanding and integration of porous flow and solid deformation. Important applications in the geosciences include environmental cleanup, petroleum production, solid waste disposal, and carbon sequestration, while similar issues arise in the biosciences and chemical sciences as well. Examples of field applications include surface subsidence, pore collapse, cavity generation, hydraulic fracturing, thermal fracturing, wellbore collapse, sand production, fault activation, and disposal of drill cuttings. The above phenomena entail both economic as well as environmental concerns.

Another important related class of problems involves CO₂ sequestration, which is proposed as a key strategy for mitigating climate change driven by high levels of anthropogenic CO₂ being added to the atmosphere. In a CO₂ sequestration project, fluid is injected into a deep subsurface reservoir (rather than being produced or extracted), so that inflation of the reservoir leads to uplift displacement of the overlying surface. As long as a CO₂ sequestration site is removed from faults, this uplift is several centimeters, while its wavelength is in tens of kilometers, so that the uplift poses little danger to buildings and infrastructure. Nevertheless the uplift displacements are of great interest for non-intrusive monitoring of CO₂ sequestration, which can be measured with a sub-millimeter precision using Interferometric Synthetic Aperture Radar (InSAR) technology. In contrast, intrusive monitoring via drill holes bored into the reservoir is expensive, with costs of several million dollars per well. Furthermore, such wells are the most likely pathway for future leakage of sequestered CO₂ back into the atmosphere. Of course, if a CO₂ sequestration site is close to a fault, one should be concerned about triggering instability leading to large surface displacements that may result in significant losses.

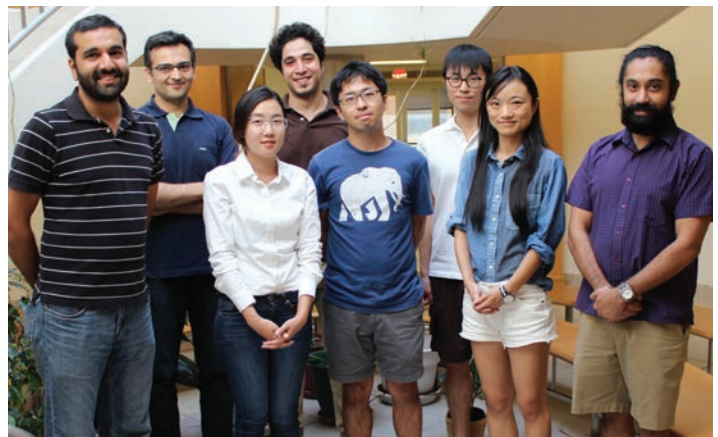


NETL: Development of Geomechanical Screening Tools to Identify Risk: An Experimental and Modeling Approach for Secure CO₂ Storage (funded by DOE)

Carbon dioxide is a reservoir pore fluid of much interest because of applications to enhanced oil recovery (EOR) and more recently because of the pressing needs for carbon dioxide geological storage as an option to reduce CO₂ emissions to the atmosphere. Although CO₂ has been used for decades in EOR, successful carbon geological storage at commercial scale requires enhanced storage efficiency and safe CO₂ containment over thousands of years.

The main objectives of this project are to:

- Measure petrophysical and hydro-mechanical properties of rocks in the presence of CO₂ in the laboratory. Perform these experiments under varying conditions of temperature and chemical reactivity of rocks with CO₂
- Develop upscaling methods for rock petrophysical and hydro-mechanical properties considering natural heterogeneity and pre-existing fractures
- Develop advanced and cost-effective coupled solvers for simulations of coupled flow and geomechanics
- Simulate numerically and perform history matching of CO₂ injection results at a field sites
- Develop schemes for quantifying the residual uncertainty after model calibration and data assimilation
- Quantify reservoir overpressure and strains caused by pore pressure, thermal and chemical loadings; show the influence of each type of loading and the occurrence of emergent phenomena
- Predict reservoir fluid composition after injection, which would serve as an input for evaluating geochemical reactivity of CO₂ at in potential leaks through fractures and faults.
- Develop guidelines to mitigate the risks of CO₂ injection in the subsurface.



Simulation of the Cranfield CO₂ Injection Site with a Drucker-Prager Plasticity Model

Coupled fluid flow and geomechanics simulations have strongly supported CO₂ injection planning and operations. Linear elasticity has been the popular material model in CO₂ simulation for addressing rock solid material behaviors. On the other hand, nonlinear constitutive models can take into account more realistic rock formation behaviors to model complex, chemically active, and fast injecting operations. For example, failure or damage may occur for rock formation near wellbores due to high fluid injection pressures or flow rates. The damaged formation near wellbores results in the changes in rock porosity or permeability, which impacts fluid flow behaviors. Such failure or damage of rock formations can be well described by the Drucker-Prager plasticity theory.

The Drucker-Prager plasticity solid mechanics module has been implemented into IPARS. The coupled poro-plasticity system is solved using an

iterative coupling scheme: the nonlinear flow and mechanics systems are solved sequentially using the fixed-stress splitting, and iterates until convergence is obtained in the fluid fraction. The application of this algorithm is new for poro-plasticity. To achieve fast convergence rates, a material integrator is consistently formulated that gives quadratic convergence rates. An enhanced parallel module for general hexahedral finite elements is also developed for IPARS for solving large-scale problems in parallel. A Cranfield CO₂ injection model is set up according to the reservoir geological field data and rock plasticity parameters based on Sandia national lab experimental results, and our model predicts both CO₂ flow and solid deformation.

This is a joint work with Ruijie Liu, Associate Professor in the Department of Mechanical Engineering at The University of Texas at San Antonio. Geomechanical data on the Cranfield Reservoir was provided by Tom Dewers at Sandia National Laboratories.

Figure 1. Comparison of elasticity (left) and plasticity (right) models with homogeneous parameters and rectangular geometry. Fluid pressure, vertical displacement, and plastic strain are shown.

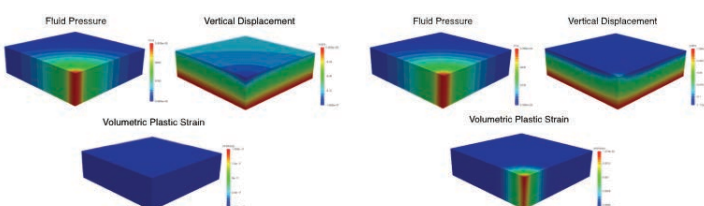
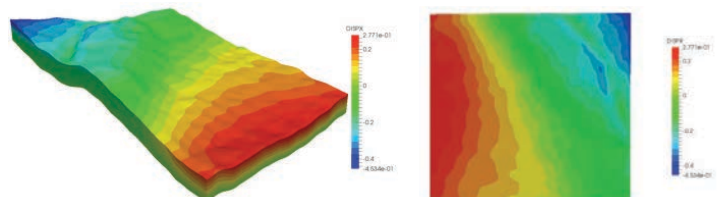


Figure 2. Elasticity model with heterogeneous Cranfield properties and geometry. 3D (left) and 2D (right) plots of the vertical displacement component at final simulation time.



Phase Field Fracture Propagation Model

The design and evaluation of hydraulic fracturing jobs are critical for efficient production from shale oil and gas fields. The efficiency depends on the interaction between hydraulic (induced) and naturally occurring discrete fractures. A rigorous fracture propagation model is therefore necessary to predict fracture growth pattern in a heterogeneous, anisotropic poroelastic medium.

We study the lower-dimensional fracture surface approximated by a phase field function, where phase field is an indicator function with diffusive crack zones, which is based on gamma-convergent approximations of free discontinuity problems. The most important advantage for using the phase field is that fracture nucleation, propagation, kinking, and curvilinear paths are automatically included in the model; post-processing of stress intensity factors and re-meshing resolving the crack path are avoided. In addition, as an indicator function we can easily couple with the reservoir simulator.

Our phase field model solves a coupled flow problem for the reservoir and fracture domains to determine pressure distribution along the fracture with fixed stress algorithm. The fracture pressure is then assumed to be in equilibrium with the normal component of the reservoir stresses at the fracture interface for both approaches. A brittle fracture theory, as originally presented by Griffith, is invoked along with its underlying assumptions to determine a fracture growth rate and failure criterion. We further extend this model with quasi-Newtonian flow and transport equation for multi physics problem employing locally conservative flow by enriched Galerkin approximation.

Figure 1. Growth of three parallel penny-shaped fractures in 3D using the active set method. The middle fracture growth is shunned by stress shadowing effect similar to those studied in 2D fracture growth (ICES Report 14-20).

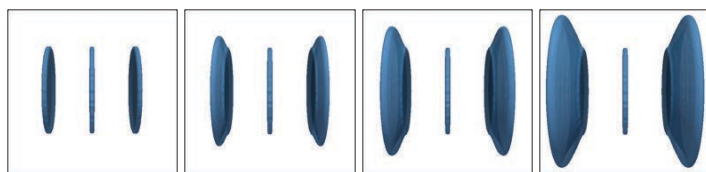
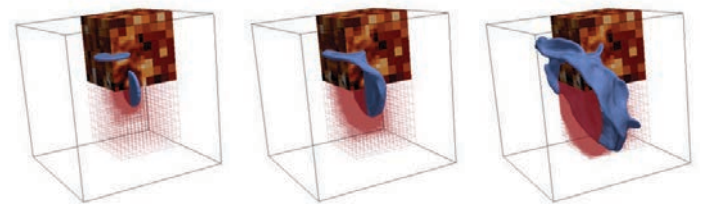


Figure 2. Fractures propagating at each time in 3D heterogeneous media. Both initial fractures grow non-planar then they join and branch. We observe the adaptive mesh around the fractures.



This development is a joint effort being carried out at the Center for Subsurface Modeling in collaboration with Andro Mikelić (Professor, at the Université Lyon 1) and Thomas Wick (Research Scientist, Austrian Academy of Sciences).

2016 Highlight: CSM Hosted a Workshop for High School Students on the Use of Science, Computations and Mathematics to Protect the Future of the Earth



In July, the Center for Subsurface Modeling hosted a workshop to inform and challenge high school students and their teachers to think about the emerging interdisciplinary role of mathematics and computational science in the simulation and solution of the Grand Challenges of Science. Sponsored by the National Science Foundation, the students addressed one of the world's "Grand Challenges for Engineering:" the build-up of greenhouse gases in the atmosphere, such as carbon dioxide (CO_2).

Included were discussions of laboratory and field experiments, mathematical modeling, numerical approximations, implementations of computational algorithms, and aspects of high performance parallel computing as applied to the environmentally important carbon storage problem. The students discussed the challenges of one solution to this problem: geologic sequestration.

Geologic sequestration is a proven means of permanent CO_2 greenhouse gas storage. However, it is challenging to design and

manage the many elements needed to properly characterize the subsurface environment, understand the complex physical and chemical processes involved, accurately assess and reduce risks and assure the permanency of geological storage of CO_2 . The students explored how mathematics and computational science have an essential role in better understanding and modeling some of these fundamental processes of earth systems as they relate to carbon storage.

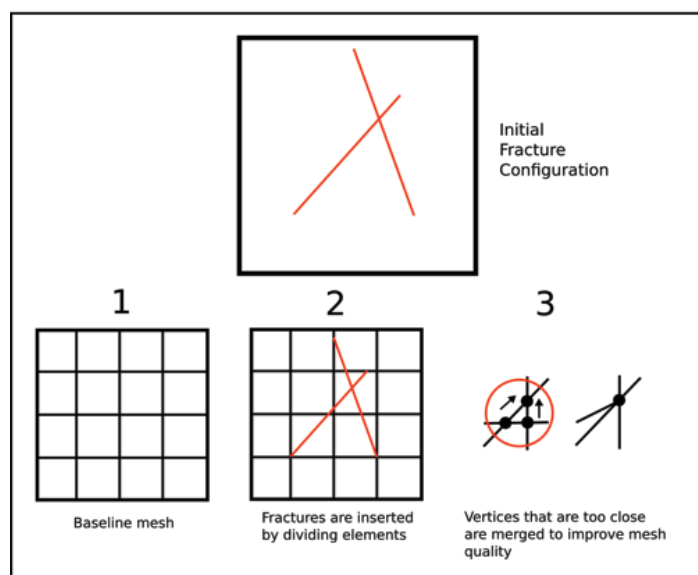
Ensemble-based Uncertainty Quantification Method for Fractured Reservoirs

Reservoir production management and optimization requires the characterization of the uncertainty in reservoir description. For fractured reservoirs, the connectivity of fracture distributions is crucial for predicting production characteristics. In this case, since the rock property fields are highly non-Gaussian, a method that combines vector-based level-set parameterization technique and ensemble Kalman filter (EnKF) or estimating fracture distributions is developed. The mimetic finite differences approach is utilized as forward model.

Mimetic finite differences approach

Modeling fluid flow through fracture networks is challenging due to the geometric characteristics of fractures. Using traditional hexahedral or tetrahedral mesh generation is not a tenable option, as it is difficult to maintain mesh quality and a reasonable number elements. In addition, the context of uncertainty quantification adds further challenges. Our approach has been to circumvent traditional mesh generation by using methods that allow for general polyhedral elements. First, a baseline rectangular grid is generated over the computational domain. Then, using an in-house utility, simple polygon division operations incorporate the fracture into the mesh. This produces a very fast and robust system for meshing complex fracture networks. The meshes are then passed into Mimpy for forward modeling of the two-phase fluid system. We refer to the fracture workflow code as MFDFrac.

Figure 1. Fast and robust polyhedral mesh generation



Parameterization using vector-based level-set method

For reservoirs with complex geology, a good estimation of the geological structures is very important for predicting and optimizing reservoir production. As the property fields of complex reservoirs are usually of bimodal or multimodal distributions, the Gaussian limitation is a major challenge for the application of the EnKF in the estimation of complex reservoirs. In order to improve the performance of the EnKF for highly non-Gaussian problems, we developed vector-based level-set parameterization method. Compared to the original multimodal distributed parameters, the transformed parameters are in better agreement with the EnKF Gaussianity limitation, which can be updated using the standard EnKF. This approach is flexible. For different types of complex geology, different parameter vectors can be used to describe the features of the reservoirs appropriately.

Applications

We apply this method on a synthetic two-dimensional two-phase fractured reservoir. After updating, the features of fracture distribution in reference field could be captured, and the matches of production data are more reliable.

In conclusion, the combination of mimetic finite differences approach, level-set parameterization and EnKF provides an effective solution to address the challenges in the history matching problem of highly non-Gaussian fractured reservoirs.

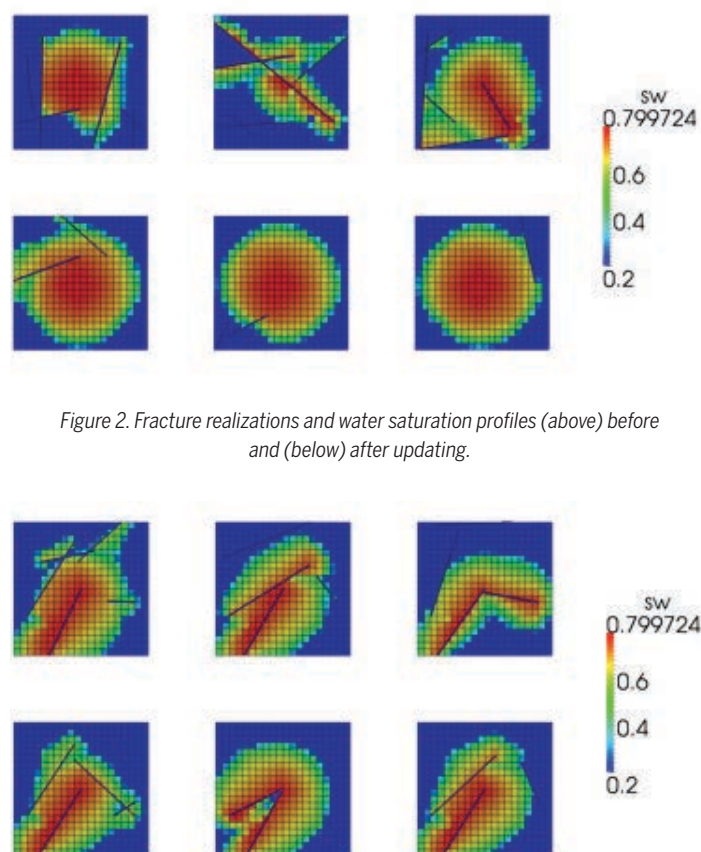


Figure 2. Fracture realizations and water saturation profiles (above) before and (below) after updating.

An Improved 3D Polymer Model

This research aims to develop a three-dimensional, shear-thinning, non-Newtonian flow model to simulate field scale polymer flooding as a tertiary oil recovery mechanism. The viscosities are calculated based upon direction dependent shear-rates. This provides an accurate representation of the non-Newtonian flow behavior in a three dimensional porous medium. The model considers a full-tensor permeability (3×3 matrix with non-zero off diagonal values) as a measure of resistance (or shearing) to flow. The shear-rate is then calculated as a function of the directional permeability and polymer phase velocity. Consequently, the shear-rate dependent fluid viscosity varies with direction resulting in an accurate physical description of shear thinning flow behavior in a three dimensional porous medium. The form of the velocity dependent permeability tensor, or in other words the coefficient in front of the gradient of pressure, is guided by a pore-scale non-Newtonian, Navier-Stokes flow solution on an assumed representative element volume (REV).

The model developments are being implemented and tested approach in IPARS (Integrated Parallel Accurate Reservoir Simulator). A multi-point-flux mixed finite element (MFMFE) scheme is further used for spatial

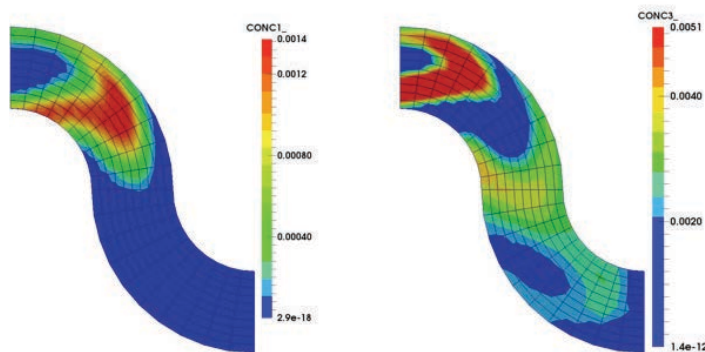
discretization of the associated partial differential equations. This scheme provides accurate fluid velocities at the faces of each element, which further improves viscosity calculations. A retardation factor, for polymer concentration, is further used to study the effect of polymer adsorption on recovery predictions. Additionally, we also consider viscosity variation due to changes in polymer concentration. Preliminary results show significant differences in sweep efficiencies due to changes in polymer front behavior, when compared to conventional models. The shear-thinning polymer viscosity is shown to decrease in a direction of low permeability and high pressure gradient (high shear rates) resulting in better sweep efficiencies. The results also show that the velocity dependent dispersion of polymer concentration is better represented due to accurate fluid velocities at the grid element faces.

This development is a joint effort being carried out at the Center for Subsurface Modeling in collaboration with Kundan Kumar (Associate Professor, University of Bergen, Norway). We also acknowledge Thomas Wick (Research Scientist, Austrian Academy of Sciences) for his deal.II fluid structure interaction toolset for solving non-Newtonian Navier Stokes flow in the REV.

Advanced Reactive Chemistry Modeling for Reservoir Flow and Transport

The local equilibrium assumption is a well-known simplification to describe instantaneous processes, with widely different time scales when compared to flow time scales. In this proposed work, we employ this assumption for modeling both volumetric and surface processes. This work aims to model physical and chemical processes, which can be broadly categorized as equilibrium and kinetic type. This classification differs from chemical equilibrium and kinetics, which strictly refer to ionic interactions. We propose to develop more general equilibrium and kinetic models, which will account for weak physical interactions such as van der Waals interactions in addition to the ionic interactions. This will allow us to predict wettability alteration due to adsorption/desorption of both polar and non-polar molecules. The model developments will be implemented in IPARS (Integrated Parallel Accurate Reservoir Simulator) under the TRCHEM reactive chemistry module. Application areas include hydrocarbon recovery prediction from low salinity water floods, reservoir characterization and diagnostic techniques using nano-particle injection engineered to mimic specific chemical species behavior.

Figure. Nanoparticle transport in a curvilinear reservoir: Nanoparticle slug injection with adsorption (left) and multiple nanoparticle slug injection (right) without adsorption.



Homogenization for Upscaling Reservoir Flow and Transport

Upscaling reservoir properties is pivotal for reducing uncertainty during parameter estimation and history matching. Further the computational cost is also lowered due to a reduced number of degrees of freedom. Upscaling single-phase flow entails estimating coarse scale, effective permeability from a given fine scale permeability distribution. However, this effective reservoir property calculation as an upscaling method holds true only for a single-phase flow process. Upscaling multiphase flow and reactive transport processes require calculation of effective coefficients which are different from known reservoir properties such as permeability, porosity etc. In this work, we use a two-scale homogenization method to evaluate these process

dependent effective coefficients. This method consistently upscales the partial differential equations associated with the flow and transport processes from fine to coarse scale in a mass conservative sense. Thus, the approach is physically accurate and mathematically consistent at both reservoir scales.

This is a collaborative effort with Hans van Duijn (Professor, Eindhoven University of Technology, Netherlands) and Dr. Andro Mikelić (Professor, University of Lyon, France).

Model selection for reservoir characterization in CO₂ sequestration

The ideal reservoir characterization is achieved from a closed-loop system that integrates geological modeling, upscaling/downscaling, reservoir simulation, history matching, and production forecasts associated with unbiased uncertainty quantification. The initial step of reservoir characterization is to identify reservoir models from all plausible geologic scenarios reflecting prior uncertainty in reservoir description. CSM has been developing model selection that implements a proxy to image flow and geomechanical responses of geologic models for CO₂ sequestration (Figure 1). A fast approximation utilizes a partial coupling scheme to obtain pressure and stress fields sequentially. A particle tracking algorithm mimics flow paths of the

models, and a stress-field solver calculates displacements of the models caused by injected CO₂. The prior models showing similar proxy responses are grouped into clusters by multi-dimensional scaling and k-means clustering. Full physics simulations are run for cluster representatives to select the best-fit cluster, which is the group whose representative exhibits the smallest discrepancy between observed and estimated responses. The models in the best-fit cluster constitute the posterior model set. In summary, the posterior ensemble incorporating geophysical time-lapse observations is more representative of the reservoir than the larger prior ensemble.

Figure 1. Reservoir characterization coupled a connectivity-based proxy within a model selection framework

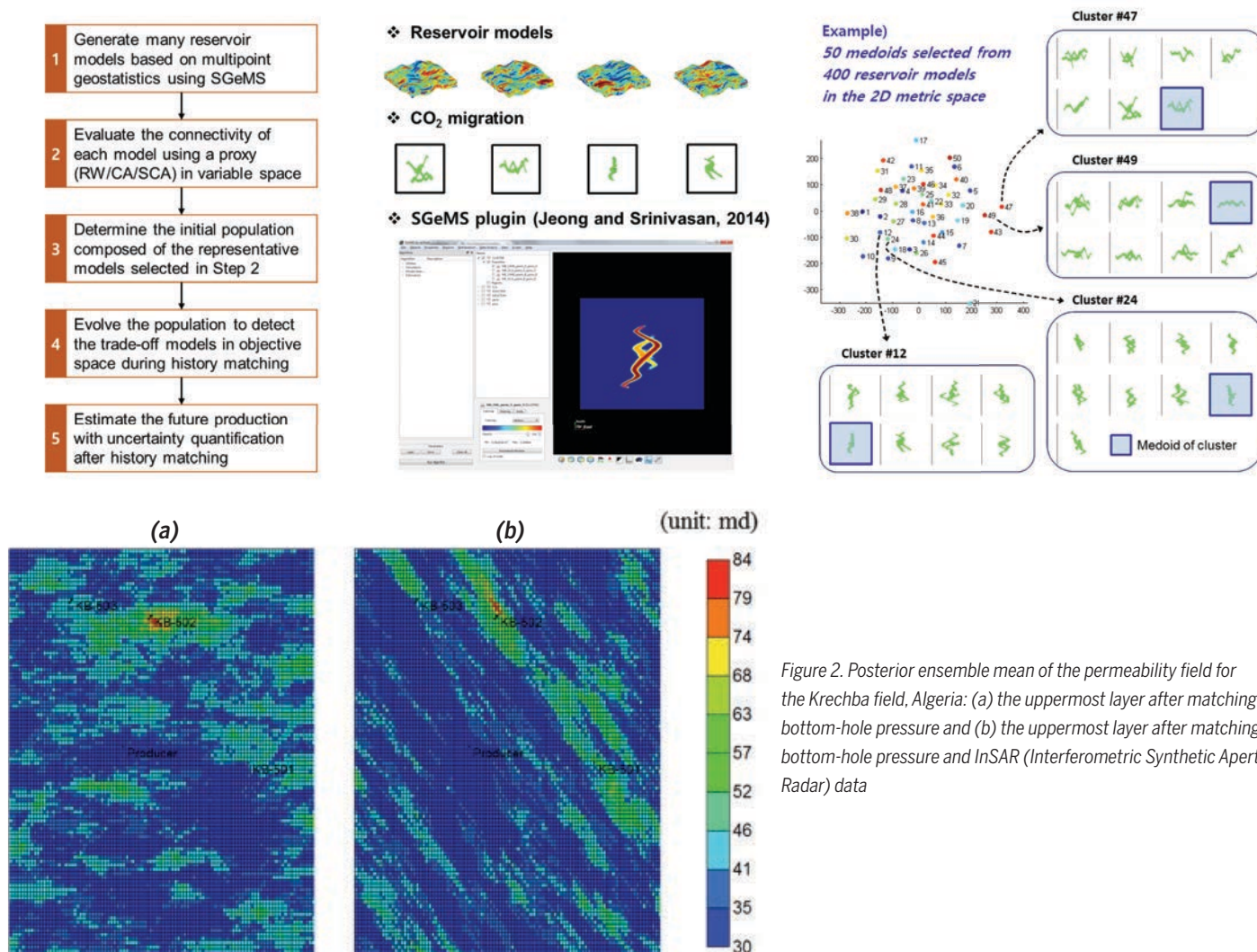


Figure 2. Posterior ensemble mean of the permeability field for the Krechba field, Algeria: (a) the uppermost layer after matching bottom-hole pressure and (b) the uppermost layer after matching bottom-hole pressure and InSAR (Interferometric Synthetic Aperture Radar) data

The CSM Staff



Connie Baxter

Sr. Administrative Associate
connie@ices.utexas.edu
Connie has been with CSM for 19 years and is responsible for day-to-day administration and event management.



Caitlyn Dambro

Sr. Office Assistant
caitlyn@ices.utexas.edu
Caitlyn has recently joined the CSM staff and is assisting with administrative duties.

Modeling Phase Behavior and Reactive Flow Occurring during Enhanced Oil Recovery Processes

The modeling of geochemical reactions is critical for managing production from reservoirs as they occur in all stages of production from an oil and gas field. Primary production from shale gas fields is modeled as adsorption reactions. Geochemical reactions also impact rock wettability that is making low salinity water flooding, an increasingly popular secondary production process. Tertiary recovery process of gas injection relies on accurate phase behavior analysis of hydrocarbon-injected gas mixture that is also impacted by geochemical reactions. A series of projects have been initiated to model the geochemical reactions for these different applications.

CO₂ injection in oil reservoirs has the dual benefit of enhancing oil recovery as well as sequestering a greenhouse gas. CO₂ injected in carbonate reservoirs, such as those found in the Middle East, can react with ions present in the brine and the solid calcite in the carbonate rocks. These geochemical reactions impact the phase behavior of in-situ hydrocarbon fluids and prediction of miscibility pressures thereby impacting oil recovery predictions from compositional simulations. Hence, it is important to model the impact of geochemical reactions on real oil during CO₂ injection.

A practical method to use the Gibbs free energy function for integrating phase equilibrium computations and geochemical reactions has been developed. This method has the advantage of combining different thermodynamic models - the hydrocarbon phase components normally characterized using an Equation of State (EOS), while the aqueous phase components usually described using an activity coefficient model.

The first project seeks to quantify how geochemical reactions impact oil recovery predictions during CO₂ injection in carbonate reservoirs. A real oil sample (Shell field courtesy * Birol Dindoruk) shall be used to show how a combination of Pitzer activity coefficient model and Peng Robinson (PR) Equation of State can result in changes in oil recovery predictions. In a separate project, the impact of geochemical reactions on the minimum miscibility pressure predictions shall be quantified using this approach. The

change in minimum miscibility pressure in the presence of geochemical reactions depends on two factors: 1) the volume ratio (and hence molar ratio) of the aqueous phase to the hydrocarbon phase and 2) the salinity of the brine. The modified phase behavior, arising out of geochemical reactions, will be implemented in our in-house reservoir simulator IPARS (Integrated Parallel Accurate Reservoir Simulator).

In a third project, the convergence properties of different activity coefficient models shall be analyzed to identify the model most suited for compositional simulation. This shall help implement the most appropriate model that can integrate phase behavior computations as well as geochemical reactions.

In addition to above research projects pertaining to gas flooding process, we are initiating projects to help explain the low salinity water flooding project. The objective is to identify and isolate the geochemical reactions that are responsible for changing rock wettability during the low salinity water flooding process. Core flood experimental data for different combination of brine ions and rock types shall be analyzed to isolate the ions that are likely responsible. In case of many ions, principal component analysis shall be used to statistically determine the main ions responsible for the process. Having isolated primary ions, the geochemical reactions responsible for the process shall be determined. An appropriate activity coefficient model shall be used to explain the observation of fluid outlet concentration. This will help make predictions on ion concentrations that should be injected to change rock wettability to enhance oil recovery.

In addition to above projects that focus on oil and gas production, geochemical reactions also have important applications in remediation of aquifers and safe disposal of nuclear wastes. The resulting changes in IPARS and TRICHEM shall be used for applications in these fields.

**This is a joint work with Birol Dindoruk at Shell Oil E&P Company.*

Detection and Quantification of Injected Gas Conformance and Breakthrough from Temperature and Pressure Measurements in Deepwater Wells during Gas EOR

Early detection of gas conformance in desired reservoir zones as well as its breakthrough from producing wells is critical for successful implementation of gas EOR projects. The installation of temperature and pressure sensors in deepwater wells are underway as they provide valuable data useful for flow analysis and quantification. Modeling using the sensor data is valuable since interventions in deepwater wells are either not possible or prohibitively expensive. In this study, temperature and pressure sensor data is used to model and monitor the conformance of injected gas. The presented model is further used for two applications 1) conformance of injected gas in an injection well and 2) identification of gas breakthrough from a production well. In this study, the production from a well producing from multiple reservoirs is modeled as a series of producing (vertical flow along with radial flow from a producing reservoir section) and non-producing (only vertical flow through the production tubing) zones. The energy balance and the momentum balance equations are coupled to quantify flow rates from individual producing reservoir sections. In addition to the sand face temperature mea-

surements, surface temperature, total surface flow rate as well as pressure and temperature measurements in the producing tubing are used as input to the model. A difference between the temperature and pressure data obtained from the sensors and that obtained from the model is used to detect and quantify gas conformance in injection well as well as gas breakthrough in production well.

The temperature data can be used to identify locations of producing and non-producing zones in the reservoir and quantify production from individual producing zones. This model will help determine the number of temperature and pressure sensors required for conformance of gas injected as well as effective detection of gas breakthrough in producing wells. The model can also be adapted to detect water breakthrough during secondary injection. The sensors along with the model have the potential to become an integral part of production monitoring for reservoir management.

Industrial Affiliates Program

The Center for Subsurface Modeling established an Industrial Affiliates Program in order to foster frequent and open communication between participating researchers and the corporate community. Over the years, this Affiliates Program has proven itself an ideal gateway for launching and conducting collaborative research efforts.

Corporate members have ready access to leading-edge research on a variety of issues in subsurface modeling, parallel processing, and high-performance computing, communicated via:

- Workshops
- Annual review meetings
- Campus visits by affiliates
- Corporate visits by faculty members
- CSM technical reports, publications and multimedia presentations of the group's activities
- Funded short-term "residences" at CSM in which members of our Affiliates' corporate staff work alongside CSM faculty, scientists and students

Corporate sponsorship yields a highly leveraged return, thanks to the large and diverse portfolio of other funding within CSM. It also provides an effective means of conducting exploratory or fundamental research that would not be feasible to perform in-house.

Membership Fees

The annual fee for membership is \$40,000. These funds are used primarily to support basic research. A small portion goes to defray the costs of annual meetings, technical reports, computational facilities and to supplement travel and other expenses for project graduate students, postdoctorates, visitors, and faculty.

In addition to their support of our general program, the following companies have engaged CSM to work on special projects:

Statoil: Fluid Structure Interaction in Porous Media

Aramco: Advanced Models and Numerical Algorithms for Reservoir Simulation

We would like to acknowledge the following companies for providing free access to their softwares for academic research:



Computer Modelling Group – CMG-GEM, CMG-STARs



Schlumberger – Petrel, Eclipse



Science Soft – S3GRAF



Program Development Co – Grid Pro

Current IAP members



The CSM Team

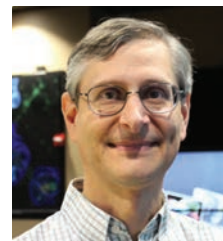


Mary F. Wheeler, Director, Ernest & Virginia Cockrell Chair in Engineering, mfw@ices.utexas.edu

Dr. Wheeler's research interests include mathematical modeling of surface and subsurface flows, mechanics, development of discretization techniques such as enriched Galerkin, multipoint flux mixed finite element method and discontinuous Galerkin and numerical solution algorithms for associated partial differential equations and its parallel computation. These include coupled multiphase flow and geomechanics modeling for fracture propagation, chemical and CO₂ enhanced oil recovery, reactive transport for carbon sequestration in saline aquifers and contaminant transport for groundwater remediation as well as modeling angiogenesis for cancer treatment.

Todd Arbogast, Professor, arbogast@ices.utexas.edu

Dr. Arbogast's areas of expertise include the numerical analysis of partial differential systems, mathematical modeling, and scientific computation. His research includes the development of a Eulerian-Lagrangian schemes for advective flow; the study of mixed methods and cell-centered finite differences for nonlinear and geometrically irregular elliptic problems; numerical homogenization, sub-grid upscaling, and domain decomposition of heterogeneous media. His work applies to the modeling and simulation of multi-phase flow through porous media, including fractured and vuggy media, petroleum production, groundwater resources, and simulation of the dynamics of the Earth's mantle.

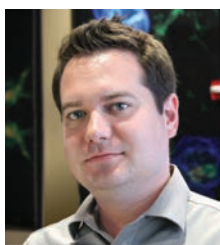
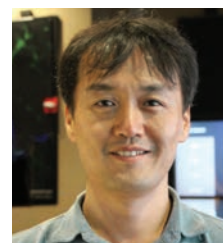


Sanjay Srinivasan, Professor, sanjays@psu.edu

Dr. Srinivasan's primary research focus is in the area of petroleum reservoir characterization and improved management of reservoir recovery processes. Some of the algorithms and methods that he has pioneered have been applied for early appraisal of ultra-deep-water plays in the Gulf of Mexico and for characterizing natural fracture networks in conventional as well as unconventional reservoirs. He has also partnered with researchers at the UT Institute of Geophysics and the Bureau of Economic Geology to develop novel schemes for integrating seismic data in reservoir models. Dr. Srinivasan is now professor of petroleum and natural gas engineering at the Pennsylvania State University and John and Willie Leone Family chair in Energy and Mineral Engineering.

Young-Ju Lee, Associate Professor, yjlee@txstate.edu

Dr. Lee's research focuses on design, analysis and implementation of numerical algorithms to solve non-Newtonian fluids flows. He has an expertise in developing fast solvers for linear and nonlinear system of equations. He also studies the modeling of wormlike micellar fluids. Recently, he developed three species models that can show the shear thickening transitions observed in wormlike micellar fluids. A shear thickening transition can have a lot of applications area. One of important applications can be found at enhanced oil recovery. He is currently a member of CSM group, led by Professor Wheeler at UT Austin, where he is interested in applying his expertise in EOR projects.

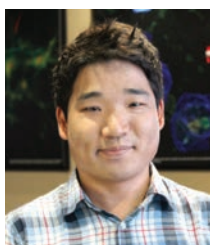


Benjamin Ganis, Research Associate, bganis@ices.utexas.edu

Dr. Ganis's most recent projects include the development of multipoint flux mixed finite element methods for non-matching hexahedral grids and the application of nonlinear plasticity for the geomechanical modeling of carbon storage reservoirs. He has many interests including domain decomposition, mortar methods, multiscale methods, uncertainty quantification, and high performance parallel computation.

Gergina Pencheva, Research Associate, gergina@ices.utexas.edu

Dr. Pencheva's research work lies in the area of large scale scientific computing with applications to porous media fluid flow. In particular, her interests include parallel domain decomposition methods for multiphase flow using multiscale mortar mixed and discontinuous Galerkin finite elements, a-posteriori error estimates and adaptivity for multiphase flow. Her recent work involves modeling of chemical enhanced oil recovering in complex reservoir geometry.

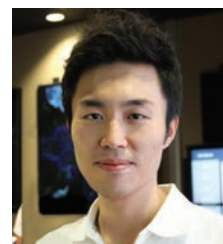


Sanghyun Lee, Research Associate, shlee@ices.utexas.edu

Dr. Lee received his Ph.D. in mathematics for non-Newtonian Navier Stokes multiphase flow with level set free boundary from Texas A&M University in 2014. His research is focusing on pressurized and fluid filled fracture propagation in three dimensional heterogeneous porous media, employing Biot system and phase field coupled by fixed stress splitting algorithm. Other interests include locally conservative flow with finite element method and transport system for multi physics applications.

Baehyun Min, Research Associate, baehyun@ices.utexas.edu

Dr. Min received his Ph.D. in Petroleum Engineering from Seoul National University in 2013. He works on the development of Pareto-optimality based evolutionary algorithm and its application to reservoir characterization, specifically, model selection, history matching, and production optimization in conventional reservoirs or in CO₂ sequestration projects.



The CSM Team - Postdoctoral Fellows



Jing Ping, Postdoctoral Fellow
jing@ices.utexas.edu

Dr. Ping received her Ph.D. in Petroleum engineering from Peking University in 2012. She works on data assimilation and uncertainty quantification. In particular, she is interested in automatic history matching of reservoirs with complex geology, such as fractured reservoirs and channelized reservoir.



Gurpreet Singh, Postdoctoral Fellow
gurpreet@utexas.edu

Dr. Singh received his Ph.D. in Petroleum Engineering from the University of Texas at Austin in 2014. His research interests include modeling coupled flow and geomechanics for fractured reservoirs, compositional flow for CO₂ EOR and sequestration and upscaling reactive flow and transport processes in porous medium.



Ashwin Venkatraman, Postdoctoral Fellow
ashwin.venkatraman@utexas.edu

Dr. Venkatraman's research focuses on modeling the thermodynamic changes as well as geochemical reactions that occur during enhanced oil recovery processes, aquifer remediation as well as safe disposal of nuclear energy. Having worked in the oil and gas industry for over six years, his research is influenced by practical problems faced by the industry.



2016 Highlight: Connie Baxter Awarded the 2016 ICES Staff Excellence Award

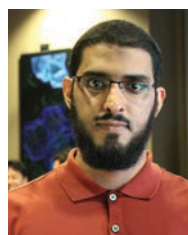
Connie Baxter, senior administrative associate and assistant to the director of the ICES Center for Subsurface Modeling (CSM), received the 2016 ICES Staff

Excellence Award "for contributions to innovation, productivity, and morale." Baxter joined ICES' predecessor, the Texas Institute for Computational and Applied Mathematics, in 1997 as an administrator for CSM, where she has remained for almost 20 years.

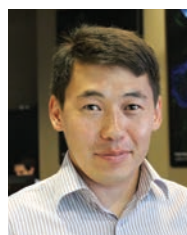
As one nominator acknowledged: "It is not an exaggeration to say that the quality of her administrative efforts have directly contributed to securing millions of dollars of funding to ICES through industrial and governmental grants."

Those she serves range from faculty to staff to students to international visitors. Despite varying needs, she manages the array of tasks and more, as a nominator affirmed: "In my experience both as a postdoc and guest, the support and involvement of Connie has been exemplary. What is more impressive is that she has often gone out of her way to help, and it is relevant to add that all the postdocs and graduate students have consensus on this."

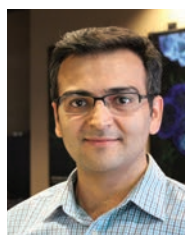
The CSM Team - Graduate Students



Tameem Almani
 multirate flow/geomechanics coupling



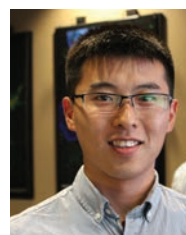
Yerlan Amanbek
 multiscale methods for flow and transport



Mohammad Reza Beygi
 gas mobility control, compositional modeling



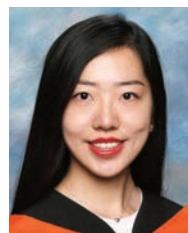
Saumik Dana
 domain decomposition for geomechanics



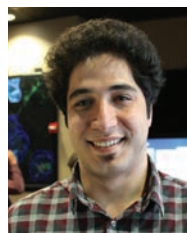
Rencheng Dong
 enriched Galerkin method for two-phase flow



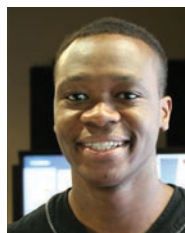
Mohamad Jammoul
 geomechanics



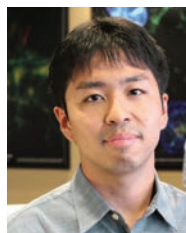
Xueying Lu
 wellbore geomechanics



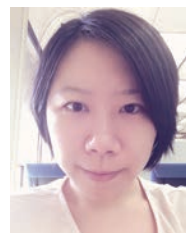
Morteza Naraghi
 stochastic reservoir characterization, data assimilation



Azor Nwachukwu
 stochastic reservoir characterization, model selection



Sogo Shiozawa
 phase field model, proppant transport



Zhen Tao
 mixed finite elements, viscosity methods



Deandra White
 plasticity coupled with fluid flow

Collaborators

Matthew Balhoff, Petroleum Engineering
The University of Texas at Austin

Silvia Barbeiro, Departamento de Matemática
Universidade de Coimbra, Portugal

Zakia Benjelloun-Touimi
IFPEN, France

Maurizio Chiaramonte, Civil and Environmental Engineering
Princeton

Thomas Dewers
Sandia National Laboratory

David DiCarlo, Petroleum Engineering
The University of Texas at Austin

Birol Dindoruk
Shell E&P Company

Hans van Duijn, Mathematics and Computer Science
Technische Universiteit Eindhoven, Netherlands

Joe Eaton
NVIDIA

Peter Eiseman
Program Development Co

Ahmed ElSheikh, Petroleum Engineering
Heriot-Watt University, UK

Anne C. Elster, Computer and Information Science
Norwegian University of Science and Technology, Norway

David Nicolas Espinoza, Petroleum Engineering
The University of Texas at Austin

Isabelle Faille
IFPEN, France

Abbas Firoozabadi, Chemical & Environmental Engineering
Yale University

Horacio Florez, Computer Science
The University of Texas at El Paso

Eduardo Gildin, Petroleum Engineering
Texas A&M University

Vivette Girault, Laboratoire Jacques-Louis Lions
Université Pierre et Marie Curie, France

Rainer Helmig, Hydromechanics and Modelling of Hydrosystems
University of Stuttgart, Germany

Nick Hayman, Institute for Geophysics
The University of Texas at Austin

Seyyed Hosseini, Bureau of Economic Geology
The University of Texas at Austin

Susan Hovorka, Bureau of Economic Geology
The University of Texas at Austin

Chun Huh, Petroleum Engineering
The University of Texas at Austin

Kirk Jordan, Data Centric Systems
IBM T.J. Watson Research Center

John Killough, Petroleum Engineering
Texas A&M University

Kundan Kumar, Mathematics
University of Bergen, Norway

Ruijie Liu, Mechanical Engineering
The University of Texas at San Antonio

Mark Mear, Aerospace Engineering & Engineering Mechanics
The University of Texas at Austin

Andro Mikelić, Mathematics
Université Claude Bernard Lyon 1, France

Chadi El Mohtar, Civil Engineering
The University of Texas at Austin

Manish Parashar, Computer Science
Rutgers University

Laxminarayan Raja, Aerospace Engineering & Engineering Mechanics
The University of Texas at Austin

Thomas F. Russell
Department of Energy

Mrinal Sen, Institute for Geophysics
The University of Texas at Austin

Shuyu Sun, Mathematics
KAUST, Saudi Arabia

Reza Tavakoli,
Chevron ETC

Martin Vohralík
INRIA, France

Thomas Wick
École Polytechnique, France

Tim Wildey, Computer Science Research Institute
Sandia National Laboratories

Gabriel Wittum, Goethe Center for Scientific Computing
Goethe University Frankfurt, Germany

Ivan Yotov, Mathematics
University of Pittsburgh

Dongxiao Zhang, Engineering
Peking University, China



Center for Subsurface Modeling

Institute for Computational Engineering and Sciences

1 University Station, POB 5.324, C0200

Austin, TX 78712

tel. 512.475.8625

fax 512.232.2445

Brochure design by Victoria Osborne

www.ices.utexas.edu/csm