Ensuring Reliability, Reproducibility and Transferability in Atomistic Simulations: The Knowledgebase of Interatomic Models (openKIM.org)

<u>Ellad B. Tadmor¹</u>

¹ Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, MN

Atomistic and multiscale simulations in materials science play a key role in realistic scientific and industrial applications. These approaches frequently use empirical interatomic models (potentials or force fields) to represent the response of the material. Modern models are fitted to reproduce electronic structure and/or experimental results for a dataset of representative atomic configurations. However, no standardized approach currently exists for quantifying the range of applicability of an interatomic model or estimating the accuracy of its predictions. This makes it difficult or even impossible to select an appropriate model for a given application. In addition, a lack of standardization in programming interfaces for models and the lack of a systematic infrastructure for archiving them makes it difficult to use interatomic models for new applications and to reproduce published results. This talk will describe a current NSF-CDI funded effort to create an open source online tool that addresses these limitations: the Open Knowledgebase of Interatomic Models (http://openKIM.org). OpenKIM will allow users to compare model predictions with reference data, to generate new predictions by uploading simulation test codes, and to download models conforming to application programming interface (API) standards which are being developed in collaboration with atomistic simulation community. In this talk I will give an overview of the KIM project and describe recent developments related to the KIM API.

The molecular simulation community is invited to participate in the KIM project and to contribute to the standardization efforts under way. Register at the KIM website.