CSM
Center for Subsurface Modeling

The Center for Subsurface Modeling
Institute for Computational Engineering and Sciences
The University of Texas at Austin

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INSTITUTE FOR COMPUTATIONAL ENGINEERING AND SCIENCES
THE UNIVERSITY OF TEXAS AT AUSTIN

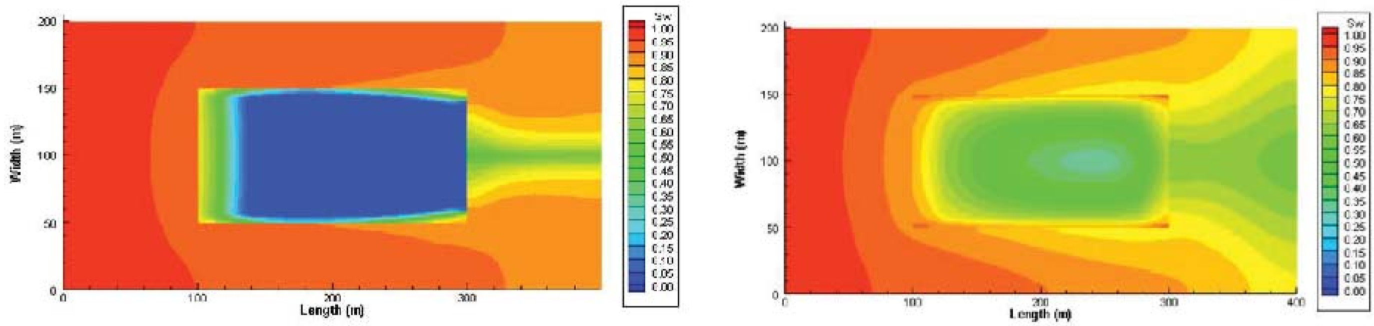
Center for Subsurfac

At the Center for Subsurface Modeling, we strive to meet today's numerical modeling challenges by bringing together mathematicians, engineers, geoscientists, and computing experts 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.

Our researchers work with visitors and industrial partners throughout the world to stay on the cutting edge of scientific advancement. We continually seek to improve existing numerical models by using better physical interpretations, better numerical techniques, and high performance computing. 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.

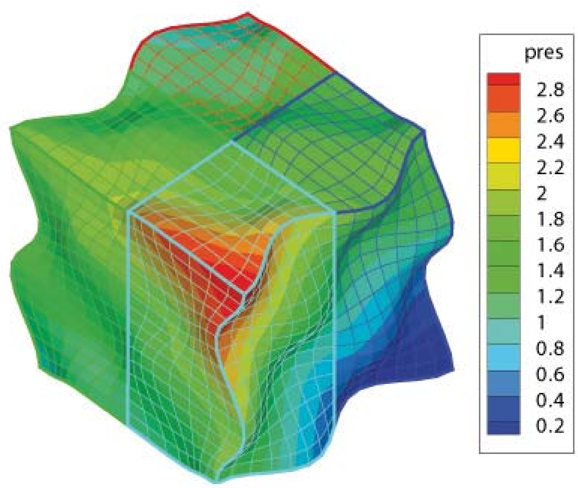
Analyzing the Effect of Capillary Pressure



Comparison of the water saturation after 10 years of injection with zero capillary pressure (**Top Left**) and nonzero capillary pressure (**Top Right**). The numerical solution was obtained using an iterative coupling formulation with a combination of mixed finite elements for the pressure and discontinuous Galerkin for the saturation. *Shuyu Sun and Mary F. Wheeler*

Multiscale Mortar Mulitpoint Flux Mixed FEM

Pressure profile (dimensionless) for the multiscale mortar mulitpoint flux mixed finite element method solution of single phase flow is shown in (**Right**) Figure. The domain is divided into four subdomains. At the interface, the mortar space uses piecewise bi-quadratic polymonials and the mortar mesh is twice coarser than the subdomain mesh. *Mary F. Wheeler, Guangri Xue and Ivan Yotov*



Brochure design and layout: Jorge Florez
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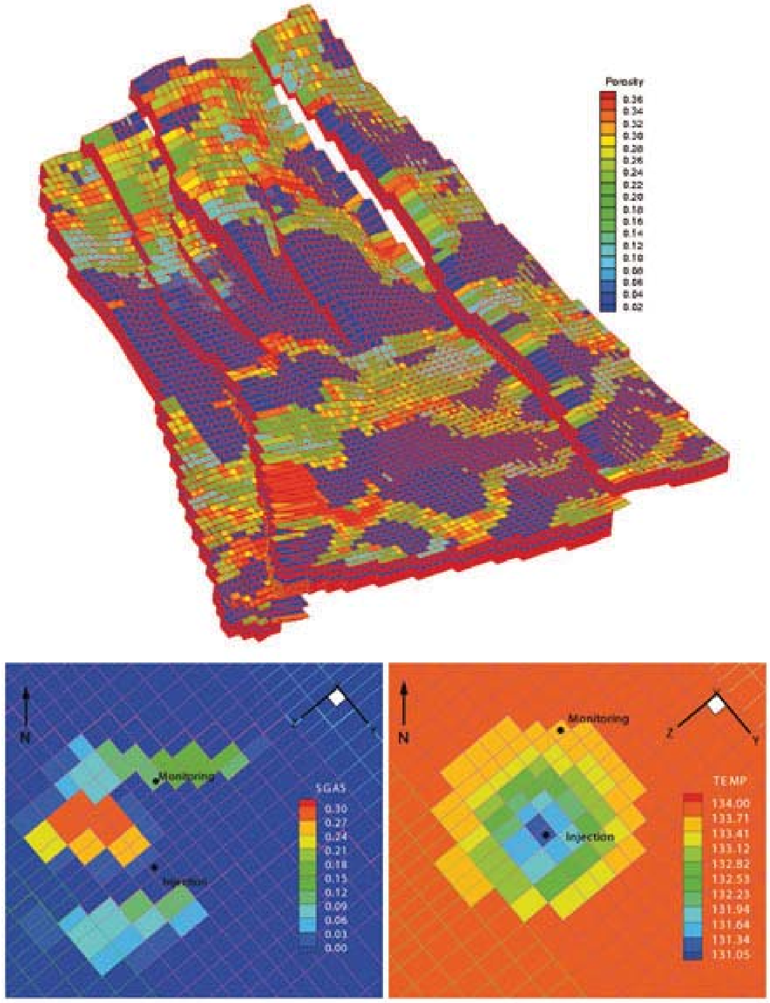
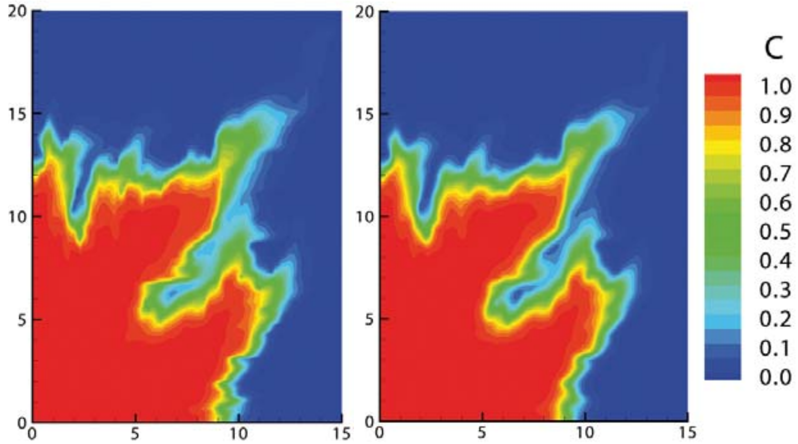
Simulation of CO_2 Sequestration at Frio

The example in this section simulates an actual field-scale CO_2 sequestration experiment conducted by the Bureau of Economic Geology (BEG) at The University of Texas at Austin http://www.beg.utexas.edu/. The bureau has conducted pilot tests for CO_2 injection off the Gulf Coast of Texas. The purpose of these pilot tests is to gather valuable data (during monitoring) and to demonstrate that large scale CO_2 sequestration can be performed with no concerns. The Frio formation is a brine-bearing sand in a well known onshore oil field with 3-d seismic and well log data available for characterization. This made it a suitable choice. Further, the existing infrastructure of wells and roads could be used for the pilot test. An existing production well was re-completed as a monitoring well, and an injection well was drilled about 30 m away, downdip. The formation is composed of two rock types-shale and sand layers. The injection took place in brine-bearing sandstone at about 1500 m (approx. 5000 ft) below the ground surface. The shale layers vary in thickness between 3 m to 15 m and separate various sandstone layers at the top of the formation. The injection target was the deepest sandstone layer (which was also the thickest) below a shale layer (in order to prevent upward drift of CO_2 due to buoyancy). The injection temperature was approximately constant and maintained at 60 F while the initial estimate of the reservoir temperature was constant at about 154.5 F. The pilot plan injected 3000 tonnes of CO_2 over a period of 12 days, after which the injection well was shut-in. Figure (**Top**) shows the porosity field. Figure (**Bottom Left**) shows the gas saturation and (**Bottom Right**) shows the reservoir temperature at 10 years. *Sunil G. Thomas, Mojdeh Delshad and Mary F. Wheeler.*



Tracer Transport with Fully Conservative Characteristic Method

Tracer transport in a heterogeneous quarter five-spot problem
Left: Godunov's method with CFL $\Delta t = 1.5$ seconds
Right: Fully conservative characteristic method with $\Delta t = 30$ seconds
Note the reduced numerical diffusion on the right.
Wenhao Wang and Todd Arbogast



The accurate and efficient simulation of subsurface phenomena requires a blend of physical and geochemical modeling of subsurface processes and careful numerical implementation. Compounding these issues is a general lack of high quality data for model calibration and verification. CSM researchers collaborate with outside experts to find suitably accurate representations of physical systems, including such processes as fluid phase behavior, particle transport and dispersion, capillary pressure effects, flow in highly heterogeneous media possibly fractured and vuggy, geomechanical response and subsidence, and well production. These and other processes must be simulated accurately so as to avoid nonphysical numerical artifacts that can cloud engineering judgment regarding risk assessment and the intervention and optimization of management objectives.

Discretization and Adaptivity

Many subsurface modeling problems involve localized phenomena, such as concentrated plumes, sharp fronts, shocks, and layers, which may also change with time. The efficient simulation of these problems requires effective, dynamic, and self-adaptive local grid refinement and coarsening guided by accurate a-posteriori error estimators and fast projections preserving important physical properties, including local mass conservation. Major objectives to achieve in this area include:

- Accurate and efficient locally conservative discretization methods on general meshes;
- Characteristic methods for transport processes;
- Robust and efficient multiblock discretization techniques for multiscale, multiphysics and multi-algorithmic implementations;
- Robust a-posteriori error estimators;
- Mesh adaptivity based on a-posteriori error estimates;
- Spatial and temporal adaptivity with goal-oriented error estimators;
- Account for and reduce upscaling error.

Multiscale Modeling

A complete subsurface characterization requires modeling a variety of processes which occur at vastly different scales, from the nanoscale and the pore scale, to the field scale, and from less than a second to millennium time scales. While a numerical simulation cannot span all of these scales, given today's computational resources, it is nevertheless necessary to incorporate relevant fine scale effects into a coarse scale model. Our group is exploring the following avenues of research:

- Subgrid upscaling and homogenization techniques for incorporating heterogeneities and other fine-scale processes within coarse grid cells;
- Computationally tractible and accurate modeling of vuggy and fractured systems;
- Pore-scale modeling of non-Newtonian fluids in granular materials;
- Physical multiscale and domain decomposition approaches;
- Coupling of stochastic and deterministic multiscale modeling;
- Goal oriented multiscale and upscaling via optimization methods;
- Utilizing a-posteriori error estimates to account for errors at different scales.

Coupled Flow and Geomechanics

Diverse geomechanical effects take place due to changes in pressure and saturation over the production lifetime of a reservoir. This is particularly critical in naturally fractured reservoirs, faulty and highly compressible formations, and in assessing borehole stability. To this end we have developed parallel scalable multiphase poroelasticity models. Theoretical analyses of stress dependent permeability has been obtained for single phase flow as well as the fomulation and implementation of a multiscale domain decomposition algorithm that allows for non-matching subdomain grids for modeling elasticity. Future work will include:

- Incorporation of plasticity models;
- Adaptive modeling using mortar multiscale domain decomposition to reduce computational costs;
- Iterative coupling to a reservoir simulator utilizing multiple time scales;
- Investigating the effects of coupling geomechanics with other subsurface processes, e.g., geochemical and thermal.

Parallel and Grid Computing

IPARS has been successfully tested on the IBM Blue Gene/P clusters, the Lonestar and Ranger clusters at the TACC, and the Bevo2 cluster at ICES, UT Austin. We are thus able to evaluate the potential of grid computing for challenging subsurface simulations at much larger scales. Some of the challenges addressed here include:

- History matching and model reduction: IPARS now has the capability to perform history matching simulations using SPSA in parallel for parameter estimation. In addition, MATLAB invoked IPARS instances have been implemented within an EnKF (ensemble Kalman filter) framework for model reduction;
- Large dataset management and integration: Pre-processors enable integration of large datasets from real-field experiments. An efficient framework distributes this data among several computing nodes. These have been tested in the simulation of the Frio CO_2 sequestration tests;
- Interactive computing and visualization: IPARS has been coupled to DISCOVER, an interactive and collaborative engine that allows for web-based portal access to our computing applications. Users can steer applications in real-time by directly altering input to the simulator, based on observed parameters (e.g., economic value) of the production process.

Objectives

Uncertainty Analysis

A significant challenge in subsurface modeling arises from the fact that properties are sparcely known. Our modeling and inverse approaches are designed to account for this source of uncertainty. By modeling and sampling known probabilistic properties of uncertain parameters, we are able to address this uncertainty and devise robust strategies that deliver optimal results, even in the presence of insufficient knowledge. Major objectives in this area include:

- Uncertainty propagation through different scales in data and models;
- Accurate and efficient parameterization of uncertainty;
- Efficient uncertainty assessment through non-intrusive approaches such as stochastic and probabilistic collocation methods;
- Stochastic domain decomposition to model non-stationary random media;
- Incorporation of a-priori information through Bayesian approaches;
- Utilization of ensemble-based methods for history matching and parameter estimation.

Solvers

Our solver effort is based on the development of efficient and scalable algorithms for solving large-scale systems of algebraic equations arising in multiphase flow and its coupling with other physical models. Efforts in this area focus on the following:

- Physics-based multilevel and domain decomposition preconditioners for solving problems in highly heterogeneous media;
- Supercoarsening and algebraic multigrid;
- Newton-Krylov and Krylov-secant methods for solving nonlinear equations;
- Iterative coupling between models;
- Utilizing multiscale information in the design of physics-based preconditioning strategies;
- Efficient solvers for discretization on general meshes;
- Efficient solvers for coupled flow and geomechanics.

Optimization and Control

The development of robust and efficient optimization is critical in parameter estimation and in the optimal management and control of reservoir systems. Our group is dedicating an important effort to the implementation of:

- Stochastic and hybrid optimization algorithms;
- Parameterization strategies to effectively cope with the curse of dimensionality;
- Model reduction for highly nonlinear and multiphysics problems;
- Improved data assimilation models;
- Metamodels to perform sensitivity analysis and improve the estimations.

Applications

Despite the above described particular algorithmic challenges for the accurate and efficient modeling of multiphase flow, chemical reactions, and geomechanics, the group has been pursuing research on a wide portfolio of applications. These efforts are in-line with the increasing interest shown by environmental agencies and the oil industry toward a much better understanding of coupled flow, geochemical and geomechanical effects in long-term simulations.

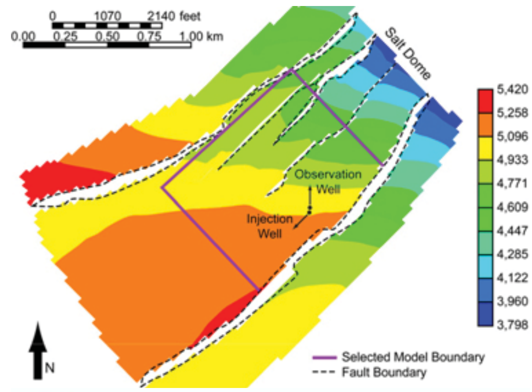
- **CO_2 Sequestration in Saline Aquifers**: Our ongoing efforts involve extending existing algorithms and the parallel computing capabilities of IPARS toward physically accurate flow models with special focus on CO_2 sequestration coupled to geochemical processes. This involves improving discretization methods and solvers for better treatment of arbitrary geometries and medium heterogeneities. For this application, a hysteresis model and a thermal energy balance have been coupled to the compositional flow model.
- **CO_2-EOR**: Our ongoing efforts involve extending existing capabilities of IPARS with special focus on CO_2 injection in oil reservoirs as combined enhanced oil recovery and CO_2 storage. The enhanced velocity mixed finite element method (EVMFEM) has been successfully implemented for compositional flow. This allows us to solve these computationally intensive problems on non-matching multiblock grids with the freedom of both choosing grid sizes, and, in a multimodel setting, using single phase flow in a majority of the computational domain. The EVMFEM has already been tested on practical problems in multiphase and compositional flow as well as flow coupled to reactive transport. For better treatment of general geometries, a robust Multipoint Flux Mixed Finite Element (MFMFE) method has been developed for the pressure equation and is being coupled to flow models.
- **Non-Newtonian Polymer Flow**: We have broadened the application of IPARS to the modeling of commercial scale polymer floods. Aqueous species such as anions, divalent cations, and polymer molecules are handled in the TRCHEM module of IPARS. High molecular weight water soluble polymers increase the viscosity of water significantly. Polymer solutions often exhibit non-Newtonian rheological behavior where the viscosity decreases as the shear rate increases. We also investigate flexible gridding, solvers, multiscale algorithms and dynamic load balancing issues that arise in parallel simulations.
- **Aqueous Chemistry**: Several published laboratory experiments have reported on the effect of potential determining ions such as Ca^{++}, Mg^{++}, and SO_4^{--} on oil recovery from carbonate chalk. We plan to model the water chemistry including rock dissolution/precipitation and the impact on wettability of carbonates and subsequent oil recovery improvement during seawater injection using TRCHEM.

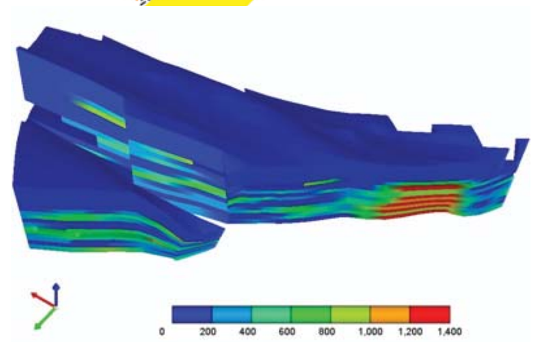
2008-09 Results

- Efficient and parallel parameter estimation based on multi-resolution parameterization, SPSA, and surrogate models via radial basis functions.
- Use of model predictive control (MPC) and ensemble Kalman filter techniques for closed-loop reservoir management.
- Development of a physics-based multiscale preconditioner for stochastic and nonlinear interface problems.
- Simulations of non-isothermal iterative compositional flow equations applied to field CO_2 sequestration experiments, such as Frio.
- Verification of a polymer module and scale-up simulations with IPARS-TRCHEM.
- Analysis of EVMFEM for non-linear single phase flow problem and flow coupled to transport on non-matching multiblock grids.
- Implementation of EVMFEM method to solve multiphase and compositional flow models and flow coupled to reactive transport on non-matching multiblock grids.
- Efficient and robust a-posteriori error estimates for multiscale mortar mixed finite elements and discontinuous Galerkin methods for incompressible single phase flow.
- Multiscale basis implementation of mortar mixed finite element method for single and two phase flow models.
- Development of a multiscale mortar MFMFE method for single phase flow.
- Development of a MFMFE in IPARS to simulate single and two-phase flows on quadrilateral and hexahedral meshes.
- Theoretical development of homogenization-based multiscale finite elements.
- Development of fully conservative characteristic transport methods for single and two-phase flows.
- Proof of convergence of a fully conservative characteristic transport method.
- Implementation of a multiscale domain decomposition algorithm with non-matching subdomain grids for modeling elasticity.
- Theoretical development of a multiscale domain decomposition method for coupling poroelasticity and elasticity.

Modeling and Simulation of CO_2 Injection in Aquifers

The objective here is to develop a physics-based simulation framework for CO_2 injection in deep aquifers. Our focus will be on coupling geomechanical, geochemical, and geobiological models with non-isothermal multiphase compositional flow. Simulations of Frio Brine field CO_2 injection test (www.gulfcoastcarbon.org) using IPARS have been successfully performed to model the CO_2 plume evolution including temperature variations and geochemical reactions on multiple processors. Figure (**Right Top**) shows the Frio experimental site within a fault bounded compartment with the injection and observation well locations. Figure (**Right Bottom**) shows the gridded reservoir model with the permeability values in md. *Sunil G. Thomas, Mary F. Wheeler, and Mojdeh Delshad*



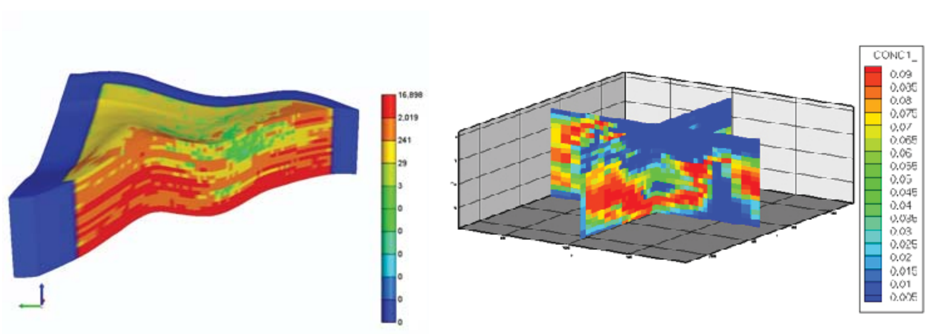


2009-10 Goals

- Advancement of model reduction methods for multiphysics problems and implementation of LABVIEW driven instances of IPARS-EnKF for history matching and parameter estimation.
- Investigation of the relationship between model reduction methods, multiscale methods, and upscaling for multiphysics problems.
- Application of multiscale physics-based, parallel AMG solvers on multicore and massively parallel platforms for multiphase and compositional flow coupled to transport.
- Development of specialized solvers for full permeability tensor discretizations based on MFMFE, Mimetic Finite Difference and/or Discontinuous Galerkin (DG).
- Utilization of a-posteriori error estimates for multiscale adaptivity, model reduction, and upscaling, and to provide stopping criteria for linear and nonlinear solvers.
- Development of multimodel implementations of compositional and single phase flow for CO_2 sequestration applications.
- Modeling and simulation of water chemistry including chalk dissolution to understand the effect on wettability and seawater flood oil recovery.
- Development of a-posteriori error estimators to accurately upscale physical properties.
- Development of efficient and reliable a-posteriori error estimators for two-phase flow.
- Development of nonsymmetric MFMFE method for highly distorted quadrilateral and hexahedral meshes in simulating multiphase flow.
- Implementation of local flux mimetic finite difference method for handling non-matching grid and also for adaptive mesh refinement allowing hanging nodes.
- Coupling MFMFE and local flux mimetic finite difference method.
- Computational development of homogenization-based multiscale finite elements and mortar methods.
- Investigation of characteristic methods for single and two-phase flows.
- Coupling MFMFE method with continuous or discontinuous Galerkin method in poroelasticity.
- Implementation of a parallel multiscale domain decomposition algorithm with non-matching grids for coupling poroelasticity with elasticity.
- Theoretical development and implementation of domain decomposition methods for coupling elasticity, poroelasticity, plasticity, and poroplasticity.

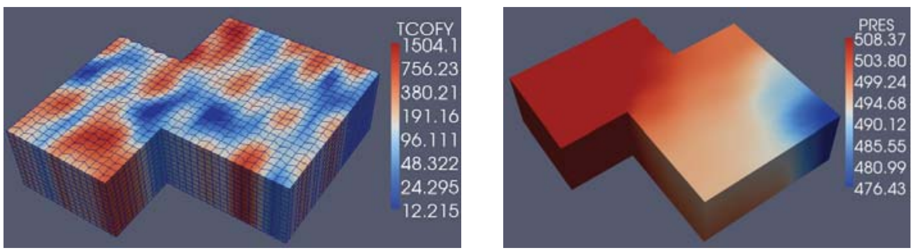
Coupling Non-Newtonian Flow with Multiphase Flow in IPARS-TRCHEM

We have implemented a comprehensive polymer module in IPARS to allow for non Newtonian viscous polymer solution for oil recovery. Very fine scale simulations are performed on up to 64 processors. The heterogeneous permeability for a grid of 86x94x19 is shown in (**Left**) Figure. Polymer concentration (wt%) at the end of the polymer flood is shown in the (**Right**) figure. *Changli Yuan, Mojdeh Delshad, Mary F. Wheeler*



Multipoint Flux Mixed FEM for Modified SPE6 Problem

The figure (**Left**) is modified SPE6 permeability field, and pressure field for the multipoint flux mixed finite element solution of two-phase flow shown in (**Right**). *Sunil G. Thomas, Mary F. Wheeler and Guangri Xue*



CSM Research

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

Dr. Wheeler's research interests include the numerical solution of partial differential systems as applied to subsurface and surface flow modeling and parallel computation. Her applications include multiphase flow and geomechanics in reservoir engineering and carbon sequestration in saline aquifers, contaminant transport in groundwater and bays and estuaries, and angiogenesis in biomedical engineering. This year, Dr. Wheeler was honored with the Society for Industrial Mathematics (SIAM) Geosciences Career Prize, as well as her third IBM Faculty Award. In July, Dr. Wheeler was awarded the Theodore von Kármán prize at the annual meeting of the SIAM, recognizing her seminal research in numerical methods for partial differential equations, her leadership in the field of scientific computation and service to the scientific community, and for her pioneering work in the application of computational methods to the engineering sciences, most notably in geosciences.

Todd Arbogast, *Associate Director*, arbogast@ices.utexas.edu

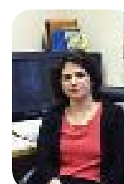
Dr. Arbogast has expertise in the numerical analysis of partial differential systems, mathematical modeling, and scientific computation. His research includes the development of a characteristics-mixed scheme for advective flow, the study of cell-centered finite differences (mixed finite element methods) for nonlinear and geometrically irregular problems, the modeling and simulation of flow through fractured and vuggy media, and the development of numerical subgrid upscaling techniques.

Clint Dawson, *Professor*, clint@ices.utexas.edu

Dr. Dawson's research interests include the development, analysis and implementation of numerical methods for flow and transport in porous media and shallow water equations. Of particular interest to him are discontinuous Galerkin schemes, finite volume schemes, and multi-algorithmic strategies. Other interests include data assimiliation and a-posteriori error estimation.

Mojdeh Delshad, *Research Associate Professor*, delshad@mail.utexas.edu

Dr. Delshad's research interests include reservoir engineering, modeling petrophysical properties, simulation of chemical and CO_2-EOR processes, modeling wettability alteration by use of chemicals to improve oil production from fractured carbonate formations, and numerical simulation of CO_2 storage in saline aquifers. She is in charge of development and user support of UTCHEM, The University of Texas chemical flooding reservoir simulator.

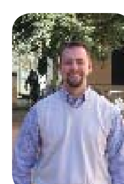


Gergina Pencheva, *Research Associate*, gergina@ices.utexas.edu

Dr. Pencheva's research work focuses on multiscale mortar mixed finite elements for large scale scientific computing with applications to porous media fluid flow. In particular, she has worked on improving the convergence of the method using balancing domain-decomposition preconditioner. Her recent work involves coupling of discontinuous Galerkin (DG) and mixed finite element methods for single and two-phase flows, domain decomposition method for linear elasticity with DG jumps and mortars, and a-posteriori error estimates for multiscales and multinumerics coupled by mortars.

Tim Wildey, *Postdoctoral Fellow*, twildey@ices.utexas.edu

Dr. Wildey's research focuses on non-intrusive stochastic methods for flow in porous media. In particular, he is interested in developing a-posteriori error estimates and adaptive methods for uncertainty quantification in reservoir simulations. Other interests include operator splitting techniques for multiscale and multiphysics applications, finite element and finite volume methods, and iterative methods for large scale problems.



Sunil G. Thomas, *Postdoctoral Fellow*, sgthomas@ices.utexas.edu

Dr. Sunil G. Thomas completed his Ph.D. in Computational Mathematics from UT Austin in August 2009 under the supervision of Prof. Mary F. Wheeler. His research interests lie in the area of parallel domain decomposition methods for multiphase flow and coupled flow-transport problems in porous media. His recent work involves the analysis and implementation of the EVMFEM for non-matching multiblock grids applied to the coupled flow-transport problem.

Team 2009-10

Guangri Xue, *Postdoctoral Fellow*, gxue@ices.utexas.edu
Dr. Xue received his Ph.D. in mathematics from the Pennsylvania State University in 2008. His current research interests include robust numerical discretizations and solvers for subsurface flow and the coupling to other physics such as geomechanics and reactive transport in general geometry.

Mika Juntunen, *Postdoctoral Fellow*, juntunen@ices.utexas.edu
Dr. Juntunen received his Ph.D. in mathematics from the Helsinki University of Technology (Finland) in 2009. He is interested in both analysis and implementation of the finite element method. His research focuses on the a-posteriori error estimation, adaptive methods, and the treatment of the boundary or interface conditions.

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Horacio Florez
Mesh generation, finite element methods

Omar al Hinai
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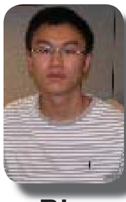
Xianhui Kong
Numerical reservoir simulation

Wenhao Wang
Characteristic-mixed methods

Jack Poulson
Distributed-memory/ GPU computing & dual state/parameter estimation



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Hailong Xiao
Applied mathematics

Nick Alger
Applied mathematics

Industrial Affiliates

Purpose

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.

Benefits of Membership

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.

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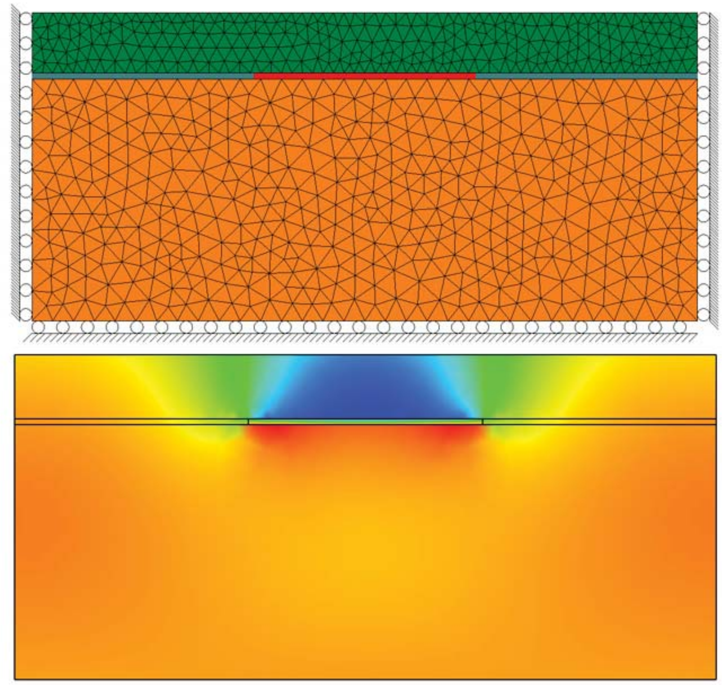
Mortar FEM Method for Poroelasticity

A reservoir compaction and subsidence synthetic model was solved using the Mortar FEM method. The pay-zone mesh, depicted in red in the center of (**Top**) Figure, is 100 x 20. Two horizontal mortars with 40 elements each and two vertical ones with 10 elements each were used. Unstructured triangular meshes were used in the surroundings to emphasize the non-matching approach. In (**Bottom**) Figure, the vertical displacement color contour is depicted showing compaction areas in blue and build-up areas in red. The results show excellent agreement with the conforming case but the computational cost is reduced by 50% due to the efficient handling of the meshes. *Horacio Florez and Mary F. Wheeler*



Svalbard Workshop

Mary F. Wheeler and Mojdeh Delshad attended the workshop in modeling and risk assessment of geological storage of CO_2 in the exotic Longyearbyen, Svalbard, in August of 2009. Longyearbyen (Latitude 78^{o}) is the northernmost settlements in the world, and is the hub for numerous polar expeditions. Recently, Svalbard has been on the news for being a pioneer not only in polar exploration, but also for its ambition of becoming a carbon neutral community using Carbon Capture and Storage (CCS) technology by 2025. This will involve the completion of new coal fired power plant and carbon storage in geological formations.

http://org.uib.no/cipr/Workshop/2009/CO2/index.htm

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