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

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Overview

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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
  $\Rightarrow$ Assign local reference frames to each atom and leverage extensive character of potential energy

$$E = \sum_i E_i$$

Overview

First step

- Local coordinate frame for each atom with atom at center

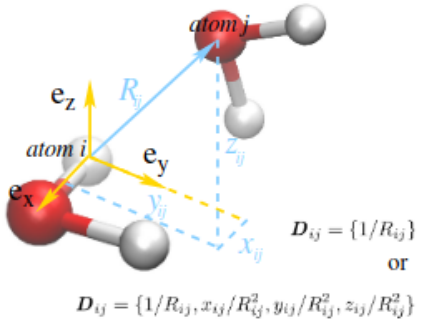
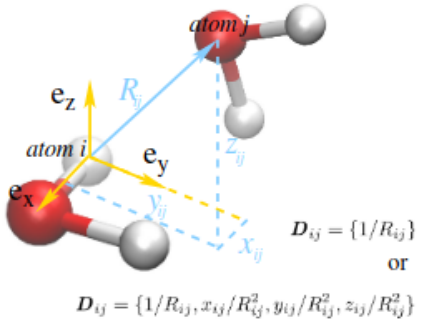


Figure: Geometry of the local coordinate frames [ZHW+18]

First step

- Local coordinate frame for each atom with atom at center
- $\mathbf{D}_i = (\mathbf{D}_{ij})_j$ input for NN, where j covers all neighbors within cutoff radius R_c, sorted by chemical species, inverse distances



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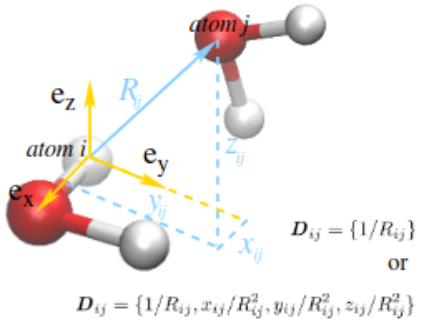
- Theoretical foundation: Embedded Atom Concept



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Second step

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

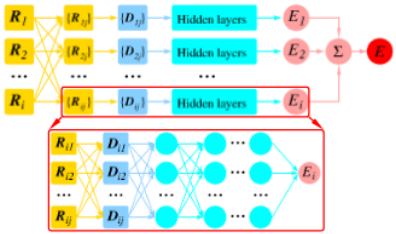

Figure: Visualisation of the NN [ZHW+18]

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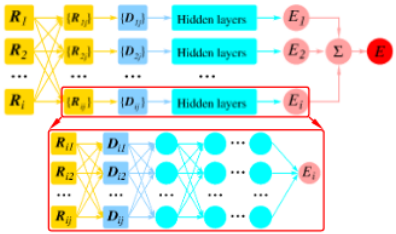

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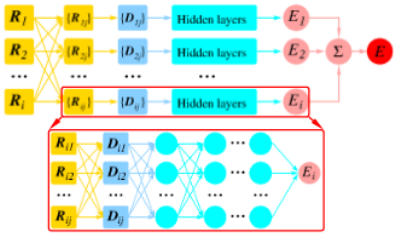

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Loss function

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

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 $\Xi = -\frac{1}{2} \sum_i \vec{R}_i \otimes \vec{F}_i$

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- Parameters p_ϵ, p_ξ steadily increased during training, p_f steadily decreased

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Disadvantages:

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

References


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