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I-FENN with DeepONets: accelerating simulations in coupled poro-mechanics problems

Mostafa Mobasher (New York University Abu Dhabi)
Diab Abueidda (New York University Abu Dhabi), Fouad Amin (New York University Abu Dhabi), Panos Pantidis (New York University Abu Dhabi)

Abstract

Coupled multiphysics problems involve highly complex and computationally expensive simulations. This research presents a novel framework integrating a deep operator network (DeepONet) with the finite element method to address coupled multiphysics problems, reducing computational costs while maintaining accuracy. By decoupling the multiphysics interactions, the integrated framework substantially reduces computational cost while offering exceptional flexibility and efficiency. DeepONet can effectively learn operators, mapping input to output functions, with a reduced generalization error and a high order of convergence. The DeepONet architecture consists of two sub-networks: the “branch” and “trunk” networks. The branch encodes the input function at fixed sensors (locations), while the trunk encodes the target output locations. The branch and trunk outputs are then aggregated to form the final DeepONet output. A gated recurrent unit (GRU) network is integrated into the branch network, enhancing DeepONet's capability to consider time dependency for mapping full-field sequential time-series inputs to their corresponding responses. The authors recently proposed the Integrated Finite Element Neural Network (I-FENN) framework, offering advancements in mechanical problems with demonstrated enhanced performance. This research introduces DeepONet to the I-FENN framework, revolutionizing its architecture and introducing extended generalizability. The proposed DeepONet model is capable of incorporating essential and natural boundary conditions, as well as body loads, in both two-dimensional and three-dimensional simulations. In addition, the DeepONet/I-FENN integration leverages the robust C++ FE library Deal.ii for optimized parallel processing on HPC systems. The validity of the proposed work is demonstrated through numerical examples explicitly focusing on thermo-elasticity and poro-elasticity, exploring computational efficiency, accuracy, and generalization capabilities. In addition, results have shown the framework's capability of solving problems with fine meshes despite being trained on coarser meshes, highlighting its potential as a scalable and high-performance solution for complex multiphysics poromechanics applications.

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Phase field modeling of hydraulic fracture in layered rock

Lingfu Liu (Cornell University)
Zahera Jabeen (ExxonMobil Technology and Engineering Company-Research), Chloé Arson (Cornell University)

Abstract

Hydraulic fracturing is a moving boundary problem: the fracture tip advances in the solid matrix, the displacement jump that separates fracture faces is not uniform, and the fluid that invades the fracture may lag behind the tip, creating a capillary interface in the fracture. The Phase Field (PF) Method is attractive because it relies on a simplified representation of interfaces: auxiliary variables are introduced to label spatial positions as one phase or another. The model is based on thermodynamic equations that provide the evolution laws of the field variables (such as stress, pore pressure and temperature) and those of the phase variables. When the PF equations are discretized in the FEM, each element is assigned one or more phases (for example, intact/damaged porous solid, liquid/gas fluid) such that each element represents a fluid-saturated continuum porous solid, and the edges of adjacent elements of different phases mark the positions of interfaces. The spatial distribution of values taken by the damage phase variable (typically, 0 for intact elements and 1 for damaged elements) determines the geometry of the fracture (all elements where the damage equals 1). PF models are computationally efficient and robust because they do not require dynamic remeshing, and they can be formulated to avoid mesh dependency. Each fracture is represented as smeared damaged zone, the size of which is dependent on an internal length parameter that enables a realistic representation of fracture geometries. The variational approach to fracture mechanics was first presented by Bourdin et al. (2008). A unified formulation was then proposed by Wu (2017). Previous studies highlighted that the parameters that influence the trajectory of hydraulic fractures in anisotropic media are mainly rock stiffness, fracture toughness, fluid viscosity, interface friction properties, geological stresses, and injection pressure or rate. But little is known on the amount of energy or work input that is needed to achieve specific propagation paths, such as propagation across and along one or more inter-layers vs. a straight path across layers. This study thus aims to understand whether it is possible to control the path of a hydraulic fracture in a layered rock mass.

Towards this goal, a hydraulic fracturing model is implemented in the Multiphysics Object-Oriented Simulation Environment (MOOSE), an open-source finite element analysis framework designed to solve complex Multiphysics problems (Giudicelli et al., 2024). The fluid lag behind the fracture tip is ignored, such that the hydraulic fracturing problem is formulated as a two-phase system: the elastic (non-damaged) fluid-saturated porous medium, and the fluid-saturated fracture, which is characterized by a rock damage field variable. A multi-physics model that couples hydraulic, mechanical, and damage-phase fields is developed. A PF fracture model is tightly coupled with a poroelasticity model, and an implicit time discretization is adopted. Residual scaling is adopted to accelerate convergence. One of the

key assumptions of the PF fracture model is the decomposition of the deformation energy stored in the solid skeleton, which can only induce damage propagation in tension or shear. The formulation of the model allows one to track the dominant fracture propagation mode at any step of the simulation. The mechanical fracture propagation criterion is expressed in terms of Biot's effective stress. Mass transport in the non-damaged porous medium is modeled by Darcy's law, with an isotropic permeability that follows Kozeny Carman's equation. Fracture permeability is expressed as a function of the characteristic crack width, the elastic porosity, and the normal to the fracture plane, which is calculated from the gradient of the damage field variable. A linear interpolation is used to calculate permeability in the transition zones between the non-damaged porous matrix and fractures. The mechanical stiffness tensor in the damaged elements is calculated as the product of the non-damaged stiffness by a degradation function, which is a function of damage.

Two-dimensional simulation results are presented. The model is first validated against analytical and benchmark numerical solutions for purely mechanical fracture propagation and poro-elasticity problems. Then, the model is compared to other numerical approaches for simulating hydraulic fracturing in a homogeneous porous medium. Next, a sensitivity analysis on the flow rate, mechanical boundary conditions, and distribution of natural fractures is presented. An example simulation result, shown in Figure 1, indicates that the model can capture the intersection of a hydraulic fracture with a natural fracture, followed by the bifurcation of the hydraulic fracture after intersection. The pore pressure in the fracture increases with the injected volume. The pore pressure drops in the damaged zone around the fracture, as the fluid invades the damaged matrix through the (micro) fracture planes. In the non-damaged matrix, the pore pressure increases with the injected volume due to the undrained boundary conditions.

Lastly, simulations are conducted to investigate hydraulic fracture propagation in a layered porous medium. The inter-layers are represented by damaged elements with higher permeability and lower stiffness and toughness than the bulk rock. The sensitivity of the trajectory of the hydraulic fracture to the biaxial far-field stress conditions and orientation of the inter-layer interfaces is assessed. Results are benchmarked against published experimental results, e.g., (Lee et al., 2015; Llanos et al., 2017) and against numerical results, e.g., (Jin and Arson, 2020). An exhaustive parametric study is used as a basis to assess in which conditions the hydraulic fracture is arrested by, offset by, crosses, or infiltrates a discontinuity. The energy input necessary to debond inter-layer interfaces under various stress and injection conditions reported in the literature for typical geomechanical reservoir operations is calculated. The distribution of energy dissipated by hydraulic fracture propagation vs. inter-layer debonding is analyzed. Together, the results presented in this study highlight the conditions in which the inter-layer interfaces debond and understand the processes that dominate the evolution of the hydraulic fracture pattern.

Figure 1. Simulation of hydraulic fracturing induced by fluid injection through a vertical notch in an elastic porous medium that contains a horizontal natural fracture. Injection rate: 1 kg/m2/s. Impermeable boundary conditions, fixed horizontal displacements at the left and right boundaries, fixed vertical displacements at the top and bottom boundaries. Top left: initial damage. Top right: final damage. Bottom left: final mean effective stress. Bottom right: final pore pressure.

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Modular Simulation of Coupled Unsaturated Flow and Geomechanics with GReS: A Pore-scale Application

Andrea Franceschini (University of Padova)
Daniele Moretto (University of Padova), Eduardo Castro (University of Padova), Massimiliano Ferronato (University of Padova)

Abstract

It is well-known that accurate prediction of geomechanical behavior is essential for the effective and safe management of subsurface resources. These systems are governed by the interplay of multiple coupled physical processes, including fluid flow, poromechanics, fault activation, heat transport, and chemical reactions, evolving over several time and space scales. While significant advances have been made in modeling individual phenomena, substantial challenges remain in achieving robust and scalable coupling of geomechanics with other relevant processes across domain boundaries and discretization schemes.

GReS (Geomechanics Reservoir Simulator) is an open-source modular simulation platform designed to support the development and prototyping of advanced numerical methods for fully coupled, multi-physics, and multi-domain problems in poromechanics. GReS is implemented in MATLAB, aiming to lower the entry barrier for researchers and facilitate rapid testing and extension of new algorithms. Its modular architecture allows for easy integration of new physical models, discretization schemes, and solver strategies.

Recent developments in GReS include the simulation of unsaturated flow by using Richards' equation discretized by a finite volume strategy. Richards' equation is particularly important in meso-scale and pore-scale simulations, where partial saturation, capillary effects, and saturation-dependent permeability can affect the effective stress and deformation of the porous skeleton. This is especially relevant in shallow subsurface processes and in materials undergoing localized compaction or collapse, such as in the case of weak or evolving porosity structures.

In addition, the multi-domain framework based on a mortar-based coupling has been generalized to support Richards' flow alongside other physics, such as single-phase flow and poromechanics, enabling the use of non-conforming meshes and heterogeneous discretizations across interconnected subdomains. This provides a flexible and robust platform for modeling complex coupled processes in partitioned domains.

To demonstrate the capabilities of GReS, we will present simulations of a pore-scale model capturing the interaction between unsaturated flow and mechanical deformation in a heterogeneous porous structure. This case highlights how the modular and extensible design of GReS enables detailed investigation of strongly coupled multiphysics problems at the pore-scale, including the role of evolving saturation in mechanical stability.

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Non-intrusive global-local method for the poroelasticity model with localized pressure effects

Hemanta Kumar (The University of Texas at El Paso), Sanghyun Lee (Florida State University), Son-Young Yi (The University of Texas at El Paso)

Abstract

In many poroelasticity applications, pressure effects are confined to a small region, making it inefficient and possibly unnecessary to solve the full system across the entire domain. Instead, we can solve the poroelasticity problem locally, where pressure effects are significant, and use a simpler linear elasticity model elsewhere. This creates an elasticity-poroelasticity interface problem with transmission conditions.

We propose a non-intrusive global-local algorithm that iteratively solves the elasticity problem in the entire (global) domain and the poroelasticity problem only in a local domain, ensuring proper transmission conditions across the interface. This approach, which extends the global-local concept to coupled multi-physics systems, significantly reduces computational cost, especially when the local domain is much smaller than the global one. Numerical experiments demonstrate the robustness and efficiency of the method, showcasing its potential for providing a scalable and efficient solution for multi-physics problems with localized effects of a single physical process.

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Physics-constrained symbolic water retention model discovery for porous media with multimodal pore size distributions

Hyoung Suk Suh (Case Western Reserve University)
Yejin Kim (Case Western Reserve University)

Abstract

Modeling water retention behavior in unsaturated porous media is crucial for predicting fluid distribution and movement under varying conditions, as it serves as a key constitutive relation for hydro-mechanically coupled simulations. However, traditional semi-empirical models, while simple and widely used, are limited to media with unimodal pore size distributions, making them unsuitable for materials with complex or multimodal pore structures. In this work, we introduce a physics-constrained symbolic regression framework that can automatically discover closed-form mathematical expressions for water retention curves directly from experimental data, eliminating the need for explicit parameter identification. Specifically, genetic programming is employed to evolve candidate symbolic expressions toward optimal mathematical models, guided by a multi-objective optimization strategy that simultaneously minimizes prediction error and penalizes violations of physical constraints. The proposed framework is validated on experimental datasets exhibiting multimodal pore size distributions, demonstrating its ability to generate interpretable, physically consistent models that may outperform traditional approaches in both accuracy and generalizability. The implementation is made publicly available to promote reproducibility and facilitate third-party applications to a wide range of porous materials.

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Simulations of two-phase flows in heterogeneous deformable porous media

Beatrice Riviere (Rice University)

Abstract

The modeling of deformable porous media arises in many fields including biomechanics and energy. 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 convection-dominated problems because they exhibit little numerical diffusion.

At each time step, mass balance and momentum equations are decoupled and the computational cost is smaller than the one for fully implicit methods. Our numerical scheme for solving the two-phase Biot problem does not require iterations over each equation for stability. 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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Coupling CFD-DEM modeling of thermo-hydro processes in fractured network media

Hoai Thanh Nguyen (The University of Utah)
Pania Newell (University of Utah)

Abstract

The use of hot dry rock (HDR) geothermal systems represents a promising solution for sustainable energy production. However, effective utilization of HDR resources requires a comprehensive understanding of coupled thermal, hydrological, and mechanical (THM) processes in fractured formations. While previous studies have provided valuable insights into single mechanisms such as heat transfer, particle transport, or fracture mechanics, the full complexity of THM interactions in interconnected fracture networks has received little attention. In this study, we developed a coupled computational fluid dynamics discrete element model (CFD-DEM) to investigate the multiphysics behavior of particle laden flows under HDR conditions. The model explicitly addresses fluid flow, heat transfer, particle dynamics and considers the effects of thermal gradients on fluid flow behavior and particle accumulation. Two injection strategies are compared: (i) direct injection of fluids and particles into fractures networks, and (ii) injection into rock formation near fracture networks. Simulation results show that high temperature conditions (e.g. 150◦C and 200◦C) increase microcapsule mobility due to reduced fluid viscosity, facilitating the microcapsule to go deeper into the fracture networks. However, at high temperature, the pressure approaching microcapsules can increase, which may lead to microcapsule to move easily and escape from
the fracture networks, which reduces sealing performance. In contrast at lower temperatures (e.g. 20◦C) microcapsules have more difficulty moving, increasing the ability of sealing. In addition, the study also highlights the importance of geometric orientation in sealing behavior. The horizontal fractures, effected by gravity, so facilitate sealing due to limited vertical space, while vertical fractures get more challenges for sealing. In terms of injection configurations, direct injection into fractures results in localized sealing near the entrance, while injection into rock formation near fracture networks causes microcapsules to accumulate below the entrance, slowing down the sealing process. These finding contribute to a better understanding of particle based sealing mechanisms in geothermal reservoirs and provide guidance for optimizing fluid injection strategies in extended geothermal systems. The proposed modeling framework provides a foundation for future multi-scale, multi-physics coupled studies in subsurface environments.

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Data-Driven Homogenization of Porous Materials: A GPU-Accelerated Neural Network Approach to Predicting Macroscale Fracture Behavior of Porous Materials

ANTON SMOLYANYY (The University of Utah)

Abstract

The analysis of the elasticity and fracture behavior of anisotropic porous materials is critical to the prediction and prevention of their brittle/semi-brittle fracture. While traditional finite element methods (FEM) can be used to solve for effective constitutive properties, these algorithms are computationally expensive and inefficient. This research investigates whether convolutional neural networks (CNN) can be trained to accurately predict the effective constitutive tensor of anisotropic porous materials by examining images of their microstructure. A pipeline of open source software packages was created to fully automate the process from creating and labeling the training data to analyzing it using a CNN model written in Python. Gmsh was used to generate mesh representations of materials with varying pore morphologies. These meshes were then used as input to a periodic homogenization algorithm in FEniCS which produced effective constitutive values to be used as labels for training. This labeled dataset was used to train the CNN to predict Young's Moduli, Poisson's Ratio, and the Shear Modulus for a given material. This neural network-driven approach significantly reduces computational time and energy, and provides an alternative to traditional FEA methods to analyze the elastic response of porous materials. The ability to accurately extract mechanical properties, enabled by CNN analysis, will give engineers in any field predictive capabilities that will transform decision-making and material design processes.

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Microscopic Origin of Hysteresis in CH4 Sorption-Induced Deformed Coal Matrix: Insights from Stepwise Hybrid GCMC/MD Simulations

Quanlin Yang (University of Alberta), Zhehui Jin (University of Alberta)

Abstract

Gas sorption hysteresis in flexible microporous materials is widely observed across both crystalline and amorphous systems and plays a critical role in applications such as gas storage, separation, catalysis, sensing, and drug delivery. While the mechanisms in crystalline materials—especially flexible metal-organic frameworks (MOFs)—have been linked to well-defined structural transitions, the origins of hysteresis in amorphous, low-permeability materials such as coal and shale kerogen remain elusive due to complex pore morphologies and compositional heterogeneity.

In this study, we employ a stepwise hybrid Grand Canonical Monte Carlo/Molecular Dynamics (GCMC/MD) simulation framework to investigate methane (CH_4) sorption hysteresis in deformable coal matrices at 313.15 K, well above CH_4's critical temperature (190.56 K). By ensuring each pressure step begins from the equilibrated configuration of the previous step, this method captures continuous pore evolution and allows us to isolate thermodynamic effects from kinetic artifacts. Our findings reveal that CH_4 hysteresis arises from local free energy minima induced by deformation of the coal matrix—rather than from capillary condensation or slow diffusion. This thermodynamic origin is shown to persist despite the relatively weak van der Waals interactions between CH_4 and the coal structure, highlighting the critical role of structural flexibility and energetic metastability.

These results provide direct atomistic-level evidence of sorption-induced deformation and hysteresis in amorphous microporous materials, offering new perspectives for interpreting experimental data. The insights gained are essential for the design and optimization of gas storage systems, CO_2 sequestration strategies, and energy recovery processes, and have broader implications for materials used in environmental remediation and advanced separation technologies.

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A Variational Phase-Field Framework for Modeling Pore-Scale Melting and Refreezing at the Ice–Ocean Interface

Junning Liu (California Institute of Technology), Xiaojing Fu (California Institute of Technology)

Abstract

Accurate prediction of ice shelf stability and long-term ice sheet evolution requires a fundamental understanding of pore-scale melting and refreezing processes at the ice–ocean interface. These processes are driven by intricate couplings between heat transport, salinity gradients, and buoyancy-induced fluid flow within the porous microstructure of ice. Capturing these interactions requires a modeling approach that can simultaneously resolve interfacial phase change dynamics, solute transport, and hydrodynamic effects at the pore scale. We present a thermodynamically consistent variational phase-field model that treats the ice matrix as a reactive porous medium. Central to our formulation is a temperature- and salinity-dependent Gibbs free energy functional, derived from alloy solidification theory, which allows accurate recovery of the seawater phase diagram without empirical freezing point relations or asymptotic approximations. The model couples the Allen–Cahn equation for phase evolution with the Cahn–Hilliard equation for solute redistribution and is extended to account for advection and diffusion under laminar flow. This enables the co-evolution of phase, temperature, and salinity fields under conditions representative of melting and refreezing at ice–ocean boundaries.

We validate the model against analytical solutions to the classical Stefan problem, confirming its ability to capture phase-front migration driven by thermal gradients. Additional validation is performed using experimental data on directional solidification and brine channel formation in sea ice and saline porous media, demonstrating the model's fidelity in reproducing key physical behaviors. High-resolution simulations reveal the model's capability to resolve complex melt–refreeze dynamics within porous ice geometries and mushy layers, capturing essential features such as brine rejection, salinity stratification, and the development of localized refreezing fronts. Notably, we show that density-driven convection can suppress local melting by exporting solutes away from the interface, thereby altering the thermodynamic balance and modulating phase change rates. This feedback mechanism illustrates the critical influence of microscale hydrodynamics on interfacial stability. Collectively, this work establishes a robust foundation for linking fine-scale thermodynamic and transport processes to emergent large-scale ice behaviors, highlighting the critical need to incorporate pore-scale physics into next-generation ice–ocean models to improve predictions of cryosphere evolution in a warming climate.

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Coupled Chemo-Mechanical Crack Propagation using a Phase-Field Approach

Giancarlo Ventura (Stanford University)
Ronaldo Borja (Stanford University)

Abstract

Understanding how fractures develop in geologic materials under the influence of both mechanical and chemical processes is critical in subsurface applications such as carbon dioxide (CO_2) sequestration and hydraulic fracturing. These processes involve prolonged interaction of reactive fluids with rock formations, often leading to mineral dissolution, and degradation of mechanical properties. As dissolution progresses, porosity increases and internal stresses redistribute, reducing stiffness and strength, making the material more prone to fracturing. These fractures may propagate even without additional mechanical loading.

This work introduces a novel finite element formulation for modeling time-dependent fracture in porous geomaterials using a fully coupled chemo-mechanical phase-field model. The formulation simultaneously solves for solid deformation, porosity evolution, and phase-field damage, with porosity governed by a strain-driven dissolution law. This formulation offers new insights into long-term rock weakening under reactive environments.

In the simulations, both creep and stress relaxation behaviors emerged naturally without imposing viscoelastic constitutive laws, demonstrating the model's ability to capture time-dependent responses driven solely by chemo-mechanical coupling. Fracture propagation continued even without additional mechanical loading, highlighting a key feature of dissolution-driven failure: chemical degradation alone can sustain and advance crack growth. As porosity increases, stress concentrations develop around evolving defects, further accelerating damage.

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The Impact of Dry Snow Metamorphism on Effective Thermal Conductivity of Porous Ice

J. Jackson Baglino (California Institute of Technology)
Adrian Moure (California Institute of Technology), Xiaojing Fu (California Institute of Technology)

Abstract

Icy porous geomaterials are ubiquitous on Earth, such as snow, firn and permafrost soil, and throughout extraterrestrial environments, such as the icy shell of Enceladus and the shallow subsurface/surface of Mars, the Moon, and some comets. Understanding the microstructural evolution of these materials is critical for predicting the response of the cryosphere to climate change, as well as for interpreting the remote sensing signatures and predicting thermo-mechanical properties of ice-bearing surfaces of other celestial objects.

Porous ice is a highly volatile material, particularly near its melting point. Driven by temperature gradients and interfacial curvature, porous ice undergoes a topological coarsening process known assnow metamorphism, which results from mass transport within the ice–vapor system. Snow metamorphism plays a central role in modifying the topology of icy porous media—enhancing connectivity, reducing specific surface area, and consequently altering the macroscopic behavior of the material [1, 2].

In this work, we investigate the pore-scale evolution of synthetic ice bead packs undergoing dry snow metamorphism. We employ a phase-field model that captures sublimation and deposition between solid ice and water vapor, enabling us to track the evolution of the ice and air phases, the temperature field, and the vapor density field under various environmental conditions [3]. High-resolution simulations of this model are then used to simulate microstructural coarsening of a virtual ice bead pack under a wide range of temperature conditions.

Next, we apply a homogenization technique to quantify the relationship between effective thermal conductivity and snow microstructure [4, 5, 6]. Using this approach, we track the evolution of the effective thermal conductivity as an ice bead pack undergoes microstructural changes due to metamorphism. Our simulation results are compared against (1) empirical relations that assume well-connected microstructures and (2) available field data [4, 5, 7].

Finally, we extend this framework to explore the behavior of larger-scale systems—such as terrestrial glaciers and ice sheets or the icy shell of Enceladus—by constructing vertically layered models composed of porous ice domains that have undergone different degrees of metamorphism. Each layer represents a distinct microstructural age, capturing the spatial variation in thermal history and structural

evolution across the depth profile of an ice pack. These results offer new insight into the thermal regulation of icy systems and contribute to a broader understanding of the heat budget in both the cryosphere and icy planetary environments.

Keywords: Snow metamorphism, phase-field/homogenization, thermal conductivity

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Modelling the Pressure Effects on Wave Dispersion and Attenuation in Fluid-Saturated Dual-Porosity Media

Fubin Chen (China University of Petroleum (East China))
Zhaoyun Zong (China University of Petroleum (East China)), Xingyao Yin (China University of Petroleum (East China)), Jiayun Li (China University of Petroleum (East China))

Abstract

When the elastic waves propagate through the fluid-saturated porous media, the wave energy dissipation occurs due to fluid flow which further leads to wave velocity dispersion. The influence of key rock physics parameters—such as porosity, water saturation, and permeability—on wave dispersion and attenuation have been extensively studied over the years. However, the effects of pressure and complex pore structure, which are prevalent in subsurface strata, remain poorly understood. Here we propose a dual-porosity acoustoelasticity model to investigate the pressure-dependent wave dispersion and attenuation in fluid-saturated porous media. The model assumes a medium containing two pore types: stiff pores and compliant cracks. We incorporate both the linear pressure effect (associated with skeleton stiffening) and the nonlinear pressure effect (related to crack closure) using acoustoelasticity and elastic piezosensitivity theories. The squirt flow (fluid exchange between stiff pores and cracks) and the global Biot flow are considered to account for the frequency dependency of wave velocity. We systematically analyze the impacts of effective pressure, frequency, and crack aspect ratio on wave propagation using the proposed model. The results reveal two distinct attenuation peaks, corresponding to squirt and global flows, respectively. Meanwhile, the increase of effective pressure results in the significant decay of wave dispersion and attenuation caused by the squirt flow, while its effect on global flow-associated dispersion is minimal. This observation may be attributed to the progressive closure of cracks under pressure. By comparing the model predictions with laboratory measurements, we demonstrate the feasibility of our model. Besides, the proposed model provides a better interpretation for measure data than the classic acoustoelasticity theory, particularly in the low-pressure regime.

2 Theory

The pore structure of a subsurface rock is usually complex. In this study, we assume that the rock contains the two types of pores, i.e., stiff pores and complaint cracks (see Figure 1). Under this hypothesis, we propose a rock physics model to calculate the wave velocities in the fluid-saturated dual-porosity media under the effect of effective pressure (i.e., the difference between the confining pressure

and pore pressure) using the dual-porosity piezosensitivity model in Shapiro (2003), the modified frame model in Gurevich et al. (2009), the poro-acoustoelasticity model in Chen et al. (2024), and the squirt flow model in Chen et al. (2025). The main steps of this method are shown in Figure 2 and its details are described below.

a) The stiff porosity ϕ_{s} and crack porosity ϕ_{c} are sensitive to the effective pressure variation, and their pressure dependency can be quantitatively described by (Shapiro, 2003)

$$\phi_{s}=\phi_{s}^{0}-(C_{drs}-C_{g})p_{e} \quad (1)$$

$$\phi_{c}=\phi_{c}^{0}\exp(-\theta_{c}C_{drs}p_{e}) \quad (2)$$

where ϕ_{s}^{0} and ϕ_{c}^{0} are the initial porosities of stiff pores and cracks of rock free of pressure, respectively, C_{g} and C_{drs} are bulk compressibility of rock grain and dry rock with no open cracks, which are the inverses of bulk modulus K_{g} and K_{drs}, respectively, θ_{c} is a bulk pressure sensitivity coefficient. From equations (1) and (2), it is shown that the stiff porosity and crack porosity are linearly and exponentially correlated with the pressure variation, respectively.

b) According to the dual-porosity piezosensitivity model in Shapiro (2003), the cracks have more significant impact on the pressure dependency of rock elasticity than stiff pores, although the cracks only occupy a small proportion of rock pore space. The pressure-dependent bulk and shear moduli of a dry rock (K_{dr} and μ_{dr}) are given by

$$K_{dr}=K_{drs}+\theta_{cK}\phi_{c}^{0}\exp(-\theta_{c}C_{drs}p_{e}) \quad (3)$$

$$\mu_{dr}=\mu_{drs}+\theta_{c\mu}\phi_{c}^{0}\exp(-\theta_{c}C_{drs}p_{e}) \quad (4)$$

where μ_{drs} is shear modulus of dry rock with no cracks, θ_{cK} and $\theta_{c\mu}$ are pressure sensitivity parameter of bulk and shear moduli, respectively.

c) A “modified frame” is introduced to calculate the elastic moduli of a fluid-saturated dual-porosity medium. The modified frame represents the rock skeleton with the dry stiff pores and fluid-saturated cracks, and its bulk and shear moduli (K_{mf} and μ_{mf}) can be written as (Gurevich et al., 2009)

$$1/K_{mf}=1/K_{drs}+(1/K_{f}-1/K_{g})\phi_{c} \quad (5)$$

$$1/\mu_{mf}=1/\mu_{drs}-4/15(1/K_{dr}-1/K_{mf}) \quad (6)$$

where K_{f} is fluid bulk modulus. To describe the wave dispersion and attenuation caused by squirt flow of fluids between stiff pores and cracks, Chen et al. (2025) derived a simple equation for the frequency-dependent fluid bulk modulus incorporating squirt flow effect, as

$$K_{f}^{*}=(1-2/\sqrt{1-k^2}+2/(1+\sqrt{1-k^2})K_{f} \quad (7)$$

where $k=1/\alpha\sqrt{-12j\omega\eta/K_{f}}$, α is crack aspect ratio, j is imaginary unit, ω is angular frequency, η is fluid viscosity. Replacing the fluid bulk modulus in equation (5) with the frequency-dependent one in equation (7), the frequency-dependent elastic moduli of modified frame can be directly obtained.

d) Chen et al. (2024) proposed the constructive equations, wave equations and plane-wave velocity equations in the poro-acoustoelastic media. We replace the dry moduli in equations (47)-(50) in Chen et al. (2024) with the elastic moduli of modified frame shown in equations (5) and (6) to obtain the velocities of the fast P wave, slow P wave and S wave in the fluid-saturated dual-porosity media.

e) Here we define the inverse of quality factor as the attenuation factor, i.e., the ratio of imaginary part of wave velocity to its real part, which can be computed with the obtained complex wave velocity straightforward.

3 Results

We use an ideal rock model to model the effect of effective pressure on the dispersion and attenuation of fast and slow P, and S waves. The basic properties of this rock model are listed here: grain bulk modulus ~ 37GPa, grain shear modulus ~ 44GPa, dry bulk modulus without cracks ~ 20.8GPa, dry shear modulus without cracks ~ 26.2GPa, fluid bulk modulus ~ 2.24GPa, fluid viscosity ~ 0.001Pa·s, initial stiff porosity ~ 0.2, initial crack porosity ~ 0.003, matrix permeability ~ 1md, tortuosity ~ 2, crack aspect ratio ~ 0.001, fluid density ~ 940kg/m3, grain density ~ 2544kg/m3. The pressure sensitivity parameters and third order elastic constants of rock model can be found in the second column of Table 1 in Chen et al. (2024).

Figures 3-5 show the influence of effective pressure on the fast P-wave, slow P-wave and S-wave velocities and the corresponding attenuation factors versus frequency, respectively. From plots, it is shown that the increasing effective pressure leads to the significant increases in the fast P-wave and S-wave velocities, but just has little impact on slow P-wave velocity, irrespective of frequency. We also see that there are two attenuation peaks in the attenuation curves, which respectively correspond to the low-frequency squirt flow and high-frequency Biot global flow. The wave attenuation induced by squirt flow gradually decays as the effective pressure increases, which is attributed to the gradual closure of cracks in theory (Alkhimenkov and Quintal, 2024; Chen et al., 2025). Besides, we notice that the attenuation factor of slow P wave is appreciably greater than that of fast P and S waves, which may explain why the slow P wave is possibly unobservable in field.

Moreover, a dataset of ultrasonic velocities of fast P and S waves in a sandstone sample measured by Fu and Fu (2018) is utilized to test our model. Figure 6 shows the comparisons of measured and modelled P-wave velocities and S-wave velocities of sandstone sample under effective pressure. It is shown that the modelled results are well consistent with the laboratory measurements.

4 Conclusions

We establish a dual-porosity acoustoelasticity model to interpret the influence of effective pressure on the wave dispersion and attenuation concurrently induced by squirt flow between stiff pores and compliant cracks, and Biot global flow. The modelling results show that the effective pressure has an appreciable impact on wave dispersion and attenuation caused by squirt flow. However, the wave dispersion caused by global flow is insensitive to the effective pressure variation. By comparing the modelled results to laboratory measurements, we illustrate the feasibility of our model. To extend the application of the proposed model in broader frequency range, the wave dispersion induced by the mesoscopic fluid heterogeneity or fluid flow should be considered in the future studies.

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Pore-Scale Dynamics in Porous Media 1

Presentation 40

A High-order Preconditioner for Pore-Scale Mechanics

Sabit Mahmood Khan (Penn State University), Yashar Mehmani (Penn State University)

Abstract

The complexity inherent to the microstructure of porous materials poses a significant challenge for the efficient simulation of mechanical deformation and failure. Such simulations are necessary to derive macroscopic behavior from fundamental descriptions of geometry and material property at the pore scale, with applications ranging from higher-precision engineering of subsurface CO2 sequestration and hydrogen storage to better designs of lightweight high-strength materials for aviation, construction, and defense. The computational bottleneck lies in the repeated solution of a large, and often ill-conditioned, linear(ized) system of equations via an iterative solver. Such solvers need preconditioning to accelerate convergence, but current preconditioners tend to fall short of achieving the kind of acceleration needed in practice. We propose a class of two-level preconditioners that are easy to construct, are parallelizable, and provide unmatched convergence rates. Building on our prior work where a low-order form of this preconditioner was developed, here, we show how to achieve even better performance by increasing the approximation order. We find the increase in order is most needed under shear or torsion loads, but not tension. We also point to a computational trade-off between the effort spent to increase order during offline calculations, and the cost savings during online calculations due to faster convergence.

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Predicting Pore-Scale Failure: Integrating Experiment with Computation

Tahmid Rakin Siddiqui (Penn State University), Yashar Mehmani (Penn State University)

Abstract

Understanding failure of porous microstructures is critical to the safety of subsurface operations aimed at storing CO2 or hydrogen, and the durability of manufactured parts used in electrochemical devices (e.g., batteries), biomedicine, construction, aviation, and defense. In this work, we integrate in-situ tension experiments performed inside an X-ray scanner on additively manufactured resins with a computational model in order to understand the interplay between pore-scale geometry and mechanical response. We use 3D-printed stereolithography (SLA) to allow for arbitrary control of geometry and to ensure experimental repeatability. Scans are acquired of structural deformation and nucleated cracks. Since SLA resin exhibits inelastic deformation prior to failure, we incorporate plasticity in our model in addition to failure. An attempt to predict observations by direct numerical simulation is made, and we present findings along with potential challenges moving forward. The experiments validate a hypothesis postulated in our prior work that claimed the dominant nucleation sites of cracks tends to coincide with geometric constrictions. The claim was the basis for the development of a rapid and scalable reduced-order model that is now given credence. Plans to curate the data as a freely available benchmark for future modeling will be outlined.

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A cross-scale characterization to bridge the observational gap between wormholes and pore networks in porous rocks

Wei Li (Stony Brook University)
Akhil Kolanti (Stony Brook University), David Sprouster (Stony Brook University), Zijie Xu (Stony Brook University)

Abstract

Flow and dissolution in soluble porous rocks often selectively enlarge some part of the pore network and result in the formation of wormholes—highly conductive, tree-shaped channels in the porous rock. These wormholes localize the flow, transitioning it from Darcy flow to pipe flow in the porous media. Understanding the origin of wormholes and their interaction with the pore network is crucial in predicting the evolution of the flow, mixing, and reaction in porous media in natural conditions and subsurface resource exploitation, such as karst formation and in-situ mining. However, gaining this understanding is challenging due to the observational gap between the millimeter-scale wormholes and micrometer-scale pore networks, which originates from the limited field of view and resolution of 3D imaging techniques. Here, we overcome this challenge by combining X-ray computed tomography (CT) and a systematic subsampling scheme, and obtain cross-scale characterizations of the wormholes and pore networks. We show that the wormholes, when observed through low-resolution CT scans, are dendritic networks and follow Horton's law of stream hierarchy, just like river networks. When observed through high-resolution CT scans, wormholes are part of the pore networks, mimicking reticulate networks that allow mixing and reactions on the pore scale. Our study offers a foundation for the modeling and upscaling of the reactive transport processes in porous rocks altered by flow and dissolution.

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Tailored Framework Designs for Improved Catalytic Efficiency of Heme-containing Proteins

Raheleh Ravanfar (Texas Tech University)

Abstract

The integration of proteins into solid-state scaffolds holds significant promise for advancing applications in biocatalysis, sensing, and therapeutic delivery. However, achieving high catalytic efficiency while preserving protein structure and function remains a fundamental challenge. In this work, we present a strategy to enhance the catalytic performance of proteins by engineering the interfacial environment between proteins and porous materials. Using a combination of experimental methods and molecular simulations, we demonstrate a precise control over protein encapsulation, stability, and activity. Our results reveal that the microenvironment within the framework plays a critical role in maintaining native-like protein conformation and facilitating efficient substrate access. This approach provides a broadly applicable platform for improving the functionality of protein-based composites and establishes design principles for the development of next-generation bioinorganic materials.

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Connecting In Situ Stress to Near-well Hydraulic Fracture Complexity with Phase-field Simulations

Fan Fei (Atmospheric, Earth, and Energy Division, Lawrence Livermore National Laboratory, USA) Yunxing Lu (Department of Civil and Environmental Engineering, University of Pittsburgh, USA), Andrew P. Bunger (Department of Civil and Environmental Engineering, University of Pittsburgh, USA), Matteo Cusini (Atmospheric, Earth, and Energy Division, Lawrence Livermore National Laboratory)

Abstract

Understanding the behavior and features of near-well hydraulic fractures is crucial for characterizing in situ stress and optimizing injection strategies in subsurface energy systems, such as enhanced geothermal systems (EGS). However, the nucleation and propagation of these fractures near the wellbore exhibit significant complexities and are commonly influenced by the factors including in situ stress, wellbore orientation, and rock heterogeneity. Motivated by this, we employ a novel phase-field formulation in GEOS---an open-source multiphysics reservoir simulator---to explore the resulting 3D features of near-well hydraulic fractures under varying in situ stress conditions and wellbore deviations. Unlike other phase-field approaches to hydraulic fracturing in porous media, the adopted model can capture both strength-based fracture nucleation and energy-based fracture propagation, making it well-suited for modeling near-well fracture behavior. In this numerical study, we systematically investigate how (i) stress orientation and magnitude, and (ii) wellbore deviation axis and angle affect three key characteristics of the near-well fracturing behavior, namely (i) fracture alignment with the wellbore, (ii) fracture shape, and (iii) fractuer nucleation location. The simulation results are categorized and compared with the experimental observations from a laboratory-scale hydraulic fracturing test under true traxial compression. To further demonstrate the applicability of this phase-field model to field conditions, we simulate a fracture injection test conducted in an EGS production well at the Utah FORGE project and compare the results with the borehole image log data. This phase-field model and the findings from the numerical study provide valuable insights for in situ stress characterization, thereby supporting the development of EGS and other subsurface energy systems.

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Molecular-Scale Analysis of Microbial Metabolism Effects on Hydrodynamics in Underground Hydrogen Storage

Aruzhan Tleubek (University of Utah)
Arvand Vedadi (University of Utah), Amin Hamed Mashhadzadeh (University of Utah), Salah A. Faroughi (University of Utah)

Abstract

Hydrogen is gaining increasing attention as a clean and sustainable energy carrier, playing a key role in the transition from fossil fuels to low-carbon energy systems. With this growing reliance on hydrogen, the need for reliable and scalable storage technologies has become critical. Storing hydrogen presents significant challenges due to its low volumetric energy density, high diffusivity, and the need for specialized infrastructure to prevent leakage and ensure safety. Among the available options, Underground Hydrogen Storage (UHS) offers a cost-effective solution for long-term, large-capacity energy storage by injecting hydrogen into geological formations such as depleted hydrocarbon reservoirs, salt caverns, and saline aquifers. However, one of the primary challenges in UHS arises from microbial activity in the subsurface. These microorganisms may produce gas impurities or form biofilms that interfere with hydrogen storage conditions. Microorganisms, including methanogens, sulfate-reducing bacteria (SRB), and acetogens utilize hydrogen as an electron donor, producing gas byproducts such as methane ($\textrm{CH}_{4}$), hydrogen sulfide ($\textrm{H}_2\textrm{S}$), and acetic acid ($\textrm{CH}_3\textrm{COOH}$) via methanogenesis, sulfate reduction, and acetogenesis, respectively. These biotic reactions alter the surface chemistry of the mineral rock and the hydrodynamic properties of the reservoir, potentially reducing storage efficiency and hydrogen recovery. Although experimental studies have investigated microbial impacts at the pore level, results remain inconsistent, and such experiments are often costly. Simulations that account for microbially induced impurities are also very limited. Therefore, evaluating these biotic effects is essential for understanding the risks associated with hydrogen loss and long-term recovery rates in UHS systems.

This study addresses these knowledge gaps by conducting molecular-scale analysis to investigate the hydrodynamics of UHS systems under realistic thermodynamics conditions. We employ non-equilibrium molecular dynamics (NEMD) simulations to investigate how microbially induced gaseous impurities influence key transport and interfacial properties, including hydrogen diffusion and the wettability of mineral surfaces representative of reservoir rock, specifically α-quartz surface. Simulations are conducted across a range of gas concentrations (10–40 vol%) and surface pH levels (5, 7, and 9), with durations of up to 10 nanoseconds. $\textrm{CH}_{4}$ induces a slight reduction in water-wettability across all examined pH levels, with contact angle measurements showing an increase up to 13° at pH 5 and 40 vol% concentration. In contrast, $\textrm{H}_2\textrm{S}$ exhibits a more complex, pH-dependent effect. It slightly reduces wettability at low pH but maintains strong water-wet

characteristics at high pH, with contact angles remaining close to zero. Despite minimal impact on wettability, both impurities significantly reduce hydrogen mobility, with $\textrm{H}_2\textrm{S}$ having a stronger effect due to its higher polarity and stronger electrostatic interactions. These findings emphasize the importance of accounting for microbial byproducts, especially $\textrm{H}_2\textrm{S}$, in the design and evaluation of UHS systems, as they can significantly impact hydrogen storage efficiency and recovery dynamics.

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Surrogate Modeling of Granular Elasto-Plasticity Using Kolmogorov-Arnold Networks with Chebyshev Polynomial Representation

Farinaz Mostajeran (University of Utah)
Aruzhan Tleubek (University of Utah), Salah A. Faroughi (University of Utah)

Abstract

Accurately modeling the nonlinear, anisotropic, and path-dependent behavior of granular materials under various loading conditions remains a significant challenge in geomechanics. Traditional constitutive models, such as elasto-plastic or critical-state formulations, are built on carefully crafted physical assumptions and empirical relations. While these models provide valuable insights, they rely on simplifying assumptions that often fail to capture the full complexity of real-world material responses. Furthermore, they require extensive calibration against experimental data, which is often scarce, noisy, or difficult to obtain, particularly for complex loading paths or heterogeneous materials. Data-driven methods, particularly those based on multilayer perceptrons (MLPs), have gained traction as alternatives to physics-based constitutive models because they can approximate complex nonlinear stress–strain relationships directly from data without relying on explicit constitutive assumptions. However, achieving high accuracy often requires deep or wide architectures, which increases the number of parameters, computational costs, and the risk of poor generalization to unseen data. While MLPs offer a flexible function-approximation framework, their black-box nature can make it challenging to extract meaningful physical insights or ensure consistency with fundamental principles, potentially limiting their use in scientific and engineering applications where interpretability and physical consistency are important.

To address these limitations, this study proposes an Elasto-Plasticity Informed Chebyshev-based Kolmogorov-Arnold Network (EPi-cKAN), a physics-informed neural network architecture designed to model complex elasto-plastic behavior of granular materials with improved accuracy, interpretability, and generalization. EPi-cKAN builds upon the strengths of Kolmogorov-Arnold Networks (KANs) and leverages augmented Chebyshev polynomials to construct expressive yet compact representations. It embeds fundamental principles of elasto-plasticity directly into the network architecture and loss function, enabling physically consistent stress–strain predictions with fewer parameters than conventional MLP-based models. Results show that EPi-cKAN achieves less than 2% error in a posteriori thermodynamic energy consistency without requiring explicit enforcement, while MLP-based models, including EPNNs, exhibit higher errors and struggle with unseen loading paths. In a blind triaxial axisymmetric loading test at $\xi = -1.75$, EPi-cKAN predicts deviatoric stress components with an error of 5%, compared to 60% for EPNN. Similarly, under a blind unloading path, EPi-cKAN achieves approximately 64% lower error than EPNN. EPi-cKAN demonstrates robustness against noisy data, achieving an error of only 1.52% in deviatoric stress predictions with 5% noise, up to six times smaller

than EPNN. These findings demonstrate that EPi-cKAN can effectively bridge the gap between data-driven and physics-based modeling approaches, offering a promising direction for the development of accurate, efficient, and physically interpretable constitutive models for granular materials in scientific machine learning. Future work will focus on extending EPi-cKAN to handle multi-axial and cyclic loading conditions beyond the axisymmetric tests explored in this study. This will enable the model to capture more complex behaviors such as shear band formation, anisotropic hardening, and strain localization. Incorporating these capabilities will enhance EPi-cKAN's applicability to real-world geomechanical problems involving diverse boundary conditions and loading histories.

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Poster Presentation 48

Pore-Scale Modeling of Two-Phase Flow in Heterogeneous Wettable Media

Arvand Vedadi (University of Utah), Salah Faroughi (University of Utah)

Abstract

Two-phase flow in porous media plays a central role in a wide range of energy and environmental systems, including enhanced oil recovery, underground hydrogen storage, and geothermal energy extraction. These systems rely on the efficient management of fluid-fluid interactions at the pore scale, where interfacial forces dominate and wettability emerges as a key control on fluid displacement and distribution. Despite its significance, numerical models frequently adopt the simplifying assumption of spatially uniform wettability, which fails to reflect the naturally occurring heterogeneity in rock-fluid interactions. In reality, variations in mineral composition, surface roughness, and fluid chemistry lead to complex wettability patterns that strongly influence the dynamics of multiphase displacement. As a result, models that ignore these spatial variations risk producing inaccurate predictions of fluid configuration, phase connectivity, and recovery efficiency. Understanding the implications of mixed-wettability systems is therefore critical, particularly under cyclic drainage and imbibition conditions where capillary forces and contact line motion are continuously evolving. Experimental studies using core-flooding or micromodels have attempted to shed light on these effects, but limitations remain. Core-flood setups are often opaque and do not allow for direct observation at the pore scale, while micromodels struggle to replicate the complexity of natural porous geometries and wettability distributions. On the modeling side, numerical simulations using Lattice Boltzmann or finite element methods have incorporated spatially heterogeneous wettability into 2D domains. However, these studies typically rely on a static contact angle, which neglects the dynamic variation that occurs as the fluid interface advances or recedes. To realistically simulate multiphase flow in such systems, both wettability heterogeneity and dynamic contact angle effects must be incorporated.

To address these challenges, this study develops a mathematical model that accounts for the dynamic contact angle, in a heterogeneous wettability system. We study this model in two dimensions across two geometries using VOF (Volume of Fluid): a T-junction, representing a single pore between three grains, and a more complex full pore-scale domain containing ordered and disordered pores. From these configurations, we investigate how fluid breakup occurs during cyclic imbibition and drainage of two-phase flow when both hybrid wettability and dynamic contact angle effects are accounted for. These results are consistent with previous studies, which showed that hybrid wettability alters the breakup behavior of droplets by introducing asymmetries in interfacial forces. In particular, differences in contact angle across surfaces were found to influence the size, speed, and timing of daughter droplet formation. Our simulations reflect these effects, revealing that hybrid wettability, when coupled with dynamic contact angle modeling, leads to irregular breakup patterns and nonuniform segmentation

during cyclic imbibition and drainage. Future extensions of this work will focus on three-dimensional domains and coupling with experimental datasets to validate droplet dynamics and flow regimes under more realistic porous architectures. Such developments will support the creation of predictive models for multiphase flow in complex natural systems.

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Modeling of Entrained Air Dissolution and Long-Term Saturation: Role of Microstructure in Emerging Cementitious Materials

Aiqing Xu (Georgia Institute of Technology), Kimberly E Kurtis (Georgia Institute of Technology)

Abstract

Freeze-thaw deterioration in air-entrained cementitious materials is primarily driven by the ingress of external moisture and the progressive saturation of interconnected capillary and air void networks. The resistance of cement-based materials to freeze-thaw deterioration is strongly influenced by the dissolution behavior of trapped air and the diffusion and saturation of water within the pore structure. Smith et al. [1] proposed a physics-based model, known as the Single Void Dissolution Kinetics (SVDK) model, to describe the dissolution of air voids under saturated matrix conditions and to capture the evolution of long-term saturation behavior. Given the differences in pore structures and transport properties among various cementitious systems, this study extends the applicability of the SVDK model to a range of cementitious material systems, including ordinary Portland cement (OPC), calcium sulfoaluminate (CSA) cement, limestone calcined clay cement (LC3), and geopolymer systems. By incorporating system-specific physical characteristics, such as porosity, tortuosity, diffusivity, and permeability, the study systematically simulates the dissolution behavior of air voids and the evolution of long-term saturation across different material systems. In addition, the influences of pore size variations and different material properties on the kinetics of dissolution, diffusion, and saturation are investigated. The results demonstrate that microstructural differences play a crucial role in determining gas transport and saturation behavior. This work provides a theoretical foundation for advancing the understanding of freeze-thaw damage mechanisms and supports the development of more durable and resilient cementitious materials.

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Using PIKAN to Track Fate and Transport of PFAS in the Vadose Zone

Nicholas Baker (University of Utah)
Farinaz Mostajeran (University of Utah), Salah A. Faroughi (University of Utah)

Abstract

Perfluoroalkyl substances (PFAS) are a class of persistent synthetic chemicals that pose significant environmental and public health risks due to their widespread use, high toxicity, and remarkable resistance to natural degradation processes. Accurately characterizing their behavior in the subsurface is essential for designing effective remediation strategies and managing long-term environmental risks. Despite ongoing research in the literature on these phenomena, accurately modeling PFAS transport remains a significant challenge. PFAS transport is governed by complex, multiscale physical processes, including sorption to porous media, interactions at the air-water interface, and the effects of PFAS acting as strong surfactants, all of which contribute to the nonlinear behavior of PFAS in subsurface environments. The long-term persistence and mobility of PFAS demand predictive models that can account for these factors and provide accurate forecasts to inform site-specific remediation strategies and regulatory decision-making. Traditional numerical methods for solving transport problems, such as finite volume and finite difference solvers, require complete knowledge of all relevant physical parameters. These methods often struggle when applied to inverse problems, where some parameters are unknown or uncertain. Furthermore, classical solvers typically rely on fine spatial and temporal discretization, which can lead to substantial computational costs, particularly when modeling PFAS fate over large domains, potentially spanning kilometers, and long timeframes, which may extend over decades. In addition, observational data from real-world geological sites are often sparse, noisy, and incomplete, further complicating the modeling process and limiting the effectiveness of traditional approaches in solving inverse problems or making reliable predictions under uncertainty. The combination of large spatial scales, long temporal scales, and complex physical interactions creates a unique challenge for numerical modeling. Physics-Informed Kolmogorov-Arnold Networks (PIKANs) offer a promising alternative to traditional solvers by leveraging machine learning to solve both forward and inverse PDE problems without requiring explicit discretization. PIKANs incorporate the governing physical laws directly into the loss function, allowing them to embed prior knowledge, enforce physical constraints, and improve generalization. These features make PIKANs particularly well-suited for data-limited environmental modeling. However, like many machine learning models, vanilla PIKAN architectures face limitations when applied to problems involving large spatial and temporal domains. Training a single, monolithic network across a large domain can lead to issues such as poor convergence, numerical instability, and degraded accuracy. The complexity of the solution space and the high dimensionality of the input further exacerbate these challenges, limiting the scalability and robustness of standard PIKAN implementations.

To address these issues, we propose a scaled and sequential PIKAN framework that leverages Chebyshev basis functions for efficient modeling of PFAS transport in subsurface environments. In this

framework, the spatial domain is scaled to align with the range of the Chebyshev basis functions, ensuring that the functions remain well-defined and that approximation errors are minimized. For temporal domains that span long durations, we partition the time domain into smaller, sequential subdomains. A separate PIKAN is trained for each temporal subdomain, and the output of one model serves as the initial condition for the next, enabling a sequential reconstruction of the full solution over time. This modular approach not only improves the stability and accuracy of the model but also enables parallel training across different temporal segments, offering significant computational advantages for large-scale and long-duration simulations. To validate the results of the scaled and sequential PIKAN framework, we have developed a traditional solver in OpenFOAM, based on established models in the literature. Preliminary results show that the scaled and sequential PIKAN approach offers improved accuracy and stability compared to standard PIKANs, particularly in modeling PFAS transport with complex boundary conditions, nonlinear source terms, and heterogeneous porous media. The findings contribute to the development of more effective computational tools for environmental management, risk assessment, and remediation planning at PFAS-contaminated sites. Future work will focus on extending this framework to tackle inverse problems, such as estimating unknown parameters like sorption coefficients, reaction rates, and permeability fields from limited observational data.

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Elastic wave propagation in fluid saturated porous media with sinusoidally varying pore geometry

Weitao Sun (Tsinghua University)

Abstract

Wave propagation in porous media plays a crucial role in seismic exploration and material design. The complex geometries of real pores in rocks pose significant challenges to accurate mathematical modeling. Existing poroelasticity theories, which typically focus on straight, thin-walled tubes, fail to capture the effects of intricate pore structures. This study develops macroscopic elastic wave equations for porous media with sinusoidally varying pore geometries. The model strikes a balance between pore structure complexity and mathematical tractability, effectively capturing fluid-solid coupling effects often overlooked by traditional models. The primary contributions of this work are twofold. First, it introduces wave equations for porous media with sinusoidal pore structures, marking a novel advancement in the field. Second, and most importantly, it derives an analytical expression for permeability—traditionally treated as an empirical parameter—directly from the sinusoidal pore geometry. Unlike previous studies where permeability is inferred from experiments or empirical models, this work establishes a direct, analytical link between the microscopic pore shape and macroscopic permeability. This breakthrough provides a new theoretical foundation for predicting permeability from first principles and paves the way for designing porous materials with geometry-driven flow control. Numerical simulations demonstrate that parameters specific to sinusoidal pore geometries significantly influence wave dispersion and attenuation. These pore structure-dependent effects on dispersion and attenuation have been largely unrecognized in prior research. This work advances the understanding of wave behavior in porous media, emphasizing the importance of complex pore structures. The results have broad implications for seismic imaging, reservoir characterization, and the design of engineered porous materials.

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Physical modeling of elastic wave propagation in fluid saturated porous media

Pinbo Ding (China Uiversity of Petroleum (Beijing)), Feng Zhang (China Uiversity of Petroleum (Beijing)), Xiang-yang Li (China Uiversity of Petroleum (Beijing))

Abstract

1 Introduction

In conventional P- wave seismic exploration, P- wave velocity and other parameters are affected by many factors, including both the rock matrix and fluid (Matsushima et al. 2016). Shear waves are mainly affected by the rock matrix, which can provide the shear wave velocity, shear modulus, and other parameters (Zhang et al. 2022) to accurately identify the geological structure of the reservoir and reduce multiplicity (Li and Zhang 2011).

Seismic forward modeling is an important method for analyzing seismic wave propagation and can simulate the processes of wave excitation and propagation in a medium (Ding et al. 2021). However, previous studies have mainly focused on physical modeling and analyzed P- wave fields, whereas wave fields excited by shear wave sources have rarely been studied.

In this study, a seismic physical model containing different types of sandstone blocks was constructed in the laboratory to simulate different reservoir parameters, such as fluids and clay. The reflection signals of P-P, SV-SV, and SH-SH waves were analyzed and compared. The sensitivity of different types of data to fluids and clay has been discussed to provide a basis for comprehensively utilizing multi-wave data for reservoir prediction and fluid detection.

2 Methods

A horizontal-layered physical model was designed with two layers (Figure 1). The overlying strata were homogeneous and isotropic. Several groups of synthetic sandstone blocks, simulating different reservoir parameters, were embedded in the second layer. The scale factor was defined as 1:10000, where 1 mm in the model represented 10 m in the field. The dimensions of the physical model were 1 m × 0.8 m × 0.14 m (length × width × height), representing 10 km in the inline section, 8 km in the crossline section, and 1.4 km depth at the field scale. In the second layer, six rows of synthetic sandstone blocks were designed, with each row of blocks representing different reservoir parameters (Figure 2). Notably, only Row 4 was used for multi-wave acquisition and analysis.

2D seismic data were acquired in the laboratory using different types of transducers, and P-, SV-, and SH- wave data were recorded along the inline direction (Figure 1b). The red dotted dashed line in Figure 1b indicates the survey line along a group of blocks with different fluids in H-1 – H-3 and CH-1 – CH-3. Because shear waves cannot propagate in water but only in solids, shear wave data were acquired on the solid surface of the physical model. Shear wave transducers were used as the source and receiver to acquire SV- and SH- data, and the polarization directions of the source and receiving transducers were

inconsistent. The polarization direction was along the survey line during SV- data acquisition and perpendicular to the survey line for SH- data acquisition.

3 Results

Based on seismic physical modeling, this study analyzed the influence of different types of wave fields on reservoir parameters, such as fluid and clay content. Shear wave data were collected on solid surfaces, SV- and SH- wave data contained large amounts of wave field information and interfering wave signals. During seismic physical model data processing, interfering wave signals, such as surface waves and multiples, were suppressed, resulting in high-quality and high signal-to-noise ratio seismic data. Hence, the accuracy of using physical modeling data to analyze the effects of fluid and clay on different types of seismic wave fields can be ensured. The seismic responses of the P-, SV-, and SH- waves were analyzed based on the seismic physical modeling results. The P- wave was more sensitive to fluids, whereas the SH- wave was not sensitive to the fluids and showed better imaging results. Compared with the SH- waves, the SV- waves were still slightly affected by the fluids, and their imaging results were not as good as those of the SH- wave. The AVA characteristics of P-, SV-, and SH- waves were extracted to distinguish reservoir parameters. A comparative analysis of the experimental results revealed that P- waves were more sensitive to fluids than SV- and SH- waves, whereas the SV- and SH- wave fields were insensitive to fluids.

As shown in Figure 3, P- wave is more sensitive to the fluids, while the SH- wave is not sensitive to the fluids and have better imaging results. The SV- wave is still affected by the fluids, and the imaging result is not as good as the SH- wave. The AVA characteristics of P-, SV- and SH- waves are extracted to distinguish reservoir parameters. P- wave AVA characteristics vary greatly and are greatly influenced by factors such as clay and fluids. The variation of SV- wave AVA characteristics is not as significant as P- wave, and SV- and SH- wave data could be more conducive to identifying whether the block contains clay. The SH- wave AVA characteristics are more reliable for seismic imaging. This study compared and analyzed the differences of different types of wave fields, the processing of shear source seismic data is simpler and more feasible than P - SV data. The results of this study show that comprehensive use of multi-wave data can better carry out seismic imaging and reservoir prediction.

4 Conclusions

In this study, we conducted a physical modeling study on seismic response characteristic analysis of P-, SV-, and SH- waves. Seismic imaging and reservoir prediction can be improved by combining P-, SV-, and SH- wave data for better hydrocarbon identification and reservoir parameter description.

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Quantifying Drying and Pore Flow in Dual-Porosity Porous Micromodels Using Micro-PIV

Yaofa Li (University of California, Riverside), Md Ahsan Habib (Montana State University), Bo Guo (University of Arizona), Diego Armstrong (Montana State University)

Abstract

Drying in porous media holds a great significance across a wide range of natural and engineering processes. Notable applications include food processing [1], pharmaceutical industries, porous building materials, soil and hydrology [2]. For instance, during CO$_2$ injection, salt precipitation due to drying reduces permeability, posing a threat to sequestration by obstructing pores. In soil, the presence of both microaggregates and macroaggregates of different pore sizes in soil creates a multiscale environment. Numerous processes, including gases and water transport, are known to be controlled by the resultant multiscale flow dynamics and inter-/intra-aggregate interaction during drying. A comprehensive knowledge of the underlying fluid physics in drying is crucial to modeling, predicting, designing and guiding the aforementioned applications.

Drying in porous media is a multiphase flow process in porous media, where the liquid phase vaporizes, causing the originally liquid-saturated pore space to be continuously displaced by the vapor phase, often described as the invasion-percolation process. Currently, drying in a homogeneous porous media is relatively well understood, which is characterized by three periods [3]. However, the drying of porous media can be significantly complicated by the multi-scale structures that exist in many porous media. Again, in soil, while the pore size in macroaggregates can be on the order of tens or hundreds of micrometers, the microscale pores in the microaggregates can be sub-micrometers. The different pore sizes in the same porous medium causes complex flow interactions between micro- and macro-pores due to their variations in capillary pressure. Our understanding of drying from porous media featuring dual porosity is thus still limited.

To that end, a novel 2D dual-porosity microfluidic device is used to study the multi-phase flow of air and water during drying, emphasizing the multi-scale interaction and role of corner film flows. In particular, the subtle interactions between drying and multiscale transport across micro- and macro- pores are carefully investigated. The microfluidic devices are created to bear the innovative three-layer glass-silicon-glass architecture, providing precise structural control and excellent optical access from both top and bottom. An innovative dual-magnification imaging technique adapted for micro-PIV and epi-fluorescent microscopy, offers insightful information about the flow dynamics at both the micro- and macro-scales concurrently. The preliminary results clearly depict the overall drying dynamics in various porous structures and show that the porous geometry and external flow conditions pose a strong control on drying rate and flow patterns.

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Damage Monitoring in Porous Concrete Via Deep Learning of Capsule Aggregate's Impedance Signals

Jeong-Tae Kim (Pukyong National University, South Korea)

Abstract

This study presents a multi-task 2D CNN model for integrated monitoring stress and damage in porous concrete structure utilizing the raw impedance signatures of capsule aggregate (CA) embedded in the structure. The fundamental theory of CA-based EMI method is presented to describe how the sensor responds to compressive loads. Next, compression tests on a CA specimens are conducted to record the stress-damage EMI responses of CA sensors under applied stresses. The multi-task 2D CNN model learned the impedance signals for predicting the porous concrete stress and damage is constructed. Consequently, the generalization and robustness of the developed model are tested against noise and untrained data.

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Probabilistic Modeling of Two-dimensional Consolidation Using the Spectral Feynman-Kac Approach

Naina Deb (Indian Institute of Technology Guwahati)
Arindam Dey (Indian Institute of Technology Guwahati), Budhaditya Hazra (Indian Institute of Technology Guwahati)

Abstract

Consolidation analysis of saturated soils remains a critical challenge in geotechnical engineering because of the inherent spatial variability of soil properties and the complexities associated with the boundary conditions encountered in real-world scenarios. Traditional consolidation analysis often assumes soil to be homogenous, considering key properties such as coefficients of consolidation, permeability, and volume compressibility as constant throughout the soil domain. However, in reality, soils are inherently heterogeneous, and these soil properties exhibit significant spatial variability. Addressing these uncertainties accurately is essential, particularly for a reliable prediction of the excess pore water pressure (EPWP) profiles and associated settlement behavior.

To incorporate these uncertainties in a probabilistic framework, this article proposes a novel meshless approach based on the spectral Feynman-Kac (SF-K) framework to address the two-dimensional consolidation problem of saturated soils. The proposed SF-K approach extends the classical Feynman-Kac formula to accommodate the spatial variability of soil properties, employing the Karhunen-Loeve (KL) expansion technique. The coefficients of horizontal and vertical consolidation (c_h and c_v) are modeled as 2D random fields to realistically capture the spatial heterogeneity of soils. These random fields of c_h and c_v are represented using a truncated KL expansion to ensure efficient spectral characterization of spatial variability. Corresponding to the governing partial differential equation (PDE) for 2D consolidation, the SF-K framework reformulates the problem into two independent stochastic differential equations (SDEs) driven by Brownian motions that generate stochastic processes in the horizontal and vertical directions. The generator SDEs are simulated using the Euler-Maruyama method within a Monte Carlo (MC) simulation framework. The solutions of EPWP profiles are approximated by taking the ensemble average of the trajectories traced by the Brownian particles, depending on the interaction of the particles with the domain boundaries.

In the present work, mixed boundary conditions representing various drainage scenarios are considered to assess their influence on the EPWP dissipation profiles and subsequent settlement of the 2D consolidation problem. Four distinct cases of boundary conditions designated as Type I, Type II, Type III, and Type IV are considered in this study. In the Type I boundary condition, the top ($z=L_z$) and the right ($x=L_x$) boundaries are pervious, facilitating drainage of pore water, while the bottom ($z=0$) and the left ($x=0$) boundaries are impervious, restricting the flow of pore water. The Type II

boundary condition deals with the pervious top, bottom, and right boundaries, enabling drainage of pore water, with only the left boundary remaining impervious. In the Type III boundary condition, the drainage of pore water is allowed by the pervious top, left, and right boundaries, while the impervious bottom boundary inhibits the flow of pore water out of the soil domain. The Type IV boundary condition allows the pore water to drain through all the pervious top, bottom, left, and right boundaries, representing a fully drained condition.

Boundary conditions are incorporated stochastically in the simulations through the interaction of the Brownian particles with the domain boundaries and by classifying the boundaries as either a Dirichlet or Neumann boundary. This mechanism mimics the physical behavior of EPWP dissipation and settlement under mixed boundary conditions. For Dirichlet boundaries corresponding to pervious or drained conditions, particles reaching the boundary exit the domain, and the trajectory of the particle is terminated. This reflects the free outflow of pore water at a Dirichlet boundary in the stochastic simulations. In contrast, Neumann boundaries representing impervious or no-flux conditions are handled by reflecting the particles reaching the boundary back into the domain. This ensures the restriction of the drainage of pore water at Neumann boundaries in stochastic simulations.

To compare and validate the accuracy of the proposed SF-K framework, a spectral finite difference method (SFDM) is developed to solve the 2D consolidation problem, incorporating the spatial variability of c_h and c_v through the KL expansion technique. The SFDM models the random fields of c_h and c_v with identical statistical properties, similar to the SF-K framework. The variations of the EPWP profiles and the settlement profiles of the 2D consolidation problem obtained from the SF-K framework are then compared against those obtained from the SFDM under the four distinct drainage cases (Type I-IV) and a uniform initial condition. The results demonstrate excellent agreement between the frameworks for all cases of drainage boundary conditions, as evidenced by low values of root mean square error (RMSE). This highlights the robustness of the RF-K framework in accurately handling the spatial variability of soils and addressing various drainage boundary cases of the 2D consolidation phenomenon. These results demonstrate the robustness of the proposed SF-K framework in accurately capturing the spatial variability of soils and handling various drainage boundary conditions within a stochastic framework that addresses the 2D consolidation problem.

Grid-based numerical methods, such as the SFDM, require a predefined spatial discretization and time step satisfying the stability criteria to ensure accuracy of the solutions. Failure to satisfy this criterion leads to numerical dispersion of the EPWP profiles and settlement profiles and inaccurate solutions. In contrast, the proposed SF-K framework is meshless, eliminating pre-processing steps such as grid generation, mesh optimization, and refinement, thereby reducing computational complexity. Moreover, the proposed SF-K framework relies on independent simulations of driftless SDEs, which further reduces the computational cost while maintaining accuracy. The study demonstrates the accuracy and computational efficiency of the proposed SF-K framework in solving the 2D consolidation of saturated soils without being constrained by strict stability conditions.

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Inelastic Poromechanics and Solitary Wave Dynamics in Fluid-Saturated Rocks

Viktoriya Yarushina (Institute for Energy Technology)

Abstract

The theory of poroelasticity began with the pioneering works of Maurice Biot [1] and Jakob Frenkel [2], who laid the foundation for understanding the coupled behavior of mechanical deformation and fluid flow in porous media. Since its beginning, poroelasticity has demonstrated its usefulness in a wide range of geophysical and engineering problems, particularly in the understanding of seismic wave propagation in the Earth's crust and the complex interactions between fluid and solid phases in geological formations. One of the key insights of poroelasticity is that the porous nature of rocks and the presence of interstitial fluid result in a more intricate mechanical response than that of purely elastic solids. For example, this theory predicts the existence of three distinct bulk moduli and three types of seismic body waves, which significantly influence wave speeds and attenuation in subsurface materials. Over time, it has become clear that the behavior of porous media is governed not only by elastic but also by inelastic mechanisms, such as viscous flow, plastic deformation, and chemical reactions. These processes, particularly in long-term geological and engineering scenarios, play a crucial role in rock compaction, fluid transport, and the development of complex structural patterns in the Earth.

Elastic models alone cannot accurately capture the time-dependent behavior of rocks under stress. Observations from both field data and laboratory experiments show that rocks undergo viscous (creep) deformation over geological time scales. Furthermore, such creep behavior is not limited to long durations; it can also manifest during the shorter timescales relevant to engineering operations, such as surface subsidence observed during petroleum extraction or geothermal energy production [3-5]. In addition, plastic failure - whether at the grain scale (microscopic) or fault scale (macroscopic) - contributes to structural transformations, permeability evolution, and localized deformation patterns [6]. Traditional linear poroelastic theory assumes that shear and volumetric deformations are uncoupled - i.e., shear deformation does not alter the volume of the porous medium. However, in real geological materials subjected to high stress, shear and volumetric processes are strongly coupled, resulting in phenomena such as shear-enhanced compaction and shear-induced dilation. To capture these effects, models must account for plastic deformation in the solid matrix. In addition to mechanical behavior, chemical reactions occurring within the pore space can alter the rock's microstructure, changing its porosity, permeability, and stiffness. This further emphasizes the need for a generalized extension of the classical Biot-Frenkel theory - one that incorporates inelastic deformation mechanisms, nonlinear rheology, and chemical interactions.

The development of such generalized models requires careful consideration of thermodynamic consistency, especially when modeling nonlinear rheological behaviors that include elastic, viscous, and plastic deformations. In our work, we adopt a framework based on nonequilibrium thermodynamics, ensuring that all model equations comply with the first and second laws of thermodynamics [7]. We demonstrate that, in the poroelastic limit, our extended equations reduce to the classical Biot model, thereby confirming the thermodynamic consistency of Biot's original theory. This result is particularly significant in light of previous literature that has questioned Biot's framework and proposed alternative models (de Boer 2000, Gurevich 2007). We critically assess these alternative formulations and demonstrate that their conclusions are based on misinterpretations of poroelastic moduli and underlying physical assumptions. To close the constitutive relations in our model, we use a micromechanical approach based on effective medium theory. We employ both newly developed analytical solutions and Galin's classical elastoplastic solution [8] for the deformation of a single cavity embedded within an inelastic solid. This allows us to derive compaction relations that account for the effects of shear stress, plasticity, viscous flow, and chemical reactions. Furthermore, consideration of a single fluid-filled pore embedded in a viscoplastic or elastoplastic solid matrix subjected to combined pressure and shear loading leads to a set of three-dimensional constitutive relations that describe both rate-dependent and rate-independent deformation of porous rocks [9]. The resulting compaction equations describe changes in the porosity, total volumetric deformation, and Darcy's flux as a function of total and fluid pressures, and reaction progress. These equations account comprehensively for elastic, viscous, and plastic components of deformation. When compared with experimental results from triaxial creep and instantaneous loading tests, our model predictions show strong agreement, validating both the physical assumptions and mathematical formulation.

We further explore the dynamic behavior of the model equations and show that the presence of viscous deformation terms enables the formation of nonlinear solitary wave solutions [10]. These porosity waves represent localized zones of elevated porosity that travel through the rock matrix while preserving their shape. In the elastic limit, these solitary waves degenerate into shock waves. The existence of these nonlinear waves depends critically on the nonlinear porosity-permeability relationship and the stress-sensitive evolution of porosity. To better illustrate the underlying physics, we analyze a simplified scenario: a vertical column of viscous/viscoplastic porous rock with uniform initial porosity that undergoes subsidence due to its own weight (Figure 1). Within this column, a solitary porosity wave forms in response to a local disturbance, then propagates upward at a constant velocity, preserving its structure. Below the wave, the rock returns to its background values of porosity and effective pressure. In this setup, the governing equations reduce to a hydraulic equation for effective pressure and a viscous/viscoplastic compaction equation for porosity evolution.

Remarkably, the reduced system of equations is mathematically equivalent to those governing the motion of a ball oscillating on a frictionless, one-dimensional curved surface. When the forces constraining the ball are removed, it moves under gravity - an elegant analogue to the evolution of porosity and pressure in the rock (see Figure 2). In this analogy, depth along the porosity profile maps to time in the ball's motion, porosity corresponds to the ball's position on the surface, and the rate of porosity change mirrors the ball's velocity. Our analysis further shows that changes in matrix rheology have a significant impact on wave behavior. In the limit of plastic deformation, the solitary wave degenerates into a sharp shock-like front. When plastic failure is coupled with viscous deformation, it induces decompaction weakening in the matrix and leads to asymmetrical wave shapes. In two-

dimensional systems, this asymmetry can produce channel-like features, which have been proposed as a key mechanism behind focused fluid flow in the subsurface [11, 12]. The inclusion of shear stresses and shear-induced dilation still facilitates the propagation of porosity waves and leads to more realistic predictions of the fluid pressure developing within the wave [9]. This finding implies that porosity waves offer a physically plausible mechanism for the formation of focused fluid flow pathways - a phenomenon observed in settings ranging from mid-ocean ridges and subduction zones to hydrocarbon reservoirs and geothermal systems.

In conclusion, the classical theory of poroelasticity, though foundational, must be expanded to incorporate the complex inelastic and chemical behaviors that dominate many subsurface processes. Our thermodynamically consistent framework, which integrates elastic, viscous, plastic, and chemical effects, provides a powerful tool for understanding and predicting the coupled mechanical and fluid transport phenomena in porous rocks. The emergence of nonlinear porosity waves and their dependence on matrix rheology highlights the importance of fully coupled models for explaining fluid migration and deformation in the Earth’s crust.

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Should seismic wave propagation in high-pressure, high-temperature media be a concern?

Wubing Deng (China University of Petroleum (East), School of Geosciences)
Li-Yun Fu (China University of Petroleum (East), School of Geosciences)

Abstract

It is widely accepted that seismic wave propagation in reservoirs subjected to high ambient pressure and temperature differs markedly from that in conventional low-pressure, low-temperature geological settings. In general, seismic velocity increases with confining pressure and decreases with temperature—an observation that holds true across a wide range of rock samples with varying mineral compositions, pore geometries, and saturation conditions. Similar trends can also be found in low-frequency forced oscillation experiments, where the dynamic Young's modulus—derived from the stress-to-strain ratio at different frequencies—also exhibits sensitivity to pressure and temperature.

However, our recent ultrasonic (1 MHz) transmission experiments conducted under controlled laboratory conditions reveal an unexpected result: the transmitted P-wave recorded under low confining pressure and ambient temperature can be nearly identical to that obtained under high-pressure and high-temperature conditions, provided that a specific relationship between pressure and temperature is maintained. This finding challenges the conventional understanding of thermo-mechanical effects on wave propagation and suggests the presence of "compensatory mechanisms" that preserve acoustic characteristics under coupled extreme conditions.

To quantitatively capture this phenomenon, we developed a physically grounded rock physics model by extending the Generalized Linear Solid (GLS) framework developed by Morozov and Deng (2016) to incorporate the effects of thermally induced stress. Specifically, thermal stress is introduced through temperature-dependent volumetric expansion, which modifies the internal stress state of the material and affects the wave propagation. This extension allows us to explain the observed equivalence in wave transmission under different pressure–temperature conditions by accounting for the coupled influence of thermal and mechanical loading. The resulting model provides a unified description of wave propagation under thermo-mechanically coupled conditions and offers new insights into the acoustic response of reservoir rocks in deep, high-pressure, high-temperature environments.

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Pore-Scale Dynamics in Porous Media 3, Conveners: Yashar, Ruby, Bo Presentation 64

Liquid-Vapor Interfaces in Pore-Scale Evaporation: Insights from Direct Numerical Simulation using Lattice Boltzmann Method

Piyush Pradhan (Department of Earth & Environmental Engineering, Columbia University)
Pierre Gentine (Department of Earth & Environmental Engineering, Columbia University), Shaina Kelly (Department of Earth & Environmental Engineering, Columbia University)

Abstract

Evaporation is a complex multiphysics process governed by the interplay of liquid–air flows, phase transitions, interfacial dynamics, and coupled heat and mass (vapor) transport mechanisms [1, 3]. In the context of porous media, evaporation plays a pivotal role in a variety of natural processes and engineering applications, including evapotranspiration in hydrology-which influences the global water cycle and long-term water balance [6], separations/crystallization and precipitation of salts due to to excessive evaporation from soils, rocks, and cements [4], phase-change electronics cooling [7], liquid water removal in proton exchange membrane fuel cells [3], curing of concrete [5], among others. In this study, we investigate evaporation dynamics under isothermal conditions in a range of three-dimensional porous media, beginning with simple sphere pack configurations and progressing to more complex porous media (soils and rocks) reconstructed from μ-CT scans. Simulations are performed using the Central-Moment (Cascaded) Lattice Boltzmann Method (CLBM) coupled with the Shan-Chen pseudopotential model to capture multicomponent, multiphase flows. The simulations are performed using an in-house, open-source, GPU-accelerated code gEOS-LB (https://github.com/piyush-ppradhan/gEOS-LB). The system is simplified to comprise of two components: a phase-changing liquid (water) and a non-condensable gas (air), following the methodology established in prior studies [3, 2]. The phase-changing component is modeled using Peng-Robinson equation of state, which has been successfully used to replicate the thermodynamic behavior of water [8]. We first validate our numerical implementation against several benchmark evaporation problems, both analytical and experimental, and show that it accurately reproduces two-component evaporation dynamics-even under conditions with high dry air mass fractions (up to 90%). Next, we explore how evaporation rates correlate with key characteristics of the wetting component including surface area, interfacial curvature, phase morphology, and connectivity in the aforementioned porous media domains (increase morphological complexity). We also compare microscale vapor flux distributions with bulk evaporation trends. Findings are analyzed for comparison with experimental observation of evaporation dynamics in porous media, which show that evaporation processes typically proceeds through multiple distinct stages: The first stage is the constant rate period (CRP), during which the liquid front remains pinned near the surface. This is sustained by capillary-driven flow from the porous region, leading to a near-constant evaporation rate. As evaporation progresses, the system enters the falling rate period (FRP), where capillary forces can no longer compensate for increasing viscous resistance. Consequently, the liquid front recedes deeper into the porous structure, and the evaporation rate begins to decline sharply.

Eventually, the process transitions into the receding front period (RFP), characterized by limited liquid connectivity and slow vapor transport, resulting in significantly reduced evaporation rates. These evaporation profiles are typically derived based on the total porous surface area and do not capture the local variations in evaporation rates at the liquid–vapor interface within the intricate and confined pore structures.

This work sets a foundation for enhancing an understanding of evaporation dynamics at the pore scale as compared to the bulk. In the long term, we seek to: (i) reveal the underlying physical mechanisms that drive observed macroscale evaporation behavior, (ii) explore in-situ hydraulic properties that can better predict CRP to FRP transition, and (iii) provide essential inputs for the development and validation of continuum-scale models through upscaling techniques. Limitations in understanding pore-scale evaporation dynamics is largely due to the challenges in resolving local evaporation dynamics within porous media, even with advanced imaging techniques. High-fidelity numerical simulations offer a valuable alternative for probing the evolution of liquid–vapor interfaces and quantifying evaporation under varying saturation conditions.

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Modeling the Initial Swelling and Capillary Contraction of Porous Materials During Wetting and Drying

Mohammadali Behboodi (University of Colorado Boulder), Yida Zhang (University of Colorado Boulder)

Abstract

The physicochemical properties of solid-fluid interface have been identified as the underlying cause of various interesting phenomena observed in porous materials during fluid intrusion. Attraction of fluid molecules toward the solid surface (i.e., adsorption) can decrease surface tension and result in a swelling of porous skeleton. This mechanism is quantitatively modeled through surface poromechanics (Behboodi et al., 2025; Zhang, 2018) which considers a system of three phases: solid, fluid, and interface where each can carry mass, momentum, and entropy. It has been demonstrated that incorporating surface properties into the solid free energy arises naturally from the system's energy balance and directly influences the response of the solid skeleton during adsorption and changes in other environmental conditions.

Experimental observations indicate that monotonic swelling is not always the case, and depending on the pore size and material type, the skeleton might experience sudden shrinkage in intermediate or high vapor pressure levels which is commonly attributed to capillary condensation. The current framework lacks the ability to account for this phenomenon. Thus, an unsaturated surface poromechanics formulation is developed to fundamentally incorporate the evolutions of interfaces among the solid, the liquid, and the gas phases. The formulation begins with a thermodynamic analysis of an unsaturated porous medium integrating the energetics of the solid-liquid (SL), solid-vapor (SV), and liquid-vapor (LV) interfaces, an adaptation from Coussy (2004) and Zhang (2018). The new formulation accounts for the physics of pore fluid phase transition between vapor and liquid, recovering the water retention characteristics curve for unsaturated porous media. Using these methodologies, two sets of constitutive equations are developed: one resolves the evolution of SL-SV-LV surface areas and the other one lumps these effects through a macroscopic capillary potential. The performance of the model is evaluated through the prediction of swelling-shrinkage-swelling observed in experiments on micro- and mesoporous materials during wetting. A hydraulic dissipation is considered as a 1st order homogeneous function to capture hysteresis in sorption and strain isotherms during wetting and drying cycles.

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A Learning-based Multiscale Model for Underground Fluid Transport Processes

Kaushik Bhattacharya (California Institute of Technology)

Abstract

Fluid transport through permeable geological formations couples various mechanical, thermal, and chemical phenomena. A critical bottleneck in building high-fidelity models to predict these complex, multi-physics transport processes is the faithful transfer of information between microscopic fluid-rock interactions and large-scale reservoir dynamics. Microscopic interactions, coupled with geochemical, biological, or hydromechanical processes, lead to continuous evolution in the properties of geologic materials. Traditional multiscale modeling approaches have been developed for particular processes to provide closure relations and pass the information across scales. However, the actual implementation of these techniques is prohibitively expensive due to the repeated solution of partial differential equations at the finer scales. \\

Here, we focus on the transport of flow through the porous medium in the presence of chemical reactions, where chemical interactions between fluids and solid structures alter the morphology of porous media at the microscale, leading to changes in transport properties and, consequently, changes in flow conditions at the reservoir scale. We specifically consider a regime where advection is dominated and the convection-diffusion equations are complicated due to fluid-rock interactions and evolving microstructure \cite{karimi2024learning}.\\

We present a methodology to overcome the challenges of traditional multiscale models by creating a high-fidelity, computationally efficient surrogate of the lower-scale behavior that can be used directly at the upper scale to prevent repeatedly solving equations (Fig. 1). Then, the surrogate serves as a closure relation by learning the history-dependent physical problem at the lower scale. This framework uses one-time, offline data generated from pore-scale simulations to train a solution to the partial differential equations over a neural network and obtain a learned surrogate. The surrogate is an inexpensive, approximate solution to the lower-scale problem, which can be used to solve the macroscopic problem without further modeling \cite{karimi2024learning}.\\

To further reduce computational costs and data generation efforts in this framework, we developed an accelerated micromechanical model for the lower-scale problem. At this scale, flow is governed by the Stokes equation, while solute transport follows an advection-diffusion equation. Our approach employs an iterative method, where each step involves either local computations or solving a Poisson equation. We use the fast Fourier transform (FFT) method, which enables spatially parallel computation and efficient implementation on accelerators such as graphics processing units (GPUs) to leverage their massively parallel architecture \cite{karimi2024accelerated}.\\

The proposed framework has the potential to bridge the gap between the micron and kilometer scales, enabling efficient information transfer and facilitating the investigation of fundamental subsurface processes. It can provide key insights into the evolution of underground formations, including carbonate structures, karst formations, the long-term behavior of injected CO$_2$ in deep geological reservoirs, and its chemical interactions with surrounding rock formations. \\

Using this framework, we study convective mixing followed by gravitational fingering in geological formations, where a denser fluid (with higher solute concentration) is placed above a lighter fluid. The flow is driven by density differences between the fluids, with gravity acting on the denser fluid, causing it to sink and displacing the lighter fluid upward. This process causes the fluid interface to become unstable, leading to the formation of finger-like patterns. We are particularly interested in investigating the gravitational fingers in the presence of chemical reactions, where the transport properties of the geological formation (i.e., porosity, permeability, and diffusivity) evolve over time due to reactions between fluid and solid structures. This process leads to the creation of preferential flow pathways and heterogeneities in the material properties of the underground formation.

We also investigate complex scenarios involving reaction-driven heterogeneities, such as upscaling multi-mineral reactive transport systems with varying reaction rates and, the effect of local curvature on chemical reactions and the formation of preferential flow pathways at the geological scale, where classical empirical relations fall short.

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Poroelastic diffusion through hydrogel membranes for fast atmospheric water harvesting

Yiwei Gao (WAVR Technologies, Inc), H. Jeremy Cho (University of Nevada, Las Vegas)
Areianna Eason (University of Nevada, Las Vegas), Yihong Zhao (WAVR Technologies, Inc)

Abstract

Water scarcity has has been increasingly dire, affecting billions of people globally. Atmospheric water harvesting (AWH) technologies offer promising solutions to provide a new source for water. Many of the existing AWH approaches utilize single-sorbent materials with. Their performance is often limited by the requirement of operating in a batch mode—cycling through water capture, storage, and release stages—and often are limited to higher relative humidity conditions than arid, water-scarce communities.

Inspired from nature—the Australian tree frog [1] —we have developed a novel AWH system that combines a hydrogel membrane with liquid desiccant. This design enables distinct and continuous water capture, storage, and release stages, allowing for significantly improved daily water harvesting efficiency, even in low-humidity environments.

Unlike many hydrogel-based AWH systems, where the hydrogel functions as both absorbent and storage medium, our design employs the hydrogel solely as a transport medium—mimic to the permeable skin of the tree frog. The liquid desiccant (saturated aqueous lithium bromide solution), serving as the absorbing and storage medium, provides a markedly lower chemical potential than the ambient air. The rate of water vapor capture in this system is determined by how rapidly vapor can diffuse through the hydrogel membrane. This process is primarily dependent on the poroelastic diffusion coefficient of the hydrogel. To better understand the capture mechanism, we employ an analogy with an electrical circuit: the chemical potential difference between ambient air and the desiccant acts as the "voltage," and the water vapor flux is the "current." Maximizing this flux requires minimizing the total "resistance" of the system, which consists of three components: vapor-phase convection resistance R_{vap}, diffusion resistance within the hydrogel membrane R_{gel}, and convection resistance in the liquid phase R_{sol}. Our analysis shows that R_{vap} is primarily dependent on environmental conditions, and R_{sol} is at least an order of magnitude smaller than R_{vap}, making it negligible. Thus, the key to maximizing water capture lies in minimizing R_{gel}, which is highly dependent on the poroelastic diffusion coefficient, $(K_{wet}* \kappa_{wet})/\mu$, where K_{wet} and κ_{wet} are the elastic modulus and the hydraulic permeability of the fully swollen hydrogel, respectively, and μ is the viscosity of water.

To determine the relationship between hydrogel stiffness, permeability, and swelling behavior, we derived a power-law model based on de Gennes' semi-dilute polymer theory. This model relates the swelling ratio to the ratio of elastic moduli between arbitrary and fully swollen states with an exponent of –9/4 [2]. Furthermore, by integrating de Gennes' theory with Darcy's law and the Kozeny–Carman equation, we established a scaling law that links hydraulic permeability to elastic modulus with an

exponent of –8/9 [3]. These theoretical foundations enabled us to develop a mathematical model for membrane diffusion resistance as $R_{gel} \propto \mu/(K_{wet} * \kappa_{wet})$. Thus, in the most ideal scenario, we would like to maximize both stiffness and hydraulic permeability simultaneously.

However, our previous research demonstrated that there is a tradeoff between the stiffness and the hydraulic permeability of the hydrogel – denser network structure leads to better stiffness but allows less water passing through. To find a sweet balance between such two properties, the traditional method was adjusting the crosslinking density of the hydrogel. Inspired by the work of Kim et al. [4], we adopted an alternative strategy: maintaining a low crosslinker concentration to preserve permeability, while enhancing mechanical stiffness through increased polymer chain entanglement. This approach enabled us to significantly lower R_{gel}, nearly reducing it to an order of magnitude below R_{vap}. By reducing the water-to-monomer ratio from 55 to 11 and crosslinker-to-monomer ratio from 3% to 0.1%, we successfully increased both stiffness and hydraulic permeability of polyacrylamide hydrogel from 7 kPa to 27.6 kPa, and from 2E-18 m2 to 7.2E-18 m2, respectively. As such, the diffusion resistance within the hydrogel membrane was successfully reduced to 7%, which is at least one order of magnitude lower than the convection resistance from the air flow. In our recent experiments, we successfully developed a stronger hydrogel membrane with almost 160 kPa stiffness modulus and around 2E-18 m2 hydraulic permeability

With such low-resistance hydrogel membranes, we successfully constructed a benchtop prototype of our high-yield water capture system using the optimized hydrogel membrane, which can be regarded as convection-limited only. Experimental results demonstrated water harvesting rates of 5.5 $kg \cdot m^{-2} \cdot day^{-1}$ at 35% relative humidity (outdoor) and 16.9 $kg \cdot m^{-2} \cdot day^{-1}$ at 58% (indoor)—performance metrics that surpass existing AWH technologies [5]. For practical application, a projected 1 m^2 device based on our system could supply sufficient daily drinking water for 2–4 adults in extremely arid regions such as Las Vegas, the driest city in the United States. Simulating based on actual weather data, the technology shows the potential to provide safely managed drinking water for billions of people worldwide.

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Shock-Like Propagation of Hydration and Dehydration Reaction Fronts in Poromechanical Systems

Stefan Markus Schmalholz (University of Lausanne, Switzerland)
Yury Podladchikov (University of Lausanne)

Abstract

We apply poro-mechanical-chemical models to investigate the propagation of hydration and dehydration reaction fronts in deforming porous rock. These (de)hydration fronts are often characterised by steep gradients in porosity and the propagation of these (de)hydration fronts is similar to the propagation of shock waves. Hydration and dehydration reactions play pivotal roles in plate tectonics and the deep water cycle, yet many facets of (de)hydration reactions remain unclear. We study first (de)hydration reactions where associated solid density changes are predominantly balanced by porosity changes, with solid rock deformation playing a minor role. We propose a hypothesis for three scenarios of (de)hydration front propagation and test it using one-dimensional hydro-mechanical-chemical models. Our models couple porous fluid flow, solid rock volumetric deformation, and (de)hydration reactions described by equilibrium thermodynamics. We couple our transport model with reactions through fluid pressure: the fluid pressure gradient governs porous flow and the fluid pressure magnitude controls the reaction boundary. Our model validates the hypothesized scenarios and shows that the change in solid density across the reaction boundary, from lower to higher pressure, dictates whether hydration or dehydration fronts propagate: decreasing solid density causes dehydration front propagation in the direction opposite to fluid flow while increasing solid density enables both hydration and dehydration front propagation in the same direction as fluid flow. Our models demonstrate that reactions can drive the propagation of (de)hydration fronts, characterized by sharp porosity fronts similar to shock waves, into a viscous medium with zero porosity and permeability; such propagation is impossible without reactions, as porosity fronts become trapped. We apply our model to serpentinite dehydration reactions with positive and negative Clapeyron slopes and granulite hydration (eclogitization). We use the results of systematic numerical simulations to derive a new equation that allows estimating the transient, reaction-induced permeability of natural (de)hydration zones. Results of this sub-study are published in Schmalholz et al. (2024).

We further present an elaborated model in two-dimensions for the dehydration of serpentinite that is deforming by simple shear and forms olivine veins. For this scenario, the solid deformation plays a dominant role. Field observations suggest that en échelon olivine veins in serpentinite mylonites formed by dehydration during simultaneous shearing of antigorite serpentinite. Here, we test the hypothesis of shear-driven formation of olivine dehydration veins with a novel two-dimensional hydro-mechanical-chemical numerical model. Our model accounts for the reaction antigorite + brucite = forsterite + water, considering significant solid density changes of approximately 25%. We assume ductile shearing, a decrease of shear viscosity with increasing porosity, and initially homogeneous total and fluid pressures

within the serpentinite stability field. Initial perturbations in porosity, and hence viscosity, cause fluid pressure perturbations during simple shearing. Dehydration nucleates where fluid pressure locally drops below the thermodynamic pressure controlling the reaction boundary. During shearing, dehydration veins grow and serpentinite transforms into olivine inside the veins. Simulations show that the ambient pressure and the relation between compaction length and porosity have a major impact on vein formation. Conversely, the orientation of the initial porosity perturbation, the pressure-insensitive yield stress, the porosity dependence of compaction viscosity, the elastic effects during compaction, and the reaction kinetics have minor impacts on the simulations. We quantify the relative contribution of the rates of solid volume change, solid density change, and reactive mass transfer to the porosity generation. Vein growth is self-limiting and eventually reaches a steady state. We discuss potential implications for natural olivine veins, slow slip and tremor, transient weakening, anisotropy generation, and formation of shear-driven high-porosity bands without a dehydration reaction. Results of this sub-study are published in Schmalholz et al. (2023).

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Effects of Pore Fluid Pressure in Extension-shear Mixed-mode Fracture in Carrara Marble and Berea Sandstone

Cate Tilley (Texas A&M University)
Casey Ruplinger (Graduate Researcher), Daniel Worley (Undergraduate Researcher), Hiroko Kitajima (Graduate Advisor), Jacob Tristan (Undergraduate Researcher)

Abstract

Pore fluid pressure in geological formations varies temporally and spatially, and elevation of pore pressure reaching near-lithostatic pressure occurs in natural processes (e.g., subduction zones) or anthropogenic activities (e.g., enhanced geothermal systems, carbon sequestration). Understanding the effects of pore pressure on fracturing processes is essential, particularly across the transition from extension-dominant to shear-dominant mixed-mode fracture at low effective stress. To understand the effects of pore pressure on extension-shear mixed-mode fractures, triaxial extension experiments on non-porous Carrara marble and porous Berea sandstone were conducted by controlling confining pressure (Pc) and pore pressure (Pp) independently to achieve the maximum effective principal stress ($\sigma_1' = Pc - Pp$) ranging from 7.5 to 130 MPa. At the same σ_1', the fracture strength of Carrara marble under Pp-controlled conditions is greater than that in dry conditions, whereas the fracture strength of Berea sandstone under Pp-controlled conditions is lower than that in dry conditions. Although the effects of pore pressure on the fracture strength are opposite between Carrara marble and Berea sandstone, the differences in fracture strength between pore pressure-controlled and dry conditions are pronounced in both rocks at extremely low effective stresses where extension mode is dominant. A series of experiments at the same effective σ_1' with different combinations of Pc and Pp confirm that the coefficient of pore pressure (α) for the fracture strength is nearly 1 on both Carrara marble and Berea sandstone. A series of experiments at various strain rates on Carrara marble reveal a positive strain rate dependence of fracture strength only under Pp-controlled conditions, implying dilatancy hardening. The elevated pore fluid pressure can contribute to the opening of microcracks and slow propagation of a macroscopic extension-dominant fracture at extremely low effective stress.

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Soft mater and novel porous media 1 Presentation 72

Impact of Interstitial Fluid Flow on Cancer Metastasis at the Bone Site

Dinesh Katti (North Dakota State University), Haneesh Jasuja (North Dakota State University), Kalpana Katti (North Dakota State University), Preetham Ravi (North Dakota State University), Sharad Jaswandkar (North Dakota State University)

Abstract

Globally, over 3.5 million people are diagnosed with breast cancer or prostate cancer each year, and about one million people die of this disease annually. The U.S. Center for Disease Control estimates that 1 in 8 women and 1 in 7 men will be diagnosed with breast cancer and prostate cancer, respectively, in their lifetime. The advent of early diagnosis and new treatment regimens has led to significant improvement in the cure of the disease if diagnosed early, and the cancer is confined to the primary sites of the breast or prostate. However, these cancers tend to metastasize, where the cancer cells from the primary site are transported to a distant organ via fluid flow through the blood vessels or the lymphatic system. Both breast cancer and prostate cancers have the prophecy to migrate to the bone, more so for prostate cancer. Once the cancers metastasize to the bone, there is no cure as of this time. We have developed the first in vitro models for prostate cancer[1-3] and breast cancer metastasis[4-7] to the bone using an innovative tissue engineering approach. The model consists of a bone mimetic tissue engineering scaffold made of polycaprolactone-insitu hydroxyapatite nanoclay composite that can differentiate human mesenchymal stem cells and regenerate bone without differentiating media. The breast or prostate cancer cells are introduced upon bone regeneration in the scaffolds. We observe mesenchymal to epithelial transition of the cells and formation of tight junction tumors, similar to those observed in bone metastasis in patients. Detailed gene expression and morphological analysis confirm that the in vitro tumors generated are identical to those in the in vivo systems, thus successfully developing cancer testbeds for bone metastasis. These cancer testbeds have been further tested with patient-derived cells from cancer tissues from a wide range of cancer types for both breast cancer and prostate cancer, validating the ability of the testbeds to accurately model bone metastasis in a clinical environment[8,9]. These testbeds have been use to identify spectral[10] and mechanical[11] biomarkers and drug candidates[12].

To more accurately simulate the in vivo conditions, a new horizontal flow bioreactor is invented to create interstitial flow conditions in the scaffolds, with flow velocities and shear stresses exerted by the flow on the cells matching the conditions in tissues in in vivo conditions[13] (Figure 1). Our work with perfusion bioreactors[14] and computational fluid dynamics simulations[15] of flow through interconnected flow through the scaffolds showed significant differences in cell proliferation, cell morphology, and gene expressions due to flow. The horizontal flow bioreactor was concurrently tuned with computational fluid dynamics simulations to model fluid flow conditions in bone tissue. Specially designed Transwell™ inserts were placed in the horizontal flow bioreactor in close proximity of the bone mimetic scaffolds. Migration assays were conducted with and without the interstitial fluid flow.

Confocal microscopy was used to quantify the migration of prostate cancer cells through the membrane towards the bone. The results indicate that the migration of prostate cancer increase several folds because of the presence of the bone, with or without the flow. The results also show that the migration of prostate cancer cells increased because of the flow. The gene expression analysis also showed significant differences between the no flow and flow conditions. Specifically, we observed the upregulation of αvβ3 and FAK expressions indicating the activation of adhesion protein, integrin to resist the fluid flow. We also observed the upregulation of several key markers related to cancer progression under flow conditions, such as the MMP9. The morphology of the cancer tumors under flow conditions were visibly affected, with the cellular boundaries in the tight junction tumoroids becoming almost indistinguishable, indicating increased cell-cell adhesion. The gene expression analysis showed upregulation of the cell-cell adhesion protein E-cadherin, confirming the mechanism for the morphological changes.

Figure 1. Image of the horizontal flow bioreactor chambers in an incubator (provisional patent)

The horizontal flow bioreactor was further used to model the circulating tumor cells and cell clusters in blood flow. The bioreactor revealed the initial adhesion and colonization of the cells and cell clusters to the bone. The bioreactors with the cancer testbeds with tissue engineering scaffolds can closely replicate the in vivo conditions of bone metastasis, providing a deep insight into the cancer progression, identification of biomarkers, and potential drug candidates that could be more effective at the bone site. These testbeds and the computational fluid dynamics used to tune the flow conditions can fill in the gaps caused by the lack of sufficient bone metastasis patient tissues for testing.

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Micromechanical Investigation of Granite Under Coupled Thermal and Saturated Conditions

Hongkyu Yoon (Sandia National Laboratories)
Ozan Altuntas (University of Utah)
Pania Newell (University of Utah)

Abstract

Granite as a primary rock type for enhanced geothermal systems is subjected to coupled thermal and hydrological conditions caused by geothermal gradients, tectonic stresses, and groundwater infiltration. These processes introduce thermal, mechanical, and chemical disturbances that can alter internal stress distributions and weaken the rock structure. Since failure and deformation begin at the microscale, understanding the factors that influence mechanical stability at this scale is important to prevent structural degradation. Despite existing research on granite under isolated thermal or mechanical loading, no study has yet addressed a combined hydro-thermal-mechanical characterization of granite at the microscale. This limits our understanding of the impact of combined environmental factors. In this study, we examined the mechanical and fracture properties of Sierra White granite at the microscale, including elastic modulus, hardness, and fracture toughness under both dry and wet conditions and at temperatures from room temperature up to 450°C. The samples were characterized using scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS), and tested using nanoindentation technique. The loading condition followed a trapezoidal load function with a linear loading segment of 5 seconds, a 2-second holding period at peak load, and a linear unloading phase over 5 seconds. Mechanical properties were derived from load-displacement curves, while fracture toughness was computed using an energy-based method. To understand how granite behaves in wet conditions, the samples were soaked in water for 24 hours before performing nanoindentation tests. The results show that after this exposure, granite loses about 60% of its strength. After drying for 12 hours under ambient conditions, a partial recovery in mechanical properties was observed. In contrast, thermal exposure up to 450°C resulted in a reduction of around 20% in hardness, modulus, and fracture toughness. The observed difference between the effects of water and heat suggests that the mechanical response of granite is more affected by water, whereas temperature-induced changes were less pronounced within the tested range. These findings demonstrate that both water and temperature influence the micromechanical behavior of granite, with a dominant role of moisture in driving nanoscale softening mechanisms. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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Modeling Consolidation of Soft Porous Core-Solid Sheath Rods

Arina Korneva (Virginia Tech)
Denis Kucherenko (Virginia Tech)

Abstract

Many engineered and biological soft porous materials, such as animal nerves, tube-based filters, and batteries, are cylindrical composites, which are anisotropic and multilayered. The model of soil consolidation initially developed by Karl von Terzaghi does not account for these complexities of porous composites. We developed analytical models to enable experimentalists to accurately measure the permeability and elastic properties of fluid-saturated soft composite rods. The model assumes affine deformation of the Hookean sheath and poroelastic core. The sheath is impermeable to the fluid, and the material properties of the composites are such that their radial deformation is much smaller than the longitudinal deformation. Moreover, in the biological applications to animal nerves, the radial permeability is negligible, and hence the flow of fluid is unidirectional, satisfying Darcy's law. The model for a Newtonian fluid can be generalized to non-Newtonian fluids like those of biological nature.

A 3D poroelastic model is reduced to a 1D model for fluid pressure by solving analytically the stress balance equations. It is shown that the consolidation of cylindrical composites depends not only on the permeability and elastic properties of the porous core but also significantly on the sheath thickness, the radius of the inner cylinder, and their material properties. A comparative analysis of the mechanical responses of transversely isotropic and isotropic poroelastic materials revealed significant differences.

When a poroelastic composite rod is laterally confined in a rigid tube while a porous piston compresses it in the composite along its axis, the consolidation changes drastically relative to that of an unconfined rod. For example, the consolidation of an isotropic confined rod is faster than that of an unconfined rod. Sets of parameters are found where the sheath does not affect the consolidation process of the poroelastic core.

When the composite cylinder is sealed and subject to uniaxial tension or compression, the rod reaction is surprisingly complex. Here, the internal stress is distributed between the sheath, the solid skeleton of the poroelastic material, and the fluid. We showed that the fluid pressure in poroelastic optic nerves of animals can be as large as one-third of the applied stress.

The analytical models are motivated by the need to experimentally measure the permeability and elastic properties of fluid-saturated soft materials. Analysis of the consolidation behavior performed herein informs the design of experiments on soft materials. We are currently validating the derived analytical model against creep experiments of pig and cow optic nerves. The results of the analytical models show that failure to select the correct model—composite or not, anisotropic or isotropic—can result in significant errors in extracting poroelastic properties of these materials.

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Decompaction Weakening as a Mechanism of Fluid Focusing in Hydrothermal Systems

Ivan Utkin (Laboratory of Hydraulics, Hydrology and Glaciology VAW, ETH Zurich, Zurich, Switzerland)
Andrey Afanasyev (Institute of Mechanics, Moscow State University, Moscow, Russian Federation)

Abstract

We present a mathematical model of nonreactive fluid flow in a compacting porous medium. The model differs from previous formulations by considering fluid transport in the frame of reference moving with the solid phase. Such an approach guarantees material balance for the fluid and solid phases not only in the small-porosity limit but also for large values of porosity. Using the numerical implementation of the proposed model, we simulate magmatic fluid transport in the Earth's upper crust. We account for the thermal softening of rocks, the plastic deformation of the solid matrix through decompaction weakening, and realistic fluid properties in a wide range of depths, including those above and below the brittle-ductile transition (BDT). We show that our simulation approach can resolve the localized flow in the ductile zone and numerous hydrothermal convection cells in the brittle zone. We investigate the influence of decompaction weakening on high-porosity channels forming in the ductile zone and their interaction with the convection in the brittle zone. We show that compaction causes magmatic fluid focusing and accumulation in high-porosity lenses beneath the low-porosity BDT zone. We show that magmatic fluid transfer through the BDT occurs mainly through the roofs of the lenses, which results in a plume of hydrothermal convection always sitting atop every lens. Other plumes between the lenses are associated with the convection of meteoric water that transfers only heat from the BDT to the surface. The simulations indicate that the lenses can be tracked by measuring certain parameters at the surface.

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Nonlinear porosity waves in elasto-visco-plastic reactive media under gravity

Yury Podladchikov (University of Lausanne)
Viktoriya Yarushina (Institute for Energy Technology)

Abstract

Large viscous porosity variations are possible if time scale is long enough to accumulate strain even with high viscosity of the solid matrix, or if its viscosity drops by one of the many weakening mechanisms. Plastic porosity changes are unlimited if fluid influx maintains fluid pressure at the yielding condition. Du to at least cubic nonlinearity of permeability-porosity constitutive relationship, large variations in porosity may propagate as nonlinear waves in addition to the Biot's linear elastodynamics waves. Rich variety of nonlinear waves types in this setting can be approximately classified into two distinct types (Connolly and Podladchikov, 2000, Connolly and Podladchikov, 2013). The first and the best-known type is manifested by formation of kinematic jumps or shocks due to nonlinearity of the advection, analogous to segregation fronts in suspensions under gravity. Similar behavior is expected in viscously compacting rock matrix under gravity during porous lower density fluid or melt escape at geological time scales (Connolly and Podladchikov, 2013). Even at much faster time scales, similar waves are expected in 'fluidized' rocks maintained at plastic yielding condition by elevated fluid pressure. The second wave type is the recently discovered soliton-like porosity waves in the viscous limit of the effective viscoelastic constitutive relationship for porosity (de)compaction. These waves in contrast to the shock waves completely detach from their source and propagate as solitary waves of constant Gaussian-like shape with velocity growing nonlinearly with amplitude of the wave (Connolly and Podladchikov, 2007). Due to difference in velocity, solitary waves having different amplitudes may collide if large amplitude wave is behind the smaller amplitude wave. Interestingly, the waves do not coalesce after collision, but propagate through each other in soliton-like fashion (Connolly and Podladchikov, 2013). Analysis of phase portraits on effective pressure – porosity plane of travelling visco-elastic solutions reveal continuous transition from elastic shock to solitary solutions with transitional spiral-like oscillations (Connolly and Podladchikov, 1998). There is a simple mechanical analogy to the phase portrait of an oscillating under gravity ball on a curved, frictionless surface (Connolly and Podladchikov, 2012, 2013, Yarushina et al. 2015).

Activation of tensile yielding or microscopic hydrofracturing leads to channels formation exhibiting both shock-like and soliton-like features. Channels are forming from soliton-like blobs at such 'ductile-brittle' transition due to 'compaction-decompaction asymmetry'. Tensile micro fracturing drops effective decompaction viscosity and results in visually flattening of upper half of the initially symmetric spherical porosity blob and stretching into a channel of the compacting lower half of the blob. All of it is due to dependence of the characteristic 'so-called compaction' length on the (de)compaction viscosity.

In summary, in nonreactive porous media, the nonlinear waves with instantaneous yielding (de)compaction rheology will be shock-like waves and with time-dependent viscous/creep rheology will be soliton-like solitary waves. Combination of both (de)compaction rheologies leads to spontaneous fluid focusing via channel formation.

Similarly, in reacting porous media even with rigid skeleton, the nonlinear waves under assumption of instantaneous local equilibrium will be shock-like waves and will be soliton-like solitary waves if reactions are controlled by kinetic rates (Omlin et al. 2017). Significant difference in dissolution versus precipitation kinetics rates leads to spontaneous fluid focusing via worm-hole-like channel formation.

Stefan problem – like front propagation in chemically reacting porous media may form even under isothermal conditions with latent heat effect replaced by densities change due to reaction (Schmalholz et al., 2024).

This type of fronts can propagate even in degenerate case of zero background interconnected porosity and permeability.

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Porous Hierarchically Ordered Hydrogels

Robert Hickey (The Pennsylvania State University)

Abstract

Cellular materials composed of a continuous solid network and voids filled with gas (i.e., foams) or liquid are commonly found in nature and have widespread use in industrial applications including thermal insulation and impact dissipation. The geometry of the pores and the composition of the pore wall directly impact the mechanical properties of the materials. Although nature has utilized cellular materials for many different purposes (e.g., wood), precisely tuning the structure and properties in synthetic porous materials is difficult. Here, the presentation will cover recent advances in porous, hierarchically ordered hydrogels where physically crosslinked spherical micelles form pore walls that surround water cavities. The mechanical response under uniaxial extension is dictated by the micrometer pores at low strain and the nanoscale micelles at high strain. Extremely low elastic moduli (< 1 kPa), high elasticity (extending more than 12-times initial length), strain-hardening, and completely reversible extension all derive from the deformation of both the micrometer-sized pores and the nanoscale micelles, which is reminiscent of natural cellular solids. Control of the material microstructure and pore orientation over many orders of magnitude (e.g., nm – μm) using bottom-up self-assembly methods reveals new possibilities for creating multiscale materials with structure dependent mechanical properties.

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Poster Presentation 79

Seismic Properties of Basal Cambrian Sandstones: Implications for Seismic Monitoring of Geological Storage and Sequestration

Douglas Schmitt (Purdue University), Anthony Wendel (Purdue University), David Diaz (Purdue University), Jason Nycz (NA Helium), Randolf Kofman (Consultant)

Abstract

Porous basal sandstones of Cambrian age lie immediately above the Great Unconformity in many basins in North America. Their often advantageous porosity and permeability, together with their great depth, make them a primary target for activities ranging from CO2 sequestration and H2 storage to geothermal extraction. Active source 4D seismic monitoring will be mandated in many of these situations, but more detailed interpretation of repeated field surveys requires knowledge of the material's seismic properties and how they evolve with changing fluid saturations and reservoir pressures. Here, measurements of the P- and S-wave velocities at ultrasonic frequencies were made on a suite of Cambrian sandstone cores extracted for helium exploration in the Canadian portion of the Williston Basin in Saskatchewan. Waveforms were collected while saturated with air, N2 gas, and liquid H2O. Confining pressures (Pc) and pore fluid pressures (Pp) reached up to 60 MPa and 17 MPa respectively, to mimic conditions at a depth of ~2.5 km. Measurements were taken with varying confining pressure and no pore pressure, with varying pore pressure and constant confining pressure (representative of in situ overburden pressure), and with confining and pore pressures varied simultaneously to maintain a constant effective pressure (Peff = Pc - Pp). Velocities display substantial pressure dependence up to effective pressures of ~30 MPa. At higher pressures, relatively high velocities for such porous rocks can exceed 4500 m/s and 2900 m/s for P- and S-waves, respectively. These speeds indicate high stiffness and rigidity under in situ conditions, which translates to relatively low sensitivity of the saturated dynamic moduli to fluid substitution. Thus, changes to density rather than frame properties will primarily control seismic detectability of fluid changes. Potential reasons for this stiffness were investigated through imaging with a scanning electron microscope and elemental analysis through x-ray diffraction. Cements present were identified as primarily siderite and dolomite. Ongoing work includes repetition of these measurements using CO2 as the saturating fluid at pressures and temperatures encompassing the triple point.

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Wave propagation in porous media 5 Presentation 82

Shock- and soliton-like porosity evolution in reacting and deforming saturated rocks

Lyudmila Khakimova (University of Lausanne)

Abstract

This work addresses how nonlinear coupling among deformation, fluid flow, and chemical reactions drives spontaneous porosity evolution and mineral alteration via a cascade of hydro-mechanical and reaction-infiltration instabilities. These coupled processes underlie key geological phenomena, flux melting, subduction-zone dehydration, and lithospheric melt migration, as well as geotechnical applications like mineral carbonation during carbon capture and storage.

Viscoelastic deformation-induced solitary waves have been proposed as a mechanism for explaining deep fluid extraction (Connolly, 1997, 2010; Yarushina et al., 2015). The transition from a viscous to an elastoplastic-brittle matrix leads to wave coalescence after collision, preventing waves from detaching from their source and causing their amplitude to decay due to geometric spreading (Connolly & Podladchikov, 1998). This loss of solitary wave solutions and fluid extraction efficiency is linked to rising viscosity as temperature decreases near the Earth's surface.

Rowan (1959) was the first to identify a positive feedback loop between dissolution and fluid flow, resulting in channel formation at the reaction front. These reactive-infiltration instabilities (as reviewed by De Wit, 2016) have since been applied to explain patterns observed in numerous geological contexts. When reactive fluid (e.g., acid or carbonic fluid) flows through porous rock, it etches pathways that increase permeability, leading to a reactive-fluid-flow instability akin to viscous fingering: the fluid preferentially moves through previously created high-permeability channels. Hinch & Bhatt (1989) examined the linear stability of this process, providing analytical solutions for extreme wavenumbers and small permeability variations, along with numerical solutions for other cases. Zhao et al. (2018, 2022) provided theoretical analysis and investigated the validity of using large-density asymptotics for studying reaction-infiltration instability in fluid-saturated rocks.

The combination of compaction-driven fluid flow and reaction-infiltration instabilities gives rise to "reactive porosity waves": mechanisms driven by reaction-induced fluid release and trapping, demonstrating that these waves can self-generate and travel long distances (Omlin et al., 2017). Malvoisin et al. (2015, 2021) demonstrated the possibility of achieving complete reactions and preserving porosity during chemical reactions such as hydration, based on natural observations. Yarushina et al. (2023) derived new constitutive relations for porosity evolution and bulk volume

changes; this closure allows volume change produced by reaction to be accommodated by matrix deformation rather than pore-space clogging.

To investigate these complex phenomena, we develop a coupled hydro-mechanical-chemical (HMC) model, constituting a critical step in bridging solid volumetric changes, porosity evolution, and (de)volatilization reactions (Khakimova & Podladchikov, 2024). The model describes reaction-driven (de)hydration and (de)carbonation front propagation, characterized by soliton-like or shock-like porosity fronts, through a viscoelastic medium. It is formulated in a fully conservative framework and implemented numerically to address two fundamental challenges in simulating reactive flow through deformable porous media. First, both the governing equations and numerical scheme rigorously enforce conservation of mass, momentum, and energy, ensuring that even trace-solute transport over geological timescales remains physically faithful. Second, as reaction-driven density or porosity changes sharpen into steep fronts or shocks, the divergence-form formulation guarantees these discontinuities are captured without spurious oscillations and that they satisfy nonnegative entropy production.

We detail the derivation of the governing equations, thermodynamic closures, and the shock-resolving numerical scheme. To demonstrate its versatility, we simulate compaction-driven fluid migration, melting reactions, (de)hydration in the antigorite–olivine system, and reactive transport in feldspar-rich rocks with neutral and charged species. Reaction-driven (de)hydration and (de)carbonation fronts, reproduced during modeling, can propagate even in the degenerate case of zero background interconnected porosity and permeability. The mathematical problem is formulated as a nonlinear, degenerate, second-order parabolic equation known to possess a family of self-similar analytical solutions (Barenblatt et al., 2000; Kalashnikov, 1987; Connolly & Podladchikov, 1998; Yarushina & Podladchikov, 2015; Schmalholz et al., 2024). These generalized analytical solutions are used to verify numerical models and assess their accuracy in predicting reaction-front propagation under coupled reaction, diffusion, and rock-deformation conditions. We also extend a unified analytical solution of the classical Stefan problem (Stefan, 1891), originally formulated for water freezing but also applied to magma crystallization (Turcotte & Schubert, 2014) and dissolution-front propagation (Coussy, 2004), according to Podladchikov & Wickham (1994). This extension covers a broader class of processes, including (de)hydration reactions in the brucite–periclase–water and antigorite–brucite–forsterite–water systems, as well as (de)carbonation in reactive rocks.

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Soft mater and novel porous media 1 Presentation 83

Field-Driven, Bioinspired Design of Porous Orthopedic Implants: Reducing Stress Shielding and Enhancing Osseointegration

Sajjad Raeisi (GenMat LLC, Irvine, CA, USA)

Abstract

Orthopedic implant failure is often linked to mechanical and biological incompatibilities with native bone. Existing implants, generally optimized for stiffness and manufacturability, disrupt bone's natural mechanical environment, resulting in stress shielding, localized bone resorption, and eventual loosening. Concurrently, mismatched porosity distribution hinders osseointegration, compromising long-term implant performance. Overcoming these limitations demands a design approach integrating biomechanical functionality, biological mimicry, and manufacturing constraints.

GenMat LLC has developed Ossevo™, a simulation-driven platform for generating patient-specific porous implants based on the principles of load-induced bone remodeling. Rooted in finite element analysis, Ossevo automates the design of orthopedic implants that adapt to local mechanical demands. In contrast to conventional approaches that rely on uniform lattices or global stiffness optimization, Ossevo employs a bioinspired, field-driven algorithm that integrates anatomical context, mechanical stimuli, and additive manufacturing constraints into a unified workflow. The method computationally mimics bone remodeling behavior by iteratively adjusting local porosity in response to strain energy density, promoting biomechanical compatibility and structural efficiency.

Ossevo's workflow begins by importing patient-specific anatomical geometries from CT scans or CAD models, which are converted into Signed Distance Fields (SDFs) to enable smooth, watertight, and robust geometric representation. Finite Element Models (FEMs) are then constructed using physiologically relevant boundary conditions—derived from gait analysis, joint mechanics, or anatomical landmarks—and can incorporate nonlinear material behavior when needed. These simulations produce mechanical field data, including strain energy density, principal stresses, and volumetric strain, which drive the subsequent field-guided optimization.

In the optimization phase, Ossevo diverges from conventional global stiffness maximization by iteratively refining material distribution to achieve a uniform local strain energy density. This field-driven adaptation promotes mechanical homeostasis, enabling effective load-sharing with surrounding bone and mitigating stress shielding. The resulting implants are functionally graded—denser in high-load regions near joints and progressively more porous in low-load zones to promote biological integration.

The optimized material layout is translated into a manufacturable lattice structure using Ossevo's implicit modeling engine, supporting both Triply Periodic Minimal Surface (TPMS) and strut-based lattices. Local lattice parameters—including pore size (500–1000 μm), porosity (10–80%), and wall thickness (200–500 μm)—are selected based on site-specific mechanical requirements and osseointegration needs. Pore geometry and distribution are controlled to support vascular and tissue ingrowth, supported by studies indicating optimal pore sizes above 500 μm for biological integration. Manufacturing constraints such as minimum feature size (≥200 μm), overhang limits, and build orientation can be embedded in the optimization process. Virtual DMLS simulations validate printability and thermal stability prior to fabrication. Final implants are exported as STL or 3MF files with implicit surface representation, ready for direct metal additive manufacturing.

Initial Finite Element validation studies show that Ossevo implants achieve the following:

- 50% reduction in stress shielding, measured by the relative decrease in strain energy density in host bone compared to solid implant benchmarks,
- 40% improvement in interface stress continuity, assessed by reduction in stress gradients and improved load transfer across the implant-bone boundary.
- Effective stiffness within 8% of cortical bone modulus (22–26 GPa), verified by numerical homogenization of the lattice structure via finite element analysis.

Initial applications focus on cranial reconstruction plates, spinal interbody cages, and mandibular implants, where anatomical complexity, variable loading, and high revision rates create demand for personalized solutions. These cases demonstrate Ossevo's ability to handle irregular geometries, localized biomechanics, and fabrication constraints in one unified platform.

Commercial platforms like nTop and Materialise Magics offer advanced and highly customizable manufacturability controls. However, their design processes are not inherently aligned with the mechanics of bone. In contrast, Ossevo’s strength lies in its biologically inspired, field-driven design approach. Rather than relying on global compliance objectives or stress constraints, which require precise load magnitudes and assume linear material behavior, Ossevo adapts implant architecture based on local mechanical stimuli, such as strain energy density, following the principles of bone remodeling. This reflects Wolff’s law: native bone responds to loading through continuous, localized adaptation, not a globally optimized shape. Thus, Ossevo replaces bone with a structure explicitly designed according to physiological principles, not merely engineering mechanics.

Additionally, Ossevo uniquely automates bioinspired material distribution without relying on simplified material models or unrealistic finite element contact assumptions. Its field-driven approach robustly adapts implant designs to uncertain loading conditions and modeling variations, resulting in implants that are both reliably manufacturable and physiologically relevant. This presentation highlights Ossevo’s capabilities in orthopedic implant design and its broader relevance to advancing the mechanics of porous biomaterials and structurally compatible implant technologies.

8th BIOT Conference on Poromechanics (BIOT-8)
October 7-10, 2025, The University of Utah, Salt Lake City, United States

Poroelastic diffusion and transient wetting of droplets on hydrogels

H. Jeremy Cho (University of Nevada, Las Vegas)
Amir Kashani (University of Nevada, Las Vegas)

Abstract

In this work, we investigate how wetting behavior can be affected by the time-dependent swelling of hydrogels. Measuring the advancing contact angles of water droplets on hydrogels of varying thicknesses, we observed thicker gels absorbed water more slowly. We also observe that, above a threshold advancing speed, water droplets collapse into a lower contact angle state on the surface. We hypothesized that this collapse threshold speed is a result of competition between the poroelastic diffusion of water into the gel and the advance of the spreading droplet, the thickness of the surface, and the diffusion of water into the gel. Taking the ratio of the poroelastic diffusion and advancing timescales results in a Peclet number with gel thickness as a characteristic length scale. Our results show that above a Peclet number of around 40, droplets will collapse on the surface across all gel thicknesses, confirming our hypothesis. This work provides simple insight to understand a complex time-dependent wetting phenomenon.

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From Linear Gassmann's Equations to Nonlinear Solitary Porosity Waves in Deforming Porous Media

Yury Alkhimenkov (University of Lausanne)

Abstract

Gassmann's equations are widely regarded as exact in the linear elastic regime, providing a cornerstone for fluid substitution in rock physics. However, natural geological processes often involve porosity evolution, viscous deformation, and plastic yielding, leading to nonlinear responses and instabilities. Elastic deformation yields shock-like solutions, viscous effects allow soliton formation, and plasticity can produce shear bands—potential indicators of fault reactivation due to fluid overpressure.

We present an extended Biot framework based on Classical Irreversible Thermodynamics, generalizing prior models by Gassmann (1951), Brown and Korringa (1975), and Detournay and Cheng (1993). We show that Gassmann's assumption of constant porosity under equal fluid and total pressure changes is not arbitrary but required for thermodynamic consistency under a diagonal second derivative energy matrix. Including off-diagonal terms yields a broader, fully consistent theory.

Through 3D numerical simulations, we explore how compaction-driven fluid flow interacts with viscoelastoplastic deformation to produce solitary porosity waves. These waves reshape flow paths and can trigger shear zones with parabolic geometries. Our results highlight the crucial role of plastic yielding in controlling flow, channel geometry, and fault stability.

GPU-accelerated computing enables high-resolution simulations at scale, advancing our ability to study nonlinear poromechanical processes in realistic geological settings.

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Simulation of Biofilm Deformation Under Flow

Ian Bourg (Department of Civil and Environmental Engineering, Princeton University)
Francisco Carrillo (Department of Chemical and Biological Engineering, Princeton University),
Mitchell Jans (Department of Civil and Environmental Engineering, Princeton University)

Abstract

Biofilms--bacterial colonies characterized by the production of extracellular polymeric substances--play important roles in many natural and engineered processes including biochemical cycling and contaminant remediation in subsurface porous media (soils, sediments, porous rocks). Experimental observations indicate that the life-cycles and impacts of biofilms in these systems are sensitive to feedbacks between fluid flow and biofilm growth and deformation. Detailed understanding of these observations remain limited by the absence of well-tested computational frameworks capable of representing the feedbacks between fluid flow (within and around biofilms) and biofilm deformation. Here, we report on our ongoing efforts to develop such a framework using simulations of biofilm growth and deformation under flow validated against microfluidic experiments. We use our tested model to explore a wide range of parameter space conditions. Our results reveal the existence of several distinct bioclogging regimes with thresholds determined by non-dimensional numbers.

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Effect of viscosity on wave propagation: poroelasticity versus viscoelasticity

Boris Gurevich (Curtin University)

Abstract

While Biot's theory of poroelasticity theory adequately describes wave attenuation in shallow marine sediments, it substantially underestimates seismic attenuation in rocks, which have much lower porosity and permeability. This is especially notable for rocks saturated with high-viscosity fluids or viscoelastic substances, which are usually described with the theory of viscoelasticity. Yet the connection between poroelasticity and viscoelasticity theories is unclear. Some insights on the connection between poroelasticity and viscoelasticity can be gained from the theory of homogenization of periodic structures. In particular, Boutin and Auriault (1990) introduced a parameter B such that a medium is poroelastic for $B << 1$ and vicoselastic when $B >> 1$. Parameter B depends on material properties only and is independent of frequency; if a particular medium is poroelastic at one frequency, it will be poroelastic at any other frequency. We show that this paremeter equals the ratio of Biot's crossover frequency and viscoelastic crossover frequency, and that the product of these characteristic frequencies equals scattering frequency squared. Since the validity of any macroscopic theory requires that the frequency be lower than the scattering frqeuency, only one of these theories can be valid for a given combination of parameters.

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Computational poromechanics 3

Presentation 92

Multiscale aggregation of smectite nanoparticles: linking microstructure, dynamics, and coupled properties

Xiaojin Zheng (Princeton University)
Ian Bourg (Princeton University)

Abstract

The aggregation of clay nanoparticles plays a critical role in governing the coupled thermal, hydraulic, mechanical, and chemical (THMC) properties of soils, sediments, and sedimentary rocks. However, the underlying mechanisms remain incompletely understood due to the challenges of characterizing clay microstructures and their interactions with water across length scales ranging from nanometers to micrometers. This study addresses these challenges through a three-part multiscale modeling approach. First, we use large-scale all-atom molecular dynamics (MD) simulations to investigate a hydrated Na-montmorillonite system composed of 27 clay nanoparticles, predicting transport properties of water–smectite mixtures across a range of temperatures and dry densities. Second, we develop and apply a new coarse-grained MD (CGMD) framework to simulate the self-assembly of up to 2,000 smectite particles, yielding insight into aggregation mechanisms and rheological properties. Third, we compact the self-assembled structures to examine emergent rock-scale properties, including tortuosity, pore size distribution, and swelling pressure. Together, these simulations bridge molecular-scale interactions and bulk properties of smectite-rich systems, providing a mechanistic foundation for understanding and modeling clay aggregation in natural and engineered settings.

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The effect of gas bubbles on the low-frequency poroelastic response of rocks

Nicola Tisato (The University of Texas at Austin)
Isabelle Lambert (The University of Texas at Austin)

Abstract

The attenuation and dispersion of seismic waves in rocks are often controlled by multiphase fluids that saturate the rocks' pores. At shallow depths (i.e., <10 km), fluids mainly comprise mixtures of brines, oil, natural gas, and carbon dioxide. Recently, hydrogen and helium have gained interest as they could be more abundant than previously thought in the subsurface. Overall, identifying the presence of exsolved fluids, either forming large patches or microscopic bubbles within the pores, is key for the geophysical exploration and monitoring of subsurface domains. The Biot theory has been used as the framework for attenuation mechanisms such as the squirt flow and the patchy saturation. However, when the bubble saturation and the center frequencies of the seismic data are below ~2% and 10 Hz, respectively, the wave-induced-gas-exsolution-dissolution (WIGED) attenuation mechanism may become predominant over those Biot-based mechanisms.

Here, we present the WIGED theory, including an exact solution for the relaxed (low-frequency) and unrelaxed (high-frequency) limits. We will also show how we derived an approximated analytical solution for WIGED and benchmarked the theory with laboratory experiments reproducing the dynamic deformation of a gas bubble in a liquid. Then, we will discuss how the effect of WIGED on the attenuation of seismic waves at low frequency is controlled by the bubble gas, the size, and the density of these bubbles (i.e., the bubble saturation). Finally, we will show how the attenuation and dispersion calculated for the WIGED theory can be used to estimate the effective dispersion and attenuation in rocks and how this can be used to predict how the seismic signals gathered by a geophysical monitoring campaign vary as bubbles form in the subsurface.

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Leveraging stochastic simulations at the pore scale to predict permeability variations during precipitation process

Zi Wang (Stanford University)
Tapan Mukerji (Stanford University)

Abstract

Solid precipitation caused by chemical reactions in porous materials leads to significant changes of porosity and permeability. Modeling such changes using full-physics simulations of flow and reactions has extremely high computational costs, especially when computations are needed for multiple digital rock samples. In this work, a geostatistical simulation method, Direct Sampling (DS), is modified to handle spatio-temporal variability, and is developed as a surrogate for generating the evolving pore microgeometry during the precipitation process. The training set is based on only one time-series dataset of digital rock geometries with dynamic precipitation computed using full-physics lattice Boltzmann simulations for coupled fluid flow and chemical reactions. The stochastic surrogate enables fast prediction of the time-evolving geometry and porosity-permeability on other similar digital rock geometries. For different initial digital rock structures, the precipitation process is generated by both LBM and DS and the evolving porosity-permeability is computed. The results show that DS successfully generates the time-evolving porous geometry similar to the ground truth and captures local precipitation morphology. The computational saving is more than 36 times, with an average relative error in permeability of less than 15%. The proposed method provides a promising, computationally efficient path for predicting variations of permeability with precipitation.

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Influence of Extraction Method and Pressure on Pore Solution Chemistry in Cement Paste

Aagya Dahal (University of Connecticut)
Kay Wille (University of Connecticut), Yifei Wang (University of Connecticut)

Abstract

Identifying how fluids are retained in the pores of cement-based materials is crucial for understanding pore solution chemistry, which can be influenced by extraction pressures. In this study, pore solution (PS) was extracted from hydrated cement paste using two methods: vacuum filtration and a high-pressure squeezing apparatus operated at varying pressure levels. The elemental composition of PS was analyzed and included measurement of calcium (Ca), potassium (K), sodium (Na), sulfur (S), aluminum (Al), iron (Fe), and magnesium (Mg) with a primary focus on Ca. Ca2+ concentrations were consistently higher in PS extracted via squeezing compared to vacuum filtration.

We observed a clear trend: increasing applied pressure led to higher Ca^{2+} concentrations. This is hypothesized to result from the progressive mobilization of fluid from smaller pores, which are retained under lower pressures due to higher capillary resistance. Smaller pores, with higher surface area-to-volume ratio, likely promote ion accumulation through stronger solid–fluid interactions.

These findings demonstrate that both extraction method and applied pressure influence which regions of the pore structure are accessed, thereby altering the measured chemical composition. By linking capillary effects and fluid mobilization, this work provides experimental insight into how pore structure governs chemical measurements in cementitious materials.

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3D GPU Simulation of Coupled Poromechanics and Two-Phase Flow

Yury Alkhimenkov (University of Lausanne)
Ruben Juanes (Massachusetts Institute of Technology (MIT))

Abstract

We present a high-performance computational framework for simulating coupled poro-elasto-plastic deformation and compressible two-phase flow in porous media. This work addresses the pressing need for scalable, high-resolution models capable of capturing nonlinear multiphysics interactions in complex subsurface environments, such as those encountered in enhanced oil recovery, carbon sequestration, and induced seismicity.

Our model incorporates large-strain poromechanical behavior, frictional plasticity, and advection- or capillary-driven two-phase flow to resolve dynamic coupling. The governing equations are discretized using a conservative finite-volume scheme. To solve the nonlinear system efficiently, we employ an accelerated pseudo-transient (APT) method that reformulates the system as a damped hyperbolic problem, enabling robust convergence without requiring global matrix assembly [1].

A distinguishing feature of our framework is its GPU-optimized implementation, which allows for massively parallel execution and exceptional computational performance. We demonstrate the ability to perform fully coupled, three-dimensional simulations on domains exceeding 100 million voxels using a single professional GPU. The solver accurately resolves non-symmetric strain localization, saturation dynamics, and pressure redistribution.

Simulation results reveal that deformation-induced pressure gradients can significantly enhance wetting-phase migration into localized shear bands. This mechanistic insight, captured through our fully coupled formulation, underscores the importance of resolving dynamic fluid–solid interactions. Unlike partially coupled or sequential solvers, our monolithic approach ensures consistency between flow and mechanics, including the evolution of porosity and capillary pressure.

Compared to traditional FEM- or FVM-based frameworks (e.g., TOUGHREACT, OpenGeoSys, COMSOL), our method achieves an order-of-magnitude increase in resolution and scalability. It is well-suited for large-scale, high-fidelity geomechanical simulations where conventional implicit solvers are computationally prohibitive.

Looking forward, we aim to extend the framework to account for gravitational forces, heterogeneous permeability, partial miscibility (e.g., CO_2 dissolution), and three-phase systems. Ultimately, this work lays the foundation for high-resolution modeling of complex coupled processes across scales, advancing the state of computational poromechanics and subsurface flow simulation.

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GPU-Accelerated Simulation of Coupled Elastic and Hydraulic Behavior in Fractured and Porous Rocks from Digital Images

Yury Alkhimenkov (University of Lausanne)

Abstract

Fractures and pore-scale heterogeneity strongly affect the elastic and hydraulic behavior of rocks, influencing seismic interpretation, geothermal energy, CO_2 storage, and subsurface fluid flow. Bridging pore-scale structure with macroscopic response remains challenging due to multiscale complexity and computational demands. We present GPU-accelerated methods for simulating poromechanical behavior in 3D digital rock volumes with unprecedented resolution and speed.

Our core solver, FastBiot_QS, is a quasi-static poroelastic code capable of solving 3D Biot's equations on voxel grids exceeding 130 million elements using a single GPU. Designed for digital rock physics, it models spatially variable fractures and pores extracted from micro-CT data. Validation confirms high accuracy, and simulations show how fracture clustering controls frequency-dependent attenuation: dense clusters enhance high-frequency losses, while sparse networks dominate at low frequencies.

We also introduce GPU-based tools for elastic homogenization and voxelwise contribution analysis, enabling rapid evaluation of anisotropic moduli in heterogeneous rocks. These tools complete problems with 7–350 million voxels in seconds to minutes.

Finally, we model wave-induced fluid flow (squirt flow) by directly simulating pore-scale geometries, capturing local hydraulic effects and frequency-dependent viscoelastic behavior. Together, these open-access tools form a high-performance digital laboratory for studying fractured, fluid-saturated media at pore-to-core scales.

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Modelling viscoelastic porosity wave/ focused fluid flow in the subsurface: its controlling factors

Lawrence Hongliang Wang (Institute for energy technology), Viktoriya Yarushina (Institute for Energy Technology)

Abstract

Seismic chimneys, prevalent along continental margins, intricately contribute to Earth's degassing processes, facilitating fluid migration from the deep Earth to the surface. This phenomenon carries significant implications for subsurface storage utilization. Among the principal mechanisms driving seismic chimney formation is the fluid flow instability within porous subsurface rocks. While numerical studies of geodynamical two-phase flow have successfully replicated vertical fluid flow structures, many of these models overlook elastic compaction, advection of solid and poro-space, and geological heterogeneity, thereby limiting their applicability in subsurface scenarios. In addressing these limitations, this study incorporates a viscoelastic rheology into the geodynamical two-phase flow model to explore the controlling factors influencing the formation of focused fluid flow. By conducting numerical models with varying Deborah number, we find elastic compaction only speed up the fluid migration slightly when the reasonable Deborah number (0~0.5) is applied for the subsurface. When lower initial fluid pressure is considered, models with high Deborah number (De>0.15) take significant more time to build up pressure and initiate the focused fluid flow. Through a comparative analysis of models with and without advection, we observe the potential importance of solid advection in fluid migration, particularly under conditions of high background porosity (≥0.1) and relatively low permeability. Further simulations involving fluid flow encountering a horizontal segment with geological heterogeneity demonstrate the potential for fluid penetration through the structure or deflection to the side, depending upon rock properties and segment size. Through our 2D models in with different shear viscosity, we find the fluid channel widths range from ~3 to ~5 compaction lengths, depending on viscosity ratio and the fluid supply. An increase of horizontal permeability over vertical permeability can further widen fluid channel to 10 δc, but the capacity of horizontal migration is still rather limited, compared to the spreading of CO2 plume at Sleipner field. This comprehensive investigation sheds light on the complex interplay of various factors influencing focused fluid flow, including geological heterogeneity, thereby contributing valuable insights to the understanding of subsurface fluid flow in real-world geological settings.

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Poster Presentation 99

Modeling the Impact of Microplasticity on Nonlinear Attenuation of Compressional and Shear Waves

Maxim Yakovlev (Lomonosov Moscow State University), Alexander Semykin (Lomonosov Moscow State University), Viktoriya Yarushina (Institute for Energy Technology)

Abstract

Nonlinear effects in seismic wave propagation are observed even at very small strain levels, where classical elastic and viscous models predict linear behavior. For example, attenuation of seismic waves at low frequencies has been found to be independent of wave amplitude — an effect that cannot be explained by standard elastic or viscous dissipation mechanisms. Frictional sliding has been proposed as a possible amplitude- and frequency-independent mechanism, but it has proven inefficient in capturing observed attenuation. An alternative explanation is microscale plastic yielding, introduced by Yarushina and Podladchikov [1], which accounts for energy dissipation through irreversible deformation at grain contacts and defects. Their work demonstrated significant attenuation of compressional waves with quality factors in the range of Q = 12–20, though it was limited to low-porosity materials where pore interaction was neglected. Importantly, experimental studies have confirmed the presence of microplastic deformation under subcritical loading during seismic wave propagation, supporting its relevance as a physical attenuation mechanism [2].

In this study, we extend that model to account for both compressional (Vp) and shear (Vs) wave attenuation in elastoplastic porous media with interacting pores. Using finite-element modeling in CAE Fidesys [3], we simulate wave-induced stress cycling in a representative volume containing multiple pores. Plastic deformation initiates locally around individual pores and expands until plastic zones merge, resulting in distributed dissipation. Numerical averaging techniques [4] are applied to compute macroscopic attenuation, revealing a nonlinear dependence on wave amplitude. We further investigate the roles of strain amplitude, effective pressure, and porosity. The results reinforce microplasticity as a viable amplitude- and frequency-independent mechanism of seismic wave attenuation in preloaded, porous rocks.

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Hydrate-bearing sediments: visco-plastic behavior

Alejandro Cardona (University of Texas at Austin), Peter Flemings (University of Texas at Austin)

Abstract

Hydrate behaves as a viscous phase within the pore space, resulting in visco-plastic behavior of the composite medium. We study this process using uniaxial strain compression experiments of natural hydrate-bearing (pressure cores) and hydrate-free reconstituted samples from Green Canyon 955 - deepwater Gulf of Mexico. Hydrate-bearing sandy silts are stiffer but have a larger uniaxial lateral stress ratio (*K₀*) than equivalent non-hydrate-bearing sediments. When the compression is paused, the stress ratio increases towards *K₀* = 1.0 in hydrate samples, whereas *K₀* remains constant with time for hydrate-free samples. We developed a geomechanical model that links these experimental observations quantitatively. The key insight of this model is that the hydrate phase and the sediment skeleton share any applied external load in proportion to their stiffnesses. Model results predict that porosity and *K₀* decreases dramatically after gas hydrate dissociation –in agreement with experimental observations. The viscoplastic behavior of hydrate-bearing sediments will impact gas production and in-situ stresses. Viscous deformation away from the production zone affects water flow, which in turn influences gas and water flow rates closer to the well. Furthermore, the time-dependent stress ratio may affect hydraulic fracturing, as the rate of pressurization impact stress evolution on the wellbore.

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A multifamily mechanical framework for non-collocated dissolution and precipitation in porous media

Yifan Yang (Northwestern University), Giuseppe Buscarnera (Northwestern University)

Abstract

A multifamily poromechanical framework is developed to extend Biot's theory: While the classic formulation effectively models porous media under both external and internal loadings, it assumes that internal loadings are isotropic and applied uniformly across all pore spaces and these assumptions limit its applicability in scenarios involving anisotropic stress sources (e.g., crystal growth) or non-collocated multiphysical processes (e.g., familywise dissolution and precipitation) in pore spaces. To address these limitations, an eigenstrain-based strategy is introduced, in which pore spaces are virtually filled with the matrix material and corresponding eigenstrains are prescribed to compensate for these alterations. This eigenstrain approach is incorporated into Biot's formalism, resulting in a generalized constitutive framework that links stress, strain, pore stress, and pore strain through homogenized tensors. A multifamily microstructure adapted from Ponte Castañeda and Willis (1995) is employed to derive these tensors analytically. Parametric studies are conducted under virtual fluid injection and crystal dissolution and precipitation scenarios, with variations in loading distributions (i.e., certain or all families), pore family volume fractions, and precipitate stiffness. The results, by revealing additional consequential effects on the multiphysical response of porous media, suggest that the proposed framework meaningfully complements the classic Biot's theory in capturing more detailed poromechanical behavior.

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Geological systems 2 Presentation 102

Evaluating Matrix–Fracture Interactions in CO_2 Geological Storage Using Dimensional Analyses and Hydro-Mechanical FEM-DEM Simulations

Shahrzad Roshankhah (University of Utah), Shivesh Shandilaya (University of Utah)

Abstract

Geological storage of CO2 and H2 in sedimentary formations are key steps towards a net-zero carbon energy economy and long-term climate stability. These geo-energy and geo-environmental applications require the injection of fluids at high rates into subsurface permeable geological formations to attain economic performance. However, high injection rates may trigger hydraulic fractures (HFs) and activate pre-existing natural fractures (NFs), depending on fluid-rock interactions in terms of the strength of energy dissipation mechanisms and fluid mass balance processes. Previous studies underscore that the distribution and properties of NFs, the stress state in the geological formation, the rock matrix permeability, and the injection rate and fluid viscosity of the working fluids are crucial factors in controlling the hydro-mechanical response. This study utilizes dimensional analyses and combined finite-discrete element method (FDEM) to understand complex interactions among hydraulic and mechanical processes in the permeable and fractured media. Considering the properties of two sandstone formations in Uinta Basin, Utah, with different matrix permeabilities, characteristics of supercritical CO2, and two different injection rates, dimensional analyses confirm that all cases fall within the toughness/leak-off-dominated regime, where fracture toughness and matrix leak-off control energy dissipation and fluid transport processes. The results of this numerical study show that sandstone formation with relatively high permeability enables rapid pressure equilibration due to high leak-off into the rock matrix, thus lowering the potential for fracture activations/propagations. The maximum mobilized pressure and the total length of generated fractures are higher with a higher injection rate, lower matrix permeability, and a higher degree of fracturedness. The study provides valuable insights into the hydro-mechanical behavior of homogeneous and fractured rock masses under various fluid injection conditions, contributing to more effective strategies for CO2 and H2 storage in sedimentary formations.

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Computational poromechanics 3

Presentation 103

Drying shrinkage of cement-based materials: study of water sorption and surface stresses in C-S-H by molecular simulations

Jingyi LENG (Laboratoire Navier (ENPC \ Institut Polytechnique de Paris, Université Gustave Eiffel, CNRS)), Laurent Brochard (Laboratoire Navier (ENPC \ Institut Polytechnique de Paris, Université Gustave Eiffel, CNRS)), Matthieu Vandamme (Laboratoire Navier (ENPC \ Institut Polytechnique de Paris, Université Gustave Eiffel, CNRS)), Patrick Dangla (Laboratoire Navier (ENPC \ Institut Polytechnique de Paris, Université Gustave Eiffel, CNRS))

Abstract

Cement-based materials shrink when drying, which can fracture the materials. A previous poromechanical model proposed by El Tabbal et al. (2020) shows that strains depend on the thickness of adsorbed water film and the surface stress at the pore surface. In the present work, we aim at investigating these two quantities with molecular simulations. First, we perform Grand-Canonical Monte Carlo (GCMC) simulations of water adsorption in two C-S-H slit mesopores that differ by their Ca/Si ratio (1.1 and 1.7) and obtain water adsorption isotherms at 6 temperatures ranging from 300 K to 525 K. We show that the variations in thickness of adsorbed layer with relative humidity can be well described with a de Boer-Zwikker equation and depend little on temperature. Second, we simulate closed and open mesopores: the pressure difference between the two configurations provides a value for the surface stress at the various water contents. The results show that surface stress of the dry C-S-H surface is on the order of several hundred mN/m and that variations of surface stress with relative humidity differ significantly from variations of surface tension with relative humidity calculated with the Gibbs adsorption isotherm.

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Geological systems 2 Presentation 104

Numerical Investigation of Particle Shape Effects on Coupled Hydromechanical Behavior in Unbreakable Particulate Packs

Ayat Alasadi (University of Utah), Shahrzad Roshankhah (University of Utah)

Abstract

Understanding the hydromechanical behavior of particulate packs is crucial for the design of the most effective proppant packs to maintain the hydraulic conductivity and mechanical stability of the activated fracture network in Enhanced Geothermal Systems (EGS). Particle shape is one of the key components governing how fluid and mechanical forces interact within densely packed particulate systems. This study offers a numerical investigation of the role of particle shape on the hydromechanical behavior of unbreakable particulate packs. A coupled Lattice Boltzmann–Discrete Element Method (LBM–DEM) framework is employed to simultaneously capture pore-scale fluid dynamics and solid-phase mechanics. The analysis begins with mechanically calibrated, dry oedometer-style simulations to establish particle shape-dependent packing behavior, which is then extended to include fluid flow under triaxial stress conditions to assess hydromechanical coupling. The results focus on tracking the evolution of micro-scale behavior, such as particle rearrangement, interlocking, and deformation pathways, and their influence on macro-scale responses, including permeability and mechanical stiffness. Outcomes are expected to inform the design of proppants for geo-energy applications.

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Surfactant transport in a thin water film covering a charged surface

Wenqian Zhang (University of Arizona)
Bo Guo (University of Arizona)

Abstract

Surfactant transport in thin water films plays an important role in physiological, industrial, and geophysical processes. However, the mechanisms governing this transport, particularly which mechanisms dominate under different surface excess conditions and water film thicknesses, remain poorly understood. We develop a mathematical model to investigate the behavior of ionic surfactants in thin water films. The model integrates lubrication theory, the Derjaguin–Landau–Verwey–Overbeek (DLVO) theory, and the Nernst-Planck-Poisson equation. Our analyses indicate that the dominant transport mechanism is governed by surface excess and film thickness. At lower surface excess and thinner films, diffusion controls surfactant transport, while Marangoni advection becomes the primary mechanism at higher surface excess and thicker films. Electromigration is significant only when the film thickness approaches the Debye length, and thus substrate charge has a notable influence on the transport process. This research offers key insights into the fundamental dynamics of ionic surfactant transport in thin water films.

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Low-frequency lab measurements: what have we learned?

Serhii Lozovyi (SINTEF)

Abstract

While ultrasonic measurements have long been the conventional method to probe dynamic rock properties in the laboratory, low-frequency measurements (based on forced-oscillation technique) are providing crucial insights into seismic wave propagation in porous media. Studies on sandstones and shales reveal pronounced velocity dispersion across seismic (sub-Hz to ~150 Hz) and ultrasonic (500 kHz) frequencies. This dispersion stems from mechanisms such as Biot flow in sands and complex viscoelastic processes involving free and bound water in clay-rich shales. One of major applications of these measurements is to bridge the gap between static and dynamic stiffness by linking responses throughout wide frequency and amplitude ranges. Furthermore, low-strain low-frequency measurements show that wave velocity stress sensitivity can be substantially higher at seismic frequencies than at ultrasonic, impacting 4D seismic interpretation and geomechanical models. Further, low-frequency data offer unique sensitivity to subtle fluid changes, like low gas saturation, often missed by higher-frequency methods. These advancements underline the indispensable role of comprehensive low-frequency laboratory data for robust rock physics models essential for subsurface characterization and monitoring.

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Capillary entry pressure of a hydrogel packing

Callum Cuttle (University of Oxford), Chris MacMinn (University of Oxford), Hangkai Wei (University of Oxford), Oliver Paulin (Max Planck Institute for Dynamics and Self-Organization)

Abstract

The capillary entry pressure of a porous medium is the applied pressure at which a non-wetting fluid will first invade the pore space by displacing the wetting fluid from the largest pore throats. For a rigid porous medium, the entry pressure is a characteristic of the two fluids, the solid material, and the pore structure. For a soft porous medium, however, the applied pressure will also compress the medium, thereby changing the pore structure and thus the entry pressure itself. This coupling complicates the basic concept of entry pressure as a material property. Here, we use experiments and modelling to study the capillary entry pressure of a model soft porous medium: a packing of hydrogel beads (diameter $\sim$1 mm), in which the individual grains are themselves soft porous media on a much smaller scale (pore size $\sim$10 nm). We show that the measurement of entry pressure provides a sensitive probe of the complex mechanics of these materials. We highlight in particular the strong interactions between entry pressure, viscoelastic creep, and stress-strain hysteresis.

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Fluid Injection-Induced Seismic Signature of Naturally Fractured Rocks with Permeable and Impermeable Matrix

Kami Mohammadi (University of Utah), Shahrzad Roshankhah (University of Utah), Shivesh Shandilaya (University of Utah)

Abstract

Induced seismicity resulting from fluid injection in subsurface geological formations poses a significant challenge to the stability and safety of infrastructures. With increasing reliance on the clean energy and environmental geosystems that involve fluid injection, such as enhanced geothermal energy recovery that involves water injection into naturally fractured granitic rocks with ultra-low permeability matrix and CO2 sequestration into naturally fractured sedimentary rocks with high permeability matrix, understanding the poromechanical mechanisms influencing induced seismicity is crucial for mitigating associated risks. This study investigates the influence of key parameters, including natural fracture density and matrix permeability, on the hydraulic, mechanical, and seismic response of model rock masses. Using the combined finite-discrete element method, the analysis captures the complex hydromechanical interactions in fractured rocks during fluid injection. Results demonstrate that significant fluid leak-off into a permeable matrix can reduce the severity of injection-induced seismicity. Moreover, the seismic signature of pre-fractured rocks due to fluid injection provides valuable insights for developing safer and more sustainable fluid injection strategies in subsurface geological formations.

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Electrochemical flow through charge-patterned wavy nanochannels

Thomas Peteresen (Sonny Astani Department of Civil and Environmental Engineering, University of Southern California, Los Angeles, CA; Department of Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, CA), Felipe P.J. de Barros (Sonny Astani Department of Civil and Environmental Engineering, University of Southern California, Los Angeles, CA), Jinwoo Im (Earth & Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CA), Pouya Golchin (Sonny Astani Department of Civil and Environmental Engineering, University of Southern California, Los Angeles, CA)

Abstract

Many applications of public utility benefit from technological improvements in controlling species transport through porous media. Surface texture along pore channels has been exploited to facilitate fluid flow and enhance scalar mixing. For instance, it is well known that mass transfer is typically enhanced along pores with wavy surface profiles. Nonetheless, exceptions exist: When both the fluctuations in aperture and the Péclet number are large, dispersion has been shown to diminish relative to flow in smooth pores [1]. Further control of flow can be exerted in electrochemical systems. The current study inspects the interplay between oscillations in geometry and surface charge density to control mixing during solute transport. The Poisson-Nernst-Planck equations are solved numerically under conditions of varying aperture profile, salt concentration, and charge placement– alternating in polarity along the channel axis. Building on the recent observation by Curk et al. [2], we show that a gating mechanism exists that transitions between regimes of electrostatically controlled and mechanically controlled flow. Upon increasing the pressure gradient along the flow marginally, the mean velocity jumps by orders of magnitude. The fluid velocity profiles are used in combination with a Brownian particle tracking algorithm to resolve the mixing statistics during transport.

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Modeling Cohesive Sediment Erosion and Transport Using a Darcy-Brinkman-Biot Framework

Mitchell Jans (Princeton University)
Ian Bourg (Princeton University)

Abstract

Cohesive sediments, i.e. sediments with elevated clay mineral content, are ubiquitous in surface sediments and play important roles in geochemical cycling, pollutant fate and transport, and fluvial and coastal geomorphic processes. Current predictive abilities in the transport of these sediments remain limited due to complex hydrologic-mechanical-chemical couplings. This work employs a multiscale Darcy-Brinkman-Biot approach, which couples fluid flow with sediment mechanical deformation and accounts for existing couplings through the implementation of swelling pressure and rheological models. We apply the framework to model cohesive sediment erosion in two key settings. First, we simulate surface deformation and erosion of a clay sediment bed in unidirectional flow in fresh and brackish waters to capture salinity's impact on riverine and estuarine sediment dynamics. Second, we use the approach to capture key mechanisms in gravity driven sediment flows that occur on lake and oceanic slopes and elucidate transitions between turbidity currents, mudflow, and slide dynamics. This work extends our knowledge of cohesive sediment transport and provides key insights across a range of salinities, sediment concentrations, and sediment mineralogies.

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An Integrated Approach to Derive Relative Permeability from Capillary Pressure

Nathan Moodie (University of Utah)
Brian McPherson (University of Utah)

Abstract

Surface tension plays a critical role in controlling fluid flow in porous media. By measuring surface tension interactions under multiphase conditions, relative permeability curves, which describe how multiple fluids interact within a porous media, can be derived. These curves are essential for modeling multiphase flow in subsurface systems, including carbon sequestration, hydrocarbon recovery, and groundwater remediation. Accurate characterization of the distribution of relative permeability in the subsurface is therefore vital.

While empirical formulas for estimating relative permeability from capillary pressure are well established, they often lack the flexibility needed to match laboratory-measured data. By expanding on existing methods, we show that both two-phase and three-phase relative permeability curves can be generated directly from capillary pressure data.

In this study, mercury intrusion capillary pressure (MICP) data from multiple lithologies, combined with interfacial tension and contact angle measurements, were used to generate relative permeability curves. These model-derived curves were calibrated against a limited set of laboratory-measured data to identify common fitting parameters. These parameters were then applied to the method to create relative permeability curves from MICP datasets lacking laboratory-derived counterparts, enabling characterization of multiphase flow behavior in a broad range of formations.

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Geological systems 2 Presentation 113

Pore pressure inhibits clustering of induced earthquakes in Western Canada

Bing Q. Li (University of Western Ontario)

Abstract

Induced earthquakes are manifestations of highly heterogeneous distributions of effective stress changes imparted by anthropogenic activities such as hydraulic fracturing and wastewater injection. It is critical to disentangle the mechanisms behind these earthquakes to better assess seismic risk. Here, a clustering methodology is applied to a catalog of 21,536 induced earthquakes detected during a 36-d hydraulic stimulation program in Western Canada. The results reveal that clustered events nucleate at short recurrence times generally less than 6 min. Notably, the clustered events are not characterized by short interevent distances as seen in regional-scale studies. Numerical modeling reveals that earthquakes cluster preferentially in regions of significantly lower pore pressure change (ΔP). Furthermore, clustered earthquakes exhibit significantly more chain-like topologies with decreasing ΔP, in agreement with laboratory studies showing that fault materials transition to rate-strengthening behavior with increasing ΔP. Proxy estimates for pore pressure change suggest these observations are consistent across Western Canada, and highlight the potential for significant temporal segmentation of induced earthquake processes.

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Numerical Evaluation of Gassmann's and Brown & Korringa (1975) Equations in 3D Settings

Yury Alkhimenkov (University of Lausanne)

Abstract

Gassmann's equations are a foundational tool in poroelasticity, linking fluid-saturated rock moduli to dry-frame properties, porosity, and fluid compressibility. While widely accepted, their numerical validation in realistic 3D pore geometries remains limited. Brown and Korringa (1975) extended this framework to multi-mineral systems by introducing additional effective moduli, yet full 3D validation of their theory has not been achieved.

We present detailed 3D finite-element simulations to evaluate both Gassmann's and Brown–Korringa's equations. The model explicitly resolves coupled solid–fluid momentum balance, using realistic pore geometries and heterogeneous solid matrices with multi-mineral inclusions. Small-amplitude harmonic boundary conditions yield drained and undrained bulk moduli, which are computed directly from volume-averaged stress-strain responses.

Results confirm that Gassmann's theory remains valid for mono-mineralic systems, with excellent agreement between numerical and analytical solutions. In contrast, its predictions deviate in multi-mineral rocks, while Brown–Korringa's equations accurately match the simulated response. The inclusion of additional moduli such as the averaged solid modulus and mixed mineral modulus is essential to capture mineralogical heterogeneity.

This study provides the first comprehensive 3D numerical validation of Brown and Korringa's theory and reinforces its consistency with Gassmann's equations in the mono-mineral limit. The developed framework enables future investigation of poroelastic behavior in complex microstructures.

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Accelerated Pseudo-Transient Method for Large-Scale Poromechanical Simulations: Unified Framework for Elasticity, Viscoelasticity, and Quasi-Static Biot Poroelasticity

Yury Alkhimenkov (University of Lausanne)

Abstract

We present a unified, matrix-free numerical framework for solving quasi-static elasticity, viscoelasticity, and coupled Biot poroelastic equations using an Accelerated Pseudo-Transient (APT) method. The method introduces pseudo-inertial terms into the governing equations, transforming elliptic PDEs into hyperbolic-type systems that efficiently converge toward steady-state solutions. Analytical dispersion analysis yields optimal numerical parameters (Strouhal number St) for rapid convergence, validated through comprehensive numerical experiments.

The matrix-free structure relies solely on local operations, enabling exceptional parallel scalability on modern GPU architectures. Ultra-high-resolution simulations demonstrate 2D strain localization on grids exceeding 10000^2 elements and full 3D simulations with complex poro-elasto-viscoplastic coupling on grids of 512^3 elements [1]. We systematically analyze the sensitivity of convergence to initial conditions, heterogeneity, boundary conditions, and nonlinearity, including plastic strain localization.

This study establishes the APT method as a robust and highly efficient tool for extreme-scale poromechanical simulations, particularly well-suited for complex subsurface problems involving coupled flow and deformation. The developed algorithms are fully reproducible, with open-source implementations provided.

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Mathematics of Sea Ice as a Porous Composite

Kenneth Golden (Department of Mathematics, University of Utah)

Abstract

Sea ice is a multiscale composite which exhibits complex structure on length scales ranging over many orders of magnitude. On the microscale, it is a porous medium of pure ice with brine inclusions whose porosity and connectivity depend strongly on temperature, and which can host algae and other microbial life. The evolution of surface melt ponds, the transport of heat, salt and nutrients through the ice, and microbial dynamics all depend critically on fluid flow through the porous brine microstructure. Here we will discuss the effective fluid and electromagnetic transport properties of this porous medium, and the mathematics of homogenization, including percolation theory and integral representations for effective transport coefficients. We'll conclude by illustrating how microscale models in mushy layer physics can be applied to ice pack dynamics on the scale of the Arctic Ocean.

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Pore network dynamics driving colloid transport in porous media: Interception history and attachment efficiency

William Johnson (University of Utah), Diogo Bolster (University of Notre Dame), Luis Ullauri (University of Utah), Bashar Al-Zghoul (University of Notre Dame)

Abstract

The focus of colloid transport in groundwater has expanded from pathogens and radionuclide-bearing clays to include engineered nanomaterials and most recently micro- and nano-plastics. For all of these and other colloid types, the following variances from expectations of Colloid Filtration Theory (CFT) have been well-demonstrated under unfavorable conditions where a repulsive barrier exists in colloid-surface interactions: a) extended tailing of low concentrations in breakthrough-elution concentration histories (BTEC) following initial elution; b) retention profiles (RP) that are non-exponential (multiexponential or nonmonotonic). We present recent experiments and simulations demonstrating that these variances from CFT arise from variations in interception history among the attached colloids. Specifically, we show that colloid concentrations decrease exponentially with distance only for colloids that attach after a single interception, whereas colloids that attach following multiple interceptions assume gamma distributions down gradient from the source with maxima at transport distances that increase with interception order. We show that all these distributions are governed by the collector and attachment efficiencies, and that the well-observed non exponential RPs result from superposition of the RPs for single- and multiple- interception attachers, wherein decreases or increases in attachment efficency with interception order yields multiexponential or nonmonotonic RPs, respectively.

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Image registration of 2D optical thin sections in a 3D porous medium: Application to a Berea sandstone digital rock image

Jaehong Chung (Stanford University)
Wei Cai (Stanford University), Tapan Mukerji (Stanford University)

Abstract

Multimodal digital rock images provide insights into pore-scale structures and upscaling properties; however, their original spatial correspondence is often unknown, and computed properties frequently differ across imaging modalities. We present a computational approach that integrates template image matching with differential evolution optimization to align 2D optical thin-section images precisely within their corresponding 3D digital rock volumes. Validation using a synthetic porous medium confirms registration accuracy. The method is then applied to a Berea sandstone sample to determine the thin-section location within the micro-CT volume, yielding a structural similarity index (SSIM) of 0.990. Registered multimodal images enable direct comparison of pore characteristics and effective elastic moduli. Thin-section images show approximately 50% higher porosity and a greater abundance of submicron pores than corresponding micro-CT images. Bulk and shear moduli derived from thin-section images are about 25% and 30% lower, respectively, indicating discrepancies due to resolution and modality differences. Additionally, thin sections reveal geological features such as cementation and mineral phases that remain unresolved in micro-CT images. These modality-dependent differences underscore the need for precise multimodal registration. Our approach leverages complementary strengths of thin-section and micro-CT imaging to improve microstructural characterization and upscaling accuracy in digital rock physics.

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Electrokinetic and Water–Mineral Interaction Effects on Nanocapillary Water Flow

Abdullah Cihan (Lawrence Berkeley National Lab), Pramod Bhuvankar (Lawrence Berkeley National Lab)

Abstract

Water transport through nanoporous materials plays a critical role in many scientific and engineering applications. While capillary flow is well characterized at microscale, its extension to the nanoscale reveals significant deviations from the existing theoretical predictions. At nanoscales, the impact of the molecular interaction forces between fluids and solids becomes increasingly significant, influencing fluid phase behavior and transport properties. Recent experimental tests show that the Lucas–Washburn equation consistently overestimates the rate of capillary filling in hydrophilic nanochannels—indicating that water advances more slowly than expected. Possible explanations for this discrepancy include induced streaming potential, the altered behavior of water near surfaces, and trapped gas bubbles, which are not accounted for in conventional models. In this study, we develop a pore-scale model based on classical density functional theory, explicitly incorporating surface tension, van der Waals, and electrostatic forces. We will present preliminary results highlighting key mechanisms that may contribute to the reduced water transport in nanochannels. These insights can improve our understanding of nanocapillary flow and guide the design of systems that rely on water transport in nanoporous environments.

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Wave-Induced Fluid Flow as a Geophysical Probe for Hydrogen Storage

Stanislav Glubokovskikh (Lawrence Berkeley National Laboratory), Seiji Nakagawa (Lawrence Berkeley National Laboratory), Mingfei Chen (Lawrence Berkeley National Laboratory), Romy Chakraborty (Lawrence Berkeley National Laboratory), Harry Lisabeth (Lawrence Berkeley National Laboratory)

Abstract

As the global energy landscape transitions toward renewables, underground hydrogen storage (UHS) has emerged as a promising solution for buffering energy supply and demand. However, the security and efficiency of UHS are vulnerable to biogeochemical transformations, particularly those mediated by hydrogenotrophic microorganisms. These microbes can catalyze geochemical reactions that not only consume stored hydrogen but also trigger corrosion, biofilm formation, and mineral precipitation—processes that impair reservoir performance and infrastructure integrity.

Our study presents a combination and experimental investigation of the dynamic poroelastic response of reservoir rocks to the presence of hydrogen gas and associated biofilms in the initially brine-saturated reservoir. The project develops an innovative, non-destructive geophysical monitoring tool to detect these microbially induced changes via wave-induced fluid flow (WIFF) mechanisms. The approach exploits how microbial growth and biofilm accumulation affect the seismic properties of porous rocks. When hydrogenotrophic bacteria form extracellular polymeric substance (EPS)-rich biofilms on grain surfaces, the altered viscosity and stiffness of the pore space change the dynamic rock response to seismic waves. Laboratory simulations indicate that both grain-scale "squirt flow" and mesoscale patchy saturation effects—driven by stress-induced fluid oscillations—can create measurable changes in seismic velocity and attenuation.

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Computational poromechanics 3

Presentation 125

Dynamics of electrolytes in nanopores under electric field

Jerry Owusu (UC Irvine)
Kevin Rosso (PNNL), Russ Detwiler (UC Irvine), Mohammad Javad Abdolhosseini Qomi (UC Irvine)

Abstract

The escalating concentration of greenhouse gases from traditional energy production poses a significant threat to environmental sustainability. Consequently, there has been a pronounced shift towards sustainable and clean energy sources. Among these alternatives, enhanced geothermal energy (EGS) has emerged as a highly promising and viable solution. In geothermal energy systems, fluids must traverse through complex networks of fractures and pores, which feature diverse surface chemistries and pore fluids. Pore fluids, comprising water and dissolved electrolytes, interact with mineral surfaces through adsorption, ion-exchange, and chemical reactions. These interactions are crucial to optimizing fluid transport and reactivity, enhancing geothermal system efficiency and sustainability. Developing a comprehensive understanding of the intricate chemical and physical interactions in subsurface fracture networks is essential for remote monitoring and predicting the geochemical evolution of the EGS.

One proven method for monitoring and measuring subsurface processes and their evolution is the application of electric field techniques, including Spectral Induced Polarization (SIP) and Electrical Resistivity (ER) methods. However, the response of electrolytes to electric fields under various nanopore surface chemistries is not yet fully understood. This gap in knowledge limits our ability to accurately interpret data from these monitoring techniques and underscores the need for further study in this area.

In this study, molecular dynamics simulations were applied to investigate the response of an electrolyte solution confined between idealized mineral nanopore surfaces with varying levels of hydrophilicity, ionophilicity, and surface charge, under different electric field strengths. Molecular dynamics simulations are capable of probing interactions at the atomistic scale, thereby revealing behaviors that are inaccessible to experiments and continuum models. Measurements of drift velocities, diffusion coefficients, and mineral surface charging revealed a significant response of electrolytes to electric fields. This response is influenced by the combined relationship between electric field strength, mineral surface chemistry, and nanopore size. The results have been parameterized into single theoretical relations, which can be applied to macroscopic simulations of the electric response of pore fluids under confinement.

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Porous Models of Thrombosis for Applications to Leaflet Thrombosis

Aaron Barrett (University of Utah)
Boyce Griffith (University of North Carolina, Chapel Hill), Aaron Fogelson (University of Utah)

Abstract

Blood clotting is a complex phenomenon that involves the interplay between biochemistry and fluid dynamics. The introduction of tissue factor and collagen can lead to the activation of platelets, which then enter a high-affinity state that promotes adhesion to the subendothelium and cohesion with other platelets. Embolization of clots can pose serious health risks, such as myocardial infarction or ischemic stroke. Clots that form near moving structures, such as near the aortic or venous valves, are at particular risk of embolization. It is essential to treat the clot as a porous medium to capture the high platelet densities observed in clots, which can often be hundreds of times greater than the background platelet concentrations. Here, we present a detailed mechanics model of clot formation that captures both the porosity of early clots and the viscoelastic stresses from the interplatelet bonds. The model is derived from a multiscale framework, where the underlying microscale bond dynamics are averaged, yielding a continuum-level description of the mechanics. We further extend this model to incorporate fluid-structure interaction using the immersed boundary method, addressing how clot formation and adhesion to moving structures occurs.

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Poster Presentation 130

Quantifying Compaction Viscosity During Compaction of Partially Molten Polycrystalline Ice: Instrument Development and Numerical Modelling

Timothy Xiong (University of Texas at Austin), Peter Flemings (University of Texas at Austin), Marc Hesse (University of Texas at Austin), Richard Ketcham (University of Texas at Austin), Nicola Tisato (University of Texas at Austin), Christine McCarthy (Columbia University), Maheenuz Zaman (Columbia University)

Abstract

The compaction viscosity of partially molten polycrystalline ice governs its compaction and affects mass and heat transport. Although it is a crucial physical property and parameter in modelling glacier and planetary icy shell dynamics, the compaction viscosity is often back-calculated or sensitivity-studied due to a lack of both experimental measurements and understanding of pore-scale mechanisms. To bridge this gap, we developed an X-ray transparent, cryogenic, triaxial loading device that allows for micro-CT imaging of geomaterials, including ice, during compaction. The device accommodates cylindrical samples with a diameter of 12.7 mm and a height of up to 55 mm. It can apply confining pressures of up to 25 MPa and axial stress of up to 33 MPa with temperature control (down to -25°C) and pore fluid flow control capabilities. We present design details and demonstrate the ability to measure permeability and Young's modulus of a clay sample. We plan to first apply isotropic loading on synthetic partially molten saline ice specimens while measuring pore pressure and deformation. To facilitate interpretation of experimental data, we have also developed 2D cylindrical, coupled, finite difference models for both poroelastic (Biot) and poroviscous (Darcy-Stokes) materials that predict different pore pressure response and porosity evolution.

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A thermo-flow-mechanics-fracture model coupling a phase-field interface approach and thermo-fluid-structure interaction

Henry von Wahl, Sanghyun Lee (Florida State University), Thomas Wick (Leibniz Universität Hannover)

Abstract

In this talk, we propose a novel approach for coupling non-isothermal fluid dynamics with fracture mechanics to capture thermal effects within fluid-filled fractures accurately. The proposed algorithm features an iterative coupling between an interface-capturing phase-field fracture method and interface-tracking thermo-fluid-structure interaction using arbitrary Lagrangian–Eulerian coordinates. We use a phase-field approach to represent fractures and reconstruct the geometry to frame a thermo-fluid-structure interaction problem, resulting in pressure and temperature fields that drive fracture propagation. We provide several numerical examples to demonstrate the capabilities of the proposed model and algorithm.

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Geological systems 4 Presentation 134

Earthquake Cycle Simulation in Poro-Viscoplastic Media: A Coupled Framework for Fault-Fluid-Inelasticity Interactions

Ahmed Elbanna (University of Southern California), Amr Ibrahim, (University of Southern California)

Abstract

Earthquake cycles, in the context of both natural and induced seismicity, are governed by complex interactions between fault slip, fluid pressure changes, and time-dependent inelastic deformation in the surrounding rock. Although existing research has advanced our understanding of fault-fluid coupling through poroelastic theory, the influence of viscoplastic processes in fluid saturated porous medium on sequences of earthquakes and aseismic slip on geological scales remains largely unexplored. Here, we develop a unified computational framework that integrates rate-and-state friction, Biot's poroelasticity, and Drucker-Prager viscoplasticity to characterize earthquake cycles in fluid-saturated, inelastic media.

We validate our implementation through comprehensive benchmark tests covering consolidation, fluid injection-production, leaky fault behavior, injection-induced slip, and poro-elasto-plastic deformation. Results demonstrate excellent agreement with analytical solutions and established numerical models, confirming the accuracy of our coupled formulation.

The framework reveals a fundamental competition between inelastic deformation, which dissipates energy and stabilizes the system, and poromechanical effects, which can either promote or inhibit instability through fluid pressurization. We demonstrate our methodology using a model of rate-and-state faults embedded within poroviscoplastic damage zones, where off-fault inelasticity influences rupture nucleation, propagation, and arrears. We explore the effects of different photomechanical parameters on seismicity statistics as well as the partitioning of deformation in the system.

This work provides new insights into the complex interplay between fault slip, off-fault inelasticity, and fluid flow across scales relevant to natural and induced seismicity. The framework establishes a foundation for future studies incorporating spatial heterogeneity and evolving damage zone properties, addressing critical questions in earthquake cycle modeling and hazard assessment.

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Poster Presentation 135

Numerical Investigation of Particle Shape and Particle Size Distribution Effects on The Mechanical Behavior in Unbreakable Particulate Packs

Ayat Alasadi (University of Utah)
Shahrzad Roshankhah (University of Utah)

Abstract

Particle shape and Particle Size Distribution (PSD) fundamentally govern the mechanical and hydraulic behavior of particulate systems, particularly under the extreme conditions encountered in Enhanced Geothermal Systems (EGS). This study numerically investigates the shape and PSD effects on the mechanical behavior of unbreakable particulate packs. The analysis includes calibrating the oedometer and direct shear tests simulations to establish shape-dependent and PSD-dependent packing behavior. The results focus on tracking the evolution of micro-scale behavior, such as particle rearrangement, interlocking, and deformation pathways, and their influence on macro-scale responses, including mechanical stiffness and permeability, which is estimated from an empirical correlation, the Kozeny-Carman relation. The results of the study show that uniform PSDs generate stable pore channels but are prone to crushing and fines generation, leading to greater permeability loss, while non-uniform PSDs produce denser packs that enhance mechanical stability but reduce permeability. At the particle scale, spherical particles display lower compressibility under uniaxial loading but limited stability under shear, resulting in lower overall permeability reduction, whereas non-spherical particles exhibit higher compressibility but greater shear resistance, leading to higher overall permeability reduction. By isolating and combining the shape and PSD effects, the work aims to clarify the role of different pack geometries on the mechanical behavior of particulate packs. Outcomes are expected to set a baseline for newly designed and manufactured proppants for geothermal applications where long-term conductivity and structural integrity are critical.

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Poster Presentation 136

Matrix–Hydraulic Fracture-Natural Fracture Interactions in EGS Reservoirs and CO2 Disposal Formations: Dimensional Analyses and Hydro-Mechanical FDEM Simulations

Shahrzad Roshankhah (University of Utah), Shivesh Shandilaya (University of Utah)

Abstract

Enhanced geothermal systems (EGS) in low-permeability igneous and metamorphic rocks and the geological storage of CO$_2$ in high-permeability sedimentary formations are key steps towards a net-zero carbon energy economy and long-term climate stability. High-rate fluid injection must be engineered in these systems to increase production in EGS through the creation of an extensive and complex network of fractures and increase storage in CO$_2$ sequestration projects through extensive fluid leak off into the far field rock mass. Without a rigorous design, high-rate fluid injection may lead to short circuiting in EGS (one or very few fractures between the stimulation and production wellbores, limiting the energy extraction), fracturing the caprock in CO$_2$ sequestration, and induced seismicity in both applications. We, therefore, study the key parameters, including the rock matrix permeability, NF characteristics (geometric and hydromechanical parameters), characteristics of the working fluids, fluid injection rate, and boundary conditions, on the overall hydraulic (pressure field and permeability evolution) and mechanical (rock mass deformation, fracture network evolution, and seismic response) behavior of sample EGS (Utah Forge) and CO$_2$ (Uinta Basin, Utah) reservoirs. We employ dimensional analyses to understand the hydraulic (leak off or storage of the fluid) and mechanical (viscous fluid drag or fracture generation dominant energy dissipation) regimes in homogeneous, isotropic rock masses. We use a hydro-mechanically coupled, hybrid finite–discrete element method (FDEM) to investigate the hydromechanical processes in naturally fractured granite and sandstone formations.

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Poster Presentation 137

Investigation of PCM-mortar under complex environment

Mohamed Morsi (The University of Utah)

Abstract

Cement mortar, a widely used construction material, is a porous medium with limited ability to buffer temperature fluctuations. Incorporating phase change materials (PCMs) offers a means to improve thermal regulation, yet this alters mechanical properties and durability. Despite numerous studies on PCM
integration, the collective impact of specimen size, curing age, and curing medium on the mechanical response of PCM-modified mortar remains poorly understood.

This study examines the mechanical properties of PCM mortar where microencapsulated PCM was incorporated through partial sand replacement and cured in different environments. Specifically, we prepared cube specimens in different sizes and evaluated compressive strength at three curing ages (i.e., 7, 14, and 28 days) and under two curing environments (i.e., air and salted water). Results show that PCM-mortar cured in salted water has the highest strength, particularly at late ages. Curing in salted media accelerated hydration and enhanced strength recovery compared with air curing, with its effects more pronounced than those of specimen size or aging alone. Smaller specimens consistently exhibited higher strength than larger ones.

These findings open opportunities for applying PCM mortar in construction under severe environmental conditions, particularly for coastal infrastructure and buildings located in or near water.

Key Words: mechanical behavior, size effect, sustainable materials.

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Does pre-existing differential pressure have an impact on poroelasticity equations?

Lynn Schreyer (Department of Mathematics and Statistics, Washington State University)
Pratap Sahay (Center for Scientific Research and Higher Education at Ensenada (CICESE), Baja California), Ryan Whitehead (Scientific Research and Technology Development, UES, a BlueHalo company, Dayton, OH)

Abstract

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 state's 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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Poster Presentation 140

Nanoindentation Study of Granite Under Elevated Temperatures and Environmental Conditions

Ozan Altuntas (University of Utah)
Hongkyu Yoon (Sandia National Laboratories), Pania Newell (University of Utah)

Abstract

Rocks are subject to thermo-hydro-mechanical (THM) conditions in most geological applications. THM conditions cause softening at the microscale in rocks and may lead to unexpected failure. Consequently, understanding the material behavior of granite, as a primary rock, at the microscale under these conditions is of a great interest to many sub-surface engineering applications, e.g., enhanced geothermal energy production. Nanoindentation offers a novel and accurate way of microscale characterization. Here, we perform nanoindentation tests on Sierra White granite under THM conditions. Dry and wet samples underwent trapezoidal linear loading (5-2-5 seconds) at temperatures from 25°C to 450°C. Samples were examined using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS) at pre- and post-indentation phases. Then the elastic modulus and hardness were derived from load-displacement curves and fracture toughness was calculated via an energy-based method. The results show that the wet samples at 25°C lost 60% of their strength, while partially recovering the original dry strength after drying. Similarly, exposure to 450°C reduced the dry and wet sample strength by 20%. These findings indicate that both temperature and liquid exposure contribute to nanoscale softening mechanisms within granite, with liquid exposure having a greater effect when thermal crack were not present. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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October 7-10, 2025, The University of Utah, Salt Lake City, United States

Poster Presentation 141

Uncovering Structure–Property Relationships in Porous Materials via Data-Driven Methods

Achyut Dhar (Postdoctoral scholar)
Pania Newell (University of Utah)

Abstract

Porous materials, whether naturally occurring or engineered, are central to a wide range of scientific and engineering applications. Understanding these systems for performance and design is challenging, as traditional experimental and high-fidelity computational methods struggle to capture the complexity of pore structures (characterized by variations in porosity and pore distribution) and their vast design space. By leveraging advances in computational power and machine learning algorithms, our goal is to discover structure–property relationships in porous materials using data-driven methods for both design purposes and optimal performance.

In this work, we employ asymptotic homogenization to compute effective elastic properties of porous materials with circular pore topologies from microscale, which are then used in phase-field fracture formulation to predict fracture response at macroscopic scale using benchmark tests. We perform both homogenization and phase-field analyses using the open-source finite element library FEniCSx, leveraging GPU-based parallelization to accelerate data generation. The resulting high-fidelity datasets are used to train convolutional neural network based regression models that map porous microstructures to their homogenized elastic responses. Representative case studies reveal how variations in the pore morphology, characterized by homogenized elastic modulus and Poisson's ratio, influence fracture behavior. These findings highlight that the resistance to crack extension has a strong dependence not just on the porosity but also on the pore morphologies for the same porosity. This integrated framework paves the way for the data-driven design and optimization of porous materials by uncovering relationships between the pore structure, elastic, and fracture behavior from a limited dataset of high-fidelity simulations.

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Poster Presentation 142

The Effect of Microscale Pore Morphology on Fracture Behavior

Ryan Nielsen (University of Utah), Pania Newell (University of Utah)

Abstract

Porous materials are found throughout nature and used extensively in the engineering field. While these materials often couple structural rigidity with other desirable traits, they are also susceptible to brittle fracture. Relative to the dimensions of an engineering structure, the scale of a porous material's underlying microstructure is infinitesimally small. This introduces difficulties in failure prediction via numerical modeling, as a single-scale domain is computationally impractical to discretize. Alternatively, brittle fracture of porous materials can be represented as a 2-scale model in which asymptotic homogenization relays microstructure-induced material anisotropy to a coarse-scale domain via a homogenized constitutive tensor, $\bar{C}$. This tensor is used in the strain energy term of a phase-field model depicting macroscale brittle fracture. To investigate how microscale pore morphology affects macroscale fracture behavior, we map different $\bar{C}$ tensors, representing various microstructures, to an edge-cracked plate in tension. Results show that although all morphologies have the same level of porosity, their corresponding macroscale crack growth varies considerably. Initial findings suggest future work should further parameterize geometric shape descriptors of a pore, such as deviation from a perfect circle and the ratio of height to width, when attempting to quantify their relation to brittle fracture in porous materials.

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Micro- and Nano-Technology Approaches to Design Bioadhesive Hydrogels for Sutureless Wound Closure

Hossein Montazerian (University of Utah)

Abstract

Bioadhesive hydrogels offer a minimally invasive alternative to sutures and staples for rapid sealing of bleeding wounds. Inspired by natural adhesives from mussels and climbing plants, catechol-based chemistries enable strong wet adhesion through phenolic interactions. However, conventional functionalization approaches often yield low catechol incorporation and limited adhesive performance. This seminar introduces new strategies to enhance both tissue adhesion and cohesive strength in polyphenolic hydrogels. Methods for integrating hemostatic efficacy and maintaining catechol stability during photocrosslinking are discussed, alongside an *in situ* polymerization approach for gelatin-based systems. A simple oxidative polymerization-coupling method is also presented for high-yield catechol attachment, producing robust, photothermally responsive, and rapidly gelating bioadhesives. These advances define a design framework for multifunctional, injectable polyphenolic hydrogels with strong wet adhesion and bioactivity, offering significant potential for clinical wound sealing and tissue regeneration.

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Additive Manufacturing of Architected Structures for Healthcare Applications

Elham (Emma) Davoodi (University of Utah)

Abstract

Additive manufacturing (AM) is transforming healthcare by enabling the precise design and fabrication of complex, customized, and multifunctional structures for diagnostics, therapy, and tissue regeneration. This presentation highlights advances in architected materials and biomanufacturing technologies developed to address clinical challenges in biomonitoring, tissue engineering, and minimally invasive therapeutics. We discuss how topology-optimized porous architectures, such as triply periodic minimal surfaces (TPMS), allow fine-tuning of mechanical, electrical, and transport properties for flexible sensors and implantable scaffolds. Examples include 3D-printed TPMS-based sensors for long-term physiological monitoring and hydrogel scaffolds supporting vascularized tissue growth. Finally, we introduce Deep Tissue In Vivo Sound Printing (DISP), a novel ultrasound-guided 3D printing technique that enables noninvasive fabrication of functional biomaterials within deep tissues, demonstrated for muscle regeneration and localized cancer therapy. Together, these innovations illustrate the convergence of material architecture, manufacturing precision, and biomedical function toward next-generation patient-specific healthcare solutions.

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Poster Presentation 155

Ionic PFAS transport along thin water films in soils

Wenqian Zhang (University of Arizona)

Abstract

Understanding how ionic surfactants migrate within thin water films is central to predicting interfacial processes in physiological, industrial, and environmental systems. We formulate a unified framework for surfactant transport in thin aqueous films overlaying charged solids, explicitly coupling interfacial thermodynamics, film hydrodynamics, and electrokinetic transport. The model extends lubrication theory to include Marangoni stresses, surface diffusion, and electrostatic migration arising from gradients in interfacial potential. Through non-dimensional analysis, we identify two key control parameters—the Marangoni number and electrostatic migration number—that govern the relative strengths of capillary and electrostatic forcing. Systematic asymptotic and numerical analyses reveal three dominant transport regimes and quantify how electrostatic coupling alters classical Marangoni-driven spreading. The resulting regime map clarifies when surface diffusion, Marangoni advection, or electrostatic migration dictates spreading behavior. This mechanistic framework provides a predictive foundation for ionic surfactant dynamics in thin films and offers new insights into PFAS migration through water films in unsaturated soils.