

# **NSF-Supported Projects Related to MoMaS Science**

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# Overview

- Searched public NSF awards database:  
<http://www.nsf.gov/awardsearch>,  
click on tab “Search All Fields”,  
enter keywords or other information
- U.S. Department of Energy is the primary funding source for some areas, e.g., nuclear engineering
- Will summarize 11 current projects

# Revolutionary Advances in Modeling Transport Phenomena in Porous Medium Systems

- Casey Miller, U. North Carolina
- Tim Kelley, North Carolina State U.
- Dorthie Wildenschild, Oregon State U.
- 4 years, 2009-13, \$1.7 million
- Cyber-enabled Discovery and Innovation (CDI) program
- First-principles theory, computation, mathematical analysis, and high-resolution experimental observation to formulate, solve, and validate multiphase flow/transport models across multiple scales
- Image analysis, continuum mechanics, thermodynamics, Lattice-Boltzmann algorithms, time/space adaptive numerics, integral methods for systems of nonlinear PDEs

# Impact of Mineral Precipitating Biofilms on the Physical and Chemical Characteristics of Porous Media

- Isaac Klapper, Montana State U.
- 4 years, 2009-13, \$750,000
- Collaborations in Mathematical Geosciences (CMG) program
- Microbially-induced  $\text{CaCO}_3$  mineralization
- Can bind/release large amounts of  $\text{CO}_2$
- Quantitative understanding of hydrobiogeochemical processes
- Lab, modeling, computational tools
- Observation of biofilm development and mineral precipitation in capillary and porous medium reactors

# Mathematical and Experimental Analysis of Reactive Transport in Discontinuous Porous Media

- Brian Wood, Oregon State U.
- 3 years, 2007-10, \$421,743
- Collaborations in Mathematical Geosciences (CMG) program
- Highly heterogeneous media
- Cloud of discrete particles representing dissolved chemical species in groundwater
- Rules to represent reactions
- Mathematical analysis, experimental validation

# Coupled Flow Phenomena in Unsaturated Clay Barriers

- Ning Lu, Colorado School of Mines
- Charles Shackelford, Colorado State U.
- 3 years, 2009-12, \$440,000
- Geotechnical Engineering program
- Coupled unsaturated fluid and chemical transport in waste containment systems
- Chemico-osmosis and membrane behavior in unsaturated clays
- Transport model including membrane; experiments for measuring membrane behavior

# Mathematical Modeling of Heterogeneous Materials

- Guillermo Goldsztein, Georgia Tech
- 3 years, 2008-11, \$170,493
- Applied Mathematics program
- Math tools for understanding & prediction of behavior & properties of heterogeneous materials
- Transport of solute & heat in porous media
- Asymptotics, homogenization, numerical simulations, modeling

# Computational Models for Evaluating Long Term CO<sub>2</sub> Storage in Saline Aquifers

- Mary Wheeler, U. of Texas at Austin
- Manish Parashar, Rutgers U.
- 4 years, 2008-12, \$2.0 million
- Cyber-enabled Discovery and Innovation (CDI) program
- Multiphase flow, rock mechanics, multicomponent transport, thermodynamic phase behavior, chemical reactions in fluid and rock, multiple space/time scales, multiphysics
- Verification & validation against field-scale experiments

# Advanced Computational Models for Geological Storage of Carbon Dioxide

- Michael Celia, Princeton U.
- Hong Wang, U. of South Carolina
- 3 years, 2009-12, \$650,000
- Collaborations in Mathematical Geosciences (CMG) program
- Large-scale injection & transport of CO<sub>2</sub>, leakage along concentrated flow paths
- New Eulerian-Lagrangian methods
- New stochastic approaches for large uncertainties

# Uncertainty Quantification for Petascale Simulation of Carbon Sequestration through Fast Ultra-Scalable Finite Element Methods

- Roger Ghanem, U. of Southern California
- Mark Adams, Columbia U.
- Kevin Long, Texas Tech U.
- 3 years, 2009-12, \$1.23 million
- Petascale Applications (PetaApps) program
- Theory
- Numerical methodology
- Computational implementation
- Scalability to petascale

# Data-Driven Stochastic Analysis of Flow in Random Heterogeneous Media

- Nicholas Zabaras, Cornell U.
- 3 years, 2008-11, \$252,000
- Computational Mathematics program
- Multi-length scale variations in properties
- Reduced-order stochastic input model
- Adaptive sparse grid collocation for stochastic PDEs
- Strategy for information passing across scales
- Low-dimensional parametrization of manifolds embedded in high-dimensional spaces

# Stochastic Models for Anomalous Diffusion

- Mark Meerschaert, Michigan State U.
- 3 years, 2008-11, \$299,945
- Collaborations in Mathematical Geosciences (CMG) program
- Particle tracking to mimic stochastic diffusion
- Fractional time/space derivatives from power law resting times / movements
- Markov process methods to obtain further pseudo-differential equation models
- Scaling limits of continuous time random walks

# Multi-Scale Data Assimilation of Soil Moisture under Heterogeneous Soil Hydraulics

- Binayak Mohanty, Texas A&M U.
- 4 years, 2006-10, \$340,792
- Collaborations in Mathematical Geosciences (CMG) program
- Shallow subsurface, data from different sources
- Range of space/time scales, predict at fine scale
- Adjoint method for conductivity at coarse scale, upscaling/downscaling techniques

# Themes of Summarized Projects

- Basic physics
- Reactive flows
- CO<sub>2</sub>
- Heterogeneity, stochasticity
- Adaptive numerics, multiscale methods, particle/Lagrangian methods
- Experimental validation