DPA4: Efficient Equivariant Interatomic Potentials with Native Short-Range Physics

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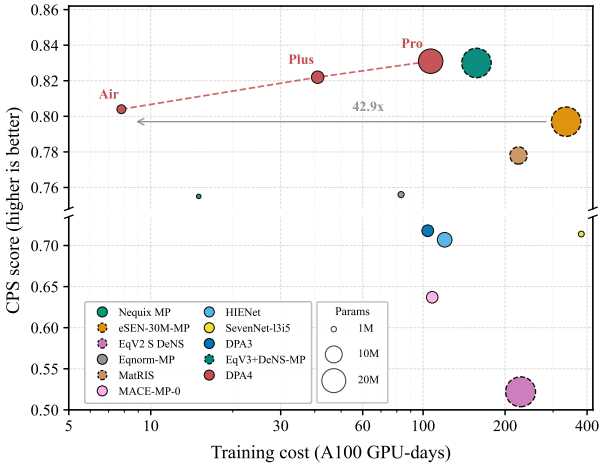

Fig. 1: Matbench Discovery CPS versus training cost. DPA4 variants form a new accuracy–efficiency frontier under conservative force training.

1. Abstract

Machine-learning interatomic potentials (MLIPs) are becoming a practical route to AI-accelerated atomistic simulation, but broad deployment still requires accuracy, training efficiency, and physical robustness beyond ordinary equilibrium data. We introduce DPA4, also referred to as SeZM for Smooth equivariant Zone-bridging Model, an equivariant MLIP architecture built for this joint objective. DPA4 combines edge-local SO(2) message passing, native analytical short-range coupling, and `torch.compile`-compatible conservative-force training. On Matbench Discovery, DPA4-Pro reaches a state-of-the-art CPS of 0.831, while DPA4-Air exceeds eSEN-30M-MP with 10.9× fewer parameters and 7.8 rather than 335 A100 GPU-days. DPA4-Plus also achieves the best aggregate accuracy on SPICE-MACE-OFF among the compared models, reducing energy and force LWAMAEs by 36% and 31% relative to the 6.5M-parameter eSEN baseline. These results place DPA4 on a new accuracy–cost frontier while preserving conservative forces and smooth short-range behaviour.

2. Approach

DPA4 keeps directional information through node features in $V_{\leq L} \otimes \mathbb{R}^C$, but performs each edge update in a bond-aligned local frame. In this frame the residual symmetry is SO(2), allowing multi-focus convolutions and radial degree coupling without the full cost of SO(3) Clebsch–Gordan tensor products used by many high-order equivariant models [1, 2]. Envelope-gated attention uses invariant scalar weights that vanish smoothly at the cutoff, while an Environment Initial Embedding injects a rotation-invariant local-environment prior into the scalar backbone.

Short-range physics is part of the same scalar energy, not a post-hoc force correction. DPA4 adds an analytical Ziegler–Biersack–Littmark branch [3] to the neural energy and uses Native ZBL Zone Bridging to freeze the direct learned pair channel in the inner zone. Forces remain conservative because both neural and analytical terms are differentiated from one total energy. For training, DPA4 traces the energy-to-force derivative path into a graph compatible with `torch.compile` [4], enabling compiled conservative-force optimisation rather than a direct-force surrogate.

3. Validation

On Matbench Discovery [5], DPA4-Pro reaches a CPS of 0.831 with 20.91M parameters, slightly above the DeNS-assisted EquiformerV3 baseline at 0.830 [6, 2]. The smaller DPA4-Air reaches a CPS of 0.804 with 2.76M parameters, exceeding eSEN-30M-MP at 0.797 while using 10.9× fewer parameters and 7.8 rather than 335 A100 GPU-days [7]. On SPICE-MACE-OFF [8], DPA4-Plus reduces aggregate LWAMAE to 0.09 meV/atom for energies and 1.77 meV/Å for forces, 36% and 31% lower than the 6.5M-parameter eSEN baseline. Controlled systems ablations show that compiled bf16 training gives a 3.1× wall-clock speedup and reduces peak memory to about 40% of the FP32 eager baseline, with MAE changes below 3%.

DPA4 also improves physical behaviour in close-contact geometries. In a C–Si dimer scan, a DPA3 model with pair-ZBL coupling develops a sharp attractive force excursion near the switching region, whereas DPA4 follows the analytical ZBL force in the inner region and joins smoothly to the learned force

outside it. This result is important for irradiation, collision, and extreme-condition simulations, where ordinary DFT training data sparsely samples the repulsive wall.

4. Significance

The present work evaluates DPA4 as a single-task, per-dataset architecture rather than as a fully pretrained large atomistic model. Even in this setting, DPA4 shows that equivariant representation design, native physical priors, and compiler-aware ML systems can be co-designed to make accurate atomistic simulation faster to train and more robust to demanding molecular-dynamics regimes.

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