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CIVIL AND ENVIRONMENTAL ENGINEERING DEPARTMENT SEMINAR & COMPUTATIONAL SCIENCE COLLOQUIUM

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Time: 4:00pm – 5:00pm EST

Location: Nord, Room 356

Zoom link: here

Machine learning enabled inverse and forward problems for polymer-bonded energetic materials

Abstract: Energetic materials are solids that can release significant energy upon stimuli. They can constitute propellants, explosives, fuels, and pyrotechnics used in aerospace, mining, and defense industries. To reduce the sensitivity of the materials and enhance safety, energy materials are often manufactured as two-phase composites, with a softer binder as the host matrix that holds the explosive crystals, such as HMX (High-melting Explosive) in place. This design, referred to as Polymer-bonded explosives (PBX), enables the molding, shaping, and uniformity of the materials, leading to improved predictable performance. Nevertheless, the characterization of the energy localization often requires a material model capable of handling extremely large deformation of phase transformation. This talk reports recent progress on forward and inverse problems for modeling the HMX and PBX enabled by machine learning. For the forward modeling problems, we attempt to create mathematical models of HMX expressed in symbolic form. To avoid the difficulty of training the Kolmogorov-Arnold network, we introduce an alternative technique to learn neural additive basis in projected feature space to control the expressivity-speed trade-off. For the inverse problem, we introduce a generative AI that enables us to create highly realistic PBX microstructures as well as the granular microstructures of crystals by separately handling the generation of grain geometry and topology of the granular structures via conditional latent diffusion and graph recurrent neural network. Benchmark numerical examples of material point simulations for shock loading in b-HMX are performed to assess the practicality of using the discovered machine learning models for high-fidelity simulations.

Bio: Dr. Sun has been an associate professor at Columbia University since 2020. He obtained his BS from UC Davis (2005), MS in civil engineering (geomechanics) from Stanford (2007), MA (Civil Engineering) from Princeton (2008), and Ph.D. in theoretical and applied mechanics from Northwestern (2011). Sun's research focuses on theoretical, computational, and data-driven mechanics for porous and energetic materials. He is the recipient of a few awards, including the Walter Huber Civil Engineering Research Prize (2023), the IACM John Argyris Award (2020), the EMI Leonardo da Vinci Award (2018), the Zienkiewicz Numerical Methods Engineering Prize (2017), and early career awards from NSF, AFOSR, and ARO.