Abstract Submitted
for the 4CS20 Meeting of
The American Physical Society

Bayesian Approach to Uncertainty Quantification of Interatomic Models in OpenKIM Database KINAMO WILLIAMS, YONATAN KURNIAWAN, CODY PETRIE, MARK TRANSTRUM, Brigham Young University — Interatomic models (IMs) are used in molecular modeling to predict material properties of interest. The development of a single IM can take anywhere from several months to years and relies on expert intuition, and yet these potentials are usually only valid for a particular application of interest. Extending existing IMs to new applications is an active area of research. Quantifying the uncertainty of an IM can tell us how much we can trust the predictions it makes. I will discuss two methods for analyzing uncertainty: Fisher Information Matrix, FIM, and Markov Chain Monte Carlo, MCMC. Using Monte Carlo methods, I sample from the posterior distribution of the parameters when trained on data. I demonstrate this method on Lennard-Jones and Morse potentials fit to triclinic crystal configurations from the OpenKIM database. In particular, IMs are often sloppy, i.e., have likelihood surfaces with long, narrow canyons and broad, flat plateaus. I will be comparing the benefits and drawbacks of the two methods.

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Date submitted: 25 Sep 2020 Electronic form version 1.4