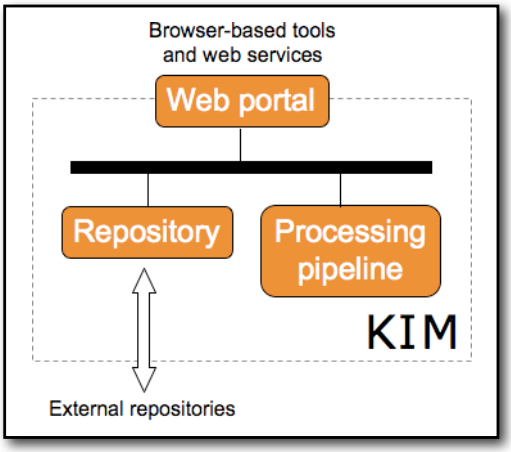
Knowledgebase of Interatomic Models

Atomistic simulations using empirical interatomic potentials are playing an increasingly important role in realistic scientific and industrial applications in many areas including advanced materials design, drug design, renewable energy, and nanotechnology. The predictive capability of these approaches hinges on the accuracy of the interatomic model used to describe atomic interactions. Modern potentials are optimized to reproduce experimental values and electronic structure estimates for the forces and energies of representative atomic configurations deemed important for the problem of interest. However, no standardized approach exists yet for comparing the accuracy of interatomic models, or estimating the likely accuracy of a given prediction. In addition, a lack of standardization in the programming interface of interatomic potentials and the lack of a systematic infrastructure for archiving them makes it difficult to use potentials for new applications and to reproduce published results. *These limitations are preventing the field of atomistic modeling from realizing its true scientific and technological potential.*

The **Knowledgebase of Interatomic Models** (KIM) is a four-year NSF Cyber-Enabled Discovery and Innovation (CDI) program which seeks to address the limitations described above in two stages:



I. Development of an online infrastructure consisting of a web portal, repository and processing pipeline. The **repository** will contain interatomic models, self-contained simulation codes that test the predictions of these models, and reference data obtained from first principles calculations and experiments. Users will be able to freely upload and download models and tests and to search the content of the repository through the **web portal.** When a new model is uploaded to the repository, the **processing pipeline** will automatically mate it with all tests already stored in the repository generating new predictions which will be stored in the repository. Similarly new tests will be mated with all models in the repository generating new predictions. In this way a great deal of information on the accuracy of interatomic models will be gathered over time. Development of the infrastructure described above will also involve the establishment, in collaboration with NIST and the research community, of terminology dictionaries, testing/benchmarking procedures, and application programming interface (API) **standards** for atomistic simulations.

II. Development of a framework for evaluating the transferability and precision of interatomic models. **Transferability** refers to the ability of a model to provide accurate predictions for properties that it was not fitted to reproduce. **Precision** refers to the error bars associated with the prediction of a particular type of model for a given property. Rigorous measures for transferability and precision will be developed based on the information stored in the KIM repository. The end goal is to develop **automatic guidelines** for the selection of appropriate models for a given scientific or technological application.

The KIM project is led by Prof. Ellad B. Tadmor (University of Minnesota), Prof. Ryan S. Elliott (University of Minnesota) and Prof. James P. Sethna (Cornell University) along with an international team of experts in model and test development. More information on KIM is available at

http://OpenKIM.org