Fall 2024 Joint Colloquium Materials Department & Materials Research Laboratory

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Data-driven constitutive relations: Multiscale modeling and experimental inference

The talk addresses the challenge of computing complex phenomena at the scale of applications. In addition to the universal laws (balance of mass, momenta etc.), these phenomena require a constitutive (closure) relation that describes the behavior of the medium at the scale of applications. Such behavior can be nonlinear, nonlocal, anisotropic, history dependent etc., and thus impossible to characterize to the desired level by the classical approach of postulating a parametrized relation and fitting the parameters to selected experiments. The talk describes two broad approaches to using data-driven methods to overcome this challenge. The first approach is multiscale modeling where one recognizes that the effective behavior at the scale of applications is determined by physics at multiple length and time scales: electronic, atomistic, domains, defects etc. The data-driven constitutive relation is obtained as a neural approximation is trained using data generated by repeated solution of the small scale problem. The second approach seeks to infer it from automated experiments that are not amenable to easy inversion. The talk will describe these approaches, challenges they raise and strategies to overcome them. The ideas will be illustrated with applications from materials science and geology.

Bio

Kaushik Bhattacharya is Howell N. Tyson, Sr., Professor of Mechanics and Professor of Materials Science as well as the Vice-Provost at the California Institute of Technology. He received his B.Tech degree from the Indian Institute of Technology, Madras, India in 1986, his Ph.D from the University of Minnesota in 1991 and his post-doctoral training at the Courant Institute for Mathematical Sciences during 1991-1993. He joined Caltech in 1993. He has received the von Kármán Medal of the Society of Industrial and Applied Mathematics (2020), Distinguished Alumni Award of the Indian Institute of Technology, Madras (2019), the Outstanding Achievement Award of the University of Minnesota (2018), the Warner T. Koiter Medal of the American Society of Mechanical Engineering (2015) and the Graduate Student Council Teaching and Mentoring Award at Caltech (2013).