THE UNIVERSITY OF BRITISH COLUMBIA
Chemical & Biological Engineering

Direct numerical simulation of flow past randomly distributed Platonic polyhedrons

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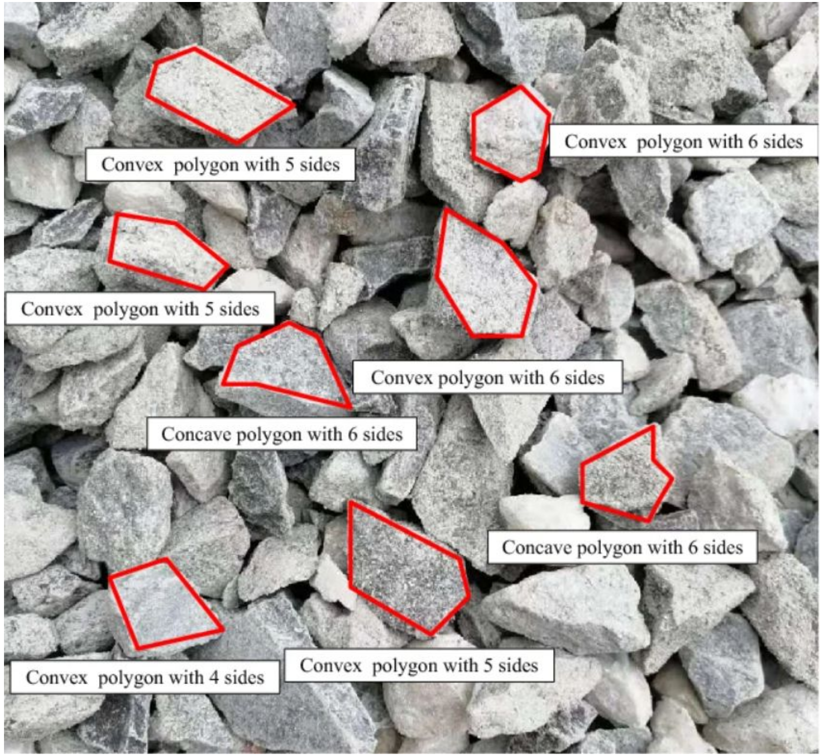
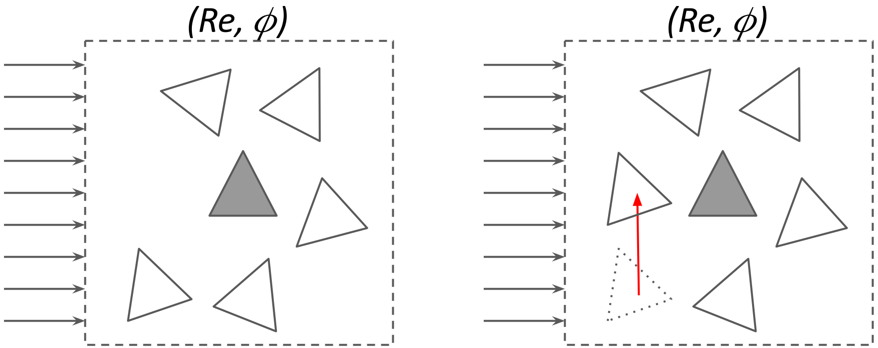
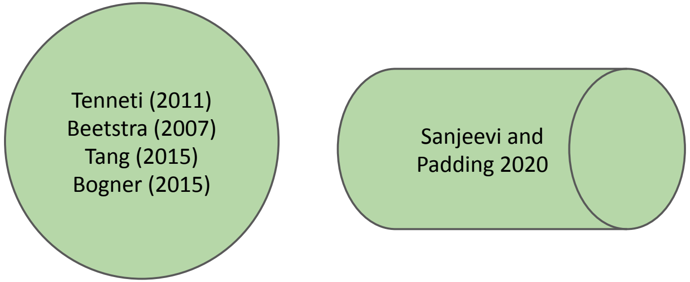
Background



Chen et al., Nature Scientific Reports, 2023

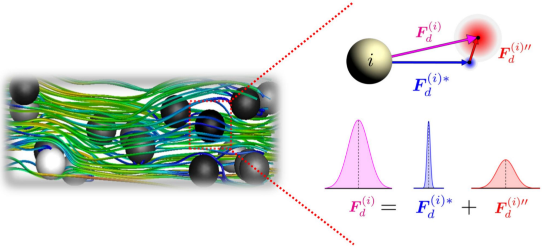


$$\boldsymbol{F}_i = \langle \boldsymbol{F}_i \rangle (Re, \phi, \kappa) + \Delta \boldsymbol{F}_i (Re, \phi, \kappa, \{\boldsymbol{r}_1, ..., \boldsymbol{r}_M\})$$



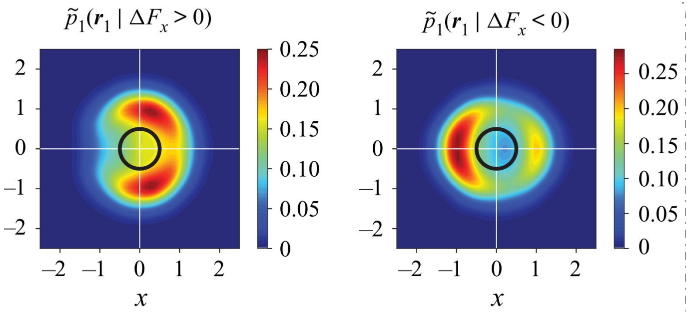
Fluctuating term models

Stochastic model



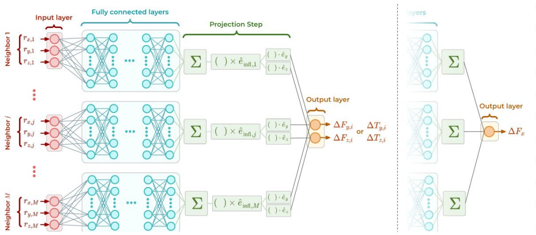
Lattanzi et al. (2022)

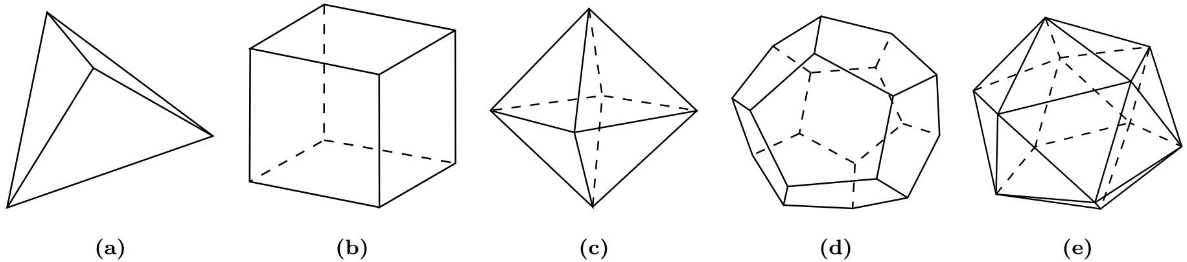
Probability driven model



$$\Delta F_{MPP}(\boldsymbol{R}, Re, \phi) = c_\alpha \, \tilde{p}\,(\boldsymbol{R} \mid \Delta F < 0) + c_\beta \, \tilde{p}\,(\boldsymbol{R} \mid \Delta F > 0)$$

NN (FNN, PINN, CNN, GNN)





Five Platonic polyhedrons with increasing sphericity κ. (a) Tetrahedron, $\kappa = 0.670$, (b) Cube, $\kappa = 0.806$, (c) Octahedron, $\kappa = 0.846$, (d) Dodecahedron, $\kappa = 0.910$, and (e) Icosahedron, $\kappa = 0.940$.

Capture particle DOFs

Accurate

Computationally expensive

Non-scalable on O(1000) cores

Particle-laden flow solver

$$\boldsymbol{\nabla}.\boldsymbol{u} = 0$$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u}.\nabla \boldsymbol{u} = -\boldsymbol{\nabla} p + \mu \nabla^2 \boldsymbol{u} + \boldsymbol{f}_b$$

+

$$\nabla^2 \approx -(1-\partial_{xx})(1-\partial_{yy})(1-\partial_{zz})$$

Converts one 3D problem into three 1D problems !!!

Step 1 → Step 2 → Step 3 → Step 4

Step 1

$$p^{*,n+\frac{1}{2}} = p^{n-\frac{1}{2}} + \phi^{n-\frac{1}{2}}$$

Pressure prediction

Step 2

$$\rho \frac{\boldsymbol{\xi}^{n+1} - \boldsymbol{u}^n}{\Delta t} - \mu \nabla^2 \boldsymbol{u}^n + \nabla p^{*,n+\frac{1}{2}} + \rho \boldsymbol{u}^n.\nabla \boldsymbol{u}^n = \boldsymbol{f}_b$$

$$\rho \frac{\boldsymbol{\eta}^{n+1} - \boldsymbol{\xi}^{n+1}}{\Delta t} - \frac{\mu}{2}\partial_{xx}(\boldsymbol{\eta}^{n+1} - \boldsymbol{\eta}^n) = 0$$

$$\rho \frac{\boldsymbol{\zeta}^{n+1} - \boldsymbol{\eta}^{n+1}}{\Delta t} - \frac{\mu}{2}\partial_{yy}(\boldsymbol{\zeta}^{n+1} - \boldsymbol{\zeta}^n) = 0$$

$$\rho \frac{\boldsymbol{u}^{n+1} - \boldsymbol{\zeta}^{n+1}}{\Delta t} - \frac{\mu}{2}\partial_{zz}(\boldsymbol{u}^{n+1} - \boldsymbol{u}^n) = 0$$

Velocity prediction

Step 3

$$\theta - \partial_{xx}\theta = -\frac{1}{\Delta t}\nabla.\boldsymbol{u}^{n+1}$$

$$\psi - \partial_{yy}\psi = \theta$$

$$\phi^{n+\frac{1}{2}} - \partial_{zz}\phi^{n+\frac{1}{2}} = \psi$$

Penalty step

Step 4

$$p^{n+\frac{1}{2}} = p^{n-\frac{1}{2}} + \phi^{n+\frac{1}{2}} - \frac{\mu}{2}\nabla.(\boldsymbol{u}^{n+1} + \boldsymbol{u}^n)$$

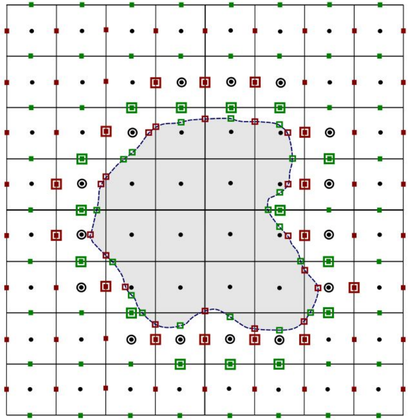
Pressure correction

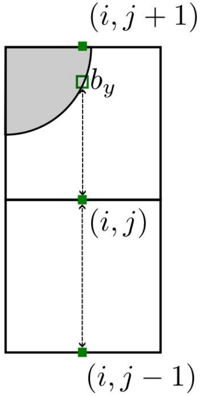
Goyal and Wachs (2023, 2024)

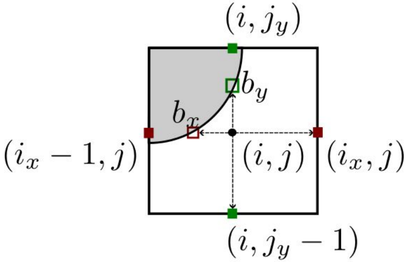
Fixed rigid bodies in solver

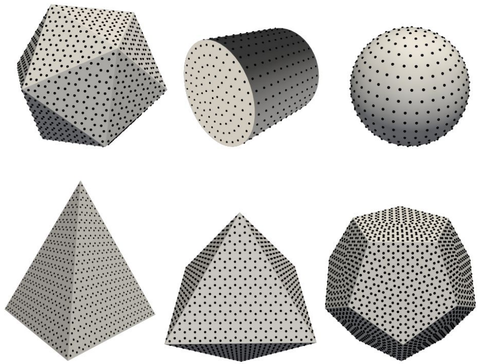
Modifications for particle-laden simulations

- Nodes presence in particles or fluid
- Diffusion stencil
- Divergence stencil
- Surface stress





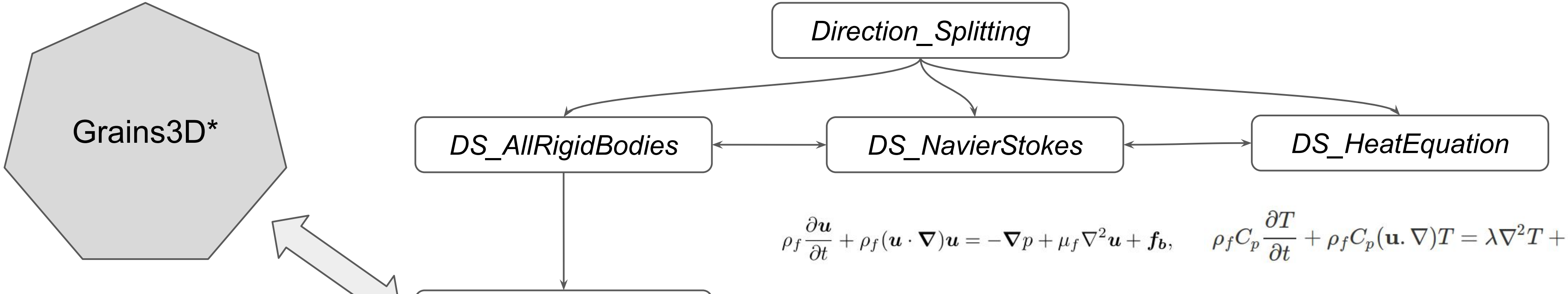




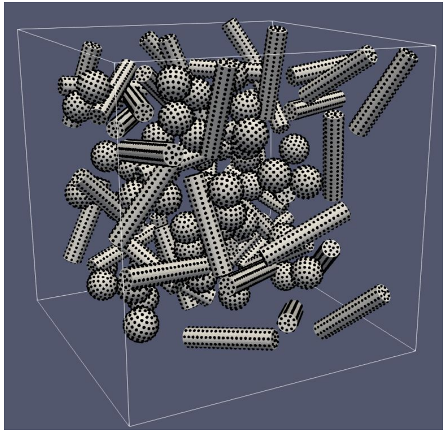
These methods can work for any particle shape.

Goyal and Wachs (2023, 2024)

Overall Framework in PacIFiC

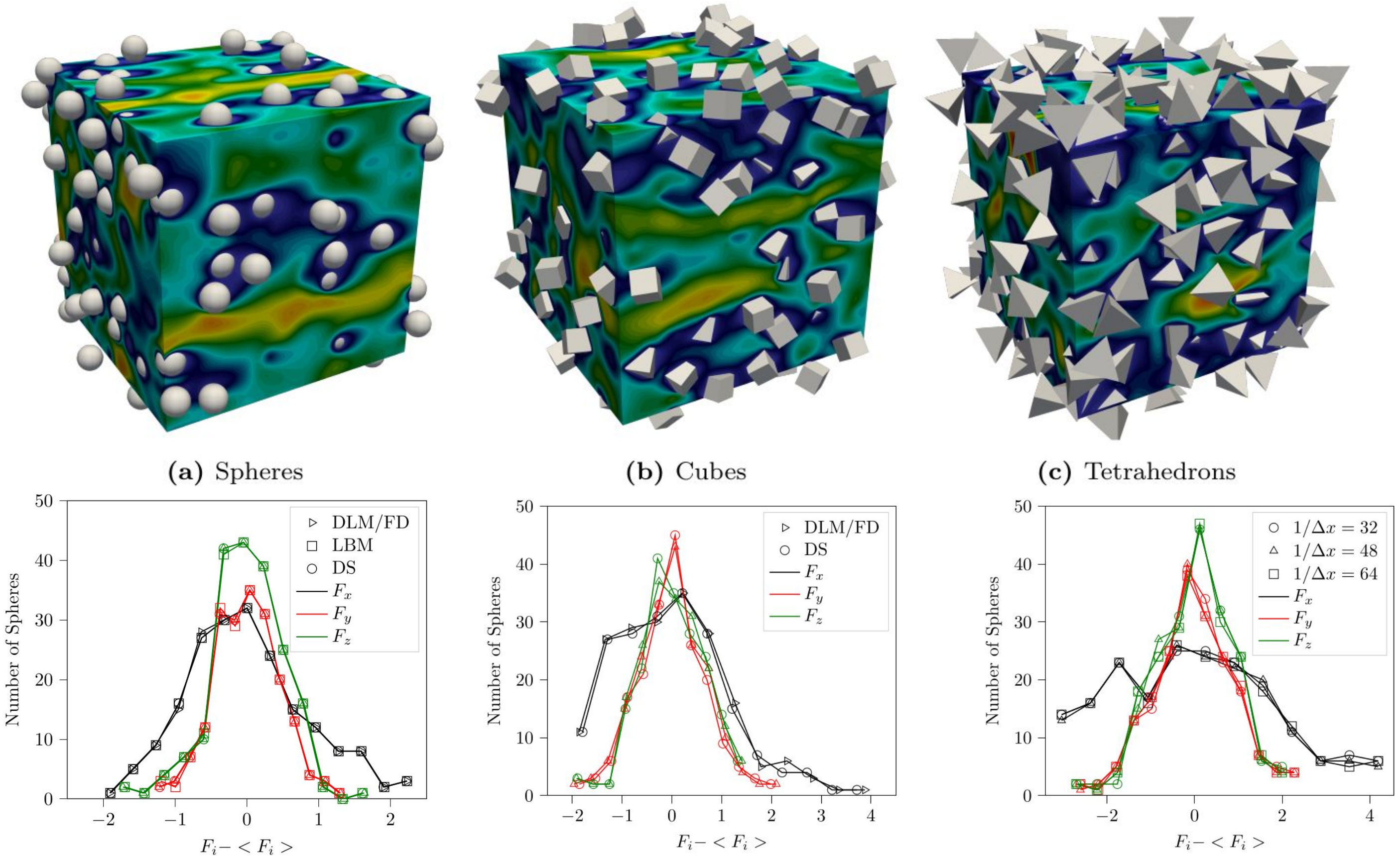


$$\rho_f \frac{\partial \boldsymbol{u}}{\partial t} + \rho_f (\boldsymbol{u} \cdot \boldsymbol{\nabla}) \boldsymbol{u} = -\boldsymbol{\nabla} p + \mu_f \nabla^2 \boldsymbol{u} + \boldsymbol{f_b}, \qquad \rho_f C_p \frac{\partial T}{\partial t} + \rho_f C_p (\mathbf{u}. \nabla) T = \lambda \nabla^2 T + Q$$



* A. Wachs et al. (2012)

Validation: Random non-spherical rigid bodies



Data generation

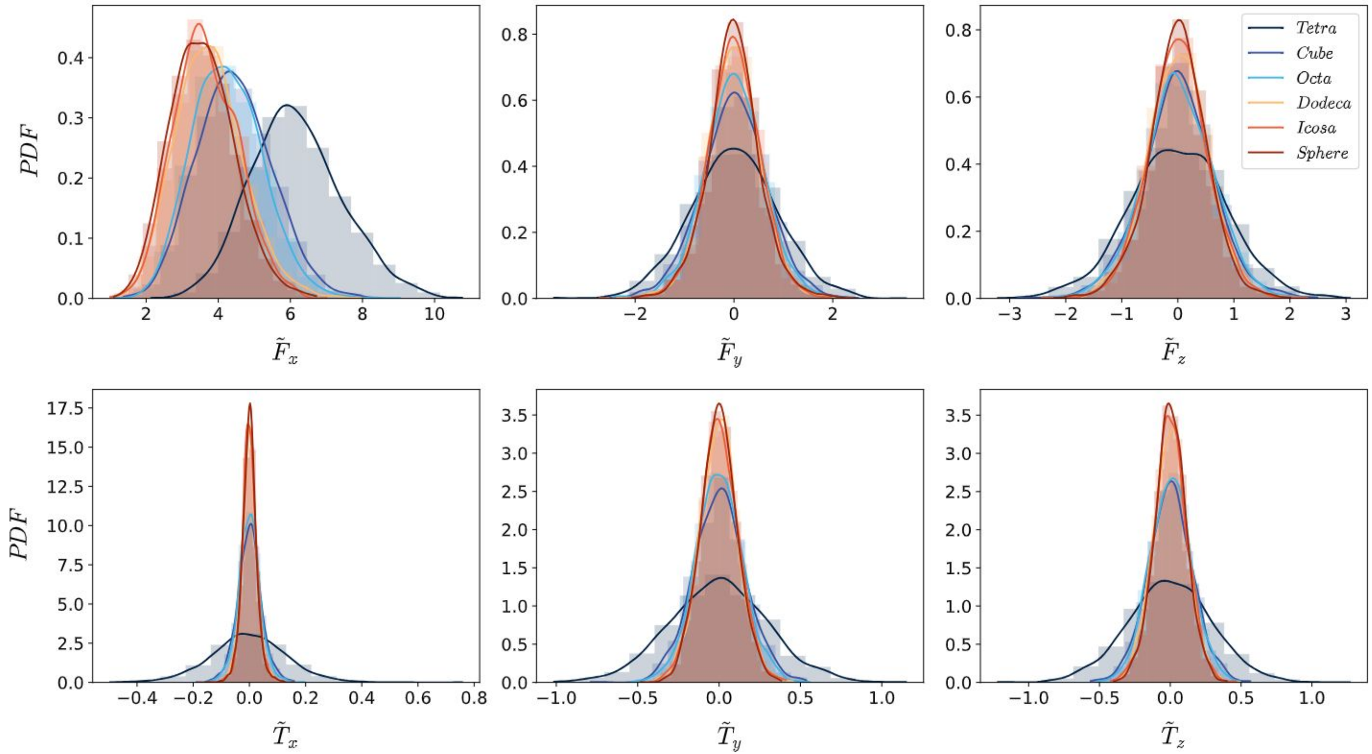
Summary of parameters used for PR-DNS of a random array of each Platonic polyhedron at $\mathcal{R}e = 1, 10, 100$.

ϕ	L	N_{RB}	$1/\Delta\tilde{x}$	FV grid cells
0.05	$23D_{eq}$	1146	32	$\sim 399 \times 10^6$
0.10	$23D_{eq}$	2292	32	$\sim 399 \times 10^6$
0.20	$18D_{eq}$	2228	40	$\sim 373 \times 10^6$

(a) Tetrahedrons (b) Cubes (c) Octahedrons (d) Dodecahedrons (e) Icosahedrons

Spatial distribution of Platonic polyhedrons in a tri-periodic box at $\phi = 0.2$.

Force and torque distributions

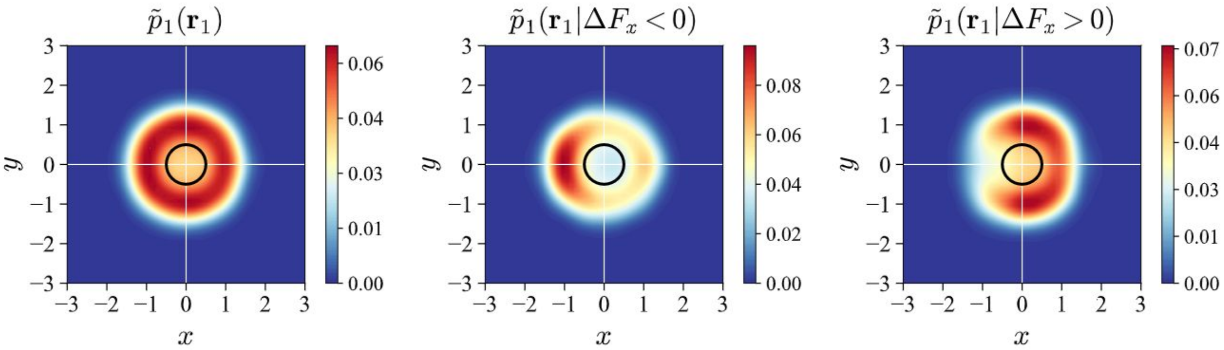


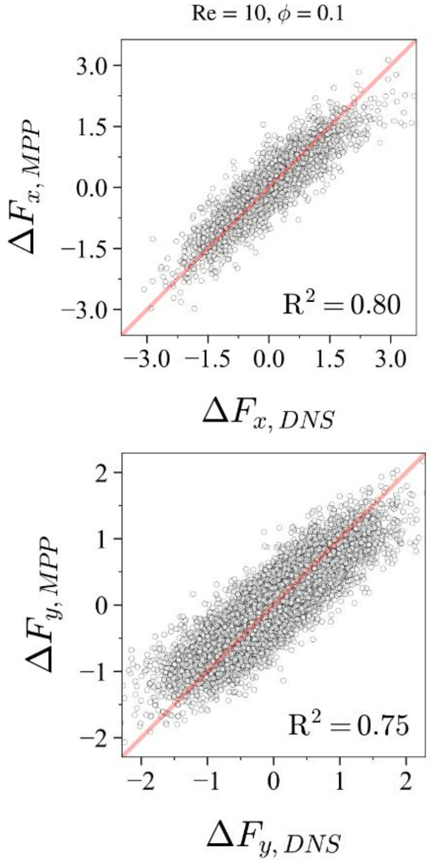
Distribution of normalized force and torque for flow past Platonic polyhedrons at $Re = 10$ and $\phi = 0.1$.

Microstructure-based Probability-driven Point-particle model

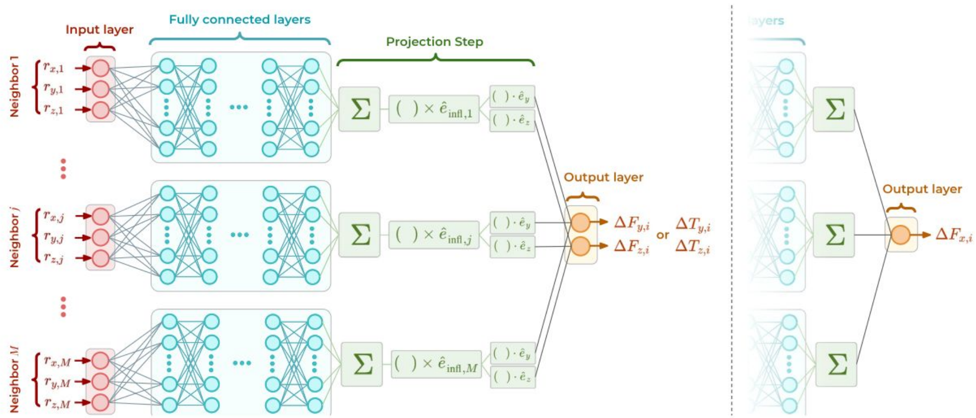
$$\Delta F_{MPP}(\boldsymbol{R}, Re, \phi) = c_\alpha\, \tilde{p}\,(\boldsymbol{R} \mid \Delta F < 0) + c_\beta\, \tilde{p}\,(\boldsymbol{R} \mid \Delta F > 0)$$

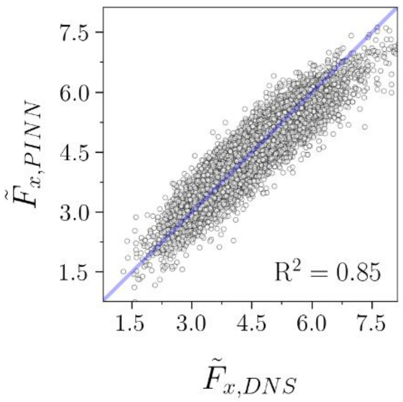
$$\Delta F_{MPP}(\boldsymbol{R}, Re, \phi) = \sum_{j=1}^{M} c_{\alpha,j}\, \tilde{p}_j\left(\boldsymbol{r}_j \mid \Delta F < 0\right) + \sum_{j=1}^{M} c_{\beta,j}\, \tilde{p}_j\left(\boldsymbol{r}_j \mid \Delta F > 0\right)$$

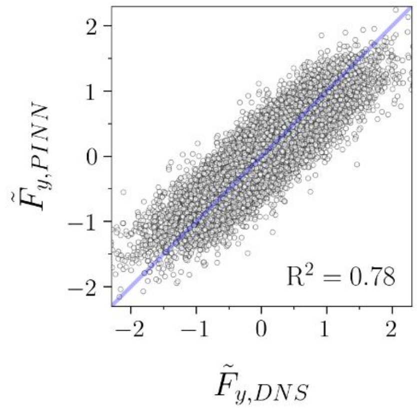




Physics Informed Neural Network (PINN)

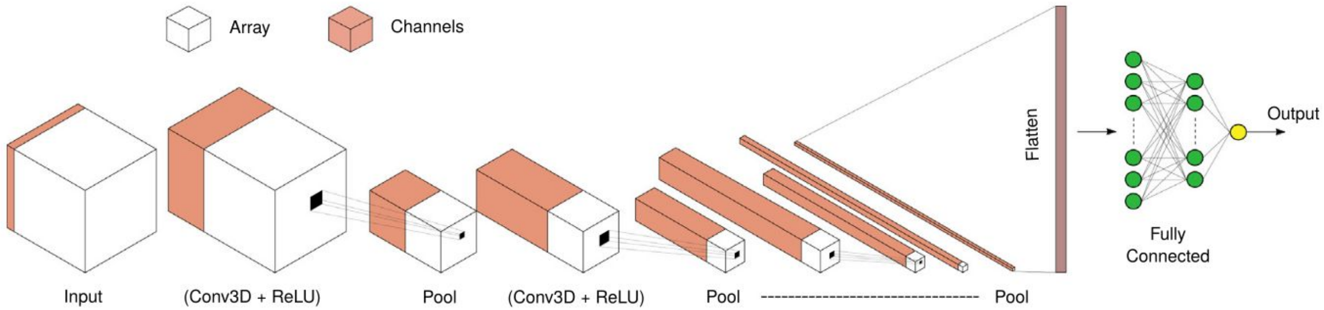


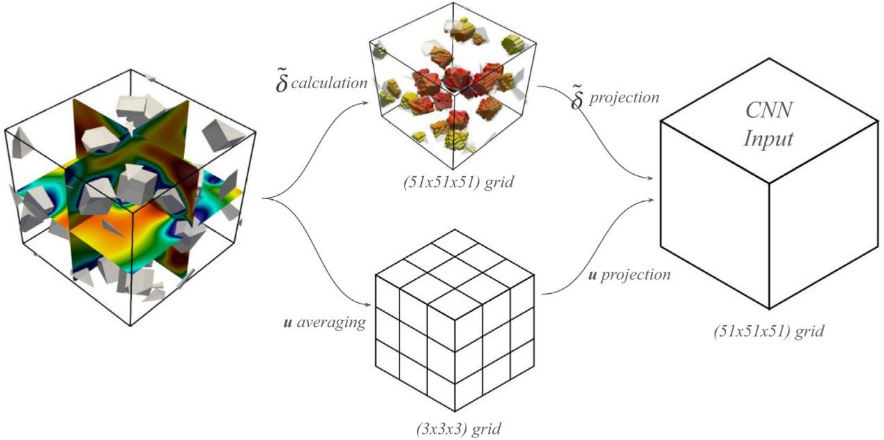


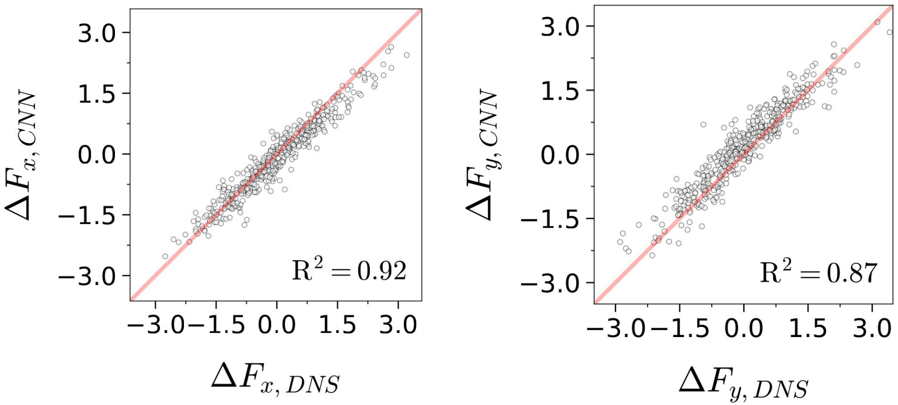


– *Each NN block handles one neighbor with three input parameters.*
– *All NN blocks share the same set of parameters.*

Convolutional Neural Network







PINN vs. CNN

PINN

ϕ	$\mathcal{R}e$	Tetrahedron $\tilde{F}_x$	Tetrahedron $\tilde{\mathbf{F}}_L$	Tetrahedron $\tilde{\mathbf{T}}_L$	Cube $\tilde{F}_x$	Cube $\tilde{\mathbf{F}}_L$	Cube $\tilde{\mathbf{T}}_L$	Octahedron $\tilde{F}_x$	Octahedron $\tilde{\mathbf{F}}_L$	Octahedron $\tilde{\mathbf{T}}_L$	Dodecahedron $\tilde{F}_x$	Dodecahedron $\tilde{\mathbf{F}}_L$	Dodecahedron $\tilde{\mathbf{T}}_L$	Icosahedron $\tilde{F}_x$	Icosahedron $\tilde{\mathbf{F}}_L$	Icosahedron $\tilde{\mathbf{T}}_L$
0.05	1	0.83	0.79	0.81	0.91	0.83	0.89	0.89	0.83	0.90	0.92	0.86	0.91	0.93	0.86	0.91
	10	0.79	0.69	0.61	0.87	0.77	0.81	0.83	0.78	0.82	0.88	0.82	0.84	0.87	0.81	0.84
	100	0.47	0.01	0.03	0.61	0.43	0.07	0.56	0.40	0.15	0.64	0.70	0.41	0.63	0.73	0.60
0.1	1	0.80	0.72	0.76	0.87	0.82	0.89	0.87	0.82	0.89	0.89	0.84	0.90	0.88	0.84	0.91
	10	0.76	0.63	0.60	**0.85**	**0.78**	**0.85**	0.82	0.76	0.84	0.86	0.79	0.86	0.85	0.78	0.88
	100	0.47	0.13	0.08	0.60	0.47	0.16	0.60	0.50	0.19	0.70	0.71	0.57	0.65	0.72	0.67
0.2	1	0.66	0.56	0.60	0.77	0.73	0.86	0.80	0.74	0.87	0.82	0.80	0.89	0.82	0.78	0.90
	10	0.65	0.50	0.47	0.77	0.70	0.80	0.80	0.71	0.81	0.81	0.76	0.86	0.81	0.75	0.87
	100	0.45	0.20	0.08	0.60	0.42	0.21	0.64	0.46	0.20	0.68	0.65	0.52	0.71	0.65	0.60

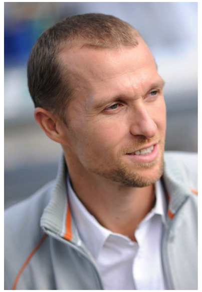
CNN

0.05	1	0.91	0.88	0.85	0.88	0.96	0.95	0.94	0.96	0.94	0.96	0.97	0.97	0.97	0.97	0.93
	10	0.92	0.73	0.66	0.95	0.93	0.87	0.94	0.92	0.87	0.97	0.94	0.90	0.97	0.94	0.82
	100	0.70	0.58	0.40	0.76	0.51	0.34	0.78	0.65	0.14	0.82	0.76	0.34	0.83	0.77	0.34
0.1	1	0.84	0.81	0.77	0.94	0.95	0.92	0.92	0.95	0.94	0.95	0.96	0.96	0.95	0.95	0.96
	10	0.84	0.75	0.63	0.92	0.87	0.86	0.93	0.90	0.90	0.95	0.93	0.91	0.95	0.95	0.92
	100	0.70	0.58	0.25	0.77	0.56	0.08	0.85	0.55	0.10	0.84	0.75	0.44	0.80	0.73	0.57
0.2	1	0.72	0.69	0.59	0.81	0.83	0.87	0.83	0.86	0.84	0.85	0.91	0.93	0.87	0.93	0.94
	10	0.72	0.61	0.52	0.80	0.81	0.81	0.84	0.83	0.77	0.85	0.89	0.88	0.86	0.87	0.90
	100	0.53	0.42	0.25	0.62	0.49	0.24	0.68	0.49	0.14	0.71	0.67	0.43	0.73	0.66	0.55

Relevant Publications

- **Aashish Goyal** and Anthony Wachs, “An accurate and scalable direction-splitting solver for flows laden with non-spherical rigid bodies - Part 1: fixed rigid bodies”, **Communication in Computational Physics** 2023
- Antoine Morente, **Aashish Goyal** and Anthony Wachs, “A Highly Scalable Direction Splitting Solver on Regular Cartesian Grid to Compute Flow in Complex Geometries Described by STL files”, **Fluids** 2023
- **Aashish Goyal** and Anthony Wachs, “An accurate and scalable direction-splitting solver for flows laden with non-spherical rigid bodies - Part 2: moving rigid bodies”, **Computers and Fluids** 2024
- **Aashish Goyal,** Gai Guodong, Zihao Cheng, and Anthony Wachs, “Flow past a random array of statistically homogeneously distributed stationary Platonic polyhedrons: Data analysis, Probability maps, and PINN model”, **International Journal of Multiphase Flows** 2024

Special Thanks !!!



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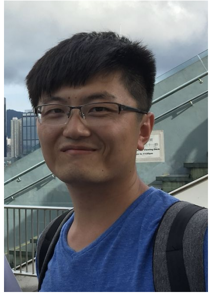

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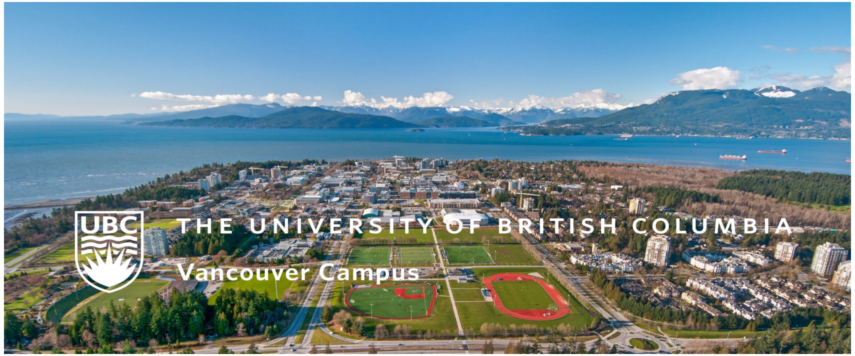

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