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Symmetry-Preserving Neural Networks

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FWAM
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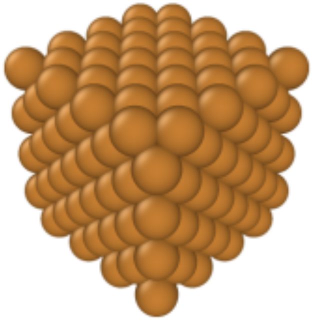
Example Problem 1: Potential Energy

Given coordinates of a group of atoms $\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n$, find its potential energy $E = E(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n)$



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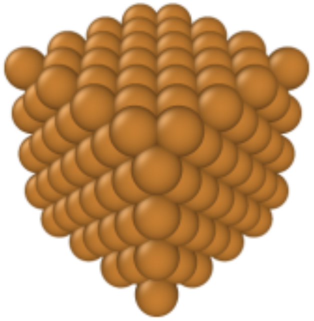

Physical Symmetries

- Translation $E = E(\boldsymbol{x}_1 + \Delta\boldsymbol{x}, \boldsymbol{x}_2 + \Delta\boldsymbol{x}, \cdots, \boldsymbol{x}_n + \Delta\boldsymbol{x})$

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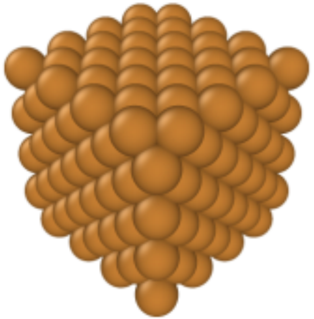

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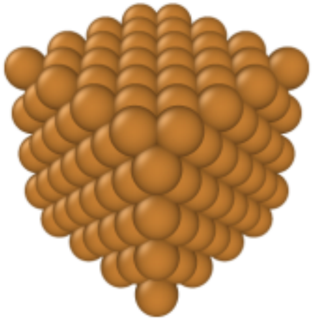

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Spatial discretization: $\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n, \boldsymbol{u}_1 = \boldsymbol{u}(\boldsymbol{x}_1), \boldsymbol{u}_2 = \boldsymbol{u}(\boldsymbol{x}_2), \ldots, \boldsymbol{u}_n = \boldsymbol{u}(\boldsymbol{x}_n),$

Consider the quantity $I := \int_\Omega c(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \approx I(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n, \boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_n)$

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- Rotation $I = I(R\boldsymbol{x}_1, R\boldsymbol{x}_2, \cdots, R\boldsymbol{x}_n, R\boldsymbol{u}_1, R\boldsymbol{u}_2, \cdots, R\boldsymbol{u}_n)$
- Permutation $I = I(\boldsymbol{x}_{\sigma(1)}, \boldsymbol{x}_{\sigma(2)}, \cdots, \boldsymbol{x}_{\sigma(n)}, \boldsymbol{u}_{\sigma(1)}, \boldsymbol{u}_{\sigma(2)}, \cdots, \boldsymbol{u}_{\sigma(n)})$

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Problem Setup

A function f maps a set of coordinates to a scalar output

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Why symmetry-preserving?

- respect the physics
- better data efficiency
- better accuracy

Related Work

- Handcrafted features, kernel method: Gaussian Approximation Potentials (GAP), Smooth Overlap of Atomic Positions (SOAP), etc.

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- Group representation: Group Equivariant Convolutional Networks, Steerable Convolutional Neural Networks, Clebsch–Gordan Nets, etc.

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Translation and Rotation Symmetry

Translation: always use relative coordinates

$$(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n) \quad \mapsto \quad (\boldsymbol{x}_1', \boldsymbol{x}_2', \cdots, \boldsymbol{x}_n') = (\boldsymbol{x}_1 - \bar{\boldsymbol{x}}, \boldsymbol{x}_2 - \bar{\boldsymbol{x}}, \cdots, \boldsymbol{x}_n - \bar{\boldsymbol{x}})$$

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$$D_{ij}' = \boldsymbol{x}_i' \cdot \boldsymbol{x}_j' \quad \text{or} \quad D' = X^\top X \ \text{ with } \ X = [\boldsymbol{x}_1', \boldsymbol{x}_2', \cdots, \boldsymbol{x}_n']^\top$$

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However, it lacks permutational invariance

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Permutation Symmetry

Deep Sets: a function f operating on a set $\{\boldsymbol{x}_i\}_{i=1}^n$ can be represented by

$$\rho(\sum_{i=1}^{n} \phi(\boldsymbol{x}_i))$$

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Example: $$z_1^2 + z_2^2 + z_1 z_2 = \frac{1}{2}(z_1 + z_2)^2 + \frac{1}{2}(z_1^2 + z_2^2)$$

Let $\phi(z) = [z, z^2]^\top$ and $\rho([a, b]^\top) = a^2/2 + b/2$

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Ansatz: parameterize ϕ, ρ with neural networks

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All Symmetries Simultaneously

Introduce a set of m embedding functions $\{\phi_k(\cdot)\}_{k=1}^{m}$

$$L_{kj} = \frac{1}{n}\sum_{i=1}^{n} \phi_k(|\boldsymbol{x}_i'|)\boldsymbol{x}_{ij}', \quad k = 1,\cdots,m,\ j = 1,2,3$$

or $\quad L = \dfrac{1}{n}G^\top X$ with $G_{ki} = \phi_k(|\boldsymbol{x}_i'|)$

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Extensions

- Guarantee equivariance if the output is

$$\text{vector: } \boldsymbol{r} = f(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n) \quad \rightarrow \quad R\boldsymbol{r} = f(R\boldsymbol{x}_1, R\boldsymbol{x}_2, \cdots, R\boldsymbol{x}_n)$$

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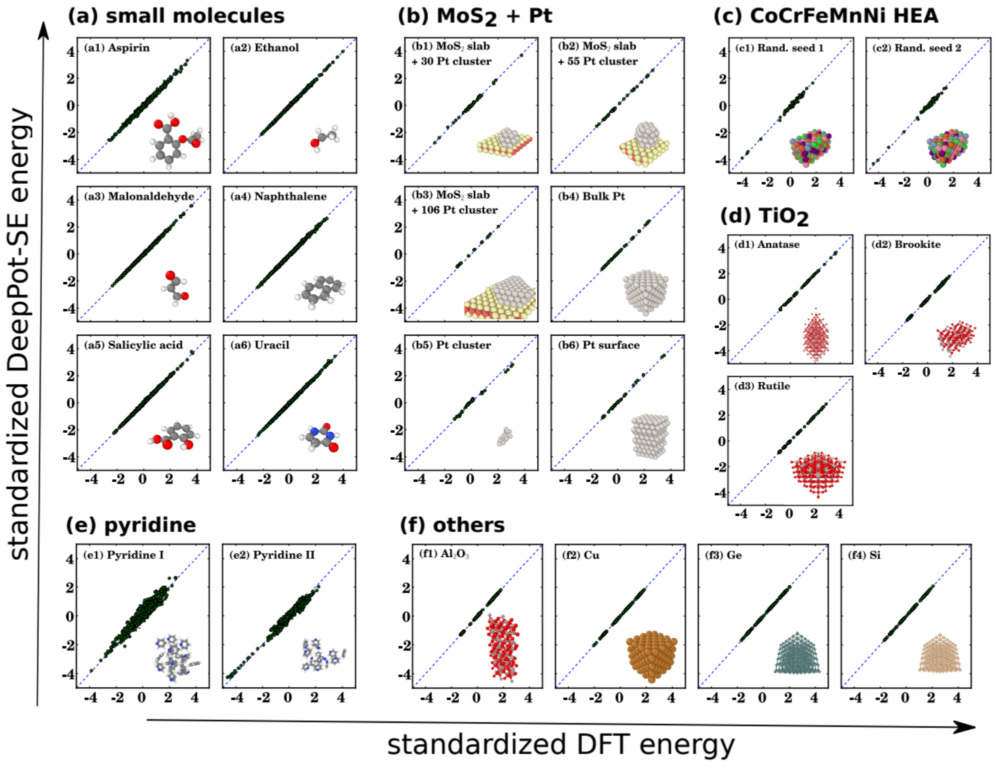
Open question: universal approximation property with practical optimality and scalability

Application: Molecular Dynamics



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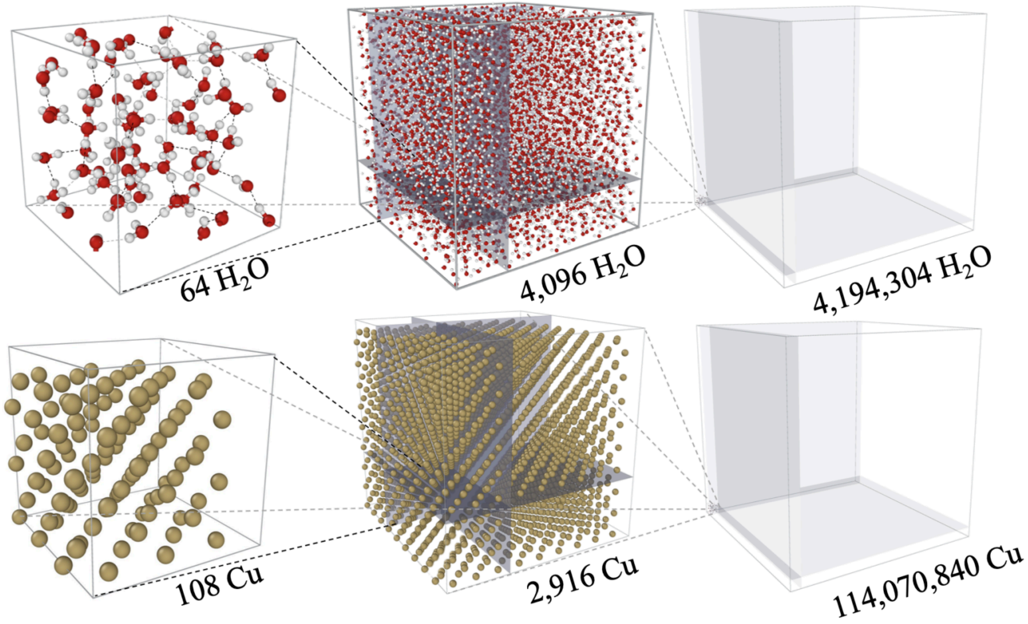

(a) AIMD + HPC; (b) DeePMD+1 GPU @ Home; (c) DeePMD+27360 GPUs @ Summit.

n is bounded as system size increased by short-range effect

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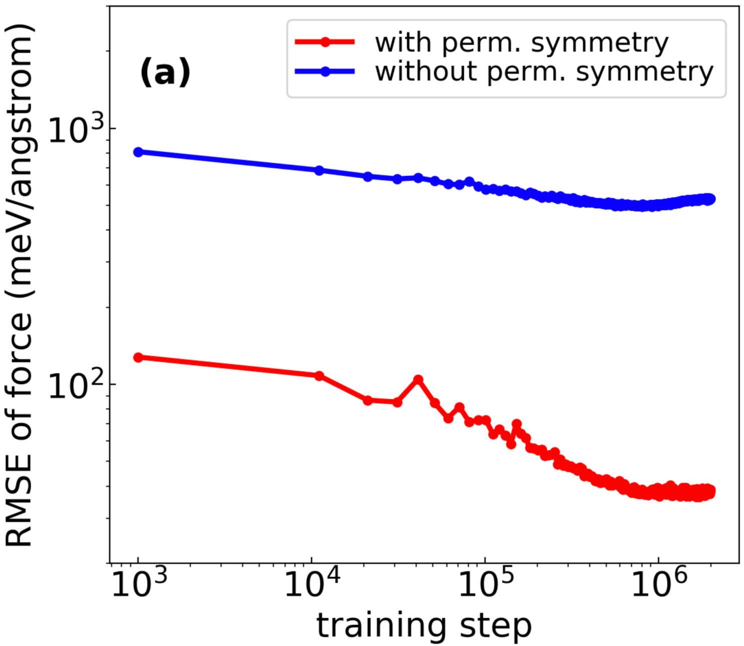
Importance of Symmetry



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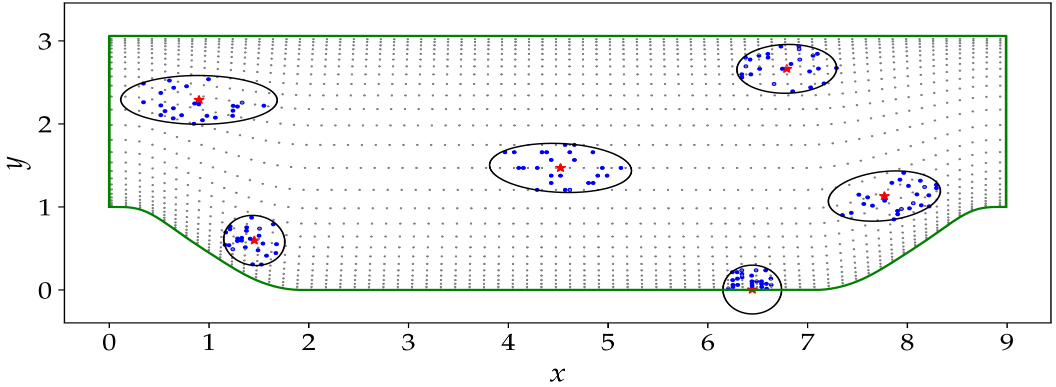
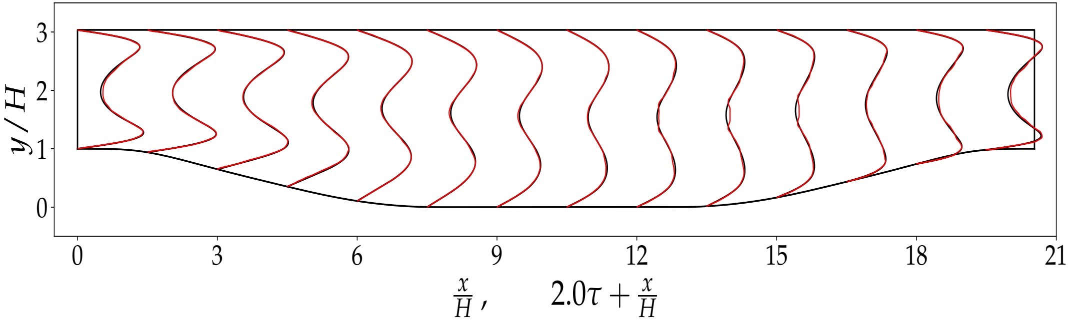
Application: Transport Equation





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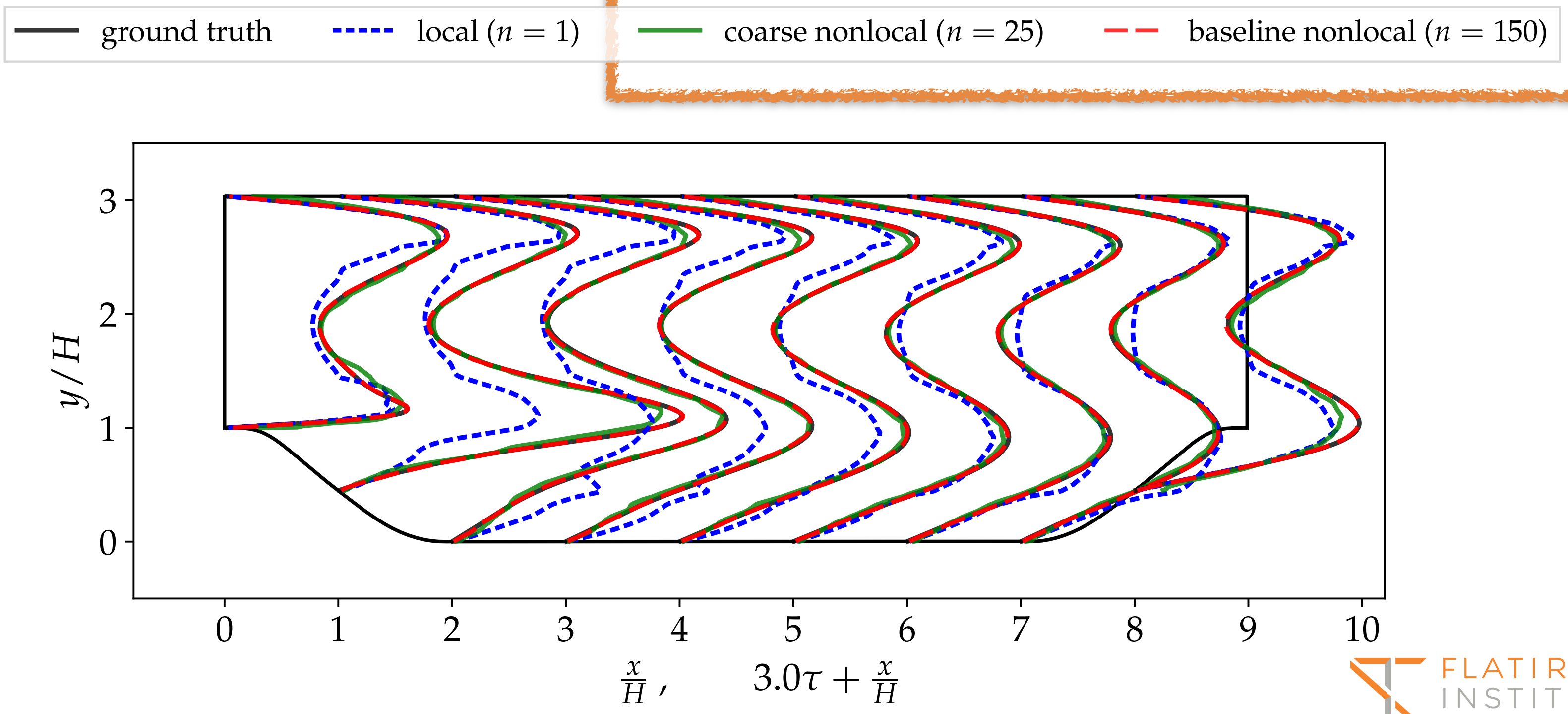
Adaptivity to Different Sizes



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  Code: https://github.com/xuhuizhou-vt/VCNN_nonlocal-constitutive-model

Thank You

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