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#### IP1

## Towards a Digital Twin for Coastal Ocean Modeling

The coastal ocean modeling community has been successful at developing high resolution physics-based models that can be used to predict and understand physical processes occurring in the coastal ocean, including tides and waves, flooding due to tropical storms, ecological studies, engineering planning and design, port operations, and many others. In the past decade, these physics-based models have been enhanced and improved by the addition of different types of data collection instruments that provide data at multiple scales. This has led to a data-driven coastal ocean modeling paradigm that merges data and physics. More recently, machine learning has come to the forefront as another tool in the coastal modeling toolbox. With these ingredients in place, it is natural to contemplate the develop of Digital Twin technology which combines these tools, algorithms, computing power, and data into a powerful whole. This talk will focus on steps taken and steps that need to be taken to realize a Digital Twin for Coastal Ocean Modeling, with specific application to coastal flooding.

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#### IP2

#### Structure Preservation in Data-driven Coarsegraining: Emergent Dynamics in Machine Learning Particle Models

Coarse-graining accelerates high-dimensional dynamical systems by reducing degrees of freedom and modifying equations to represent unresolved effects. The associated information loss induces dissipation even for reversible systems, with missing physics manifesting as emergent nonequilibrium stochasticity and memory. Efforts to machine learn models for these physics often fail, as conventional supervised models often fail to preserve the geometric structure underpinning stochastic behavior. We present a geometric ML framework for data-driven coarse-graining based on metriplectic dynamics that enforces structure preservation. Learned models obey the first and second laws of thermodynamics, fluctuation dissipation balance, and conservation principles. Because entropic state variables are unlabeled, we propose a self-supervised method to learn emergent structural variables jointly with the dynamics. Applications to star-polymer coarse-graining and to particle models learned from high-speed video of colloidal suspensions capture linkages between local structure and stochastic behavior. These studies highlight open challenges relevant to geophysical flows, including multiscale bridging, suspension interactions such as lubrication and electrostatics, and separating physical stochasticity from experimental noise. We provide an open-source Py-Torch and LAMMPS implementation to support inference of learned models at exascale.

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#### IP3

Simulating Our Way to CO2 Storage at Climate-

#### relevant Scales

CO2 storage is a proven climate technology, with over 200 million tons stored globally across numerous projects. Simulation plays a critical role in managing industrialscale projects throughout their operational lifespan. Practitioners utilize simulation techniques at various scales, from lab-scale data analysis to field-scale plume migration and basin-scale pressure modeling. Advances in numerical methods, high-performance computing, and scalability have enabled simulations at unprecedented fidelity. However, balancing complexity and computational efficiency remains essential. To this end, high-fidelity models of coupled processes provide vital benchmarks for testing new advancements in efficient mathematical models and numerical methods. Reducing model complexity can accelerate field-scale simulations, though ensuring reliability and robustness remains challenging. This keynote reviews recent computational developments in CO2 storage simulation, highlighting sub-grid modeling of CO2-specific processes, such as convective mixing and fault-related fluid flow, as an efficient way to capture the impact of fine-scale processes on coarse grids. Additionally, innovations in scientific machine learning, where neural networks are embedded into reservoir simulators, offer promising improvements in solver performance and solution accuracy. These advancements pave the way for more efficient and reliable CO2 storage simulations, ultimately accelerating the path to large-scale deployment.

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#### IP4

#### The Mathematics of Sustainability

The continual increase in the human population, magnified by increasing per capita demands on Earth's limited resources, raises the urgent mandate of understanding the degree to which these patterns are sustainable. The scientific challenges posed by this simply stated goal are enormous, and cross disciplines. What measures of human welfare should be at the core of definitions of sustainability, and how do we discount the future and deal with problems of intra-generational and inter-generational equity? How do environmental and socioeconomic systems become organized as complex adaptive systems, and what are the implications for dealing with public goods at scales from the local to the global? How does the increasing interconnectedness of coupled natural and human systems affect the robustness of aspects of importance to us, and what are the implications for management. What is the role of social norms, and how do we achieve cooperation at the global level? All of these issues have parallels in evolutionary biology, and this lecture will explore what lessons can be learned from ecology and evolutionary theory and the mathematical challenges for addressing the problems posed in achieving a sustainable future.

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#### IP5

Numerical Simulation of Biot's Model by an Iterative Coupling Solution Method Based on an

#### Oscillation-free Numerical Scheme

Biot's model describes the coupling of fluid flow and mechanical deformation within a porous media. The numerical solution of this multiphysics model has received a lot of attention during the last decades since such a coupling plays an important role in many relevant applications like geothermal energy extraction, CO2 storage, hydraulic fracturing, and cancer research, among others. Numerical difficulties in the solution of Biot's model can appear in both the discretization and the solution methods. On the one hand, the uniform stability and the possible appearance of non-physical oscillations in the numerical pressure field are issues that have to be taken into account when choosing an appropriate discretization scheme. On the other hand, the solution of the large sparse systems arising after discretization may became a bottleneck when complex real problems are solved. In this work, we address all these numerical issues by proposing a novel uniformly stable scheme that provides numerical solutions without spurious oscillations and also allows us to iterate the fluid and mechanics problems in a fashion similar to the well-known fixed-stress split method but without the necessity to stabilize the iteration. We demonstrate the parameter-robust convergence of the proposed iterative coupling method, and show the optimality of this method for one-dimensional problems and their good behavior in higher dimensions.

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#### SP1

SIAM Activity Group on Geosciences Career Prize Lecture - Interface-controlled Multi-field Processes in Porous Media Coupled with Free Flow From Pore to REV Scale

Flow and transport processes in domains composed of a porous medium and an adjacent free-flow region appear in a wide range of industrial, environmental, and medical applications. The overall behavior of these coupled systems is determined by the character, geometry and dynamics of different types of fluid-fluid and fluid-solid interfaces, not only on the targeted characteristic scales, but especially on small scales. To what extent interfaces and the associated interface-controlled mass, momentum and energy processes on different scales influence the effective behavior of single and multiphase processes in coupled porous media / free flow systems and how this can be integrated into existing model concepts is the focus of this presentation. The lecture will use selected examples to give an overview of our work in recent years on coupling concepts and multi-scale (hybrid) approaches with a focus on interfaces from the pore to the REV scaler, that play an important role in this context.

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#### SP2

SIAM Activity Group on Geosciences Early Career Prize Lecture - Iterative Coupling Methods for Poroelasticity: From Design to Analysis through a Unified Thermodynamical Approach

Poroelasticity describes the two-way coupling of fluid flow

and geomechanics in permeable and deformable porous media. This coupling is crucial for applications such as CO2 sequestration, geothermal energy, and ground water extraction. The mathematical models governing these processes are often strongly coupled, necessitating robust and efficient numerical solution strategies for effective simulations. Iterative coupling methods have proven highly successful, enabling the integration of different simulators for subproblems and the development of state-of-the-art preconditioners for large-scale simulations. In this lecture, I will present a unified thermodynamical interpretation of poroelasticity models, focusing on the generalized description of energy dissipation through generalized gradient flows. This approach naturally leads to iterative splitting schemes derived from alternating minimization applied to the energetic formulation of poroelasticity. Additionally, this framework provides a comprehensive basis for the theoretical convergence analysis of these splitting methods, offering sharp convergence rates. This analysis extends the generalization of alternating minimization methods to nonsmooth and non-convex problems, which are common in poroelasticity.

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#### CP1

## Numerical Investigations of Spontaneous Imbibition in Layered Porous Media

The spontaneous imbibition in a homogeneous porous medium follows the diffusive Washburn's law. However, for a heterogeneous porous medium such as fractured petroleum reservoirs consisting of two or more layers, the capillary-controlled displacement deviates from the Washburn's law. For two-layered media, we show at Darcy scale how different properties of the layers affect the crossflow between the layers and consequently change the flow behaviour. We used MATLAB Reservoir Simulation Tool to investigate the flow dynamics of wetting fluid, where a substantial amount of residual oil is left behind in the layers of a porous reservoir. The results of our study demonstrate that crossflow between the layers is not confined to the region near the imbibition front. Comparing imbibition in the interacting and non-interacting porous layers, we show that (a) due to permeability contrast, the saturation profiles of the layers approach the saturation profile observed in an averaged permeability porous medium, (b) capillary pressure variation results in cross-flow in different directions at different locations to equalize capillary pressure between layers, and (c) when both capillary pressure and permeability are correlated, an anomalous behaviour is observed where the low permeability layer exhibits the leading front. These results offer insights to develop a new model to predict the overall behaviour of spontaneous imbibition in layered porous media.

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#### CP1

Physics-Based Adaptive Mesh Refinement for Effi-

#### cient Multiphysics Simulation in Porous Media

This work investigates physics-based adaptivity in the finite element framework for simulating multiphysics processes in porous media using a posteriori error estimates. Leveraging MOOSEs adaptive mesh refinement, the study focuses on independently refining mesh structures for distinct physical phenomenaflow, energy, transport, and mechanics within coupled systems, enhancing computational efficiency and accuracy. Mesh refinement is particularly critical for complex geometries and localized phenomena, such as fractures, where solution accuracy benefits from targeted resolution enhancement. Strategies include hrefinement (element subdivision), p-refinement (higherorder basis functions), r-refinement (node repositioning), and hp-refinement (combined h- and p-adaptivity). A posteriori error estimatorsresidual-based, recovery-based, and goal-orientedguide mesh refinement by quantifying solution errors. The implementation of independent physics-based adaptivity is demonstrated in poroelastic systems, decoupling mechanics from fluid flow, with refinement driven by error estimators. For CO2 sequestration, error estimators optimize mesh refinement for transport and fluid flow, ensuring precise, resource-efficient simulations. This approach significantly improves solution accuracy while reducing computational overhead, providing a robust framework for high-fidelity porous media simulations.

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#### CP1

## Statistical Integro-Differential Fracture Model (Sid-Fm) for Subsurface Flow and Transport

Highly conductive fractures act as fluid conduits that significantly influence subsurface flow patterns. However, the distribution of these fractures is highly uncertain, and their length scales may be comparable to the domain of interestmaking it impossible to define a representative elementary volume (REV); especially in cases with isolated fractures. Models that explicitly resolve each fracture are computationally expensive, even for a small number of fractures, and the cost of Monte Carlo studies is exorbitant and often prohibitive. Therefore we propose a novel model for simulating expected flow and transport in fractured porous media. This model targets the ensemble-averaged solution directly, using fracture statistics as input, thereby bypassing the need for costly Monte Carlo simulations. It captures the non-local interactions between fractures and the porous matrix through kernel functions, leading to a system of integro-differential equations. Numerical experiments with statistically one-dimensional test cases show good agreement with reference Monte Carlo data; in terms of pressure, flow rates and transport. This is encouraging in view of further developments towards a Sid-FM simulator for practically relevant 3D formations.

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#### CP1

#### Fracture Displacement Basis Function Method for Fast Geomechanical Simulations of Fractured Rock

In reservoir engineering, computations of stress and displacement fields, shearing, and tensile opening are essential for predictive simulations of flow, transport, and seismicity. In our approach, we model rock deformation by assuming the rock to be homogeneous with linear elastic behavior and the fractures to have predefined slip and tensile opening profiles. For isolated fractures these profiles are elliptic with a linear relationship between maximum slip and induced stress. We employ these single-fracture displacement solutions as basis functions in our model. Overall stresses are obtained by mapping and superimposing these basis functions to the fracture ensemble of interest. The resulting stress field combines far-field- and all displacementinduced stresses, constraining maximum slip and tensile opening along each fracture while considering local force balance constraints. The resulting matrix equation only has two degrees of freedom per fracture - one for shear slip and one for tensile opening. To more accurately represent interacting and intersecting fractures, additional S-shaped basis functions and related degrees of freedom are introduced. Despite this addition, the approach remains highly efficient, requiring only few degrees of freedom to represent complete displacement and stress fields, as well as shearing and opening of fractures. We illustrate the methods capability for single, parallel, and intersecting fractures, as well as for complex fracture networks.

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#### CP

# Compositional Reservoir Simulation with a High-Resolution Compact Stencil Adaptive Implicit Method

The adaptive implicit method (AIM) is the mainstream approach for compositional reservoir simulation. In its standard form, AIM uses single-point upwinding to reconstruct the interfacial fluxes, and this leads to substantial numerical diffusion and loss of accuracy. Previous efforts to improve the accuracy of AIM focused on using

high-order schemes to reconstruct the interfacial fluxes; those schemes introduced additional numerical nonlinearities to the system of equations or compromised the accuracy of the Jacobian by neglecting the high-order terms in its construction. We describe a high-resolution compactstencil (HRCS) AIM that, in addition to the mixed implicit/explicit time discretization of standard AIM, also uses a mixed space discretization. Specifically, we blend low- and high-order fluxes according to a well-defined rule that uses a high-order reconstruction in the explicit regions of the domain and a low-order reconstruction in the implicit regions. This strategy ensures that additional nonlinearities introduced by the high-order reconstruction do not impact the Jacobian matrix, thus preserving the algebraic structure of standard AIM. The HRCS AIM method is demonstrated using several compositional problems. The results indicate substantial gains in accuracy with a small additional computational cost compared with standard AIM. Additionally, HRCS AIM is more robust and has a smaller computational cost compared with its full highresolution counterpart.

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#### CP1

Explicit Hyperbolic System for Coupled Buoyant Two-Phase Flow and Transport in Heterogeneous Porous Media

Recently, a new approach for simulating buoyant two-phase flow and transport in porous media, which is based on a coupled hyperbolic system, was proposed. This new scheme incorporates Darcys law by adding a source term to the isothermal Euler equations plus an extra equation for phase transport. The system allows for explicit simulations and is solved in its hyperbolic form with a finite volume scheme employing an approximate Riemann solver to obtain the numerical fluxes. Since all required operations are local, for many problems this method has significant advantages over previous ones in terms of computational cost and parallelizability. Here, this approach is generalized for heterogeneous porous media, which has implications for the numerical solution algorithm. In particular, it is crucial that the source terms are considered by the Riemann solver, otherwise the results get contaminated by numerical errors. To achieve this, a new Rankine-Hugoniot-Riemann (RHR) solver is devised. It accounts for the source terms by introducing consistent Rankine-Hugoniot jumps in each finite volume cell (separately in all coordinate directions) while still honoring conservation. Numerical results with shale layes confirm that the new RHR solver is effective and that the explicit hyperbolic solution approach to coupled buoyant flow and transport in heterogeneous porous media is computationally efficient and leads to accurate results.

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#### CP2

An Adaptive High Order Finite Element Solver for the Shallow Water Equations with Irregular Bathymetry

We present an adaptive finite element solver for the shallow water equations, which inherits the efficiency and robustness properties of the semi-implicit methods of [Casulli, Int. J. Numer. Methods Fluids 2009]. We restrict our attention to a second order IMEX time discretization that treats the pressure gradient term explicitly, while applying an implicit method to the friction term. Within a high order Discontinuous Galerkin method we focus on a robust and accurate treatment of the bathymetry, nowadays available with higher resolution than the mesh in coastal areas. This poses a series of challenges for higher order methods that work on coarse meshes: the mesh may not be aligned to large bathymetric gradients and the finite element method should be able to handle such gradients within an element. We choose as prognostic variable the free-surface elevation which is smooth and for which we employ a finite element representation. The bathymetry at the quadrature node is directed evaluated from the reference data without any modification. We discuss some numerical implications of this approach, concerning massconservation with wetting/drying and the discretization of a passive tracer. We show the robustness in presence of an irregular bathymetry also with under-resolved features at the grid scale. In this framework, we test static and dynamic Adaptive Mesh Refinement handled with the deal.II library to simulate the tidal circulations in complex coastal environments.

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#### CP2

Beyond Trade-Offs: Robust, High-Accuracy, High-Performance Operations in Spherical Geometry

In geoscientific modeling, remapping accurately transfers physical quantities between grids with varying resolutions and coordinate systems. Locally conservative remapping, which preserves the locality of remapped quantities, requires mass transfer only between overlapping cells, demanding accurate geometric calculations on spherical surfaces, particularly intersection of grid lines. Accurate, efficient, and robust algorithms for spherical computational geometry are difficult to define. Exact arithmetic maintains precision and robustness but is too computationally expensive for large-scale applications. Conversely, typical geoscience software prioritizes performance with floating-point arithmetic, introducing accuracy and robustness issues. This presentation describes an algorithm for spherical intersection calculation that preserves all three properties.

We characterized the asymptotic behavior of floating-point errors across regimes, identifying conditions causing significant precision lossup to half the working precisionand derived relative error bounds. In problematic cases where errors propagate through operations, simple formula adjustments proved inadequate. We developed a robust algorithm using an enhanced intersection formula and extended error-free transformation techniques, ensuring numerical stability and achieving machine epsilon accuracy comparable to exact arithmetic, with no added computational cost when vectorization and parallelization are enabled.

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#### CP2

## A Depth-averaged Multipoint Method for Landslide Simulations

Among the most dangerous natural phenomena for the safety of people, landslides are one of the most problematic: not only because of their potentially catastrophic nature in terms of human and economic loss, but also because of their intrinsic unpredictability. In this work, we show some recent results on the simulation of landslide evolution immediately following the phase of initiation of the landslide front[M. Fois, C. de Falco, L. Formaggia, A Semi conservative depth-averaged material point method for fast flow-like landslides and mudflows, Comm. in Nonlin. Science and Num. Simul., 2024]. The basic mathematical model used to describe gravity-driven free surface flows is the depth-integrated equations derived from the Navier-Stokes equation for an incompressible fluid. We propose a semiconservative variant of the Depth-Averaged Material Point Method (DAMPM), which is a depth-integrated version of the Material Point Method (MPM). The effectiveness of the procedure will be demonstrated by several real life tests.

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#### CP2

#### Alternating-Implicit Dynamically Orthogonal Runge-Kutta Schemes for Geosciences Applications

We employ our family of implicit integration methods for the dynamical low-rank approximation, the alternatingimplicit dynamically orthogonal Runge-Kutta (ai-DORK) schemes. Explicit integration often requires restrictively small time steps and has stability issues; our implicit schemes eliminate these concerns in the low-rank setting. We incorporate our alternating iterative low-rank linear solver into high-order Runge-Kutta methods, creating accurate and stable schemes for a variety of previously intractable problems, including stiff systems. Fully implicit and implicit-explicit (IMEX) ai-DORK are derived, and we perform a stability analysis on both. The schemes may be made rank-adaptive and can handle ill-conditioned systems. To evaluate nonlinearities effectively, we propose a local/piecewise polynomial approximation with adaptive clustering, and on-the-fly reclustering may be performed efficiently in the coefficient space. We demonstrate the ai-DORK schemes and our local nonlinear approximation on an ill-conditioned matrix differential equation, a stiff, two-dimensional viscous Burgers' equation, the nonlinear, stochastic ray equations, the nonlinear, stochastic Hamilton-Jacobi-Bellman PDE for time-optimal path planning, and the parabolic wave equation with low-rank domain decomposition in Massachusetts Bay.

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#### CP2

## Fast-Slow Dynamics of the Quasi-Geostrophic Approximation

This work is devoted to investigating the rotating Boussinesq equations of inviscid, incompressible flows with both fast Rossby waves and fast internal gravity waves. The main objective is to establish a rigorous derivation and justification of a new generalized quasi-geostrophic approximation in a channel domain with no normal flow at the upper and lower solid boundaries, taking into account the resonance terms due to the fast and slow waves interactions. Under these circumstances, We are able to obtain uniform estimates and compactness without the requirement of either well-prepared initial data or domain with no boundary. In particular, the nonlinear resonances and the new limit system, which takes into account the fast waves correction to the slow waves dynamics, are also identified without introducing Fourier series expansion. The key ingredient includes the introduction of (full) generalized potential vorticity.

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#### CP3

# Reinforcement Learned, Bidirectional Stochastic Hamiltonian Operators for Efficient History Matching

While history matching methods have demonstrated the ability to infer subsurface geometric and material properties that reproduce observed well logs and production time series data, their use of brute-force inversion is extremely time consuming with large budgets of full-forward physics simulations and hence limited to low uncertainty inference in smallish regions surrounding existing wells. We present a novel history matching method with progressive forward and inverse, reinforcement learned stochastic Hamiltonian operators that accomplishes the inverse Bayesian refinement of subsurface properties, by simultaneous training both stochastic operators, and in accelerated time. The reservoir's flow dynamics state is continuously and progressively embedded in a low-dimensional latent dynamic phase space where Hamiltonian dynamics are governed by a learned energy functional, guaranteeing symplectic, volume-preserving, and time-reversible evolution. Inverse active inference from each well expands local high-fidelity subsurface property regions yielding uncertainty minimized subsurface properties with path-wise guided stochastic Hamiltonian dynamics control. Our progressive forward-inverse stochastic Hamiltonian framework using point-wise estimates along guided paths sharply reduces reliance on full-physics runs, retains physical consistency with lower uncertainty quantification, and integrates seamlessly into existing reservoir workflows.

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#### CP3

## A Numerical Strategy for Electromagnetic Inversion

This work deals with the reconstruction of the subsurface composition of the earth, by recorded measurements taken at the surface. We focus on an electromagnetic sounding method that consists of placing magnetic dipoles above the surface. The response electromagnetic fields can be used to determine the underground conductivity profile, by means of an inversion procedure. By assuming that the local subsurface structures are composed by horizontal homogeneous layers, integral representation of the response fields can be derived in terms of Hankel transforms. Having at disposal reliable quadrature rules to evaluate this kind of integrals (Denich et al., "A fast and accurate numerical approach for electromagnetic inversion"), we deal with the inverse problem of computing the model parameters. The assumption on the subsoil model leads to a severely ill-conditioned inverse problem, in which the conductivity profile solution is represented by a piecewise constant function. We present a quite heuristic minimization strategy (Denich et al., "A numerical strategy for electromagnetic inversion), based on a preprocessing analysis for the location of a set of initial guesses. We exploit a linear approximation of the model and the theory of the best  $L^2$  approximation attainable with a piecewise constant function, that allow to work without assuming to have relevant information about the subsoil composition. We present realistic experiments based on river levees conductivity models.

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#### CP3

#### Conditional Diffusion Models for Hydrogeologic Parameter Estimation

Estimating hydrogeologic parameters from time-lapse Electrical Resistivity Tomography (ERT) monitoring data is challenging due to the inherent nonuniqueness and ill-posed nature of mapping measured geophysical responses to subsurface flow and transport properties. In this work, we present an AI-driven methodology employing conditional

diffusion models to robustly estimate hydrogeologic simulation parameters while explicitly quantifying uncertainty. Our approach uses a reverse diffusion process that starts with a Gaussian random vector and gradually denoises it conditioned on high-dimensional time-lapse ERT monitoring data to recover a 29-dimensional parameter vector. A goodness-of-fit metric assesses the accuracy and precision of the uncertainty distribution for each parameter, thereby avoiding unreliable or overconfident solutions. Experimental results demonstrate that the recovered parameters produce simulated ERT data in close agreement with the given conditional ERT data, highlighting that conditional diffusion models offer a robust, uncertainty-aware solution for geophysical inversion.

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#### CP3

## Dual Implicit Neural Representations for Fwi with Salt

Full Waveform Inversion (FWI), a data-driven approach inverting for earth model properties from seismic data is often the first step in seismic processing used to characterize both hydrocarbon reservoirs as well as reservoirs for carbon sequestration. FWI is an inverse problem involving a PDE with earth model properties as its coefficients. FWI is a nonlinear inverse problem and is well known for non-unique solutions, which necessitates having a good initial model. Some areas within the earth have complex salt structures where building an initial model can often be a manual time-consuming process. Our inverse problem now consists of two coupled subproblems: determining the salt geometry and determining the earth model sediment properties. We will show an approach that evolves the salt geometry simultaneously with sediment updates, by representing both the geometry and sediment properties as implicit neural networks. We specifically use SIREN network which is characterized by sine activation functions. We will show this PINN method can successfully invert for both salt structure and sediment properties in 2D with no prior model. We leverage the JAX framework which makes it easy to compose different operators and allows us to leverage the power of auto differentiation. We will also show some examples that indicate that our method can scale to 3D real field applications. This technique bridges geomodeling and geophysics disciplines, potentially enhancing collaboration.

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#### CP3

#### Water Exposure Time Distributions Controlled by Freshwater Releases in a Semi-Enclosed Estuary

Freshwater diversions manage water shortages, salinity, and floodwaters by redirecting river flows; however, their full ecological and hydrological impacts remain uncertain. This study applies a hydrodynamic model coupled with Lagrangian particle tracking to quantify how diversion operations (open, closed) and tributary discharge levels (low, median, high) affect water exposure time in a diversion-influenced estuary (Lake Pontchartrain Estuary, USA). Ex-

posure timethe cumulative duration water resides in a specified region of interest (ROI), including re-entrywas evaluated using  $E_{50}$ ,  $E_{75}$ , and  $E_{90}$  metrics, defined as the exposure times for 50%, 75%, and 90% of tracked particles, respectively. To identify zones vulnerable to poor water quality due to stagnant water, the spatial heterogeneity of exposure time was evaluated at system-wide (the entire system) and localized (a smaller, defined (ROI) scales. Results show that exposure time distributions vary considerably, spatially and across discharge regimes, highlighting the complexity of transport dynamics. For example, low tributary discharge produced large zones of recirculation and prolonged retention, whereas, high discharge created direct flow paths of diversion-sourced water through tidal inlets, short-circuiting the system, inducing flow separation. These findings establish a framework for identifying transport mechanisms influencing exposure time and highlighting areas vulnerable to poor water quality.

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#### CP4

## Recent Advances in Stabilization-Free Polytopal Methods

This talk focuses on recent advances in the field of polytopal methods for solving partial differential equations, particularly focusing on the family of Virtual Element Methods (VEMs). In the literature, it has been shown that these methods are robust, capable of addressing problems characterized by high geometrical complexity, and can be easily integrated into already developed Finite Element routines. Traditionally, the discretized bilinear form associated with polytopal methods comprises two operators: one for ensuring polynomial consistency and the other for enforcing stability. However, in many application, it has been shown that the isotropic nature of the stabilization term can introduce non-physical perturbations into the model. Recently, a new line of research has grown, studying the possibility of designing bilinear forms that preserve the structure of the problem operator, characterized by polynomial approximation operators that are both consistent and stable. In particular, this presentation focuses on stabilization-free VEM schemes for elliptic equations and shows their application to problems of interest.

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#### CP4

Entropy Generation and Heat Transfer Analysis in Mhd Casson Hybrid Nanofluid Flow over a Permeable Stretching Sheet with Nonlinear Solar Radiation and Varying Viscosity As Well As Thermal Conductivity

This study presents a numerical analysis of entropy generation in the two-dimensional MHD flow of a Casson hybrid nanofluid over a permeable stretching sheet, incorporating the effects of nonlinear solar thermal radiation, heat source/sink, and mixed boundary conditions. In this study, we have used two distinct base fluids are considered: (i) 30% ethylene glycol (EG) + 70% water  $(H_2O)$ and (ii) 50% ethylene glycol + 50% water, in which copper (Cu) and ferric oxide  $(Fe_2O_3)$  nanoparticles are suspended to formulate two hybrid nanofluids. In order to provide a realistic view on the behavior of nanofluids under a varying thermal situations, the study takes into account temperature-dependent viscosity as well as thermal conductivity. The governing non-linear coupled PDEs are transformed into non-linear coupled ODEs by using the appropriate similarity variables and solved numerically using MATLAB solver bvp4c. The numerical outcomes are validated with semi-analytical outcomes obtained through the homotopy analysis method, and they are also compared to available literature as a limiting case. The influence of non-dimensional parameters on skin friction coefficient, local Nusselt number, flow and thermal profiles is discussed with the assistance of graphs and tabular data. A comparative analysis of  $Cu + Fe_2O_3/EG(30\%) + H_2O(70\%)$ and  $Cu + Fe_2O_3/EG(50\%) + H_2O(50\%)$  reveals significant variations in heat transfer performance and entropy generation.

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#### CP4

#### Microscopic Perspective of Ice Nucleation of Soot Particles from Turbofan Engine

Aerosols are small particles like soot, ash and desert dust in the atmosphere, also known ?as ?particulate matter. They have a net cooling effect on climate, but to what extent is still a mystery. ??The range runs from 0.2 to even 0.9 degrees Celsius dampening influence on global ?warming. ?These emitted ultrafine particles from aero-engines are affecting the climate both directly via ?reflection and absorption of sunlight, ?and indirectly by acting as a starting point for cloud ?formation. Followed by the ice nucleating mechanism, the microscopic perspective of these ??particles is a huge challenge of nowadays, since its deeply related to the ?design ?of ?pilot engines under SDGs regulations.? ?Hence, the target of this work is to provide a multiphase simulation framework capable of ?tracking the thermal fatigue and heat ?wave ?divergences surrounding the nucleic soot, besides the ?temporal passive/active ?ice nucleation and the phase change during the capillary?condensation.? To do so, ?(1) the mechanism of ice nucleation associated with flow trajectory ?will be highlighted in straight

minichannels, considering ?the interference of isobaric cooling. ??(2) The ?growth and departure of aggregated soot will be analyzed to quantify the mass ??transfer enhancement. (3) The ?dynamics of soot compression ?during antigravitational injection ?will be identified, based on the nonlinear energy flow and thermal desorption.? This work will strenghen the path of green aviation.?

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#### CP5

#### Derivation and Investigations of Effective Dispersion Models for Electroosmotic Flow in An Evovling Thin Strip

Dispersion is one of the key parameters in transport in porous media. We derive novel effective dispersion models for reactive transport of electrically charged chemical species in a thin, potentially evolving strip by formal asymptotic expansion. These models include Taylor-Aris, electroosmotic induced dispersion and their cross coupling effects. We prove existence and uniqueness of strong solutions in the fixed geometry setting. Moreover, we numerically investigate scenarios for both the fixed and evolving geometry situation. We study the limits of vanishing channel width, precipitation layer thickness, and molecular diffusion and show convergence of the solutions to the corresponding limit cases such as a hyperbolic model or the fixed geometry case.

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#### CP5

#### Viscous Dissipation Effects on Thermal Convection in Bidispersive Porous Media with Inertial Effect and Vertical Throughflow

This study delves into the problem of thermal convection in a bidispersive porous medium (BDPM), with the impact of viscous dissipation, inertial effect, and throughflow via linear and nonlinear theoretical frameworks. The flow behaviour is characterized through Darcys law and the Oberbeck-Boussinesq approximation, with local thermal equilibrium between the fluid and solid phases. The temperature field depends solely on the vertical coordinate in the basic solution. The model may well align with packed bed reactors and thermal insulation as a practical application. Stability analysis carried out using normal mode technique for linear and nonlinear (via energy method) analyses. The numerical solutions to the eigenvalue problem for both linear and nonlinear theories are obtained using the bvp4c routine, and the influence of various physical parameters on the stability behaviour of the system has been explored. The effect of viscous dissipation on the onset of convection can only be seen for significant throughflow. The effective permeability ratio stabilizes the system with upward throughflow and vice versa with downward throughflow. The Gebhart number does not influence the sub-critical region, whereas the sub-critical region increases with the permeability ratio and momentum transfer coefficient. Further, heat transfer is studied using weakly nonlinear analysis.

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#### CP5

## Does Pre-Existing Differential Pressure Have An Impact on Poroelasticity Equations?

The existing formulation of quasistatic poroelasticity for saturated porous materials relies on the assumption that differential pressure, defined to be the difference between the confining and liquid pressures, is zero at the reference state. This assumption can be problematic in problems involving swelling media, such as clay, and deep underground where preexisting pore pressure may differ from the total pressure. Here, the quasistatic poroelastic equations are derived from only the conservation of mass for each phase and the Terzaghi effective stress principle for the case when there is a nonzero reference differential pressure. In the process, a dynamic equation for the porosity is derived, and one additional parameter representing a dimensionless reference differential pressure is introduced. Although the form of the quasistatic poroelastic equations remains the same, the poroelastic compressibilities change with the reference states nonzero differential pressure. The changes in these compressibilities are systematically outlined, and the impact on more specific classes of material is examined. The altered compressibilities imply, among other changes, that the compressional velocity is a function of the preexisting differential pressure, which is useful to account for in dynamic measurements, but that the dependence is weak for materials with low compressibilities.

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#### CP5

#### Efficient Basis Function Method for Pressure-, Streamline-, and Flow Calculations in Fractured Reservoirs

Fractured porous media are an important area of research as fractures can significantly alter the flow and transport properties. Hence, to achieve accurate simulations, ideally all fractures should be resolved. However, this often is not feasible due to huge numbers of fractures. Smaller fractures often are upscaled into the matrix properties, while larger fractures are explicitly represented. Here we present a meshless method as an alternative. The method is based on the idea that a fracture acts as a combination of sources and sinks. Close to the fracture we use a numeric approximation, while far away one can use an analytical continuation; we call this the basis function. For a formation with many fractures we can superimpose the basis functions to compute pressure, velocities or the streamlines. Since the basis functions only have to be computed once, the computational cost of the method reduces to determining the summation weights. We present numerical experiments and compare the results of the new method against classical high-fidelity solutions for a variety of fracture geometries. Pressure and velocity fields as well as streamlines are excellent agreement, even for complex formations with many fractures.

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#### CP5

# Rigorous Upscaling of the Unsteady Stokes Equations in Heterogeneous Porous Media under Time-Varying Boundary Conditions

Understanding large-scale flow behaviors through heterogeneous porous media is essential for optimizing many subsurface engineering applications. To study these behaviors efficiently at practical scales, macroscopic flow models can be developed through rigorous upscaling techniques to accurately predict a systems large-scale responses to external forces (e.g., fluid injections, buoyancy due to temperature gradients). However, such techniques often rely on assumptions that oversimplify the complexities of real-world systems (e.g., steady state, periodic microstructures, negligible system-scale boundary effects). Recently, we developed and validated the Method of Finite Averages (MoFA), an upscaling methodology for singlespecies advective-diffusive transport that rigorously accommodates heterogeneous microstructures, system-scale time-dependent boundary effects, and a wide range of transport regimes. In this work, we apply MoFA to singlephase Stokes flow in heterogeneous porous media under system-scale, time-varying boundary conditions, and analytically derive upscaled momentum balance equations with a priori error guarantees. We then perform numerical validation of the derived model against fully resolved pore-scale simulations. We also apply MoFA to advectivediffusive-reactive transport in heterogeneous porous media. The results show that MoFA is an effective, general technique for constructing coarse-scale models for diverse physical processes in complex systems.

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#### CP5

An Adaptive Homotopy Continuation Solver for

#### Incompressible Two-Phase Flow in Porous Media

Accurate modeling of flow in porous media relies on an appropriate selection of constitutive laws. However, nonlinearities in the constitutive lawse.g., in the relative permeability and capillary pressure functionshave been identified as one of the main causes of slow or nonconvergent nonlinear solvers. To address these challenges, various methods such as trust-region methods and specialized flux discretizations have been proposed. For highly complex numerical flux functions with multiple nonlinearities, such methods can be challenging to implement. In this work, we employ homotopy continuation (HC) as a flexible method to enhance the robustness of two-phase flow simulations with severe nonlinearities. The method first solves a simpler problemwith linear constitutive lawsand then iteratively traces a solution curve toward the target problem. To efficiently trace the solution curve, we leverage a posteriori error estimates. The numerical error estimate is decomposed into discretization, HC, and linearization components. By balancing all three components, we develop an HC algorithm that converges robustly at large time steps while minimizing the total number of nonlinear iterations. We demonstrate robustness and efficiency of the new method on relevant simulations of varying complexity. Finally, we discuss the application of our method to machine-learned constitutive laws.

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#### CP6

## Solving Earthquake Frictional Contact As a Variational Inequality

We formulate the frictional contact problem of crustal dynamics as a variational inequality in the PyLith framework, and apply scalable nonlinear solvers from the PETSc libraries. We aim to apply this formulation to crustal problems drawn from Alaskan tectonics.

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#### CP6

## Rigorous Upscaling of Nonlinear and Coupled Systems in Heterogeneous Porous Media

Reactive transport through heterogeneous porous media continues to challenge modeling efforts focused on subsurface engineering systems. Rigorous upscaling techniques can be employed to derive efficient and reliable models (i.e., models that come with a priori error estimates and applicability conditions, or physical conditions under which the error estimates are satisfied) for such systems, but they often depend on a number of methodological assumptions (e.g., diffusion-dominated physics and periodic geometries at finer scales, scale separation, and negligible effects from the boundaries of a system) that limit their applicability to idealized scenarios. Previously, we developed a novel upscaling methodology called the Method of Finite Averages (MoFA) that avoids the aforementioned assumptions while retaining a priori error estimates and applicability conditions. In this presentation, we develop a strategy for applying MoFA to nonlinear and coupled systems in an efficient manner. We detail the strategy and implement it to model advective-diffusive transport systems experiencing nonlinear reactions. We then highlight the benefits of using the strategy and compare the strategy to applying MoFA directly to model nonlinear and coupled systems.

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#### CP6

## Coupled Thermo-Hydro-Mechanical Uncertainties for Co2 Storage Integrity Assessment

The Aramis project in the Netherlands is a key initiative in CCS, where industrial actors aim to reduce CO2 emissions by capturing and storing it in a depleted offshore gas field under the North Sea. This study focuses on geomechanical risk assessment in a realistic setting, considering both the depletion and injection phases. The geological domain includes a depleted reservoir bound by fault surfaces and a prominent salt body, which adds complexity due to stress reorientation around its structure. The problem is modeled using a non-isothermal, compositional two-phase flow model, fully coupled to a linear thermo-poro-elastic formulation. This coupling ensures that variations in pore pressure and temperature directly influence the mechanical behavior of the rock and vice versa. A scenario representing a realistic quasi-operational framework is considered, with 40 years of hydrocarbon depletion followed by 20 years of CO2 injection and 180 years of post-injection monitoring. The simulations were performed using GEOS, an open-source platform designed for multi-physics modeling of coupled flow and geomechanics. This study aims at exploring the effect of parameter variability on the uncertainty ranges affecting the prediction of the maximum admissible pressure, but also to assess the impact of different meshing strategies on the vertical displacements and integrity criteria evolution over time.

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#### CP6

# End-to-End Uncertainty Quantification for CO<sub>2</sub> Injection-Induced Seismicity Via Multifidelity Estimators and Data-Driven Approaches

Injection of carbon dioxide (CO<sub>2</sub>) into subsurface geological formations increases pore pressure, which can trigger seismic events due to fault reactivation. Such injectioninduced seismicity poses considerable risks to the urban population near injection sites, potentially leading to structural damage and endangering public safety. Several factors contribute to these hazards, such as the rate and amount of CO<sub>2</sub> being injected, as well as the poromechanical properties of the injection site. The large range and uncertainty in these problem inputs is reflected in a large spread in the resulting risk of injection-induced seismicity. To quantify the amplification of background seismicity in light of this uncertainty, we use Monte Carlo sampling to build cumulative distribution functions for key quantities of interest. By leveraging multifidelity estimators that combine simulations from the open-source, multiphysics simulator GEOS with data-driven model predictions, we propose an efficient end-to-end uncertainty quantification framework that can inform the decisions of site operators so as to minimize injection-induced earthquakes. We present results for a flexible data-generating validation case with one or multiple faults, and discuss the generalizability of our surrogate models. Next, we show some initial results for real-world cases to demonstrate scalability, and highlight planned future steps to further improve the efficiency of our workflow.

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#### CP7

#### Asymptotic Analysis of Thin Elastic Plate-Visco-Elastic Thick Layer Interaction

The paper is devoted to an asymptotic analysis of a problem on interaction between a thin purely elastic plate and a thick viscoelastic layer described by the Kelvin-Voigt model. Such a problem appears in modeling of the earth crust-magma interaction. The small parameter is the ratio of the thicknesses of the elastic part and the viscoelastic one. At the same time the plate has a high Young's modulus, that is, an inverse to the third power of the small parameter. The complete asymptotic expansion of the solution is constructed. The error estimate is proved for the difference of the exact solution and a truncated expansion. The limit problem is the Kelvin–Voigt equations with a special boundary condition. This limit problem is solved numerically by a finite element scheme. The difference between the initial and limit problems is studied theoretically and by numerical computations. The talk follows paper by F. Chardard, A. Elbert, G. Panasenko, Asymptotic analysis of a thin elastic plate viscoelastic layer interaction, SIAM Journal Multiscale Model. Simul., 16, 3, 2018, 1258-1282

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#### CP7

## Signal Processing of Non-Stationary Spherical Data. From Real Life to Mathematical Challenges

In signal processing the time-frequency analysis of nonlinear and non-stationary processes, as well as the determination of the unknown number of active sub-signals of a blind-source composite signal are, in general, challenging inverse problem tasks. If we consider data sampled on a sphere, things get even more complicated. This is the reason why just a few techniques have been developed so far to study this kind of data. However, much real-life data is of this nature, like in Geophysics and Physics. The idea is to extend the Iterative Filtering (IF) algorithm to work on the sphere. IF is a non-stationary signal decomposition method proposed a decade ago [1] to address the problem of extracting time-varying oscillatory components from a nonstationary multicomponent signal. This method proved to be really valuable in many applications, see [2] and references therein, and it was accelerated in what is known as Fast Iterative Filtering (FIF) [3] by leveraging the Toeplitz matrix theory. In this talk, we introduce the generalization of IF to handle spherical data and show how we can address the question about its convergence [4]. We conclude with some examples of application to geophysical data. [1] L. Lin et al. Adv. in Adap. Data An., 2009. [2] G. Barbarino et al. Lin. Alg. and its Appl., 2022. [3] A. Cicone et al. Num. Math., 2021. [4] G. Barbarino et al. Lin. Alg. and its Appl., 2024.

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#### CP7

## An Adaptive High-Order Locally-Nonhydrostatic Ocean Solver

To simulate and study ocean phenomena involving complex dynamics over a wider range of scales, from regional to small scales (e.g., thousands of kilometers to meters), resolving submesoscale features, nonlinear internal waves, subduction, and overturning where they occur, nonhydrostatic (NHS) ocean models are needed. The main computational burden for NHS models arises from solving a globally coupled 3D elliptic PDE for the NHS pressure. To address this challenge, we start with a high-order hybridizable discontinuous Galerkin (HDG) finite element NHS ocean solver that is well suited for multidynamics systems. We present a new adaptive algorithm to decompose a domain into NHS and HS dynamics subdomains and solve their corresponding equations, thereby reducing the cost to compute NHS pressure. The NHS/HS subdomains are adapted based on new numerical NHS estimators, such that NHS dynamics are resolved only where needed. We evaluate the costs and accuracy of the adaptive NHS-HS solver using three idealized 3D NHS dynamics test cases: (i) idealized internal waves (ii) tidally-forced oscillatory flow over seamounts and (iii) bottom gravity currents. We then complete more realistic NHS-HS simulations of subduction dynamics by nesting with our MSEAS operational data-assimilative HS ocean modeling system. Finally, we discuss DG-FEM-based numerical techniques to stabilize and accelerate the high-order ocean solvers by leveraging the high aspect ratio characteristic of ocean domains.

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#### CP7

#### Bounds-Constrained Methods for Time-Dependent Partial Differential Equations with Applications to Overland Flow

The solutions to partial differential equations frequently satisfy bounds constraints. When using finite element or finite difference methods, if one wishes to construct an approximate solution that satisfies these same bounds, great care is required. In a finite element context, one can replace a discrete variational problem with a discrete variational inequality. This allows for the selection of an approximate solution from a set of functions which satisfy the bounds constraints. Solving nonlinear optimization problems, though incurring a practical expense, bypasses known order barriers for linear problems and allows for the possibility of high-order and uniformly bounds-constrained finite element methods. It is difficult to work with the entire set of bounds-constrained polynomials. However, the polynomials whose coefficients, when represented in the Bernstein basis, satisfy the bounds constraints form a convenient subset with which to work. Selecting an approximation from this set via a variational inequality, one obtains an approximation which is uniformly bounds-constrained, independent of the mesh used. This approach may be extended to collocation-type Runge-Kutta methods. Using a stage-value formulation, the collocating polynomial can be cast in the Bernstein basis to enforce bounds constraints uniformly in time. Examples are shown in which optimal order accuracy is observed, and these methods are applied to a problem from the study of overland flow.

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#### CP7

#### Modeling Atmospheric Lamb Waves Generated by the 2022 Hunga-Tonga Volcanic Eruption

Atmospheric Lamb waves are low-frequency acoustic gravity waves that can be generated by large scale events such as volcanic eruptions or earthquakes. On January 15th, 2022 the undersea volcano Hunga Tonga-Hunga Haapai (HTHH) located near the South Pacific island of Tonga violently erupted. The resulting atmospheric Lamb wave was tracked by multiple sensors around the globe and

has been modeled by several different researchers. We model the Lamb Wave using the shallow water approximation proposed by [Amores et al., "Numerical simulation of atmospheric Lamb waves generated by the 2022 Hunga-Tonga volcanic eruption.", Geophysical Research Letters 49.6 (2022)]. In this model, temperature in the troposphere is related to a bathymetry term in the shallow water model. We present the results of a numerical simulation using high resolution finite volume methods and adaptive mesh refinement.

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#### CP7

## Stochastic Hamiltonian Fluids : Structure-Preserving Schemes

We construct numerical schemes for stochastic fluid dynamics models based on stochastic variational principles, designed to preserve the underlying geometric structures of the equations. Combining recent advances in finite element discretizations for fluid flows with a stochastic midpoint variational integrator on Lie groups, the method ensures the discrete conservation of key quantities such as Kelvins circulation and Casimir functions. As a first application, we implement the method for the stochastic rotating shallow water equations and the stochastic incompressible Euler equations with variable density. Numerical experiments demonstrate the effectiveness of the integrators in preserving geometric properties in a stochastic setting. In future work, we aim to apply this approach to concrete geophysical fluid models, incorporating unresolved small-scale motions as stochastic components.

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#### MS2

#### Well-posedness of Surface-atmosphere Turbulent Flux Algorithms in Earth System Models

Accurate computation of surface turbulent fluxes is vital for the coupling of surface and atmosphere components of Earth system models. At present, Earth system models apply iterative methods such as fixed point iterations to approximate surface fluxes without any consideration of whether the equations underlying the turbulent flux parameterization are well-posed. We demonstrate that under certain meteorological conditions, the underlying equations associated with some turbulent flux algorithms over oceans and sea-ice have no solution or have more than one solution. In this scenario, we present regularization techniques to ensure existence and uniqueness of the computed turbulent fluxes and discuss overall model impacts.

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#### MS2

#### Leveraging Surrogate Models for Efficient Time-Stepping of Geophysical Systems

Many geophysical simulations involve dynamical systems that are so complex and require such high fidelity that they become computationally impractical. Model order reduction, machine learning, and other types of surrogate modeling techniques offer cheaper ways to describe the dynamics of these systems at the cost of additional approximation errors. To overcome the individual limitations of the full and surrogate models, this talk presents new timestepping strategies that intelligently combine both models. The inexpensive surrogate model is integrated with a small timestep to guide the solution trajectory, and the full model is treated with a large timestep to occasionally correct for the surrogate model error and ensure convergence. We provide numerical experiments on the quasi-geostrophic equations to show that this approach can be significantly more efficient than using only the full or surrogate model for the integration.

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#### MS2

## Flexible Implicit Flux Coupling for Atmosphereland Interactions in E3SM

For over 30 years, Earth system models have used one of two methods for transmitting energy, mass, and momentum between their surface and atmospheric components. Explicit flux coupling, analogous to explicit time integration, evaluates fluxes between components using the current state of the Earth system. This is simple to implement and does not require components to use the same horizontal grid or temporal discretization, but is susceptible to numerical instability. Implicit flux coupling evaluates fluxes using a predicted future state, and is derived using a monolithic view of atmosphere-surface coupling, where a semi-implicit method is applied to reduce the calculation of fluxes to the solution of a band-diagonal system, which in turn is treated as a block-diagonal system to divide computational work between components. This is more stable, but also complex to implement and forces components to use compatible semi-implicit methods and compatible discretizations. This study introduces a novel predictor-corrector approach to implicit flux coupling, which is flexible enough to accommodate components with heterogeneous approaches to spatial and temporal discretization. This approach can piggyback off of the existing iterative solvers typically used in atmosphere-surface coupling to avoid significant increases in cost. We show in Energy Exascale Earth System Model that this approach is effective in preventing numerical instability without harming model performance.

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#### MS2

## Challenges and Opportunities in Multiphysics Simulation

Along with increasing capabilities of computing systems, there has been a commiserate increase in simulation capability with single physics simulations giving way to multiphysics and multiscale simulations. While significant progress has been made in developing numerical methods to bring high order accuracy and highly efficient numerical methods to these complex simulations, significant challenges remain. In this talk I will give a brief overview of the challenges and opportunities faced in multiphysics and multiscale simulation and discuss where near and longer

time opportunities exist. The talk will end with a discussion of various ways breakthroughs in numerical methods can be inserted into multiphysics simulations with some observations of best practices.

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#### MS3

#### High-Resolution Hydrodynamic Modeling of Texas Coastal Bend to Evaluate the Performance of Nature-Based Solutions

The presentation will showcase an application of the advanced circulation (ADCIRC) model for the Texas Coastal Bend. We emphasize the high resolution of the finite element meshes upon which the shallow-water equations are solved in hydrodynamic simulations of tides under different sea-level rise scenarios. This high resolution affords the capture of finer channels and tidal creeks that feed and run through the wetlands. In addition, the high resolution provides flexibility to resolve physical features into the model for the performance evaluation of nature-based solutions (NBS). The importance of high resolution in the ADCIRC simulations extends to the coupling with other models in this case with marsh equilibrium model for such NBS performance evaluations. In the Texas Coastal Bend, short-term priorities are evaluated by modeling the elevation response trajectories under sea-level rise for two restoration strategies in Nueces Delta: lump sum of sediment versus thin-layer placement. Longer term priorities are evaluated in terms of when supplemental (engineered) sediment delivery will be required to sustain elevation capital for different rate of sea-level rise.

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#### MS3

#### Bathymetry Reconstruction Via Optimal Control in Well-Balanced Finite Element Methods for the Shallow Water Equations

The reconstruction of bathymetry from known free surface elevation via numerical solution of the shallow water equations (SWE) is an ill-conditioned and generally ill-posed inverse problem. Without proper regularization, a method may fail to converge, or steady-state topography may exhibit spurious oscillations. The presence of noise in the data, or a poor choice of discretization techniques aggravates such issues. To filter out perturbations caused by ill-conditioning and/or presence of unresolvable fine-scale features, a numerical method for the inverse SWE problem must be equipped with carefully designed stabilization operators. In this work, we discretize the two-dimensional shallow water equations using continuous linear finite elements. Physical admissibility is enforced using a wellbalanced and positivity-preserving algebraic flux correction (AFC) scheme. The steady-state bathymetry is calculated via time marching. Two approaches are used to cure the lack of well-posedness and avoid oscillations. The first one adds an artificial diffusion term to the conservation law for the water height. In the second approach, the regularization term consists of numerical fluxes that are constructed using a new optimal control method. An optimization problem is formulated for scalar flux potentials with the aim of minimizing the perturbation of the discretized shallow water equations and deviations from the measured free surface elevation.

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#### MS3

#### Bound Preserving Fem Methods for Shallow and Dispersive Shallow Water Equations for Coastal Louisiana Ecosystem Modeling

Marsh terraces are man-made structures designed to restore and protect coastal wetlands by reducing wave energy and promoting sediment accumulation. Ecosystem benefits include erosion prevention, habitat restoration and carbon sequestration. Numerical modeling of marsh terraces involves challenges like complex geometry and boundary conditions and coupled physical systems spanning a wide range of spatio-temporal scales. This study presents cases of bound preserving finite element methods to analyze wave- hydrodynamic behavior of marsh terraces using the shallow water equations (SWEs). Linear, chevron and circular shaped terrace configurations are modeled. A local refinement strategy based on bathymetry gradients is employed to optimize the mesh. Preserving physical bounds of positivity of water elevation is essential when modeling SWEs. Another numerical constraint is the presence of dynamically wet and dry elements. We discuss highorder DG schemes and flux correction techniques for SWEs. An advection-diffusion model softly coupled with SWEs is made to evaluate the geomorphological behavior. Presence of sharp physical gradients and dominance of advection violate maximum principles, leading to spurious oscillations or nonphysical negative concentrations. A flux-corrected transport (FCT) scheme maintaining a high order accuracy is employed. This modeling framework offers a valuable tool for optimizing terrace design and placement in future marsh restoration projects.

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#### MS4

## A Multiscale Flow Model for Faults with Asymmetric Damage Zones

This work presents a multiscale flow model for faults with asymmetric damage zones, improving the representation of fault complexity in subsurface reservoirs. Traditional models often simplify faults as planar barriers, overlooking their internal heterogeneity. Here, faults are represented as volumetric features composed of a core and asymmetric damage zones, each with distinct hydraulic and mechanical properties. Using field data from the Moab Fault (Utah, USA), we analyze fracture networks statistically to inform a hybrid upscaling method for deriving anisotropic equivalent permeability tensors. Monte Carlo simulations, based on scanline data, capture spatial variability and directional bias within the damage zones. These properties are integrated into coupled flow and geomechanical simulations to assess how geometric asymmetry, fault offset, and dip affect reservoir pressurization and fault stability. Results show that asymmetric architectures strongly influence pressure compartmentalization and stress distribution, potentially promoting fault slip or seal degradation. The findings underscore the importance of geologically realistic and stresssensitive fault models in applications such as CO2 storage.

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#### MS4

## Coupling Phase Field and Enriched Galerkin for Hydro-Mechanical-Reactive Flow

Acid stimulation is a common acidizing treatment in which an acid solution under formation fracture pressure is utilized to dissolve a low permeability matrix and connect isolated fractures thus resulting in increased formation permeability and bypassing damaged areas around the wellbore. This is especially important in enhancing production in carbonate reservoirs. Some well-known experimental observations include: (1) An optimum acid injection rate for different fluid and mineral systems at which the amount of acid to breakthrough is minimum is fairly well understood; (2) Various dissolution patterns can be created by different acid injection rates and acid types; (3) Most experimental studies are limited to the core scale and numerical simulation is essential for addressing scaling up to the field. Here we present a hydro-mechanical-reactive flow phase field model for realistic acidizing operations. A fixed stress algorithm is used where displacements, phase-field, pressures and concentrations are solved in a staggered sequence. We employ an enriched Galerkin (EG) method to simulate acidizing in fractured carbonate reservoirs based on a two-scale continuum model for the acid transport. The coupled flow and reactive transport systems are spatially discretized by EG methods; the mechanics by continuous Galerkin finite elements. This model development represents an extension of recent work by Lee, Wheeler, and Wick for thermo-hydro-mechanical propagating fractures.

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#### MS6

## The Ontology of Scale in Mathematical Descriptions of Flow

In this talk, we will explore how scale underpins fundamental notions that form the basis of transport descriptions in porous media, and how inadvertent neglect of this essential factor can undermine predictiveness, particularly in complex environments that deviate significantly from idealized systems. We will briefly review non-equilibrium models and discuss the necessity of non-locality in the conservation of momentum to extend steady-state macroscale formulations to near-steady and unsteady flow regimes. This modeling approach rests on two key observations: first, that time and space are inherently related through the transport equation; and second, that Darcys law, along with

experimentally derived fluid mobility and constitutive relations, is fundamentally based on steady-state conditions. This is true regardless of the experimental method used to measure the constitutive functions: the method can be unsteady, but the estimation is still based on steady-state assumptions. In practice, however, macroscale models are routinely applied to simulate dynamic, unsteady conditions. Consequently, there is a need to upscale local saturation information to a characteristic length scale where the near-steady flow assumption holds scale that can be extracted directly from observations of stable or unstable flows, rather than treated as a fitting parameter.

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#### MS6

#### Pore-Scale Modeling of Geologic Carbon Storage

Pore-scale models, supported by advancement in imaging and computational techniques, have been adopted for characterizing complex multiphase flow processes in porous media. The objective of this study is to leverage lattice Boltzmann simulations and investigate the coupled effect of wettability heterogeneity and pore geometry on the pore-scale dynamics of CO2-brine system applicable to geologic carbon storage. Different pore-scale displacement patterns were characterized by changing the wettability from strongto weak-wet conditions. As the wetting conditions shift from strong drainage to imbibition, a transition from burst events to corner flow was observed. The impact of wettability heterogeneity on the drainage relative permeability, capillary pressure curves has been investigated. The simulation results demonstrated that spatial distribution of wettability controlled CO2 trapped clusters residually trapped during brine flooding.

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#### MS6

## Gas Shielding Effect in Multiphase Reactive Flow in Porous Media

Acid dissolution of carbonate formations is ubiquitous in nature and relevant to many important engineering applications. The dynamics of dissolution reactions are complex and strongly depend on either the flow properties or sample mineralogy and are further complicated by the production of carbon dioxide gas bubbles making the reaction multiphase. Under appropriate pH conditions carbonate dissolution can lead to the formation of CO2 bubbles, which can shield the reactive surface and significantly slow down the overall reaction. In this work we combine physics-based models and machine learning with microfluidics experiments to quantify, at high temporal resolution, the impact that gas shielding effects have on effective reaction rates. We also extract a relationship between the latter and gas saturation. Our findings show good agreement between the experimentally observed relationship and our analytical predictions.

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#### MS6

#### Pore-Scale Modeling of Foam Transport

Foams are dispersions of gas bubbles within a liquid. They often generate in porous and fractured media during coinjection of gas and liquid in the presence of surfactants that stabilize foam bubbles. Since foam viscosity is much higher than the constituent gas and liquid phases, they are used for diverting fluid to less permeable subsurface formations in applications such as enhanced oil recovery or carbon dioxide storage. Pore geometry, thermodynamic conditions, molecular structure and behavior of stabilizing agents such as surfactants or nanoparticles near fluid/fluid or fluid/solid interfaces all affect stability and regeneration of foam in porous media. We have developed and validated a new 2D/3D model for foam propagation that incorporates fundamental mechanisms within the detailed geometry of a porous medium. The foam propagation is modeled using a lattice Boltzmann model that couples the momentum equation for liquid flow and the advection-diffusion equation for gas diffusion. To our knowledge, this is the first model with the foam flow driven by pressure gradient in a fractured / porous medium. Depending on the injection conditions, we correctly capture foam bubble wiggling or splitting (into multiple bubbles) through pore throats as compared to the micromodel experiments in literature, and run a series of numerical simulations to quantify the behavior in the parametric space of capillary number and normalized pressure.

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#### MS7

#### Malady: Multiclass Active Learning with Auction Dynamics on Graphs

Active learning enhances the performance of machine learning methods, particularly in low-label rate scenarios, by judiciously selecting a limited number of unlabeled data points for labeling, with the goal of improving the performance of an underlying classifier. In this work, we introduce the Multiclass Active Learning with Auction Dynamics on Graphs (MALADY) algorithm which leverages an auction dynamics technique on similarity graphs for efficient active learning. In particular, the proposed algorithm incorporates an active learning loop using as its underlying semi-supervised procedure an efficient and effective similarity graph-based auction method consisting of upper and lower bound auctions that integrate class size constraints. We also introduce a novel active learning acquisition function that incorporates the dual variable of the auction algorithm to measure the uncertainty in the classifier to prioritize queries near the decision boundaries between different classes. Overall, the proposed method can efficiently obtain accurate results using extremely small labeled sets containing just a few elements per class; this is crucial since labeled data is scarce for many applications. Moreover, the proposed technique can incorporate class size information, which improves accuracy even further. Lastly, using experiments on classification tasks and various data sets, we evaluate the performance of our proposed method and show

that it exceeds that of comparison algorithms.

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#### MS7

#### Weighted Matrix Completion: Applications to Compressive Hyperspectral Imaging

This paper introduces and studies a least-squares weighted matrix completion framework, offering a practical alternative to nuclear norm minimization with significantly lower computational cost and comparable accuracy. We focus on compressive hyperspectral imaging to demonstrate its effectiveness in real-world remote sensing applications. The reconstruction proceeds in a slice-by-slice manner, enabling real-time streaming of pushbroom-acquired data. A key advantage of this framework is its ability to gradually gain prior subspace information as streaming progresses, allowing for improved denoising and reconstruction without requiring prior knowledge at the outset. To address the challenge of parameter tuning during recovery, we incorporate machine learning models trained on NASAs HICO hyperspectral dataset to guide weight selection. We also provide theoretical guarantees, including reconstruction error bounds and sampling complexity requirements. The results establish this approach as a fast, accurate, and theoretically grounded method for large-scale data reconstruction in streaming and remote sensing environments.

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#### MS7

#### Hyperspectral Band Selection via Tensor Low Rankness and Generalized 3DTV

Hyperspectral band selection plays a key role in reducing the high dimensionality of data while maintaining essential details. However, existing band selection methods often encounter challenges, such as high memory consumption, the need for data matricization that disrupts inherent data structures, and difficulties in preserving crucial spatialspectral relationships. To address these challenges, we propose a tensor-based band selection model using Generalized 3D Total Variation (G3DTV), which utilizes the power of L1 norm to promote smoothness across spatial and spectral dimensions. Based on the Alternating Direction Method of Multipliers (ADMM), we develop an efficient hyperspectral band selection algorithm, where the tensor low-rank structure is captured through tensor CUR decomposition, thus significantly improving computational efficiency. Numerical experiments on benchmark datasets have demonstrated that our method outperforms other state-of-the-art approaches.

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#### MS9

#### Methods for Downscaling from Global Climate Scales to Coastal Scales for Risk and Adaptation

Coastal flood hazards have increasingly become a central concern across the planet, as the changing climate and our understanding of it renders our historical knowledge of the risk to life and property increasingly insufficient. The study of future risk to coastal flooding requires input from a host of climate models, a robust way to evaluate future storm and sea-level rise scenarios, and in-depth knowledge of the local environments, especially in urban settings. Methods for tackling this problem must run over large ensembles, represent complex physics, and handle the inherent uncertainties. This talk will outline some of these challenges and ways we are attempting to address these issues through both mathematical and computational approaches with a focus on multiple modeling and data approaches are integrated to solve these complex problems.

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#### MS9

## Advancing Continential-Scale Hydrologic Modeling: the National Hydrology AI Digital Twin

Understanding water availability, predicting droughts and floods, requires a top-to-bottom accounting of the water cycle from treetops to bedrock. Groundwater supports half the global population, 60% of crop production, and a wide array of ecosystems. Yet, it is so sparsely observed that it cannot be simulated solved by data-driven statistical or machine-learning approaches. This limitation can be addressed with physics based models at great computational costs. We lack high fidelity physically accurate models that capture the entire hydrologic cycle. The CONUS2.1 platform is a high-resolution, physically-based models that couple surface and subsurface hydrology, enabling the simulation of complex processes such as groundwater-surface water interactions, evapotranspiration, and land-atmosphere feedbacks. We are evolving this platform into the first digital twin of the terrestrial hydrologic cycle across the United States. This model is continuously updated and improved with new information from remote sensing products and gauge observations. This platform is based on the ParFlow integrated hydrology model and is accelerated by modern solution techniques, excellent code architecture and a dedicated development community. In addition to presenting the digital twin, this talk will focus on a number of recent advancements that leverage GPU acceleration, machine learning emulation and dynamic downscaling of physical processes to accelerate this platform.

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#### MS9

## The Most Efficient N-split Second-order Operator-splitting Methods

Operator-splitting methods are widely used for the time integration of differential equations, especially those that arise from multiscale or multiphysics models, because a monolithic approach may be inefficient or even infeasible. By far, the most common operator-splitting methods have been derived for N=2 operators. Only two OS methods are known for the general case of N operators: the Lie-Trotter (or Godunov) and Strang (Strang-Marchuk) methods. In this talk, we enumerate all N-split second-order operator-splitting methods that are the most efficient in terms of sub-integrations. We derive a conjugate pair of complex-valued OS methods that can be interpreted as a composition of the Lie-Trotter method that we call the complex Lie-Trotter method. We also construct a new oneparameter family of second-order N-split methods with strictly real coefficients (for which Strang is a special case) as well as sets of conjugate pairs of complex-valued secondorder N-split methods that consist of Strang and complex Lie-Trotter methods. These methods can be further used as building blocks to obtain third-order methods through composition and represent the only known third-order Nsplit operator-splitting methods with positive real parts; indeed such methods are not possible with strictly real coefficients. We report on the performance improvements of these methods relative to standard implementations on benchmark problems from geophysics.

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#### MS9

#### Coupling MFEM with Structured AMR Software Libraries for Geophysical Multiphysics Simulations

Modern geophysics simulations can involve solving two or more models that capture subsets of the overall set of physical processes. Each model can have different unknown fields (e.g., momentum vs velocity) and different discretization approaches (e.g., structured vs unstructured meshing). Toward the goal of enabling the simulation of atmosphere flow on a structured mesh driving wind turbine stress on an unstructured mesh, recent developments have been made in the MFEM library to support coupling with structured mesh libraries. One such feature is the ability to transfer fields between the element-based adaptive mesh refinement framework in MFEM and the patched-based AMR framework in structured mesh libraries. Another feature is the generalization of the 2:1 AMR capability in MFEM to support the N:1 refinement common in structured mesh libraries. Results coupling MFEM with the PISALE library will be presented, with results for other structured mesh libraries possible. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-2005423.

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#### **MS10**

# A Finite Volume Method for Elastic Wave Propagation in Fractured Media with Fracture Contact Mechanics

Numerical modeling of elastic wave propagation is important for subsurface applications such as geothermal energy production, CO2 storage and wastewater disposal. We consider the problem of elastic wave propagation in fractured media, where the medium is modeled using a mixeddimensional discrete fracture-matrix approach. Fracture deformation is governed by a Coulomb friction law for fault slip, and a non-penetration condition which prevents the fracture surfaces from intersecting. We discretize the elastic wave equation in space using the cell-centered finite volume Multi-Point Stress Approximation with weak symmetry, which is a geometrically flexible and locally conservative method well-suited for handling anisotropies, heterogeneities and fractures. For time discretization, we use the Newmark method, and to minimize artificial boundary reflections, we apply first order absorbing boundary conditions. We present results from numerical simulations in both two and three dimensions for fractured, heterogeneous and anisotropic media. These results highlight the methods capability to model wave propagation and fracture deformation within complex geological structures such as anisotropic and heterogeneous rock.

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#### **MS11**

Integrated Groundwater Flow and Saltwater Intrusion Modeling Using Machine Learning and Airborne Electromagnetic Resistivity in the Mississippi River Valley Alluvial Aquifer

This study presents an integrated, two-way coupled groundwater flow and saltwater intrusion modeling framework for the Mississippi River Valley Alluvial Aquifer (MRVA), developed through the novel integration of Airborne Electromagnetic (AEM) resistivity data, borehole logs, and water samples using machine learning to en-

hance the understanding of groundwater dynamics. A high-resolution MODFLOW 6 model was developed for the entire Mississippi Embayment Aquifer System (MEAS), reducing uncertainty in boundary conditions while enabling detailed simulations within the MRVA, guided by machine learningsupported data integration. The coupled flow and solute transport model incorporates variable-density flow to simulate the upconing of deep saline water driven by increased groundwater withdrawals. Aguifer characteristics were delineated using hierarchical clustering and cokriging of AEM resistivity and borehole data, transforming discrete measurements into spatially continuous hydrogeological zonations. Initial chloride distributions were derived from AEM and water samples using deep learning algorithms. Model calibration was performed using the Iterative Ensemble Smoother (iES). The model produced risk-based maps highlighting areas vulnerable to saltwater intrusion and groundwater depletion. This integrated approach represents a significant advancement in regionalscale aquifer modeling and provides a robust decisionsupport tool for sustainable groundwater management

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#### **MS11**

Integrated Lithologic, Airborne EM Resistivity, and Groundwater Modeling to Advance Hydrogeological Characterization in the Lower Mississippi-Gulf Region

The coastal lowlands (CLAS) and Mississippi embayment (MEAS) aguifer systems are vital freshwater sources in the Lower Mississippi-Gulf (LMG) region but lack the highresolution subsurface characterization needed for informed groundwater management. This study presents a detailed 3D lithologic model constructed by integrating horizon restoration with indicator kriging, using around 157,000 drillers and 8,400 electrical logs across 14 hydrogeologic units. The model validates airborne EM resistivity data and reveals key hydrostratigraphic features and potential saline sand zones, particularly in Louisiana and eastcentral Arkansas. It also delineates recharge zones, assesses lithology-based MAR suitability, and classifies surface watergroundwater connections based on depth relationships, revealing strong spatial patterns, especially in the Yazoo Basin. Mapping of salinity risk is guided by the distribution of low-resistivity zones, indicating potential upward brine migration, fault leakage, and upconing. To simulate regional flow, an unstructured-grid model was developed using MODFLOW 6 with parallel computing, comprising 9.5 million cells divided into 23 sub-models along HUC watershed boundaries, with inter-model exchange files that preserve hydraulic continuity. This integration of highresolution geologic modeling, salinity assessment, and efficient numerical groundwater flow simulation offers a robust framework for advancing groundwater sustainability in the LMG region.

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#### **MS11**

3D Geostatistical Interval Kriging for Large-Scale Subsurface Characterization of the Mississippi River Valley Alluvial aquifer

The Mississippi River Valley alluvial aquifer (MRVA) in the U.S. is crucial for national food security and global agricultural supply. However, the subsurface structure of the aquifer is still poorly understood. Therefore, developing a high-fidelity 3D hydrostratigraphy of the MRVA is critical for a coherent understanding of subsurface geology to support groundwater studies. The large-scale hvdrostratigraphic model, integrating a sand and fine-grain lithofacies model and a graveliferous top surface model, is built upon more than 73,000 boreholes, including drillers logs, geotechnical logs, and electric logs. This study applies a novel and efficient 3D geostatistical methodinterval krigingto conduct large-scale hydrostratigraphic modeling with big data. Interval kriging is a best linear unbiased estimator for irregular interval supports. Interval kriging considers 3D anisotropies between a horizontal plane and a vertical axis, with the minimized smoothing effect. A novel 3D interval semivariogram is developed. The minimization of estimation variance is regulated with an additional regularization term. The comparison of four geostatistical methodsinterval kriging, 2.5D indicator kriging, 3D indicator kriging, and the MPS algorithm (SNESIM)is conducted. This comparison suggests that interval kriging is an effective and efficient 3D geostatistical method that can capture structural complexity and spatial connectivity while significantly reducing computational time.

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#### **MS11**

Reservoir Capacity and Pressure Response in Multi-Well CO2 Injection: A Numerical Study of the Mokelumne River Formation in Sacramento Basin

In the United States alone over 100 carbon capture and storage projects are pursuing commercial-scale, dedicated CO2 storage in the deep subsurface; multiple of these projects plan to inject into the same reservoir in spatial proximity. In this study, we developed a geological model

for the Sacramento Basins Mokelumne River Formation using public data and performed basin-scale simulations with the open-source GEOS reservoir simulator. We first conducted a parametric study, varying the number of injection wells and injection rate to evaluate the long-term response of the reservoir via average pressure increase and amount of dissolved CO2 in surrounding brine. From this analysis, we derived a closed-form equation to predict those two quantities after extended injection. Next, we assessed pressure interference by operating wells at prescribed injection pressure while varying inter-well distance. While hydraulically connected injection operations can impact injectivity and storage interval pressure, results indicate that it appears feasible to design well spacing and injection schedule to accommodate multi-megaton-per-year injection into the Mokelumne River Formation. However, a thorough assessment of its suitability would require consideration of geomechanical and geochemical effects, which were not evaluated in this analysis. LLNL-ABS-XXXXXX. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 Release Number: LLNL-ABS-2007575

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#### **MS12**

## Simulation of Pore Scale Mineral Reaction Rates in Gas Storage Systems

Mineral reactions can result from introduction of a gas into a porous, subsurface geologic formation for temporary or permanent storage. Such reactions result from gas-fluidmineral interaction at pore scales and impact macroscopic properties (porosity and permeability). Accurate simulation of mineral reaction rates, however, is limited by a poor understanding of mineral reactive surface area its evolution. Mineral accessible surface area, the physical mineral surface area participating in the reaction, is a noted means of improved reactive surface area quantification. Here, a combined imaging, laboratory experimental, and numerical simulation approach is used to enhance understanding, quantification, and predictability of mineral accessible surface area of sandstones. Mineral accessibility and accessible surface area are quantified for samples with varied properties and composition and the impact of pore connectivity, clay coating, and flow conditions on accessible surface area considered. Results indicate accessible surface area is reduced as compared to traditional specific surface area estimations and has some predictability from formation properties. The evolution of accessible mineral surface area is notable different than traditional means of simulating specific surface area evolution. Flow conditions are also important where new observations about the role of flow and reaction regime in controlling mineral accessibility are presented.

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#### MS12

# Assessing the Limits of Direct Pore-Scale Modeling for Dual Permeability/Porosity Systems Using FEM

The interplay between the two different characteristic scales possessed by dual-porosity and dual-permeability systems can create a complex behavior, often related to different physical processes that are dominant in one region versus another which can make modeling a challenge. Various methods have been developed for modeling these systems, such as the Brinkman equation which augments the Darcy's equation for microporosity with traditional fluid mechanics approach for macroporosity. Alternatively, advances in computing and image-based modeling techniques enable direct modeling of multiscale systems, capturing all length scales via direct pore-scale modeling. In this work, we probe the limits of direct modeling of dual-permeability systems using unstructured tetrahedral meshing and the finite element method for fluid flow coupled with stochastic particle tracking for solute transport. Mesh generation performed using open-source and in-house algorithms, emphasize the impressive capabilities of modern mesh generation algorithms for control and adaptation of meshes to geometries from CAD and digital images. Flow validation is performed against analytical results in micro-ducts and complex geometries using grid refinement tests. Results show good accuracy in velocity, even at coarse P2P1 meshes but show a degradation in the microporosity below a critical size ratio. These results help define situations that can be considered for direct modeling of dual-scale porous materials.

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#### MS13

## Accurate Boundary Condition Enforcement in Shifted Boundary Methods

Immersed boundary methods offer a useful alternative to traditional boundary-conforming approaches, particularly for cases with complex geometry. Traditional cell-cutting methods often require specialized quadrature operations and careful management of "small cut-cells." The Shifted Boundary Method (SBM) addresses these challenges by eliminating cut cells altogether, via use of surrogate domains with fully intact elements. The true boundary conditions are shifted onto the location of the surrogate boundary by way of field extension operators constructed with Taylor expansions. Optimal convergence rates have been demonstrated for essential boundary conditions, where the solution and its gradient are readily accessible (in the case of P1 interpolation functions). Shifting Neumann boundary conditions poses additional challenges, as the higherorder terms in the Taylor expansion are unavailable. The aim of this work is to construct an approach that achieves optimal convergence for shifted Neumann boundary conditions without intrusive modification to the computational domain, just as it would with Dirichlet conditions. This is accomplished by introducing extension terms to the variational statement evaluated on the Neumann boundary, which provide approximate integration over the gap between the true and surrogate boundaries. We show how these modifications provide a stable and accurate scheme for embedded finite element computation involving Neumann boundary conditions.

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#### MS13

#### A Fast and Accurate Hybrid Numerical Method to Incorporate Non-uniform Mixing in Porous Media Flows During Shear-thinning Polymer Flooding

We will present a fast and accurate hybrid numerical method for modeling flows of shear-thinning polymers in porous media. It is usually assumed that the polymer is uniformly mixed in the aqueous phase in space and time. However, this is rarely the case after an initial period of flow through the porous media. Even though there does not exist any theory of how the non-uniformity in mixing develops in time and space, we propose a modeling approach to include initial non-uniform distribution of polymer in the aqueous phase. We perform numerical simulations of shear-thinning polymer flooding using a fast and accurate hybrid method [J. Comp. Phys., 335, pp. 249-282, 2017 to evaluate the effect of such non-uniform mixing of shear-thinning polymer [Physics of Fluids, Vol. 35, 046606 (2023)]. We will present results for several levels of non-uniform mixing for two polymers at multiple injection rates and initial polymer concentrations.

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#### **MS13**

Equivalent Polynomials Implementation of Higher-Order Immersed and Embedded Finite Element Methods for Multiphase Flow.

Fluid-fluid and fluid-solid coupling in multiphase flows have distinctly different requirements for numerical discretization methods that make implementation of effective methods for air-water-solid models difficult to achieve. One source of these difficulties arises from the different physics at fluid-solid interfaces and fluid-fluid interfaces. Another is the difficulty of robustly and accurately integrating along

these moving interfaces. The equivalent polynomials technique provided an elegant approach to represent integration of Heaviside and Direct distributions exactly for common cell types cut by moving interfaces. That approach was used recently to implement and extend at CutFEM method developed for the Oseen problem to incompressible fluid-solid interaction problems where the CutFEM method is convenient for enforcing the fluid-solid jump conditions for rigid solids with a stabilized Nitsche method. In this work we extend the approach to include a second incompressible fluid. For the jump conditions between the fluids, the method is convenient as it allows representation of discontinuous viscosity, density, and pressure across the interface without introduction of extra degrees of freedom or ghost penalties that would be required by a Nitsche method. We present details of the complete three-phase method and application to granular media.

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#### **MS13**

## Fast Methods for Shear-Induced Droplet Formation in Co-Flowing Fluids.

These surface tension driven phenomena have been deeply explored using interface tracking and interface capturing approaches. For applications with a symmetrical structure of droplet formation, a one-dimensional model with the interface tracking approach is advantageous in terms of computational costs. We consider a one-dimensional model for shear-induced droplets that estimates droplet sizes for an environment with co-flowing fluids. The presented model is derived using asymptotic expansion and a front-tracking method to simulate the droplet interface. The model is then discretized using the Galerkin finite element method in the mixed form. However, the jumps in the solution gradients are discontinuous and can grow faster due to the highly convective pinch-off process. This leads to an erroneous droplet interface and incorrect curvature. Therefore, the mesh must be sufficiently refined to capture the interface accurately. The mixed form of the governing equation naturally provides smooth interface gradients that can be used to compute the error estimate. The computed error estimate is then used to drive the adaptive mesh algorithm.

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#### MS15

## Recent Results in Parameter Reconstruction for Nonlinear PDEs

In this talk, we will discuss several recent results in the analysis of parameter reconstruction algorithms for nonlinear PDEs. In particular, we will introduce several related algorithms and present some unifying principles for their convergence analyses.

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#### **MS15**

## Equation Discovery Via Continuous Data Assimilation

We demonstrate an equation discovery/model identification method which relies on near-continuous partial observations of the state of the system in question. Not only is the method relatively easy to implement (and even derive), but it is rigorously justified under certain reasonable assumptions in finite dimensional systems. The utility of this method is shown via several numerical examples, and a sketch of the rigorous justification will be provided.

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#### **MS16**

## Including Nonlinear Behavior in Sph Fluid Structures Interaction Models

Characterizing fluid-solid interactions has been a grand challenge in physical, numerical, and cyber-physical simulations. Coastal engineering problems are representative of the mathematical challenge to integrate a precise alignment of physical laws and numerical simulation methods for two-way fluid-structure interaction (FSI). These problems have a critical time-dependent nature often neglected when characterizing the response of fluid-soil-foundationstructure interactions under currents and waves. The performance of numerical tools to model solid or fluid behavior falls short of capturing the combined nonlinear behavior of the different components of the FSI system. To accurately account for two-way FSI while considering the progressive structural loss of resistance, it is necessary to implement, calibrate, and validate an algorithm capable of representing the mechanical non-linear behavior of common civil engineering materials. This algorithm is currently being implemented into DualSPHysics, a particle-based open-source software that uses the SPH method to solve the Navier-Stokes equations. By integrating constitutive laws that capture progressive damage and cumulative effects beyond the elastic limit, this work aims to improve the assessment of structural durability and behavior under cyclic and dynamic loading. After calibration and validation using data recorded during an experimental campaign, the algorithm will be used to train machine learning models for cyberphysical simulations. It will also be made available to the DualSPHysics community, ultimately enabling the efficient design of resilient coastal infrastructure against natural disasters.

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#### **MS17**

#### Controlling Irrigation in a Unsaturated Flow Framework by Physics Informed Neural Networks

We propose a PINN architecture with a Chebychev-type loss function to solve an optimal control problem related to Richards' equation in a 2D spatial domain. This approach would provide a theoretical framework to optimize irrigation according to crop needs and soil hydraulic properties. We also discuss convergence results relative to the

Gradient Descent method, showing numerical evidence of such a method applied to different soil settings.

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#### **MS17**

# Standards-Based Model Interoperability Framework to Enhance Collaboration and Speed Development

Interoperable performant models expand prediction capabilities and take advantage of domain science expertise. However, identification of performant coupled models requires evaluations in a controlled testing environment. Differences in model structure and input requirements impede interoperability and make fair inter-comparison difficult. Together with other federal partners, the NOAA/NWS, Office of Water Prediction has embarked the Next Generation Water Resources Modeling Framework (NextGen Framework). The Framework uses the Basic Model Interface (BMI) for model coupling. It also uses the OGC Water ML (v2.0) Hydrologic Features (HY\_Features) conceptual data model to describe hydrogeomorphology. Hydro-relevant land features in this conceptual data model include catchment boundaries, one- or two-dimensional "flowlines", twoor three-dimensional "water bodies", and connectors between these features called "nexuses". Models that expose variables and operation through the BMI and use the HY\_Features data model to derive their network properties (topology) and inputs (georeferenced physiography to estimate parameters) are compatible with the NextGen Framework. The Framework also includes a BMI forcing engine and regridder to provide forcing inputs to models. Domain science model developers are free to apply their own internal discretizations and solvers. This presentation provides example use cases and an update on the status of NextGen Framework development.

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#### **MS17**

## Perspectives of Algebraic Multigrid Methods for Handling Water Flow Models in Porous Media

We present a scalable, GPU-accelerated framework coupling finite-volume discretization with Algebraic Multigrid (AMG) solvers to quantify uncertainty in steady groundwater flow governed by

$$\nabla \cdot (K(\mathbf{x}) \, \nabla h(\mathbf{x})) = Q \, \delta(\mathbf{x})$$

in randomly heterogeneous porous media. Log-conductivity  $K(\mathbf{x}) = \exp(Y(\mathbf{x}))$  is modeled as a Gaussian random field with prescribed variance and correlation length. For each Monte Carlo realization, the resulting sparse linear system is solved using AMG preconditioners

with different coarsening strategies (PMIS, aggressive aggregation) and smoothers (Chebyshev, Jacobi-L1, Gauss-Seidel). We compare two Dirac-regularizations (smoothed 4-point cosine and Gaussian-like kernels) and evaluate convergence via  $L_2$ -error and mean absolute error across mesh refinements. Three case studies (moderate, low, and high variance) demonstrate that AMG with PMIS coarsening and Chebyshev smoothing, combined with the 4-point cosine source regularization, achieves the fastest convergence and lowest error. Statistical moments (mean, variance, skewness, kurtosis) of the hydraulic head stabilize within 400 realizations for moderate heterogeneity and within 100 for low variability. Our results indicate that AMG-based solvers enable efficient, high-fidelity uncertainty quantification in groundwater flow, laying the groundwork for realtime inversion and hydrogeophysical data assimilation.

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#### **MS17**

## Multiphase Modeling Across Spatial Scales: A Community-Driven Approach

Multiphase flow in porous media is governed by complex interactions at the pore scale, yet traditional macroscale models fail to explicitly capture interfacial behavior know to be important at the microscale. As a result, traditional models rely on empirical closure relations that are highly nonlinear and hysteretic. The thermodynamically constrained averaging theory (TCAT) has been used to formulate a model that is consistent between the microscale and the macroscale and closed using theoretically based evolution and state equations. We advance a communitydriven macroscale model that approximates the solution of the TCAT two-phase model. We present a suite of benchmark problems designed to rigorously test and compare macroscale multiphase flow models. These test problems are designed to evaluate the limitations of existing models, identify knowledge and modeling gaps, and support iterative model improvement. By providing a shared platform for code verification and model validation, we aim to accelerate the development of the next-generation macroscale models that more fully resolves the inherent complexity of multiphase flow in porous media.

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#### **MS18**

# A Semi-Discrete Lagrangian-Eulerian Approach with Enhanced Generalized Multiscale Finite Elements for Three-Phase Flows in High-Contrast Multiscale Porous Media

In this work, we will discuss how integrating a novel class of semi-discrete Lagrangian-Eulerian Schemes subject to a new weak CFL stability condition with enhanced generalized multiscale finite elements for two-phase flow and threephase flow simulations in high-contrast multiscale porous media. No dimensional splitting technique is employed. In the case of multidimensional hyperbolic systems of conservation laws, we also show that the Lagrangian-Eulerian scheme also satisfies the weak version of the positivity principle proposed by P. Lax and X.-D. Liu. We also found a connection between some of the results of A. Bressan, in the context of local existence and continuous dependence for discontinuous ODEs and the no-flow curves (now also viewed as a forward vector field with locally bounded variation). We review computational strategies aiming to solve multiscale nonlinear coupled model reduction in highcontrast porous media environments, presenting an innovative semi-discrete Lagrangian-Eulerian approach for the hyperbolic-transport subproblem and discussing a novel design, proof-of-concept GMsFEM approach, for the elliptic pressure-velocity-flow subproblem. Numerical experiments are undertaken to evaluate the performance of features of the proposed integrated multiscale method. If time allows, we will also briefly present some preliminary numerical results for the Lagrangian-Eulerian approach in the context of high-performance parallel computing via a MPI environment.

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#### MS18

#### Model Order Reduction of Seismic Applications via the Laplace Transform

In this talk we propose a model order reduction approach to speed up the computation of seismograms for different model parameters. This is highly relevant for seismic applications such as full waveform inversion, seismic tomography, or monitoring tools of seismicity that are computationally challenging as the discretized (forward) model has often a huge number of unknowns and needs to be solved many times for different model parameters. Our approach achieves a reduction of the unknowns by a factor of ap-

proximately 1000 for various numerical experiments for a 2D subsurface model of Groningen, the Netherlands. Moreover, when using multiple cores to construct the reduced model we can approximate the (time domain) seismogram in a lower wall clock time than an implicit Newmark-beta method. To realize this reduction, we exploit the fact that seismograms are low-pass filtered for the observed seismic events. Therefore, we consider the Laplace-transformed problem in the frequency domain and restrict ourselves to the frequency range of interest thus avoiding the high frequencies that would require many reduced basis functions to reach the desired accuracy. Instead, we can prove for our ansatz that for a fixed subsurface model the reduced order approximation converges exponentially fast in the frequency range of interest in the Laplace domain.

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#### **MS18**

## Stable Localized Orthogonal Decomposition in Raviart-Thomas Spaces

In this talk, we discuss a computational multiscale method for the mixed formulation of a second-order linear elliptic equation subject to a homogeneous Neumann boundary condition, based on a stable localized orthogonal decomposition (LOD) in Raviart-Thomas finite element spaces. In the spirit of numerical homogenization, the construction provides low-dimensional coarse approximation spaces that incorporate fine-scale information from the heterogeneous coefficients by solving local patch problems on a fine mesh. The resulting numerical scheme is accompanied by a rigorous error analysis, and it is applicable beyond periodicity and scale-separation.

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#### **MS19**

#### Advancing Fluvial Geomorphology Research Through Ai-Enhanced Multi-Physics Modeling and Autonomous Systems

The evolution of rivers, lakes, and reservoirs drives complex responses in hydrodynamics, sediment transport, and ecosystem services. To improve predictive capabilities, my research integrates hybrid deep learning models with multiphysics simulations, supported by autonomous field platforms. I develop Computational Fluid Dynamics (CFD) models utilizing Large Eddy Simulation (LES) and Detached Eddy Simulation (DES) to resolve interactions between anisotropic turbulence, sediment dynamics, and morphodynamic processes. These high-fidelity models enhance the development of reduced-order solvers for sed-

iment transport and riverbed evolution. Field data collection is accelerated through the deployment of intelligent autonomous systems, including self-driving boats equipped for underwater mapping, significantly increasing sampling efficiency and spatial coverage. Future efforts will integrate real-time data from Unmanned Aerial Systems (UAS) and robotic platforms with adaptive AI models such as Long Short-Term Memory networks (LSTMs), Transformers, Generative AI, and Knowledge-Augmented Neural Solvers (KANS). This research advances real-time flood risk assessment, sediment transport forecasting, and riverine system management. By fusing physics-based and AI-driven approaches, it lays the foundation for adaptive, self-learning Earth system models capable of perceiving and reasoning across complex geomorphologic environments.

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#### **MS19**

#### Modeling the Growth of a Vegetated River Delta

Understanding how young, fluvially dominated deltas grow is a key step in predicting fine-grained sediment capture at coastlines and developing engineering solutions to enhance coastal resilience. A network of channels spaced by vegetated inter-channel embayments or islands conveys flow and sediment on the delta top. These islands trap sediment and sustain the production of organic mud through plant senescence. However, integrating vegetation progression, sediment trapping, and organic mud production in models of delta morphodynamics remains an open problem. We build upon an existing one-dimensional framework of river delta growth that explicitly accounts for channel formation and development to model vegetation dynamics and sediment trapping on islands and embayments. We initially focus on a single species with variable density across the delta top. Vegetation density is set to vary with inundation frequency based on field data collected along the Louisiana coast and is limited by plant mortality. Sediment capture is then modeled as a function of vegetation density. In this way, vegetation progression also causes a change in fine sediment deposition rate on the delta top with a consequent impact on the geometry of the delta. Modeling island colonization by multiple vegetation types is a future goal to develop a tool that can help with a variety of applications that include predicting ecological succession and the long-term sequestration of carbon.

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#### **MS19**

## Modeling Changes in Sand Transport Along the Middle Mississippi River

Understanding changes in sand transport along the Mississippi River is important for comprehending the geomorphological processes that shape the river and sustain its

delta. To enhance our understanding of the changes in sand transport along the middle Mississippi River (MMR), I developed two one-dimensional hydrodynamic models. The first model represents a less engineered river channel circa 1900 and the second model represents the highly engineered present-day channel. These models were used to parameterize the Engelund and Hansen total load transport equation to estimate sand transport capacity of the MMR for these reference conditions. Since 1950, the decadal average suspended sand loads have ranged from 12 to 26 MT/yr-1, with the present-day load (2010s) estimated to be approximately 15 MT/yr-1. The modeled sediment-transport capacity for the entire MMR averaged around 18 MT/yr-1 for present-day conditions and about 9 MT/yr-1 for historic conditions. The difference in average sediment-transport capacity is attributed to river engineering efforts that focused flow into a narrower and deeper single-thread channel (60%) and changes in river flows (40%). These findings indicate that 20th-century river-channel engineering and changes in river flows have substantially enhanced the sand-transport capacity through the MMR.

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#### MS20

#### Nonlinear Reduced Order Probabilistic Emulation for High-Dimensional Thermospheric Density Using SINDYc

This work demonstrates the first successful application of SINDYca framework for the sparse identification of governing equations in nonlinear dynamical systems with controlto modeling thermospheric density. It also marks the first use of SINDYc on a high-dimensional system, significantly exceeding the complexity of prior applications in the literature and highlighting its practical and scientific value. The model is developed in a data-driven framework based on the TIE-GCM model for the Thermosphere-Ionosphere system. The analysis covers altitudes ranging from 100 km to 450 km. The thermospheric density state is represented by a tensor  $\rho(t) \in \mathbb{R}^{24 \times 20 \times 16} \sim \mathbb{R}^{7680}$ , and dynamical modeling with SINDYc is performed in a reducedorder space obtained via SVD of the original state. Building upon previous Dynamic Mode Decomposition (DMDc) approaches with nonlinear inputs, we show that SINDYc outperforms DMDc by over 70% during geomagnetic storm conditions, such as the October 30, 2003 event. Moreover, the SINDYc model accurately tracks the dynamical evolution of the density state, matching or exceeding the fidelity of current operational models along the CHAMP satellite trajectory during the Halloween storm. The framework's seamless transition between discrete and continuous formulations further underscores its versatility, making this advancement significant for both scientific exploration and operational applications.

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#### MS20

#### Neural Network Approaches for High-Dimensional Optimal Control and Transport Problems

We present neural network approaches for highdimensional optimal control and optimal transport problems. The Neural-HJB method approximates optimal policies, enabling real-time control while alleviating the computational burden of traditional approaches. Similarly, the COT-Flow method applies DNNs to solve dynamic conditional optimal transport problems, which is critical for applications like sampling and density estimation in Bayesian inference. Empirical results highlight the effectiveness of both methods, showcasing their performance compared to state-of-the-art alternatives.

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#### **MS21**

## Estimating High-Dimensional Covariance Matrices with Hierarchical Rank Structure

Ensemble data assimilation relies on a sample-based estimate for the prior covariance matrix associated with forecasting the evolution of a high-dimensional dynamical system. Practical constraints on the ensemble size mean that this covariance matrix must usually be estimated from a number of samples which is far less than the system dimension. To address this problem, it is common to reduce sampling error by forming a covariance estimate that is spatially localized. This talk will instead present techniques for computing high-dimensional covariance estimates that are hierarchically rank structured. Whereas spatial localization assumes that long-range correlations are near-zero, hierarchical rank structure corresponds roughly to the situation where long-range correlations vary more smoothly than short-range ones. We will begin the talk by investigating, from both theoretical and empirical perspectives, the circumstances under which this type of structure arises. We will then present theory and algorithms which show how to estimate a high-dimensional, hierarchically rank structured covariance matrix from limited samples. Through numerical experiments with a variety of dynamical systems, we will demonstrate that these techniques are effective at reducing sampling errors in the covariance.

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#### **MS21**

## Estimating Cloud Parameters with Ensemble Conjugate Transform Inversion Methods

One of the major challenges in cloud and precipitation modeling is the presence of bounded quantities. For example, precipitation amounts are inherently non-negative and often exhibit highly skewed distributions near their lower bounds. Similar constraints apply to cloud microphysical parameters, which govern the evolution of cloud processes in Earth system models. As a result, parameter estimation methods based on linear/Gaussian assumptions frequently struggle to accurately calibrate these microphysical param-

eters from cloud-sensitive observations. In this talk, we investigate the feasibility of a newly developed inversion algorithm the Ensemble Conjugate Transform Inversion (ECTI) for estimating microphysical parameters within a column cloud model. ECTI builds on a recent generalization of Kalman filter theory to non-Gaussian distributions (Chipilski 2025: https://doi.org/10.1175/JAS-D-24-0171.1) and leverages invertible transport maps. We will highlight the advantages of ECTI implementations that incorporate normalizing flows, a class of generative AI methods, and compare their performance against the benchmark Ensemble Kalman Inversion (EKI) as well as other nonlinear generalizations.

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#### MS21

#### Simple and Sophisticated Localization for Ensemble-based Data Assimilation

Covariance estimation is a key step in ensemble-based data assimilation, such as the ensemble Kalman filter (EnKF). In geophysical applications, where state spaces are highdimensional and sample sizes are small, the sample covariance is known to be a poor estimator, and the EnKF can be sensitive to these covariance estimates. Covariance localization is implemented to address this issue, modifying the sample covariance by tapering covariances as a function of distance. Traditional localization is often implemented via a compactly-supported correlation function of a single length scale which tapers long-range correlations that are assumed to be spurious. While this method of localization is widely successful, with the increase in observations, more complex models, and additional computational power, one may ask whether localization should also become more sophisticated. In this talk, we carefully explore this issue. We compare various covariance localization techniques, ranging from simple to sophisticated to statistical in the cycling EnKF on test problems of moderate complexity. Our experiments show that traditional, distance-based localization leads to a massive error reduction. More sophisticated schemes can lead to additional error reduction, though the impacts are only marginal, if any at all. These results confirm existing linear, non-cycling theory and suggest that sophisticated localization schemes may not lead to drastic improvements over simpler approaches.

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#### MS21

## On the Inadequacy of Nudging for Non-Dissipative Systems $\,$

In this talk, we investigate the performance of the

AzouaniOlsonTiti nudging algorithm for continuous data assimilation when applied to non-dissipative dynamical systems. We focus on three dynamical systems: the 2D incompressible Euler equations, the classical Kortewegde Vries (KdV) equation in 1D, and a partially dissipative variant of the Lorenz 1963 system. We demonstrate that the absence of the finite determining Fourier modes property leads to the existence of infinitely many solutions that are indistinguishable from a limited set of observations for all three of the systems we consider. Our computational study confirms that while the AOT algorithm recovers solutions accurately for the damped and driven KdV equation, it fails for non-dissipative and partially dissipative regimes. These results highlight fundamental limitations in the application of nudging for systems lacking inherent dissipativity, motivating the need for alternative data assimilation strategies in such contexts.

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#### **MS23**

## Operator Learning for Multiphysics Coastal Hydrodynamics

The Shallow Water Equations (SWE) is a set of nonlinear conservation laws that describe the large-scale physics of a fluid layer and have proved useful in predicting the behavior of fluids in the atmosphere, oceans, rivers, and estuaries. Hence, accurate real-time forecasting of hydrodynamic processes in these physical systems under a variety of flow conditions is essential for infrastructure planning and forecasting natural hazards. We introduce the Multiple-Input Temporal Operator Network (MITONet) [1], a novel autoregressive neural operator framework that can efficiently emulate high-dimensional numerical solvers for complex, nonlinear systems, described by time-dependent, parameterized PDEs. Although the MITONet framework is problem-agnostic, we showcase its capabilities by forecasting the evolution of two real-world flow problems governed by the two-dimensional, depth-averaged SWE. These examples represent (a) regional, multi-driver coastal dynamics and (b) natural inflow-induced riverine hydrodynamics with variable initial conditions, boundary conditions, and domain parameters. We discuss MITONet's longterm forecasting and generalization capabilities as well as the potential to extend to multi-physics applications. [1] Rivera-Casillas, P., Dutta, S., Cai, S. et al., 2025. A Neural Operator-Based Emulator for Regional Shallow Water Dynamics. arXiv preprint arXiv:2502.14782.

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#### MS23

# Differentiable Modeling for Computational Hydrodynamics: Bridging Physics-Based and Data-Driven Modeling

Physics-based modeling and data-driven modeling are the two major approaches for modeling in science and engineering. Traditionally, computational hydraulics models numerically solve the governing partial differential equations. Data-driven approach uses data, which embed the physics, and learn system dynamics. Recently, the combination of both physics-based and data-driven modeling approaches has gained increasing popularity due to the rapid development of machine learning and artificial intelligence. Among many of the proposed hybrid strategies, differentiable programming has emerged as a very promising path forward. There are several approaches to make a model differentiable, e.g., building a differentiable surrogate or re-writing the model using a differentiable programming language. This presentation will give an overview of these different approaches and then some examples. These examples include parameter inversion and scientific machine learning. One important application is the combination of the shallow water equations (SWEs) and neural networks (NN), termed universal shallow water equations (USWEs). SWEs are the backbone of all hydraulic models such as ADCIRC, AdH, HEC-RAS, and SRH-2D. In USWES, NN replaces part of the governing equation, which is hard to determine, not well understood, or simply unknown. NN learns the unknown parameterization and dynamics from data. Due to the differentiability, the training of NN includes the hydrodynamic solver in the loop.

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#### **MS23**

#### Multi-Dimensional Flood Modeling of An Extreme Rainfall Event in Norway

Public availability of large high-resolution datasets and advancements in computational capabilities have made the use of partial differential equation based numerical models in hydrology an effective tool for predictions of extreme events and management of water supplies. These developments combined with climate change driven increases in extreme hydrologic events, such as flooding, has generated a need for more accurate and informed water management and prediction tools. As a test case Hans, an extreme storm event in 2023, that saw 100-139mm of precipitation over a large interior area of Norway in a short time frame was modeled. To improve future responses and preparation to

these types of events this study aims to create more accurate and informed runoff model based on finite element discretizations of surrogates to the shallow water equations. These surrogates include the Diffusive Wave Approximation, and the multi-dimensional Kinematic Wave Approximation. In the present work, we develop finite element approximations of these shallow water surrogates. Our focus in the development of a model that utilizes the elevation and landcover data for the Nesbyen catchment and precipitation data from the Hans event as input and model data. Focus is given to the validation of the developed approximations utilizing the diffusive wave model, whereas a novel 1D-2D coupled model utilizing the kinematic wave equation is also presented.

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#### MS24

#### Non-Linear Reduced Order Modeling on Manifolds for Fast Reservoir Simulation

Sustainable hydrocarbon production considering a decarbonization paradigm demands complex decision-support strategies involving fast risk assessment and optimal injection-production scheduling. At the core of these decisions is the prediction of reservoir performance, usually done by running computationally demanding complex simulators. As a fast substitute, physics-aware machine learning (ML) techniques have been used to endow data-driven proxy models with features closely related to the ones encountered in nature, especially conservation laws. They can lead to fast, reliable, and interpretable simulations used in many reservoir management workflows. In this talk, I will build upon our recently developed nonlinear manifold deep-learning-based reduced-order modeling framework for fast and reliable proxy for reservoir simulation, especially for C02 sequestration and storage. I will show advances in data-driven model reduction using Physics Informed Neural Nets (PINNs) to heterogeneous stratified saline aquifers, where CO2 migration is governed by highly discontinuous, multi-valued flux functions. I will also show examples of Dynamic Mode Decomposition (DMD) and Operator Inference (OpInf).

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#### **MS24**

Coupled Flow and Geomechanics in Edfm-Type Models: Incorporating Fracture Surface Roughness Effects

We investigate the Embedded Discrete Fracture Model (EDFM) with geomechanical coupling and introduce a novel methodology to incorporate fracture stress sensitivity into flow simulations. Departing from conventional frictional contact models, we integrate the influence of fracture surface roughness using the Barton framework, characterized by the Joint Roughness Coefficient (JRC) and Joint Compressive Strength (JCS). This approach provides a physically motivated regularization for the normal contact stress response and is coupled with a nonlinear hyperbolic law that captures the relationship between normal traction and fracture closure. The resulting formulation enables a more realistic representation of fracture deformation under evolving stress conditions. The proposed EDFM-geomechanics coupling dynamically updates transmissibilities associated with non-neighboring connections to account for variations in overburden stress and pore pressure. This dynamic capability is essential for accurately capturing the influence of stress-induced fracture aperture changes on fluid flow behavior. Numerical simulations of reservoir depletion and CO2 injection are performed to assess the impact of these couplings.

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#### MS25

#### Approximation of Degenerate Parabolic Problems Using Weno Methods

We discuss approximation of the degenerate parabolic PDE  $u_t - \nabla \cdot [D(u)\nabla b(u)] = 0$  using multilevel weighted essentially nonoscillatory (ML-WENO) finite volume discretizations. The solution may exhibit steep fronts, which are difficult to approximate even in one space dimension, since the derivative is essentially a delta function distribution. Finite volume discretizations require a mesh or submesh of spacing  $\delta$ , so the derivative will be approximated by a value that is  $O(1/\delta)$ , independently of the equation being approximated. We present analytical and numerical studies of the problem. We determine the true flux across the steep front, and show that, although the computed flux may be inaccurate, over a few time steps there is little effect on the computed solution. We then present an overall ML-WENO procedure using a modified numerical flux function that gives an accurate approximate function for

both smooth and nearly discontinuous solutions. An analysis of stability and accuracy of the scheme in one space dimension is given.

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#### MS25

# Impact of Portlandite Dissolution on the Self-Healing of Concrete Microfractures by Calcite Precipitation

Water-bearing microfractures in concrete exhibit the ability to heal without additives, leading to the closure of the fracture. Since concrete cracks provide passage for chemical compounds that can lead to the deterioration of the cementitious matrix and reinforcements, this self-healing capability is an important feature, enhancing the durability and longevity of concrete. One of the most important self-healing mechanisms is the precipitation of calcium carbonate. This is the result of an intricate interplay between fluid flow, the concomitant transport of chemical species, and chemical reactions within the fluid and at the fluidsolid interface. We aim to gain a better understanding of the coupled hydraulic and chemical mechanisms underlying self-healing through calcite precipitation. To this end, we have developed a numerical model which simulates the relevant processes within the fracture void space in two dimensions, i.e. along the plane of the fracture. FEniCS is used to solve flow equations (incorporating the cubic law) and transport equations for 6 chemical species, and Reaktoro is used to quantify the chemical equilibrium and mineral kinetic reactions. The simulation results underline the importance of portlandite dissolution as the main driver of calcite precipitation, as it increases calcium concentration and pH, and triggers a shift towards carbonate in the carbonic acid-lime system within the fracture water, leading to pronounced calcite precipitation.

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#### MS25

## Coupled Free Flow and Degenerate Porous Medium Flow

Fluid flow in coupled systems, consisting of a free-flow region and an adjacent porous medium, occurs in a wide range of environmental and industrial applications. In this work, we investigate the mathematical formulation of such systems, modeled by a coupled Stokes-Darcy system with interface conditions governed by the Beavers-Joseph-Saffman law. We specifically address the case where the porosity in the Darcy region vanishes, representing pore clogging phenomena. To handle this degeneracy, we rescale the pressure and velocity with respect to the vanishing porosity, following the framework introduced by Arbogast and Taicher (SIAM J. Numer. Anal., 2016). This approach leads to a transformed Stokes-Darcy system with appropriately rescaled interface conditions. We establish the existence and uniqueness of solutions to the transformed

system by employing the theory of mixed variational problems, suitably adapted to the degenerating porosity and weighted function spaces.

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#### MS25

#### Snow is a (multiscale) Evolving Porous Medium

We consider modeling the metamorphosis of (dry) snow as a mixture of ice and air phases which evolve due to phase change between ice crystals undergoing sublimation and deposition. At the interface scale, our model is a coupled system of (Tp) energy equation for temperature solved in ice and air, and (M) mass conservation for water vapor solved in the air phase only; these are coupled by latent heat terms on the interface. Even though the process is well known, our approach using a parabolic variational inequality for (M) is new and very flexible. It also allows upscaling to Darcy scale and further modeling of snow consolidation. In the talk we will also compare these models to our other results on upscaling heat and flow in ice and liquid in permafrost soils.

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#### MS26

#### Modeling the Impacts of Dam Construction on Channel-Floodplain Dynamics in Andean Rivers

Andean foreland rivers are characterized by high sediment fluxes that drive rapid rates of channel migration, riverfloodplain exchanges, and create diverse floodplain morphologies, however, they represent preferential sites for hydroelectric dam construction. Dams alter fluvial water and sediment supply with expected morphodynamic and environmental impacts over decades to centuries. To study the long-term impacts of dams in Andean rivers, we apply an innovative hydro-morphodynamic model that accounts for flow, sediment transport, and channel-floodplain morphodynamics, including bend migration, dynamic vegetation, and channel abandonment. The model reproduces realistic rates of channel migration, cut-off formation and avulsions similar to observations from Andean Rivers. Our simulations demonstrate that Andean foreland rivers will undergo significant vertical and lateral erosion within less than 100 years following dam construction, with persistent or irreversible effects. This erosion leads to the formation of an entrenched inner secondary floodplain, which diminishes floodplain inundation extent and frequency. Net erosion volume, and associated hydrologic changes, depend on predam river characteristics with highly active rivers before dam construction experiencing the largest changes. Our simulations underscore the significant role of geomorphic channel-floodplain interactions in driving fluvial reorganization and ecological adaptation to dams over centuries.

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#### **MS26**

## Leveraging Exascale Computation for Studying Environmental Hydrodynamics

Computational power of the largest supercomputers in the United States have breached the Exascale, creating an opportunity for studying important riverine and coastal hydrodynamics problems at an unprecedented scale and resolution. In the current talk, first we will present spectral element method (SEM) based computational solver NekRS, that can been used to leverage these modern Exascale supercomputers. Next we will illustrate the usage of the solver through examples from riverine and coastal hydrodynamics. The talk will end with discussing potential future problems that can be explored, facilitating novel insights about the complex turbulent structures.

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#### MS26

## Vegetation-Geomorphology Feedbacks in the Louisiana Coastal Master Plan Model

Changing environmental conditions prompt shifts in coastal vegetation species. The speed of these changes and the resulting vegetation response can be the difference between vegetation death and subsequent land loss or vegetation transition and land maintenance. Since vegetation impacts both sediment and hydrologic processes, including vegetation changes is key to modeling coastal land evolution. We integrate satellite imagery and in-situ observations from the Louisiana Coastwide Reference Monitoring System (CRMS) to initiate and drive vegetation coverage modeling with the Louisiana Vegetation Model (LAVegMod v3). We calculate the coastwide model performance and examine the role of salinity change magnitude and duration on vegetative transitions. LAVegMod is a regional model and a part of the Integrated Compartment Model used to develop the Louisiana Coastal Master Plan. LAVegMod provides feedback that drives changes in organic accretion, impacting the rate of land loss or gain. Capturing the vegetation response to drivers with different temporal scales is important to obtaining accurate predictions of coastal landscapes and allow for more informed policy and management decisions.

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#### **MS26**

Investigation of the Environmental Impact of Annual Sea Level Rise Variability on the Deltaic Landscape Evolution in Estuarine Environments

Traditional deltaic landscape evolution models often simplify sea level rise (SLR) as a smooth curve to represent the impact of long-term increase in sea level. However, annual variability in SLR can significantly impact these dynamic ecosystems. This study employs a computationally efficient biophysical model to investigate the effects of varying SLR scenarios on Barataria Basin, a complex estuarine environment. Simulations were conducted using three smoothed SLR estimates (2m, 1.1m, and 0.6m by 2100) and four additional scenarios incorporating annual variability around each of the smoothed curves. Our findings suggest that Barataria Basin could experience substantial land loss, potentially ranging from 50,000 to 70,000 acres between 2030 and 2070 due to annual variability in SLR. These results underscore the critical need to consider SLR variability in coastal planning and management strategies to mitigate the impacts of rising sea levels.

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#### **MS27**

# The Suitability of the Black Oil PVT Model for Modeling Commercial-Scale CO2 Storage in Saline Aquifers

The SPE 11th Comparative Solution Project (CSP) consisted of three Carbon Capture and Storage (CCS) problems to compare the numerical aspects of different approaches and simulators. Each of the three problems has different facies properties, geometry, and fluid properties. Problem A is a 2D experimental scale problem based on a sandpack experiment and numerical benchmark project under isothermal conditions. Problem B is a scale-up of problem A, with an increase in domain size to typical field values and changes to properties such as permeability, porosity, and capillary pressures to values commonly observed in the North Sea fields, and includes the impact of heat transfer. Finally, Problem C extends Problem B by extruding its geometry in an extra dimension, leading to a complex 3D geometry. The Black-Oil (BO) is a PVT model used to describe the oil and gas phase behavior and is widely used in reservoir simulation models in the oil industry due to its simplicity and more efficient computational cost. In this work, the oil in the BO is replaced by an aqueous phase and the model is extended to account for thermal effects using enthalpy tables and PVT tables for different temperatures. The model is compared to other approaches used in CCS, such as the equilibrium ratios in thermal cases, and gas solubility tables or Henrys law for the isothermal cases. Results demonstrate that the BO model accurately simulates CCS processes while improving numerical results.

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#### **MS27**

## The 11th Society of Petroleum Engineers Comparative Solution Project: Summary Report

The 11th Society of Petroleum Engineers Comparative Solution Project benchmarked simulation tools for geological CO2 storage. A total of 45 groups from leading research institutions and industry across the globe signed up to participate, with 18 ultimately contributing valid results. This talk summarizes the SPE11. A comprehensive introduction and qualitative discussion of the submitted data are provided, together with an overview of online resources for accessing the full depth of data. A global metric for analyzing the relative distance between submissions is proposed and used to conduct a quantitative analysis of the submissions. This analysis attempts to statistically resolve the key aspects influencing the variability between submissions. The study shows that the major qualitative variation between the submitted results is related to thermal effects, dissolution-driven convective mixing, and resolution of facies discontinuities. Moreover, a strong dependence on grid resolution is observed across all three versions of the SPE11. However, our quantitative analysis suggests that the observed variations are predominantly influenced by factors not documented in the technical responses provided by the participants. We therefore identify that unreported variations due to human choices within the process of setting up, conducting, and reporting on the simulations underlying each SPE11 submission are at least as impactful as the computational choices reported.

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#### **MS27**

# Grid Convergence and Triggering of Mixing Dynamics in the 11th Spe Comparative Solution Project

We report on a systematic grid refinement study carried out for Case B from the 11th SPE Comparative Solution Project (SPE11). We assess the convergence behavior of key observables used to compare simulation results across participants. The study is conducted on structured grids using standard discretizations, and includes both global and local metrics relevant for storage security assessment. In the second part of the talk, we investigate how different grid types and flux discretizations affect the simulation of convective mixing beneath the CO2 plume. We find that the onset and strength of dissolution fingers are strongly influenced by local grid geometry and numerical inconsistencies at the interface. These findings highlight the need for careful grid and method selection when modeling fine-scale mixing processes in subsurface CO2 storage.

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#### MS27

## A Sub-grid Model for Convective Mixing Applied to the 11th SPE Comparative Solution Project

Solubility trapping, involving the dissolution of supercritical CO2 into resident brine, is crucial for geological carbon storage. Density-driven convective mixing enhances solubility trapping but is challenging to model in standard reservoir simulations due to its centimeter-scale nature. We present a sub-grid model for convective mixing in geological carbon storage, designed for coarse-grid simulation. This model includes a dynamic partitioning algorithm to relax phase equilibrium assumptions in large cells and an effective transport component to enhance sub-scale unstable flow and transport modeling. The approach is implemented in the Open Porous Media (OPM) Flow simulator and has previously been validated on 2D field-scale geometries in a simple setup. Our study applies this model to the 11th SPE Comparative Solution Project (SPE 11), addressing simulation challenges in CO<sub>2</sub> storage operations within geologically complex settings. The sub-grid model is used in SPE 11B and C, 2D and 3D geometries at realistic operational conditions, showcasing its utility in enhancing CO<sub>2</sub> dissolution estimates and exploring parameter sensitivities for realistic storage projects. The impact of dispersion and grid resolution on convective mixing is discussed. This study improves geological carbon storage project assessments by considering both dispersion and upscaling effects on convective mixing.

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#### MS28

#### Ensemble Score Filter with Image Inpainting for Data Assimilation in Tracking Surface Quasi-Geostrophic Dynamics with Partial Observations

Data assimilation is crucial for understanding and predicting turbulent systems in geoscience and weather forecasting, addressing key challenges such as high dimensionality, nonlinearity, and partial observations. Recent machine learning (ML)-based approaches have shown promising results. In this work, we develop an Ensemble Score Filter (EnSF) that integrates image inpainting to handle partial observations. The EnSF uses a training-free diffusion model to tackle high-dimensional, nonlinear data assimilation problems and has demonstrated strong performance under full observations. However, because it does not model covariances between observed and unobserved variables, extending EnSF to partial observations is nontrivial. To address this, we incorporate image inpainting techniques to predict unobserved states during assimilation. At each filtering step, we first apply the diffusion model to estimate observed states using likelihood-informed score functions, then predict unobserved states via inpainting. We validate the EnSF with inpainting on the Surface Quasi-Geostrophic (SQG) model under various scenarios, demonstrating its potential to advance data assimilation methods for geoscience and weather forecasting applications.

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#### MS30

#### Domain Decomposition for Enhancement of Reduced-Order Models

Decision-support systems for environmental management of coastal areas must account for brine and seawater dynamics. Physics-based models of these phenomena are computationally expensive, which limits their usefulness for decision-making under uncertainty. Data-driven modeling techniques, such as extended dynamic mode decomposition (xDMD), ameliorate these challenges. We demonstrate that xDMD, equipped with a novel domain decomposition component, effectively represents a validated, realworld, coupled nonlinear seawater inundation model. It serves as an efficient surrogate of process-based simulations, capable of accurate reproduction and reconstruction of missing pressure and salinity data in the interpolation regime. It accurately predicts low-rank pressure distributions (repeated dynamics) but struggles to forecast longterm salinity dynamics (cumulative evolution). The addition of domain decomposition improves the robustness and accuracy of xDMD, with the overlapping domain approach outperforming the nonoverlapping one in the projection accuracy. In our experiments, xDMD is 1700 times faster than the process-based model and requires 800 times less storage, while efficiently capturing pressure and salinity dynamics.

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#### MS30

## Modeling Crop Irrigation by Machine Learning Tools

Precision irrigation is a key element for ensuring sustainable water resource management, especially in agricultural contexts where water stress and soil salinity pose significant challenges, thus motivating the interest in deepening the forecast of these variables. This study examines high-frequency soil monitoring data collected from an experimental agricultural site in Gallipoli, Italy, to investigate sustainable irrigation with treated wastewater. The dataset includes measurements taken every 15 minutes from sensors installed at depths of 30 cm and 60 cm, which monitor soil moisture, temperature, and electrical conductivity under various irrigation and fertilization treatments. These time-series data provide the basis for developing predictive models aimed at optimizing irrigation timing and quantities, reducing water consumption, and enhancing resource use efficiency. The research focuses on creating predictive models using both traditional statistical methods, such as the Holt-Winters method, and machine learning techniques. . Traditional univariate time-series mod- els, such as VARIMA, are compared to data-driven approaches for forecasting soil water dynamics up to 72 hours ahead. The temporal analysis addresses key challenges such as dealing with missing data, integrating external variables such as irrigation events, and incorporating physical constraints from soil-water interaction models.

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#### **MS30**

#### Geometric Shallow Water and Diffusive Wave Approximation for Basin Scale Coupled Surface-Subsurface Hydrological Simulations

Shallow water models of geophysical flows must be adapted to geometric characteristics in the presence of a general bottom topography with non-negligible slopes and curvatures, such as mountain landscapes. In this work, we derive an intrinsic formulation for the diffusive wave approximation of the shallow water equations, defined on a local reference frame anchored on the bottom surface. We then derive a numerical discretization by means of a Galerkin finite element scheme intrinsically defined on the bottom surface. We aim to analyze the differences between the diffusive wave approximation and the shallow water model, both defined within a geometrically intrinsic framework and with a focus at the basin scale. Basin scale simulations on synthetic test cases show the importance of taking into full consideration the bottom geometry even for relatively mild and slowly varying curvatures.

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#### **MS30**

#### Domain and Spectral Localization for Square Root Filters and Their Applications

This work develops projection-based localization for the ETKF. An overview of Kalman Filter techniques is presented, and the framework for dimension reduction and localization is then described. Through projections generated by matrices, identifications are made to the inputs of the ETKF algorithm to create a scheme with reductions in dimension. To showcase this generalization of localization, we consider the Lorenz '96 model to generate testing data. We test a domain localization approach, in order to showcase how the scheme can generalize standard Schur product-based localization schemes. In addition, we provide experiments in which the localization is spectral in nature. To do this, we employ a POD-based approach, in which we look at the SVD of a so-called "Snapshot Matrix". Extensive numerical results are given for these two approaches, showcasing various improvements in dimension reduction and accuracy as we change the experimental parameters. The findings highlight the generality of the algorithm, and provide a way to implement other schemes to reduce the dimension of the Kalman Filter.

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#### MS31

Upscaling and Symbolic Deduction: Model Discovery for Multiscale Modeling of Multiphase Flow and Reactive transport in Porous Media through Symbolic-Numeric Software's

Modeling flow and transport in the subsurface continues to be a major open challenge in computational physics since the relevant scales of interest can easily span 10 orders of magnitude. Despite advances in the development of multiscale models, significant challenges remain in the rigorous derivation of continuum models themselves, and their numerical implementation and verification, particularly in presence of systems of realistic complexity. The derivation and numerical implementation of macroscopic models from their fine-scale counterpart through formal upscaling techniques can take many years of concerted efforts between applied mathematicians, modelers and computational physicists to develop. Recent works have shown that symbolic deduction, implemented in a sofware called Symbolica, can be used to augment and boost human deductive capabilities through the automation of rigorous upscaling theories. Allocating to the machine such procedures allows one to speed up the time to derive upscaled equations by 5 orders of magnitude, compared to the same calculations performed by a human. We show some of Symbolicas capabilities in deriving macroscopic equations for multiphase flow and for complex reactive transport problems. We also develop the first fully integrated symbolic-numerical framework to automatically transform the equations generated by Symbolica into numerical codes which can be written and run with minimal human interaction.

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#### MS31

#### Multiscale Finite Element Methods for Advection-Diffusion Problems

The Multiscale Finite Element Method (MsFEM) is a finite element (FE) approach that allows to solve partial differential equations (PDEs) with highly oscillatory coefficients on a coarse mesh, i.e. a mesh with elements of size much larger than the characteristic scale of the heterogeneities. To do so, MsFEMs use pre-computed basis functions, adapted to the differential operator, thereby taking into account the small scales of the problem. We consider here multiscale advection-diffusion problems in the convection-dominated regime. When the PDE contains dominating advection terms, naive FE approximations lead to spurious oscillations, even in the absence of oscillatory coefficients. Stabilization techniques (such as SUPG) are to be adopted. In the multiscale context considered here, we discuss different ways to define the MsFEM basis functions, and how to combine the approach with stabilization-type methods. In particular, we show that methods using suitable bubble functions and Crouzeix-Raviart type boundary conditions for the local problems turn out to be very effective (see [R. Biezemans, C. Le Bris, F. Legoll and A. Lozinski, CMAME 2025]). Joint work with R. Biezemans, C. Le Bris (ENPC and Inria) and A. Lozinski (Univ. Franche-Comte).

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#### MS31

Physics-Preserving Impes Based Multiscale Methods for Immiscible Two-Phase Flow in Highly Heterogeneous Porous Media

In this presentation, we introduce a novel physicspreserving multiscale approach to tackle the challenge of immiscible two-phase flow problems. These are typically described as a coupled system comprising Darcy's law and mass conservation equations. Physics-preserving IMplicit Pressure Explicit Saturation (P-IMPES) scheme, is designed to uphold local mass conservation for both phases while remaining unbiased. Notably, when the time step is kept below a certain threshold, the P-IMPES scheme ensures bounds-preserving saturation for both phases. For velocity updates, we employ the Mixed Generalized Multiscale Finite Element Method (MGMsFEM), a highly efficient solver that operates on a coarse grid to compute unknowns. We adopt an operation splitting technique to manage the complexities of two-phase flow, utilizing an upwind strategy for explicit saturation iteration, while employing the MGMsFEM to compute velocity via a decoupled system on a coarse mesh. To validate the effectiveness and robustness of our proposed method, we conduct a series of comprehensive experiments. Additionally, we provide a rigorous analysis to establish the theoretical underpinnings of the method, which are corroborated by our numerical findings. Both simulations and analysis demonstrate that our approach strikes a favorable balance between accuracy and computational efficiency.

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#### **MS32**

#### Impacts of Gold Mining on River Morphodynamics

The meandering sand-bed Madre de Dios (MDD) River, headwater tributary of the Amazon River located in Peru, is heavily impacted by unregulated alluvial gold mining. Mining activities within the watershed include surface mining in large swaths of the upper mountain slopes, pit mining from the active floodplain, and suction mining on the riverbed. Suction mining dredgers scoop or suction materials directly from the riverbed, removing enormous amounts of gravel that are then redeposited on riverbanks and within channels. The extensive material-moving and removal of vegetation resulting from the mining activities have pushed these river systems to a state of disequilibrium in terms of the physical processes. This study evaluates the alteration of natural migration and hydrodynamic patterns in the MDD river within an impact mining area. Preliminary numerical simulations with a fixed bed show that for higher discharge ( 3000 cms) the hydrodynamic patterns were altered by changes in flow direction and magnitude. These hydrodynamic patterns could increase rates of erosion in the outer bank, and consequently increase the planform migration rate. These results confirm, at least to some extent, the impacts of gold mining in the natural migration process of the MDD River. Additional numeric simulations will focus on improving the representation of mining in the model and perform simulations with bedload and suspended sediment transport.

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#### **MS32**

Oxbow Lake Sediment Flux Driven by Unsteady Establishing Vegetation in Salt Marshes and in

#### Flow

Classic models of neck cutoff evolution depict a relatively rapid transition from active meandering to oxbow lake formation, driven by sediment plug development at the cutoff entrance and exit. However, field observations from a 2014 neck cutoff on the White River (Arkansas, USA) challenge this paradigm. Nearly eleven years post-formation, the cutoff remains hydrologically connected, with ongoing inflow and incomplete sediment plugs at the oxbow-main channel junctions. This geomorphic configuration reflects a prolonged transitional stage characterized by hydraulic bifurcation, sediment bypass, and partial infill a state not fully captured by existing models. Integrating observations from aerial imagery, field datasets, and numerical modeling, we demonstrate that during this stage of oxbow lake disconnection, an intermediate condition between active channel and lacustrine isolation, has important implications for sediment routing, habitat dynamics, and floodplain connectivity. Our findings highlight the role of unsteady flow conditions on fine-grained sediment flux into the oxbow lake and the complex patterns of long-term sedimentation that emerge.

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#### MS32

Hydrodynamic and Inundation Characteristics in the Atchafalaya Basin Under Varying Streamflow and Tidal Conditions for Vegetation Establishment Assessment

Hydrodynamic and geomorphological conditions in active delta systems are governed by various factors, including river inputs, vegetation, and tides. The Wax Lake and Atchafalaya Deltas (WLAD) are located in the Mississippi River Delta and represent actively prograding deltas with expanding vegetation cover. The deltas experience varying flow velocities and inundation patterns in deltaic islands depending on the river stage, storm surges and vegetation roughness. We use a calibrated 2D hydrodynamic model (finite volume method-based solver, named ANUGA) for WLAD under varying river discharge and tidal scenarios to assess inundation times and flood frequencies of deltaic wetlands. The model uses a non-uniform triangular mesh incorporating different land coverages (e.g., open water, swamp, and vegetation), resulting in spatially variable friction coefficients of seasonal vegetation cover (spring and fall). We simulated scenarios with a systematic increase in the river discharge and tidal forcing for the seasonal vegetation coverages, showing a spatially-varying increase in inundation area and flooding periods. The model results are used to compare inundation patterns with results from exploratory delta models to assess model performance and habitat suitability. Future work will focus on the coupling with a dynamic vegetation model of multiple species to explore the feedback between hydrodynamics and vegetation establishment in coastal Louisiana.

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#### MS32

#### Open-source Models

Hydrodynamic models that include a morphology component, such as Delft3D, are used widely for understanding the evolution of coastal systems, and they inform strategies for coastal protection and ecosystem preservation. Vegetation growth is often an important factor in coastal morphology, and even though some models may include vegetation via a roughness parameter, they do not have builtin capabilities for modeling dynamic vegetation processes. In recent years, several biophysical models with coupled dynamic vegetation processes have been developed, but few are open-source and compatible with non-proprietary software, hindering community development. This work presents a simple, open-source Python model that has been coupled dynamically with Delft3D FM to represent colonization, growth, and mortality of multiple species of vegetation in coastal environments. The model includes detailed vegetation processes with colonization and mortality as functions of hydromorphodynamic conditions and species-specific growth curves, resulting in spatial and temporal updates of friction effects in Delft3D FM. The code is designed to prioritize accessibility for all user levels and allow for smooth implementation of additional structures and processes. We present a comparison to previously validated dynamic vegetation models and demonstrate the models adaptability and potential for community development and future coupling with other hydro-morphodynamic models.

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#### MS33

#### Nonlinear Domain Decomposition Preconditioning for Efficient Simulation of Underground Thermal Energy Storage

Underground thermal energy storage (UTES) offers significant potential for large-scale energy storage, such as utilizing waste heat and balancing renewable energy sources like wind and solar power. Thermal subsurface flow exhibits distinctly different temporal scales, from rapid, advection-dominated flow in wellbores and fractures to slow, conduction-dominated flow in solid rock. The governing equations for mass and energy conservation are also strongly coupled due to pressure- and temperaturedependent fluid properties. Therefore, simulation technology for these systems requires robust nonlinear solution strategies that ideally can resolve processes at their intrinsic timescales, especially during abrupt temperature changes in the near-well region at the onset of charging and discharging. The nonlinearities in UTES are mainly localized spatially (in faults/fractures and near wellbores) and temporally (at the onset of charging/discharging). This work demonstrates how we can utilize this by devising nonlinear domain decomposition strategies for rightpreconditioning of Newtons method in the open-source, fully differentiable JutulDarcy simulator. We demonstrate the method on real and realistic UTES scenarios, and discuss how the temporal resolution can be adapted in space and time to achieve high accuracy without compromising performance.

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#### MS33

#### Solving Poroelasticity by Coupling Opm Flow with the Two-Point Stress Finite Volume Method

The interaction between fluid flow and solid mechanics plays an important role in reservoir engineering applications such as CO2 storage, in which large pressure changes are artificially induced. Simulating such systems efficiently and accurately remains a computational challenge, especially on the regional scale. This is partially due to the numerical methods that are historically used for the different physics problems. Finite-volume methods are predominantly chosen for simulating fluid flow whereas the solid mechanics is typically modeled using the finite element method. However, finite elements are not directly applicable to the complex corner-point grids commonly used in reservoir models. As an alternative, the Two-Point Stress Approximation (TPSA) method has recently been proposed as a consistent finite-volume method for solid mechanics. In this talk, we show how the TPSA method can be coupled to a reservoir simulator such as OPM Flow. We highlight the benefits of employing two finite-volume methods on the same grid. In particular, the information passed between the flow and mechanics solvers consists of only one value per cell, without the need for interpolation operators. Moreover, optimized solvers designed for the two-point flux finite-volume method can be reused to efficiently solve the TPSA system. Different coupling techniques are discussed, and we demonstrate the applicability of the method through several case studies on the regional

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#### MS33

#### An Optimal Stabilization Strategy for Gibbs and Saddle-point Oscillations Relevant to Subsurface Applications

This work investigates numerical instabilities in subsurface simulations using piecewise linear interpolation on tetrahedral grids. We apply the Physical Influence Scheme (PIS) to derive stabilization terms for mean stress and pore pressure fields, effectively eliminating both Gibbs and saddle-point instabilities. Linear elasticity and poroelasticity models are solved using primal and mixed formulations, with emphasis on different stabilization strategies. A key focus is on the element characteristic length, h, which appears in the stabilization terms. We propose interpreting has a quantity used to approximate the Laplacian of a general function, and compute it by solving an optimization problem per element. To reduce the associated computational cost, a machine learning model is introduced to predict the optimal h. Results show that for linear elasticity, mean stress oscillations arise not only in nearly incompressible cases (saddle-point) but also in regions with sharp gradients (Gibbs). The proposed stabilization removes both. Similar improvements are observed in poroelasticity problems, where pressure oscillations are also mitigated. Comparison with other common calculation of the characteristic length, the proposed optimized h ensures just enough numerical diffusion to stabilize the solution without sacrificing accuracy.

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#### MS33

## Vertically Integrated Modelling of Stress Sensitive Fault Leakage

Vertical CO2 migration along faults is a risk in geological carbon storage operations. During the development of a storage site this risk must be thoroughly understood and quantified. Appropriate mitigation strategies must also be developed. Leakage along faults is dominated by the fracture networks within the fault damage zone. The properties of those fracture networks including those that impact flow are difficult to constrain with data and are highly sensitive to stress conditions. Here, we present a vertically integrated modelling framework that accounts for vertical migration along faults through a stress dependent source term and an adapted transmissibility across the fault. The framework is physically consistent and supported by fine-scale simulations of representative scenarios. We discuss implementation details, physical implications of the capillary barrier, and its stress sensitivity. We then illustrate the application of the method to identify representative scenarios and quantify uncertainty in a Monte Carlo approach thanks to the computational efficiency of the method.

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#### MS34

Gaussian Process Emulator for Modeling and Pre-

#### diction of Mosquito Population

Dengue, one of the most rapidly spreading diseases in the world, is predominantly carried by the Aedes aegypti mosquito. Hence, having a digital twin that emulates the dynamics of the mosquito population is of paramount importance for the development of appropriate strategies and public policy to control the dengue epidemic. To address this need, we employ a data-driven Gaussian process (GP) framework that respects the natural physical constraints as a surrogate to forecast and model the evolution of the mosquito population. This framework leverages output transformation and variational inference to ensure physical admissibility of the population variable. It also employs statistical learning and model discovery algorithms to identify GP structures that achieve metric-based optimal fitting or prediction of the measured population data under different environmental conditions. The proposed framework can be applied and extended to a wide range of biological systems, paving the way for uncertainty-informed decision making and real-time data generation.

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#### **MS34**

## Digital Twins for Investigating Co2 Storage Capacity in Composite Confining System

Assuring secure containment of stored CO2 is of paramount importance for climate change mitigation. Regional seals, such as those sealing petroleum accumulations, have proven to be effective for securing CO2. However, the goal of permanent sequestration can also be satisfied with composite confining systems consisting of multiple, possibly discontinuous flow barriers that, in aggregate, create a system with very high permeability anisotropy and effectively retard the vertical migration of CO2. This study focuses on investigating various barrier characteristics necessary for effective containment of CO2, by developing digital twins for physical flow experiments. There are three stages: (1) emulate, via training machine learning models with modified invasion percolation simulations, the fluid flow dynamics of the experiments in tank-scale synthetic domains; (2) determine the sensitivity of quantities of interest (such as CO2 leakage rate, leakage volume, storage capacity) to the parameters that characterize the effective barriers within composite confining systems (e.g., barrier shape, length and gradation); (3) solve the inverse problem to identify the underlying parameters in the ground-truth physical experiments. The constructed digital twins can be used to inform the development of new screening criteria for characterization and effectiveness of composite confining systems in CO2 storage.

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#### MS35

## Simulation of Compositional Flow in Geothermal Applications with PorePy $\,$

PorePy is an open-source Python package for prototyping multiphysics models in deforming, fractured porous media. With active development going on since 2017, PorePy has a wide range of capabilities for meshing and representing

porous media, with fractures embedded as explicit lowerdimensional objects. Capabilities in multiphysics modeling include coupled single-phase flow, thermo-poroelasticity and fracture contact mechanics. Recent developments have added support for modelling multiphase, multicomponent fluids with a strong focus on thermodynamically consistent modelling of fluid properties. In this talk we demonstrate PorePys modelling framework, which leverages Python's multiple inheritance to provide a flexible sandbox for introducing various physics into the model as mixed-dimensional equations. We propose an objectoriented representation of the mathematical abstractions needed for solving the equilibrium problem in compositional multiphase mixtures. This extends PorePy to effectively address non-isothermal, compositional multiphase problems. Finally, we present a solution strategy to solve the resulting highly non-linear and tightly coupled system using nested flash algorithms in the global numerical scheme.

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#### MS35

#### Gres: A Novel Multi-Physics and Multi-Domain Prototyping Platform for Coupled Geomechanics in Porous Media

The accurate prediction of geomechanical behavior is essential for the sustainable management of underground resources, where complex interactions among fluid flow, poromechanics, fault activation, thermal transport, and chemical reactions occur across multiple spatial and temporal scales. While significant progress has been made in modeling individual processes, coupling geomechanics with other phenomena at appropriate scales remains an open challenge. GReS is a novel open-source modular platform designed to facilitate the development and prototyping of numerical algorithms for fully coupled multiphysics, multidomain geomechanical problems. The computational domain can be partitioned into possibly non-conforming subdomains, allowing different physical models and discretizations to coexist. Built on MATLAB, GReS reduces the entry barrier for users and fosters rapid testing of new algorithms. Its modular structure supports contributions at various levels, from solvers to physical models. Despite being a prototyping tool, it interfaces with efficient low-level linear algebra libraries. We present the current status of GReS, including recent advances in the mortar-based coupling for non-matching meshes, and provide benchmark results highlighting its capabilities.

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#### MS35

## OPM Flow: Scaling Up an Open-Source Simulator for Industrial Application

OPM Flow is an open-source reservoir simulator that has been under development for over a decade, with the goal of full operational deployment. It supports a broad range of fluid models and advanced well models used in industry, while also offering nonlinear and linear solvers fresh from research. The simulator scales to models with hundreds of millions of cells on HPC systems, and GPU support is currently in development. As the simulator has matured, the focus has shifted from the initial development of standard flow models towards supporting a wide variety of model options and additional features required for real-world applications, all while minimizing runtime. Other areas of focus included improving error reporting, documentation, and the integration with pre- and post-processing tools to streamline connection with industrial workflows. Scaling up the simulator has also involved managing a geographically distributed team and balancing diverse stakeholder interests, raising important questions about governance and decision-making processes. This presentation will explore how OPM Flow has navigated these challenges, highlighting both successful design decisions and instances where unforeseen consequences arose. These lessons offer valuable insights for others working to scale open-source simulators for industrial readiness.

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#### MS35

#### Geos: An Open-Source Simulator for Subsurface Multiphysics on Exascale Hardware

Subsurface energy and storage technologies such as geological carbon storage, enhanced geothermal systems, and hydrogen storagerequire predictive simulation tools to evaluate site suitability in terms of both capacity and safety. In this context, freely available, open-source software is essential for ensuring quality control, enabling repeatability of simulations, and facilitating open review of simulation strategies. With this goal in mind, we present GEOSan open-source simulation tool designed as a computational engine for subsurface energy and storage applications. We summarize the multi-institutional development of GEOS and the goals of the supporting projects. Key components discussed include the data infrastructure, guidelines for constructing and solving single- and multi-physics problems, and strategies for achieving performance portability across hardware platforms. We also describe the development process that governs the integration of new physics capabilities into the main codebase, including coding standards, review procedures, and testing requirements. Results from large-scale simulations are presented, with emphasis on GPU performance and weak scaling. Finally, we discuss plans for future GEOS user and developer support.

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#### **MS36**

#### The Rise of Voluntary Carbon Credit Markets in the Transition to a Circular Economy

The economy of the world is changing from linear to circular as we begin to evolve beyond carbon dioxide emissions. This evolution is occurring without the impetus of comprehensive environmental legislation with the change occurring from within the private sector rather from than the public sector, at least within the United States. Within this voluntary reduction movement, carbon accounting has become central as most private companies seek ways to avoid, minimize and mitigate carbon emissions. Within the mitigation segment, registries such as BCarbon which was formed out of a stakeholder group at the Baker Institute at Rice University write protocols for various naturebased carbon capture concepts such soil, forest and coastal blue carbon storage along with plugging oil and gas wells that are abandoned and idle and leaking methane. Collectively, these various abatement methods have the potential to remove billions of tons of carbon dioxide equivalent emissions each year, leading to this voluntary carbon credit market promising to be a major part of the long-term carbon abatement strategy.

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#### **MS36**

# Connecting Environmental Uncertainty to Environmental Interest Rates: Advances in Mathematical Understanding

Environmental Impact Bonds are novel financial instruments becoming an increasingly popular mechanism for financing environmental restoration. The interest rate on these bonds is often tied to well established financial instruments plus additional premium for projects that are successful or overperform, also called pay-for-performance. Interest rates are a critical mechanism by which investors are rewarded for taking on risk, with a positive correlation between risker projects and higher interest rates. Prior efforts from Brand et al., 202 focused on developing a more precise quantification of an "environmental interest rate" fundamentally tied to a risk model which predicts the likelihood of bond failure as a result of environmental variability. This effort, however, generated interest rates considered much too low for projects with large uncertainties when compared to the overall bond market. This talk will focus on the prior efforts at connecting environmental uncertainty along with new efforts to more rigorously connect environmental variability to financial risks, both from theoretical frameworks and empirical analysis.

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#### **MS36**

# Leveraging Ecosystem Modeling and Metrics to Advance Conservation Finance Projects

Scaling effective conservation finance solutions is dependent on the intersection of ecosystem process-based and statistical modeling, economic valuation, and financial

structuring. While conservation finance is a growing opportunity to support critical environmental resilience efforts in the face of increasing wildfire and flood risks, the sectors growth remains constrained by challenges in rapid, cost-effective quantification of ecological outcomes at multiple scales. Through case studies, we explore diverse payor-benefit relationships in conservation finance projects - including utilities, corporations, insurance, and the public sector - with a focus on the modeling frameworks required to support long-term capital commitments. This talk will introduce conservation finance, supporting ecosystem models, and gaps in current capabilities that can provide the data-driven foundations needed to develop successful, scalable, and investable projects.

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#### MS36

# Bringing Payors to Coastal-Estuarine Restoration Projects That Deliver Ecosystem-Service Cobene-

As coastal ecosystems experience impacts from rising seas and more intense storms, land managers must explore a suite of proactive techniques to promote wetland resilience. Coastal wetland position relative to sea level is maintained by surface elevation and driven by accretion, an accumulation of sediment, and plant roots. We collaborated with an interdisciplinary group of scientists, reserve managers, and restoration specialists to explore how management options could help maintain or increase coastal wetland surface elevation in Northeast Florida. Critical to this work was the design of a coastal vulnerability index (CVI) tailored to the estuarine context that incorporates factors such as boat wake exposure and changes in natural habitat distribution and function. This talk will describe a process for identifying ecosystem restoration interventions, such as living shorelines and mangrove establishment, that help wetlands keep pace with rising sea levels. Our research enabled land managers to prioritize sites of concern and stakeholders to consider the potential of four wetland elevation strategies for flood protection and other ecosystem services. The evaluation of restoration benefits is a crucial step in securing funding and innovative finance for these projects.

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#### MS37

#### A Geometric Lagrangian-Eulerian Formulation for the Intrinsic Shallow Water Equations on General Topography

We present a geometrically adapted Lagrangian-Eulerian finite volume formulation for the intrinsic shallow water equations (ISWE) in the case of spatially variable bottom geometry, also in the presence of localized discontinuities. Using a local curvilinear reference system anchored on the bottom surface, we develop an effective first-order and high-resolution time-space discretization of the no-flow surfaces. The method is based on a two-step evolution-remap building block: i) a solution of a Lagrangian initial value problem describing the evolution of the balance laws (Lagrangian step); ii) a remapping to the original surface (Eulerian step). The resulting scheme maintains monotonicity

and captures shocks, without providing excessive numerical dissipation also in the presence of non-autonomous fluxes. Moreover, this is an effective method to account for localized discontinuities in the bottom topography, without major modifications of the (global) system of equations. We provide a representative set of numerical examples to illustrate the accuracy and robustness of the proposed formulation for two-dimensional surfaces with general curvatures and discontinuous initial conditions.

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#### **MS37**

#### An Posteriori Error Estimate for the Transport Equation Discretized with SUPG-Stabilized Virtual Element Method

Convection-dominated problems are known to be challenging, both theoretically and computationally. Indeed, the discretization of such problems leads to unstable solutions with spurious oscillations if the velocity field is high. One way of preventing solution instabilities is to employ a stabilization technique. In a previous work, we presented a virtual element discretization of the steady transport equation stabilized with the Streamline-Upwind/Petrov-Galerkin (SUPG) technique. However, in the case of discontinuous solutions in a convection-dominated regime, the SUPG stabilization is not sufficient to avoid oscillations at the discontinuities. For this reason, we worked on an adaptive mesh refinement strategy for our problem. This presentation thus aims to present the derivation of the a posteriori error estimate in the steady case, expose the refinement strategy, and see how it adapts to the unsteady case, specifically in the case of an advancing front of densitv.

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#### **MS37**

## A Polyhedral Discretization Method for Compositional Multiphase Poromechanics

This work presents a novel approach to generalized finiteelement discretizations by integrating the Hybrid Mimetic Finite Difference (MFD) method and the Virtual Element

Method (VEM) for compositional multiphase poromechanics. The approach supports arbitrary polyhedral grids, including elements with coplanar and planar polygonal faces, thereby enabling flexible meshing of complex and irregular geometries. General support for distorted cells is provided, and accuracy and convergence properties are established under the assumption of planar faces. A local pressurejump stabilization technique is employed to prevent spurious pressure oscillations in the incompressible regime, enhancing numerical stability. The approach is implemented within GEOS, an open-source multiphysics simulator, facilitating immediate practical application. The capabilities of this numerical scheme are demonstrated through its application to challenging polytopal partitions and complex fluid behavior, highlighting its robust performance in poromechanical simulations.

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#### **MS37**

## Interior Penalty Discontinuous Galerkin Methods for Two-Phase Flows in Poroelastic Media

The modeling of poroelastic deformation arises in many fields including biomechanics, energy and environmental engineering. We propose a discontinuous Galerkin method for solving the two-phase poroelasticity equations. Discontinuous Galerkin methods (DG) have been successfully applied to multiphase flows in rigid porous media because of their flexibility resulting from the lack of continuity constraint between mesh elements. DG methods are locally mass conservative, they allow for polytopal meshes, local mesh refinement and local high order of approximation; and they are well suited for the solution of convectiondominated problems because they exhibit little numerical diffusion. Our numerical scheme for solving the two-phase Biot problem does not require iterations over each equation for stability. At each time step, mass balance and momentum equations are decoupled and the computational cost is smaller than the one for fully implicit methods. We apply the proposed method to three-dimensional problems and we study the impact of heterogeneities (regions with different capillary pressures) and loading on the propagation of the fluid phases in the medium.

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#### MS38

## Development of Sequentially Coupled Hydro-Mechanical Approaches in Pflotran

Numerical modeling of enhanced geothermal systems (EGS) requires the coupling of key subsurface processes, including fluid flow, heat transfer, and geomechanical deformation. The governing equations describing the system can be solved simultaneously using a fully coupled approach, which is computationally expensive. Alternatively, a sequential coupling strategy can be employed, offering flexibility in implementation and an overall improved computational efficiency. In this work, efforts to enhance the modeling capabilities for EGS using PFLOTRAN focus on a sequential coupling approach. The approach leverages process model coupling framework in PFLOTRAN, which allows for the combination of different discretization schemes for each process model, as well as the application of appropriate solvers and timestep strategies. In this work, we aim to present the development of the sequential coupling approach for modeling poro-elasticity problems and describe several operator splitting strategies that have been implemented. These strategies range from simpler, more intuitive methods such as the drained split and fixed strain split methods to increasingly stable alternatives, including the undrained split and fixed stress split approaches. We also explore the effectiveness and applicability of these strategies in capturing key subsurface interactions within enhanced geothermal systems, highlighting potential improvements to model accuracy and computational efficiency.

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#### **MS38**

#### An Optimization-Based Domain Decomposition Approach for DFN Simulations and 3D-1D Coupled Problems

A PDE-constrained optimization approach is proposed for flow simulations in complex discrete fracture networks (DFNs). The method is based on a three-field domain decomposition approach, in which independent variables are introduced at fracture intersections. The combination of domain decomposition and optimization-based coupling results in a novel method robust to geometrical complexities, which can handle non-conforming meshes and which ensures local mass conservation at fracture intersections. The same approach also addresses 3D-1D coupled problems, arising from dimensionality reduction of 3D-3D problems with thin inclusions. Possible applications span different research areas, from geosciences (a system of wells

in a reservoir, the interaction between tree roots and soil) to biomedicine (capillary networks, tubular medical implants). Unlike DFNs, the definition of interface conditions is not straightforward, as no bounded trace operator is defined between manifolds with codimension higher than one. However, the issue can be overcome by proper assumptions on the regularity of the solutions, and once a well posed mathematical formulation is derived, all the advantages of the three-field PDE-constrained optimization framework are retained. Combining the method with an eXtended Finite Element discretization, optimal convergence rates are preserved also in presence of very strong gradients around the thin inclusions, without the need of mesh refinement.

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#### **MS38**

#### A Unified Compositional Model for Simulating Multiphase High-Enthalpy Geothermal Reservoirs

Simulating high-enthalpy geothermal reservoirs is challenging due to complex interactions between multicomponent, multiphase fluids under extreme pressure and temperature. These conditions induce non-ideal fluid behavior, complex phase transitions, and mineral precipitation due to high salinity and dissolved solids, requiring rigorous thermodynamic modeling. We propose a unified compositional flow model that integrates mass and energy conservation across predefined phases using advanced equations of state and a consistent thermodynamic framework. The formulation maintains a persistent set of primary variables and equations, enabling the natural treatment of phase transitions without manual switching, improving numerical stability and computational efficiency. Full flash calculations are replaced by an operator-based linear approximation built from precomputed flash data, reducing computational cost. Implemented in the open-source Python framework PorePy, the model is validated through simulations covering a wide range of high-enthalpy geothermal conditions, from single-component, single-phase to multicomponent, multiphase systems. We also extend the model to fractured reservoirs via the discrete fracture-matrix (DFM) approach, capturing fracture-matrix interactions. Numerical results present valuable insights into phase behavior, heat transfer, and component transport, and show strong agreement with benchmark cases from the commercial geothermal simulator CSMP++.

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#### **MS39**

# Geodetic Investigation of Coastal Subsidence Dynamics Using Long-Term GPS Observations

Southeast Louisiana is a rapidly subsiding coastal region, influenced by natural and anthropogenic processes. This research investigates the spatial and temporal characteristics of land subsidence using long-term Global Positioning System (GPS) data from Continuously Operating Reference Stations (CORS). These high-precision measurements reveal substantial variability in vertical land motion, with rates exceeding 10 mm/year in some areas. Sediment compaction emerges as a dominant natural driver, especially within Holocene deltaic deposits rich in organic material and moisture, where compaction occurs as pore water is expelled. GPS data confirm the persistence of this trend, particularly in zones with thick sediment accumulation across the Mississippi Delta. Additional contributors include tectonic activity, isostatic adjustment, groundwater withdrawal, and hydrocarbon extraction. Integrating GPS observations with sediment compaction models enhances our understanding of cumulative subsidence in Louisianas coastal zone. This integration supports the development of Digital Twin frameworks that simulate real-time and future ground deformation, improving predictive capabilities for infrastructure risk assessment, coastal restoration, and resilience planning. The study highlights the essential role of GPS-based geodetic monitoring in advancing sustainable coastal zone management through a deeper understanding of subsidence processes.

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#### **MS39**

#### Modeling Groundwater Withdrawal-induced Land Subsidence in Baton Rouge, Louisiana Using MODFLOW 6: Implications for Groundwater Management

Land subsidence driven by excessive groundwater extraction and active faults constitutes a major geomechanical hazard, with profound implications for aquifer sustainability and infrastructure resilience. This study advances a comprehensive, integrated framework that couples a groundwatersubsidence model with extensometer records, GPS data, and TS-InSAR analysis to investigate the mechanisms driving subsidence in the Capital area of Louisiana. This multidisciplinary methodology enables precise quantification of subsurface compaction within the Southern Hills aquifer system and delivers a comprehensive assessment of the long-term geomechanical consequences associated with unsustainable groundwater exploitation and active fault displacement. This study identifies the Industrial District as the area most affected by ongoing subsidence, despite reduced pumping, due to irreversible compaction that permanently reduces aquifer storage capacity. This study further highlights the Baton Rouge fault and the Denham Springs-Scotlandville fault as active tectonic features that amplify the coupling between intensive groundwater extraction and surface deformation processes, resulting in spatially heterogeneous subsidence patterns and heightened structural vulnerability in adjacent urban areas. These findings establish a critical framework for advanced subsidence risk management and deliver practical insights for policymakers tackling groundwater depletion in fault-prone areas.

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#### MS40

# Numerical Modeling of Fault Stability in Co2 Geological Sequestration: a Real-World Case Study in Italy

The analysis of fault stability in the geological sequestration of CO2 is a key issue for the safety and feasibility of the storage project. The simultaneous simulation of frictional contact mechanics for the fault behavior and multi-phase fluid flow in geological media is a coupled multi-physics process, with the aperture and slippage between the contact surfaces driving the potential CO2 leakage and the pressure variation perturbing the stress state in the surrounding medium. In this presentation, we focus on realworld case study of a CO2 geological sequestration project in an exhausted reservoir in Italy with the objective of investigating the fault behavior as a consequence of the storage activities. A blended finite element/finite volume method is used, where the porous medium is discretized by low-order continuous finite elements with nodal unknowns, cell-centered Lagrange multipliers with a stabilization are used to prescribe the contact constraints, and the multiphase fluid flow is described by a classical two-point flux approximation scheme. Multiple grids are used in order to optimize the accuracy of the discretization for the specific analysis at hand.

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#### MS40

# Leakage Dynamics of CO2, H2, and Compressed Air Storage in Aquifers

Underground hydrogen storage and geologic CO2 sequestration in saline aquifers are promising technologies for transitioning to a cleaner energy future. Compressed Air Energy Storage in aquifers is a promising technology for smoothing power fluctuations and intermittency associated with renewable sources such as wind and solar power. However, a wide-scale adoption of these technologies has been hampered by the risk of leakage of these gases. Leakage pathways may activate through stress-induced shear failure

of faults and tensile failure/shear dilation of fractures in the caprock. It is unclear how one leakage mechanism affects the risk profile of the other mechanism and its implications for the distribution of stress and fluids in the subsurface. We investigate the interplay of the leakage mechanisms by utilizing 3D coupled flow-geomechanics models that integrate a stress-dependent Barton-Bandis model for caprock fracturing with a Coulomb frictional failure-induced fault permeability model. We also investigate the ground surface deformation signature associated with different leakage pathways, which can inform real-time monitoring efforts at these storage sites.

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#### MS40

## Use of Soreide-Whitson Model for the Prediction of Co<sub>2</sub> Solubility in a Depleted Gas Reservoir

This study focuses on modelling the injection of carbon dioxide (CO2) into depleted gas reservoirs for CO2 sequestration, considering the presence of light gases such as methane and hydrogen sulfide. The model employs a twophase gas-water system, emphasizing the solubility of gas components in the water phase. To achieve this, the Sreide-Whitson (SW) equation of state (EoS) is used. This EoS strikes a balance between reasonable accuracy and simplicity, effectively incorporating the influence of salinity while requiring minimal modifications compared to more complex EoS such as models based on the statistical associating fluid theory (SAFT). In this work, we use publicly available measured data for validation and calibration. Adjustments to some correlations are applied to ensure accurate predictions of species solubility in water. We apply the model to simulate CO2 injection, beginning with small synthetic models to verify implementation accuracy and robustness. These tests confirm the models reliability. We apply the model to a large North Sea reservoir to assess its industrial applicability in a CO2 sequestration pilot. The results confirm the model's ability to predict the solubility of components in water accurately. It also evaluates the impact of impurities in the water phase on CO2 trapping. Additionally, the model demonstrates efficiency and applicability for full-field settings, reinforcing its value for large-scale CO2 sequestration projects.

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#### **MS40**

Coupled Flow and Geomechanics Modeling of Subsidence and Uplift in the Wilmington Field, CA,

#### 1936-2020

Since the 1930s, there has been approximately 2.5 billion barrels of oil produced and ten times as much water injected in the Wilmington oil field, Los Angeles Basin, California. This history, together with extensive structural and geophysical data of the basin, provides a unique opportunity to assess the long-term impacts of reservoir operations on seismic hazard. Here, we assess (1) the influence of the initial stress state on ground deformation, and (2) the evolution of fault stability. We develop a suite of numerical models that include a detailed representation of faults in and around the field, monthly production and injection history, and the effect of permanent (plastic) deformation. We show that the stress regime and initial deviatoric stress levels control the amount of plastic deformation that can be achieved. We document the evolution of fault stability using two history-matched models, with homogeneous and heterogeneous initial stress states, respectively, and discuss the implications of uncertainty in the stress state on seismic hazard assessment during subsurface operations. We conclude by documenting the link between computed stress changes and historical seismicity, including a series of seismic events observed during operations at Wilmington.

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#### **MS41**

#### Real-Time Bayesian Inference at Extreme Scale: A Digital Twin for Tsunami Early Warning Applied to the Cascadia Subduction Zone

We present a digital twin (DT) for tsunami early warning in the Cascadia subduction zone (CSZ). This DT assimilates pressure data from seafloor sensors into an acousticgravity wave equation model, solves an inverse problem to infer spatiotemporal seafloor deformation, and forward predicts tsunami wave heights. The entire end-to-end data-toinference-to-prediction computation is carried out in real time through a Bayesian framework that rigorously accounts for uncertainties. Creating such a DT is challenging due to the enormous size and complexity of both the forward and inverse problems. For example, a discretization of the spatiotemporal seafloor velocity in the CSZ the parameter field to be inferred gives rise to a system with one billion parameters. Using current methods, computing the posterior mean alone would require more than 50 years on 512 GPUs. We exploit the shift invariance of the parameter-to-observable map and devise novel parallel algorithms for fast offline-online decomposition. The offline component requires just one adjoint wave propagation per sensor; the PDE solver is implemented with MFEM and exhibits excellent scalability to 43,520 GPUs on LLNLs El Capitan system. Fast Hessian applications are enabled by an FFT-based algorithm for the resulting block Toeplitz matrices. Using this framework, the Bayesian inverse solution and wave height forecasts are computed in 0.2 seconds, representing a ten-billion-fold speedup over state-of-the-art methods.

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#### MS41

# Machine-Precision Neural Networks for Multiscale Dynamics

Deep learning techniques are increasingly applied to scientific problems where the precision of networks is crucial. Despite being deemed as universal function approximators, neural networks, in practice, struggle to reduce prediction errors below a certain threshold even with large network sizes and extended training iterations. We developed an algorithm to tackle this issue and demonstrate that the prediction error from multi-stage training can nearly reach the machine precision of double-floating point (Wang and Lai, JCP 2024). This mitigates the longstanding accuracy limitations of neural network training and can be used to address the spectral bias in multiscale problems. I will discuss an application where neural networks are used to solve geophysical inverse problems, leveraging large-scale Earth observations to uncover constitutive laws for polar ice (Wang, Lai et al., Science 2025).

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#### MS42

#### Discontinuous Polytopal Methods for Multi-Physics Differential Problems

We present the library lymph for the finite element numerical discretization of coupled multi-physics problems. lymph is a Matlab library for the discretization of partial differential equations based on high-order discontinuous Galerkin methods on polytopal grids (PolyDG) for spatial discretization coupled with suitable finite-difference time marching schemes. The objective of the talk is to introduce the li-

brary by describing it in terms of code structure, high-lighting – when necessary – key implementation aspects related to the method. We show the results obtained for several differential problems, namely the Poisson problem, the heat equation, the elastodynamics system, and a multiphysics problem coupling poroelasticity and acoustic equations. Through these examples, we show the convergence properties and highlight some of the main features of the proposed method, i.e. geometric flexibility, high-order accuracy, and robustness with respect to heterogeneous physical parameters. Finally, some applications in the context of geophysical simulations, e.g. thermo-hydro-dynamics and wave propagation problems, are presented.

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#### MS42

#### How to Achieve the Reproducibility of Simulation Results

Ensuring the reproducibility of simulation results necessitates the sustainable archival and accessibility of research software artifacts. While the importance of research software in contemporary scientific workflows is widely acknowledged, establishing long-term reproducibility remains a complex and ongoing challenge. In this talk, we conceptualize research software artifacts as time-stamped representations of research progress and as essential components in a sustainable cycle of development, experimentation, and dissemination. Building upon this understanding, we propose a set of requirements and recommendations aimed at enhancing the archiving, accessibility, and reusability of research software. To address the diversity of reuse scenarios, we introduce a multi-modal representation framework for software artifacts. We examine how corresponding representations can facilitate reproducibility by supporting different levels of user engagement and technical requirements. Furthermore, we highlight the role of robust archival infrastructure in enabling these reuse modes. Drawing on insights from a pilot initiative at the University of Stuttgart, we reflect on the practical challenges associated with implementing sustainable software archival strategies. These experiences inform a broader discussion on how institutional efforts and community practices can converge to support the reproducibility of simulation-based research.

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#### **MS42**

#### JutulDarcy.jl - a Fully Differentiable Reservoir Simulator Written in Julia

Differentiable simulation is gradually becoming the norm in computational science, both for inverse problems where parameters are calibrated against observations and for optimization of controls for already calibrated models. Reservoir simulation models are notoriously difficult to differentiate, however, as practical models of interest have a large number of parameters per degree of freedom and require the solution of multiple ill-conditioned linear systems for each time-step. In this talk, we present JutulDarcy.jl, an open-source, high-performance, fully differentiable reservoir simulator written in Julia. We give an overview of how the software was designed to use automatic differentiation in a way that both allows for high flexibility in terms of discretizations and governing equations while also retaining commercial grade performance, and detail how this design allows for an efficient and accurate adjoint implementation for inverse problems for any model parameter. Examples from different types of multi-phase, multi-component flow will be given, including compositional reservoir simulation, CO<sub>2</sub> storage and geothermal energy recovery. We will also discuss how the code leverages the Julia software ecosystem to produce high-quality documentation, examples and tests, and give an assessment of Julia itself for complex scientific applications.

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#### MS43

### Simulation of Flow and Transport in the Partially Molten Mantle of the Earth

Partial melting in the Earth's mantle is an important process in the generation of oceanic and continental crust, and in determining the large-scale separation and deposition of minerals in the Earth. We present a framework for large-scale simulation of two-phase, two-component partial melting processes. The mechanics of flow is modeled by a degenerate elliptic Darcy-Stokes system modeling the slow Stokes creep of the mantle and the Darcy flow of melt. This subsystem is degenerate since the Earth's fluid component and porosity is due solely to melting and may be solid (i.e., nonporous) in some regions. It is discretized by mixed finite element methods that maintain accuracy in the degenerate regions of a single solid phase. The parabolic/hyperbolic transport of heat energy and two mineral components (olivine and orthopyroxene) that are miscible in the fluid phase are modeled. This is discretized by multilevel weighted essentially non-oscillatory (ML-WENO) finite volume discretizations. Eutectic phase behavior is incorporated to model thermodynamic equilibrium, and to determine the Earth's porosity. These three framework modules are combined in an operator splitting technique based on using a partition function approach. We present numerical results illustrating the framework and the evolution of the Earth.

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#### MS43

#### The Enriched Galerkin Method for Elastic Wave Propagation in Fractured Media

The enriched-Galerkin method (EGM) combines the advantages of spectral-element and discontinuous-Galerkin methods. This method offers significant advantages for the propagation of elastic waves, especially if the domain includes fractures. We present a grid-dispersion analysis of EGM and show that, using an enriched basis of low polynomial order, the results are polluted with grid-dispersion error. This error can be minimized using high-order enrichment. We also show that the stability conditions of EGM are significantly higher than those of the discontinuous-Galerkin method. Our analysis gives insight into the accuracy of EGM as a function of the order of the enriched basis functions.

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#### MS43

# The Impact of Locally Conservative Methods and Compatibility in Coastal and Hydraulic Process Modeling

As mathematical modeling expanded into increasingly complex coupled processes and practical modeling applications over the last two decades, basic notions like convergence algorithms and asymptotic convergence rates for solution variables have in some cases become secondary to debates about what methods are practically optimal. Around the turn of the century Dr. Wheeler's work was central to debates over the local mass conservation, and the spirit of that debate continues to inform work on other critical model properties, such as bounds preservation. In this talk I will review some of the history on continuous and discrete conservation properties, the notion of compatibility introduced by Wheeler and coauthors, and some simple and fast algorithms for recovering local mass conservation that have had practical impacts in near-surface environmental modeling.

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#### **MS43**

Ai-Driven Automation for Electrochemical Analy-

#### sis in Energy Applications

This presentation explores how artificial intelligence (AI) is transforming electrochemical analysis, with a focus on developing corrosion inhibitors. Electrochemistry underpins critical technologies from batteries and sensors to coatings and corrosion mitigation. Traditional experimental workflows for inhibitor development are systematic but slow, offering limited insight into complex material interactions. We introduce an enhanced AI-driven platform that integrates generative models and physics-based equations to identify corrosion drivers, reduce experimental redundancy, and improve prediction accuracy. Unlike black-box ML models, this approach embeds scientific principles, enabling more interpretable, transferable insights. The upgraded platform provides contextual recommendations, automates data analysis, and supports laboratory practitioners with detailed reports and guidance. Powered by a Large Language Model (LLM) assistant, the no-code system accelerates experimental design, shortens development cycles, and redefines innovation in materials science. Join us to explore how this AI-augmented framework sets new benchmarks in electrochemical research and energy applications.

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#### **MS44**

## Thermo-Poromechanics in Highly Fractured Porous Media

Multi-physics modeling in deformable porous media with complex fracture networks presents significant computational challenges. The convergence of nonlinear solver strategies for non-smooth contact mechanics, coupled with flow, heat transfer, and deformation in the matrix, is non-trivial due to the inherent non-smoothness, coupling, and nonlinearity of the problem. In this talk, I will more closely explore the impact of fracture topology complexity and the coupling strength between different sub-physics on the challenges of solving contact mechanics with a semi-smooth Newton's method.

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#### **MS44**

#### A Hybrid High-Order Method for Phase-Field Modeling of Fracture Propagation

Fracture propagation is a challenging problem in computational mechanics, especially with complex crack patterns and localized physical phenomena. We develop a Hybrid High-Order (HHO) method [Di Pietro and Ern, 2015] within a phase field framework [Miehe et al., 2010; Bourdin et al., 2000; Bourdin et al., 2008] to model fracture evolution. The phase field method offers a diffuse fracture representation, avoiding explicit crack tracking. A continuous scalar field transitions from 0 (intact) to 1 (fully broken), with the crack as a thin transition zone. This enables intricate crack networks and bypasses issues linked to discontinuous representations. A key advantage of HHO methods in this context is their ability to efficiently handle non-conforming meshes. Since fractures localize damage in narrow regions and evolve over time, adaptive meshing is essential. The flexibility of polytopal methods allows for localized mesh refinement without the need for mesh conformity, making HHO particularly well-suited for fracture modeling. To validate our approach, we implement and test the method using the open-source HArD::Core library [Di Pietro and Droniou], which supports HHO schemes in 2D and 3D. Though used in other models, its potential for fracture mechanics remains unexplored. We propose to extend it to handle coupled displacement-phase field formulations, demonstrating its effectiveness through comparisons with classical Finite Element methods and benchmark simulations.

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#### **MS44**

#### A Mortar Method for Coupling Discontinuous Subdomains in Hydro-Mechanical Simulations of Faulted and Fractured Domains

Accurate simulation of hydro-mechanical processes in faulted and fractured subsurface formations is crucial for applications like carbon sequestration, geothermal energy storage, and subsidence risk assessment. These simulations are challenging due to complex multi-physics interactions and nonlinearities. A key issue is coupling non-conforming subdomains with distinct discretization schemes for different processes, limiting the modeling of local phenomena. We propose a mortar method for efficiently coupling subdomains with different discretizations, such as finite elements for momentum equations and finite volumes for mass transport and thermal processes. This method is extended to model discontinuous mechanics in fault and fracture zones, incorporating Karush-Kuhn-Tucker (KKT) conditions to simulate sliding and non-compenetrability between fractures. The approach is implemented in GReS, an opensource platform for fully coupled, multi-physics, multidomain geomechanical simulations. This talk will introduce the mortar method, its extension for fracture modeling, and its application to hydro-mechanical simulations in complex subsurface formations. Benchmarks will demonstrate its effectiveness. We will also discuss challenges related to interpolation and coupling across non-conforming subdomains, relevant to methods like polytopal discretization. Future work on large-scale subsurface simulations and potential applications will be explored.

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#### **MS44**

# Space-Time Finite Element Methods for a Poromechanical Model with Memory Effects

In this talk, we consider a poromechanical model with memory effects, known as the BiotAllard model. We derive an equivalent formulation where the memory effects are represented by an auxiliary partial differential equation. The system is then rewritten as a first-order system in time and well-posedness is proven using Picard theory. The equations are then discretized by continuous Galerkin methods in time and equal-order finite element spaces in space. Error estimates are proven and the convergence is studied numerically.

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#### **MS45**

#### The Arctic Coastal Erosion Model: Overview and Calibration at Drew Point, Alaska

We present the Arctic Coastal Erosion (ACE) model a simulation tool that couples oceanographic/atmospheric boundary conditions with a multi-physics, finite element based terrestrial domain to capture the thermo-mechanical dynamics of erosion along permafrost coastlines at stormresolving time steps. It solves 3D heat conduction with phase change (thermal problem), and stress/strain development according to a plasticity material model (mechanical problem). The mechanical material properties like elastic modulus are dependent on the local ice content determined by the thermal problem this couples the thermal and mechanical dynamics of the permafrost evolution. Oceanographic and atmospheric boundary conditions applied to the terrestrial domain provide time-dependent temperature, salinity, and water level information. Erosion is captured via mesh element removal according to stress, strain, and kinematic related criteria such as tensile and compressive yield and strain limit of the material. This enables failure from any allowable deformation such as block failure and thermal denudation, making it novel in its ability to simultaneously capture these erosional processes whilst being sensitive to terrestrial variability and responsive to transient environmental drivers. Model calibration from a 2018 summer field campaign at Drew Point, Alaska with sub-daily observations of thermo-denudation and thermo-abrasion demonstrates accurate daily simulation of both erosional processes.

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#### MS45

### Upscaling with Geometry Non-Conforming Finite Elements

Creating meshes for use in the finite element method can be a challenging task in complex 3D domains such as porous media at the micro-scale. In the context of upscaling, body-fitted meshes will resolve many details that will be averaged away while structured voxel-based grids may not conform to the geometry. Even in the case where a geometry non-conforming structured grid is sufficient, sometimes the size of the structured grid is required to be quite small in order to resolve the correct pore structure. In this case, convergence of the numerical solver may be quite slow and techniques such as multigrid difficult to implement. In this talk, we explore representing the geometry using implicit level sets in combination with finite elements using a hierarchical basis.

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#### MS45

# Reducing Uncertainty in Arctic Carbon Dynamics with the TEM-DART Data Assimilation System

Rapid environmental changes in the Arctic, including rising temperatures, permafrost thaw, and shifting vegetation patterns, demand accurate ecological forecasting to support effective climate adaptation and mitigation strategies. However, substantial uncertainties remain in carbon

cycle projections, limiting predictive confidence. To address this, we present TEM-DART, the first terrestrial data assimilation system developed explicitly for Arctic ecosystems. TEM-DART couples the Dynamic Vegetation ModelDynamic Organic SoilTerrestrial Ecosystem Model (DVM-DOS-TEM) with the Data Assimilation Research Testbed (DART). By integrating field observations, remote sensing products, and process-based modeling, TEM-DART reduces uncertainties in terrestrial carbon balance estimates and improves predictions of permafrost dynamics under changing climate conditions. Through assimilation of key ecological variables such as leaf area index and above-ground biomass, the system refines both surface and subsurface state estimates, leading to more accurate forecasts of soil and vegetation carbon dynamics. Initial single-site experiments at Bonanza Creek demonstrate the systems capability to significantly improve model perfor-

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#### eja-

#### MS45

#### Coupled Soil-snow Model

We model heat conduction in snow and soil, both nonlinear, and coupled across an interface. We discuss two approaches: (i) a fully coupled system of nonlinear PDEs for both domains, and (ii) a lumped snow model, a single algebraic snow model resulting in a nonlinear Robin-type boundary condition for the soil. Both models involved over n=13 environmental parameters including the albedo of surface, effects of radiative transfer, and more. For (i), we consider a domain decomposition strategy, with interface conditions to ensure the continuity of temperature and the conservation of heat flux. For (ii), we consider efficient Neural Network parametrizations which can be applied in a decoupled or fully coupled model. Our simulations and analyses contribute to the understanding of the response of the soils in the Arctic to the weather data and help to assess the reliability of the model.

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#### **MS46**

# Operator Inference Applications for Rapid Reservoir Simulation

The quest for fast simulation models has spurred innovation in computational methodologies, driving the development of reduced-order models leveraging machine learning architectures through data-driven simulations. Although

successful implementation of non-intrusive techniques has emerged in reservoir simulation, it still poses challenges related to its generalizations and interpretability. In this paper, we propose a novel approach to Operator Inference (OpInf), which is a nonintrusive method to compute projection-based reduced-order model from snapshot (simulated or measured) data. In this talk, I will demonstrate how to write the single and two-phase flow equations in a quadratic bilinear formulation which is the building block for construction the surrogate model. I will also show the feasibility of our method using a 3D single-phase and a 3D two-phase flow model.

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#### **MS46**

#### Salt Rock Integrity Assurance Using Thermohydro-viscoplastic Models and Iterative Coupling

This work uses a thermo-hydro-viscoplastic model to assess the integrity of salt rock under seasonal loadings in natural gas, Hydrogen and CO2 storage/disposal applications. Salt (halite) exhibits a long-term, time-dependent mechanical response under deviatoric stresses. Salt mechanics are tightly coupled to temperature, pressure, and mechanical transients across multiple time scales. Our model formulation incorporates J2 viscoplasticity and uses the Finite Element Method for spatial discretization, with fixed-stress iterative coupling to capture the material response to reservoir dynamics. We validate the model using well-established numerical simulators. Our results indicate that the transient-state response of salt bodies significantly dissipates deviatoric stresses within the operational timeframeranging from weeks to monthsbefore approaching the steady-state asymptote. We use a parametric study to investigate the time constant of the system strongly as a function of the model parameters. These numerical estimates suggest that projects cannot rely on a steady, hydrostatic stress state in salt bodies, but should expect a residual deviatoric component after transient loads. We show a parametric study that can be extended to broader cases, such as the deviatoric destressing of salt caprocks subjected to high injection pressures in Enhanced Oil Recovery (EOR) applications.

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#### **MS46**

Convergence of DG Methods for Miscible Displace-

#### ment with Low Regularity

Numerical simulation of miscible flows in porous media is of critical importance in many engineering applications such as decontamination of groundwater flows, hydrocarbons production, and storage of carbon dioxide. Thanks to the increase in computational power, scientists are able to model flows in heterogeneous and complex media. In this case, however, the solution to the mathematical equations characterizing miscible flows is no longer smooth and the derivation of a priori error estimates is not possible. Convergence of the numerical scheme is obtained by using a compactness argument. In this talk, we review the class of discontinuous Galerkin (DG) methods with or without hybridization for solving the miscible displacement. We present the convergence of both interior penalty DG and hybridizable DG methods under low regularity. Proofs rely on special functional analysis tools for discontinuous polynomial spaces.

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#### **MS47**

#### Bound Preserving Methods for Infiltration Applied to Nature-Based Stormwater Infrastructure

Nature-based infrastructure systems, such as rain gardens and bioswales, are backfilled by engineered soils that enhances infiltration to the subsurface. The subsurface infiltration process can be simulated using the parabolic Richards Equation (RE), which is notorious for its strong nonlinearity. The standard discretization methods often fail to possess local maximum principle which results in non-physical oscillations. Several stabilization techniques such as mass lumping and upwinding are employed to generate stable monotone numerical solution which results in creating lower order accurate results. The Flux Corrected Transport (FCT) Method combines high order accuracy with the ability to limit nonphysical oscillation near sharp fronts. In this work, the Flux-Corrected Transport (FCT) implementation of Richards Equation (RE) will be employed to simulate nature-based infrastructure systems such as rain gardens and bioswales under different boundary conditions, including rainfall and ponding. The seepage flux through the bioswale media and into the drainage system will be explicitly calculated as part of the modeling effort. Furthermore, contaminant transport processes, specifically the migration of nitrogen through the bioswale soil matrix, will be simulated using a random walk particle tracking method to capture the complex interaction between water flow and solute transport.

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#### **MS47**

Simulating Coastal River-Subsurface Seawater Intrusion Using Coupled Density-Dependent Navier-Stokes Flow and MODFLOW 6 with a Corrected

#### **Darcy-Brinkman Equation**

Seawater intrusion into the Mississippi River increasingly threatens the drinking water supply for New Orleans and coastal communities in Plaquemines Parish. However, the dynamics of the saltwater wedge, influenced by upstream river flow and downstream sea levels, are not fully understood. Additionally, the interactions between the river and groundwater, and their effects on saltwater intrusion, remain unclear. This study develops a two-dimensional numerical model coupling density-dependent Navier-Stokes flow, Darcys flow, and salinity transport to investigate river-groundwater interactions, with a focus on saltwater wedge dynamics and hyporheic flow. Hyporheic flow, water that infiltrates into the subsurface and returns to surface water, is a central component to the model, especially at the river-groundwater interface. A corrected Darcy-Brinkman equation is applied to simulate hyporheic dynamics and saltwater wedge behavior. Surface water is modeled by solving the incompressible Navier-Stokes and salinity transport equations, while groundwater flow is simulated using MODFLOW 6 developed by the U.S. Geological Survey. Iterative coupling of the surface water model with MODFLOW 6 captures the evolution of the saltwater wedge and buoyancy effects on velocity and salinity fields. Results highlight the importance of effective viscosity in the corrected Darcy-Brinkman formulation and offer new insights into Mississippi River salinization and coastal aquifer management.

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#### **MS47**

#### Capturing Groundwater Interactions in Fast Flood Inundation Model

Many physics-based pluvial flood inundation models adopt relatively simplistic parameterizations of infiltration or assume that the soil is fully saturated, in order to predict flood hazards especially during extreme events. Fully coupled surface-subsurface models allow for rigorous modeling of rainfall runoff, including variable soil moisture, which is particularly important for runoff estimation but usually at prohibitively high computational costs. Here we present a novel flood inundation model formulation and GPU-accelerated implementation in which infiltration is sensitive to depth-to-groundwater as an indicator of surface soil saturation, and changes to the depth-to-groundwater are tracked over time including their role in driving seepage into nearby water bodies. Model applications are presented demonstrated levels of process representation, accuracy and speed.

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#### **MS47**

Residence Times in Layered Composite Media with Full Coupling to Advective-dispersive Boundary Compartment: A Hydrological Example and its Solution

Solute transport in stream corridors is governed by advection and dispersion, as well as diffusive exchange between the stream and sediment bed that controls tailing and reaction extent. In many cases the transport within the bed is governed by vertical diffusion with depth-dependent diffusion coefficient and reactivity. Here we take a simple approach of discretizing the bed into two layers, the benthic biolayer and the hyporheic zone, each with constant diffusion and reaction properties. To quantify reach-scale solute dynamics, we solve the fully-coupled three-domain transient transport problem with each domain structured on age, or not. The solution is closed-form in double Laplace space (for both time and age) and the steady-state agedistribution in each domain can be obtained as a limit in the time-Laplace variable. By changing which domains are age-structured, the same overall solution gives the agedistribution per domain or any combination. Then to estimate reaction extent e.g., in the case where reactions take place only in the biolayer subdomain, one computes the reaction extent for all ages within the biolayer RTD and then sums them, weighted by that RTD. We will present a preliminary application to data pertaining to nitrate in the Missouri Flat Creek within the Cook Agronomy Farm near Pullman, WA.

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#### MS48

# A Thermomechanical Model for Frost Heave and Subglacial Frozen Fringe

Ice-infiltrated sediment is responsible for phenomena such as frost heave, ice lenses and meters of debris-rich ice under glaciers. Understanding frozen fringes is important as frost heave is responsible for damaging infrastructure at high latitudes and sediment freeze-on at the base of glaciers can modulate subglacial friction, influencing the rate of global sea level rise. Here we describe the thermomechanics of liquid water flow and freezing in ice-saturated sediments, focusing on the conditions relevant for subglacial environments. The force balance that governs the frozen fringe thickness depends on the weight of the overlying material, the thermomolecular force between ice and sediments across liquid premelted films and the water pressure required by Darcy flow. We combine this mechanical model with an enthalpy method that conserves energy across phase change interfaces on a fixed computational grid. The force balance and enthalpy model together determine the evolution of the frozen fringe thickness. Our model accounts for premelting, partial ice saturation of the pore space, water flow through the fringe, thermodynamics and vertical force balance. We explicitly account for the formation of ice lenses, regions of pure ice that cleave the fringe at the depth where the interparticle force vanishes. Our model results allow us to predict the thickness of a frozen fringe and the spacing of ice lenses in subaerial and subglacial sediments.

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#### **MS48**

Physics-based Simulations of Hydrologic Processes in Permafrost-affected Regions: Progress and Remaining Challenges

High-resolution process-resolving simulations of coupled thermal hydrologic processes are important tools for understanding the evolution of permafrost landscapes in a warming Arctic. Such models are designed to bridge from the scales of laboratory and site-scale investigations to the coarse scales of Earth system models. We summarize progress in simulating integrated surface/subsurface thermal hydrology of degrading permafrost landscapes with the Amanzi-ATS code. The permafrost modeling capability in Amanzi-ATS combines surface energy balance models, a nonisothermal variant of Richards equation that includes freezing/thawing for pore water, a nonisothermal extension of the diffusion wave equation for surface water, and snow thermal models. Time-stepping is by the backward Euler method with custom globalization algorithms to stabilize the iterative solution around the water/ice phase change. An intermediate-scale variant of Amanzi-ATS also includes the effects of subsidence and microtopographic evolution caused by melting of unevenly distributed ice bodies in the subsurface. Efforts to evaluate these simulation capabilities against field observations will be described. Multidecadal projections suggest microtopographic evolution will accelerate drying of tundra landscapes in a warming climate. Remaining modeling challenges and uncertainties will be discussed.

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#### MS48

### Solvers for Permafrost Soil Models at Multiple Scales

We study solvers for the nonlinear heat equation with phase change between liquid and ice where the energy to change phase is given by the enthalpy-temperature relationship  $w \in \alpha^{(m)}(\theta)$ , considered at multiple scales, e.g., for  $m \in \{pore, Darcy\}$ . At the pore-scale, this relationship is single-valued when considered between  $(\theta, \chi)$  and w. At Darcy scale in we allow this relationship to be

multi-valued (P\* model) close to 0 due to the presence of macro-pores, but away from zero is essentially smooth due to the Gibbs-Thomson effect leading to a continuum distribution of freezing temperatures. Our numerical model is implicit in time and based on Finite Volume in space, and requires both global and local nonlinear solvers which face challenges due to nonsmoothness of  $\alpha$ . We discuss robustness and efficiency of various solvers including Newton-Anderson. We also show convergence based on newly developed analytical solutions.

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#### MS48

#### A Tensor-Train Stochastic Finite Volume Method for the Uncertainty Quantification in Advection-Dominated Pdes

Many problems in physics and engineering are modeled by systems of partial differential equations such as the shallow water equations of hydrology, the Euler equations for inviscid, compressible flow, and the magnetohydrodynamic equations of plasma physics. The initial data, boundary conditions, and coefficients of these models may be uncertain due to measurement, prediction, or modeling errors. The stochastic finite volume (SFV) method offers an efficient one-pass approach for assessing uncertainty in hyperbolic conservation laws. The SFV method has shown great promise as a weakly-intrusive PDE solver for uncertainty quantification. However, in many relevant applications, the dimension of the stochastic space can make traditional implementations of the SFV method infeasible or impossible due to the so-called curse of dimensionality. We introduce the Tensor-Train SFV (TT-SFV) method within the tensor-train framework to manage the curse of dimensionality. This integration, however, comes with its own set of difficulties, mainly due to the propensity for shock formation in hyperbolic systems. To overcome these issues, we have developed a tensor-train-adapted stochastic finite volume method that employs a global WENO reconstruction, making it suitable for such complex systems. This approach represents the first step in designing efficient tensor-train techniques for uncertainty quantification in hyperbolic systems and conservation laws involving shocks.

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#### **MS49**

Uncertainty Quantification for Interactions Across Lake, Atmosphere, and Land Model Components in the Great Lakes Region

In this work we formulate a neural network surrogate-based method to assess the uncertainty associated with interacting physics parameterizations across the lake, atmosphere, and land surface within a high-resolution regional climate model of the Great Lakes region. Small perturbed physics ensembles of the model during the 2018 summer are used to train the surrogate model to predict lake surface temperature and near-surface air temperature. We present our findings of the estimated magnitude of uncertainties, how these vary spatiotemporally, and the dominant sources of uncertainty – atmosphere, lake or land parameterizations or their interactions - which are deduced from the surrogate model. We also discuss some limitations of the methodology, such as the small number of ensembles used to train the surrogate model and how representative it can be of the true model uncertainty. In addition, we address specific structural model biases in the lake that are identified when compared to observations, which cannot be accounted for by our physics uncertainty setup.

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#### MS49

#### Calibration and Uncertainty Quantification for Atmospheric Gravity Wave Parameterizations in Global Climate Models

Improved simulations of the stratosphere, including the properties of the QBO and polar vortex variability, will depend, amongst other things, on the representation of gravity waves in climate models (gravity wave parameterization, or GWP). In this work, we will present a) attempts to replace existing physics-based GWPs with ML methods, including those that represent lateral propagation of GWs, b) the application of calibration techniques (Ensemble Kalman methods and approximate Bayesian methods) to calibrate parameters in GWPs to observed properties of the QBO, and c) uncertainty quantification for both physics-based and ML-based GWPs.

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#### **MS49**

# Modeling Fire-Driven Pyrocumulonimbus: New Uncertainty Quantification Opportunities

A clear increasing trend in large-scale wildfire events has recently been observed across many regions worldwide. These large wildfires can intensify and trigger extreme pyrocumulonimbus (PyroCb) convection, which, in terms of total aerosol emissions, is comparable to moderate volcanic eruptions. Such events can result in significant socioeconomic losses. PyroCb involves complex, multi-scale physical processes, including fire emissions, plume devel-

opment, aerosol-cloud interactions, lightning generation, and smoke transport. However, the underlying mechanisms of PyroCb remain poorly understood, contributing to large uncertainties in its modeling. Here we enhanced the PyroCb simulation within the Energy Exascale Earth System Model (E3SM) by improving key processes: the non-hydrostatic regionally refined mesh (RRM), plumerise scheme, fire-induced water vapor transport, and highresolution fire forcing. The efficient RRM mesh design and tracer advection enable wildfire simulations to achieve high computational efficiency, supporting multi-year ensemble simulations, which are essential for robust quantification of model uncertainties. We will demonstrate several uncertainty quantification (UQ) approaches using a low-resolution E3SM ensemble of approximately 100 simulations in conjunction with satellite observations. Furthermore, we will highlight new opportunities and requirements for UQ that arise from pyroCb case simulations with our new E3SM-RRM wildfire framework.

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#### MS50

# A Multigrid Reduction Framework for Scalable Multiphysics Simulations

This talk presents recent advancements in the multigrid reduction (MGR) method tailored for solving large-scale linear systems arising in coupled multiphysics simulations. The extended MGR framework has been enhanced to support a broader range of applications, including thermal and isothermal compositional flow, multiphase poromechanics, and simulations involving fractured reservoirs. Designed with both performance and portability in mind, the method has been fully integrated into the hypre library, enabling efficient execution on modern CPU and GPU architectures, including hardware from NVIDIA and AMD. Extensive validation using the GEOS simulator demonstrates the methods robustness and scalability, even in the presence of strong multiphysics coupling and highly heterogeneous materials. The results highlight the capability of the enhanced MGR framework to efficiently handle problems with billions of unknowns, establishing it as a powerful solver technology for complex multiphysics applications.

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#### **MS50**

Progress and Challenges in Multiphysics Simulation of Enhanced Geothermal Systems with PFLO-

#### TRAN and PETSc

Vast and untapped potential sources of geothermal energy are widespread, but naturally occurring geothermal systems are comparatively rare, requiring a fortuitous combination of hot rock, fluid saturation, and hydraulic permeability. Enhanced geothermal systems (EGS), in which humans inject fluid into the subsurface to establish open, well-connected fracture systems through which fluid can be continuously circulated, might greatly increase the amount of usable geothermal energy. A major challenge in making EGS viable is the ability to predict and, ultimately, control rock behavior and fluid movement within an EGS reservoir. We will discuss development of capabilities in PFLOTRAN for simulating reactive flow and transport in EGS as well as real-time monitoring of stress-permeability evolution through time-lapse electrical resistivity tomography. This involves solving "inner loop" multi-physics forward simulation problems surrounded by an "outer loop" in which simulated and observed monitoring data are used to perform multi-physics joint inversion for the time evolution of 3D permeability and porosity. Such calculations present some special challenges for the underlying algebraic solvers. We will discuss some of the approaches we have adopted so far using the PETSc library's composable nonlinear and linear solvers and preconditioners as well as speculate on future approaches they may be promising.

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#### MS50

# Evaluating Multi-Physics Preconditioning Strategies for Ice-Sheet Dynamics in Albany Land Ice

The development of robust and efficient multi-physics preconditioners is crucial for drastically improving the computational performance of large-scale, thermo-mechanically coupled ice-sheet models. The primary challenge in simulating ice sheets at scale is solving the linear system associated with a thin, high-aspect ratio mesh. This problem is exacerbated by the coupling of first-order Stokes, a nonlinear elliptic problem for ice velocity, with the enthalpy formulation, an advection dominated problem. In this presentation, we show the performance of various multi-physics preconditioning strategies to assess a viable strategy for simulating the large, coupled ice-sheet model on large GPU supercomputers such as Perlmutter and Frontier.

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#### MS51

From Emulation to Explanation: Compressing Climate Models and Geospatial Data with Machine Learning

We present two machine learning approaches that reduce

the complexity of large-scale climate simulations and enable interpretable predictions in geospatial data. First, we present ISEFlow, a neural network-based surrogate model that emulates computationally expensive ice sheet models for sea level projection. By compressing the dynamics of complex physics-based models into a lightweight neural architecture, the ISEFlow emulator enables scalable exploration of climate scenarios, while preserving uncertainty estimates via deep ensembles and normalizing flows. Second, we describe a prototype-based neural network architecture that enhances model interpretability by learning a reduced set of representative training instances that are embedded directly in the models prediction logic. This compressed, instance-based representation enables scientifically meaningful explanations for model predictions in high-dimensional spatiotemporal climate data. Together, these techniques demonstrate how data-driven compression through emulation and prototype learning can accelerate geophysical modeling and transform large-scale geospatial data into scientific insights.

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#### MS51

#### Discovering Complex Seismic Wave Physics using Compact and Interpretable Deep Learning

Seismic wavefields are naturally multiscale due to the complex wave propagation in a heterogeneous Earth medium. While conventional approaches to wavefield simulation incorporate a low-order complexity obtained by seismic tomographic methods, seismologists tend to simulate broadband seismic wavefields by superimposing a stochastic time series to represent unexplained, short-wavelength phenomena. The densification of seismic networks and the emergence of technologies, such as Distributed Acoustic Sensing (DAS), highlight the shortcomings of this hybrid approach by recording more complexity in the real seismic signals. We develop a new deep learning framework to simultaneously predict the three pillars of seismological data: geospatial wavefields, earthquake source parameters, and simplified Earth structural models, from input seismograms (time series) of sparse sensor networks. The novel method incorporates multi-scale reconstruction in both frequency and space using multi-resolution shallow recurrent decoders (MrSHRED), an interpretable latent space constrained by sparse identification of nonlinear dynamics (SINDY), effectively a lossy compression of wavefield data. We develop the elements of this framework on 3D numerical simulations of seismic wavefields and test it on distributed acoustic sensing and broadband seismic data.

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#### MS51

## ZFP: A Compressed Array Representation for Efficient Computations and Storage

With the growth in acquired and simulated science data rapidly outpacing advances in storage, the geoscience community is turning to lossy data compression as a means to keep data volumes manageable. However, lossy compression introduces additional error that needs to be understood and controlled so that compression errors do not adversely impact data analysis and scientific conclusions. We present ZFP, one of the leading compressors for numerical data, and detail efforts to analyze biases, correlations, distributions, and bounds on compression errors and their impact on geoscientific data analysis. ZFP not only serves as a compact format for offline storage but also provides random-accessible, read-write array primitives that make it suitable as a compressed in-memory representation for numerical computations. We provide examples of using ZFP arrays for visualization, data analysis, and numerical computations like PDEs, where data is decompressed ondemand and re-compressed as needed to reduce not only storage but also data movement, which increasingly dictates performance and power usage in high-performance computing applications.

#### Peter Lindstrom

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#### MS52

# Solvability of a Predator-Prey Model with Mixed Boundary Conditions: Theoretical and Numerical Framework

The study of prey-predator models provides great insights about the dynamic relationships between species in an ecosystem, providing key insights into population fluctuations, ecological balance, mutual co-existence, and strategies for biodiversity conservation. Consideration of the spatial distribution pattern of species captures the realistic nature of the population interaction. This article establishes the existence of a unique weak solution for the prey-predator model in a three-dimensional bounded domain with mixed boundary conditions on the Lipschitz boundary using Schauder's fixed-point theorem. Further, a finite element scheme is proposed for the prey-predator model comprising Galerkin finite element discretization in space and implicit CrankNicolson discretization in time. Numerical simulations are performed to validate the proposed numerical scheme, and the impacts of prey-tactic sensitivity and diffusion coefficients in the prey-predator system are explored.

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#### MS52

#### Modeling Soil Formation and Vertical Accretion in Coastal Wetlands Through a Flexible Coupling Framework

Coastal wetland sustainability depends on the balance between vertical soil formation processes and external environmental forces. This work presents a modeling framework focused on simulating the vertical accretion of coastal marshes by coupling hydrodynamic and sediment inputs with a simplified soil dynamics model. The framework emphasizes the representation of inorganic sediment deposition and organic matter accumulation as key drivers of marsh surface accretion. The model tracks as soil cohorts the successively buried surface loadings with an accounting of the downcore processes over time. Flexibility is built into the system, enabling the use of interchangeable drivers from either model-based outputs or field-based observations to support accretion simulations. Initial applications focus on point-based simulations at selected CRMS sites near the Atchafalaya and Terrebonne basins, using observed tidal and sediment conditions. This approach provides a computationally efficient tool for exploring soil column dynamics, marsh resilience to sea-level rise, and responses to sediment supply shifts, supporting broader efforts to integrate biogeochemical and ecological processes into wetland modeling.

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#### **MS52**

#### Forecasting Mosquito Ecology in Maricopa County Using Climate Factors and Bayesian Techniques

Climate change is expected to alter the large-scale distribution of mosquito populations and disease patterns, making predictive modeling increasingly essential due to its complexity. Using a 10-year time series (20142024) of weekly mosquito abundance and West Nile Virus (WNV) prevalence data collected in Maricopa County, we investigated how local climate variations influence mosquito population dynamics and disease transmission. We developed a mechanistic model of WNV dynamics driven by daily temperature and 30-day accumulated precipitation to predict mosquito populations and WNV prevalence. Our statistical forecasting framework leveraged climate factors to improve predictive accuracy by integrating adaptive modeling techniques and Bayesian methods to infer precise model parameters. To achieve this, we applied the Ensemble Kalman Filter (EnKF) method to estimate both timevarying and static parameters. Using generalized additive models (GAMs), we forecasted these time-varying parameters on a two-week basis, incorporating precipitation and temperature as covariates. These forecasts were used as inputs for a mechanistic ordinary differential equation (ODE) model, which predicted mosquito abundance and WNV prevalence while capturing associated uncertainties. This enhanced methodology provides actionable insights for public health decision-makers, supporting resource allocation and improving mosquito-borne disease prevention outcomes.

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#### **MS53**

Addressing Uncertainty in the Relationship Between the Quasi-Biennial Oscillation and Convection in E3SM

The quasi-biennial oscillation (QBO) is the leading mode of variability in the stratosphere, with effects on weather patterns and temperature in both the tropics and midlatitudes. Observations show that the QBO influences deep convection in the tropics and modulates another mode of variability called the MaddenJulian oscillation (MJO). We investigate the QBO representation in E3SM, focusing on its influence on deep convection and the MJO. Our analysis is based on cloud regimes and uses nudging of the zonal winds to produce a more consistent QBO.

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#### MS53

Probabilistic Projections of the Amery Ice Shelf Catchment, Antarctica, under Conditions of High Ice-Shelf Basal Melt

Antarctica's Lambert Glacier drains about one-sixth of the East Antarctic Ice Sheet and is stable thanks to buttressing by the Amery Ice Shelf. Earlier projections showed significant mass loss would require near-total ice-shelf removal, unlikely with modest ocean warming before 2100. Yet climate models now project abrupt ocean warming after 2100 as plausible. We quantify parametric uncertainty in the Lambert Amery systems response to such warming using a perturbed-parameter ensemble of the MPAS-Albany Land Ice model at 420 km resolution. Six parameters (basal friction, ice stiffness, calving rate, and ice-shelf basal melt) were sampled via 200-member space-filling Sobol sampling scheme. We build Gaussian process emulators for efficient exploration and calibrate parameters against observations of mass balance, grounding-line, and calving-front movement with expert priors. A subset of simulations is projected to 2300 under low- and high-emission scenarios using climate-forcing data. Multivariate emulators combining GP regression and PCA emulate sea-level contribution time series. After calibration, posterior distributions yield greater mass loss and reduced variance versus priors. Uncertainty remains large until 2130, making scenarios indistinguishable early in the century; projections diverge within decades following rapid warming. This study offers efficient Bayesian calibration and uncertainty propagation workflow.

<u>Sanket Jantre</u> Brookhaven National Laboratory sjantre@bnl.gov

#### **MS53**

### Uncertainty Quantification under Model Misspecification: The Sandwich Estimator

In this talk I will review basic elements of Frequentist inference, specifically maximum likelihood (ML) and Mestimation to point out a critical flaw of Bayesian methods for model training and uncertainty quantification. Under model misspecification, the sensitivity and variability matrices of the ML model parameter values provide conflicting information about the observed Fisher information of the data. As a result, the ML parameter covariance matrix does not simplify to the inverse of the observed Fisher information, as suggested by naive ML estimators and Bayesian methods but amounts instead to the so-called sandwich matrix  $\widehat{\mathcal{G}}_n^{-1}$  where the observed Godambe information  $\widehat{\mathcal{G}}_n$  is the fundamental currency of data informativeness under model misspecification. The sandwich matrix is a metaphor for a meat matrix  $\widehat{\mathbf{B}}_n$  between two

bread matrices  $\widehat{\mathbf{A}}_n$ . I will demonstrate the implications of the sandwich variance estimator using different case studies involving simple statistical distributions and dynamic models of the rainfall-discharge transformation. Then, I will introduce a new recipe of sandwich-adjusted MCMC simulation, which yields asymptotically valid sandwich parameter estimates under misspecification.

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#### MS54

## High-Performance Preconditioning for Matrix-Free Contact Mechanics Simulations

Matrix-free iterative solvers have emerged as a promising approach in the fluid dynamics and solid mechanics communities as a memory-efficient alternative to traditional sparse matrix approaches, where memory traffic is often the primary bottleneck. This work explores matrix-free techniques for contact mechanics under quasi-static conditions on semi-structured grids. To enhance the convergence of iterative solvers, we introduce a geometric multigrid preconditioner with all components the smoother, restriction, and prolongationimplemented in a fully matrix-free manner. We present performance results of these matrix-free operator kernels, demonstrating superior performance compared to matrix-based counterparts on GPU architectures.

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#### MS54

# Adaptive Conservative Time Integration (ACTI) for Efficient and Accurate Simulation of Reactive Transport in Heterogeneous Porous Media

Modeling reactive transport in heterogeneous porous media is challenging, particularly when fast reactions amplify the effects of numerical diffusion. We present a modified version of Adaptive Conservative Time Integration (ACTI) scheme that eliminates the sorting step of the original formulation, thereby improving the computational efficiency. We extend the use of ACTI to cases with fast reactive transport and demonstrate a significant reduction in spurious numerical diffusion relative to both conventional implicit and explicit schemes. Moreover, by selecting timesteps near the local stability (CFL) limit in each control volume, the method achieves substantial computational savings compared to standard explicit approaches that are bound by a global stability limit. These developments provide a foundation for scalable and accurate simulation of reactive multiphase systems in energy and environmental applications.

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#### MS54

#### Robust Preconditioners for the Coupled Stokes-Darcy Problem

We develop reliable simulations for the Stokes-Darcy coupled problem, which models the interaction between free flow and porous medium flow. The complexity of interface coupling often degrades the performance of standard numerical methods. To address this, we design parameterrobust preconditioners within the operator preconditioning framework, specifically tailored to multiphysics problems like the Stokes-Darcy system. Our approach combines rational approximations for fractional operators, deflation techniques to address near-kernel spaces, and specialized multigrid methods to enforce interface constraints. We establish theoretical guarantees for the parameter-robustness of the proposed preconditioners and validate their effectiveness through numerical experiments. The results demonstrate the scalability and practical applicability of our methods in complex, real-world scenarios.

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#### MS54

### Adaptive Nonlinear Domain-Decomposition for Scalable Reservoir Simulation

We recently proposed a method to accelerate convergence in nonlinearly stiff reservoir simulations by prepending local subdomain solves to each global Newton iteration, improving initial guesses and reducing the need for global corrections. Our implementation in the open-source, operational OPM Flow simulator employs MPI/OpenMP parallelization of the resulting two-level partitioning: the global Newton step is distributed across MPI ranks, each managing multiple subdomains. Nonlinear stiffness leads to highly localized computational cost for subdomain solves, many of which can be bypassed adaptively based on convergence history and solution changes. This approach has demonstrated significant speedup for industry-grade  ${\rm CO2}$ storage and oil recovery models. Through examples, we highlight the resulting challenges in load balancing and partitioning, as the cost of the global solve depends on the number of cells per rank, while local solve costs vary spatially due to nonlinear stiffness.

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#### MT1

#### **GEOS Simulation Framework**

GEOS is an open-source code for modeling subsurface processes, with applications in carbon storage, hydrogen storage, geothermal energy, and oil and gas recovery. This minitutorial provides an introduction to using, understanding, and extending GEOS, making it accessible to both new users and developers interested in contributing to its capabilities. The session is structured into three parts: 1. Getting Started with GEOS A hands-on tutorial on installing and running GEOS, following best practices from the online documentation. Participants will learn how to set up and execute basic simulations. 2. Understanding the Core Physics and Numerics An overview of the governing equations and numerical methods in GEOS, including how the finite element method is used to model geomechanical deformations and how the finite volume method is applied to flow and transport. 3. Extending GEOS: Developing New Physics Modules A brief guide to implementing new physics capabilities within GEOS. This section will cover the softwares modular design and provide an introduction to adding new capabilities to the code. By the end of this tutorial, attendees will have a practical understanding of how to use GEOS, a conceptual grasp of its underlying numerical methods, and insights into developing new features within the code. The session is ideal for researchers, engineers, and developers working in subsurface energy and storage applications.

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#### MT2

PETSc the Portable Extensible Toolkit for Scien-

#### tific Computation

PETSc, the portable extensible toolkit for scientific computations, is used as an algebraic backend in many scientific libraries around the world. It has been deployed on various architectures, from laptops to large exascale systems. In the tutorial, we will cover the basics of PETSc, moving quickly to the solution of linear, nonlinear, and time-dependent systems arising from PDE. We will also present some other advanced capabilities, for example, using its sister libraries SLEPc and TAO, to solve eigenvalue problems, compute singular value decompositions, and solve bound constrained optimization problems. We will focus on examples drawn from geoscience, implemented live, in either C, Fortran or Python, depending on the attendees preference

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#### MT2

## PETSc the Portable Extensible Toolkit for Scientific Computation

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#### MT3

#### UM-Bridge (UQ and Modeling Bridge)

Uncertainty Quantification (UQ) plays a crucial role in geoscience. Uncertainty propagation allows trustworthy predictions in the face of measurement errors. Conversely, Bayesian inference determines model parameters from observed data, discovering model ambiguities and the influence of data quality. Despite its scientific value, UQ is held back by a need for interdisciplinary expertise as well as the technical complexity of integrating simulators with advanced UQ codes and (possibly) high-performance computing (HPC). This tutorial introduces UM-Bridge [1], a universal software interface that facilitates seamless integration of complex simulation models with an entire range of leading UQ packages. Separating concerns between simulation and UQ, UM-Bridge allows rapid development of cutting-edge applications. UM-Bridge further enables scaling workflows to HPC and cloud. UM-Bridge supports 10 UQ packages, more than 20 scientists across ;15 institutions contributed to UM-Bridge's UQ benchmark library, and early industry adoption is taking place. In the tutorial, participants integrate UQ in simulation workflows using UM-Bridge, including advanced UQ software controlling simulations on live cloud clusters. We explicitly encourage participants to bring their own simulators and UQ codes to try out during the hands-on exercises. [1] L. Seelinger, A. Reinarz, et al, Democratizing uncertainty quantification, JCP, 2025

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#### MT3

#### UM-Bridge (UQ and Modeling Bridge)

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#### PP1

### Numerics-Informed Neural Networks for Parabolic PDEs

We investigate numerics-informed neural networks (NINNs) for two-dimensional parabolic partial differential equations (PDEs), focusing on Backward Euler (BE) time-stepping as both a classical baseline and a neural surrogate. In the NINN formulation, a compact U-Net learns step-by-step updates while training on the BE residual, and the method enforces Dirichlet boundary conditions through boundary lifting. Using manufactured trigonometric and Gaussian solutions under parabolic h), we benchmark NINNs against time scaling (?t finite-difference Backward Euler solvers. The BE method provides a stable baseline, while NINNs achieve comparable accuracy and, on finer grids, occasionally surpass it with faster convergence. We also study sensitivity to time-step size, training schedules, and optimization parameters. Together, these results highlight the reliability of classical BE schemes and demonstrate the promise of NINNs as lightweight neural surrogates for time-marching diffusion problems.

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#### PP1

#### Fast Iterative Filtering Decomposition of Non-Stationary Signals. Energy Conservation and Orthogonality of the Decompositions

Fast Iterative Filtering (FIF), an alternative algorithm to Empirical Mode Decomposition (EMD), has been successfully applied, in recent years, in various applied fields of research, see for instance [1] and references therein. However, its mathematical framework is not complete. In particular, it is still an open question if FIF can be guaranteed a priori to preserve the energy of the original signal during a decomposition. The fact that a signal s in  $L^2$  is decomposed by FIF in a set of Intrinsic Mode Functions (IMFs) which are non-orthogonal, makes this method not that attractive from a mathematical perspective and raises the concern, from an applied point of view, that the method could possibly introduce spurious oscillations which are not present at all in the original signal. In this poster, we introduce a new definition of energy of the signal s that is conserved in its decomposition into IMFs via FIF, and we leverage it to introduce a new definition of orthogonality that can be applied to the IMFs derived via FIF. [1] G. Barbarino, A. Cicone. Conjectures on spectral properties of ALIF algorithm. Linear Algebra and its Applications, Volume 647, pages 127-152, 2022.

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#### PP1

# Numerical Modelling of Fracture Growth Using Periodic Quadratic $C^1$ B-Splines

The geometry of growing fractures is modelled using sequences of  $C^1$  periodic quadratic B-splines in three dimensions. Displacement equations are solved on the polygonally discretised geometry of fractured medium and the fracture growth is determined based on stress intensity factors obtained from solutions to linear elastic deformation equations. As growth advances, multiple adapting  $C^1$  Bspline curves are generated and combined to construct a periodic and differentiable NURBS surface. The NURBS surface further enables a smooth approximation of the displacement solution using least-squares method, which is  $C^1$ continuous across the fracture front. As opposed to triangular representations, the proposed parametric approach captures smooth fracture growth by eliminating geometric errors from polygonal discretisation and enabling continuous stress field variation through increased solution field continuity. This approach also supports straightforward refinement in radial and transverse directions and smooth solution mapping during simulation. The proposed approach reduces geometric modelling cost whilst preserving detail in multi-fracture three-dimensional fracture network growth simulations, in order to support coupled multi-physics simulations in fractured or fracturing media. Examples of growth at the 10- and 100-meter scale are shown, with systems of up to 6,400 simultaneously growing explicit fractures.

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#### PP1

### Semi-Lagrangian Exponential Integrators: Numerical Foundations and Possibilities

Governing equations modeling atmospheric circulation are dominated by nonlinear advective processes and stiff linear waves, which impose stability restrictions. With these conditions, special numerical methods are required; in this work, we further explore the semi-Lagrangian exponential method proposed by Peixoto and Schreiber (2019). To construct this class of methods, it is necessary to investigate Exponential Integrators and semi-Lagrangian methods, as well as their coupling. Here, we explore the numerical foundations of the semi-Lagrangian exponential method, explaining the main properties of exponential integrators, particularly their effectiveness when handling stiff linear problems, and also investigating semi-Lagrangian methods, which are known for their greater stability when compared with explicit finite difference methods for advection problems. We will present the general construction of semi-Lagrangian exponential methods and apply them to prototype hyperbolic partial differential equation problems, discussing further possibilities to increase the methodology to higher accuracy orders, extending the recent work of Stein et al 2025.

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#### PP1

#### Forecasting Operational and Non-Operational Flows in River Diversions with Convolutional Neural Networks

Forecasting flow through hydraulic infrastructure, such as freshwater diversions, remains a critical yet underdeveloped component of large-scale water management systemsparticularly during periods when structures are not actively in use. During these non-operational periods, flows such as leakage through diversion structures can still meaningfully influence downstream hydrology, yet are often excluded from predictive modeling efforts. This study applies a data-forward approach to forecast both operational and non-operational flows from river diversion structures utilizing a convolutional neural network (CNN), using the Bonnet Carr Spillway (USA) within the Mississippi River Basin as a case study, where diversion flows are orders of magnitude smaller than basin-wide flows. Historical leakage volumes from the spillway are estimated using a modified, broad-crested weir equation to refine stage-discharge relationships that may have been previously underestimated. The CNN is trained on multi-source time series inputsincluding upstream discharge and meteorological patternsto predict the timing and magnitude of non-operational flows, as well as the probability of diversion operation events,

days to weeks in advance. While developed for the Bonnet Carr Spillway, this approach provides a tool for other engineered diversion where forecasting both operational and non-operational flows is critical for flood risk mitigation, water quality management, and resource planning.

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