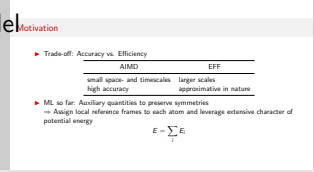
Deep Potential Molecular Dynamics: a scalable model with the accuracy of quantum mechanics - A summary [ZHW+18]


Motivation

- Trade-off: Accuracy vs. Efficiency

AIMD	EFF
small space- and timescales	larger scales
high accuracy	approximative 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, empirica FF: based on approximations and experimental dataData: Atomic configurations and corresponding potential energies, learn this functional dependencereal 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: extened periodic systems

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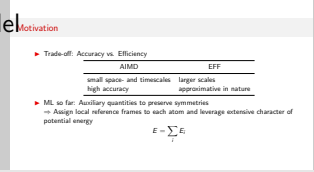
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Convection: transfer of heat by the movement of the fluid
Natural: motion generated by density differences, not by external sources
Applications: Nuclear reactor design, cooling of electronic eqiupment, heating and ventialtion in the design of buildings
Goal: Identify different flow patterns and investigate which method is suited better

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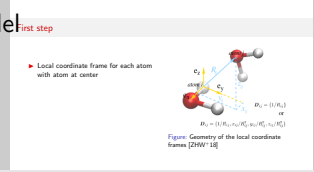

Embedded Atom Concept: Energy sum of functions of seperation of atom and neighbors. Reciprocal distances: Reduce weight of distant neighbors- Figure: Water, e x O-H bond, e z perpendicular to plane of water molecule other option for D i j angular information as well x ij cartesian coordinates of R i j

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The model

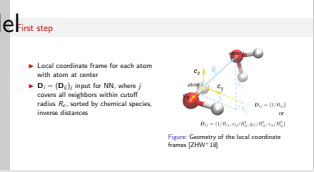

Figure: Geometry of the local coordinate frames [ZHW+18]

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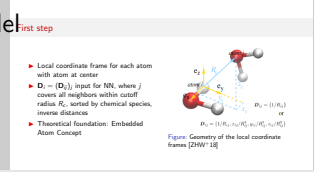

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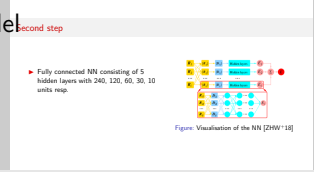

Figure: Visualisation of the NN [ZHW+18]

NN: fixed input size, append 0s potentially

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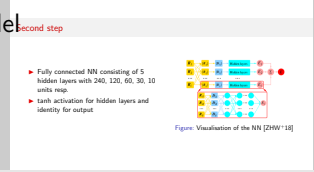
└The model



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The model

second step

- Fully connected NN consisting of 5 hidden layers with 240, 120, 60, 30, 10 units resp.
- tanh activation for hidden layers and identity for output
- Adam optimizer

Figure: Visualisation of the NN [ZHW+18]

NN: fixed input size, append 0s potentially

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Loss function

$$L(p_\epsilon, p_f, p_\xi) = p_\epsilon \Delta\epsilon^2 + \frac{p_f}{3N} \sum_i |\Delta \vec{F}_i|^2 + \frac{p_\xi}{9} |\Delta \Xi|^2$$

Δ : Difference between prediction and training data, N : number of atoms, ϵ : 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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└The model

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- Key difference: Inclusion of forces and virial tensor for regularisation
- Parameters p_ϵ, p_ξ steadily increased during training, p_f steadily decreased

Virial: comparison of kinetic, potential energy

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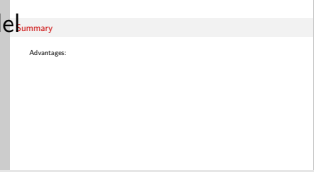

GDML: gradient domain machine learningnot chemically accurate, since still approximative, but way better than empirical FFsCoulomb: electrostatic forces over distances outside curoff radius

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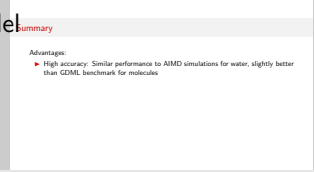

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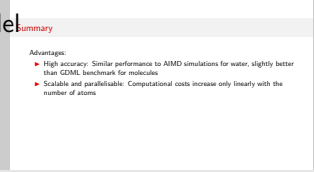

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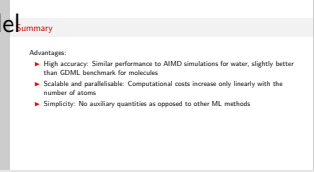

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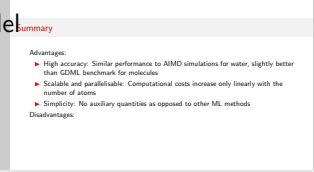

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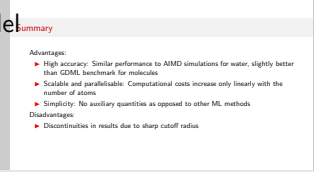

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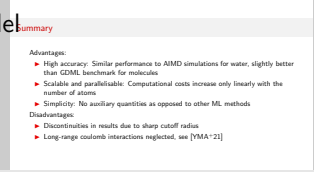

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