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Improving reproducibility and automation in atomistic simulations

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ABSTRACT

Atomistic simulations, such as molecular dynamics, are becoming more widely used in a variety of areas, including industrial research and development. However, there are still barriers to the broad use of these methods, both on their own and as part of an Integrated Computational Materials Engineering or multiscale/hierarchical approach. One of the major challenges relates to reproducibility of interatomic potentials and simulations. In this discussion, we will discuss our efforts in the area of interatomic potential evaluations and simulation automation. We will also discuss how this fits into the Materials Genome Initiative and highlight major issues identified in the annual NIST "Atomistic Simulations for Industrial Needs" workshops that are designed to facilitate interactions between industrial and academic researchers.