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Point-particle drag, lift, and torque closure models using machine learning: hierarchical approach and interpretability

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Acknowledgments: The Office of Naval Research (ONR) as part of the Multidisciplinary University Research Initiatives (MURI) Program, under grant number N00014-16-1-2617.

The views contained herein are those of the authors only.

Outline

- Introduction
- Problem description
- Hierarchical approach
- Universal force & torque predictions
- Interpretability
- Conclusions and Future Work

Euler-Lagrange Methodology

- The carrier phase, generally fluid, is considered in Eulerian frame of reference.
- The dispersed phase, particles in this work, is considered in Lagrangian frame of reference as point-particles.
- Governing equations for an incompressible, isothermal fluid with particles in thermal equilibrium with the surrounding fluid.
- Particle phase:

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}$$

$$M_p \frac{d\mathbf{V}}{dt} = \mathbf{F_h} + \mathbf{F_c} + \mathbf{F_b}$$

where,

$\mathbf{F_h}$ - Hydrodynamic force

$\mathbf{F_c}$ - Collisional force

$\mathbf{F_b}$ - External body force

Obtained from models (Analytical or Data-driven)

- Fluid phase:

$$\nabla \cdot \mathbf{u} = -\frac{1}{\phi^{(f)}}\frac{D\phi^{(f)}}{Dt}$$

$$\rho^{(f)}\frac{D\mathbf{u}}{Dt} - \nabla \cdot \sigma^{(f)} = \frac{\mathbf{f_{pf}}}{\phi^{(f)}}$$

$$\sigma^{(f)} = -p\,\mathbf{I} + \mu^{(f)}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

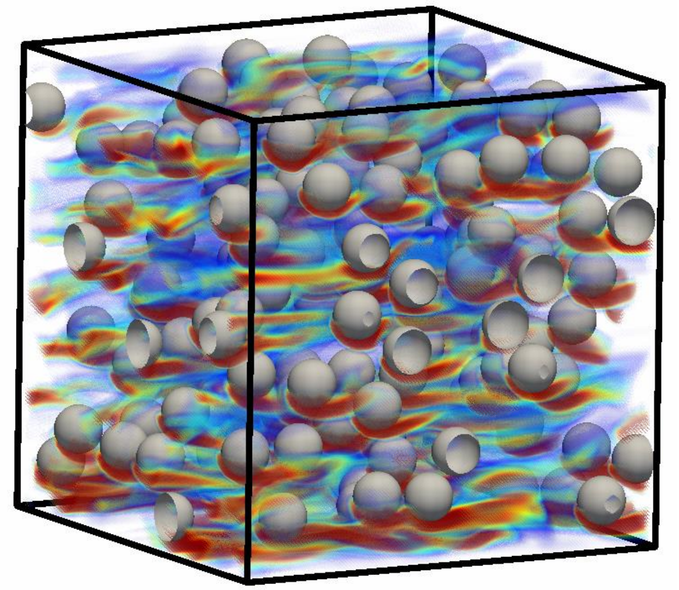
where,

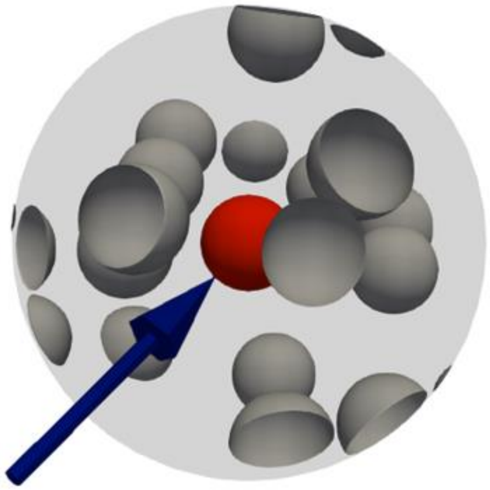
$\mathbf{f_{pf}}$ - particle-fluid coupling force

- Particle-fluid coupling force at a Eulerian grid point is formulated based on Hydrodynamic force of many point-particles in its vicinity.

Problem Description

- Predict **force** and **torque** acting on a particle based on volume-averaged Reynolds number, particle volume fraction, mean-flow direction, and exact location of influential neighbors.
- Data generated using particle-resolved direct numerical simulation (PR-DNS) in a triply-periodic box for **stationary particles**.





Inputs:

$$Re_i, \phi_i, \hat{\hat{\boldsymbol{e}}}_i,$$

$$\{\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_M\}$$

Output:

$$\boldsymbol{F}_i, \boldsymbol{T}_i$$

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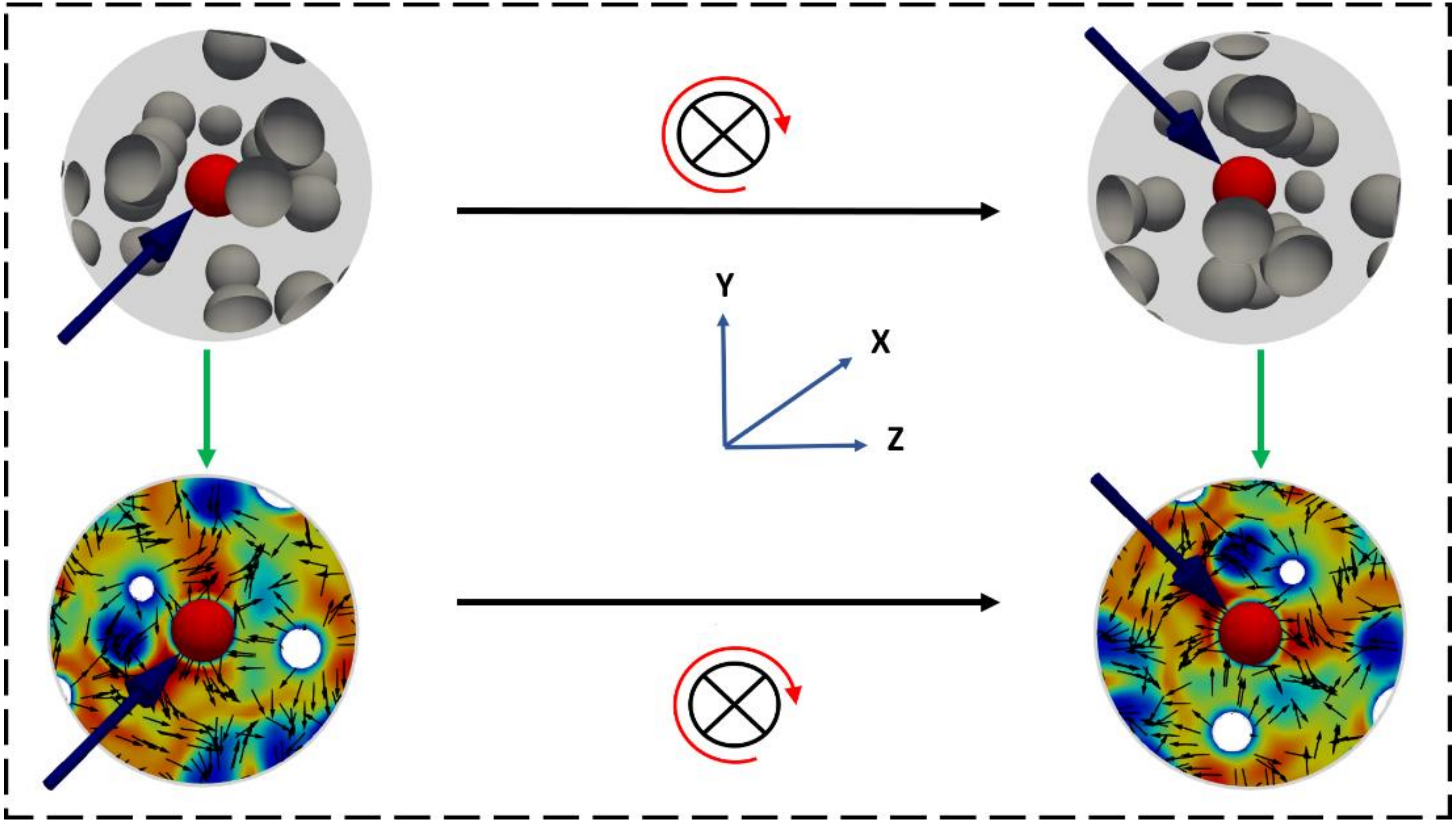
Symmetry



Previous data-driven studies for this N-body problem

- Moore et al., JCP 385 (2019): 187-208 (Hybrid PIEP model).
- He et al., Powder technology 345 (2019): 379-389.

$$\boldsymbol{F} = MLP(Re, \phi, \{\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_M\})$$

An MLP is made up of multiple layers of the following constitutive block:

$$b_n = \sigma(w_{mn}\, a_m + d_n)$$

Where $\boldsymbol{a}$ is the input array in the above definition, $\boldsymbol{b}$ is the output array, and σ is an activation function.

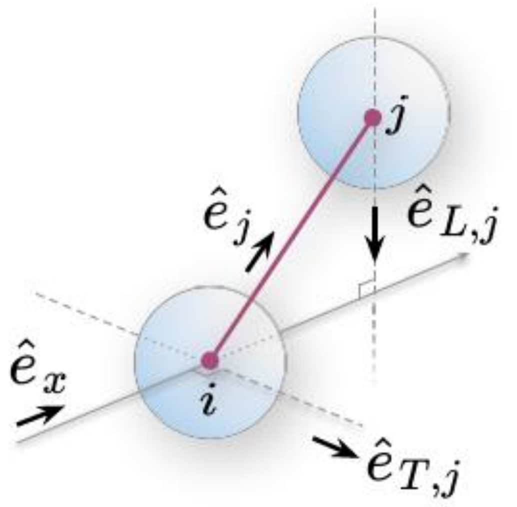
- Seyed-Ahmadi et al., JFM 900 (2020).

Pairwise-interaction Approach

- Recently, A. Seyed-Ahmadi, and A. Wachs (2022), Computers & Fluids 238 , proposed a systematic and robust NN model based on **pairwise interaction**, Akiki et al., JFM 813 (2017): 882-928.

$$\Delta \boldsymbol{F}_D = |\boldsymbol{u}| \sum_{j=1}^{M} w_j \; MLP_1(\boldsymbol{r}_j)\hat{\boldsymbol{e}}_x$$

$$\Delta \boldsymbol{F}_L = |\boldsymbol{u}| \sum_{j=1}^{M} w_j \; MLP_2(\boldsymbol{r}_j) \frac{\hat{\boldsymbol{e}}_x \text{x} \, (\hat{\boldsymbol{e}}_x \text{x} \, \boldsymbol{r}_j)}{\|\hat{\boldsymbol{e}}_x \text{x} (\hat{\boldsymbol{e}}_x \text{x} \, \boldsymbol{r}_j)\|}$$



Seyed-Ahmadi et al., Computers & Fluids 238 (2022)

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Hierarchical Approach

$$\boldsymbol{F}_i(Re_i, \phi_i, \{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_M\})$$

$$= \boldsymbol{F}_{1i}\,(Re_i, \phi_i)$$

Unary Model

$$+ \sum_{j=1}^{M_2} \boldsymbol{F}_{2i}(Re_i, \phi_i, \boldsymbol{r}_j)$$

Binary-interaction Model

Trinary-interaction Model

$$+ \sum_{j=1}^{M_3-1} \sum_{k=j+1}^{M_3} \boldsymbol{F}_{3i}(Re_i, \phi_i, \boldsymbol{r}_j, \boldsymbol{r}_k) + \cdots$$

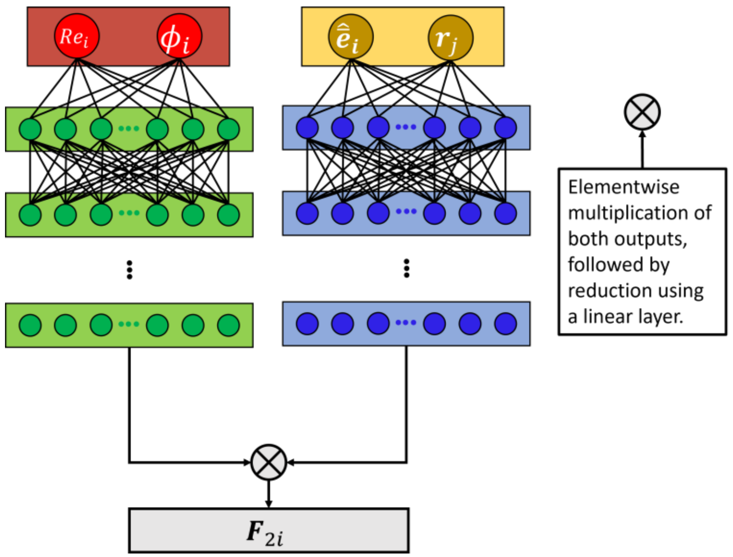
Symmetry-preservation using E(3)-NN

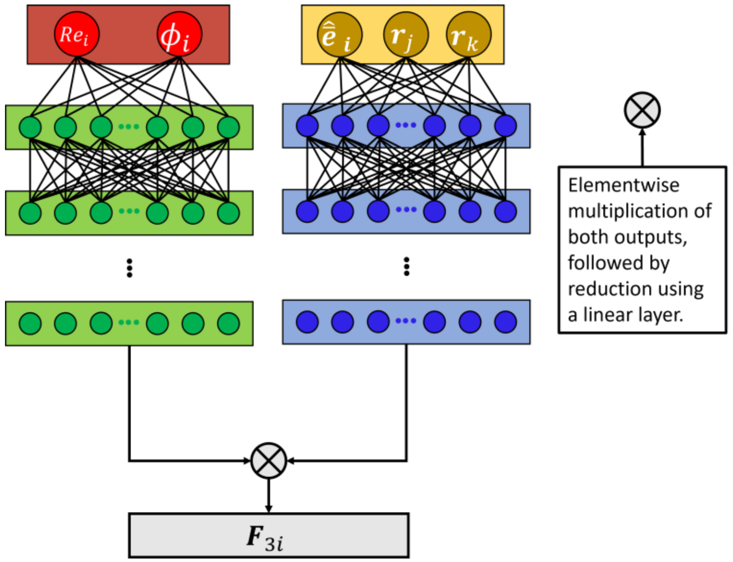
- An equivariant neural network is built using the following constitutive block:

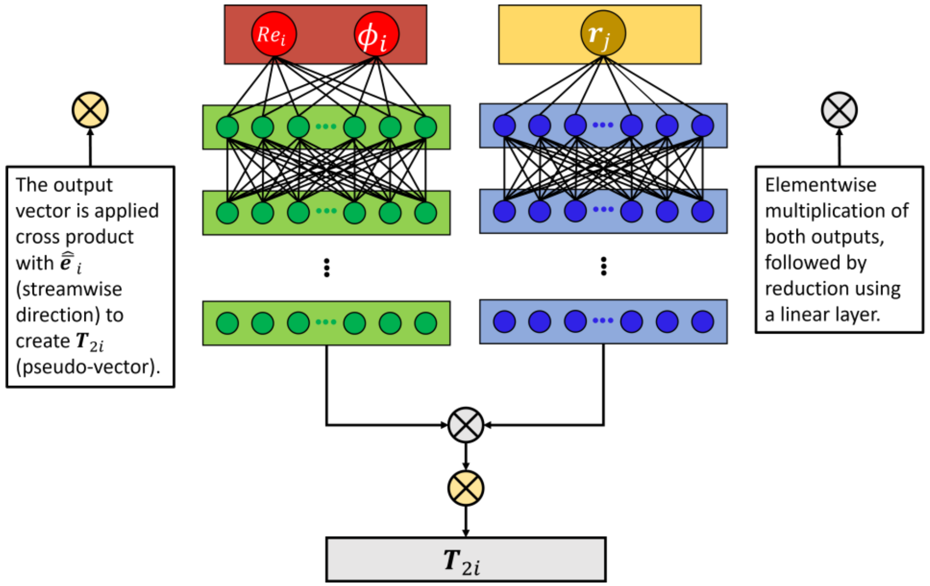
$$\boldsymbol{b}_n = \frac{\sigma(\|w_{mn}\,\boldsymbol{a}_m\| + d_n)}{\|w_{mn}\,\boldsymbol{a}_m\|}(w_{mn}\,\boldsymbol{a}_m)$$

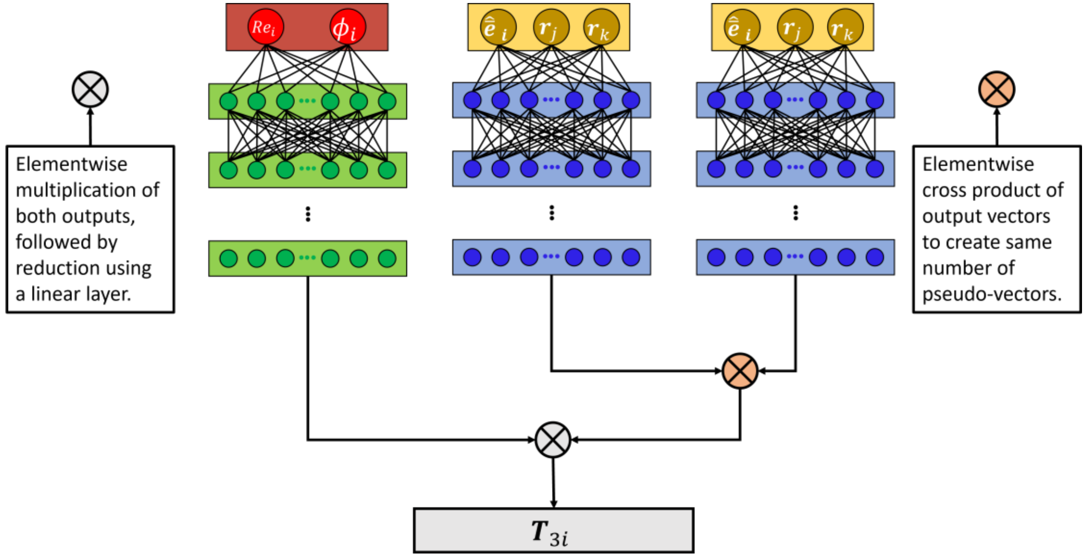
- Where $\boldsymbol{a}$ is the input list of vectors, $\boldsymbol{b}$ is the output list of vectors, and σ is an activation function.

Scalable architectures for universal predictions









Datasets

$\langle Re \rangle$	$\langle \phi \rangle$	$\lvert\langle \boldsymbol{F} \rangle\rvert$	σ_{Drag}	σ_{Lift}	$\sigma_{\text{Torque},\parallel}$	$\sigma_{\text{Torque},\perp}$	N
9.86	0.10	2.76	0.7823	0.4661	0.2407	0.9253	1000
121.36	0.10	9.55	3.1110	1.4986	0.5043	1.3689	1000
6.95	0.21	4.03	0.9581	0.7454	0.4195	1.2987	1000
73.40	0.21	9.51	2.7987	1.6178	0.6441	1.7103	1000
27.81	0.40	12.68	2.0613	1.5028	0.6734	2.0589	1000
73.42	0.40	19.14	3.6087	2.4135	1.0285	2.5955	1000
2.20	0.10	2.63	0.5425	0.3973	0.2375	0.9241	2984
10.92	0.10	3.28	0.7351	0.4839	0.2405	0.9838	3000
165.96	0.10	9.48	2.4191	1.5662	0.4339	1.1972	2984
0.25	0.20	4.42	0.7971	0.6737	0.4295	1.4509	3055
2.48	0.20	4.47	0.8116	0.6707	0.4217	1.4465	3000
49.78	0.20	7.72	1.8194	1.2608	0.5078	1.6549	3055
187.25	0.20	14.24	3.6989	2.6873	0.8446	2.0219	3055
3.25	0.40	11.75	2.7535	2.1329	1.0256	2.4789	2578
64.35	0.40	19.67	5.0963	3.6885	1.3063	2.9899	2578
245.65	0.40	36.62	9.5692	7.1215	2.0385	3.9776	2578

Datasets are gathered from two different sources.

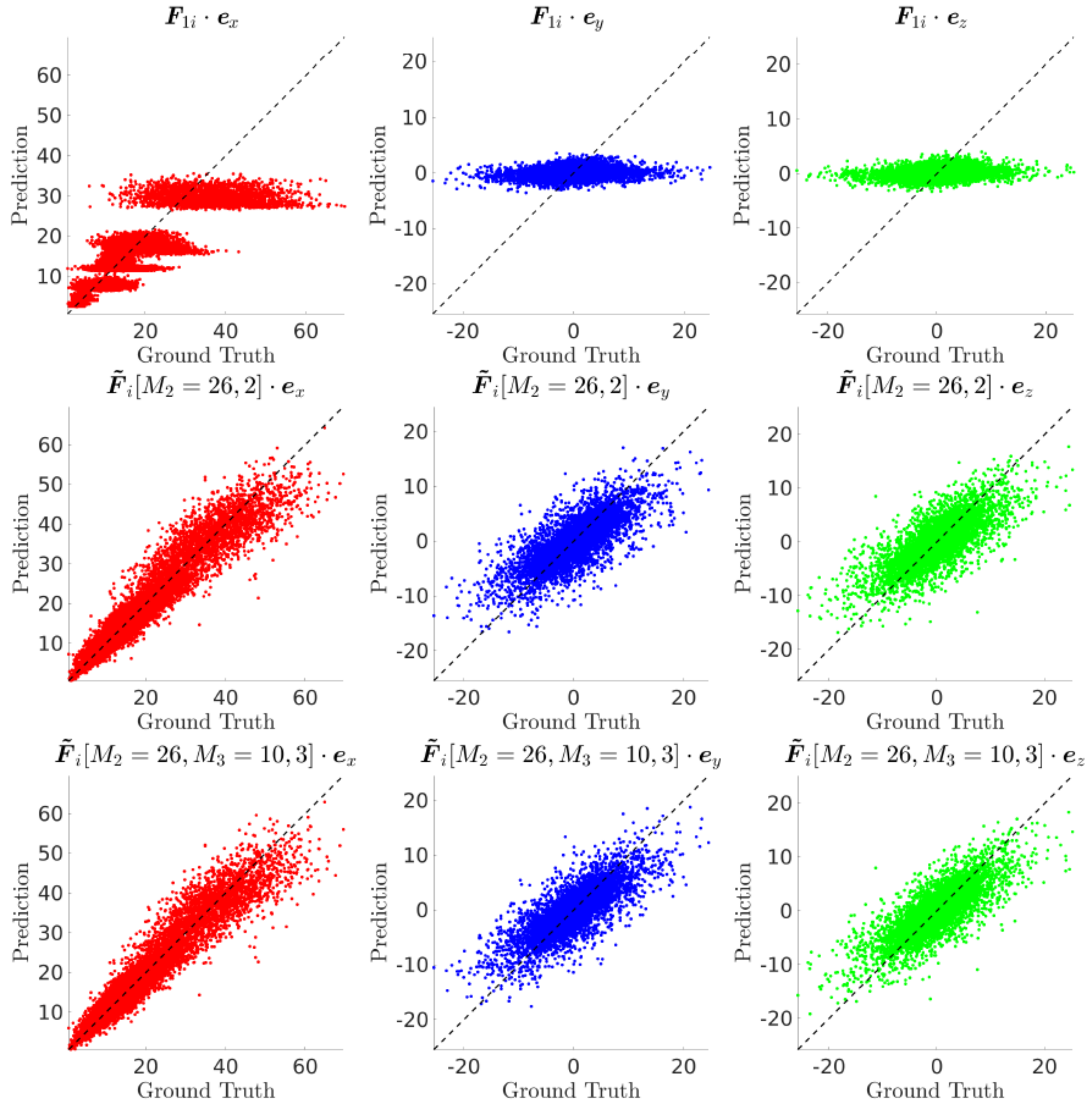
Model Interaction-truncation

$$\widetilde{\boldsymbol{F}}_i[M_2, 2] = \boldsymbol{F}_{1i}\,(Re_i, \phi_i) + \sum_{j=1}^{M_2} \boldsymbol{F}_{2i}(Re_i, \phi_i, \boldsymbol{r}_j)$$

$$\widetilde{\boldsymbol{F}}_i[M_2, M_3, 3]$$
$$= \boldsymbol{F}_{1i}\,(Re_i, \phi_i)$$
$$+ \sum_{j=1}^{M_2} \boldsymbol{F}_{2i}(Re_i, \phi_i, \boldsymbol{r}_j) + \sum_{j=1}^{M_3-1} \sum_{k=j+1}^{M_3} \boldsymbol{F}_{3i}(Re_i, \phi_i, \boldsymbol{r}_j, \boldsymbol{r}_k)$$

Universal Force Predictions

$\boldsymbol{F}_{1i}(Re_i, \phi_i)$



$\tilde{\boldsymbol{F}}_i[M_2 = 26, 2]$

$\tilde{\boldsymbol{F}}_i[M_2 = 26, M_3 = 10, 3]$

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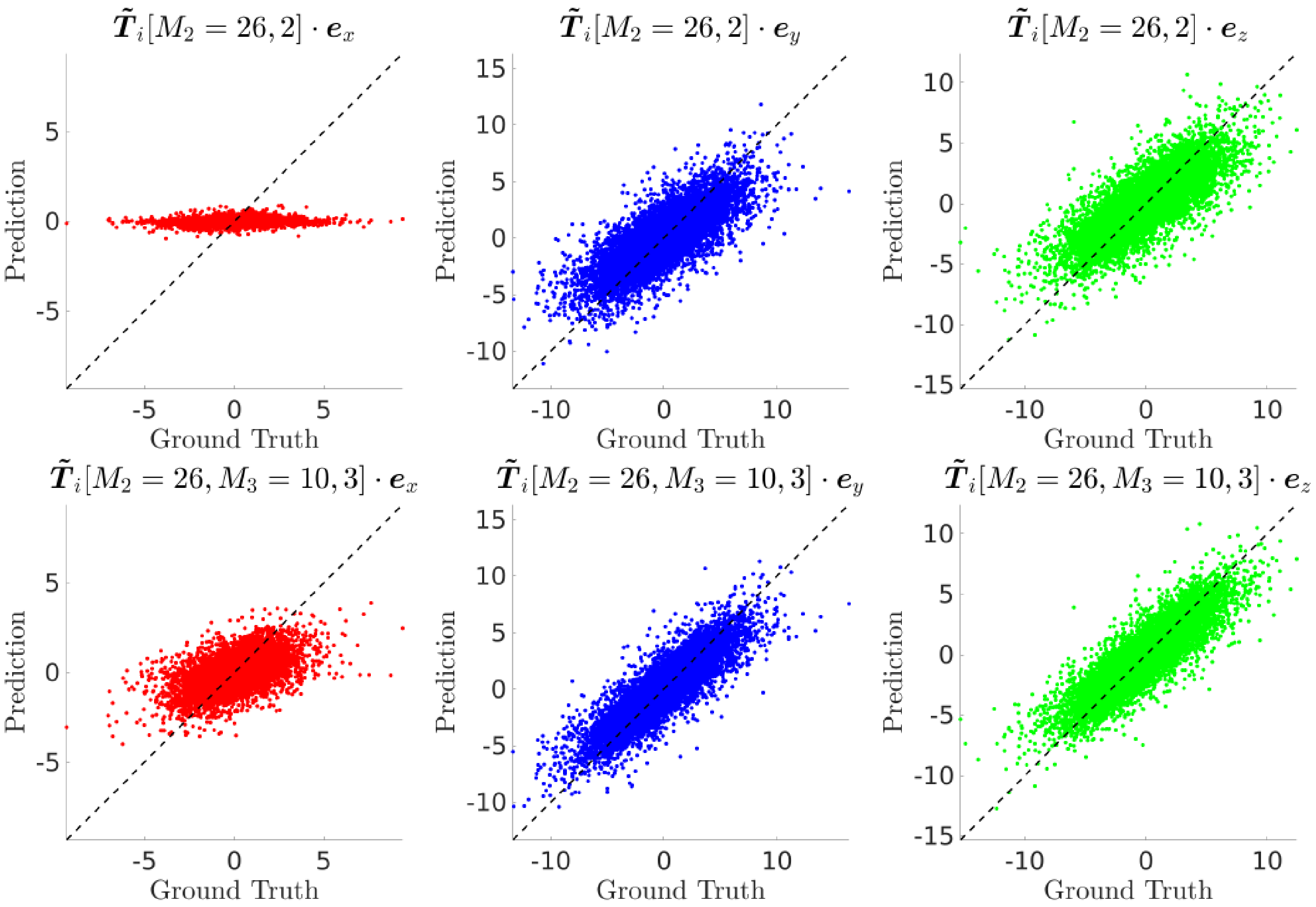
Universal Torque Predictions

$\widetilde{\boldsymbol{T}}_i[M_2 = 26, 2]$



$\widetilde{\boldsymbol{T}}_i[M_2 = 26, M_3 = 10,3]$

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Performance Evaluation Metric

$$R^2_{\text{Drag}} = \frac{\sum_{\text{Test samples}}\left(F_{i,(x,\text{PR})} - \Delta F_{i,(x,\text{NN})}\right)^2}{\sum_{\text{Test samples}}\left(F_{i,(x,\text{PR})} - \langle F_{i,(x,\text{PR})}\rangle\right)^2}$$

$$R^2_{\text{Lift}} = \frac{\sum_{\text{Test samples}}\left(F_{i,(y,\text{PR})} - F_{i,(y,\text{NN})}\right)^2 + \left(F_{i,(z,\text{PR})} - \Delta F_{i,(z,\text{NN})}\right)^2}{\sum_{\text{Test samples}}\left(F_{i,(y,\text{PR})} - \langle F_{i,(y,\text{PR})}\rangle\right)^2 + \left(F_{i,(z,\text{PR})} - \langle F_{i,(z,\text{PR})}\rangle\right)^2}$$

- $R^2 = 1$ means a perfect model that captures the fluctuations.
- $R^2 = 0$ means the model is not capturing any fluctuations at all.
- R^2 can also be negative.

Force Results, R^2

$\langle Re \rangle$	$\langle \phi \rangle$	$\tilde{F}_i[M_2 = 26, 2]$				$\tilde{F}_i[M_2 = 26, M_3 = 10, 3]$			
		Drag		Lift		Drag		Lift	
		Train	Test	Train	Test	Train	Test	Train	Test
9.86	0.10	0.775	0.740	0.797	0.776	0.842	0.762	0.862	0.803
121.36	0.10	0.685	0.645	0.707	0.696	0.787	0.650	0.805	0.701
6.95	0.21	0.816	0.809	0.812	0.800	0.853	0.817	0.862	0.827
73.40	0.21	0.757	0.728	0.746	0.739	0.818	0.745	0.833	0.772
27.81	0.40	0.807	0.788	0.795	0.784	0.837	0.809	0.841	0.823
73.42	0.40	0.759	0.738	0.754	0.738	0.807	0.769	0.817	0.786
2.20	0.10	0.837	0.833	0.803	0.800	0.854	0.838	0.842	0.826
10.92	0.10	0.810	0.807	0.812	0.808	0.826	0.815	0.861	0.851
165.96	0.10	0.624	0.611	0.715	0.718	0.679	0.615	0.759	0.732
0.25	0.20	0.756	0.747	0.757	0.753	0.769	0.758	0.773	0.764
2.48	0.20	0.780	0.773	0.764	0.758	0.791	0.782	0.791	0.784
49.78	0.20	0.747	0.743	0.716	0.719	0.772	0.754	0.795	0.787
187.25	0.20	0.662	0.656	0.668	0.671	0.698	0.661	0.731	0.711
3.25	0.40	0.698	0.672	0.592	0.567	0.722	0.679	0.625	0.584
64.35	0.40	0.744	0.727	0.655	0.643	0.764	0.739	0.717	0.696
245.65	0.40	0.661	0.632	0.574	0.558	0.698	0.649	0.654	0.611

Training and testing performance of binary-interactions and trinary-interactions included force models.

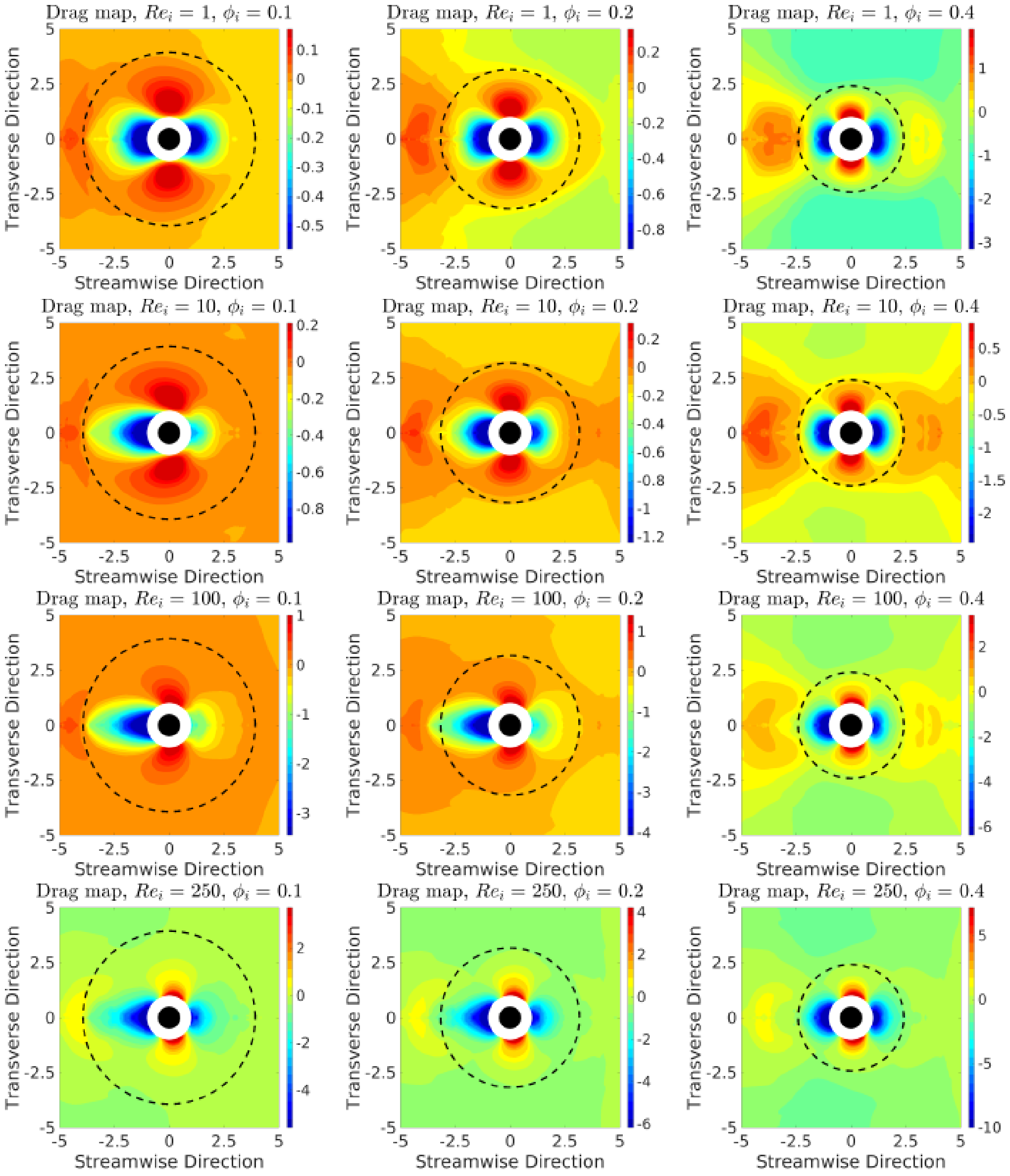
Torque Results, R^2

$\langle Re \rangle$	$\langle \phi \rangle$	$\tilde{\boldsymbol{T}}_i[M_2 = 26, 2]$ Torque,$\perp$		$\tilde{\boldsymbol{T}}_i[M_2 = 26, M_3 = 10, 3]$ Torque,$\parallel$		Torque,$\perp$	
		Train	Test	Train	Test	Train	Test
9.86	0.10	0.752	0.751	0.602	0.469	0.933	0.899
121.36	0.10	0.308	0.285	0.467	0.011	0.835	0.618
6.95	0.21	0.827	0.825	0.699	0.610	0.951	0.929
73.40	0.21	0.496	0.486	0.458	0.234	0.868	0.774
27.81	0.40	0.657	0.647	0.658	0.544	0.937	0.897
73.42	0.40	0.435	0.434	0.571	0.437	0.864	0.804
2.20	0.10	0.899	0.898	0.678	0.630	0.969	0.962
10.92	0.10	0.798	0.794	0.583	0.549	0.928	0.918
165.96	0.10	0.533	0.541	0.181	0.047	0.793	0.741
0.25	0.20	0.896	0.895	0.673	0.647	0.954	0.949
2.48	0.20	0.898	0.896	0.665	0.653	0.958	0.954
49.78	0.20	0.713	0.717	0.415	0.363	0.876	0.864
187.25	0.20	0.595	0.595	0.192	0.120	0.793	0.758
3.25	0.40	0.820	0.813	0.661	0.598	0.916	0.886
64.35	0.40	0.694	0.685	0.451	0.408	0.806	0.777
245.65	0.40	0.565	0.564	0.305	0.208	0.768	0.715

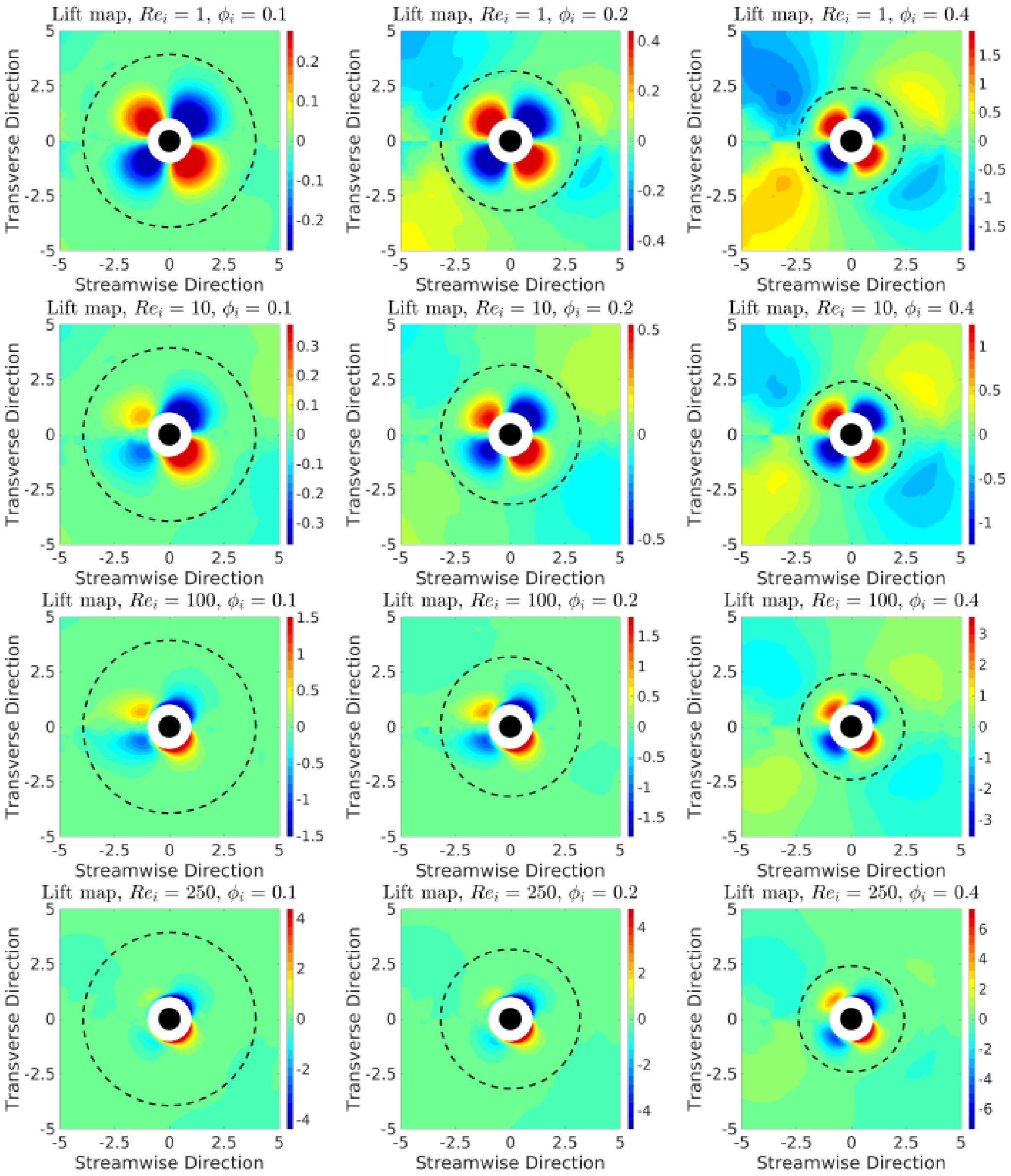
Training and testing performance of binary-interactions and trinary-interactions involved torque models.

Interpretability-Binary Force Maps

Drag Maps



Lift Maps



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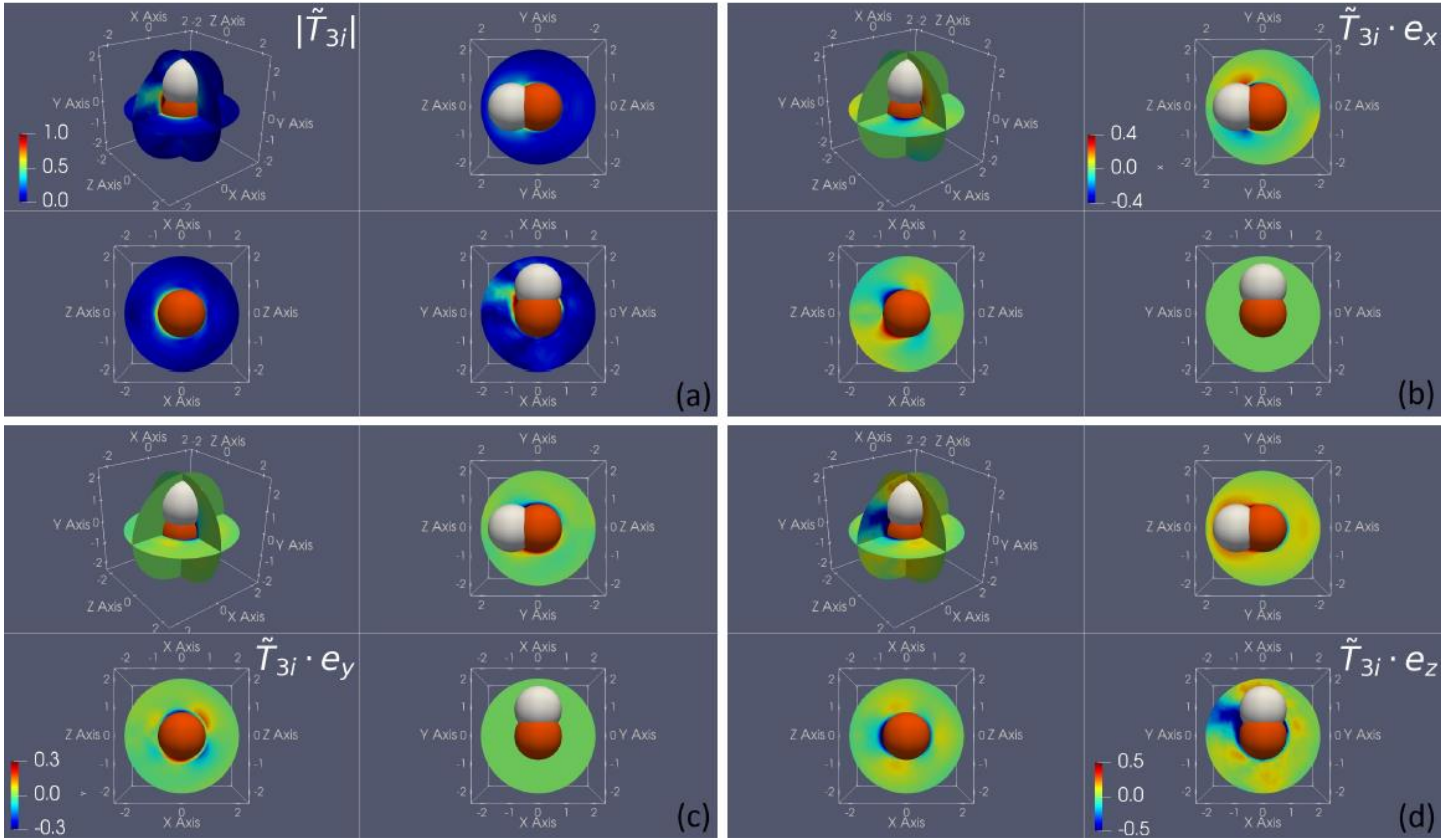
Trinary-interaction Torque Map



First neighbor (white) is at (0, 1.1, 0) relative to reference particle (red). Flow direction is along +*x*.

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Conclusions and Future Work

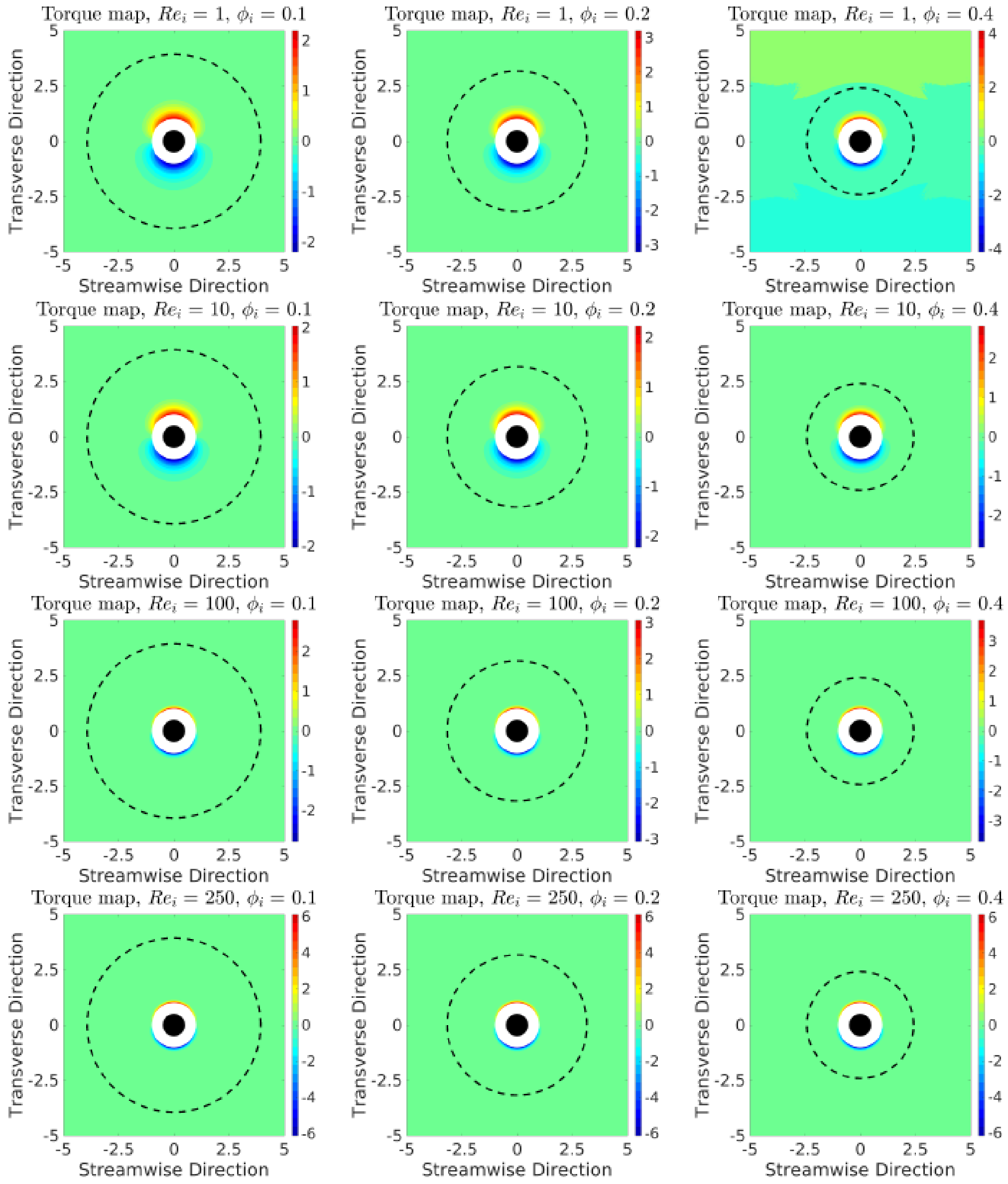
- Building symmetries into neural models makes them robust and generalizable.
- Systematic hierarchical approach (unary, binary, trinary) brings interpretability.
- Extending to moving particle simulations.
- Model deployment in large scale Euler-Lagrange simulations.

Thank You!

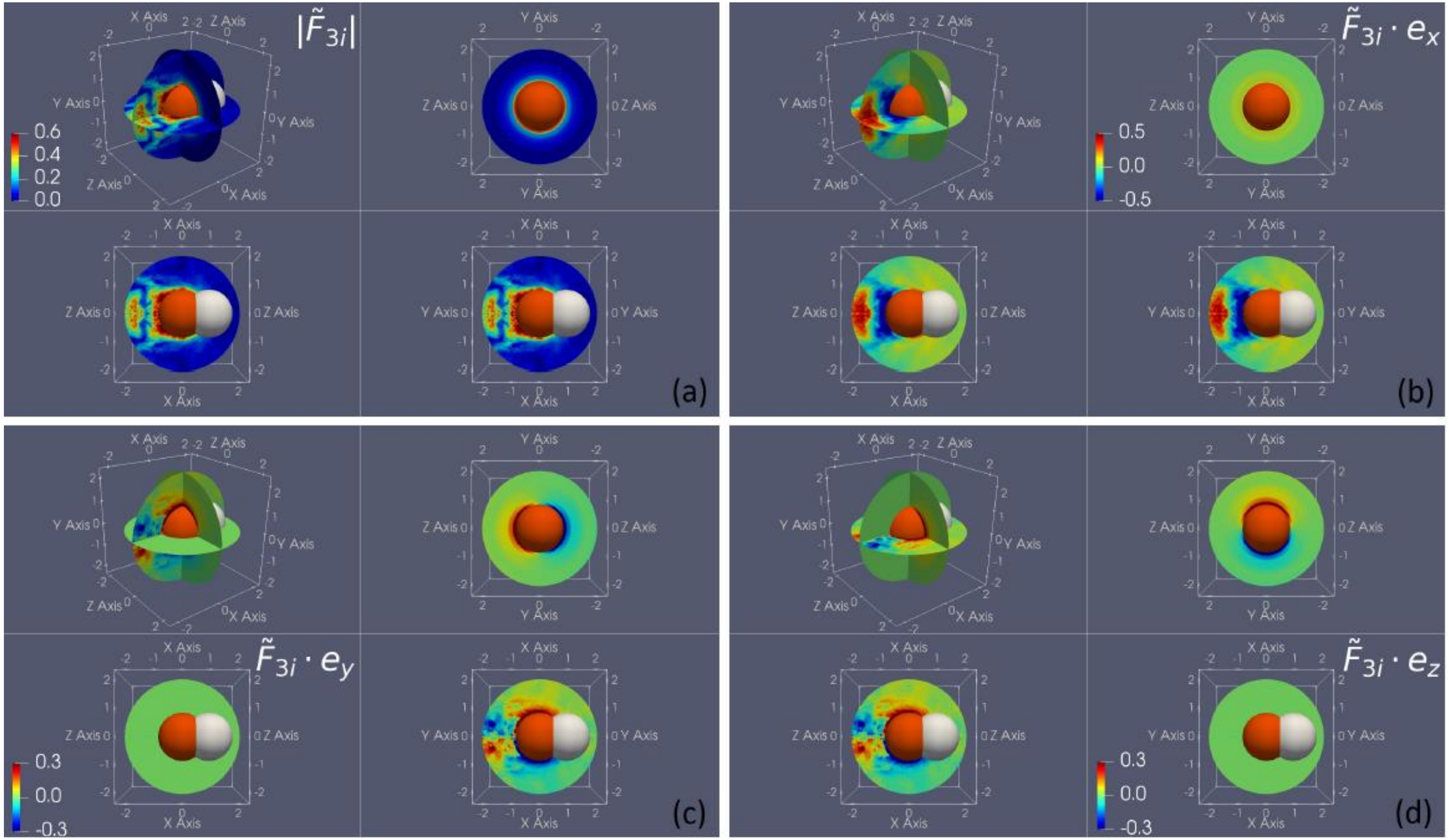
Questions?

Additional Slides

Binary Torque Maps



Trinary-interaction Force Map



First neighbor (white) is at (1.1, 0, 0) relative to reference particle (red). Flow direction is along +*x*.

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