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Improved Uncertainty Quantification of Interatomic Models using Sloppy Model Analysis[1] DYLAN BAILEY, MARK TRANSTRUM, YONATAN KURNIAWAN, CODY PETRIE, Brigham Young University — Interatomic models (IMs) are useful in predicting material properties of interest. However, The development of a single IM can take months to years and relies on expert intuition, and is then normally only valid for a singular application. Extending existing IMs to new applications is an active area of research. Uncertainty quantification (UQ) can help to inform us how well an IM predicts in a new regime to which it was not trained. The predictions of many IMs are insensitive to large, coordinated changes in many of their parameters, a phenomenon known as sloppiness. Our previous work has shown that sloppiness poses challenges both for the implementation and interpretation of traditional UQ analysis. To address these issues we use the Manifold Boundary Approximation Method to systematically remove sloppy parameters and perform UQ on the reduced model. I report on our progress on a model of MoS_2 monolayer using the Stillinger-Weber potential. We find that in comparison to the original the confidence region of the reduced model becomes less sensitive to the choice of confidence level.

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