

**University of Stuttgart**

Cluster of Excellence EXC 2075 „Data-Integrated Simulation Science“

Faculty 2: Civil and Environmental Engineering

**Place:**

Pfaffenwaldring 7, Room 2.157

**Thursday, 12 September 2024**

09:00 – 09:45 am

Dr. Sidian Chen

11:15 – 12:00 pm

Nikita Bondarenko

02:00 – 02:45 pm

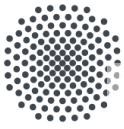
Dr. Lluís Saló-Salgado

04:15 – 05:00 pm

Dr. Catherine Spurin

Scientific  
Colloquium

Hydromechanics



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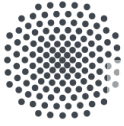
I will present two example problems to discuss the critical role of non-equilibrium fluid flow, chemical transport, and thermodynamics in porous materials. The first example addresses PFAS contamination in the vadose zone. PFAS migration in vadose zones is significantly slowed down by their accumulation at air-water interfaces (AWIs) in water-unsaturated soils—including bulk AWIs and thin-water-film AWIs (>90%). It remains unknown how the accessibility of thin-water-film AWIs and the mass transfer in thin water films will control PFAS downward migration. I address this challenge by developing a pore-scale model that considers PFAS-specific processes such as adsorption at AWIs, diffusion along AWIs, and mass transfer in thin water films. Modeling results highlight the importance of above physical mechanisms on PFAS transport in soils. The second problem focuses on shale gas recovery. Existing field-scale models often fail to predict gas production due to abnormal thermodynamic phase changes and nonequilibrium flow in the nanoscale pore spaces in shale rocks. I tackle this problem by developing pore-scale models that represent the realistic pore spaces and molecular-level physical processes therein. I will discuss how these micro-scale phenomena influence macro-scale behaviors in rock samples and how they can be integrated into field-scale predictions. Overall, my research aims to harness non-equilibrium porous media physics for addressing environmental and energy challenges.

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Nonequilibrium  
Phenomena in  
Multiphase Flow,  
Transport, and Phase  
Change in Porous Media:  
Pore-Level Physics,  
Network Modeling, and  
Upscaling

**Dr. Sidian Chen**

Stanford University, USA



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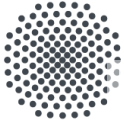
Injection of carbon dioxide (CO<sub>2</sub>) into deep underground formations is a promising approach to mitigate accelerating greenhouse gas emissions. However, it affects the state of stress in the subsurface, potentially making it more favorable for fault reactivation and earthquakes.

In this presentation, the results of laboratory testing are combined with high-performance numerical modeling to assess the risk of induced seismic response during CO<sub>2</sub> injection at IBDP site in Illinois Basin. The conducted experiments address strength, poromechanical response, single- and two-phase permeability of tight rock specimens from reservoir, basal sealing, and crystalline basement formations at representative conditions. High-resolution numerical modeling allows to consider the stratigraphy of injection site and reconstruct three-dimensional state of stress and its evolution during the injection, highlighting role of local stratigraphy and heterogeneity in creation of critically stresses zones in crystalline basement.

## **Geomechanical Assessment of Induced Seismicity During CO<sub>2</sub> Injection in Illinois Basin**

**Nikita Bondarenko**

University of Illinois  
Urbana-Champaign, USA



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Mitigating climate change, enhancing water security, and improving energy access require the development of subsurface systems at an unprecedented scale.

Subsurface systems, however, are complex, with fractures and faults as key structural discontinuities. These structures control the movement of fluids, and are responsible for geohazards including earthquakes, groundwater pollution, or geomechanical deformation. The scientific challenge lies in *quantifying* and *reducing uncertainty* in the behavior of subsurface systems—necessary to scale up operations, but difficult due to limited access and heterogeneity.

In this talk, I will present the development of a computational framework to tackle this challenge by means of (1) an improved description of fault hydraulic behavior, and (2) its application in uncertainty quantification forecasts. First, I will describe a new methodology to model multiphase flow properties of fault zones, including anisotropy and uncertainty. Second, I will present how this methodology is being applied in flow and geomechanics simulation models to assess and mitigate fault CO<sub>2</sub> migration hazard during Megatonne-scale geologic carbon storage.

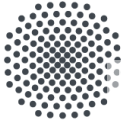
I will conclude the talk by describing a paradigm-shift in the description of faults and fractures in subsurface simulation environments, my proposed research program to make this shift a reality, and how this will enable sustainable development of the subsurface.

## Sustainable Development of Complex Subsurface Systems at Scale: A Defining Challenge of the 21<sup>st</sup> Century

**Dr. Lluís Saló-Salgado**  
Harvard University, USA

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Subsurface fluid flow is ubiquitous in nature, and understanding the interaction of multiple fluids as they flow within a porous medium is central to many geological and environmental processes. It is assumed that the flow pathways of each phase are invariant when modelling subsurface flow using Darcy's law extended to multiphase flow; a condition that is assumed to be valid during steady-state flow.

However, X-ray imaging of porous media has revealed intermittent fluid flow pathways, even during macroscopically steady-state flow. These intermittent connections influence the propagation and trapping of the fluids, thus influencing the migration of a CO<sub>2</sub> or hydrogen plume in the subsurface. Changes in connectivity of the fluid phases can be correlated to the pressure drop across the core, although this correlation is non-trivial due to the non-local nature of fluctuations. Fluid flow has also been observed to be heavily influenced by small-scale heterogeneities, which are not considered in large-scale models.

While imaging has revealed important physics about fluid movement in the subsurface, large-scale models rely on averaged pressure values. What information are we losing by averaging the pressure data, and can we explore the impact of the small-scale heterogeneities using the pressure data? I show ways that we can explore the underlying dynamics using the pressure data, with the aim to include these findings in field-scale models.

## **Investigating the Upscaling of Subsurface Multiphase Fluid Flow Dynamics Using Pressure Data: From Pore-Scale Observations to Field-Scale Applications**

**Dr. Catherine Spurin**  
Stanford University, USA

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