Simple machine-learned potentials enable accurate billion-atom simulations

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Machine learning (ML) has revolutionised the field of atomistic simulations of materials by providing increasingly accurate and generalisable interatomic potentials. ML potentials are now being routinely and rapidly developed both for highly accurate simulations of targeted materials and for somewhat less accurate but broad screening of materials from arbitrary elements of the periodic table. I will present and focus on a pragmatic approach to ML potentials we developed and used extensively in the last five years, aiming for truly practical and useful simulations of various materials. Specifically, I will show highlights from the development and use of tabulated Gaussian approximation potentials (tabGAP https://gitlab.com/jezper/tabgap) for metals, alloys, and semiconductors. The tabGAP method is by design a simple and computationally extremely efficient ML potential, enabling large-scale molecular dynamics simulations with GPU acceleration and competitive accuracy. Highlights from recent applications include billion-atom radiation damage simulations of fusion reactor materials, understanding ordering and segregation in high-entropy alloys, prediction and experimental verification of novel radiation-resistant alloys, and mapping the phase diagram of silicon carbide.