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Symmetry-Preserving Neural Networks for Scientific Computing

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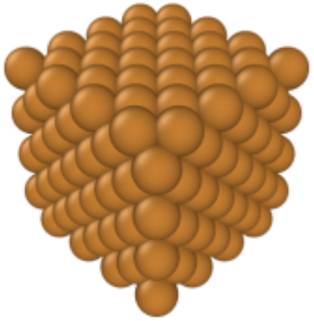
Example Problem 1: Potential Energy

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



Physical Symmetries

- Translation $E = E(\boldsymbol{x}_1 + \Delta \boldsymbol{x}, \boldsymbol{x}_2 + \Delta \boldsymbol{x}, \cdots, \boldsymbol{x}_n + \Delta \boldsymbol{x})$
- Rotation $E = E(R\boldsymbol{x}_1, R\boldsymbol{x}_2, \cdots, R\boldsymbol{x}_n)$
- Permutation $E = E(\boldsymbol{x}_{\sigma(1)}, \boldsymbol{x}_{\sigma(2)}, \cdots, \boldsymbol{x}_{\sigma(n)})$

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Example Problem 2: Transport Equation

$$\Delta c(\boldsymbol{x}) - \nabla \cdot (\boldsymbol{u}(\boldsymbol{x})c(\boldsymbol{x})) + S(c(\boldsymbol{x})) = 0$$

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

Physical Symmetries

- Translation $I = I(\boldsymbol{x}_1 + \Delta\boldsymbol{x}, \boldsymbol{x}_2 + \Delta\boldsymbol{x}, \cdots, \boldsymbol{x}_n + \Delta\boldsymbol{x}, \boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_n)$
- 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 $I = I(\boldsymbol{x}_{\sigma(1)}, \boldsymbol{x}_{\sigma(2)}, \cdots, \boldsymbol{x}_{\sigma(n)}, \boldsymbol{u}_{\sigma(1)}, \boldsymbol{u}_{\sigma(2)}, \cdots, \boldsymbol{u}_{\sigma(n)})$

Problem Setup

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

$$y = f(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n)$$

Supervised learning: fit this function from data and preserve all the symmetries simultaneously

Why symmetry-preserving?

- respect the physics
- better data efficiency
- better accuracy

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Related Work

- Handcrafted features, kernel method: Gaussian Approximation Potentials (GAP), Smooth Overlap of Atomic Positions (SOAP), etc.
- Behler-Parrinello neural network (BPNN)
- Learned features: Deep Potential/Vector Cloud Neural Network, SchNet, etc.
- 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

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

Rotation:

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

However, it lacks permutational invariance

Permutation Symmetry

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

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

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

Ansatz: parameterize ϕ, ρ with neural networks

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

This leads to symmetry-preserving feature matrix $D = LL^\top = \frac{1}{n^2}G^\top XX^\top G$

Map to the final output through a general function $\rho(\mathrm{vec}(D))$

Ansatz: parameterize ϕ, ρ with neural networks

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Extensions

- Guarantee equivariance if the output is

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

$$\text{or tensor: } Q = f(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n) \quad \rightarrow \quad RQR^\top = f(R\boldsymbol{x}_1, R\boldsymbol{x}_2, \cdots, R\boldsymbol{x}_n)$$

- Guarantee invariance and equivariance if we have additional scalar/vector/tensor features attached to each point

- Use high-order information to do embedding

Open question: universal approximation property with practical optimality and scalability

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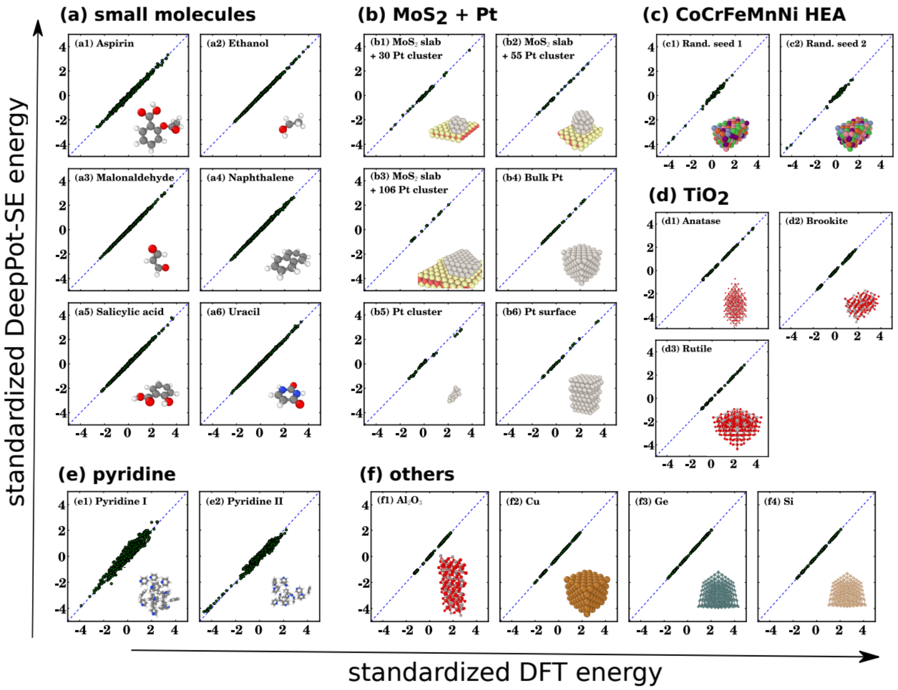
Application: Molecular Dynamics

Deep Potential for molecular dynamics



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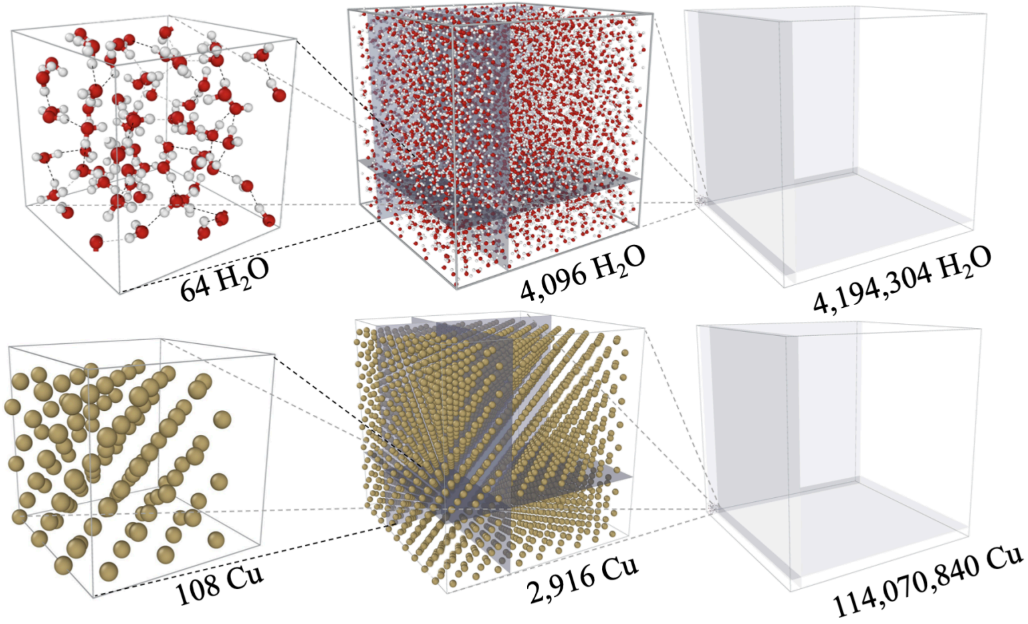
Application: Molecular Dynamics



(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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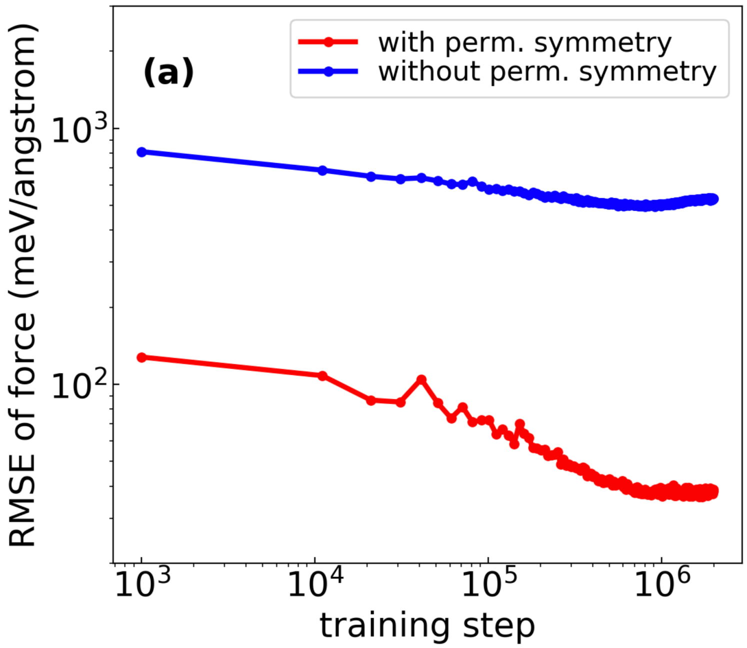
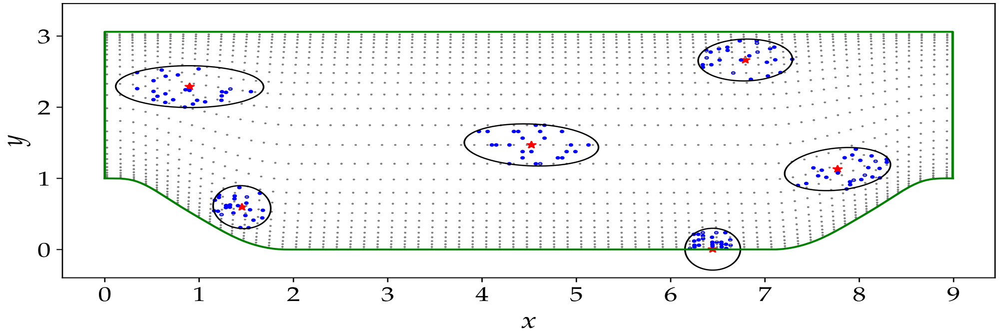
Importance of Symmetry

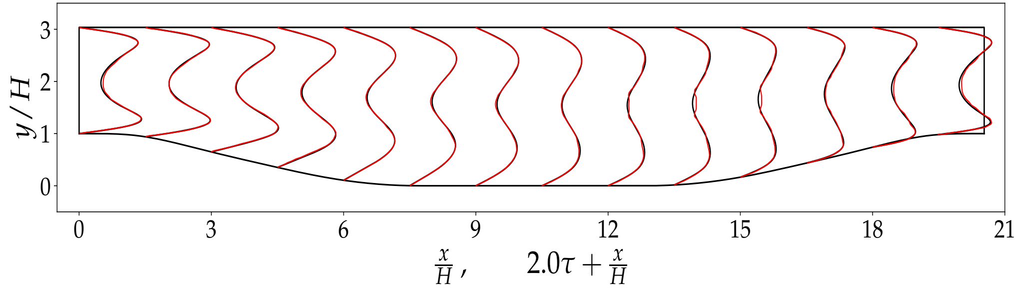


Application: Transport Equation

Vector-Cloud Neural Network (VCNN) for nonlocal modeling



$$\Delta c(\boldsymbol{x}) - \nabla \cdot (\boldsymbol{u}(\boldsymbol{x}) c(\boldsymbol{x})) + S(c(\boldsymbol{x})) = 0$$



Solve $c(\boldsymbol{x})$ at any point $\boldsymbol{x_0}$ from the velocity field $u(\boldsymbol{x})$ around $\boldsymbol{x_0}$ (nonlocal relationship)

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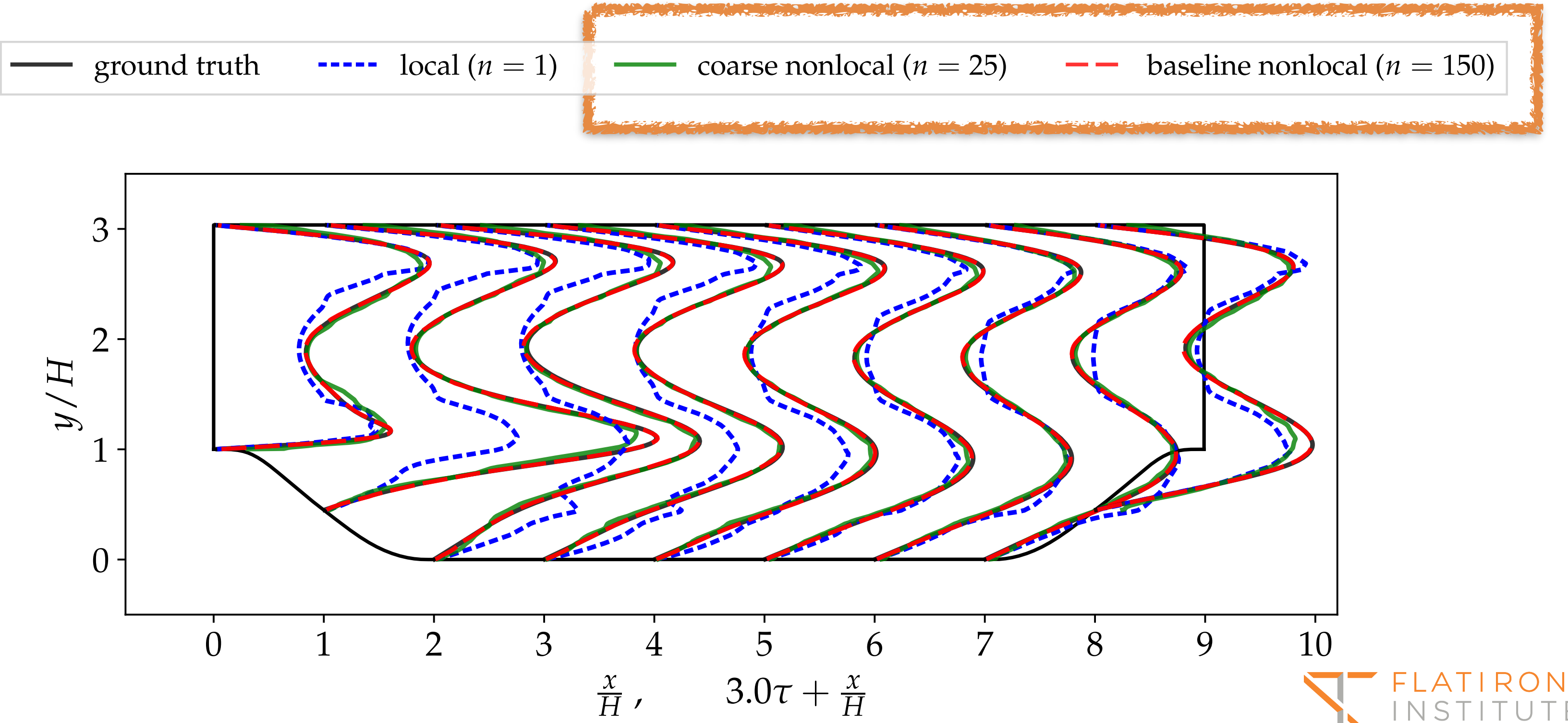
Adaptivity to Different Sizes



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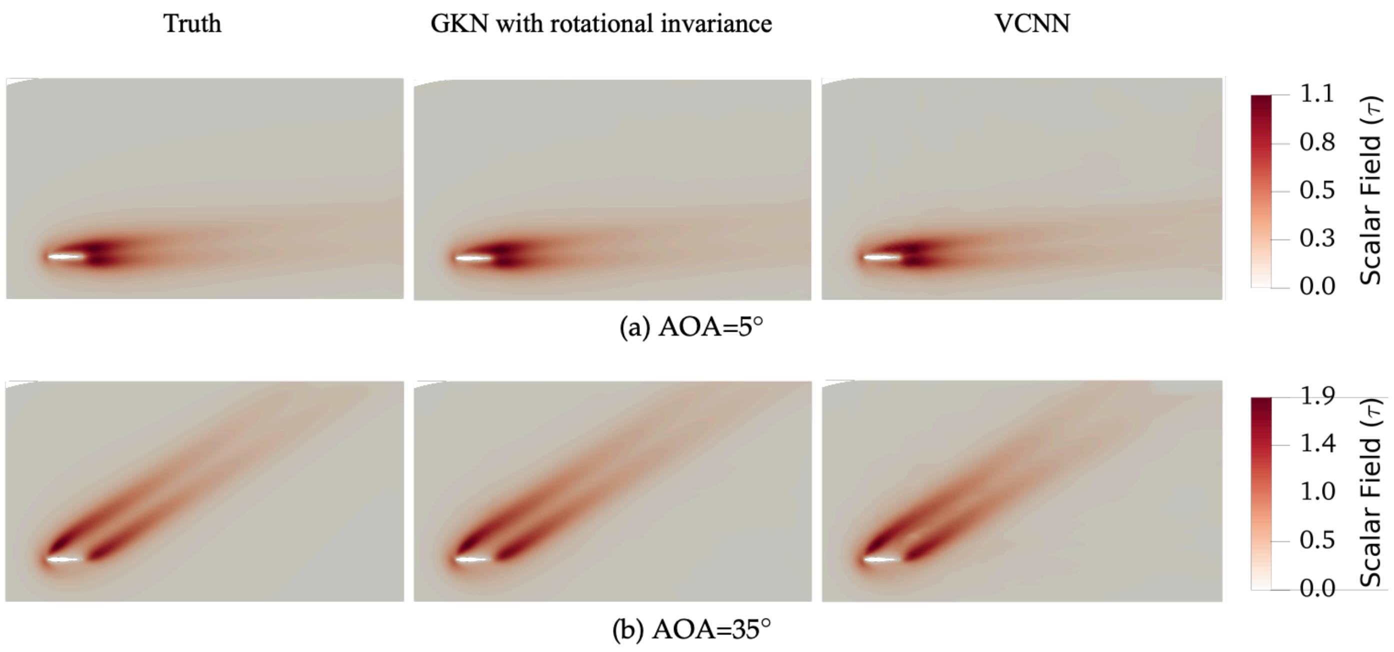
Evaluation in Different Frames



Importance of Frame Invariance

(a) True concentration field

(b) Reference frame rotation = 0°

(c) Reference frame rotation = 35°

(d) Reference frame rotation = 70°

(e) Reference frame rotation = 90°

(f) Reference frame rotation = 180°

Prediction by an operator based on graph neural networks without rotation symmetry. The results are highly sensitive to the angles of the reference frame.

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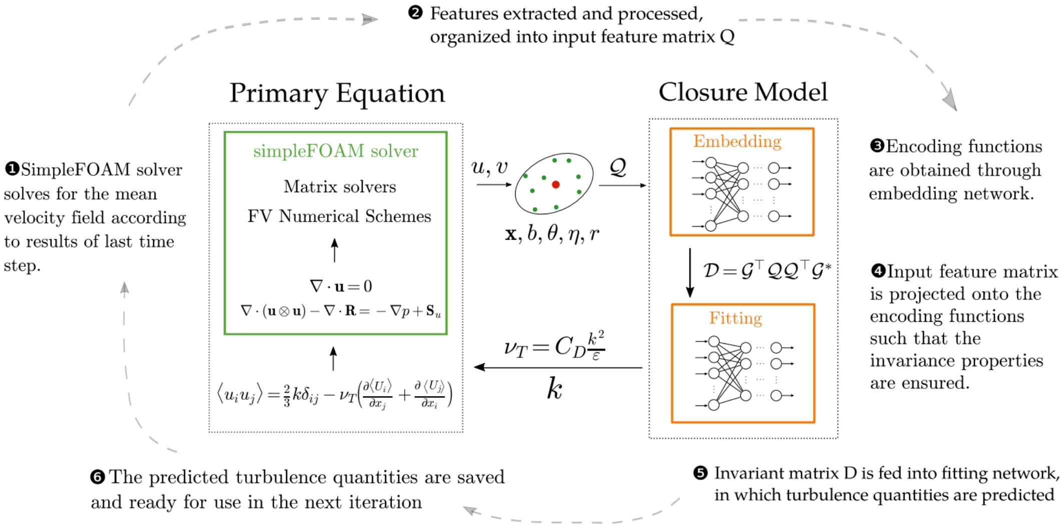
Closure Model for RANS equations

$$\frac{\bar{D}\langle U_j\rangle}{\bar{D}t} = \nu\nabla^2\langle U_j\rangle - \frac{\partial\langle u_i'u_j'\rangle}{\partial x_i} - \frac{1}{\rho}\frac{\partial\langle p\rangle}{\partial x_j},$$

$$\langle u_i'u_j'\rangle = \frac{2}{3}k\delta_{ij} - \nu_T\left(\frac{\partial\langle U_i\rangle}{\partial x_j} + \frac{\partial\langle U_j\rangle}{\partial x_i}\right),$$

Constitutive relationship for *k*?

Use vector-cloud neural network to model *k*



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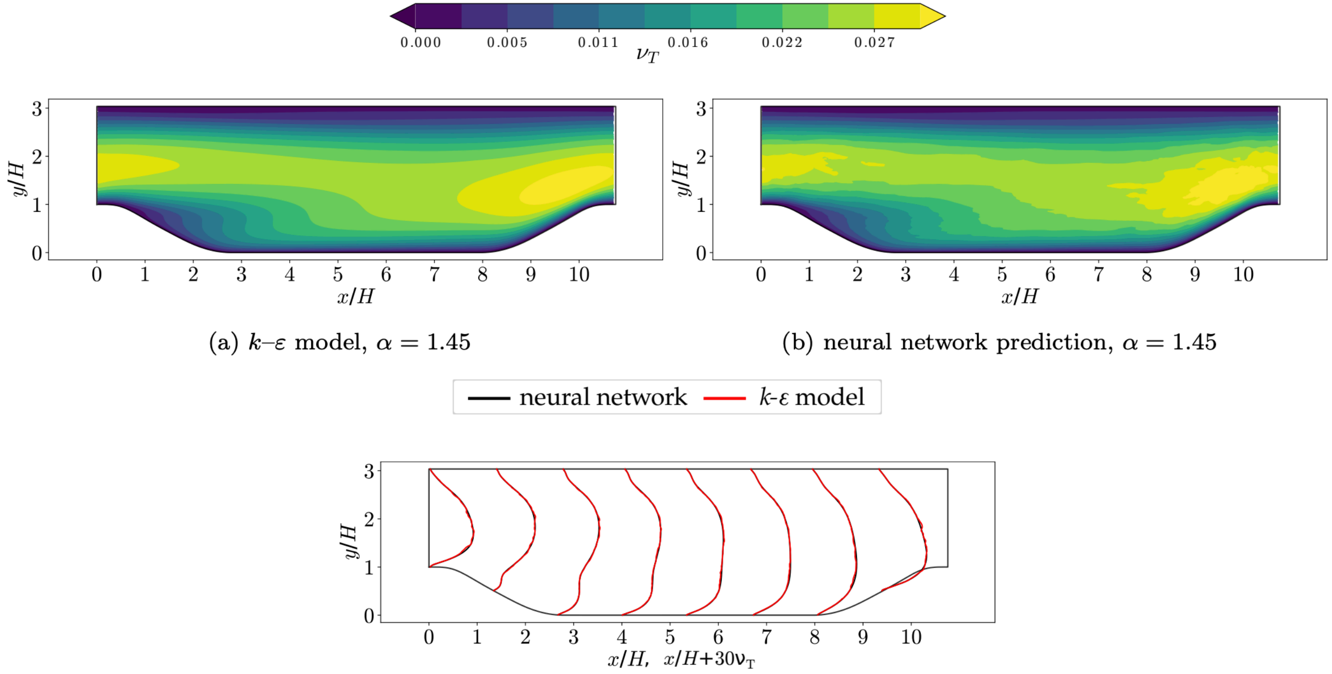
Closure Model for RANS equations



(a) k–ε model, $\alpha = 1.45$

(b) neural network prediction, $\alpha = 1.45$

(c) neural network prediction, $\alpha = 1.45$

References

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Thank You

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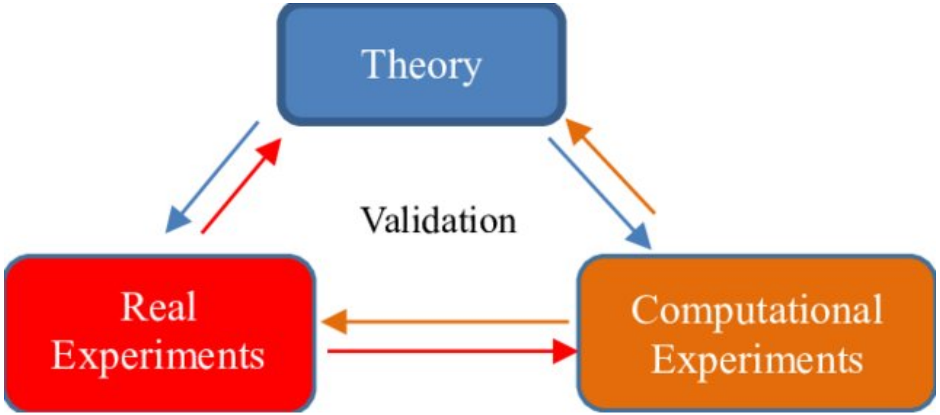
“Third Pillar” of Science

Together with theory and experimentation, computational science now constitutes the “third pillar” of scientific inquiry.

— President’s Information Technology Advisory Committee report (2005)



About Flatiron Institute

The institute, an internal research division of the Simons Foundation, is a community of scientists who are working to use modern computational tools to advance our understanding of science, both through the analysis of large, rich datasets and through the simulations of physical process.

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