Indirect learning of interatomic potential for accelerated materials simulations

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Machine learning (ML) interatomic potentials are emerging tools for materials simulations but require a trade-off between accuracy and speed. We show one ML potential can be used to train another by using an existing, accurate, but more computationally expensive GAP model to generate reference data (labels and locations) for faster “indirectly-learned” MTP potentials. Extensive datasets are easily generated without quantum-mechanical computations at the indirect learning stage. The additional data significantly improve the predictions of fast potentials with less flexible functional forms.

We apply the technique to disordered silicon, including million-atom simulations of vitrification and polycrystalline grain formation. Compared to indirectly-learned potentials, fitting directly to DFT-labelled data leads to unphysical predictions for large systems not apparent in smaller simulations ($\leq 10^4$ atoms). This emphasises the importance of validating ML potentials chemically, not only via numerical error measures. Our work provides conceptual insight into learning interatomic potentials and enables accelerated simulations of nanostructured materials.