2024 CSM Industrial Affiliates' Meeting

March 21, 2024

Time:	Speaker:	Topic
9:00 am	Dr. Sanghyun Lee	"Phase Field Fracture Propagation for Subsurface Applications"
9:30 am	Dr. Mary Wheeler	"Modeling Frac-Hits by Employing Reservoir Geomechanics and Phase Field Finite Element Simulations"
10:00 am	Dr. Ali Dogru	"Large-Scale Numerical Simulation of Multiphase Flow in Porous Media"
10:30 am	Dr. Mohamad Jammoul	"Numerical Modeling of CO2 Storage: Applications to the FluidFlower Experimental Setup"
11:00 am	Break	
11:30 am	Dr. Faruk Omer Alpak	"Less-Intrusive Consistent Discretization Methods For Reservoir Simulation On Cut-cell Grids: Algorithms, Implementation, and Testing"
12:00 pm	Dr. Todd Arbogast	"A high order, finite volume, multilevel WENO scheme for multidimensional flows"
12:30 pm	Dr. Robert Podgorney	"High-Performance Computing Approaches for Coupled Thermal-Hydraulic-Mechanical Reservoir Simulation of Injection/Production at the Utah FORGE EGS Site"
1:00 pm	Lunch	Catered by Central Market in 6.102 for registered attendees only (down the hallway to the left)
2:00 pm	Panel-Drs. Hector Klie, Fredrick Saaf, Eduardo Gildin, and Manish Parashar	Panel discussion: Recent and future trends in energy resources and simulation
2:30 pm	Dr. Ahmed Almetwally	"Enhanced Geothermal Systems (EGS) Modeling Using Finite-Element Phase-Field and Porous Media Multiphysics; Application: Forge Geothermal Project"
3:00 pm	Dr. Roy Stogner	"An Introduction to MOOSE: Multi-physics Object-Oriented Simulation Environment"
3:30 pm	Dr. Thomas Hughes	"Phase Field Fracture : From the Small to the Large"
4:00 pm	Break	
4:30 pm	Dr. Mojdeh Delshad	"Energy Production and Storage"
5:00 pm	Dr. Bruno Fernandes	"Hydrate Risk Assessment during CO2 Storage in Depleted Gas Reservoirs"
5:30 pm	Dr. Nicola Tisato	"Detecting multiphase fluids in the subsurface: the importance of seismic waves attenuation."

Start Time: 9:00 am

Speaker: Dr. Sanghyun Lee

Title: “Phase Field Fracture Propagation for Subsurface Applications”

Abstract: In this work, we review and describe our computational framework for solving multiphysics phase-field fracture problems in porous media. Therein, the following six coupled nonlinear physical models are addressed: displacements for geo-mechanics, a phase-field variable to indicate the fracture position, a pressure equation for the porous media flow, a crack width problem, a proppant concentration transport equation, and/or a saturation equation for two-phase fracture flow, and finally a recently developed temperature equation. The overall coupled problem is solved with a staggered solution approach, known in subsurface modeling as the fixed-stress iteration. A classical linear continuous Galerkin finite elements are employed for the displacement-phase-field system and the crack width problem. Locally conservative Enriched Galerkin formulations are used for the pressure, the proppant and/or saturation, and the temperature equations. A robust and efficient quasi-monolithic semi-smooth Newton solver, local mesh adaptivity, and parallel implementations allow for competitive computational cost. Several numerical examples will illustrate two- and three-dimensional examples considering different scenarios. The resulting program is an in-house code named IPACS (Integrated Phase-field Advanced Crack Propagation Simulator) and is based on the finite element library, deal.II.

Start Time: 9:30 am

Speaker: Dr. Mary Wheeler

Title: “Modeling Frac-Hits by Employing Reservoir Geomechanics and Phase Field Finite Element Simulations”

Additional Author: Dr. Ahmed Almetwally, The University of Texas at Austin

Abstract: Infill well development has become a widely used strategy for hydrocarbon production in unconventional reservoirs with an increasing number of "infill" wells being drilled offset to one or more existing producers. However, the proximity of these new wells ("child" wells) to existing producers ("parent" wells) often leads to negative impacts on production due to fracture interactions or "frac hits". The severity of the impact depends on factors such as well spacing and the age of the parent, and impacts are highly variable between different shale plays. To address these issues a geomechanical model was constructed to simulate Frac-Hit events by considering geological, reservoir, and fracturing parameters for multiple horizontal

wells in a drilling spacing unit. The model was validated against recorded micro-seismic events and used to simulate different scenarios and combinations of operational parameters.

Start Time: 10:00 am

Speaker: Dr. Ali Dogru

Title: "Large-Scale Numerical Simulation of Multiphase Flow in Porous Media"

Abstract: This presentation will cover progress in large scale simulation using massively parallel simulators for multiphase, multi component compressible flow in hydrocarbon reservoirs and basins. The presentation will also cover Co2 sequestration in saline aquifers, simulation of geothermal reservoirs and hydrogen storage in aquifers. A brief description of mathematical formulation and numerical solutions will be presented.

Start Time: 10:30 am

Speaker: Dr. Mohamed Jammoul

Title: "Numerical Modeling of CO2 Storage: Applications to the FluidFlower Experimental Setup"

Abstract: A major concern in carbon storage projects is the prediction of plume movement due to the uncertainty in the subsurface and the complexity of the physical processes. Numerical simulations can resolve the aforementioned challenge, provide better assessment of the associated risks, and facilitate more informed decision making. In this talk, I will describe a benchmark study for CO2 storage in porous media. The study aims to evaluate the uncertainties that arise in modeling subsurface processes. The numerical simulations were conducted using the in-house reservoir simulator (IPARS) and the results were validated against the FluidFlower experimental setup.

Start Time: 11:30 am

Speaker: Dr. Faruk O. Alpak

Title: "Less-Intrusive Consistent Discretization Methods For Reservoir Simulation On Cut-cell Grids: Algorithms, Implementation, and Testing"

Additional Authors: Drs. Mohamad Jammoul and Mary F. Wheeler, The University of Texas at Austin

Abstract: Consistent discretization methods are a natural fit for the novel cut-cell gridding technique for reservoir simulation, which preserves the orthogonality characteristic in the lateral direction. Both uniform (global) and novel hybrid (local) variants of consistent discretization methods are implemented and tested in the vicinity of fault representations on cut-cell grids. Novel consistent discretization methods, which do not require major intrusive changes to the solver structure of industrial-grade reservoir simulators, are investigated in this work. Cell-centered methods such as multi-point flux approximation (MPFA), average multi-point flux approximation (AvgMPFA), and nonlinear two-point flux approximation (NTPFA) methods fit naturally into the framework of existing industrial-grade simulators. Thus, cut-cell compatible variants of AvgMPFA and NTPFA and their novel hybridizations with TPFA are implemented and tested. An implementation of the relatively more computationally expensive MPFA is also made to serve as accuracy reference to AvgMPFA and NTPFA. AvgMPFA and NTPFA multiphase simulation results are compared in terms of accuracy and computational performance against the ones computed with reference MPFA and TPFA methods on a set of synthetic cut-cell grid models of varying complexity including conceptual models and a field-scale model. It is observed that AvgMPFA consistently yields more accurate and computationally efficient simulations than NTPFA on cut-cell grids. Moreover, AvgMPFA-TPFA hybrids run faster than NTPFA-TPFA hybrids when compared on the same problem for the same hybridization strategy. On the other hand, the computational performance of AvgMPFA degrades more rapidly compared to NTPFA with increasing "rings" of orthogonal blocks around cut-cells. Auspiciously, only one or two "rings" of orthogonal blocks around cut cells are sufficient for AvgMPFA to deliver high accuracy.

Start Time: 12:00 pm

Speaker: Dr. Todd Arbogast

Title: "A high order, finite volume, multilevel WENO scheme for multidimensional flows"

Additional Authors: Dr. Chieh-Sen Huang, National Sun Yat-sen University (Taiwan), and Chenyu Tian, The University of Texas at Austin

Abstract: We develop a novel and general framework for solving partial differential equations (PDEs) using finite volume weighted essentially non oscillatory (WENO) techniques on general computational meshes. Such techniques are able to handle both advective and (degenerate) diffusive behavior, even when the solution develops shocks or steep fronts. We overcome the restrictions and difficulties of using current WENO techniques on general meshes in multiple space dimensions by resolving two fundamental issues. First, polynomial approximations on general stencils of elements can be of poor quality, even for what appear to be geometrically nice stencils. We present a robust and efficient procedure for producing accurate stencil polynomial

approximations. Second, by their design, current WENO reconstructions combine only stencil polynomials of exactly two different degrees. This fact restricts the types of stencil polynomials that can be used and also effectively precludes using single element stencils. We develop a novel and efficient finite volume, multilevel WENO (ML-WENO) reconstruction that combines stencil polynomial approximations of various degrees. The nonlinear weighting biases the reconstruction away from both inaccurate oscillatory polynomials of high degree (i.e., those crossing a shock or steep front) and smooth polynomials of low degree, thereby selecting the smooth polynomial(s) of maximal degree of approximation. We apply these new ML-WENO reconstructions to develop a finite volume scheme for solving Richard's equation governing an air-water hydrological flow in porous media.

Start Time: 12:30 pm

Speaker: Dr. Robert K. Podgorney

Title: "High-Performance Computing Approaches for Coupled Thermal-Hydraulic-Mechanical Reservoir Simulation of Injection/Production at the Utah FORGE EGS Site"

Abstract: The Frontier Observatory for Research in Geothermal Energy (FORGE) site is a multi-year initiative funded by the U.S. Department of Energy for enhanced geothermal system research and development. The site is located on the margin of the Great Basin near the town of Milford, Utah. Modeling and simulation are playing a critical role at the site and is considered as a general scientific discovery tool to elucidate behavior of enhanced geothermal systems and as a deterministic (or stochastic) tool to plan and predict specific activities. This paper will provide an overview of the research site and discuss recent modeling and simulation activities.

Start Time: 2:00 pm
Speaker: Drs. Hector Klie, Fredrick Saaf, Eduardo Gildin, and Manish Parashar

Panel Topic: Recent and future trends in energy resources and simulation

Start Time: 2:30 pm

Speaker: Dr. Ahmed Almetwally

Title: "Enhanced Geothermal Systems (EGS) Modeling Using Finite-Element Phase-Field and Porous Media Multiphysics; Application: Forge Geothermal Project"

Abstract: This work presents a novel finite-element simulation technique specifically designed for EGS applications, addressing the coupled multiphysics challenges present in the Forge project. Our approach leverages the strengths of both the Enriched Galerkin (EG) method for accurate fluid flow and energy conservation calculations, and the Continuous Galerkin (CG) method for efficient mechanics modeling. Crucially, this framework integrates a phase-field approach for simulating dynamic fracture initiation, propagation, and width estimation. This hybrid methodology exhibits superior local mass conservation and computational efficiency compared to traditional CG or Discontinuous Galerkin (DG) methods. Its applicability is demonstrated through the simulation of coupled thermoporoelastic behavior relevant to EGS. Focusing on the Forge geothermal site in Utah, we utilize the proposed approach to model hydraulic fracturing processes. We employ a fixed-stress split approach, extending its use to efficiently simulate fully coupled fracturing multiphysics. The EG scheme ensures mass and energy conservation while capturing the abrupt pressure and temperature jumps at the matrix-fracture interface. Additionally, a variational phase-field method eliminates the need for continuous re-meshing during fracture propagation. Moreover, a diffraction system seamlessly transfers mass and energy between the matrix and fracture along the interface. The capabilities of this framework are validated through the simulation of two analytical problems and a 3D triaxial geothermal experiment replicating the Forge scenario. This experiment incorporates pressure-driven fracture propagation and comparison with microseismic data. The compelling results confirm the suitability of our approach for field-scale EGS applications like Forge, paving the way for optimized reservoir development and enhanced geothermal energy extraction.

Start Time: 3:00 pm

Speaker: Dr. Roy Stogner

Title: “An Introduction to MOOSE: Multi-physics Object-Oriented Simulation Environment”

Abstract: A discussion of the MOOSE framework for solving computational engineering problems, the design goals and user needs which are met by MOOSE and its “herd” applications, and the design philosophies which have evolved to meet those goals. The framework will be examined from the perspective of engineering users, of application developers, as well as from the perspective of developers of the framework itself and of its underlying mathematical analysis and high-performance computing libraries.

Start Time: 3:30 pm

Speaker: Dr. Thomas Hughes

Title: “Phase Field Fracture : From the Small to the Large”

Abstract: It seems phase fields are everywhere in engineering analysis these days. There are two types of phase fields in common usage: *binary phase fields* and *continuous phase fields.*

Perhaps the most prevalent binary phase field in engineering is "trim" in computer-aided design (CAD), in which geometrical objects are trimmed to prescribed geometric requirements by introducing two phases, one having value 1.0 for material and the other having value 0.0 for void, where the material has been cut away. The analysis version of trim appears in "immersed methods," where objects are placed in a background mesh and the actual geometry cuts through the elements of the background mesh. Although immersed methods have existed seemingly forever, they have only come into prominence recently due to breakthroughs that dramatically increased the accuracy they can attain, which rivals that of the classical boundary-fitted meshing approach. As in CAD, in immersed methods, the material body is a phase of 1.0 and the part of the background mesh unoccupied by materials is phase 0.0. Topology optimization utilizes the same binary phase concept, material is 1.0, and void is 0.0.

In continuous phase fields, the phase field parameter is typically a real number, that, for example, can vary between 1.0 and 0.0. Continuous phase fields are essential technologies in additive manufacturing (aka 3D printing), analysis of multiphase flows, and, last but not least, *fracture mechanics.*

Phase-field fracture has its origins in image processing. It was observed that the Mumford-Shah functional of image processing had essential features in common with the Griffith theory of brittle fracture. Ambrosio and Tortorelli showed that the Mumford-Shah theory could be obtained as the limit of a functional involving a continuous phase-field. The analog for Griffith theory opened the way for computing fracture solutions through finite element methods. The phase field in this framework has value of 1.0 for undamaged material and 0.0 at a fracture, and varies continuously in between. The zone of transition is referred to as the "process zone" and its thickness is a length scale that can be determined from material properties.

Phase field fracture has captured the imagination of the theoretical and computational mechanics communities, but there are issues that challenge its widespread utilization. A prominent one is the process-zone size. For real materials it can be very small. For example, for aluminum it is about 0.06 mm. To achieve an accurate solution, the mesh length scale, say h, needs to resolve the process zone, meaning for aluminum that h must be much smaller than 0.06 mm. The upshot is that it takes a prohibitively large mesh to solve a full-scale engineering structure. That has been a showstopper until recently. In my talk today, I will describe recent work that renormalizes a phase field fracture theory so that it can be efficiently applied to large engineering structures.

Start Time: 4:30 pm

Speaker: Dr. Mojdeh Delshad

Title: "Energy Production and Storage"

Abstract: Hydrogen has the potential to play a significant role in the energy transition as a clean energy carrier and storage medium to mitigate the seasonality of renewable energy supply and demand. Underground hydrogen storage in porous geological formations is essential for a large-scale hydrogen economy, particularly for lowering the cost of hydrogen as it can enable hydrogen producers to take advantage of seasonal energy and feedstock availability and prices. However, technology and knowledge barriers remain to be addressed for industrial-scale deployments. These barriers include quantifying the effect of heterogeneities on injection and recovery, hydrogen leakage pathways, and loss mechanisms. Our research aims to advance further our understanding of the underlying fundamental mechanisms involved in hydrogen storage in real geological models of depleted gas reservoirs and saline aquifers. Our insights on trapping and loss mechanisms produced hydrogen purity, wettability, petrophysical properties, and cushion gas will be discussed.

Start Time: 5:00 pm

Speaker: Dr. Bruno Fernandes

Title: "Hydrate Risk Assessment during CO2 Storage in Depleted Gas Reservoirs"

Abstract: The study aims to quantitatively assess the risk of hydrate formation within the porous formation and its consequences to injectivity during storage of CO_2 in depleted gas reservoirs considering low temperatures caused by the Joule Thomson (JT) effect and hydrate kinetics. The aim was to understand which mechanisms can mitigate or prevent the formation of hydrates. The key mechanisms we studied included water dry-out, heat exchange with surrounding rock formation, and capillary pressure. A compositional thermal reservoir simulator is used to model the fluid and heat flow of CO_2 through a reservoir initially composed of brine and methane. The simulator can model the formation and dissociation of both methane and CO_2 hydrates using kinetic reactions. This approach has the advantage of computing the amount of hydrate deposited and estimating its effects on the porosity and permeability alteration. Sensitivity analyses are also carried out to investigate the impact of different parameters and mechanisms on the deposition of hydrates and the injectivity of CO_2. Simulation results for a simplified model were verified with results from the literature. The key results of this work are: (1) The Joule-Thomson effect strongly depends on the reservoir permeability and initial pressure and could lead to the formation of hydrates within the porous media even when the injected CO_2 temperature was higher than the hydrate equilibrium temperature, (2) The heat gain from underburden and overburden rock formations could prevent hydrates formed at late time, (3)

Permeability reduction increased the formation of hydrates due to an increased JT cooling, and (4) Water dry-out near the wellbore did not prevent hydrate formation. Finally, the role of capillary pressure was quite complex, where it reduced the formation of hydrates in certain cases and increased in other cases. Simulating this process with heat flow and hydrate reactions was also shown to present severe numerical issues. It was critical to select convergence criteria and linear system tolerances to avoid large material balance and numerical errors.

Start Time: 5:30 pm

Speaker: Dr. Nicola Tisato

Title: "Detecting multiphase fluids in the subsurface: the importance of seismic waves attenuation"

Abstract: The detection of multiphase fluids in the subsurface is crucial in understanding processes related to natural hazard mitigation and industrial activities. For example, the formation, coalescence, and migration of bubbles magmatic chambers pre-cursor volcanic eruptions, and carbon dioxide sequestration and hydrogen storage in the subsurface are becoming critical industrial activities. Therefore, seismic methods are key to monitor the formation and migration of bubbles in the subsurface. I will show laboratory experiments and numerical results illustrating how the presence of bubbles in the fluids saturating rocks can largely attenuate seismic waves. The developed theory should be used to improve subsurface monitoring to help mitigate hazards and seismic imaging to boost exploration.