Addressing Industrial Needs for Atomistic Simulations through OpenKIM

Ellad B. Tadmor[1]

[1] Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, MN 55455, USA, tadmor@umn.edu, https://dept.aem.umn.edu/~tadmor/

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Atomistic and multiscale simulations using empirical interatomic potentials (IPs) promise to address real-world industrial needs by reaching technologically-relevant length and time scales. This is particularly true with recent developments of high-accuracy machine learning IPs. However, to be trusted in industry, atomistic simulations must be reliable both in their predictive ability and reproducibility. These issues are addressed by the Open Knowledgebase of Interatomic Models project (https://openkim.org) [1-2]. OpenKIM curates IPs with full provenance control, issues them DOIs so that they can be cited in publications and retrieved for reproducibility needs, ensures their coding correctness using "Verification Checks," and tests them exhaustively using "KIM Tests" that compute a host of material properties. OpenKIM is integrated into major simulation packages (including ASE, DL_POLY, GULP, LAMMPS, and Quasicontinuum) allowing users to seamlessly use OpenKIM IPs and query their predictions (stored on openkim.org) in simulation pre- and post-processing steps.

REFERENCES

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