## Research Statement

My long-term career goal is to become a scholar who makes long-lasting contributions to mechanics and computations of natural and man-made materials. Computational poromechanics is a field concerned with using computer simulations to predict how multi-phase materials with pores filled by one or more fluids react to external loading and changing environmental conditions. I use a combination of first principles and phenomenological observations to predict the evolution of internal microstructures. I also derive, implement, verify and validate mathematical frameworks for macroscopic poromechanics problems. An overarching theme of my research, is to develop new methods that accurately, and efficiently, capture porous media responses to fluid-infiltration under the influence of changing stress, deformation, temperature, chemical and flow regimes, in order to predict when, and how, porous media fail under extreme environmental conditions. Predictive computer simulations of porous materials are critical for numerous engineering applications, including those concerning nuclear waste disposal, hydraulic fracture, and near-surface explosions.

Conventional geomechanics modeling research often focus only on constitutive laws at a material point. These constitutive models (e.g. critical state plasticity, Gurson models) often evolve around phenomenological internal variables in Lie groups (e.g. damage, rotation, porosity). Yet, multi-physical coupling effects often originate from evolutions of internal microstructures (e.g. void collapse, grain rearrangement) and phase transitions (e.g. twinning, crystal growth, melting) that exhibit size effects. Understanding and numerically replicating these mechanisms requires more precise descriptors that are essentially non-Euclidean (e.g. connectivity graphs of granular assembles, pore network for fluid flow). Since joining Columbia University in January 2014, my research group has focused on developing new and practical ways to overcome these technical barriers. As of August 2020, I have published more than 55 peer reviewed articles in the top journals of my research field, been the recipient of 3 career or young investigator awards from NSF, AFOSR and ARO, raised over $20M in research funding and $5.6M in research expense as a PI, and helped three of my PhD students and two of my postdocs to secure tenure-track positions in well-known research institutions. The following paragraphs contain summary highlights and key results of my funded research projects since 2014, and a statement on my future research directions.

Multiphysics Modeling of Porous Media

Models of coupled physics present a unique challenge for numerical methods, in the sense that the prime field variables, such as displacement, pore pressure, or temperature, can evolve at different spatial and temporal scales. For instance, the injection of hot water into frozen soil can lead to growth of both the temperature and pressure plumes, but the growth rates of each can differ by several orders of magnitude [14]. However, many computer models used to investigate problems such as this often employ the same finite element discretization and basis functions for all variables in order to simplify model implementation, which can lead to spurious oscillating results. By considering the kernel space of the coupling operators and defining the product normed space of the scalar fields (e.g. temperature and pore pressure), I have identified the necessary condition to maintain stability of mixed finite element implementations, i.e. a two-fold inf-sup condition [8, 9, 18, 19]. I have also introduced a variety of numerical inf-sup tests for multiphysics problems to detect numerical stability issues, and proposed a corresponding stabilization procedure to eliminate the onset of spurious oscillations that plague many poromechanics problems under non-isothermal conditions [9].

The inf-sup stable finite element framework has provided the cornerstone for my group to develop new models that bring important insights into many challenging civil engineering problems, such as brittle-ductile transitions in geological formations [17, 21, 23, 24, 27, 34] phase-transition behaviors of porous

WaiChing Sun, Associate Professor, Civil Engineering and Engineering Mechanics,
500 West 120th Street 614 S.W. Mudd MC: 4709 New York, NY 10027
212-851-4371 Fax 212-854-6267 http://poromechanics.org Last update: 8/1/2020

media, including freezing and thawing of soils and concrete [18], and potential leakage due to crystallization-induced damage for CO2 geological disposal [25]. In the work of the frozen soil modeling, for example, my group's goal is to combine pre-melting theory with thermodynamic restrictions to formulate a multi-phase model that captures how ice crystallization and thawing impact the shear strength of the soil body. In a related ARO supported project, I am also working on analyzing the formation of ice lenses using a phase field formulation in porous media and studying how ice lenses might induce damage to civil infrastructures in cold regions. Meanwhile, I have also published a series of papers to explain fluid-driven plasticity, and damage fracture in fluid-infiltrating porous media [3, 5, 7, 15, 16, 20, 29, 33]. In particular, my work introduces a configurational (material) force framework that predicts different types of energy dissipation (e.g. damage, fracture, and plasticity) that affect the failure mode and constitutive responses (see Figure 1). To increase the efficiency of the simulations, I derived a new configurational force for the fluid-infiltrating porous media and used as the criterion for mesh adaption for Lie-group internal variables [4, 34, 37].

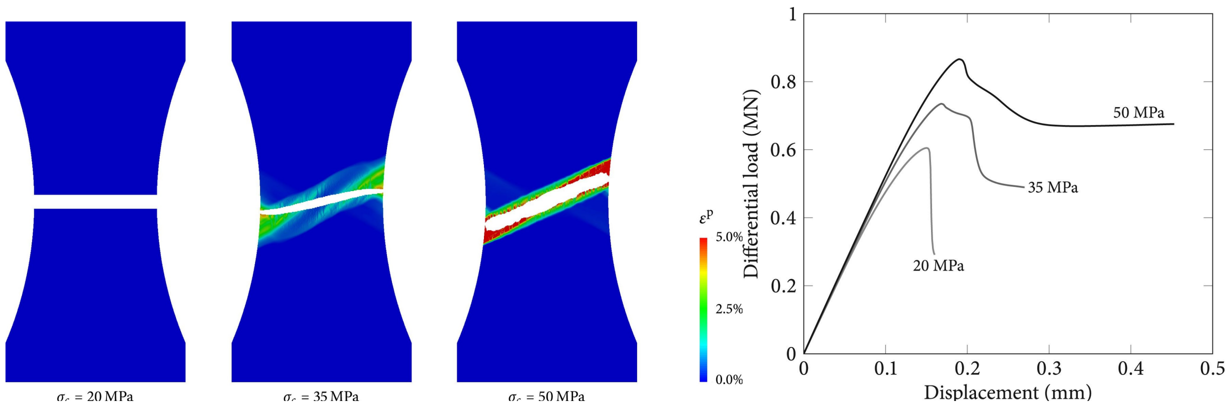


*Figure 1: A phase field/plasticity model for brittle-ductile transition. With different lateral tractions, the material may exhibit brittle fracture, quasi-brittle failures, shear localization and diffusive failures. Furthermore, our model is also able to predict the influence of anisotropy for failure mode – by changing the orientations of the anisotropic materials may also lead to change of failure modes from fracture/damage dominated to plastic dominated.*

Multiscale Modeling of Porous Media

A major challenge of many poromechanics problem is the proper upscaling and homogenization of fluid infiltrating porous media at appropriate spatial and time scales [1, 2, 6, 13, 26]. While previous multiscale frameworks often relied on the validity of the scale separation to enable sub-scale simulations as replacements of incremental constitutive updates, my group's research on computational homogenization has shown that using a discrete element model as a replacement for constitutive laws in the post-bifurcation regimes can lead to spurious mesh dependency. To resolve this issue, I introduced a new phase-field-based, adaptive Arlequin multiscale model for poromechanics [19]. While the classic Arlequin method uses the partition of unity on the energy functional to couple small- and large-scale models in a predefined handshake domain, our group's new model leverages the strength of a phase field model to keep track of the domain of interest (e.g. crack tip, shear band) and adaptively assign the appropriate enhanced constitutive laws for non-polar and micropolar continua. By overcoming the computational barrier due to coupling effects across length scales, the concurrent multiscale model provides a fresh insight into understanding the fundamental role of the pore-fluid in the formation of localized bands and cracks propagation in porous media with defects, flaws, and other small-scale geometrical features [8, 12, 13, 16, 22, 27, 28, 31, 36].

In the area of hierarchical multiscale frameworks, my unique contribution is the introduction of the micropolar DEM-FEM model, which is designed specifically to capture size effects in wetted granular materials using a high-order homogenization procedure, where the constitutive updates of higher order

WaiChing Sun, Associate Professor, Civil Engineering and Engineering Mechanics,
500 West 120th Street 614 S.W. Mudd MC: 4709 New York, NY 10027
212-851-4371 Fax 212-854-6267 http://poromechanics.org Last update: 8/1/2020

kinematics (displacement and micro-rotation) and kinetics (the non-symmetric force stress and couple stress) are obtained from representative elementary volumes. In another situation where faulting and fracture lead to evolving discontinuities, I introduced a modified Hill-Mandel lemma such that the interfacial solid and fluid responses (i.e., the effective cohesive zone law and anisotropic permeability) can be obtained [15, 22, 29].Furthermore, in the case where a porous medium is both fractured and fissured, I introduced a modified homogenization suitable for a multi-permeability system (e.g. fractured and fissured porous media). The multi-permeability homogenization problem is designed to overcome the limitations of the single-permeability model, where characterizing the hydraulic responses with one single effective permeability may lead to significant errors for leakage predictions, which is crucial for the nuclear waste disposal. In such cases, I proposed the idealization which decomposes the entire pore space into a finite number of interacting pore spaces (e.g. cracks, grain boundary, fissure and connecting pore in bulk volume). The effective permeability tensors of these interacting pore spaces are computational homogenized individually, and the mass exchanges among these spaces, are characterized through additional constitutive laws identified via inverse problems. Since the effective permeability tensors of these pore spaces are not necessarily co-axial and the eigenvalues can be of orders of magnitudes, this multi-permeability multiscale effective medium model can replicate complex hydro-mechanical responses that cannot be efficiently captured otherwise [6, 10 , 22, 29].

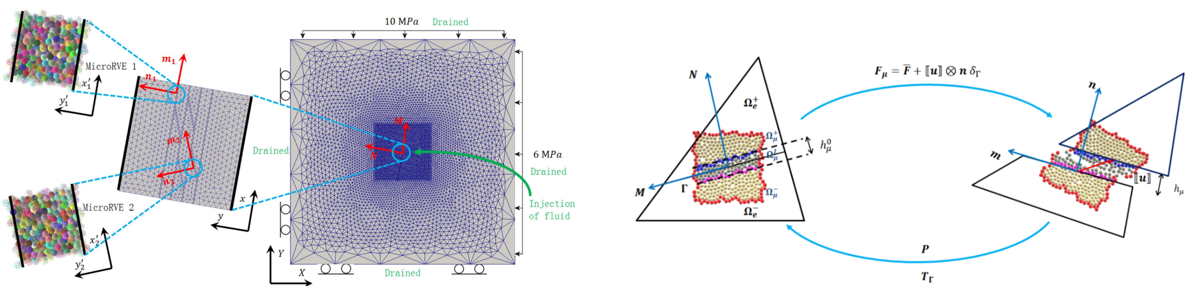


*Figure 2: Recursive homogenization enabled by machine learning (LEFT), the embedded strong discontinuity methods for multi-permeability problems (RIGHT).*

One of the major drawbacks of common hierarchical multiscale methods, is that running the RVE simulations, which are used to replace the macroscopic constitutive laws, can be computationally costly. Hence, in many cases, surrogate models are derived such that sub-scale hydro-mechanical models are merely used as tools to generate auxiliary data for material parameter identification [12, 16, 32]. However, deriving, implementing, verifying and validating surrogate models can also be very time-consuming. Hence, I introduced a new approach in which I employ concepts from graph theory to model the actions that a modeler takes to write a surrogate model. In particular, constitutive models are conceptualized as information flow in directed graphs that link a source (e.g. strain history) to the sink (e.g. stress) with physical quantities. The action a modeler takes to create, verify, validate, but also falsify or disprove a constitutive law (e.g. deciding the size and shape of yield function(s), hardening laws, identification of slip system, plastic flow directions) are then formulated in a decision tree. Using this approach, meta-modeling can be formulated as a Markov decision process with well-defined states, actions, rules, objective functions, and rewards, i.e. a game [30, 32]. By using deep neural nets to estimate values of combinatorial decisions, the computer agent I designed is able to efficiently self-improve the constitutive model it generated through self-playing, while also learning the essence of strategies used previously by both human and AI modelers to improve its own modeling skills, as shown in Figure 3 [30]. This idea is in sharp contrast with previously reported black-box neural network constitutive laws, in the sense that the predictions of stress are built based upon the principle of combinatorial generalization, i.e., the predictions of complex behaviors using easier and simpler predictions as building blocks. **While tensor calculus and differential geometry have enabled revolutions in engineering mechanics for decades, the potential of discrete mathematics, such as graph theory and combinatorics, for applications in engineering mechanics has not yet fully**

**unleashed. My work in this area represents a beginning of this, potentially powerful, new research trend.**

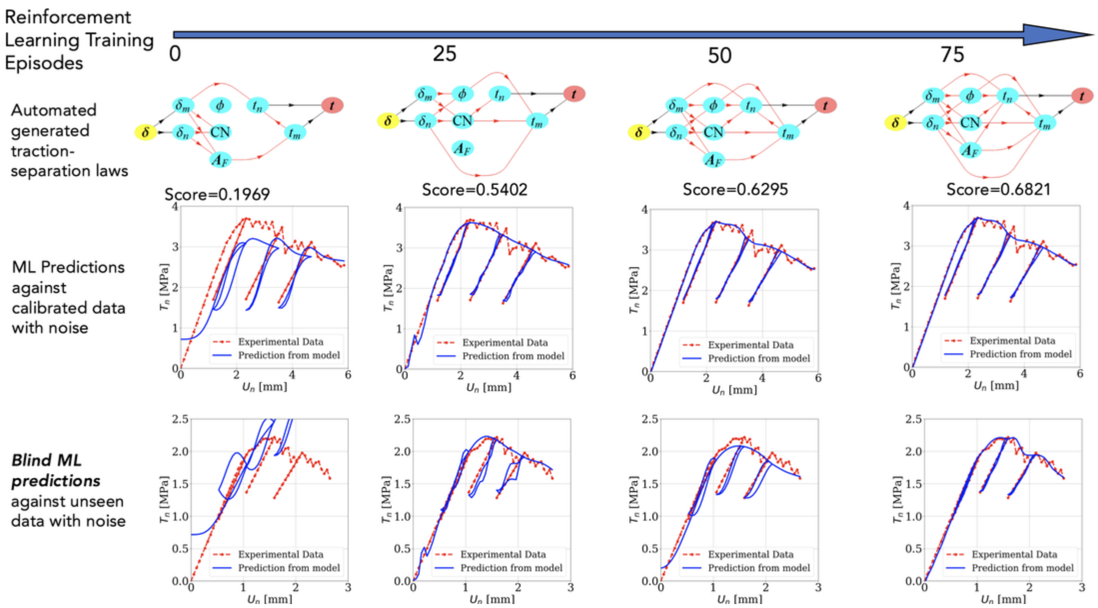


*Figure 3: The progress of the AI made while learning to write traction-separation law via reinforcement learning method. The performance of blind predictions and calibrations are similar.*

<u>Future Vision</u>

Numerical methods, such as finite element methods, have revolutionized multiple engineering disciplines during the past 40 years. This success is largely due to the coordinated efforts of countless engineers, mathematicians and computer scientists. Their contributions have made it possible to convert physical phenomena described by partial differential equations into systems of algebraic equations, where a computer may perform repetitive arithmetic operations in order to deliver important insight and predictions. While this computational approach is nearing maturity, many of the recent engineering challenges faced by humanity have become so complex that this traditional methodology is no longer viable due to excessive computational costs (e.g. during direct simulations of localized turbulence), large sets of unknown parameters (e.g. during subsurface and reservoir modeling), and lack of complete knowledge (e.g. during simulations of explosive or biological process).

My career goal is to make a real difference in the field of computational mechanics, which does not only limit to advancing computational approaches, conducting repetitive arithmetic operations and solving large matrix systems (e.g. FEM, FVM), but also explore new path where we may leverage computers for inductive reasoning, cognitive computing, combinatorial optimizations and decision making.  I envision a new wave of computational mechanics approaches and discoveries that will make use of the increasingly large and diversified data sets generated from new types of simulations (e.g. MD simulations), experiments (micro-CT imaging, digital image correlation) and field data across scales (e.g. seismic tomography), as well as new forms of data representations, such as graphs and manifolds (see figure below).

WaiChing Sun, Associate Professor, Civil Engineering and Engineering Mechanics,
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212-851-4371    Fax 212-854-6267    http://poromechanics.org Last update: 8/1/2020

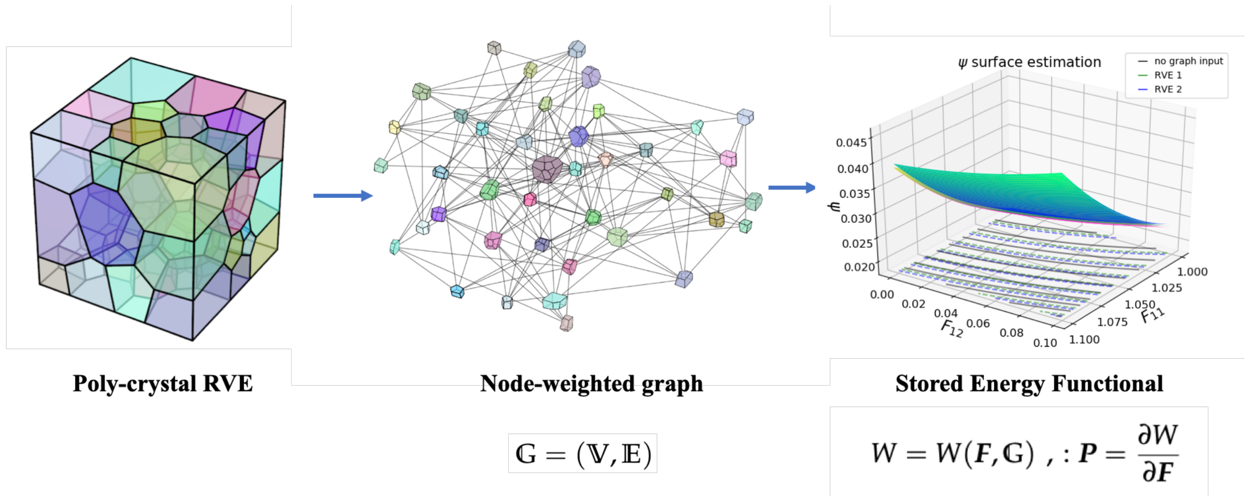


*Figure 4: Incorporation of non-Euclidean microstructural data of polycrystal contact graph to predict stored energy functional for representative elementary volume done by Sun Group (cf. Vlassis, Ma and Sun [38], in preparation (manuscript available upon request).*

My research group has carefully planned and uniquely positioned itself to tackle next-generation challenges for computational mechanics and poromechanics problems, as evidenced by the depth and breadth of the knowledge displayed in our publications and presentations. My vision is to become a major force in creating a new school of thought in which true knowledge can be gained from new innovative ways to create, harvest, analyze and incorporate new types of data into new modeling frameworks. Through developing new approaches to incorporate elements traditionally underutilized in computational mechanics (e.g. game, graph and group theories, machine learning, and non-Euclidean descriptors), I am confident that my students and I can make a positive, impactful difference for years to come.

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