

**CP1****Analyzing Multiphase Flows with An Eye Toward Enhanced Oil Recovery**

In this talk, we will provide results of our stability studies on multi-layer multiphase flows which are relevant at fundamental level for enhancing oil recovery. We will also discuss an interplay between heterogeneity effects and viscosity driven instability effects by using an approximate model to quantify their relative importance.

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**CP1****Variable Relaxation Schemes for Two-Phase, Multi-Component Flows**

We present a new relaxation scheme for the simulation of two-phase, multi-component flows in porous media. The governing equations are weakly hyperbolic and strongly nonlinear. We reformulate the problem as a linear strictly hyperbolic system with a nonlinear source term that is effectively dealt with using operator splitting. The dissipative error introduced by this reformulation is effectively reduced by locally adapting the relaxation matrix. The scheme is a computationally attractive alternative to Riemann-based solvers.

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**CP1****The Structure of Conservation Laws Modeling Four-Component Three-Phase Flow**

Modeling carbon dioxide sequestration in water-flooded oil reservoirs requires four components in three phases, to allow components to partition between the phases. We study the characteristic equations for the system of three conservation laws that model compositional flow in this system in one dimension. We discuss the loss of strict hyperbolicity in the three-phase region, as well as shock constraints. Finally we demonstrate several analytical solutions for carbon dioxide injection into an oil reservoir.

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**CP1****A Level Set Method for Determining Critical Curvatures for Drainage and Imbibition**

An accurate description of pore level immiscible displacement mechanics could significantly improve macroscopic parameter predictions in real porous media. We present a simple but robust model based on the level set method for determining critical events for drainage and imbibition.

The method arrives at geometrically and topologically correct interfaces and is independent of the pore space complexity. We describe its extension to nonzero fluid-fluid-solid contact angles.

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**CP2****Scaling Up of Sources Terms with Random Behavior**

We study the transport and migration of contaminants in aquifers from a "sources site" made of a large number of "local sources". The "local sources"  $f^\varepsilon$  are periodically repeated and lying on a plan. Moreover the release starting time and the release time evolution, of each local source, are both random. Our aim is to give a mathematical model describing the global evolution of such a system, with only one "global source"  $F$ . Numerical simulations of a long-lived nuclear waste underground repository, are presented, demonstrating the accuracy of the theoretical results.

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**CP2****Couplex Test Cases Calculations Using Finite Element-Finite Volume Code**

We present the results of Couplex benchmarks for the simulation of radionuclide transport around a nuclear waste repository. They are obtained with a finite-element-finite volume code where the diffusive terms (flow and transport) are discretised with finite element method and the convective term with the Godunov type FV method. Calculations are made on structured meshes that fulfil Delaunay and cotangents criteria. Some comparisons between mono- and multi-domain calculations are also included.

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**CP2****Approximation of Compressible Two Phase Flows in Porous Media Combining Mixed Finite Element and Finite Volume Methods**

We solve a system of coupled parabolic equation and nonlinear convection-diffusion equation. The MFE method is employed for the parabolic equation. A Godunov-type FV method is applied for the convective term and a conforming FE method with piecewise linear elements is used for the

dispersion term. The results of convergence as well as  $L^\infty$  and  $BV$  estimates are shown. Numerical simulations are given for a 2D problem related to nuclear waste repository.

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## CP2

### Modeling of Solute Transport In Randomly Heterogeneous Porous Media Via Exact Simulation Of Diffusions

It is well known that a advection-dispersion equation (ADE) can be interpreted as forward-Kolmogorov equation, also called Fokker-Planck equation, of a diffusion process given by a stochastic differential equation. Such solute transport can be simulated by generating paths of this process. We use a new method (*A. Beskos and G.O. Roberts*, Exact simulation of diffusions, The Annals of Applied Probability 2005, vol. 15(4), 2422-2444) to obtain a 'particle solution' of the ADE. We compare the results with those obtained by the forward reverse method of *Milstein et al.* (Bernoulli 2004, vol. 10(2), 281- 312) for transition density estimation. Finally we adress the problem of sensivity analysis of exceedance probabilities with respect to variations of the transmissivity field, porosity and dispersivity.

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## CP2

### Mimetic Finite Difference Methods on Polyhedral Meshes

A mimetic finite difference (MFD) method preserves essential properties of the continuum differential operators, such as conservation laws, solution symmetries, and the fundamental identities and theorems of vector and tensor calculus. In the talk, I present the MFD method for solving the diffusion problem with tensor coefficients on unstructured polyhedral meshes consisting of arbitrary elements: tetrahedrons, pyramids, hexahedrons, degenerated and non-convex polyhedrons, generalized polyhedrons, etc. The MFD method uses simple geometric characteristics like normals and areas of mesh faces; therefore, it can be applied to AMR meshes with hanging nodes in exactly the same manner as to tetrahedral meshes.

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## CP2

### Improvement of Chemical-Transport Coupling Code: From Parallelism to Non Linear Gradient Algorithm

In the context of the software platform Alliances, ANDRA and CEA have developed a code coupling approach for reactive transport simulation. In order to improve the performance of the method different approaches have been investigating: parallel distribution of the chemical computations, implementation of a non linear gradient algorithm instead of the classical sequential iterative approach, initialization of the coupling algorithm via linear projection.

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## CP3

### Optimizing History Matching in Oil Reservoir Using Kullback Leibler Distance in Bayesian Framework

In oil reservoir engineering, integrating dynamic data into the geomodel is a major issue. Due to the cost of data acquisition, it is essential to optimize the design of field experiments, so to quantify the value of data. Using a Bayesian framework, we build an objective function, which relies on both the Fisher information matrix and the Kullback-Leibler distance. Its minimization permits to quantify the value of the information brought by new observations and thus enables to characterize the optimal sampling for a reliable production forecast. This quantification significantly enhances the decision making process within an uncertain framework.

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**CP3****Deconvolution Using B-Splines**

In this work we develop a methodology based on B-splines and least-squares for the solution of the Volterra equation of first kind. We utilize B-splines for representing the unknown function under the convolution integral. We use either constant piecewise or Laplace transformable functions for the kernel function. For dealing with noisy sets of data we implement a regularization algorithm in our methodology. We apply the new algorithm on a deconvolution problem arising in petroleum engineering.

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**CP3****Deterministic Sensitivity Analysis for a Model for Flow in Porous Media**

Uncertainties can be obtained by probabilistic methods, which give good results and are relatively easy to implement. The deterministic method investigated here is much less demanding in computing time but gives only a local information. It is based on the singular value decomposition of the Jacobian matrix of the mathematical model of the problem. The 3D flow follows Darcy's law. The Jacobian matrix is computed through analytical formulas, following the adjoint state method. We will compare performances and results obtained through probabilistic and deterministic methods.

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**CP3****Parameter Estimation: A New Approach to Weighting a Priori Information**

We propose a new approach to weighting initial parameter misfits in a least squares optimization problem for linear parameter estimation. Parameter misfit weights are found by solving an optimization problem which ensures the penalty function has the properties of a  $\chi^2$  random variable with  $n$  degrees of freedom, where  $n$  is the number of data. This approach differs from others in that weights found by the proposed algorithm vary along a diagonal matrix rather than remain constant. In addition, it is assumed that data and parameters are random, but not necessarily normally distributed.

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**CP3****Simulation and Optimal Design in Bioventing**

Bioventing is a subsoil cleanup technology. Bacteria biodegrade the contaminant and the needed oxygen is provided by air injection wells. A mathematical model based on theory of fluid dynamics in porous media and on bacteria population dynamics will be used for the simulation of the physical phenomenon. The optimal design problem consists of determining the number, the positioning and the pumping rates of the air injection wells so to maximize the biodegradation rate.

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**CP3****Wavelet Analysis and Filtering to Identify Principal Directions of Permeability Anisotropy**

An accurate representation of permeability anisotropy is needed to correctly model the rate and direction of groundwater flow. Wavelet analysis can be used to characterize principal directions of permeability anisotropy; however, if the permeability field contains regions with different principal directions, wavelet analysis may only identify the principal directions of the primary region. We present a combined wavelet analysis and filtering method to characterize primary and secondary principal directions of permeability anisotropy.

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**CP4****Modelling of Near-Wellbore Formation Damage**

Drilling induced formation damage has a huge impact on well productivities. In this paper, we present a numerical approach to study the impact of formation damage on well performance. In this approach, a small scale two-phase flow model taking into account near-wellbore formation damage is first developed, then the degree of formation damage is characterized by skin factors using an optimization method, and finally large scale reservoir simulations are used with the specific skin factors to calculate oil productions. Some examples are given to illustrate this approach. Using this approach allows to limit the risks of formation damage and to maximize well productivities.

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**CP4****The Mathematical Theory of Thermal Oil Recovery**

In this work, we review ongoing progress on the Riemann solution for thermal problems in multiphase flow in porous media extending the classical Buckley-Leverett theory, so we can study heavy oil recovery. There are non classical

waves, some to be expected such as combustion and condensation waves, other unexpected, such as evaporation waves. We present a general framework to study the systems of balance equations arising in such problems, and discuss open problems.

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#### CP4

##### **Analysis of Finite Element Methods for Coupled Hydro-Mechanical Problems**

This work is concerned with the finite element approximation of non-stationary Hydro-Mechanical models. An a posteriori error analysis is performed, leading to space-time error indicators from which time and space discretization errors can be estimated separately. The reliability and the optimality of the error indicators are investigated. Numerical experiments using the industrial finite element software Code\_Aster (developed at Électricité de France, freely available at [www.code-aster.org](http://www.code-aster.org)) are exposed.

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#### CP4

##### **Modeling the Early Evolution of Hypogene Karst Systems by Dissolution and Fracture Growth in Hydrothermal Systems**

Fracture dissolution in the early stages of karstification under hypogene conditions is investigated using a coupled model of fluid flow, heat transfer and reactive transport in the multi-component  $\text{H}_2\text{O}-\text{CO}_2-\text{CaCO}_3$  system with temperature-dependent solubility and kinetics. The behavior of aperture growth at early time can be described by an ODE whose solution predicts the occurrence of a "maturation time" at which there is a dramatic increase in fracture transmissivity. In variable-aperture fractures, a stochastic analysis is used to predict fracture transmissivity growth. We discuss the relevance of this model to the evolution of hot spring and thermal cave systems in karst formations.

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#### CP4

##### **Well Modeling Incorporating Non-Isothermal Effects and Asphaltene Precipitation**

A comprehensive flow model which incorporates compositional and non-isothermal effects to predict asphaltene precipitation in advanced well completions is proposed. An available asphaltene model is incorporated into a two-phase multi-segment network model. The network model is used to compute the overall pressure and temperature profiles in the well. The compositional asphaltene model is then used where asphaltene precipitation is most likely to occur to calculate temperature and predict asphaltene precipitation using an isenthalpic-flash, three-phase equilibrium model.

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#### CP5

##### **Sensitivity Analysis for Shallow Water Equations**

Adjoint sensitivity methods have been successfully applied in a variety of fields. In the field of meteorology, its use has been extensive, including data assimilation techniques, parameter estimation, stability analysis and synoptic studies. The shallow water equations, being simple statements for mass and momentum, exhibit many of the properties associated with the horizontal dynamical component of atmospheric models. We consider linear shallow water equations and its adjoint. These equations are solved numerically using high-order methods and the adjoint variables are analyzed to understand the sensitivity of the perturbation of the main variables.

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#### CP5

##### **Matrix-Free Interpolation and Scattered Data Approximations on the Sphere**

We construct interpolation nodes and a minimal quadrature rule and corresponding interpolation bases for a space that allow two fast Fourier transform type matrix-free formulas for interpolating functions on the sphere. We also construct a quasi-interpolatory approximation for a large dataset in the latitudinal and longitudinal directions, with a longitudinal symmetry condition. We prove and demonstrate that the quality the operators are same as that of the classical two dimensional spectral interpolation. This is a joint work with H.N. Mhaskar.

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**CP5****Assimilation of Time-Averaged Observations for Paleoclimate Reconstruction**

Paleoclimate observations are typically available only with very limited temporal resolution, such as accumulated precipitation. Here we explore a technique for assimilating time-averaged observations with the goal of constraining low-frequency climate variability. Our method is an extension of the ensemble Kalman filter, applied to a quasi-geostrophic atmospheric jet model. Accurate analyses are produced, with errors smaller than observation error, especially in the time-averaged quantities.

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**CP5****Quadrilateral Grids and Finite Volume Methods for the Sphere**

A logically rectangular computational grid is mapped to the sphere in such a way that the ratio of largest to smallest cell sizes is bounded by 2. The use of this grid makes it easy to apply the high-resolution finite volume methods implemented in CLAWPACK, including adaptive mesh refinement, to problems such as shallow water equations on the sphere. Analogous three-dimensional hexahedral grids will also be presented for studying problems in a spherical shell (e.g. the atmosphere) or in a solid sphere (e.g. geodynamics).

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**CP5****Introduction of the Reduced Spectral Transformation into Jma-Gsm**

JMA-GSM is a hydrostatic global spectral atmospheric model. It is used for operational weather forecasts at Japan Meteorological Agency. In the conventional JMA-GSM, there are a lot of redundant grid-points and insignificant wavenumber components especially in the high-latitudes. This redundancy leads to large wastage of computational resources. In order to improve the computational efficiency of JMA-GSM, we introduce the reduced spectral transformation into the model. We will present the computational performance of the model.

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**CP5****Numerical Modeling of Atmospheric Pollutant Transport with Spatial Reduction Algorithm**

Atmospheric chemical dynamics computational modeling presents an enormous challenge associated with its multiscale (ten orders) nature and large number of chemical compounds used. We offer a dynamically adaptive spatial reduction numerical method for atmospheric chemical evolution equations which diagnoses chemical dynamics on-line, and partitions the region into different domains where, a properly reduced chemical model is used. This allows reducing computational cost by at least an order of magnitude for typical atmospheric chemical kinetics.

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**CP6****Frechet Kernels for Multiscale Seismic Inversion**

Waveform inversion for subsurface seismic velocities is often studied from the perspective of PDE constrained optimization. A multiscale approach is essential to stabilise the inversion. We compare sensitivity functions for iterative optimization from different forward modeling engines. Classical discretization of the full wave equation is compared with ray theoretic modeling based on the Maslov asymptotic approximation to distinguish contributions of refracted and scattered energy within the inversion. This approach makes 3D seismic waveform inversion feasible.

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**CP6****Grid Dispersion and Stability Analysis of the Numerical Methods for Seismic Wave Propagation**

We will present the grid dispersion and stability analysis for the Finite Differences (FD) and Finite Elements (FE) methods that have become the most popular for seismic wave propagation, including staggered-grid FD and Spectral FE. We derive an approach based on a generalized eigenvalue formulation to analyze the dispersive behavior of FE acoustic and elastic wave propagation that overcomes the difficulties due to irregular node spacing and high order polynomials, as used in Spectral FE.

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### CP6

#### Intel Mkl-Based Trust-Region Solvers: Performance and Applications in Geosciences

Trust-Region (TR) algorithms are relatively new iterative algorithms for solving nonlinear optimization problems. High efficiency of TR methods was demonstrated in a number of recent papers and books [A. R. Conn, N. I.M. Gould, P. L. Toint. Trust-Region Methods. SIAM Society for Industrial and Applied Mathematics, Englewood Cliffs, New Jersey, 2000.]. They have better local super convergence, when compared to Newton-type methods, commonly used for solving Inverse Problems [M.M.Lavrentiev, A.V.Avdeev, M.M.Lavrentiev, Jr., V.I.Priimenko. Inverse Problems of Mathematical Physics. VSP Publ., The Netherlands, 2003]. TR techniques are used in a number of well-known SW libraries such as IMSL, TAO, GALAHAD, LANCELOT, etc. Highly-optimized Trust-Region solvers developed for Intel Math Kernel Library [Intel Math Kernel Library - <http://www.intel.com/cd/software/products/asm-na/eng/perflib/mkl/index.htm> ] allow to solve: nonlinear least squares problem (without and with bound constraints) system of nonlinear equations (without and with bound constraints) problem of functionals minimization (without constraints) The auxiliary routines provide calculation of Jacoby and Hessian matrices as well as gradient vector. TR solvers are implemented with OpenMP support and can be used in multiprocessing mode. They show excellent performance vs. competitors (VNI IMSL Fortran library v5.0 and TAO v1.8.1) - on benchmark tests TR give average 10 times speed-ups vs. IMSL and 5 times average speed-ups vs. TAO. TR effective usage in a number of applied geophysical problems will be presented.

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### CP6

#### A Mixed Unsplit-Field PML-Based Scheme for Total Wavefield Inversion in the Time-Domain

We discuss the inverse problem of PDE-parameter identification in PML-truncated semi-infinite heterogeneous domains, when given partial information. We use total wavefields in the time-domain, under a PDE-constrained optimization framework: to satisfy the ensuing first-order optimality conditions, we solve initial-value state, final-value adjoint, and a time-independent control problem to iteratively update the unknown PDE parameters. We report on a mixed finite element implementation of the inverse problem based on new unsplit-field PMLs, and present results in one and two dimensions.

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### CP6

#### An Iterative Approach to Seismic Moment Tensor

### Inversion

We present a new approach to seismic moment tensor inversion. This approach uses properties of Toeplitz matrices which give the ability to work on large data sets through the implicit storage of the Green's functions. Iterative inverse techniques, such as the Conjugate Gradient Least Squares method, are easily adapted to use Toeplitz multiplication, and explicit regularization is introduced for extra stability. This method is demonstrated on volcano data from Mount Erebus, Antarctica.

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### CP6

#### Refraction Travel-Time Tomography Based on Adjoint State Techniques

Standard refraction travel-time tomography based on ray tracing techniques has difficulties to handle large datasets that come from current seismic acquisition surveys. To overcome this problem we suggest a refraction tomography method based on adjoint state techniques to derive the gradient of the travel-time misfit function. We use the eikonal equation for the forward modeling, and iterate with a conjugate gradient method. Numerical examples demonstrate the efficiency of the method.

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### CP7

#### A Stochastic Differential Equation Model Of Multiphase Flow In Heterogeneous Porous Media

This research explores the use of stochastic differential equations (SDEs) in modeling multiphase flow in heterogeneous aquifers, specifically the flow of NAPL in saturated soils. The proposed method results in a nonlinear stochastic differential equation describing the position of the non-wetting phase fluid particle. In this presentation six aspects of the model are covered, each of which addresses a different component of the SDE model deemed important either by experimental tank results or on theoretical

considerations.

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### CP7

#### Scaling Behavior of Stochastic, Multiphase Flow in Porous Media

Subsurface formations are heterogeneous at all length scales, and even fine scale heterogeneities, particularly in the permeability field, can have a significant impact on large scale flow. Due to the difficulty in complete and certain characterization of these heterogeneities, stochastic representations of subsurface geologic properties have become commonplace. As a result, the flow equations have stochastic coefficients, and must also have stochastic solutions. Thus predictions of flow outcomes are inherently stochastic. We examine multiphase flow in stochastically described heterogeneous porous media. The study centers on the interplay between nonlinearity and heterogeneity in determining fluid mixing dynamics. Monte Carlo simulations are used for a quantitative analysis of this mixing. Different flow regimes, identified by the large time scaling behavior of the mixing dynamics, are characterized. This characterization provides significant guidance for uncovering effective methods (and their limits) for the scaling-up of multiphase flow systems to scales suitable for computationally inexpensive yet accurate fluid flow simulations.

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### CP7

#### Three-Phase Flows in Heterogeneous Formations

We are concerned with the accurate numerical simulation of three-phase flows in heterogeneous, multiscale porous media. An operator splitting technique combines a second order central scheme for the approximation of a hyperbolic system with mixed finite elements for the numerical solution of elliptic and parabolic problems. The new scheme is validated against semi-analytic results. Moreover, our simulator is used to show that transitional waves, which have been identified in one-dimensional problems, also appear in heterogeneous two-dimensional formations.

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### CP7

#### Approximation of the Richards Equation by Discontinuous Galerkin Methods

We investigate Discontinuous Galerkin methods to approximate the Richards equation which describes unsaturated flow in porous media. We compare an approach based on

the mixed form with local flux reconstruction to another approach based on the primal form. We present different methods in one and two space dimensions to discretize time-derivative and to treat non-linearities. Several test cases for unsaturated and unsaturated-saturated flows will be exposed.

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### CP7

#### Stochastic Analysis of the Displacement Front in Three-Dimensional Heterogeneous Porous Media

The problem of two-phase flow of immiscible fluids in randomly heterogeneous porous media is studied. Using improved perturbation theory we consider the effects of medium heterogeneity and nonlinearity together. This enables us to obtain the expression governing the front shape during the propagation and this shape is related to the permeability distribution and the frontal mobility ratio. Performing the averaging we obtain the mean saturation distribution near the front as well as the saturation variance.

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### CP7

#### Compositional Space Parameterization for Flow in Porous Media

Phase behavior is the most time consuming kernel of modeling multiphase multi-component flow in porous media. We present methods based on parameterization of the compositional space where the tie-lines and their geometry are the key parameters. A table look-up or a CSAT (Compositional Space Adaptive Tabulation) approach may be used to take advantage of this special parameterization. Using a variety of challenging test cases with large numbers of components, we demonstrate that the parameterization approach results in significant gains (e.g., at least an order of magnitude) in computational efficiency compared to existing methods.

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### CP8

#### Adaptive Discontinuous Galerkin Methods for Modeling Transition Flows

We consider time-dependent advection-diffusion equations with a spatially varying diffusion tensor modeling highly heterogeneous media. The mathematical behavior of the model imposes certain interface conditions between regions of advection or diffusion dominated flow. Such transition regions can be difficult to accurately model and may produce erroneous numerical solutions. We propose several variants of a discontinuous Galerkin method in an effort to adaptively capture the solution behavior in a stable and accurate manner. A priori error estimates are derived for each variant and are validated by numerical results. Our results also address the behavior of each variant with particular attention paid to the transition regions.

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### CP8

#### New Decomposition Method for Solving Multi-Species Reactive Transport Problems Coupled with First-Order Kinetics

A new method for decomposing of multiple solute transport equations, coupled by first-order reactions, is developed. The approach is based on the semigroup theory and reduces the multi-species problem to single-species equations with various initial and boundary conditions. Analytical formulas are derived for all reactants. This new method overcomes some of the limitations that were implicit in previously published algorithms. The proposed approach is flexible for solving one-, two- or three dimensional advection-dispersion systems. The methodology is demonstrated on the reductive biodegradation of chlorinated solvents, such as tetrachloroethylene(PCE) and trichloroethylene(TCE).

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### CP8

#### A Posteriori Error Analysis of Discontinuous Galerkin Schemes for Reactive Transport in Porous

### Media

The Discontinuous Galerkin scheme is particularly useful to simulate pollutant transport in groundwater flows. Reliable and efficient calculations often require adaptive meshes. We develop a residual-type a posteriori error analysis yielding two error components - the actual residual and a conforming error measuring the distance to continuous functions. Numerical results and adaptive meshes are presented to show the performance of the error indicators.

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### CP8

#### Inertial Influence on Pore-scale Dispersion in Porous Media

Although it has been recognized for some time that inertial effects can influence the observed conductivity (or, equivalently, friction factor) for fluid flow through porous media, the influence that inertial flows have on dispersion has not been as widely realized. We report on the prediction of the effective dispersion tensor for a simple 3D unit cell, and focus on the influence inertial effects (at large values of the particle Reynolds number) have on the predicted dispersion tensor. Our results indicate that inertial effects have a small effect on the longitudinal component of the dispersion tensor, but the transverse component is dramatically affected.

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### CP8

#### Multidimensional, Locally Conservative, Eulerian-Lagrangian Finite Element Methods for a Semilinear Parabolic Equation

Several locally conservative Eulerian-Lagrangian mixed finite elements of a two-dimensional convection-dominated diffusive process governed by a semilinear parabolic equation will be described. The simplest, low-order method is based on  $RT_0$  finite element method and post-processing procedures utilize the approximate flux variable to improve the approximation to the scalar variable. In addition, we discuss higher-order methods based on the  $BDFM_2$  finite element method. We present convergence proofs and experimental results.

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### CP9

#### Dispersion Minimizing Stencil for the Wave Equation

We have developed a new 41-point diamond-shaped stencil for the acoustic wave equation in 2D. The numerical error in the group velocity is minimized to get a stencil that works down to four gridpoints per wavelength. The elements in the stencil are polynomials in the cfl-number and is stable for cfl-numbers up to 0.707. Computations have been made up to 1000 wavelength with good results. A similar 129-point diamond-shaped stencil has also been derived in 3D.

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### CP9

#### Elastic and Acoustic - The Absorbing Boundary Condition

The elastic and acoustic wave equations are computed in finite regions. To control spurious reflections at the model boundaries we consider the Cerjan sponge as a method of choice and compare to the widely popular perfectly matched layer method. The sponge method is considered to be a numerical method, but new analysis shows that it has a suitable analytical basis.

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### CP9

#### Nonlinear Uncertainty Analysis in Reservoir Seismic Modeling and Inverse Problems

Forward modeling and inverse problems in reservoir seismic can be enhanced by nonlinear uncertainty analysis to quantify the range of expected outcomes. This requires capturing the a priori uncertainties in the model, parameter and data domains, and nonlinear sampling to produce realizations of each quantity. Application of the forward modeling or inverse operators to the realizations generates a posteriori uncertainty distributions, from which statistical measures of uncertainty can be calculated.

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### CP9

#### Incomplete Block Factorization for the Complex Helmholtz Equation

The lecture deals with a system of linear equations  $(A+iB)x=f$  where  $A$  is a symmetrical positive definite matrix and  $B$  is a diagonal matrix with elements of fixed sign. Method correctness is proved and spectre estimates are provided.

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### CP9

#### Elastic and Acoustic Wave Phenomena

This paper presents two and three-dimensional finite difference modeling of elastic and acoustic waves to identify different modes of elastic waves. The numerical formulation for the wave equation uses velocity-stress components in the modeling code. We review criteria necessary to generate Rayleigh waves in 2-D and 3-D for application to shallow surface-wave data imaging and analysis. The results of modeling study for the propagation of Rayleigh waves affected by heterogeneity of the medium are also presented. Examples of wave propagation and surface waves will be illustrated in movie loops.

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### CP10

#### Geological Pattern Recognition

The purpose of this paper is to determine the maximum volume in which a uniform upscaling can be performed. Any high change in geology occurring within a sufficiently large area, prevents to use only one single volume of averaging; the homogenized tensor is "non uniform". One way to discriminate the different regions is to group the "flux classes". The guess is then that the change of "flux class" corresponds to the change of region.

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### CP10

#### Comparison of Dominant Scales of Subsurface Flow and Transport Using Wavelet Analysis

Wavelet analysis is an integral transform method that can be used to extract local information about dominant scales of a spatial data set. We perform wavelet analysis on simulated data sets of aquifer properties (e.g., permeability) and on the head and concentration distributions resulting from flow and transport simulations in these aquifers. The results are used to identify relationships between dominant scales of aquifer properties and the dominant scales of flow and transport.

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**CP10****Multiscale Basis Optimization for Darcy Flow**

Simulation of flow through a heterogeneous porous medium with fine-scale features can be computationally expensive if the flow is fully resolved. Coarsening the problem gives a faster approximation of the flow but at a cost of some detail. We propose an algorithm that obtains the fully resolved approximation but only iterates on a sequence of coarsened problems. The sequence is chosen by optimizing the shapes of the coarse finite element basis, and converges superlinearly.

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**CP10****Numerical Solution of Porous Flow and Transport in Fractal Media**

Soils and rock are generally very heterogeneous, and contain structure over many scales. In order to capture the effect of this multiple scale structure in numerical models of flow and transport through permeable media, an integration of the governing partial differential equations with fractal coefficients has been developed. Statistics of the porous medium guide selection of the fractal coefficients. Examples are given for two and three dimensional applications.

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**CP10****A Tall-Block Model for Miscible Displacement in Fractured Media**

The effects of turbulent mechanical mixing of non-stationary, incompressible, two-component, miscible displacement in a fractured medium with tall blocks is studied. In that medium, there is an interconnected system of fracture planes dividing the porous rock into a collection of tall blocks. The fracture planes form paths of high permeability. Most of the fluids reside in tall blocks, where they move very slow. Let  $\epsilon$  denote the horizontal to the vertical size ratio of the tall blocks and let permeability, gravity and width ratios of tall blocks to fracture planes be of the orders  $\epsilon^2$ ,  $\epsilon^0$  and  $\epsilon^0$  respectively. The equations for the two-component, miscible displacement in fractured media converge to a dual-porosity model as  $\epsilon$  tends to 0. In this talk, we shall explain the dual-porosity model.

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**CP11****Wave Propagation Algorithms and Adaptive Re-****finement for Tsunami Modeling**

Modeling global tsunami propagation as well as local inundation requires resolving diverse flow regimes and spatial scales. The shallow water equations, a commonly accepted governing system, are hyperbolic conservation laws—a class of PDEs which ideally should be treated with specialized numerical methods. I will describe the extension of a type of finite volume method and adaptive refinement algorithms developed for such systems to the application of tsunami modeling. Together these methods allow transoceanic propagation modeling and local inundation modeling in single global-scale computations.

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**CP11****Perturbation Dynamics of a Planktonic Ecosystem**

Planktonic ecosystems provide a key mechanism for the transfer of CO<sub>2</sub> from the atmosphere to the deep ocean. Linear theory is used to predict how an ecosystem in a steady state will respond to a small perturbation and to solve for the perturbation that will result in an optimal response at a fixed time under some norm, such as carbon export. Results will be discussed.

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**CP11****Large Eddy Simulation of Stratified Mixing in a Dam-Break Problem**

Mixing in both coastal and deep ocean is an important process for the transport of pollutants, sediments, and biological species, as well as for the global thermohaline circulation. The oceanic observations and most coastal and general circulation models can only provide partial information about oceanic mixing processes. A new class of physically-based large eddy simulation (LES) models is proposed as an investigation tool to complement observational and large-scale modeling efforts.

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#### CP11

##### **Towards Understanding Coastal Ocean Internal Tides Via SUNTANS**

Monterey Bay (MB) experiences large internal tides and unexplained elevated dissipation. To understand what causes these phenomena, we developed **Stanford Unstructured Nonhydrostatic Terrain-following Adaptive Navier-Stokes Simulator (SUNTANS)** with the ultimate goal towards understanding connections between internal tides and enhanced dissipation. High resolution simulations of MB identify the main source region of the internal tides, and show the three-dimensional nature of the internal tidal field. These unique results improve our understanding the internal tide evolution.

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#### CP11

##### **Generalized Quasi-Geostrophy for Spatially Anisotropic Rotationally Constrained Flows: Non-Hydrostatic Flows**

Large-scale geophysical flows often exhibit balanced motions that reflect an underlying reduced dynamic contained within the primitive equations. In this talk closed reduced equations analogous to the quasi-geostrophic equations are derived in the extratropics for small Rossby numbers and vertical scales that are comparable to or much larger than horizontal scales. On these scales, significant vertical motions are permitted and found to couple to balanced geostrophic dynamics. These equations are derived by a systematic exploration of different aspect ratios, and Froude and buoyancy numbers, and offer advantages similar to the standard quasi-geostrophic equations but for studies of smaller-scale rotationally constrained processes. Their potential relevance to open ocean deep convection will be discussed.

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#### CP11

##### **Numerical Simulation of An Asymptotically Reduced System for Rotationally Constrained Convection**

Numerical simulation of Navier-Stokes equations for rotationally constrained convection is severely limited by thin Ekman boundary layers and fast inertial waves. To investigate convection in this regime, we employ numerical simulation of an asymptotically reduced system of nonlinear PDEs valid in the limit of small convective Rossby number. Simulations exhibit strong qualitative agreement with physical experiments. Such simulations have potential to provide insight into ocean deep convection, and pathways to improved mixing parameterizations.

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#### CP12

##### **An Information-Theoretic Observation Targeting Algorithm for An Ensemble Forecast System**

This work presents an efficient multiple targeting algorithm incorporated with an ensemble forecast system. The impact of each additional observation on the verification site is computed by that of a fictitious observation taken at the verification site back on the search space, which significantly reduces the number of times that the computationally expensive ensemble updates must be performed. Numerical simulations using an idealized chaos model are presented to validate the advantage of the proposed algorithm.

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#### CP12

##### **Toward an Optimal Reduced Order Control Strategy in 4D-Var Data Assimilation**

Order reduction in atmospheric four dimensional variational data assimilation is implemented using the proper orthogonal decomposition (POD) method. A reduced second order adjoint model provides Hessian matrix information and is used to assess the efficiency of the POD-based optimization. Optimal data collection and development of a reduced order control strategy that accounts for the characteristics of the data assimilation system are discussed. Numerical experiments are presented with a finite volume global shallow-water model.

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#### CP12

##### **A Kalman Filter Methodology for Non-Gaussian Errors**

Kalman filtering is an assimilative technique for correcting predictions of linear models using data related to the model states. Kalman techniques assume white noise distributions for model and measurement errors. A distribution-free Kalman filtering exists but its predictions are affected by outliers. In addition, normality of the errors is lost when extending by linearization Kalman methodology to nonlinear models. We present a Kalman filter methodology for dispersion exponential family distributions that avoids these problems.

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#### CP12

##### **The Impact of the Numerical Discretization on Targeted Observations**

The problem of targeted observations in numerical weather prediction is considered in the context of 4D-Var data assimilation. Adjoint sensitivity and singular vectors methods are implemented for the Lin-Rood flux-form semi-Lagrangian shallow-water model on the sphere. Identification of the target area is shown to depend on the specification of the subgrid distribution in the 1D finite-volume

transport operators. Results are presented for the piecewise linear and piecewise parabolic schemes.

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#### CP12

##### **Path Integral Approach to Data Assimilation**

I describe a path integral approach, based on a hybrid Monte Carlo method, for data assimilation. The method can be used for such tasks as computing a smoother solution, parameter estimation, data/model initialization. Since it makes no assumptions on linearity in the dynamics, or on Gaussianity in the statistics, it permits consideration of very general estimation problems. This estimation method exploits gradient-following sampling and nonlocal decorrelation strategies to achieve a significant reduction in computational costs, as compared to basic Monte Carlo sampling. An application to Lagrangian data assimilation in fluid flow and an application to hydrology will be used to illustrate the method's capabilities.

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#### CP12

##### **A Weighted Total Least-Squares (wtls) Approach to Geophysical Time-Series Regression Analysis**

Standard regression allows for measurement noise only in the response variable whereas random errors in the regressors are neglected. We present an approach based on the Weighted Total Least-Squares principle that properly handles such errors in all variables. This approach is highly beneficial, as we demonstrate using data from a recent article (EOS, 87/24) by M.E.Mann and K.A.Emanuel where they tried to link atlantic hurricane trends to climate change. (Joint work with Andreas Wieser).

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#### MS1

##### **Modeling Flow and Deformation Processes in Porous Media**

Bio-tissue, highly-interacting soils such as clay, and swelling polymers such as what are used for drug delivery

systems are all examples of swelling porous materials for which the coupling of flow and deformation may be of interest. Here we examine the assumptions of the traditional formulation (Darcy's law and the Terzaghi stress principle) and develop a thermodynamically admissible generalization of these two equations for swelling porous media.

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### MS1

#### **Strong Ellipticity for Anisotropic, Nonlinear Elastic Material Bodies**

Nonlinear hyperelasticity is an appropriate setting in which to model the large deformation behavior of many materials of geological relevance. The stability of such deformations to small perturbations is a central issue from the physical, computational and mathematical perspectives. Various notions of convexity of the strain energy function (e.g. polyconvexity, quasiconvexity and strong ellipticity) play key roles in studying these stability issues. There are good arguments that strong ellipticity is the physically most compelling condition to consider. This talk presents a survey of results concerning both necessary and sufficient conditions for strong ellipticity to hold for strain energy functions of certain novel sets of strain invariants characterizing isotropic or orthotropic constitutive behavior recently introduced by Criscione et al that are particularly well-suited to fitting real material data.

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### MS1

#### **Iterative Coupling of Multiphase Flow and Mechanics in Porous Media**

The modeling of coupled flow simulation and mechanical deformations is important in addressing the response of reservoirs located in structurally weak geologic formations. In this presentation we present an iterative coupling algorithm of poroelasticity. In treating the multiphase flow we use a discretization which involves a fully implicit mixed finite method for multiphase flow and a Galerkin method, either discontinuous or conforming, for elasticity. Theoretical convergence results and computational examples are presented.

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### MS1

#### **Estimating the Elastic Moduli and Permeability of Porous Materials from Two-Dimensional Pore Space Images**

Physical properties of porous media are estimated from two-dimensional pore images. The permeability prediction uses the hydraulic radius approximation to estimate the individual pore conductances, and Kirkpatrick's effective medium approximation to upscale to the core-scale permeability. The elastic moduli prediction uses a scaling law based on the perimeter and area to estimate individual pore compressibilities, and then uses the differential effective medium theory to upscale to the core-scale elastic moduli. Good agreement is obtained with permeability and moduli measurements on various sedimentary rocks and ceramics.

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### MS2

#### **Beyond Homogenization - New Scaling Approaches for Stable and Unstable Density Dependent Flows through Heterogeneous Media**

A practicable solution of density-dependent problems for field application requires consideration of the influence of natural heterogeneity and thus up-scaling. Generic aquifers with different geostatistical properties of the permeability distributions are looked at, following the concepts developed in Held et al. [2005]. First, a stability analysis combined with a generalized two-scale expansion is proposed to investigate the stability of density dependent flows on geological scales. So far only stability criteria for density dependent flows in homogeneous media exist. Our new approach, however, allows to predict the onset of instabilities of density driven flows in heterogeneous media. Second, to determine effective parameters for density dependent flows in heterogeneous aquifers, a systematic analysis of heterogeneity impacts is carried out here based on a new approach which homogenization combined with a filter method called Coarse Graining. The new approach allows to overcome the limitation of standard homogenization which is the assumption of scale separation. We will present explicit results for scale dependent effective parameters in the case of stable as well as unstable flow configurations.

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### MS2

#### **pH-Dependent Transport of Zinc at Cape Cod, Massachusetts**

Land disposal of sewage effluent at Cape Cod, Massachusetts resulted in contamination of the aquifer with zinc (Zn). Adsorption of zinc was apparently correlated with pH-values of the groundwater. A correlation between the pH-value and a referring K<sub>d</sub>-value could be derived from sorption experiments with zinc and sediment material from Cape Cod. 2-D and 3-D models have been set-up using the transport code r3t. It was possible to reproduce

the essential features of the measured zinc distribution.

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## MS2

### Advanced Numerical Methods for Transport and Reaction in Porous Media

Precise numerical solutions for systems of partial differential equations modeling the flow, transport and reaction in porous media have to overcome several nontrivial difficulties - complex geometries that imply applications of unstructured grids, the different scales of the advection, diffusion-dispersion and reaction models that require very general algorithms, and the sensitivity of computations to unphysical oscillations that demands robust numerical schemes. In this talk, some advanced numerical methods that fulfill such challenging requirements will be presented. Additionally, new applications of level set methods in problems of flow and transport in porous media will be presented.

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## MS2

### Effect of Single-Species Reactive Solute Transport on Thermohaline Groundwater Flow in Fractured Porous Media

A three-dimensional numerical model has been developed to solve coupled fluid flow, heat and single-species reactive mass transport with variable fluid density and viscosity. The focus was put on a single reaction between quartz and its aqueous form silica. Results of a long-term (100 years) simulation indicate that coexistence of dissolution and precipitation leads to self-sealing of fractures. Salt mass fluxes through fractures decrease significantly due to major fracture aperture reduction in the precipitation zone.

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## MS3

### Estimation Theory and Data Assimilation for Transport Processes

A brief overview of some recently developed estimation and data assimilation methods will be given. Specific applications to transport processes will be presented.

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## MS3

### Upscaling Reactive Transport Processes From the Pore- to Continuum-Scale Using the Lattice Boltzmann Method

Reactive transport processes with different reactions in various synthetic structured and real porous medium geometries

obtained with computed microtomography (CT) are simulated at the pore scale using the lattice Boltzmann (LB) method. The results are volume averaged over a REV (representative elemental volume) and fit to multiscale continuum models. It is shown that the LB model enables the computation of macroscopic parameters needed in the continuum formulation, and the determination of the most appropriate continuum formulations (single, dual, or multiple continua). It is noted that the detailed pore-scale information obtained from the LB simulation may help explain the observed discrepancy between laboratory and field derived reaction rates by accounting for multiscale process at the continuum scale with explicit representation of distinct transport domains through separate interacting continua.

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## MS3

### Hybrid Models for Multiscale Simulation of Subsurface Biogeochemical Processes

Many subsurface flow and transport problems involve coupled flow, transport, and reactions in heterogeneous media. Experimental research has revealed details about the physical, chemical, and biological mechanisms involved in these processes at a variety of scales ranging from molecular to laboratory scales. However, integration of quantitative process models across these scales remains a significant challenge. We will present examples illustrating these challenges and outline a hybrid multiscale approach as applied to this problem.

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## MS3

### Efficient Numerical Methods for Uncertainty Analysis with Multiscales

Many physical systems, such as natural porous media, are highly heterogeneous and characterized by parameters that are uncertain due to the lack of sufficient data. This uncertainty (randomness) occurs on a multiplicity of scales. In this talk we will investigate numerical solvers to deal with such kind of problems. The focus is on the efficiency and accuracy of the algorithms and their applicability to practical applications.

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#### MS4

##### Upscaling DNAPL Dissolution Mass Transfer in Porous Media

Dissolution of NAPL takes place at the pore scale while remediation technologies are applied at the field scale. Building models that effectively represent the pore scale processes requires developing techniques for quantifying these processes and their impact on large-scale mass transfer rates. We present an integrated experimental and computational approach to quantitatively investigate the role of pore structure, entrapped NAPL distribution and hydrodynamic conditions on pore scale mass transfer rates.

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#### MS4

##### Comparison of Particle, Grid- Based and Lattice Boltzmann Methods for Multiphase Fluid Flow in Fractured and Porous Media

Particle (smoothed particle hydrodynamics and dissipative particle dynamics) grid based (Navier Stokes equation solvers with volume of fluid and level set interface tracking) and lattice Boltzmann models have been developed and applied to multiphase fluid flow in porous media, fractured porous media and fractured impermeable media. The results of simulations of multiphase fluid flow in fractured and porous media will be presented, and the relative strengths and weaknesses of the models investigated will be discussed.

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#### MS4

##### Smoothed Particle Hydrodynamics Model of

##### NAPL Flow and Dissolution

A smoothed particle hydrodynamics model was developed to simulate the flow of mixtures of aqueous and non-aqueous phase liquids in porous media and the dissolution of the non-aqueous phase in the aqueous phase. The model was used to study the effects of pore-scale heterogeneity and anisotropy on the steady state dense non-aqueous phase liquid (DNAPL) saturation when gravity driven DNAPL displaces water from initially water saturated porous media.

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#### MS4

##### Simulation of Particulate Flow at the Pore Scale using Embedded Boundary Volume of Fluid Methods

We present a simulation capability for transport of colloidal-sized particles at the pore scale. Particulate is represented by a bead-rod polymer model and is fully-coupled to a Newtonian solvent. Finite differences are used to discretize the interior of the domain; a Cartesian grid embedded boundary / volume-of-fluid method is used near boundaries and interfaces. Electrochemical interactions are included in the particle model. We demonstrate this capability on particulate flow in a spatially-resolved packed bed column.

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#### MS5

##### New Approaches for Model Reduction for Reservoir Flow Simulation

Adjoint-based optimal control techniques are well suited for optimizing the performance of oil reservoirs, though these methods require that numerous simulation runs be performed, which can be very expensive with large reservoir models. The goal of this work is to investigate the use of model reduction procedures for this problem. Our approach uses a large set of "snapshots," generated from detailed reservoir simulations, and then applies a hybrid technique that combines Centroidal Voronoi Tessellation and Proper Orthogonal Decomposition to efficiently generate low-order models. We show that these low-order models are able to capture the behavior of the detailed model with a reasonable degree of accuracy even in the case of varying well rates and pressures, which indicates that this approach is indeed suitable for use in well control optimiza-

tion.

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## MS5

### Low-Order Approximation Methods for Oil Reservoir Simulation and Control

Great effort has been devoted to constructing high-order reservoir models for improved oil recovery. Several models of varying complexity have already been tested and understood. Additionally, the use of novel multivariable optimization techniques, optimal control, and sensor technology in the oil industry has increased the potential for greater oil recovery, and therefore, enhanced reservoir management and profitability. However, these models entail large amounts of computational effort in order to obtain accurate solutions in a reasonable time. This work compares several linear and nonlinear model order reduction techniques for the simulation and design of low-dimensional optimal controllers for flow in porous media.

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## MS5

### Kernel Principal Component Analysis for a Reduced Order Differentiable Parameterization of Multi-Point Geostatistics

This work describes a novel approach for creating an efficient, reduced differentiable parameterization of large-scale non-Gaussian, non-stationary random fields (represented by multi-point geostatistics) that are capable of reproducing complex geological structures such as channels. Such parameterizations are appropriate for use with gradient-based algorithms applied, for example, for history-matching or uncertainty propagation. In earlier work we showed that the standard Karhunen-Loeve (K-L) expansion (also called linear principal component analysis, PCA) could be used as a differentiable parameterization of input random fields defining the geological model. The standard K-L model is, however, limited in two respects. Specifically, it requires an eigen-decomposition of the covariance matrix of the random field, which is prohibitively

expensive for large models. In addition, it preserves only the two-point statistics of a random field, which is insufficient for reproducing complex structures. In this work, we apply kernel PCA to address the limitations associated with the standard K-L expansion. Kernel PCA is widely used in machine learning applications but does not appear to have found much if any application for geological model parameterization. With kernel PCA, an eigen-decomposition of a small matrix called the kernel matrix is performed instead of the full covariance matrix. The method is thus much more efficient than the standard K-L procedure. Through use of higher order polynomial kernels, which implicitly define a high-dimensionality feature space, kernel PCA further enables the preservation of arbitrarily high-order statistics of the random field, instead of just two-point statistics as in the K-L method. The kernel PCA eigen-decomposition proceeds using a set of realizations created by geostatistical simulation (honoring two-point or multi-point statistics) rather than the analytical covariance function. We demonstrate that kernel PCA is capable of generating differentiable parameterizations in terms of a small number of random variables that reproduce the essential features of complex geological structures represented by multi-point geostatistics. The kernel PCA representation is then applied to history match a water-flooding problem. This example demonstrates that kernel PCA can be used with gradient-based history matching to provide models that match production history while maintaining multi-point geostatistics consistent with the underlying training image.

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## MS5

### Enablers for Low Dimensional Galerkin Models for Control and Observation in Fluid Dynamics

The proper orthogonal decomposition (POD, and close variants) method is extremely efficient in compressing empirical flow data, such as from an attractor, but is notorious for the fragility of resulting models when transient dynamics are of interest. We shall review a suit of enablers for maintaining the efficiency of the Galerkin approximation, which is essential in applications such as feedback control or real time estimation, while expanding the dynamic range of the model and improving its effective use. A key enabler, reported earlier, is the inclusion of a generalized mean field model. We shall demonstrate that, indeed, base flow dynamics are locally represented by a single flow mode, which varies slowly along natural and actuated transients. This mode can be extracted empirically, or from linearized flow equations. Geometrical methods will be used to capture by interpolation the continuous deformation of dominant flow modes along transients. Thus, dynamic representation of transients is achieved at the cost of an added nonlinearity (due to mode interpolation) but without an increase in dimension, when compared with a model obtained from a single operating point or orbit. Interpolation methods include the use of both a posteriori empirical data (e.g., POD modes) or a priori linear stability analysis. They are established as viable tools also for accommodating changing geometries (e.g., an airfoil angle of attack) and flow conditions (e.g., the Reynolds number). The flow space geome-



try is a critical component in POD mode extraction. We shall present variations based extensions of the observability Gramian, to extract the most observable (or relevant) modes.

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### MS6

#### **Optimizing Tetrahedral Element Quality Through the Use of Mesh Smoothing Techniques for Studying Near Surface Phenomena**

An algorithm for rapid, large-scale mesh generation will be presented in the context of studying near-surface phenomena. The output of black-box mesh generation software is post-processed with a mesh-smoothing technique to ensure quality tetrahedral elements in the final mesh. The result is an optimization problem with more than 100k degrees of freedom. The entire procedure will be presented with a specific focus on the smoothing algorithm, the optimization problem, and the treatment of buried objects.

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### MS6

#### **Some Derivative-Free Approaches to a Hydraulic Capture Benchmarking Problem**

We discuss some derivative-free optimization techniques applied to a hydraulic capture problem proposed in the literature for benchmarking purposes. This application is an example of simulation-based optimization. We discuss several aspects of the problem which effect the minimization including the capture constraint formulation and inclusion of fixed costs which leads to a mixed-integer problem. We include results obtained with several sampling methods and also consider a multi-model approach and the use of surrogate models to help with the expensive simulations involved.

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### MS6

#### **Application of Optimization Techniques to Large-scale Groundwater Problems for Model Calibration**

The Engineer Research and Development Center models groundwater flow and transport for monitoring and remediation purposes. Physics based models for some of these sites are very large and require parallel computer resources. Data provided for these sites such as borehole data, head values, and concentration values are spatially sparse. Optimization techniques have been applied to these parallel numerical models that utilize the sparse data to provide the best estimates of the model input parameters.

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### MS6

#### **POD Methods for Model Calibration**

Abstract not available at time of publication.

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### MS7

#### **Dispersion in Deformable Media**

Swelling porous media such as clays and many polymers are ubiquitous and consequently a proper understanding of how chemicals are transported within such systems is critically import. Here we review several of our attempts to model anomalous dispersion in these systems over a hierarchy of scales.

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### MS7

#### **Modeling Leakage of Carbon Dioxide from Underground Storage Sites**

Reduction of atmospheric greenhouse gas is of great current interest. One mechanism for reducing carbon dioxide emissions is to capture and reinject these gases into abandoned reservoirs. Regulators must then be able to determine whether these buried gases will leak back out into the atmosphere or into underground "assets" such as active hydrocarbon reservoirs or aquifers with unusable drinking water. We will discuss a simple modeling study to begin to answer questions of CO2 leakage.

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**MS7****Theoretical Investigation of the Effects of Consolidation on Contaminant Transport in Composite Contaminant Barriers**

Consolidation of clayey contaminant barriers such as land-fill liners has been advocated as a cause of early breakthrough of contaminants. This paper theoretically investigates this proposition. We propose a sophisticated one-dimensional, large deformation model of coupled mechanical consolidation and solute transport. This new model is a generalization of existing coupled consolidation and solute transport models described in the literature taking into account both nonlinearities of the geometric relations as well as of the constitutive relations.

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**MS7****Advective Transport in Porous Media: A Calibration of Computational**

The calibration of computational approaches to modelling of the advective transport in a fluid saturated porous media invariably use a classical one-dimensional solution with constant flow velocity, where the front has a discontinuous profile, resulting in a restrictive criterion for unconditional stability. This paper calibrates the computational performance of the stabilized schemes through several recently developed analytical solutions, which take into consideration time-dependent velocities and the influence of processes resulting from natural attenuation.

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**MS8****Title Not Available at Time of Publication**

Abstract not available at time of publication.

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**MS8****On the Role of Transversal Dispersion in Density Dependent Flow and Transport in Heterogeneous Porous Media**

Abstract not available at time of publication.

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**MS8****Title Not Available at Time of Publication**

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**MS9****A Globally Coupled Method for Reactive Transport in Porous Media**

Reactive transport with equilibrium reactions leads to a system of advection-diffusion PDEs, coupled with algebraic equations. We investigate a global solution method, formulated in terms of total mobile and total immobile concentrations, and we propose to solve the nonlinear problem with a Newton-Krylov method. In contrast with the more traditional direct substitution approach, we keep chemistry distinct from the transport equations, leading to a formulation with a smaller number of unknowns, where evaluating nonlinear function requires solving a chemical problem at each grid point.

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**MS9****Reformulation of Multicomponent Transport-Reaction Equations for the Reduction of the Problem Size, and Treatment of Mineral Reactions as a Complementarity Problem**

The talk is about a reformulation of multicomponent transport-reaction equations which can be used to reduce the size of the corresponding nonlinear system of equations. This leads to a reduction of cpu time, while the system of PDEs, ODEs and algebraic equations is still treated fully implicitly without splitting. Special emphasis will be laid on the handling of equilibrium mineral reactions. They are formulated as a *Complementarity Problem*. Hence, the full nonlinear problem can be solved by the *Semismooth Newton method*.

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**MS9****Dissolution and Precipitation in Porous Media: Analytical and Numerical Results**

We consider a pore scale model for dissolution and precipitation in porous media. Ions transported by a fluid flowing through the pores may react and form a precipitate layer that is attached to the surface of the grains. Conversely, dissolution is also possible, leading to a possible change in the geometry of the pores. We present some analytical and numerical results, and focus on the occurrence of dissolution and precipitation fronts.

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**MS9****Modeling Mixing-Controlled Biogeochemical Reactions from the Pore to Continuum Scale**

Several studies have demonstrated the important role played by transverse mixing and dispersion along the fringes of chemical plumes in porous media. These studies have also demonstrated that the length scale of transverse mixing zones can be very small, often on the order of centimeters or less. In order to study dispersion, mixing and reaction at this scale we are using pore-scale numerical modeling and micro-model laboratory experiments. The numerical modeling framework consists of the following: (a) geometric construction of a packed bed of grains; (b) solution for the steady flow field by the lattice-Boltzmann method; and (c) solution for the steady-state distribution of reactive chemicals using a finite-volume code. For the case with microbially-mediated reactions, there is an additional step that uses a rules-based approach to simulate biofilm growth. The simulation results show good agreement with the experimental data. The numerical model also shows how the overall reaction rate depends upon pore-scale geometry. Comparing the pore-scale results with continuum models shows that transverse mixing is adequately quantified using classical hydrodynamic dispersion coefficients. This is contrary to other results in the literature for longitudinal mixing. Extension to field scales will also be discussed. In this case, macro-dispersion coefficients that model spreading due to sub-grid scale heterogeneity cannot be used to model reactant mixing.

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**MS10****Particle Suspension Transport in Porous Media: Einstein-Smoluhowskii and Boltzmann Models**

Suspension transport in porous media is accompanied by particle capture, mainly by size exclusion and attachment. The conventional mathematical model assumes that parti-

cles move with the carrier water velocity. Nevertheless, size exclusion remove particles mostly from thin pores, causing increase of particle speed. On the contrary, attachment is proportional to free surface area, particles are removed mostly from large pores, causing particle speed decrease. We take two different approaches - that of Einstein-Smoluhowskii (population balance models resulting in continuous Markov chains) and that of Boltzmann - to resolve the paradox. Unknowns for both models are particle and pore size distributions. Several exact solutions allow for averaging of both micro scale models. The averaged models significantly differ from the conventional model. Particle averaged speed is different from water velocity.

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**MS10****Lattice Boltzmann Simulations of Multi-Component Reactive Transport in Porous and Fractured Media at the Pore Scale**

A lattice Boltzmann (LB) pore-scale model for simulating multi-component reactive transport process in porous and fractured media is presented. The model takes into account advection, diffusion, homogeneous reactions among multiple aqueous species, heterogeneous reactions between the aqueous solution and minerals, ion exchange and surface complexation reactions at the fluid-solid interface, as well as the resulting geometrical changes in pore space. Simulation results with different reactions in various synthetic structured and real porous and fractured media are presented.

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**MS10****Residual Fluid Blobs and Contact Angle Measurements from X-Ray Images of Fluid Displacement**

We consider the measurement of fluid-fluid and fluid-solid surfaces in X-ray computed tomographic images of two phase (oil-water) displacement at residual fluid conditions in a Berea sandstone sample. 3D reconstructions of the residual fluid blobs show qualitative behaviour which is in agreement with conventional wisdom. We consider the measurement of fluid-solid contact angle via such images and elucidate the challenge in identifying triple points (points with three phases in contact). We develop an algorithm for contact angle measurement. Results from application of the contact angle algorithm indicate the ability to distinguish wetting and non-wetting fluid blobs and reveal satisfactory agreement with experimental wettability measurements.

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### MS10

#### Computational Rock Physics: Pore Scale Simulations in Realistic Granular Microstructures

Pore-scale process simulation is moving towards more complex geometries. The construction of physics-based, realistic rock microstructure is needed to better understand geologic processes. We are working on granular media simulations to create rock geometries and couple them with simulations of various transport processes. Rock microstructure created from physics-based modeling using Discrete Element Method serves as an input to Lattice Boltzmann flow simulation.

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### MS11

#### Model Reduction from Input/Output Measurements

In many applications no explicit model of a given process is available. Instead input/output measurements of the process exist. The problem therefore consists in computing an appropriate approximate (reduced-order) model directly from these measurements. In this talk we will propose a method for achieving this objective. The main tool is the Loewner matrix. We will also show that this method can be extended to deal with passivity preserving model reduction. Numerical experiments verifying the theoretical considerations will also be provided.

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### MS11

#### Robust Model Reduction for Contaminant Transport Applications

Robust reduced-order models, i.e. those able to approximate full-scale outputs over a wide range of parameters, have an important role to play in making tractable large-scale optimal design, optimal control, and inverse problem applications. We pose the task of determining appropriate training sets for reduced-basis construction as a sequence of optimization problems and show that these problems

have a closed-form solution under certain assumptions. We present an efficient model-construction algorithm that scales well to systems with a large number of parameters.

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### MS11

#### The Use of Reduced Order Models to Accelerate the Iterative Solution of Systems of Equations

We developed a method to use reduced-order models for solution acceleration of systems of equations using iterative solvers in time stepping schemes for reservoir simulation. We assessed the efficiency of this technique for large-scale linear and nonlinear systems. The acceleration is achieved by determining an improved initial guess for the iterative process based on information in the solution vectors from previous time steps, through the use of proper orthogonal decomposition (also known as Karhunen-Love decomposition, principal component analysis or the method of empirical orthogonal functions). The algorithm basically consists of two projection steps: 1) projecting the governing equations onto a subspace spanned by a low number of global empirical basis functions extracted from previous time step solutions, and 2) solving the governing equations in this reduced space and projecting the solution back on the original, high dimensional one. We applied the algorithm to implicit-pressure explicit-saturation schemes and fully implicit schemes using Newton and Picard iteration. We achieved a substantial reduction in the number of iterations and an associated acceleration of the solution. Our largest test problem involved 93,500 variables, in which case we obtained a maximum reduction in computing time of 67%. The method is particularly attractive for problems with time-varying parameters or source terms.

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### MS11

#### Balanced Reduction with a Parameter Free ADI-like Method

Balanced reduction provides a means to approximate a linear time invariant dynamical system with a reduced order system that has excellent approximation properties including a global a priori error bound and preservation of asymptotic stability. To construct the transformations required to obtain balanced reduction, large scale Lyapunov equations must be approximately solved in low rank factored form. We have developed a new method for solving Lyapunov equations that is essentially a synthesis of the approximate power method (APM) and the alternating direction implicit (ADI) algorithm. Problems on the order of 1 million state variables can be solved on a high end workstation. The new algorithm is provably convergent and does not require the selection of parameters (as in the ADI

method). It is, therefore, a promising candidate for developing into reliable mathematical software. An extension of this approach has been developed that will simultaneously solve the two Lyapunov controllability and observability equations to obtain the balancing transformation. This can be a considerable improvement when only one of the two equations admits a very low rank approximate solution.

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#### MS12

##### **Small-scale Computational Modeling of Vuggy Porous Media**

We discuss computational techniques for small-scale simulation of flow and transport in interconnected vugs, i.e., cavities. Flow is governed by Darcy's law in the rock matrix and Stokes' equations in the vugs, with the Beavers-Joseph condition on the interface. We develop a code for simulating the 3-D Darcy-Stokes flow with a multi-grid method and modified Uzawa smoother to solve the ill-conditioned linear system. We compare our computational predictions to field and laboratory experiments.

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#### MS12

##### **Discontinuous Finite Elements for Ground Water/Surface Water Coupling**

We discuss mathematical and numerical issues related to the modeling of flow and transport in coupled ground water and surface water domains. Particular issues which arise include the appropriate choice of models within each domain, and the determination of boundary conditions at the coupling interface. Numerically, ground and surface water flows often occur at very disparate spatial and temporal scales. We will present recent results on the application of discontinuous Galerkin methods for these models.

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#### MS12

##### **High Resolution Multi-Scale Storm Surge Modeling for Southern Louisiana**

Coastal Louisiana is characterized by low-lying topography and a network of sounds, estuaries, bays, marshes, lakes, rivers and inlets that permit widespread inundation during hurricanes. A basin to channel scale implementation of the ADCIRC unstructured grid hydrodynamic model simulates hurricane storm surge, tides, river flow and wave-radiation-stress setup in this complex region. This is accomplished by defining a domain and computational resolution appropriate for the relevant processes, and implementing accurate, robust, and highly parallel algorithms.

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#### MS12

##### **Coupling of Flow and Transport for Surface Water-Groundwater Systems**

We discuss a mathematical and numerical model for contaminant transport in surface water-groundwater systems. The Stokes-Darcy flow system is coupled with a transport equation. Beavers-Joseph-Saffman interface conditions are imposed. Stability and error estimates are established for a finite element discretization based on conforming or discontinuous elements for Stokes flow, mixed finite elements for Darcy flow, and local discontinuous Galerkin elements for transport. The formulation utilizes a Lagrange multiplier to impose the interface conditions. A non-overlapping domain decomposition algorithm is developed for the flow equations which reduces the coupled algebraic system to an interface problem for the normal stress. Each interface iteration requires solving Stokes and Darcy subdomain problems. The properties of the interface operator are analyzed. Numerical results are presented.

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#### MS13

##### **Geomechanics of Fractured Reservoirs**

Most rocks in the crust are fractured, and both their fluid flow characteristics and their geomechanical behavior are strongly affected by the fractures. A semi-analytical model for random polycrystals of porous laminates permits detailed calculations of both geomechanical and transport coefficients for model reservoirs. This approach also enables the use of rigorous error estimates (or bounds) of the Voigt, Reuss, and Hashin-Shtrikman types. The resulting comparisons provide insights into expected behavior of fractured reservoirs.

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#### MS13

##### **Advanced Constitutive Model for Unsaturated Soils Including Double-Sided Hydro-Mechanical Coupling**

An advanced constitutive model for unsaturated soils, including a double-sided hydro-mechanical coupling is presented. It answers the need for a complete behavioural model, adaptable to a large panel of geomaterials with a reasonable number of parameters. It offers a unified modelling solution for several engineering problems such as dimensioning of earth dams. The model formulation derives directly from the understanding of mechanisms of behaviour of partially saturated material submitted to combinations of mechanical and hydraulic loading in laboratory. A performing saturated model based on two plastic mechanisms has been extended to deal with partially sat-

urated states, leading to the so-called ACMEG-S model. The adopted stress framework is a Bishop-type effective stress for the mechanical part and the matric suction for the hydraulic part. The many simplifications brought by the effective stress representation versus traditional net stress and suction representation are exposed and related to the definition and multiple use of the loading collapse curve. One pre-eminent contribution of the study lies in the modelling of the hydraulic response, termed soil water retention curve, by the means of a simple elastoplastic isotropic model rendering both the hydraulic hysteresis and the dependency of the soil water retention curve on void ratio. The coupled effects of mechanical history on the hydraulic response are quantified experimentally with an unsaturated oedometer. By integration via a custom numerical tool, several experimental hydro-mechanical test paths from the literature are successfully simulated with the ACMEG-S model, highlighting the major implications of the comprehensive hydro-mechanical framework.

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### MS13 Brinkman-Darcy Models of Porous Media

Single-phase flow through fissured porous media is described by a system of partial differential equations with components of Brinkman and Darcy types. These are suited to the simulation of flow in fissures and pore structure, respectively, and we study the solution regularity properties of these systems.

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### MS13 Two-Scale Modeling of Deformable Porous Media with Applications to Clays

A two-scale asymptotic analysis for flow in an elastic porous media is considered. The influence of the microscale interfacial phenomena on the effective behavior of clays is studied.

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### MS14 Carbon Dioxide Storage Capacity in Deep Saline Formations: Concepts and Optimization

Saline formations are expected to have a very large capacity to store carbon dioxide in a dense super-critical phase. This paper explores the underlying physical concepts that influence storage capacity, including hysteretic relative permeability curves, formation heterogeneity, and buoyancy

driven flow. In light of these fundamental processes, options for optimizing storage capacity are evaluated, including injection depths, well configuration, number of injection wells and formation properties. These studies are carried using properties of the Frio Formation in Texas, but general conclusions for a variety of storage sites are provided.

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### MS14 Residual Trapping in Sloping Aquifers

An estimate of the area invaded by the CO<sub>2</sub>-plume is of interest for site selection. During plume migration, CO<sub>2</sub> is trapped as residual gas in the wake of the plume. We present a simple model of a plume spreading in a horizontal a sloping aquifer with residual trapping. In a sloping aquifer the vertical sweep efficiency of the CO<sub>2</sub>-plume increases, this leads to a decrease of the maximum up-dip migration distance with increasing aquifer slope.

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### MS14 Application of a Locally Conservative Variational Multiscale Method for the Simulation of Geological CO<sub>2</sub> Storage in Highly Heterogeneous Formations

We present a variational multiscale mixed finite element method for flow in porous media. The method enables inexpensive simulations that capture the fine-scale heterogeneities that control buoyancy-driven flow. We simulate CO<sub>2</sub> migration with an IMPES multiscale strategy, in which the pressure equation is solved implicitly on a coarse grid, and the saturation equation is solved explicitly on the fine grid. We illustrate the formulation with synthetic and realistic cases, and discuss ongoing work to account for compressibility and hysteresis in relative permeability and capillary pressure.

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#### MS14

##### **Onset of Convection in a Gravitationally Unstable Diffusive Boundary Layer, in a Porous Medium**

We present a linear stability analysis of density driven, miscible flow in porous media in the context of CO<sub>2</sub> sequestration in saline aquifers. CO<sub>2</sub> dissolution into the underlying brine leads to a local density increase that results in a gravitational instability. The physical phenomenon is analogous to the thermal convective instability in a semi-infinite domain due to step change in temperature at the boundary. We present a solution, based on the dominant mode of the self-similar diffusion operator, which can accurately predict the critical time and the associated unstable wavenumber. This approach is used to explain the instability mechanisms of the critical time and the longwave cutoff in a semi-infinite domain. For large times, both the maximum growth rate and the most dangerous mode decay as  $t^{1/4}$ . The instability problem is also analyzed in the nonlinear regime by high accuracy direct numerical simulations. The nonlinear simulations at short times show good agreement with the linear stability predictions. A dimensional analysis for typical aquifers shows that for a permeability variation of 1 - 3000mD, the critical time can vary from 2000 yrs to about 10 days while the critical wavelength can be between 200m and 0.3 m.

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#### MS15

##### **Dynamics of 3D Atmospheric Mountain Gravity Waves**

Abstract not available at time of publication.

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#### MS15

##### **Urban Atmospheric Boundary Layer Dynamics**

Abstract not available at time of publication.

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#### MS15

##### **High Resolution Simulations of Stratospheric Clear Air Turbulence**

Abstract not available at time of publication.

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#### MS15

##### **Lagrangian Coherent Structures and Clear Air Turbulence**

Abstract not available at time of publication.

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#### MS16

##### **A Fully Mass and Volume Conserving Implementation of a Characteristic Method for Transport Problems**

The characteristics-mixed method transports mass along the characteristic curves of the hyperbolic part of the equation, and thereby produces little numerical dispersion, conserves mass locally, and can use long time steps. Since the shape of a trace-back region is approximate, its volume may be incorrect, giving inaccurate concentration densities. We present a simple modification that conserves both mass and volume of the transported fluid regions. Theoretical convergence results and several numerical examples are given.

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#### MS16

##### **Upscaling of Two-Phase Flow Transport in Heterogeneous Porous Media**

I will discuss a multiscale technique for simulation of porous media flows in a flow-based coordinate system. Flow based coordinate system allows us to simplify the scale interaction and derive the upscaled equations for purely hyperbolic transport equations. We discuss the applications of the method to two-phase flows in heterogeneous porous media. For two-phase flow simulations, the use of flow based coordinate system requires a limited global information, such as the solution of single-phase flow. Numerical results show that one can achieve accurate upscaling results using flow-based coordinate system. This is a joint work with T. Hou and T. Strinopoulos.

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#### MS16

##### **Iterative Coupling for Multiscale Methods for Multiphase Flow in Porous Media**

We discuss a multiscale mortar mixed finite element

method (MMFE) for multiphase flow that employs an iterative coupling scheme at each time step. Iterative coupling is an operator splitting technique that decouples the multiphase flow system into pressure and saturation equations. At each time step a series of iterations are computed that involve solving both pressure and a linearized saturation equation using specific tolerances that are iteration dependent. Concentrations are updated using mass balance equations. This approach is locally conservative and computationally more efficient than fully implicit.

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### MS16

#### Multiscale Mortar Domain Decomposition for Flow in Porous Media

We develop multiscale mortar mixed finite element discretizations for second order elliptic equations. The continuity of flux is imposed via a mortar finite element space on a coarse grid scale, while the equations in the coarse elements (or subdomains) are discretized on a fine grid scale. The polynomial degree of the mortar and subdomain approximation spaces may differ; in fact, the mortar space achieves approximation comparable to the fine scale on its coarse grid by using higher order polynomials. Our formulation is related to, but more flexible than, existing multiscale finite element and variational multiscale methods. We derive *a priori* error estimates and show, with appropriate choice of the mortar space, optimal order convergence and some superconvergence on the fine scale for both the solution and its flux. We also derive efficient and reliable *a posteriori* error estimators, which are used in an adaptive mesh refinement algorithm to obtain appropriate subdomain and mortar grids. Numerical experiments are presented in confirmation of the theory.

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### MS17

#### Physics-Based Deflation Preconditioners for Flow in Porous Media

This work describes a physics-based deflation preconditioner approach for solving porous media flow problems characterized by high permeability contrasts. The approach relies on rearranging the linear system coefficients in high- and low-permeability blocks. The procedure is labeled as physics-based 2-Stage deflation preconditioner

(2S-DP). Numerical experiments reveal that the P2DP is a powerful alternative to solve non-symmetric pressure systems arising in fully-implicit formulations.

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### MS17

#### Domain Decomposition Methods for Multiscale Elliptic PDEs

In this talk we will discuss domain decomposition preconditioning for linear systems arising from finite element approximation of symmetric elliptic problems with highly variable coefficients. The work is motivated by problems arising in the computation of flow through heterogeneous media. We will give condition number bounds which demonstrate how the subdomains and coarse space basis functions should be designed in order for the methods to be robust to both the heterogeneity of the media and the mesh parameters. In particular, we give a rigorous connection between low energy basis functions and robustness to heterogeneity. The results are illustrated by examples showing the benefits of using multiscale finite element interpolation as a coarsener.

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### MS17

#### Flexible GMRES with Deflated Restarting with Application for the Solution of the Helmholtz Equations

In this talk we will describe a flexible Krylov subspace method that enables the preconditioner to change from one iteration to the next. It is referred to Flexible GMRES-DR due to its close resemblance with the GMRES-DR method by R. Morgan in the way it recycles some spectral information at each restart. Numerical experiments for the solution of the Helmholtz equations using the multigrid scheme by Riyanti et al as preconditioner will be reported.

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#### MS17

##### **Deflation Acceleration of ICCG for Porous Media Flow**

In this paper it is proven that the number of small eigenvalues of the IC preconditioned matrix is equal to the number of high permeable domains, which are not connected to a Dirichlet boundary. It appears that the Deflated ICCG method annihilates the effect of these small eigenvalues. A method is given to construct the corresponding projection vectors in an efficient way. It appears that the implementation of the deflation acceleration is important. The efficiency of the DICCG method is illustrated by numerical experiments.

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#### MS18

##### **Elucidating Model Inadequacies in Parameterizations by Use of An Ensemble-Based Calibration Framework**

Every parameterization contains structural model errors, but the sources of these errors are difficult to pinpoint because of complicated nonlinearities and feedbacks. Ensemble-based parameter estimation is proposed as a method to elucidate model inadequacies. Rather than striving to find the single best set of parameter values, the output is instead an ensemble of parameter sets. The resulting ensemble can help uncover model deficiencies and structural errors that might not otherwise be easily revealed.

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#### MS18

##### **Data Assimilation and Ensemble Forecasting**

Abstract not available at time of publication.

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#### MS18

##### **Ensemble Kalman Filtering for Severe-Weather Prediction**

While global numerical weather prediction has seen steady progress over the last 40 years, forecasting for smaller scales (below, say, 100 km) remains difficult. Small scale phenomena, such as hurricanes and thunderstorms, unfortunately also account for much of severe and damaging weather. Data assimilation, or estimating the atmospheric state at small scales given observations, is a key obstacle to useful numerical prediction of severe weather, since accurate forecasts require accurate initial conditions. The ensemble Kalman filter addresses many of the difficulties of small-scale atmospheric state estimation. It employs a general, Monte-Carlo-based covariance model that can spread information from limited observations spatially, temporally and to unobserved variables. It does not require linearization or adjoints of complex and strongly nonlinear physical processes such as those surrounding the formation and evolution of cloud and rain. It also facilitates subsequent probabilistic forecasts, which are necessary at small scales because of the very short predictability times, by producing an ensemble (or sample) of initial conditions. I will review recent progress in employing the ensemble Kalman filter at small scales in the atmosphere, with emphasis on the assimilation of Doppler radar observations of severe thunderstorms and the initialization of hurricane forecasts. Multiple spatial scales and dynamics, typically involving the small-scale weather elements and a larger-scale environment, is a key open issue.

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#### MS18

##### **Title Not Available at Time of Publication**

Abstract not available at time of publication.

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#### MS19

##### **Biphase Poroelastic Models for Deformation in the Cellular Microenvironment of Articular Cartilage**

Articular cartilage can be idealized as a biphase poroelastic mixture that is comprised of a solid extracellular matrix saturated with interstitial fluid. Cartilage extracellular matrix is maintained by a sparse population of cells whose metabolic activity is highly dependent upon mechanical characteristics of the pericellular environment. We present computational models for poroelastic deformation at the cellular scale in a cartilage layer subjected to dynamic loading. Implications for modeling osteoarthritis and tissue engineering are discussed.

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#### MS19

##### **Mechanisms of Coupling of Deformation, Contamination, Dissolution and Precipitation in Porous Media**

The ways deformation and chemical mass change influence one another are addressed. We investigate mechanisms and identify key variables at different scales that control the rate and the amount of mechanical changes induced by chemical processes. The focus of this paper is on irreversible changes in porous media as expressed via chemoplasticity. A primary role of so called compensatory mode of chemical softening plays in producing plastic strain due exclusively to chemical processes at constant stress.

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#### MS19

##### **A Hybrid Mixture Theoretic Approach to Modeling Two Time-Scale Multiphase Flow in a Deformable Medium**

A two time-scale model for flow in a swelling porous medium developed via hybrid mixture theory will be presented. The theory defines connected and unconnected bulk phases of liquid and vapor phases at the mesoscale to create a dual porosity model at the macroscale. One example application is the modeling of an unsaturated swelling system. The results will be compared with previous models; implications and measurement issues associated with the model will be discussed.

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#### MS19

##### **Three Regime Model for Drug Delivery Systems: Flow and Transport Models**

Darcy's law and Fick's law are combined with conservation of mass equations to obtain flow and transport models for a swelling drug delivery system. The model identifies three distinct regimes based on experimental evidence and makes the appropriate simplifying assumptions for each regime, resulting in a set of highly non-linear, coupled, partial integro-differential equations. The model accounts for polymer swelling and dissolution and drug dissolution and diffusion even in the case of low-solubility drugs.

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#### MS20

##### **Field-scale Optimization of WAG Injection for Coupled CO<sub>2</sub>-EOR and Sequestration**

The effect of relative permeability hysteresis on both CO<sub>2</sub> storage and oil recovery for the water-alternating-gas (WAG) injection process has been studied for heterogeneous 2-D cross sectional and 3-D field-scale models. Compositional simulations were performed to study the effect of WAG ratio, CO<sub>2</sub> slug size and reservoir heterogeneity with hysteresis modeled to optimize the CO<sub>2</sub> storage and oil recovery. The relative permeability and capillary pressure models were selected for three representative sandstone rock types. The parameters in the hysteresis model are based upon experimental data from the literature. The EOS model and fluid characterization were based upon experimental PVT data for a West Texas crude oil so that multiple-contact miscibility could be predicted accurately. A grid refinement study was performed to evaluate the convergence behavior of simulation model with the hysteresis option included. Physical dispersion was modeled with small grid blocks and a second order finite-difference method in an attempt to capture the mixing phenomena as accurately as possible. The trapped gas saturation has a very large effect on the amount of gas that can be sequestered in the reservoir. Experimental design was applied as a tool to perform a comprehensive study of this and other important parameters. Statistical analysis was performed to determine the most influential factors on both oil recovery and CO<sub>2</sub> storage. Optimization was carried out and response surfaces were constructed to quantify the effect of each parameter.

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#### MS20

##### **Performance Assessment of CO<sub>2</sub> Storage in Saline Aquifer**

Long-term CO<sub>2</sub> storage in aquifer may well be an interesting option to mitigate atmospheric CO<sub>2</sub>. However, detail site characterisation must be carried out prior to any long-term storage. Key to performance assessment of such storage are the multiphase fluid flow simulators. Such simulators must account for permeability (intrinsic and relative) heterogeneities but also the pressure temperature effect on CO<sub>2</sub> as a free or trapped phase (supercritical or gaseous) or dissolved within the aquifer. Given the time-scale of CO<sub>2</sub> storages in aquifer (over a 1000 years), several additional driving forces must be modeled, i.e., diffusion and dispersion within the aquifer and its geosphere (cap-rock and overburden), but also the role of pressure and temperature gradients both natural and induced during the injection process (short-term). Coupled to these hydrodynamical forces, geochemical and geomechanical influence should be carefully modeled to assess the long-term behavior of the CO<sub>2</sub> plume. A sequential approach coupling two reaction-

transport sub-models with a prediction-correction scheme is implemented in COORES, the research code from IFP. The code is used to model the performance of a CO<sub>2</sub> storage in a saline aquifer.

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## MS20

### Seismic Monitoring of CO<sub>2</sub> Sequestration: Imaging and Inversion Issues

Seismic is useful for monitoring subsurface CO<sub>2</sub> injection and storage. The physical properties of CO<sub>2</sub>-saturated rocks can vary significantly, so the resulting seismic wavefields can be rich and complex, posing challenges to obtain accurate images and inversion results. We discuss the rock and fluid properties of CO<sub>2</sub>-saturated rocks, the effects of CO<sub>2</sub> injection in realistic models on FD seismic data, and compare to real seismic images and inversion results at operational CO<sub>2</sub> sequestration sites.

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## MS20

### Multi-Scale Processes in Geologic Storage of Greenhouse Gases

Injection of CO<sub>2</sub> and other greenhouse gases underground induces coupled processes of fluid flow, heat transfer, and chemical and mechanical interactions between rocks and fluids. The long-term fate of stored CO<sub>2</sub> is affected by processes that involve positive as well as negative feedbacks on a broad range of space and time scales. We present results of numerical simulations aimed at developing effective descriptions and parameters for large-scale field studies of CO<sub>2</sub> storage systems.

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## MS21

### Application of the ECCO-MITgcm Adjoint Modeling Framework for Global Ocean State Estimation and Sensitivity Analysis

Since the end of the 1990's the ECCO (Estimating the Circulation and Climate of the Ocean) Consortium has embarked on applying mathematically rigorous methods of state estimation and optimal control in the context of the global ocean circulation at decadal time scales. As formulated, an automatic differentiation (AD) tool is used to derive the adjoint code of the MIT general circulation model (MITgcm) with respect to a 10<sup>8</sup> dimensional control space comprising initial conditions and time-varying surface boundary fluxes, and the method of Lagrange multipliers is used to render the problem one of unconstrained least-squares minimization. At the present time the solution represents a misfit to about 410 million separate observational constraints covering the period of the World Ocean Circulation Experiment (WOCE), and including among other data, satellite altimetry from TOPEX/POSEIDON, Jason-1, ERS-1/2, ENVISAT, and GFO, a global array of

profiling floats from the Argo program, and satellite gravity data from the GRACE mission. Major problems today lie less with the numerical algorithms than with interpreting the residual model/data misfits in terms of remaining data, model and representation errors. Besides the OSE problem, example applications of adjoint sensitivity studies are given in the MITgcm framework, covering subgrid scale mixing processes, coupled ocean sea-ice modeling, and biochemical studies. An outlook on AD tool requirements and model development is given.

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## MS21

### Newton-Krylov Methods for Fast Dynamical Spinup of Ocean General Circulation Models

Numerical models of the climate system play an important role in efforts to understand climatic variability on centennial to millennial timescales. In many studies, climate models are driven by forcings that are either time-independent or that vary periodically (seasonally) and it is often highly desirable to obtain equilibrium solutions of the model. Due to the long timescale for dynamical adjustment of the ocean, the conventional method of computing an equilibrium solution by direct forward integration is prohibitively expensive. Here, we present a novel solution technique based on transforming this time-dependent "spinup" problem into a nonlinear algebraic equation that can be solved using matrix-free Newton-Krylov (MFNK). This approach can be applied to any dynamical system defined via a (legacy) time-stepper. Preliminary results from a sector configuration of the MIT ocean model show that the MFNK method is both robust and competitive in comparison to conventional methods. However, due to its matrix-free nature, preconditioning of the linear Newton equation is nontrivial, and remains an outstanding challenge.

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## MS21

### Adjoint Sensitivity Analysis of the California Current Circulation and Ecosystem Using the Regional Ocean Modelling System (ROMS)

The adjoint of the Regional Ocean Modeling System (ROMS) coupled to a four component nitrogen-based trophic model has been used to explore the sensitivity of various physical and biological aspects of the California Current to linear variations in different attributes of the system. Those aspects of particular interest are characterized by suitably defined indices of variability, and include measures of coastal upwelling, eddy kinetic energy, baroclinic instability and biological activity.

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### MS21

#### Fully-Implicit Techniques for Ocean Circulation Problems

Recent advances in methods for solving sparse linear systems bring fully-implicit ocean models within reach. This class of models can be used to address a variety of problems that cannot be solved using conventional time-stepping codes. In this talk I will present results of fully-implicit model calculations applied to problems of the stability of the Meridional Overturning Circulation (MOC). The equilibrium structure of the MOC will be examined using bifurcation analysis, while its linear stability will be addressed using an eigenvalue analysis. In addition, initial results will be presented of fully-implicit adjoint calculations

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### MS22

#### Multiscale Mixed/Mimetic Methods – Generic Tools for Reservoir Modeling and Simulation

The combination of multiscale mixed finite element methods and mimetic finite difference methods is a particularly versatile tool for modeling subsurface flow. The method is based on a hierarchical grid approach, where basis functions with subgrid resolution are computed numerically to correctly account for subscale features from an underlying (fine-scale) geomodel when solving the global flow equations on a coarse grid. The coarse grid can in principle be any partition of the subgrid, where each coarse block is a connected collection of subgrid cells. This feature allows the method to naturally adapt the grid in regions of particular importance, such as near-well regions (to avoid near-well upscaling) and regions with large pressure gradients to accurately account for compressibility effects.

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### MS22

#### Anomalous Dispersion: Angstroms to Kilometers

Super-diffusion in the atmosphere, oceans, and the sub-surface, or the super-diffusive behavior of motile microbes under a microscope, and the sub-diffusive behavior of molecules in confined nano-films can all be modeled within the same basic framework. The Fokker-Planck equations are always of the same integro partial-differential form, only the kernels change. We present the basic form of the Fokker-Planck equation for all the above processes and compare its solution with experimental data.

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### MS22

#### A Multiscale Finite Volume Method for Multi-Phase Flow in Porous Media: Black Oil Formulation for Compressible, Three-Phase Flow with Gravity and Capillary Pressure

The multiscale finite volume (MSFV) method has been established as an efficient and accurate way to solve coupled flow/transport problems in reservoir flow simulation. In this paper the MSFV method has been extended to standard black oil formulation (i.e., three phase, compressible flow with solution gas and gravity/capillarity). An operator splitting is employed to decompose the pressure equation into elliptic part, buoyancy/capillary force dominant part, and inhomogeneous part with source/sink (wells) and accumulation. Flow and transport equations are decoupled and solved sequentially. An accurate coarse grid operator is derived for the flow equation (pressure and velocity) and a local fine grid solution is reconstructed via basis functions. In addition, adaptive computation is extensively implemented for numerical efficiency. The MSFV method of black oil formulation allows us to study a large class of practical problems. We analyze the numerical efficiency of MSFV and demonstrate the robustness and computational efficiency of the MSFV, using large heterogeneous reservoir models.

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**MS22****Title Not Available at Time of Publication**

Abstract not available at time of publication.

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**MS23****Deflation in Two-Phase Flow Through Multilevel Upscaling**

The operator hierarchy defined by a robust variational multigrid method implicitly defines an operator-induced deflation process that accurately captures the low-energy modes of the solution. We extend our earlier work on a multilevel upscaling framework for single-phase flow, to provide a deflation process for two-phase flows. We focus on the accuracy and mass conservation of the hierarchical velocity field. Comparisons with multiscale finite element approaches demonstrate the effectiveness of this method.

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**MS23****Recycling Krylov Basis Methods**

Abstract not available at time of publication.

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**MS23****Domain Decomposition Methods and Deflated Krylov**

The balancing Neumann-Neumann (BNN) and the additive coarse grid correction (BPS) preconditioner are fast and successful preconditioners within domain decomposition methods for solving partial differential equations. For certain elliptic problems these preconditioners lead to condition numbers which are independent of the mesh sizes and are independent of jumps in the coefficients (BNN). Here we give an algebraic formulation of these preconditioner. This formulation allows a comparison with another solution or preconditioning technique - the deflation technique. By giving a detailed introduction into the deflation technique we establish analogies between the balancing, the additive coarse grid correction and the deflation technique. We prove that the effective condition number of the deflated preconditioned system is always, i.e. for all deflation vectors and all restrictions and prolongations, below the condition number of the system preconditioned by

the balancing preconditioner and the coarse grid correction preconditioner. This implies that the conjugate gradient method applied to the deflated preconditioned system is expected to converge always faster than the conjugate gradient method applied to the system preconditioned by the coarse grid correction or balancing. Moreover, we prove that the A-norm of the errors of the iterates built by the deflation preconditioner is always below the A-norm of the errors of the iterates built by the balancing preconditioner. We also compare different implementation techniques of deflation based preconditioners. Numerical results for porous media flows emphasize the theoretical results.

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**MS23****Robust Coarsening for Multiscale PDEs**

We consider two-level overlapping domain decomposition preconditioners for piecewise linear finite element approximations of elliptic PDEs with highly variable coefficients, as they arise in practice, for example, in the computation of flows in heterogeneous porous media, in both the deterministic and (Monte-Carlo simulated) stochastic cases. We propose and analyse new robust coarsening strategies for these problems, e.g. based on smoothed aggregation and multiscale finite elements, and study different ways of combining the coarse solve with the local solves (i.e. additive, multiplicative and deflation). We will use and extend a recently developed general framework for analysing the resulting preconditioners to show their robustness for a variety of model situations, but we will also focus in this talk on linear algebra and parallelisation aspects. Numerical experiments will be used to illustrate the robustness and efficiency of the proposed methods and the sharpness of our theoretical results.

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**MS24****Solving the Nonlinear Shallow Water Equations on**

### the Sphere Using Radial Basis Functions

Three test cases are conducted to assess the RBF methodology for solving the shallow water wave equations in spherical geometry: 1) global steady-state flow, where the initial velocity and height fields are also the solution for all time, 2) a zonal flow over an idealized mountain that generates a downstream wave train, shedding vortices in its wake, and 3) Rossby-Haurwitz waves - these solutions move from west to east, resembling the horizontal structure of large-scale weather systems.

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### MS24

#### Divergence-Free Radial Basis Functions on the Sphere

This talk presents a new tool for fitting a divergence-free vector field tangent to a two dimensional orientable surface in  $\mathbf{R}^3$  (e.g. a sphere) to samples of such a field taken at scattered sites on the surface. This method, which involves a kernel constructed from radial basis functions, has applications to problems in geophysics, and has the advantage of avoiding problems with poles. Numerical examples testing the method on the sphere are included.

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### MS24

#### Multi-Domain Radial Basis Functions

Instead of considering the global operator obtained using a direct RBF discretization of a PDE, or system of PDEs, on a domain  $\Omega$ , we consider the case of a partitioning into sub-domains  $\Omega_i$  such that  $\Omega = \cup_i \Omega_i$ . The problem consist now into finding boundary conditions making the individual subproblems compatible with the global PDE. For elliptic problems, this is the Steklov-Poincaré operator while, for hyperbolic PDEs, this is the usual characteristic decomposition at the cell interfaces. In this talk, exploratory work will be presented.

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### MS24

#### Transport Schemes on the Sphere Using Radial Basis Functions

The RBF implementation for modeling transport (pure advection) on the sphere is discussed. We show that the RBF formulation of the advective operator in spherical coordinates is completely singularity-free. We then present results for two classical test cases: linear advection and deformational flow. Compared to other commonly used spectral methods, we find that RBFs require a much lower spatial resolution to achieve the same accuracy, while being able to take unusually large time-steps.

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### MS25

#### Computational Methods for CO2 Leakage Estimation

One of the most likely pathways for leakage of injected CO<sub>2</sub> is abandoned wells, especially in North America, where millions of wells have been drilled over the past century. The large disparity in length scales between overall CO<sub>2</sub> plume size and localized leakage along wells, and the high uncertainty about materials within old wells, make the problem of leakage estimation very challenging. In this presentation, a range of computational methods will be explored to estimate CO<sub>2</sub> leakage.

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### MS25

#### Analytical Modeling and Experimental Investigation of Physical Mechanisms

Of the candidates for geological sequestration, the physics of transport and sequestration in coal is the least well understood. We investigated the physics involved in flow in coalbeds through a combination of experiments and analytical modelling. We will discuss experimental investigation of adsorption and desorption paths, as well as 1-D displacement experiments for a variety of gas injection mixtures, and analytical solutions for multicomponent, multiphase, convective transport with adsorption using the method of characteristics.

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### MS25

#### The Influence of Interfaces and Instabilities on Multiphase, Multicomponent Flows in Porous Media

Please enter your abstract here. Seventy-five (75) word maximum. Do not include self defined TeX commands. We present a model concept that is capable of describing the flow and transport processes of CO<sub>2</sub> sequestration in aquifer systems due to advection and diffusion in the reservoirs. We further consider the mutual solubilities of CO<sub>2</sub> and water/brine as well as the influence of phase composition on the fluid properties in the CO<sub>2</sub>-water system. The influence of the heterogeneities and instabilities of the front propagation will be discussed.

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### MS25

#### Application of Semi-Analytical Methods for Leakage Estimation and Risk

Estimation of the flow and migration of CO<sub>2</sub> during the injection phases of a CO<sub>2</sub> storage operation is greatly complicated by the presence of large numbers of abandoned wells. These wells act as potential conduits for leakage. This presentation covers the development of fast semi-analytical solutions to CO<sub>2</sub> migration in systems of several aquifers connected by abandoned wells, and uses this semi-analytical framework to analyse a sample injection operation from a risk assessment perspective.

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### MS26

#### Flow and Transport at WIPP

The geology and hydrogeology at the Waste Isolation Pilot Plant in New Mexico has been extensively studied. The main transmissive feature in the area is a continuous thin layer of Culebra Dolomite rock. Measurements of the transmissivity and hydraulic head are available at approximately 40 locations. The talk will discuss the problem of estimating the time for a tracer released at a borehole in the middle of the site to travel to the boundary of the region, given the available data.

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### MS26

#### Efficient Linear Solvers for Stochastic Groundwater Simulations

We consider groundwater flow governed by Darcy's law with uncertain conductivity data. The resulting stochastic saddlepoint problem is discretized by the stochastic finite element (SFEM) method, employing Raviart-Thomas elements for the deterministic part of the problem and polynomial spaces in random variables for the stochastic part. The uncertain conductivity data is modelled as a random field and expanded in a Karhunen-Loeve series in independent random variables, which is truncated after sufficiently many terms for discretization. Using a suitable basis for the stochastic degrees of freedom, the stochastic variables may be uncoupled, resulting in a large block diagonal system, in which each block is a parametrized saddlepoint problem. We solve each block system using a preconditioned Krylov subspace method, in which a preconditioning scheme for the deterministic groundwater flow problem due to Powell and Silvester is incorporated. In the talk we report on our experiences using Krylov subspace recycling techniques, which attempt to reuse approximation subspaces across several of the block systems.

tioned Krylov subspace method, in which a preconditioning scheme for the deterministic groundwater flow problem due to Powell and Silvester is incorporated. In the talk we report on our experiences using Krylov subspace recycling techniques, which attempt to reuse approximation subspaces across several of the block systems.

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### MS26

#### Stochastic Krylov Methods for Flow in Random Porous Media

Generally, the porous media is highly heterogeneous with contrasts defined by different geological arrangements and intrinsic rock properties. Hence, uncertainty assessment under non-stationarity assumptions is emerging as a subject of intensive research. This work combines Krylov subspace methods with Karhunen-Loeve moment equation methods to provide an efficient characterization of fluid flow on non-stationary random porous media. Numerical comparisons are established with other Krylov-based stochastic methods to assess uncertainty on porous media.

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### MS26

#### Stochastic Simulation of Flow and Solute Transport in Heterogeneous Porous Media

Abstract not available at time of publication.

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### MS27

#### Smooth Division and Rough Division in Wave-Equation Imaging Conditions

Recovering seismic reflectivity in the process of seismic reflection imaging calls for taking a ratio of the reflected and incident wave fields. Division of oscillatory wavefields is a particular form of inversion and can be greatly improved by employing the method of regularization. I show how different forms of regularization can serve different tasks in seismic imaging: increasing the image resolution, reducing imaging artifacts, and compensating for uneven reflector illumination.

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MS27

**Optimal Illumination for Array Imaging in Random Media**

I will introduce the problem of optimal illumination for array imaging and propose a number of algorithms for doing the optimization while dealing with the random inhomogeneities in the background. In addition to showing results of numerical simulations I will outline a mathematical theory for analyzing the optimization problem. This is joint work with L. Borcea and C. Tsogka.

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MS27

**Deterministic Imaging in a Random World**

This talk will overview the mathematical basis of contemporary seismic imaging algorithms in the harmonic analysis of partial differential equations. Partly because of data bandwidths, the images produced by these algorithms are limited in resolution. The Earth structure at nonresolved scales may usefully be viewed as random. Despite nonlinear coupling between scales, in at least some cases large scale structure may be estimated deterministically in the presence of randomness in small scale structure.

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MS27

**Adaptive Coherent Interferometric Imaging**

I present a coherent interferometric approach for array imaging in cluttered media, in regimes where the recorded traces have long and noisy coda due to the multiple scattering of the waves by the inhomogeneities. Coherent interferometry is an efficient statistical smoothing technique exploiting the spatio-temporal data coherence to obtain stable images. The delicate balance between having stable images and achieving the optimal resolution depends on two clutter-dependent parameters that are estimated during image formation. The robustness of the method is illustrated with several results.

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MS28

**Pore to Continuum Upscaling and Coupling Using Mortars**

In this work pore-scale network models are coupled to adjacent media using mortars. While mortars have been used in the past to couple subdomains of different models, physics, and meshes, they are extended here for the first time to pore-scale models. The approach is demonstrated by modeling single-phase flow in coupled pore-scale models, but the methodology can be utilized in the future to model dynamic processes and perform multiscale modeling in 3D continuum simulators.

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MS28

**On the Heterogeneous Multiscale Method with Various Macroscopic Solvers for Linear and Nonlinear Problems**

The heterogeneous multiscale method (HMM) is a general method for efficient numerical solution of problems with multiscales. It consists of two components: an overall macroscopic solver for macro variables on a macro grid and an estimation of the missing macroscopic data from the microscopic model. In this talk the speaker presents a state-the-art review of the HMM with various macroscopic solvers, including finite differences, finite elements, discontinuous Galerkin, mixed finite elements, control volume finite elements, nonconforming finite elements, and mixed covolumes. The HMM with these macroscopic solvers for nonlinear and random homogenization problems is also presented.

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MS28

**Time-Decomposition Methods as Multiscale and Physics-Preserving Algorithms for Applications in Transport-Reaction Processes in Porous Media**

Abstract not available at time of publication.

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MS28

**An Component-Based Formulation for Compositional Flow and Transport**

Compositional models describe the simultaneous transport of multiple components flowing in coexisting phases through porous media. Because each component can transfer through different phases, the mass of each phase or a component within a particular phase is no longer conserved. Instead, the total mass of each component among all the phases must be conserved, leading to very large, strongly coupled systems of transient nonlinear advection-diffusion equations. These equations are closely coupled to a very large set of constraining equations, which are strongly nonlinear, implicit functions of phase pressure, phase temperature, and mole fractions. We present a component-based formulation for compositional flow and transport and corresponding computational results with traditional simulators.

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### MS29

#### High Performance Flow Simulation in Discrete Fracture Networks

Natural fractured media are highly unpredictable because of existing complex structures at the fracture and at the network levels. Fractures are by themselves heterogeneous objects of broadly-distributed sizes, shapes and orientations that are interconnected in large correlated networks. We generate stochastic discrete fracture networks and run numerical flow simulations, using a mixed finite element method. We achieve large scale simulations by using appropriate numerical libraries and parallel computing.

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### MS29

#### Simulation of Water-Gas Flow Processes in Fractured-Porous Systems

Water-gas flow processes in fractured-porous media occur in number of environmental and engineering applications. Special difficulties have to be dealt with if the fractures are highly permeable. One example is given by rainfall induced surface-runoff which fast infiltrates via macropores into the subsurface. Another example is given by tube-like failures in dikes caused by animals or dead roots where water can fast infiltrate or exfiltrate. It will be investigated to which extend the 'classical' combined model approach (discrete fracture as 1D-element embedded into a 2D matrix) for two-phase flow in fractured-porous media which amongst others assumes the validity of the Darcy law is suitable for modeling the above-mentioned processes or whether other model concepts should be preferred. The simulations will be compared to laboratory experiments.

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### MS29

#### A 3D Discrete Fracture Network Flow and Transport Simulator for the Characterization of Fractured Reservoirs

The presence of fractures at various scales affects the flow dynamics within a reservoir, thus casting uncertainty on the assessment of the field productivity and reserves. Methodologies and tools are now available (i) to construct geologically-realistic models of the fault/fracture network (ii) to turn these models into simplified conceptual models usable for field-scale simulations of multi-phase produc-

tion methods. However a critical intermediate step remains that of validating the geometry of the geological fault/fracture network and characterizing it in terms of flow properties. This paper presents an original and multi-purpose 3D Discrete Fracture Network simulator enabling one to fulfil this hydraulic characterization step.

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### MS29

#### Continuum Transport Parameters from Discrete Fracture Networks

Traditional approaches to modeling flow in fractured porous media can be subdivided into discrete and continuum method. Due to the fact that commercial simulators only work at the continuum scale, it is important to be able to predict effective flow parameters from discrete information. In this paper we show two procedures for obtaining full tensor parameters. The first method requires solution of transport equation on the network; the second relies on the effective medium theory.

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### MS30

#### A High-Order Conservative Climate Model

A high-order conservative dynamical core for climate modeling has been developed. This is a conservative option for NCAR's climate modeling HOMME framework. The horizontal aspects of the model is based on high-order inherently conservative discontinuous Galerkin method. The vertical discretization rely on a 1-D Lagrangian method and associated vertical remapping is done by a conservative cell-integrated semi-Lagrangian method. Preliminary results with idealized baroclinic tests are encouraging and we hope to present more recent and advanced test results in the seminar.

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### MS30

#### Time-Stepping for High-Order Nonhydrostatic Models

In this talk, efforts are directed towards a general and effi-

cient linearly semi-implicit time-stepping technique adaptable to a large class of problems. Using Rosenbrock-W methods an efficient time-stepping procedure is constructed. Simple approaches for preconditioning the resulting linear system are discussed and an application to a high-order discontinuous Galerkin nonhydrostatic mesoscale model is presented.

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### MS30

#### **A Comparison of Dissipation Mechanisms (Filtering, Viscosity and Hyper)**

Not available at time of publication.

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### MS30

#### **Aquaplanet Simulations with the NCAR Spectral Element Dycore**

Abstract not available at time of publication.

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### MS31

#### **Lattice Boltzmann Modeling and Image Analysis for Multiphase Porous Medium Systems**

Multiphase lattice Boltzmann (LB) techniques provide an opportunity to quantitatively study pore-scale processes in realistic, three-dimensional porous media. We use high-resolution three-dimensional LB simulations to evaluate the behavior of disconnected non-wetting phases in water wet systems. Equilibrium conditions are evaluated at the microscale and macroscale and image analysis tools developed to study such systems are described and applied to the resultant LB simulation data. The simulation results are interpreted in light of recently derived averaging results for two-fluid-phase multiphase systems.

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### MS31

#### **Porous Micro-Models: Local Versus Global Interfacial Energy Density**

In a porous medium containing two immiscible fluids, prior to breakthrough, there are strong local variations and gradients in saturation and interfacial area per volume (IAV) within a sample. Yet traditional approaches to measuring saturation mainly obtain global averaged values over the porous medium sample. We observed that the interfacial energy density function of local averages at a single capillary pressure is identical to the function of global averages over many different capillary pressures.

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### MS31

#### **Thermodynamically Constrained Averaging Theory Formulation of Two-Phase Flow in Porous Medium Systems**

Classical macroscale models of fluid flow and transport in porous media lack rigorous connection to the microscale physics. Using averaging procedures, one can systematically integrate from the microscale to produce macroscale quantities and equations with explicit relations to microscale counterparts. Averaging carries the overhead burden of requiring closure relations for the derived conservation equations. Building upon the general thermodynamically constrained averaging theory (TCAT), we present the approach, complicating issues, and governing equations for a two-fluid-phase system.

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### MS31

#### **Potential and Limitations for Using X-Ray-Based Micro-Imaging to Characterize Multi-Phase Flow**

### in Porous Media

A remaining hurdle in using x-ray microtomography to describe fluid flow in porous media is adequate quantification of the results. Many highly quantitative studies are made difficult by the complexities in processing the resulting grey-scale data into information such as pore network geometry, phase saturations, and interfacial areas. The potential and limitation in applying microtomography to fluid flow problems are partially controlled by our ability to improve image processing techniques for segmentation of grey-scale tomographic images.

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### MS32

#### Incorporation of Global Effects in Upscaling of Two-Phase Flow and Transport in Heterogeneous Formations

We present a methodology that efficiently incorporates large-scale global flow in two-phase upscaling. The method integrates two basic quasi-global approaches. The upscaled single-phase transmissibility, computed using an adaptive local-global procedure, accounts explicitly for a specific global flow; while the subgrid models for two-phase parameters, determined using effective flux boundary conditions, accounts approximately for the global effects (via generic global flows). The accuracy of the overall method is demonstrated for several examples involving flow and transport.

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### MS32

#### Multiscale Finite Element Methods Using Limited Global Information for Subsurface Flows

In this talk, I will describe multiscale finite element methods for flows in heterogeneous porous media. The main idea of multiscale finite element method is to construct finite element basis functions that can capture the small scale information. I will present an extension of multiscale finite element method that uses some type of limited global information to take into account the connectivity of the media. I will also briefly mention the extension of the method to nonlinear partial differential equation (pseudomonotone operators). This is a joint work with T. Hou, V. Ginting and R. Ewing.

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### MS32

#### From Homogenization with a Continuum of Scales to Electrical Impedance Tomography with Incom-

### plete Boundary Measurements

We show how homogenization theory (upscaling) for divergence form elliptic operators can be rigorously extended to situations where the medium is not stationary at small scales and characterized by a continuum of scales. Next we consider inverse homogenization (downscaling); although this problem is ill posed and highly non linear we deduce that it can be reduced to the search for an optimal solution within a linear space. We show how these results can be applied electrical tomography with incomplete boundary data. Parts of this talk are joint works with Lei Zhang, Roger Donaldson, Mathieu Desbrun and Yiyang Tong.

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### MS32

#### Reservoir Modeling with Global Scaleup

Global scale-up uses global fine-scale flow solutions to scale-up effective permeabilities for a coarse reservoir model. It has been recognized in various studies that global scale-up leads to more accurate coarse models than commonly used local scale-up methods. Various ways of incorporating global flow information into the scale-up process has been studied in recent years. In this presentation, we review a global scale-up method that was first proposed about two decades ago and analyzed recently by Wu, Efendiev, and Hou. Then, we discuss the advantages and challenges in applying this method to practical problems. Numerical examples will be given.

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### MS33

#### Coherent Imaging in a Random Medium

In this presentation, we consider a problem of imaging a point reflector in a random medium. We introduce a new coherent imaging functional, which is a generalization of the previously proposed coherent interferometric functional. We show that in right scale regimes, it yields a statistically stable image of the reflector. The performance of this functional is checked for a variety of settings ranging from a single receiver to a collection of apertures.

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### MS33

#### Extended Imaging Conditions for Seismic Data

The imaging condition commonly used for seismic imaging uses simple cross-correlation of two wavefields reconstructed from the sources and receivers. Although robust, this imaging condition ignores spatial and temporal coherency of reconstructed wavefields and, therefore, can lead to artifacts in migrated images. This presentation outlines an imaging condition extension that alleviates this problem

and enables other applications that have not been conventionally designed for the imaging step.

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### MS33

#### Extracting the Green's Function from Ambient Fluctuations for General Linear Systems

It is known for several years that for acoustic or elastic waves the Green's function can be extracted from the recordings of ambient fluctuations. This principle can be extended to a much larger class of linear systems that include the diffusion equation and the advection equation. These equations are not invariant for time-reversal, this indicates that time-reversal invariance is not needed for the extraction of the Green's function.

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### MS33

#### Title Not Available at Time of Publication

Abstract not available at time of publication.

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### MS34

#### Kuznetsov-Repin Hexahedral Mixed Finite Elements and Their Application to the 3-D Andra Benchmark

We first present the 3-D Andra benchmark, and then discuss our numerical methods. We consider general hexahedral meshes since many engineers prefer to use them instead of tetrahedral meshes. However standard Raviart-Thomas-Nédélec mixed finite elements do not converge on general hexahedral grids for second order elliptic problem. So we present the Kuznetsov-Repin hexahedral mixed finite element and show its convergence theoretically and numerically. This method is used for calculating Darcy flow as well as for diffusion-dispersion in transport calculations. Numerical results are shown for the benchmark.

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### MS34

#### Numerical Zoom and Applications to Nuclear Waste Repository Sites

Nuclear waste repository site assessment requires multi-

scale simulations with scales ranging from kilometers to centimeters. Every engineer zoom in a detail and redo the simulation in the restricted domain, but what is the error associated with such procedure? We shall answer this question by relating it to Rappaz's numerical patches and Schwarz' domain decomposition method. Error estimates will be given for Darcy's problem and the linear convection diffusion parabolic problem of nuclide concentration.

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### MS34

#### Aitken-Schwarz Domain Decomposition for Darcy Flow

The potentiality of the adaptive Aitken-Schwarz domain decomposition method to simulate the transport of fluids in heterogeneous underground mediums even with a randomly distributed hydraulic conductivity is shown. The slow linear convergence of the Schwarz on this non separable problem, can be accelerated adaptively with a posteriori estimates by Aitken acceleration of convergence. Hence the difficult computing of optimal parameters for the transmission conditions at interfaces is avoided. Performance comparisons with other solvers will be provided

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### MS35

#### Meshing Fractured Porous Media

In order to perform detailed numerical studies of fluid flow in geometrical complex geological systems, flexible meshes are necessary. Recently, an algorithm was presented by Persson and Strang for generating high quality meshes iteratively. We present extensions to this algorithm that enables mesh adaptation to internal boundaries such like fractures. The results of applying the extended algorithms to benchmark examples are given.

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### MS35

#### Flow in Porous Media with Fractures: Modeling Forchheimer Fractures as Interfaces

In this article we consider the case of a fractured porous medium in which flow in the matrix is governed by Darcy's

law but flow in the fractures is more accurately described by Forchheimer's law. A model in which the fractures are represented by interfaces,  $n-1$  dimensional surfaces, between subdomains of porous medium, is presented. In this model exchange between the fractures and the surrounding medium is taken into account. Numerical results will be shown.

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### MS35

#### Modelling Fractured Systems: Geo-Statistical Analysis and Deterministic-Stochastic Fracture Generation

We will present a concept for the modelling of single- and multi-phase flow processes in a fracture-matrix system. Following a discussion of the generation of fractures and the matrix, we will then describe a new interface condition which allows us to include in the matrix a lower-dimensional fracture with a locally conservative finite-volume scheme.

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### MS35

#### Analytical and Numerical Study of a Preconditioner for Fractured Porous Media

Fractures in a porous medium may be modelled as interfaces between neighboring subdomains. Then a domain decomposition method, in which the transmission conditions are continuity of the pressure and Darcy flow along the fracture, is formulated. We study a preconditioner for the resulting interface problem, that is a combination of the Neumann-Neumann preconditioner, widely used when the fractures are passive, and of the inverse of the flow operator along the fracture. We carry out an analytical study in a simple geometry, and show numerical results in more complex situations.

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### MS36

#### Dynamically Adaptive High-Order Simulation of Decaying 2D Navier-Stokes Flow

GASpAR is a spectral-element solver that employs dynamically adaptive mesh refinement (AMR; Rosenberg et al. 2006, *J. Comp. Phys.*). Turbulence at high Reynolds number (ratio of nonlinear to viscous accelerations) is characterized by strongly spatiotemporally localized features that may be amenable to high-order AMR simulation. We will present an application of GASpAR to 2D Navier-Stokes decaying fluid dynamics, including exact solutions, few-vortex interaction tests and turbulence initialized by a given power spectrum with random mode-phases.

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### MS36

#### Spectral Element and Discontinuous Galerkin Semi-Implicit Nonhydrostatic Atmospheric Models

Spectral element and discontinuous Galerkin methods continue to prove their worth in all fields of fluid dynamics. Recently, however, they have begun to emerge as a viable technology for constructing atmospheric and ocean models. The attractive features of these methods is that they offer high-order accuracy, geometric flexibility to use unstructured adaptive grids, and unparalleled scalability on distributed-memory computers. However, without semi-implicit time-integrators, it makes very little sense to propose these methods for operational-type models (such as those used in numerical weather prediction). In this talk we shall show results for our high-order models using thermal bubbles, hydrostatic and nonhydrostatic mountain waves, and density current problems. The solutions obtained with these new models compare favorably with existing state-of-the-art mesoscale models while using extremely large time-steps. We shall comment on the future direction of this research.

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Abstract not available at time of publication.

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tba

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**MS36****Towards an Adaptive Discontinuous Galerkin Method for Mesoscale Modeling**

Current mesoscale models have successfully simulated local as well as national weather systems. However, increases in resolution are limited to global decrease in spacing. Severe events such as tornadoes and squall lines are on much smaller scales than the current 4km spacing. In order to accurately capture them, adaptive gridding and high-order discretization are desirable. This presentation will concentrate on building blocks for a new adaptive high-order discontinuous Galerkin method for the non-hydrostatic equation set based on past experience with the adaptive spectral element method.

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**MS36****EULAG: A High-Resolution Computational Model for Research**

EULAG is a computational model for simulating thermo-fluid flows across wide ranges of scales and physical scenarios. It is noteworthy for its non-oscillatory semi-implicit integration algorithms, robust elliptic solver, and generalized coordinate formulation enabling grid adaptivity technology. Here we summarize the mathematical and numerical model design and illustrate its capabilities for high Reynolds number flows: canonical decaying turbulence in a triply-periodic box, breaking of internal gravity waves in the Earth's atmosphere and turbulent solar convection.

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**MS37****Preferential Growth of Biofilms in Heterogeneous Porous Media**

A *Pseudomonas aeruginosa* culture was inoculated into columns of glass beads. Growth substrate utilization and permeability changes were used to track growth, and post-experiment in situ staining of biomass provided visual evidence of colonization and growth. Permeability was reduced noticeably in each experiment. In an analogous ex-

periment in a heterogeneous bead pack, biofilm was prolific in the high permeability layer, but surprisingly sparse in the lower permeability layer. A history match of the tracer effluent histories indicated a four-fold reduction in porosity in the coarse beads. We speculate that a form of quorum sensing may become active as microbe communities become established within the bead pack. This conjecture raises interesting challenges for modeling reactive transport in biologically active soils and sediments.

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**MS37****Reactive Transport and Aperture Alteration in Single Fractures and Discrete Fracture Networks**

We have developed a parallel computational model of reactive fluid flow through variable aperture fractures in which the small-scale variability of the fracture aperture is represented explicitly. Direct comparison to dissolution experiments demonstrates that this model effectively simulates the experimentally observed behavior over a range of the dimensionless Peclet and Damkohler numbers ( $Pe = \text{advective}/\text{diffusive transport}$ ,  $Da = \text{surface reaction rate}/\text{advective transport}$ ). A series of fracture dissolution simulations in which we varied  $Pe$ ,  $Da$  and fracture size demonstrate that the length scale required for development of distinct dissolution channels increases for larger  $Pe$  and smaller  $Da$ . Furthermore, the spacing of distinct dissolution channels scales with the length of the longest channels. These results suggest the potential for the development of generalized scaling relationships to quantify the channeling induced by reactive fluid flow in variable aperture fractures.

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**MS37****Evolution of the Mechanical and Transport Properties of Fractures: Interactive Feedbacks of Stress**

## and Chemistry

The mechanical and transport properties of fractures are strongly nonlinear, with important feedbacks between mechanical and reactive chemical processes. Mechanical processes include fracture closure and dilation with applied shear and normal loads, the extension of micro-cracks, and augmentation of reactive surface area and activity by stress-corrosion and other mechanisms of micro-cracking. Chemical processes include precipitation, dissolution, reaction and transformation some of which take advantage of the modified mechanical state, and may be augmented and accelerated by stress effects. These observations have been made on fractures in novaculite, limestone, diorite and tuff, and illustrate a broad range of behaviors under differing mechanical and chemical regimes. We illustrate the interaction of these processes and demonstrate a variety of different behaviors: regimes where permeabilities increase with net dissolution, then enigmatically switch with no apparent change in experimental conditions; and regimes where wear products from deformation dominate the response. We examine these behaviors using models for the interaction of two rough surfaces in contact, as both lumped parameter systems, and as distributed parameter systems using Lagrangian-Eulerian models for dissolution-precipitation and transport. Observed and modeled responses are upscaled into constitutive models to represent the interaction of stress and chemistry in the evolution of transport properties at the continuum scale, and with appropriate feedbacks. These are accomplished through the application of both weakly-coupled and strongly-coupled models to represent these responses, and to follow behavior. Applications of these models are to contemporary issues of reservoir engineering in geothermal systems, and in the safe isolation of high-level radioactive wastes.

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### MS37

#### Lagrangian Particle Model for Reactive Transport and Mineral Precipitation in Porous Media

Lagrangian particle methods such as Smoothed Particle Hydrodynamics have several advantages for modeling pore-scale flow and transport as they allow complex physical and chemical processes such as reactions and phase transitions to be simulated through simple interparticle interactions. SPH reactive transport model was used to study the effect of porosity, pore scale heterogeneity and Damkohler and Peclet numbers on transport and precipitation and to estimate effective transport properties of porous media.

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### MS38

#### A Multiscale Well Model for Reservoir Simulation

We present a variational multiscale mixed finite element method for the solution of Darcy flow in porous media, in which the permeability field displays a multiscale character. The formulation is based on a multiscale split that leads to a rigorous definition of a (global) coarse problem and a set of (local) subgrid problems. One of the key issues for the success of the method is the proper definition of the local boundary conditions for the subgrid problems. The main contribution of the present paper is the development of a well model, which accounts for subgrid heterogeneity and radial flow regime in a consistent fashion, without compromising the local mass conservation property.

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### MS38

#### Analytical Upscaled Permeability and First Order Homogenized Approximation for Flow in Porous Media

Please enter your abstract here. SevenWe present a closed analytic form for the upscaled permeability, and for the first order homogenized approximation to linear and nonlinear flow equations defined in bounded subdomain of  $\Omega \subset \mathbb{R}^n$ , and such that the permeability coefficients are periodic and rapidly oscillating and can be defined as step functions describing inclusions in a main matrix. We illustrate the procedure by considering permeability ratios between the matrix and the inclusion of 1:10, 1:100 and 1:1000, respectively. The new contribution comes from deriving an analytical approximation in  $L^p(\Omega)$  for the solution of the periodic cell problem, obtained by a two-scale asymptotic expansion of the respective heterogeneous equations. In this way, an analytical upscaled permeability rendering the zero<sup>th</sup> in  $W^{1,p}(\Omega)$  and first order approximations in  $L^p(\Omega)$  are readily obtained. The zero<sup>th</sup> order approximation gives the macroscopic behavior of the flow whereas the first order approximation describes the macroscopic plus microscopic features. The known results of harmonic average in 1-D, and harmonic and arithmetic averages for layered media are obtained as particular cases. We demonstrate numerically the convergence properties in  $L^2$ -norm of these approximations as the scale parameter,  $\varepsilon$ , goes to zero, by applying the results to problems of interest in flow in porous media.

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### MS38

#### Operator-Based Multiscale Method for Compressible Flow

A scalable and extendible Operator Based Multiscale Method (OBMM) will be discussed in this talk. OBMM is cast as a general algebraic framework of the multiscale

method. It is very natural and convenient to incorporate more physics in OBMM for multiscale computation. In OBMM, two multiscale operators are constructed: prolongation and restriction. The prolongation operator can be constructed by assembling basis functions, and the specific form of the restriction operator depends on the coarse-scale discretization formulation (e.g., finite volume or finite element). The coarse-scale pressure equation is obtained algebraically by applying the prolongation and restriction operators on the fine-scale flow equations. Solving the coarse-scale equation results in a high quality coarse-scale pressure. The fine-scale pressure can be reconstructed by applying the prolongation operator to the coarse-scale pressure. A conservative fine-scale velocity field is then reconstructed to solve the transport equation. As an application example, we study multiscale modeling of compressible flow. We show that the extension of modeling from incompressible to compressible flow is straightforward for OBMM. No special treatment for compressibility is required. The efficiency of multiscale methods over standard fine-scale methods is retained by OBMM. The accuracy of OBMM is demonstrated by several challenging cases including highly compressible multiphase flow in a strongly heterogeneous permeability field (SPE 10). This is a joint work with H. Zhou.

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### MS38

#### **A Parallel Multiscale Mixed Method for Multiphase Flow and Reactive Transport in Porous Media**

We will focus on the mortar mixed finite element method for multiphase flow. The effects of chemical reaction, advection and diffusion-dispersion are implemented using a time-split algorithm. We solve the reaction system using ODE theory, the advection using a higher order Guodonov approximation and the diffusion-dispersion using a mixed finite element approximation, with a full tensor for physical dispersion. For non-matching grids, suitable projections are defined to account for the different grids in adjacent sub-domains. We present theoretical a priori and a posteriori estimates and computational results.

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### MS39

#### **On Building Parallel Algorithms and Software for Hydraulic Tomography**

Future basin-scale hydraulic tomography inevitably involves millions of degrees of freedom, making parallel computing the only viable approach. We advocate a subdomain-based approach for building both parallel numerical algorithms and the resulting software. More specifically, each subdomain is a relatively independent computing unit, making use of existing serial algorithms and software. To enforce the needed inter-subdomain collaboration, a global controller and related communications can be implemented as reusable parallel libraries.

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### MS39

#### **Informed Sampling Strategies for Hydraulic Tomography**

Measurements used in hydrogeologic imaging are usually collected without a governing purpose or design and with incomplete record of ambient conditions. Background noise makes it difficult to extract the information that could have been conveyed in the measurements. E.g., pressure measurements may have been affected by unknown recharge or boundary conditions. We argue for protocols for the collection of measurements that convey maximum information, through proper sampling and noise elimination.

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### MS39

#### **Trajectory-Based Methods for Estimating Hydraulic Conductivity**

Given the increasing data flow associated with characterizing and modeling natural hydrological systems there is a need for efficient data analysis tools. In this talk I discuss trajectory-based methods for integrating transient head, tracer, and multi-phase flow data. The techniques, which are similar to ray methods in geophysics, may be motivated by the method of multiple scales. Several examples are used to illustrate the methodology and to highlight the advantages and limitations of the trajectory-based approach.

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### MS39

#### **CAT-Scanning Groundwater Basins**

The theme of this talk is to promote the idea of collecting data intelligently and analyzing data smartly for characterization of the subsurface at high resolutions beyond the capabilities of current technology. Specifically, fusion of passive basin-scale tomographies are suggested that exploit recurrent natural stimuli as sources of excitations, along with implementation of sensor networks that provide long-term and spatially distributed monitoring of signals on the land surface and in the subsurface.

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### MS40

#### **Fluid and Electrical Transport in Sea Ice**

Brine flow through sea ice, which carries salt, heat, and nutrients and facilitates key geophysical and biological processes, is controlled by the vertical permeability  $k$ . Measurements of  $k$  are sparse, as are theoretical works. Here we present a multifaceted theory for  $k$ , based on rigorous



bounds, continuum percolation theory, hierarchical models, network simulation, and microstructural analysis. The results agree closely with laboratory and Arctic field data.

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#### MS40

##### Ice Sheet Modeling with a Remapping Transport Scheme

Most ice sheet models use the shallow-ice approximation, in which velocity is diagnosed from thickness, and thickness is prognosed using an advection scheme. Advection schemes in current models can promote numerical noise and are not monotonic. To alleviate these problems, a 2D incremental remapping advection scheme is applied in Glimmer, a state-of-the-art ice sheet model. The remapping scheme gives improved fields of thickness, temperature, and ice age.

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#### MS40

##### Modeling Arctic Sea Ice

Arctic pack ice moves and deforms in response to winds and currents because of concentrated deformations at leads. An elastic-decohesive constitutive model for pack ice has been developed that explicitly accounts for leads. The constitutive model is based on elasticity combined with a cohesive crack law that predicts initiation, orientation, and opening of leads. A numerical technique called the material-point method (MPM) shows promise for treating problems with explicit leads.

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#### MS40

##### Stochastic Aspects of Glacier Sliding

Glacier flow is sensitive to properties of the basal interface. When the driving force is large enough, the finite strength of asperities at the interface is exceeded, and the ice begins to slide. This behavior, which is similar to yielding in materials, is explored using a 2D plasticity model. The model is used to describe the dependence of the yield point on the asperity distribution function and to explore the possibility of self-organizing critical behavior.

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#### MS41

##### Convergence and Monotonicity Properties of MPFA Methods

Convergence and monotonicity properties are discussed for the MPFA O-methods and L-method on quadrilateral grids. Only physical space discretizations show the desired convergence behavior on rough grids, but symmetry

is then lost on general grids. The L-method has optimal monotonicity properties, but at the cost of a directional sensitivity.

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#### MS41

##### A Node Reconnection Algorithm for Mimetic Finite Difference Discretizations of Elliptic Equations on Triangular Meshes

Despite its simplicity, node reconnection methods (we call them *c*-adaptation methods) are seldom analyzed apart from other adaptation methods, even in applications where severe limitations are imposed on topological operations with a mesh. In this talk, we demonstrate that *c*-adaptation alone can significantly reduce the discretization error. We develop and numerically analyze a new *c*-adaptation algorithm for mimetic finite difference discretizations of elliptic equations on triangular meshes.

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#### MS41

##### Enriched Multipoint Flux Approximation

This talk will present the enriched multi-point flux approximation (EMPFA), which is able to reduce or eliminate numerical oscillations in the pressure solutions. The key step in this approach is to improve the consistency and accuracy in local flux calculations through the introduction of new temporary unknowns and better pressure interpolation techniques. EMPFA can be used for modeling general multiphase flows in 2-dimensional or 3-dimensional reservoir models, and the grid can be Cartesian, Voronoi, or even arbitrary. Simulation results will demonstrate the difference among EMPFA, MPFA, TPFA and other locally conservative schemes, e.g., the classical mixed finite element method.

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#### MS41

##### Grid Generation for Improved Monotonicity of MPFA on Unstructured Grids

The inverse of the linear operators resulting from MPFA discretization on unstructured grids can suffer from loss of monotonicity at medium to high permeability anisotropy ratios leading to oscillatory pressure solutions. This behavior can be linked to the interplay of permeability and grid geometry. In this talk we develop the mesh criteria for monotonicity and present an approach for optimal grid generation and parameterization in 2 and 3D which attempts to eliminate spurious oscillations.

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#### MS42

##### A Stability Analysis of Finite-Volume Advection Schemes Permitting Long Time Steps

A Von Neumann stability analysis of Eulerian flux-form and cell-integrated semi-Lagrangian advection schemes developed in the meteorological community is given. The main finding is that the dissipation and dispersion properties of Eulerian flux-form schemes are sensitive to the choice of inner and outer operators applied in the schemes that can lead to increased numerical damping for large Courant numbers. To explain these properties a conceptual interpretation of the flux-based Eulerian schemes is provided.

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#### MS42

##### Using Spherical Centroidal Voronoi Tessellations in Climate System Modeling

Spherical Centroidal Voronoi Tessellations (SCVTs) offer great potential to improve climate system model simulations. The powerful aspect of centroidal Voronoi point-sets is their ability to produce variable-resolution grids that maintain a high degree of local uniformity. Often the important length scale of interest varies substantially throughout the domain. Examples will be provided to demonstrate that SCVTs do an exceptional job in allowing us to place resolution where we need it, while producing a

locally-uniform grid.

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#### MS42

##### Accuracy and Efficiency Considerations for Euler Equations Solvers Applied to the Atmosphere

Large-scale atmospheric models often filter horizontally-divergent modes. This filtering, while appropriate at large scales, is detrimental to resolving meso-scale dynamics until very high resolutions are reached ( $\Delta h < O(10)$  km). We examine some existing formulations with respect to this issue. Additionally, meso-scale and cloud-scale structures that appear as resolution is increased are crucial to improved simulations. These features are at the margins of resolution, hence the marginal resolving power of a model is a more important model property than order of accuracy or convergence rate, and it is the accuracy measure that should be used in an efficiency (accuracy/cost) measure.

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#### MS42

##### Measuring the Characteristic Length Scale of Basis Functions

The spatial resolution of eigenfunctions of Sturm-Liouville equations in one dimension is frequently measured by examining the minimum distance between their roots. This technique does not work well for eigenfunctions in higher dimensions that are not tensor products of one-dimensional eigenfunctions. In this talk we propose an alternative measure of estimating the characteristic length scale that does not require knowing collocation or optimal interpolation points and show it does well in one and two dimensions.

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#### MS43

##### Using Lie Groups to Construct Similarity Solutions

The presentation will begin with a brief review of the basic method of symmetry analysis. The method can be used to find the symmetries of almost any system of differential equations and the knowledge of these symmetries can be used to construct similarity variables and corresponding similarity solutions. Several illustrative examples will be described.

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**MS43****Lock-Exchange Flows in Horizontal Porous Media**

We present a family of similarity solutions to lock-exchange flows in two-dimensional horizontal porous media of finite depth. We consider the evolution of two homogeneous fluids of different density and viscosity. New similarity solutions are presented for the case where the step in the interface does not extend over the entire depth of the porous layer. We discuss the effects of the viscosity ratio and a simple model of residual trapping on the solutions.

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**MS43****Injection of Fluids into Confined Aquifers - Stability Analysis and Application**

We consider injection of partially miscible fluid (in our application CO<sub>2</sub>) into an initially water-filled aquifer. Using sharp interface assumptions we are able to derive ordinary differential equations in a similarity variable for the CO<sub>2</sub>-water front, as well as a second front associated with evaporation of the residual saturation of the water behind the invading CO<sub>2</sub> front. This secondary front therefore separates 'wet' CO<sub>2</sub> from 'dry' CO<sub>2</sub>, and is referred to as the drying front. We show stability of the fluid fronts, thereby validating the use of the similarity solution for a range of parameters. Applications to carbon dioxide storage for the purpose of climate-change mitigation are discussed.

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**MS43****CO<sub>2</sub> Dispersal in Confined Aquifers - Analytical Models**

Abstract not available at time of publication.

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**MS44****Coarsening of Three-Dimensional Structured and****Unstructured Grids for Subsurface Flow**

We present a generic, semi-automated algorithm for generating non-uniform coarse grids for modeling subsurface flow. The algorithm is applicable to arbitrary grids and does not impose smoothness constraints. The approach should therefore allow users to specify the simulation grid dynamically to fit available computer resources, and, e.g., use the original geomodel as input for flow simulations. This is of great importance since coarse grid-generation is normally the most time-consuming part of an upscaling phase, and therefore the main obstacle that has prevented simulation workflows with user-defined resolution. We apply the coarsening algorithm to a series of two-phase flow problems on both structured (Cartesian) and unstructured grids. The numerical results demonstrate that one consistently obtains significantly more accurate results using the proposed non-uniform coarsening strategy than with corresponding uniform coarse grids with roughly the same number of cells.

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**MS44****Correction Functions for a General Multiscale Modeling Framework**

Abstract not available at time of publication.

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**MS44****Transmissibility Upscaling with Compact, Spatially Varying Multi-Point Flux Stencils**

In this talk, we describe a new single-phase transmissibility upscaling method, called VCMP, that uses spatially varying and compact multi-point flux stencils. In this method, fluxes are approximated by multi-point stencils that are adaptively chosen from neighboring pressure values to maximize compactness and ensure monotonicity. The accuracy of this approach is demonstrated for two-dimensional Cartesian cell-based anisotropically refined (CCAR) grids with challenging fine-scale permeability distributions. We also show that VCMP is consistent.

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#### MS44

##### **Improving the Robustness of the Multiscale Finite Volume Method**

The multiscale finite volume method (MSFV) is a promising approach for efficiently simulating porous media flows. The success of the method is due, in part, to its ability to accommodate full-tensor anisotropy in a coarse-scale pressure equation. Unfortunately, in cases with challenging fine-scale permeability heterogeneity and/or high aspect ratio grids the computed pressure fields may lack monotonicity. We will analyze monotonicity issues and develop a new compact MSFV method with improved robustness.

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#### MS45

##### **Hydraulic Tomography at the Boise Hydrogeophysical Research Site**

Hydraulic tomography field and modeling methods are being developed to provide three-dimensional distributed-parameter estimates of permeability ( $k$ ) for heterogeneous aquifers such as the fluvial aquifer at the Boise Hydrogeophysical Research Site (BHRS). We conduct a series of pumping tests from intervals in one well while measuring pressure changes with time in multiple intervals in nearby observation wells, and then we use these transient observations as the basis for tomographic inversion to estimate the  $k$  distribution.

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#### MS45

##### **Analysis of Tomographic Pumping Tests with Regularized Inversion**

I present the analysis of a set of tomographic pumping tests in an alluvial aquifer using regularized inversion. This approach allows the data to determine the amount of detail

required in the estimated hydraulic conductivity ( $K$ ) field, subject to imposed smoothness constraints. Regularization techniques explored include truncated singular value decomposition inversion and Tikhonov regularization. I also discuss the associated model resolution matrices, which describe the inherent blurring of  $K$  variation induced by the inversion.

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#### MS45

##### **Multi-Method and Multiscale Validation of Hydraulic Tomography in a Laboratory Aquifer with Deterministic Heterogeneity**

Hydraulic tomography potentially is a viable technology that facilitates subsurface imaging of hydraulic heterogeneity. To date, a comprehensive validation of the hydraulic tomography has not been done either at the laboratory or field scales. The main objective of this study is to examine the accuracy of the hydraulic conductivity ( $K$ ) and specific storage tomograms ( $S_s$ ) obtained from various hydraulic tomography algorithms developed by Yeh and Liu [2000] and Zhu and Yeh [2005, 2006]. We first obtain reference tomograms through the inversion of synthetic cross-hole test data generated through numerical simulations to examine the ability of the algorithm to image the heterogeneity pattern under optimal conditions without experimental errors and with full control of forcing functions (initial and boundary conditions as well as source/sink terms). Parallel to the generation of synthetic data, we conduct hydraulic tests at multiple scales in a laboratory aquifer with deterministic heterogeneity to generate data that are used to validate the  $K$  and  $S_s$  tomograms from hydraulic tomography. Generated data consisted of multiple  $K$  estimates from core, slug, single-hole and cross-hole tests as well as several steady-state flow-through experiments obtained within the sandbox. Estimates of  $S_s$  were obtained from single- and cross-hole tests. Validation of the tomograms involved a multi-method and multiscale approach proposed by Illman et al. [in review] and Liu et al. [in review] which included: 1) visual comparisons of  $K$  tomograms to the true sand distributions and the reference  $K$  tomogram; 2) testing the ability of the  $K$  and  $S_s$  tomograms to predict the hydraulic head distribution of an independent cross-hole test not used in the computation of the  $K$  and  $S_s$  tomograms; 3) comparison of the mean and variance of local  $K$  and  $S_s$  from the tomograms to the sample mean and variance of results from other measurements; 4) comparison of local  $K$  values in  $K$  tomograms to those from the reference tomogram; 5) cross-comparisons of  $K$  and  $S_s$  values in the tomograms obtained from steady and transient hydraulic tomography and 6) comparison of local  $K$  and  $S_s$  values in the tomograms to those obtained from other data including cores and single-hole tests. We recently also attempted to compare the flow rate through the entire sandbox from forward simulations using the  $K$  and  $S_s$  tomograms and measured rates from the flow through experiments and evaluated the tomograms also with available tracer tests. The multi-method and multiscale validation approach proposed herein further illustrates the robustness of steady-state and transient hydraulic tomography in subsurface heterogeneity delineation.

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#### MS45

##### Hydraulic Conductivity Distributions from Pulsed Signals

Hydraulic conductivity ( $K$ ) is a measure of how easily water moves in an aquifer. We have been using pulsed signals (a sine wave) and measure the change in phase and amplitude between the source and receiver well. If the area between the source and receiver locations is assumed to consist of blocks of material with a constant  $K$ , a system of linear equations to be solved for the block  $K$  values can be formed.

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#### MS46

##### Iterative Methods for Solving a Boundary Inverse Problem in Glaciology

The problem is to find the basal velocity of a glacier using the over-determined boundary conditions on the surface. We consider two-dimensional flow, described by a non-linear Poisson equation. This equation treats a first-order approximation to flow in a longitudinal cross section or full-order flow through a transverse cross section of a glacier. We solve the inverse problem using several iterative methods such as a Kozlov–Maz’ya method, Landweber iterations and other modifications of gradient methods.

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#### MS46

##### Well-Posedness and Instability in an Equilibrium Model of Temperature-Dependent Ice Sheets

The problem of the shape of a steady shallow ice sheet flowing under its own weight, given an accumulation map, has a variational inequality formulation similar to the  $p$ -Laplacian obstacle problem. Numerical experiments sug-

gest that adding a coupled conservation of energy model produces strong instabilities (“spokes”). I will address well-posedness (especially existence and continuity) of solutions when there is a nonconstant temperature field within the ice, and then speculate on the spokes.

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#### MS46

##### Models for Ice Streams from Coulomb Slip

Ice sheets exhibit localization of ice flow into ice streams, or well-defined narrow bands of fast flow. This rapid flow occurs due to slip at the base of the ice. Modern empirical and theoretical evidence points to Coulomb friction laws as parameterizations of basal slip. We analyze a family of ice-flow models capable of incorporating Coulomb slip, with particular emphasis on the effect of regularizing the strict Coulomb friction law.

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#### MS46

##### What is the Minimum Mathematical Model of Ice Sheet Dynamics?

The central problem of glaciology and its impact on the earth system is understanding the mass balance of polar ice sheets. Time series analysis of modeled ice volume indicates that the nature of the forcing can impact the cyclic behavior of mass balance. We use various novel forcings of accumulation fields on traditional and newly formulated simple ice sheet models to investigate the minimal mathematics necessary to capture the essential dynamics of ice sheets.

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#### MS47

##### Lagrangian Averaged Turbulence Model for Ocean Circulation

Lagrangian averaging is an alternative to the LES and RANS approaches to modeling turbulence, not a subset. We discuss the derivation and some test results for the Lagrangian averaged fluid equations with stratification and rotation. Being derived from Lagrangian averages, these “alpha-model equations possess a Bjerknes theorem for their total circulation, which allows buoyancy to be a source of subgrid-scale turbulence. Taylor’s hypothesis

provides the closure.

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#### MS47

##### **A Study of the NS- $\alpha$ Model for Two-Dimensional Turbulence**

For spatial scales smaller than  $\alpha$ , there are three possible power laws for the NS- $\alpha$  model stemming from the three possible dynamical eddy turnover time scales of the model equations: one from the smoothed velocity field, the second from the rough field, and the third from the combination of the two. Our numerical simulation of two-dimensional NS- $\alpha$  model shows that the energy spectrum of the smoothed velocity field follows a power law corresponding to the time scale of the rough velocity field.

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#### MS47

##### **The Effect of Small-Scale Regularization on Large-Scale Dynamics**

Regularization of small scales is considered as an ad hoc approach to modeling the effects of unresolved mesoscale eddy activity in the context of geostrophic turbulence. Numerical simulations show that not all such regularizations are equally effective. Analysis of cases where such regularization is effective suggests that the small-scale regularization leads to a change in stability characteristics, allowing for an enhanced inverse cascade of energy (compared to the unregularized case) and thus modifying the larger scales.

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#### MS47

##### **The LANS-Alpha Model of Sub-Grid Scale Turbulence in the POP Ocean Model**

We introduce a new implementation of the POP ocean model that uses the LANS-alpha model. Results from an idealized ACC test case which invokes the baroclinic instability shows that POP-alpha improves measures which depend on the resolution of meso-scale eddies, such as vertical temperature profile, kinetic energy, and eddy kinetic

energy. In some cases these improvements are comparable to a doubling of horizontal resolution.

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#### MS47

##### **Fluid and Numerical Stability in the LANS-Alpha Model**

In this talk we present two stability results for the LANS-alpha model. The first result shows that the LANS-alpha model's regularization moves the baroclinic instability to lower wave numbers while preserving all the classical baroclinic instability theorems. The second result shows that the LANS-alpha model, for the fastest waves in climate models, can take a larger maximum allowable time step.

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#### PP0

##### **Krylov Subspace Methods in Geophysical Tem Simulation**

Transient electromagnetic (TEM) fields have become a widely used geoelectric prospecting technique. The simulation of subsurface TEM phenomena requires the solution of an initial value problem for the quasistatic Maxwell's equations. Difficulties arising here include the stability constraints on the time-step for explicit methods and the expensive solution of the large indefinite linear systems of equations which arise in each time step of an implicit method. We discuss two alternative solution schemes, both based on Krylov subspace methods. The first, also known as the Lanczos Spectral Decomposition Method, approximates the matrix exponential multiplied with the initial data vector by a Krylov projection method. The second is based on the frequency domain formulation, resulting in a time-harmonic Maxwell equation for the range of frequencies present in the solution. We employ a model reduction technique based on a Krylov subspace generated by one or more full problems, solving the remaining time-harmonic problems in this reduced form. We present numerical re-

sults for and comparisons between both approaches.

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#### PP0

##### **On Linear Model Uncertainty Computation in Electrical Imaging**

Image appraisal is of increasing importance in quantitative electrical imaging. We here compare two widely used linear expressions of model uncertainty based on error propagation and a posteriori model covariance calculation. Although often overlooked, the two variants yield spatial distributions of parameter variance with inverse qualitative behavior. However, this actually is in agreement with their original definitions. Independent Monte-Carlo simulations, accounting for the non-linearity of the problem, indicate the limitations of a linear approach.

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#### PP0

##### **Numerical Models for the Interaction of Volcanic Flows with Water**

Modeling a pyroclastic surge interacting with a body of water requires a coupling of compressible gas dynamics for a hot dusty gas with fluid equations for the liquid, ideally including heat transfer and phase change as well as penetration of the water by the solid phase. An approach to this problem will be presented based on high resolution wave propagation algorithms for a dusty gas developed by Pelanti and LeVeque and previously used to model volcanic jets and plumes.

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#### PP0

##### **Hydropower Plant Reservoir Flow Simulations:**

#### **Preconditioners Comparison**

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#### PP0

##### **Darcy Multi-Domain Approach For Integrated Surface/Subsurface Hydrologic Models**

The main processes governing hydrological cycle at the catchment scale may be divided in surface and subsurface processes, two kind of processes strongly coupled. Until recently, hydrologic models assumed a weak coupling, essentially for numerical reasons. We present in this work a global model based on a Darcy multi-domain approach where the water dynamics on ground surface and in vadose and saturated zones, is described through a single Darcy nonlinear equation with domain-dependent parameters. We show how this equation is solved numerically and applied to different catchment hydrologic situations.

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#### PP0

##### **Parameter Estimation in Spatially Varying and Heterogeneous Soils**

Soil hydraulic properties are commonly modeled with the Van Genuchten equation which contains fitting parameters. These parameters and their corresponding statistics are well understood for specific soil types. However, parameter estimates will vary spatially across a watershed with heterogeneous soils. One way to account for this variability is through parameter uncertainty. In our approach we use known parameter values and uncertainties for homogeneous soils as initial estimates and combine them with soil moisture measurements from pits in the Dry Creek Watershed. We combine them by minimizing data and initial parameter estimates in a weighted least squares sense. Data weights are chosen to be the inverse of the variance of measurement errors, but do not assume normally distributed data. To account for heterogeneous soils, the parameter misfit weights are found by solving an optimization problem which ensures the penalty function has the properties of a chi-square random variable. The result is a dense weighting matrix which does not smooth parameter estimates. This approach gives consistent parameter estimates, and their corresponding uncertainties, which account for spatially varying and heterogeneous soils.

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**PP0****The Problem of the Separation of the Information and the Construction of Models from Seismological Time Series**

We study the problem of separating the stochastic and deterministic information and the construction of models from seismological time series, working with concepts and methods arising from nonlinear and stochastic dynamics. We construct a weave of interwoven methods with the aim of pre-processing, characterizing and modelling data from time series. The relations between methods depend on dynamical and static criteria, which allow for an evolution to an optimal analysis state of the available information.

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