A non-cooperative game for creating, validating and falsifying predictive polycrystal and granular materials with non-Euclidean internal variables

ABSTRACT: Many machine learning models used in computational mechanics employ supervised and unsupervised learning techniques to make predictions with little or no interpretability. This black-box approach makes it difficult to assess and manage risks for engineering applications. In this talk, we present a new framework in which multiple AIs assigned to different roles (experimentalist, modeler) are participating and interacting in the scientific discovery process where plausible knowledge of constitutive mechanisms is represented by directed graphs and directed multigraphs. As such, both human and machine learning process are re-cast as the procedure of finding a directed graph that links the input and output data with the optimal set of edges that maximize the reward (the objective function that measures the prediction qualities) while fulfilling mechanics principles (e.g. convexity, material frame indifference, thermodynamic laws, symmetry and invariance).

Based on the performance of the modelers, two experimentalist AIs are then design experiments, one rewarded by actions that enhance the blind prediction quality, another one rewarded by actions that expose the weakness of the models. Through competitions, the three modelers repetitively practice and improve their skills of completing their corresponding tasks via the Edisonian scientific approach without consuming human time. We demonstrate that the proposed algorithm is able to discover new hidden hierarchical structures of mechanics knowledge, rediscover well-known mechanics knowledge without any human intervention, spot the weakness of existing models and create new approach to incorporate non-Euclidean data traditionally excluded in constitutive laws to make predictions more accurate and robust.

BIOGRAPHICAL SKETCH: Professor Sun obtained his B.S. from UC Davis (2001); M.S. in civil engineering (geomechanics) from Stanford (2007); M.A. degree 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 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), among others.