

EXPERT PROGRAMMER NEEDED FOR THE DEVELOPMENT OF KIM: THE KNOWLEDGBASE OF INTERATOMIC MODELS

UNIVERSITY OF MINNESOTA, TWIN CITIES

Atomistic simulations in materials science and nanotechnology play a key role in many scientific and industrial applications. However, the predictive capability of these approaches hinges on the accuracy of the mathematical models used to describe atomic interactions. Modern models are optimized (fit) to reproduce quantum mechanical values for the forces and energies of representative atomic configurations deemed important for the problem of interest. However, no standardized approach currently exists for quantifying the range of applicability of an interatomic model or estimating the accuracy of its predictions. The result is that the field of atomistic modeling struggles with the unknown and uncontrolled capacity of its models to predict phenomena outside the fitting database, keeping this field from fully realizing its scientific and technological potential. This problem will be addressed by creating the Knowledgebase of Interatomic Models (KIM); an interactive, self-extending, database of interatomic models, self-contained simulation codes that test the predictions of these models, and reference data. The knowledgebase will be driven by a *Processing Pipeline* that is the analytical workhorse of the KIM system. The processing pipeline will be responsible for automatically matching tests with compatible models and generating the corresponding prediction to be stored in the KIM system. This online resource will allow users to rapidly compare model predictions with reference data, to generate new predictions by uploading their own tests, and to download models conforming to community standards developed as part of this project.

The KIM project is funded through the NSF Cyber-enabled Discovery and Innovation (CDI) program and is a broad collaborative effort led by Professors Ellad B. Tadmor (U. Minnesota), Ryan S. Elliott (U. Minnesota), James P. Sethna (Cornell U.), Ronald E. Miller (Carleton U., Canada), and Dr. Chandler A. Becker (NIST). The project also includes interactions with Pennsylvania State U.; U. of Edinburgh (UK); the Technical University of Denmark; Los Alamos, Sandia, Lawrence Livermore and Argonne National Laboratories; NASA Ames; and Intel Corp.

We are seeking a postdoctoral fellow to work on the development of the processing pipeline in the KIM infrastructure. The creation of this key component of the KIM system will require exceptional programming skills at both the system and application levels. Experience with the development, packaging, and support of software systems written in multiple scientific programming languages is required. Experience in the development of standards to define Application Program Interfaces (APIs) is beneficial but not required. In addition, some experience in molecular simulation in materials science, chemistry, physics, or biology is desirable. The position is available immediately. Applications will be considered until the position is filled.

Interested individuals are encouraged to contact Professor Tadmor (tadmor@aem.umn.edu). However, all applicants must also apply online in order to be considered part of the official applicant pool. To apply online, please visit <https://employment.umn.edu> and search for Requisition Number 162470.

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