

Deep Potential Molecular Dynamics: a scalable model with the accuracy of quantum mechanics - A summary [ZHW⁺18]

└ Motivation

Motivation

► Trade-off: Accuracy vs. Efficiency

AIMD	EFF
small space- and timescales high accuracy	larger scales approximate in nature

- ML so far: Auxiliary quantities to preserve symmetries
 → Assign local reference frames to each atom and leverage extensive character of potential energy

$$E = \sum_i E_i$$

AIMD: First principles, quantum mechanics, DFT. Computational costs: 100 ps, 100s of atoms, empirical FF: based on approximations and experimental data. Data: Atomic configurations and corresponding potential energies, learn this functional dependence. System invariant to permutations, translations, rotations, so model needs too. Auxiliary quantities: Symmetry functions (describe local geometric environment, problem: ad hoc), coulomb matrix entries: distinct inverse distances between all atoms, problem: extended periodic systems

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Convection: transfer of heat by the movement of the fluid

Natural: motion generated by density differences, not by external sources

Applications: Nuclear reactor design, cooling of electronic equipment, heating and ventilation in the design of buildings

Goal: Identify different flow patterns and investigate which method is suited better

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└ The model

First step

► Local coordinate frame for each atom with atom at center

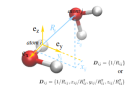


Figure: Geometry of the local coordinate frames [ZHW⁺18]

Embedded Atom Concept: Energy sum of functions of separation of atom and neighbors. Reciprocal distances: Reduce weight of distant neighbors-
Figure: Water, e_x O-H bond, e_z perpendicular to plane of water molecule
other option for D_{ij} angular information as well $\times ij$ cartesian coordinates of R_{ij}

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└ The model

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- Local coordinate frame for each atom with atom at center

- $D_i = [D_{ij}]_i$ input for NN, where j covers all neighbors within cutoff radius R_c , sorted by chemical species, inverse distances

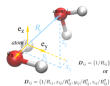


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- Local coordinate frame for each atom with atom at center
- $D_i = [D_{ij}]_i$ input for NN, where j covers all neighbors within cutoff radius R_c , sorted by chemical species, inverse distances
- Theoretical foundation: Embedded Atom Concept

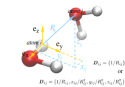


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└ The model

Second step

► Fully connected NN consisting of 5 hidden layers with 240, 120, 60, 30, 10 units resp.



Figure: Visualisation of the NN [ZHW⁺18]

NN: fixed input size, append 0s potentially

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- Adam optimizer



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Loss function

$$\mathcal{L}(\rho_e, \rho_f, \rho_\epsilon) = \rho_e \Delta e^2 + \frac{\rho_f}{3N} \sum_i |\Delta \vec{F}_i|^2 + \frac{\rho_\epsilon}{9} |\Delta \Xi|^2$$

Δ : Difference between prediction and training data, N : number of atoms, e : energy per atom, \vec{F}_i : Force on atom i , Ξ : Virial tensor $\Xi = -\frac{1}{2} \sum_i \vec{R}_i \otimes \vec{F}_i$

Virial: comparison of kinetic, potential energy

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- Key difference: Inclusion of forces and virial tensor for regularisation
- Parameters ρ, ρ_L steadily increased during training, p_T steadily decreased

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Advantages:

GDML: gradient domain machine learning not chemically accurate, since still approximative, but way better than empirical FFs
Coulomb: electrostatic forces over distances outside cutoff radius

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- Long-range coulomb interactions neglected, see [YMA⁺21]

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