Some applications of graph theory in data-driven multiscale mechanics

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Abstract: In this talk, we will share our experience in using undirected and directed graphs to solve computational solid mechanics problems with a variety of deep neural networks. In the first half of the talk, we will focus on the usage of undirected weighted graphs that represent the microstructures. We will demonstrate 1) how to effectively represent microstructures such as polycrystals, granular assemblies and composites as node-weighted graphs, a network of nodes with assigned attributes connected by edges, 2) how to create low-dimensional topological descriptors via graph convolution neural network that exhibits spatial and rotational invariance properties and 3) how these topological descriptors can be used to enhance the accuracy and robustness of the forward predictions and generalize the surrogate constitutive models generated via semi-supervised learning. In the second half of the talk, we will examine the application of directed multi-graphs that represent causality/relational knowledge of material laws. By idealizing the process of modeling constitutive laws as a multi-player game, we will examine 4) how the process of writing, validating and falsifying a constitutive law can be formulated as a Markov decision process, and 5) how a model-free deep reinforcement learning paradigm can introduce artificial intelligence (AI) modelers and experimentalists that learn to create hand-crafted-like constitutive models through competitions and repeated trial and errors. Examples will be provided to illustrate how these self-interacting, self-improving AI agents discover new hidden hierarchical structures of mechanics knowledge, spot the weakness of existing models and create new approaches to incorporate non-Euclidean data traditionally excluded in constitutive laws to make predictions more accurate and robust.

Bio: Dr. Sun is an associate professor in the department of civil engineering and engineering mechanics department at Columbia University. He obtained his B.S. from UC Davis (2005); M.S. in civil engineering (geomechanics) from Stanford (2007); M.A. (Civil Engineering) from Princeton (2008); and Ph.D. in theoretical and applied mechanics from Northwestern (2011). From 2011 to 2014, he worked at the Mechanics of Materials department at Sandia (Livermore), first as a postdoc, then senior MTS. Sun's research focuses on theoretical, computational and data-driven mechanics for porous media and geological materials. He is the recipients of the IACM John Argyris Award, NSF CAREER Award (2019), the EMI Leonardo da Vinci Award (2018), the Zienkiewicz Numerical Methods Engineering Prize (2017), AFOSR Young Investigator Program Award (2017), Dresden Fellowship (2016), ARO Young Investigator Program Award (2015), and the Caterpillar Best Paper Prize (2014).