Developing drag models for non-spherical particles through machine learning

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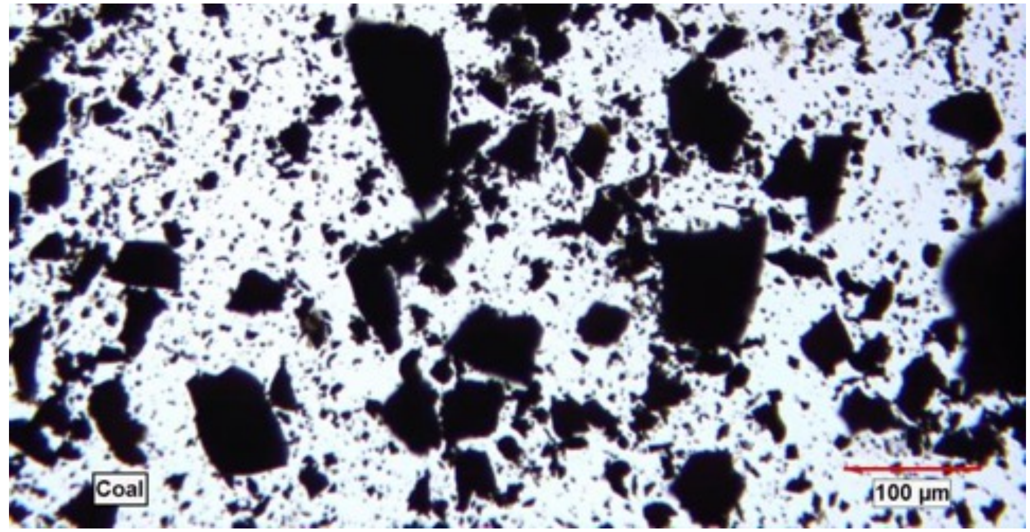
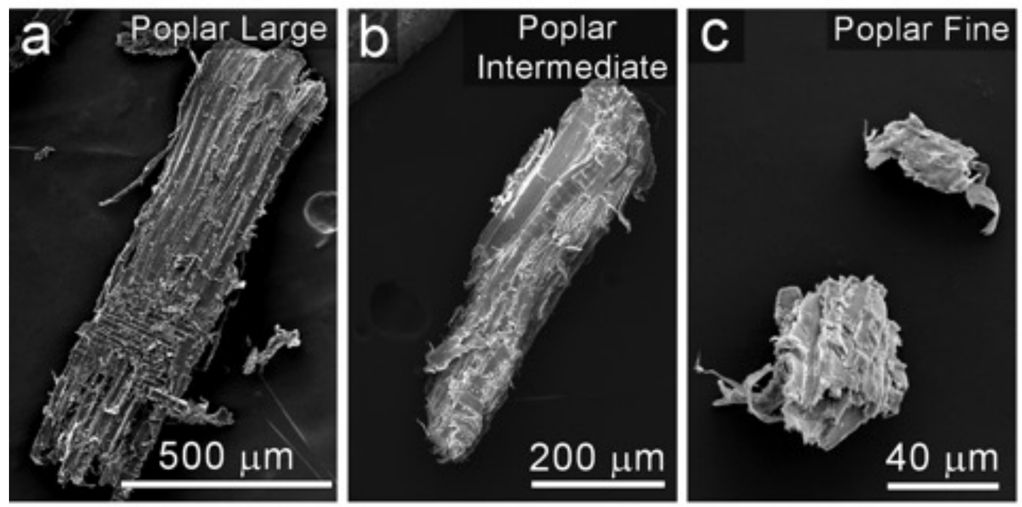
We would like to thank William A. Rogers, Cheng Li, Xiongjun Wu, Avinash Vaidheeswaran, Mehrdad Shahnam, Jordan Musser, Jeff Dietiker, and many others in the Multiphase Flow Science group at NETL

Motivation: coal and biomass gasification

- Thermal conversion systems are very challenging to model:
  - Particles have complex shapes, a broad range of sizes, shapes and density.
  - Non-spherical particle interact with other particles.
  - Force closures are needed for non-spherical particles, i.e. drag and lift (maybe even other unsteady forces such as added mass and history force)

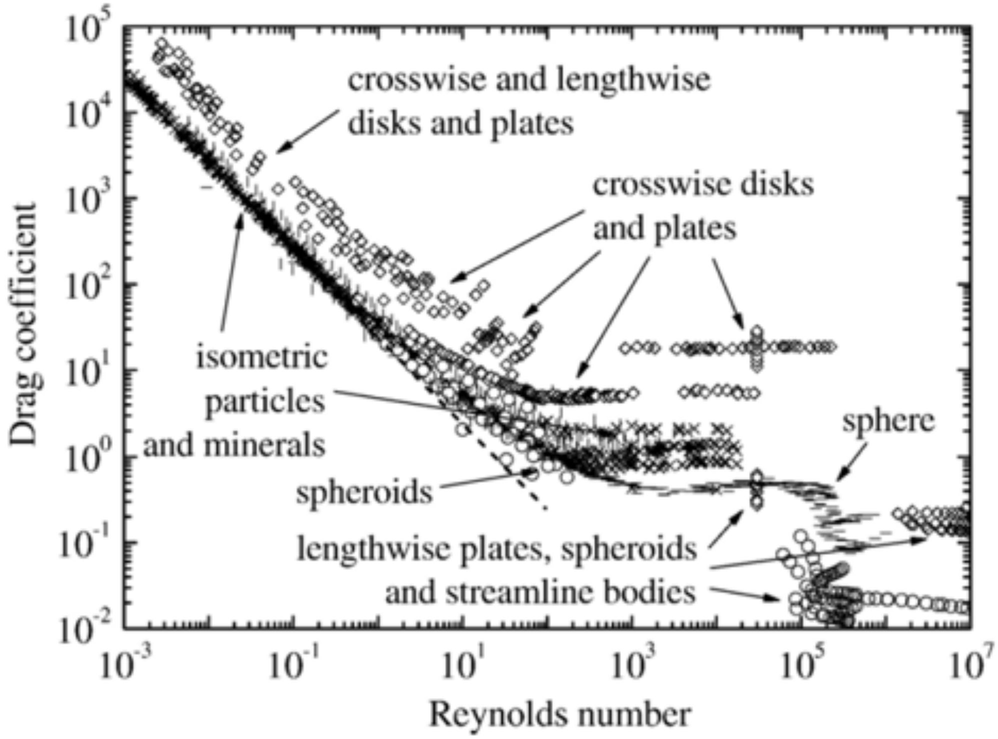




Objective: develop validated drag models for non-spherical particles

Drag Coefficient on Single Spherical and Non-Spherical Particle

Different drag correlations proposed by different groups based on the Reynolds number and sphericity (Φ) projected to different directions.



A. Hölzer, M. Sommerfeld / Powder Technology 184 (2008) 361–365

Sphere (Stokes flow): $c_D = \dfrac{24}{Re}$

Non-spherical particle (Stokes flow):

$$c_D = \frac{8}{\mathrm{Re}}\frac{1}{\sqrt{\Phi_\perp}} + \frac{16}{\mathrm{Re}}\frac{1}{\sqrt{\Phi}}$$

D. Leith, Aerosol Sci. Tech. 6 (1987) 153

Non-spherical particle ($Re < 10^5$):

$$\frac{c_\mathrm{d}}{K_2} = \frac{24}{\mathrm{Re}K_1 K_2}\left(1 + 0.1118(\mathrm{Re}K_1 K_2)^{0.0567}\right) + \frac{0.4305}{1 + \frac{3305}{\mathrm{Re}K_1 K_2}}$$

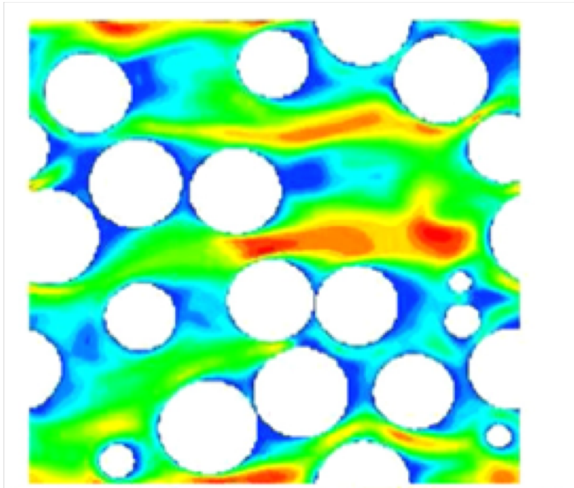
$$K_2 = 10^{1.8148(-\log\phi)^{0.5743}}$$ (Newton factor)

G. H. Ganser, Powder Technol. 77 (1993) 143

Non-spherical particle ($Re < 10^5$):

$$c_D = \frac{8}{\mathrm{Re}}\frac{1}{\sqrt{\Phi_\parallel}} + \frac{16}{\mathrm{Re}}\frac{1}{\sqrt{\Phi}} + \frac{3}{\sqrt{\mathrm{Re}}}\frac{1}{\Phi^{\frac{3}{4}}} + 0.4210^{0.4(-\log\Phi)^{0.2}}\frac{1}{\Phi_\perp}$$

Drag Coefficient on Packed Spherical Particle

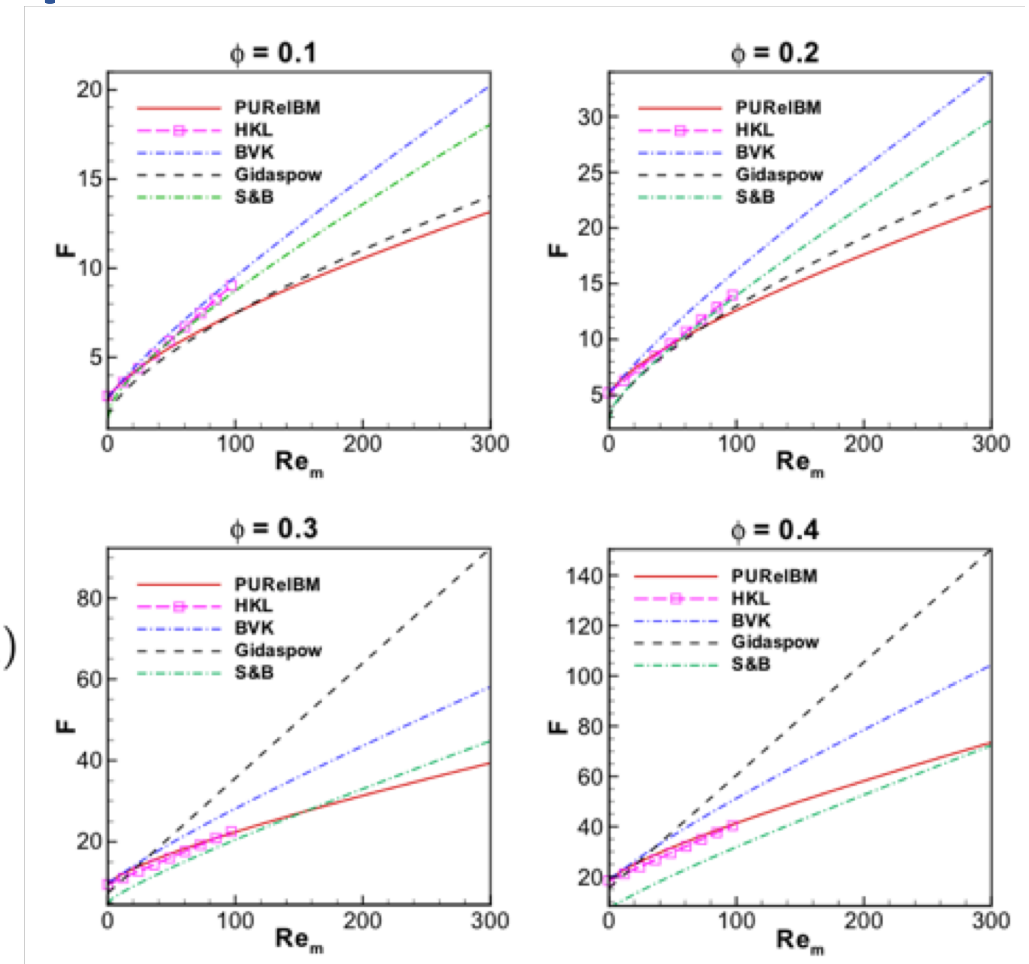


Tenneti et al. (2011)

$$F(\phi, \mathrm{Re}_m) = \frac{\boxed{F_{\mathrm{isol}}\left(\mathrm{Re}_m\right)}}{(1-\phi)^3} + F_\phi(\phi) + F_{\phi,Re_m}(\phi, \mathrm{Re}_m)$$

$$F_\phi(\phi) = \frac{5.81\phi}{(1-\phi)^3} + 0.48\frac{\phi^{1/3}}{(1-\phi)^4}$$

$$F_{\phi,\mathrm{Re}_m}(\phi, \mathrm{Re}_m) = \phi^3\,\mathrm{Re}_m\left(0.95 + \frac{0.61\phi^3}{(1-\phi)^2}\right).$$

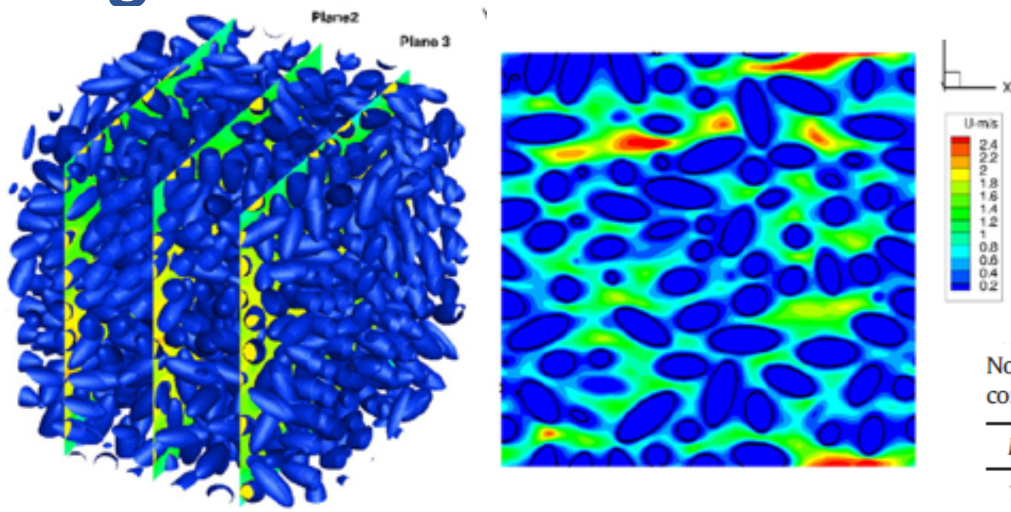


Tenneti et al. (2011)

Wen & Yu (1966) for dilute suspensions and Ergun's equation (Ergun 1952) for denser systems are the earliest experimental efforts.

Tenneti et al. (2011);
Hill et al. (2001);
Beetstra et al. (2007);
Gidaspow (1986);
Syamlal and O'Brien (1987);

Drag Coefficient on Packed Non-spherical Particle



L. He et al. / Powder Technology 313 (2017) 332–343

$$F(\phi, \mathrm{Re}_m) = \frac{\boxed{F_{\mathrm{isol}}(\mathrm{Re}_m)}}{(1-\phi)^3} + F_\phi(\phi) + F_{\phi,Re_m}(\phi, \mathrm{Re}_m)$$

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$$F_{\phi,\mathrm{Re}_m}(\phi, \mathrm{Re}_m) = \phi^3\,\mathrm{Re}_m\left(0.95 + \frac{0.61\phi^3}{(1-\phi)^2}\right).$$

Normalized mean drag force from current simulation compare to F&H, T&H and T&Z correlation.

Re	Φ	IBM	F&H	% diff	T&H	% diff	T&Z	% diff
10	10%	3.58	2.78	−22.51%	3.65	1.99%	3.49	−2.72%
50		5.82	5.66	−2.80%	6.26	7.47%	5.92	1.67%
100		8.46	8.76	−3.58%	9.14	8.14%	8.29	−1.96%
200		14.10	14.45	2.53%	14.60	3.61%	12.32	−12.62%
10	20%	6.87	4.39	−35.10%	6.57	−4.34%	6.30	−8.37%
50		11.13	8.95	−19.66%	10.43	−6.28%	9.88	−11.29%
100		15.81	13.66	−13.57%	14.74	−6.75%	13.41	−15.16%
200		24.97	22.02	−11.78%	22.89	−8.30%	19.47	−22.01%
10	30%	13.14	7.46	−43.18%	11.98	−8.81%	11.57	−11.89%
50		20.20	15.38	−23.83%	18.38	−9.02%	17.56	−13.06%
100		27.58	23.29	−15.56%	25.59	−7.21%	23.63	−14.31%
200		42.82	36.77	−14.11%	39.34	−8.13%	34.27	−19.97%
10	35%	19.38	10.85	−44.01%	16.41	−15.32%	15.99	−17.46%
50		26.83	21.42	−20.16%	25.02	−6.75%	24.20	−9.83%
100		36.59	34.39	−6.01%	34.81	−4.86%	32.66	−10.75%
200		57.76	60.34	4.46%	53.52	−7.34%	47.64	−17.53%

$$\boxed{c_D = \frac{8}{\mathrm{Re}}\frac{1}{\sqrt{\Phi_\parallel}} + \frac{16}{\mathrm{Re}}\frac{1}{\sqrt{\Phi}} + \frac{3}{\sqrt{\mathrm{Re}}}\frac{1}{\Phi^{\frac{3}{4}}} + 0.4210^{0.4(-\log\Phi)^{0.2}}\frac{1}{\Phi_\perp}}$$

$F_{\mathrm{isol}}(\mathrm{Re}_m)$ is the isolated drag model.

Human Learning versus Machine Learning

Human Learning

Sphere (Stokes flow): $c_D = \frac{24}{Re}$

add non-spherical shape

Non-spherical particle (Stokes flow):

$$c_D = \frac{8}{\mathrm{Re}} \frac{1}{\sqrt{\Phi_\perp}} + \frac{16}{\mathrm{Re}} \frac{1}{\sqrt{\Phi}}$$

D. Leith, Aerosol Sci. Tech. 6 (1987) 153

add large Re

Non-spherical particle ($Re < 10^5$):

$F_{\text{isol}}\left(\mathrm{Re}_m\right)$

add concentration

$$F(\phi, \mathrm{Re}_m) = \frac{F_{\text{isol}}\left(\mathrm{Re}_m\right)}{(1-\phi)^3} + F_\phi(\phi) + F_{\phi,Re_m}(\phi, \mathrm{Re}_m)$$

Machine Learning

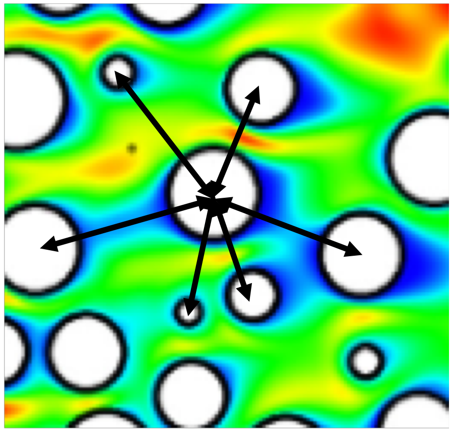
$$\boldsymbol{F}_i = \langle \boldsymbol{F}_i \rangle (Re, \phi) + \Delta \boldsymbol{F}_i(Re, \phi, \{\boldsymbol{r}_{j=1}, \ldots, \boldsymbol{r}_{j=M}\}),$$
$$\boldsymbol{T}_i = \Delta \boldsymbol{T}_i(Re, \phi, \{\boldsymbol{r}_{j=1}, \ldots, \boldsymbol{r}_{j=M}\}),$$

Seyed-Ahmadi and Wachs (2020)

Neighbor configuration

input features for ANN

$[Re, \phi, x_1, y_1, z_1, x_2, y_2, z_2 \ldots x_n, y_n, z_n]$



He and Tafti 2019

Still spherical particles

Problems

Curse of dimensionality:
As the number of features or dimensions grows, the amount of data we need to generate grows exponentially.

1 neighbor Input: $\boldsymbol{r}_j = (x_j, y_j, z_j)$ Output: F_d, c_d $D_1 = 3, \quad N_1 = 1000$

15 neighbor Input: $15 \times 3 = 45$ Output: F_d, c_d $D_2 = 45, \ N_2 = N_1^{D_2/D_1} = 1000^{15}$

Table 1
Number of spherical particles tested at each solid fraction.

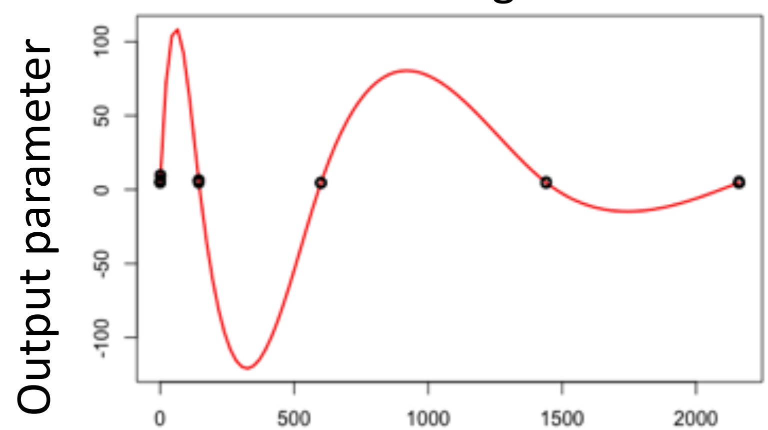
Number of particles (N)	$\phi = 0.1$	191
	$\phi = 0.2$	382
	$\phi = 0.3$	573
	$\phi = 0.35$	669

each particle are collected, to yield 21,780 data points. All forces are further normalized using the Stokes-Einstein relation:

The input is a vector containing 47 features (1 Reynolds number, 1 solid fraction, relative distance in(x,y,z) from the nearest 15 neighboring particles).

He and Tafti 2019

Overfitting



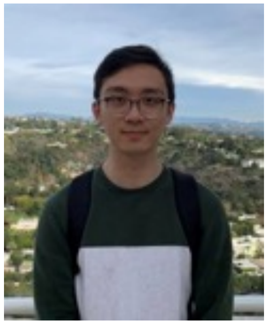
Input parameter

1. Reduce the number of dimensions
2. Increase the sample size

Introduce our team and methodology

Subteam 1: Experiment

Rui Ni



Xu Xu

Subteam 2: Simulation

Gretar Tryggvason

Jiacai Lu

Diagnostic methods

Drop tower (Re, Φ)

Dimension reduction

Particle-resolved DNS

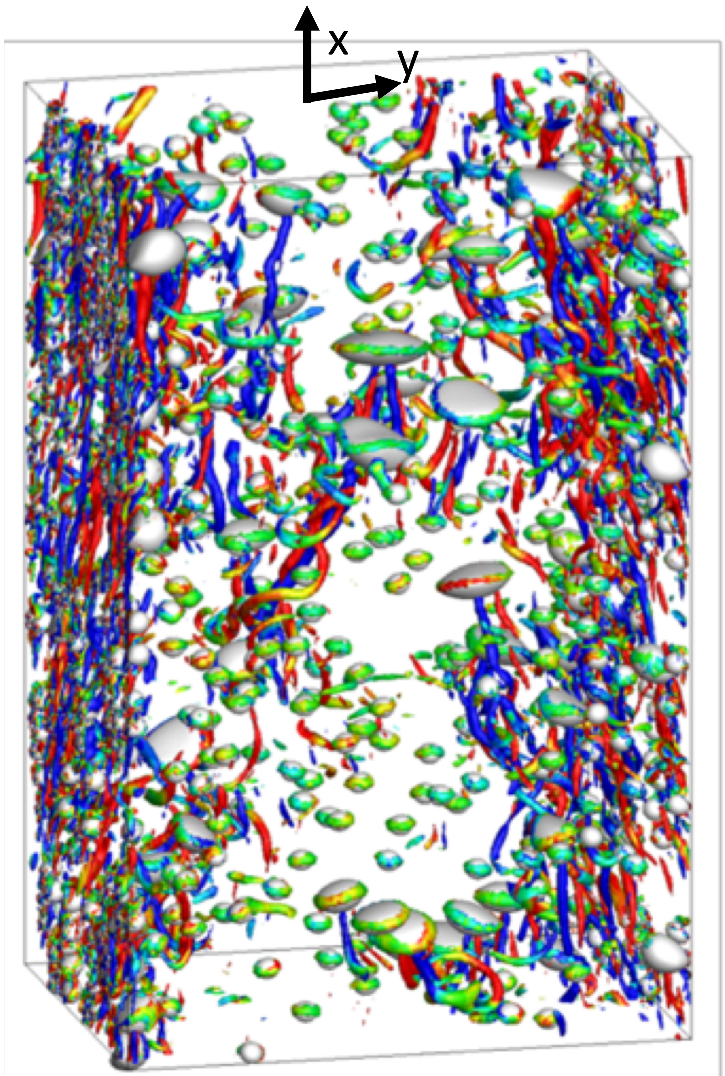
Training

Training

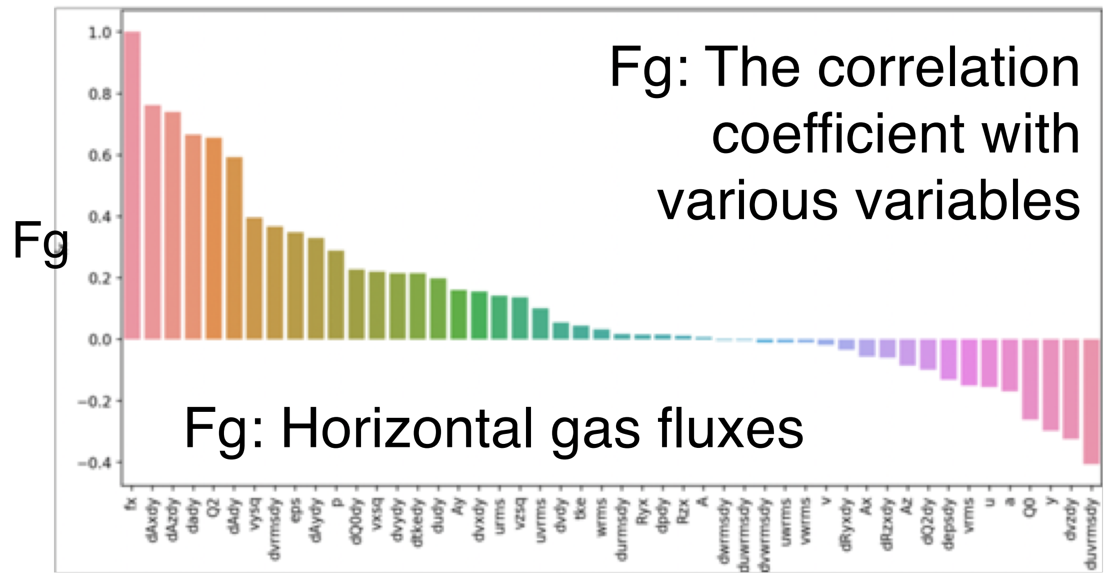
Validation

Validation

Using Machine Learning for closure terms in multiphase flow modeling

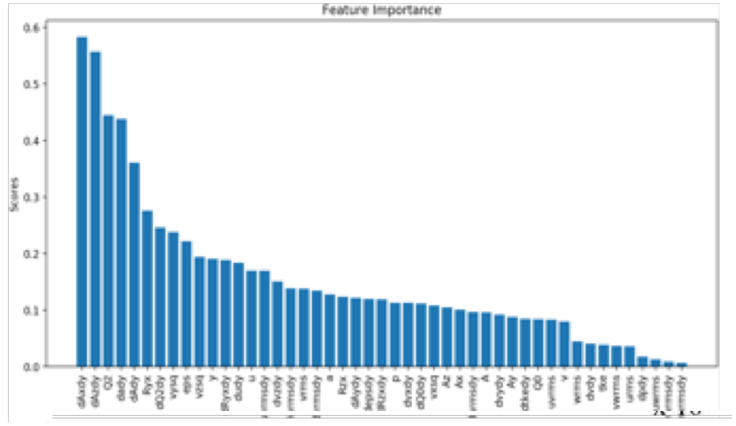


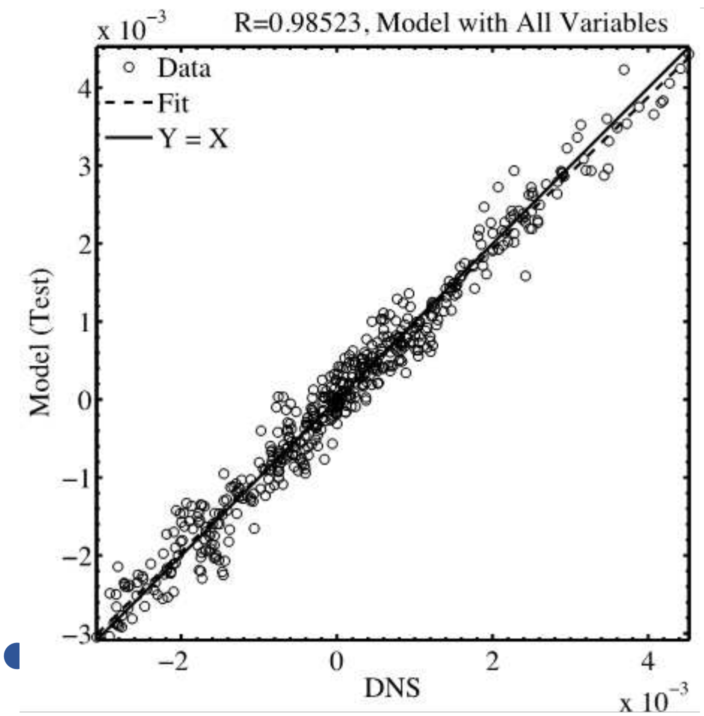
For turbulent flow, the fluxes depend both on resolved variables like void fraction and vertical velocity and on variables describing the average state of the unresolved state.

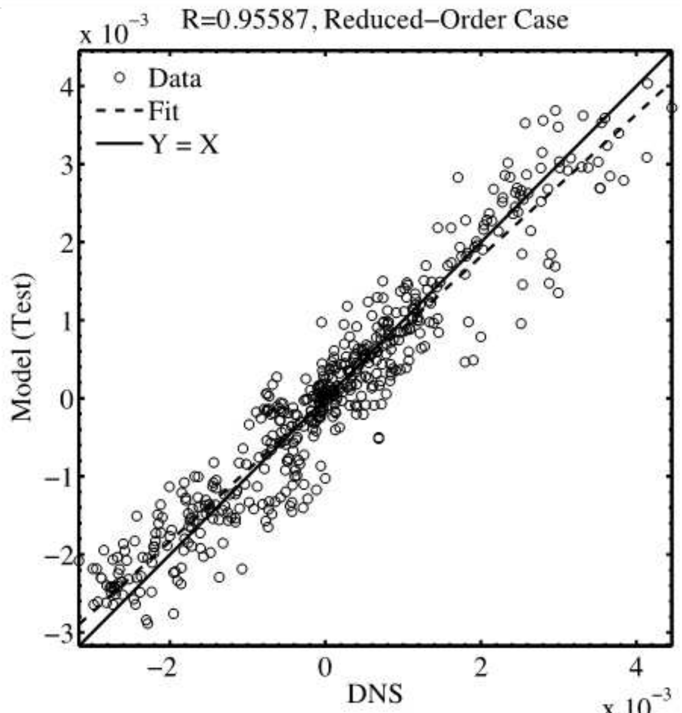


Using Machine Learning for closure terms in multiphase flow modeling

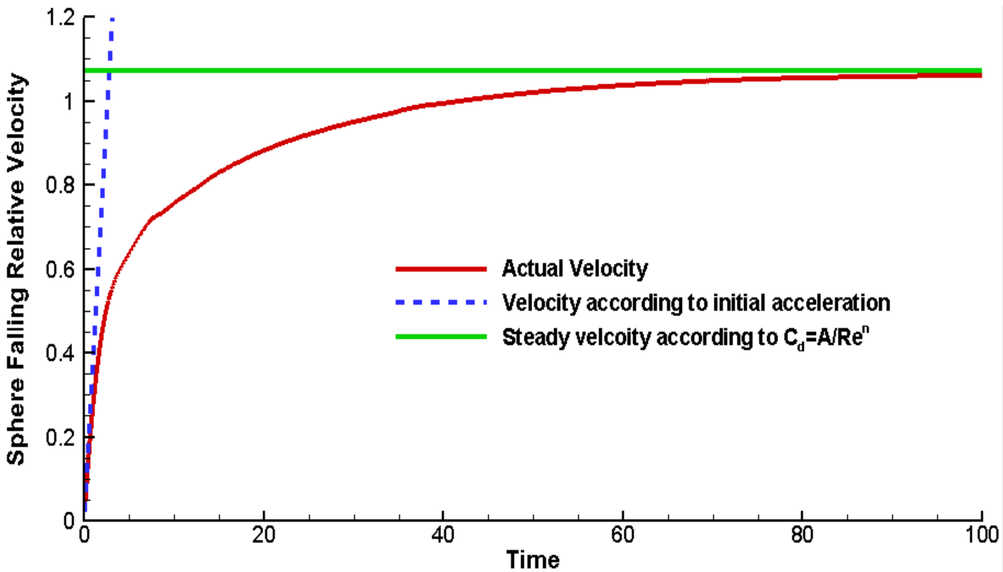
Fg: The importance of various features as measured by the Gini coefficient

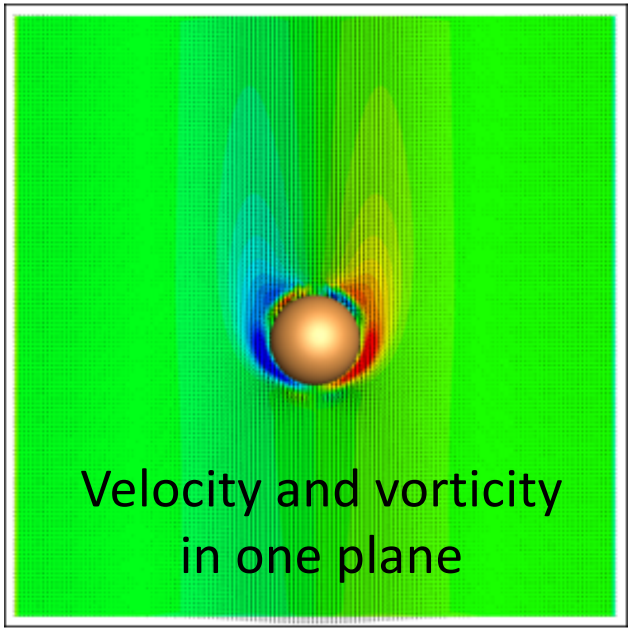






Flow around a falling solid sphere



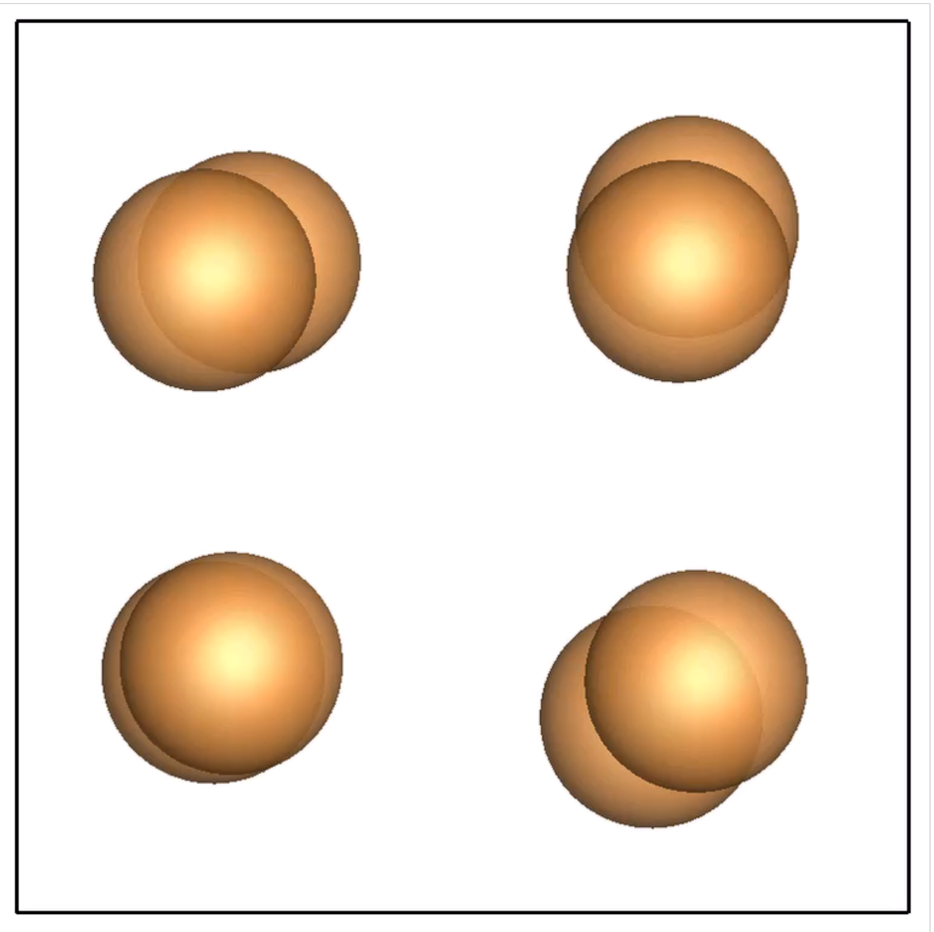


Solid motion is computed by solving the fluid equations for the whole domain, with the correct density in the solid and the fluid.

A solid body motion is imposed in the solid by correcting the velocity in an iterative manner.

Collision is accounted for by adding repulsion forces. Proximity is determined using index functions on the grid used for the solving the fluid equations.

Falling solid spheres

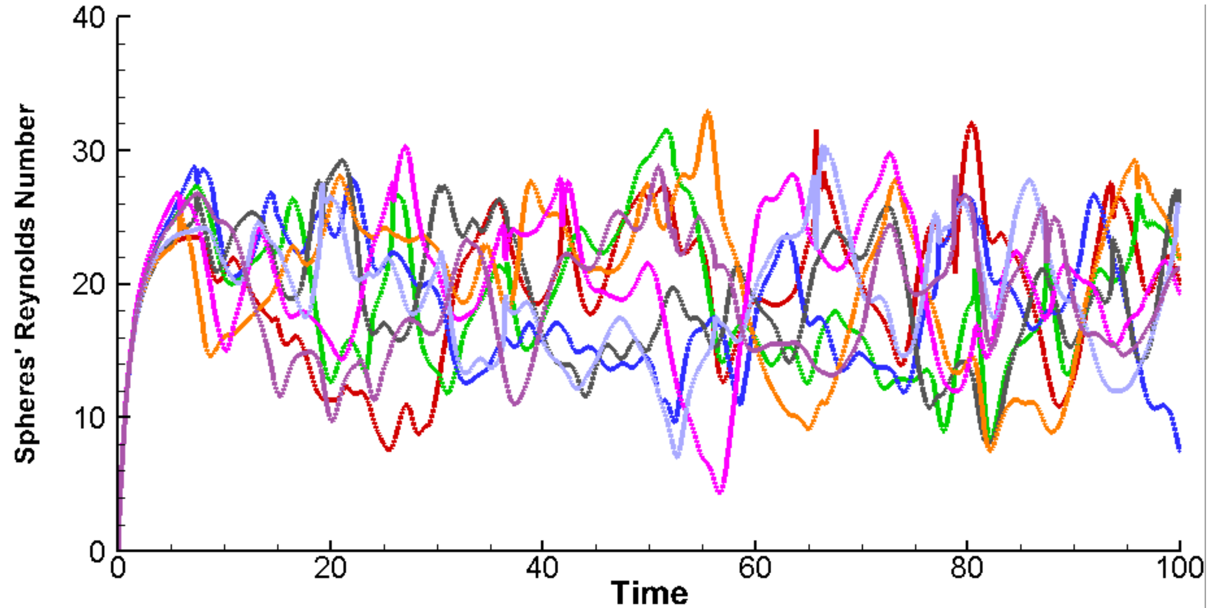


The unsteady motion of 8 spheres in a periodic domain, viewed from above

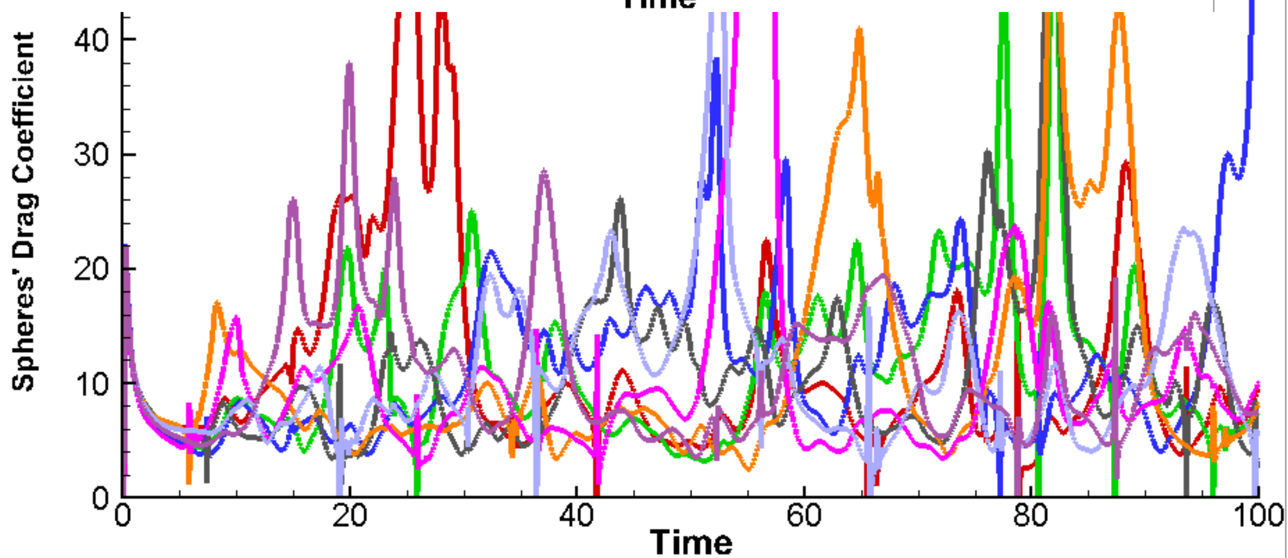
The trajectories of the centroids of spheres in a periodic domain viewed from above. The circles denote the initial conditions. Trajectories leave and enter the domain

Falling solid spheres

The Reynolds number of 8 solid spheres falling in a periodic domain versus time



The instantaneous drag coefficient of each sphere versus time, computed from the slip velocity and the acceleration of each sphere



Falling solid spheres

Domain Size: 2.0 x 2.0 x 2.0;

Resolution: 180 x 180 x 180;

Gravity: 0.6081;

Fluid/solid density: 1.0 / 10.0

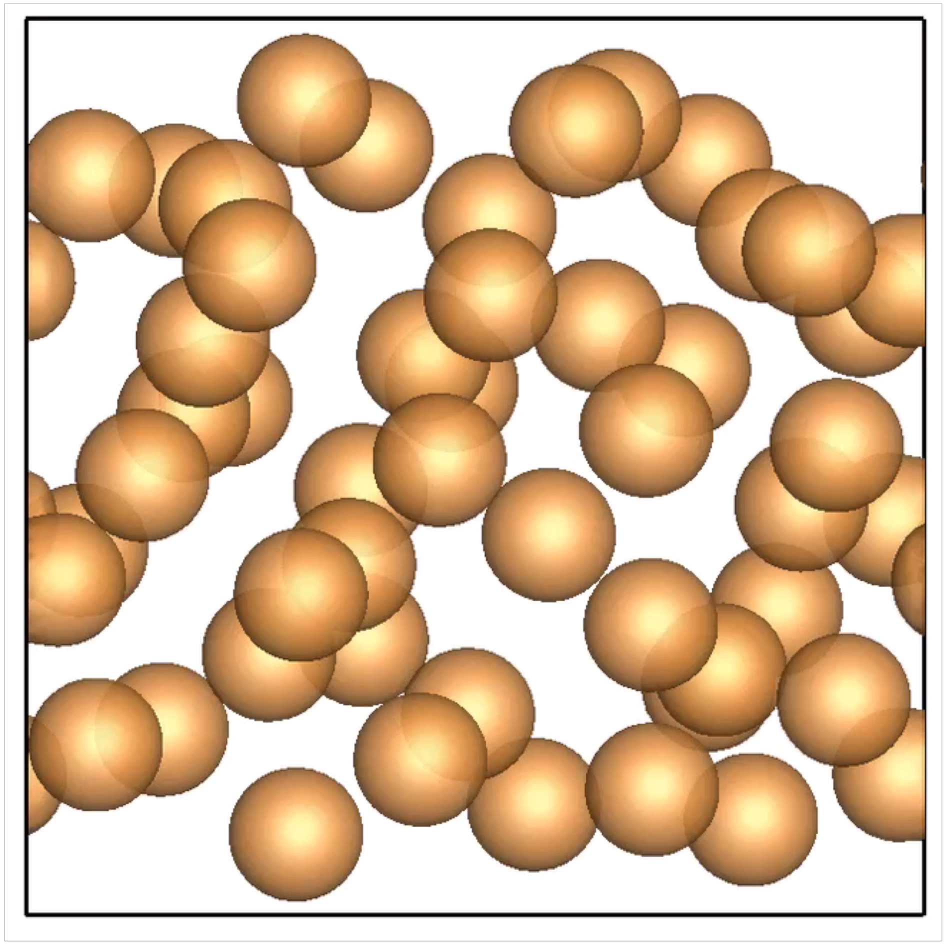
Fluid viscosity: 0.005

Number of Solid Spheres: 50

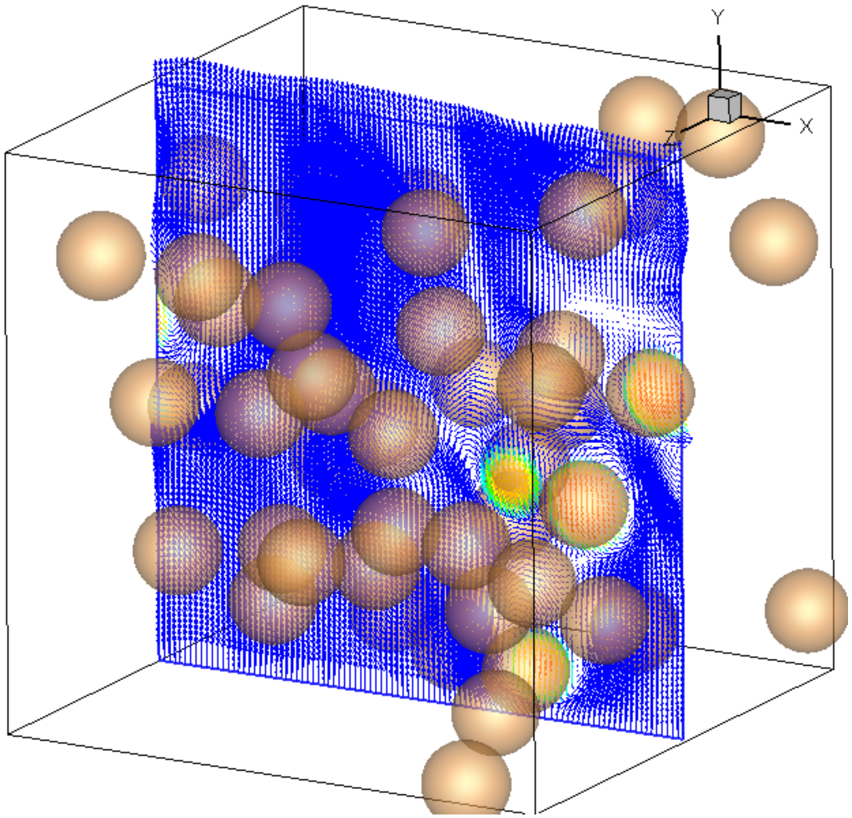
Diameter of Spheres: 0.30

Volume Fraction of Solids: 8.84%

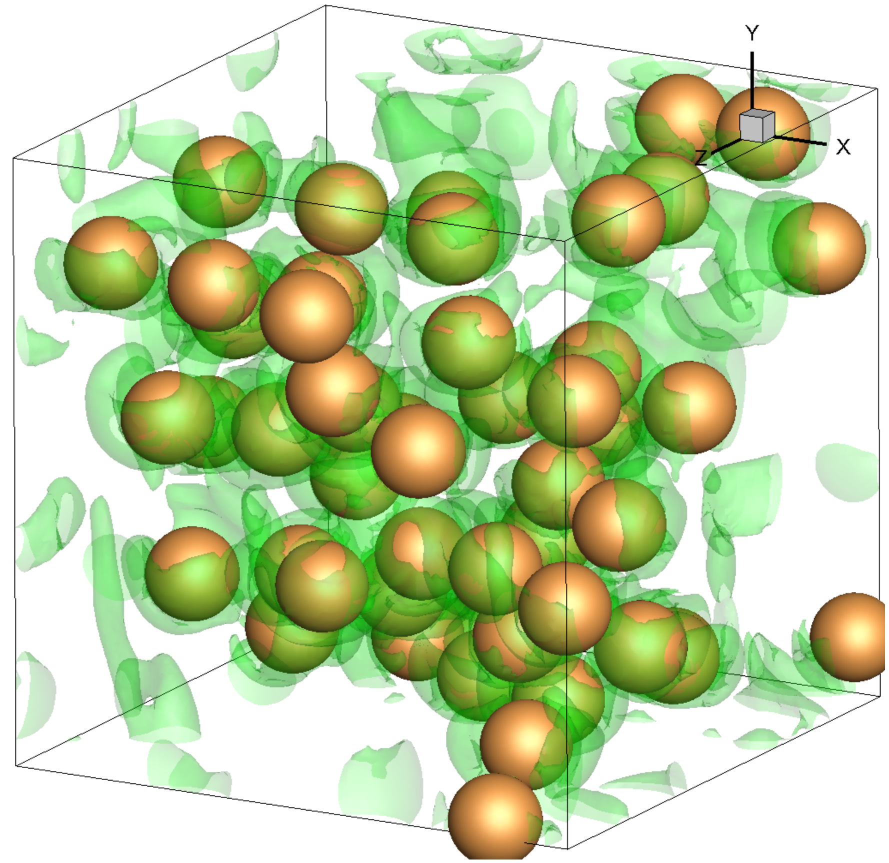
The volume fraction is high, so the spheres collide frequently



Falling solid spheres



The spheres and the fluid velocity in one plane



The vorticity around the spheres, visualized by the λ_2= -4.0 contour

Falling solid ellipsoids

Domain Size: 2.0 x 2.0 x 2.0;

Resolution: 200 x 200 x 200;

Gravity: 0.6081;

Fluid/solid density: 1.0 / 10.0

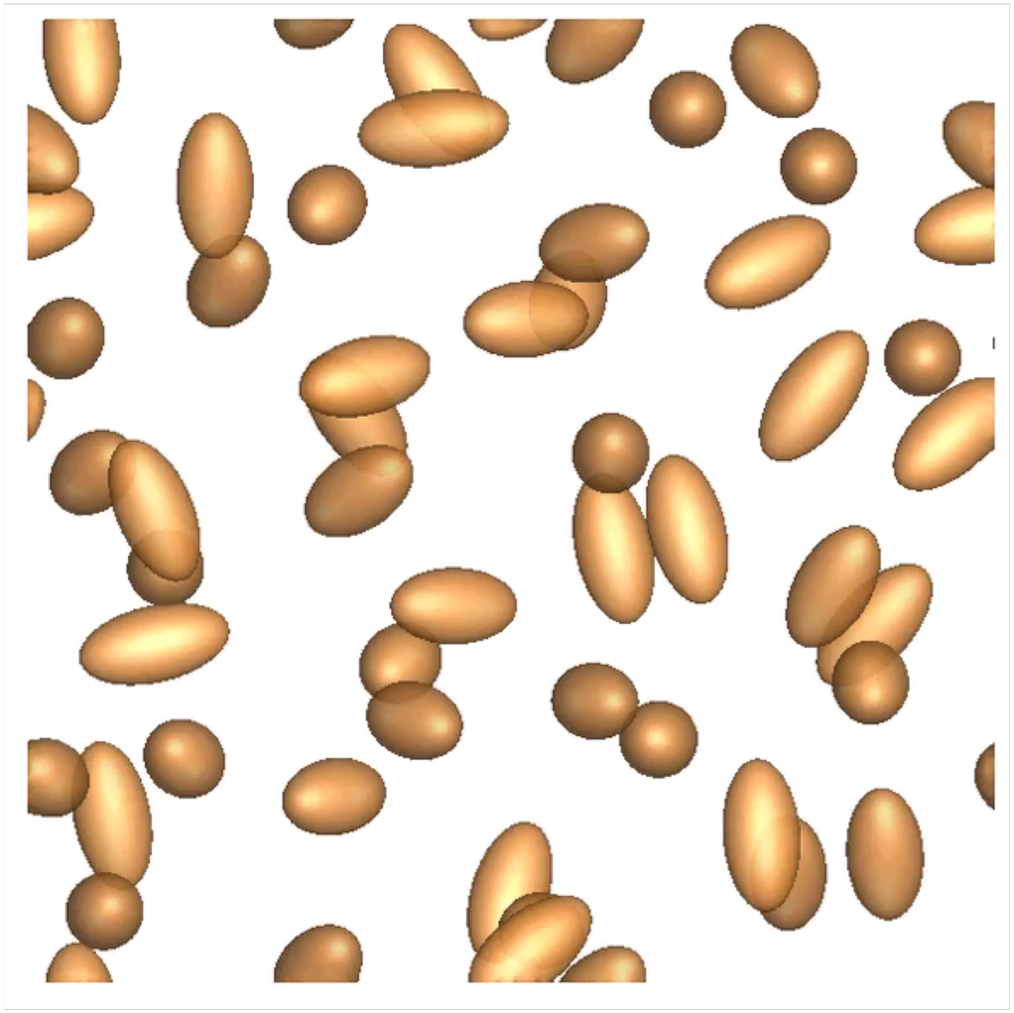
Fluid viscosity: 0.005

Number of Solid Spheres: 50

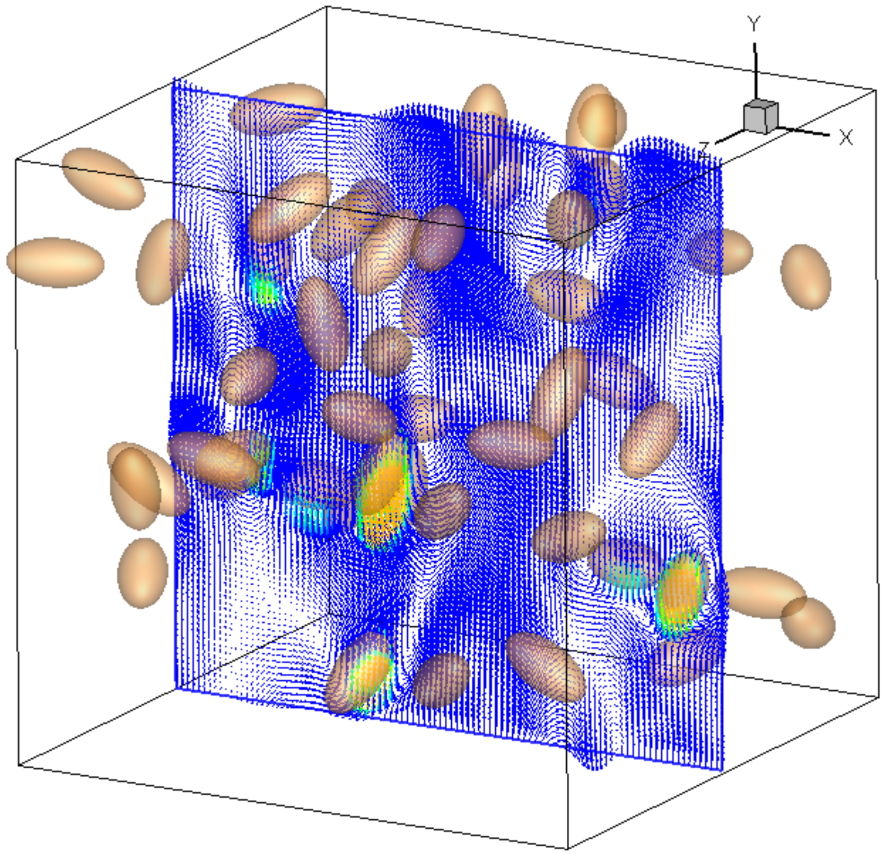
Size of Ellipsoids: 0.32 x 0.16 x 0.16

Volume Fraction of Solids: 2.68%

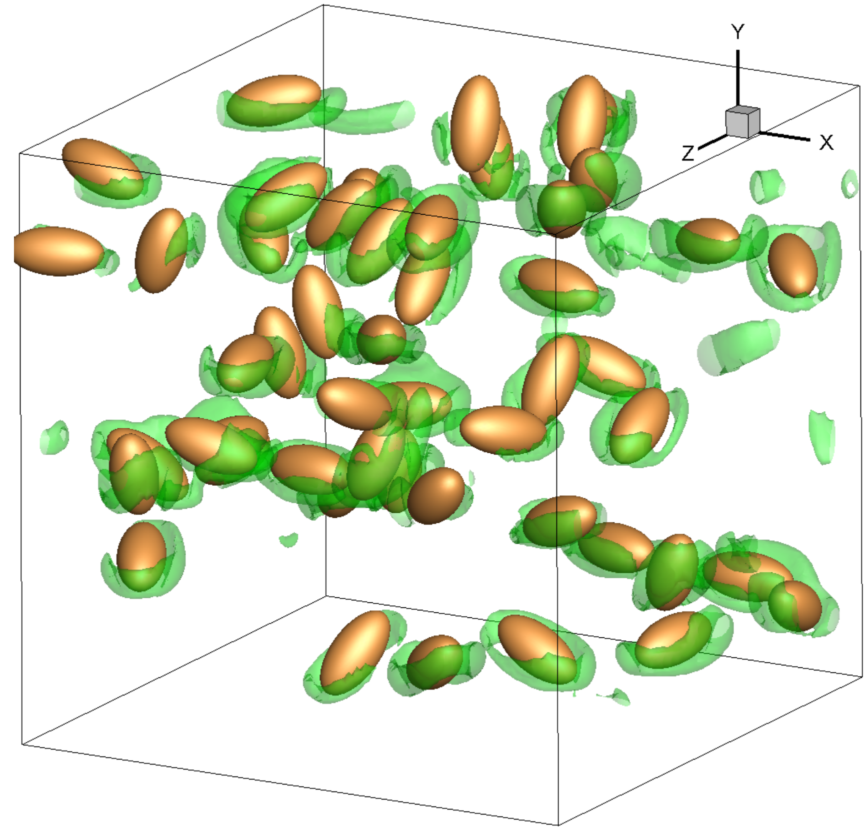
Notice that the volume fraction is lower than for the spheres. Although many fall broadside on, not all do



Falling solid ellipsoids

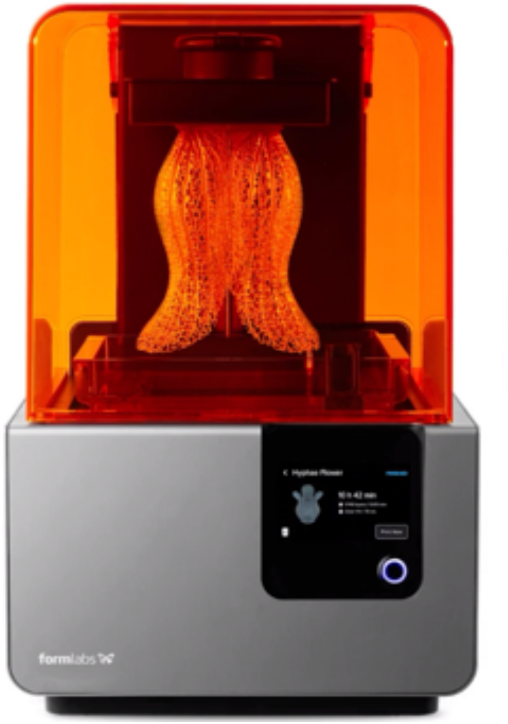


The ellipsoids and the fluid velocity in one plane



The vorticity around the ellipsoids, visualized by the λ_2= -4.0 contour

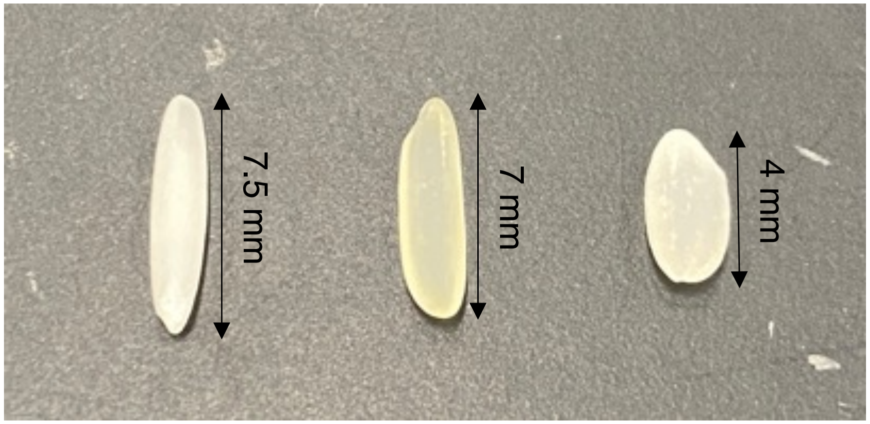
Non-spherical particles



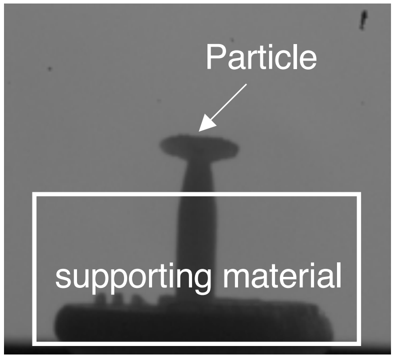
Formlabs Form2 3D printer

- Stereolithography technology
- 145 × 145 × 175 mm build volume
- 25 μm minimum layer thickness

Non-spherical particles also exist in nature

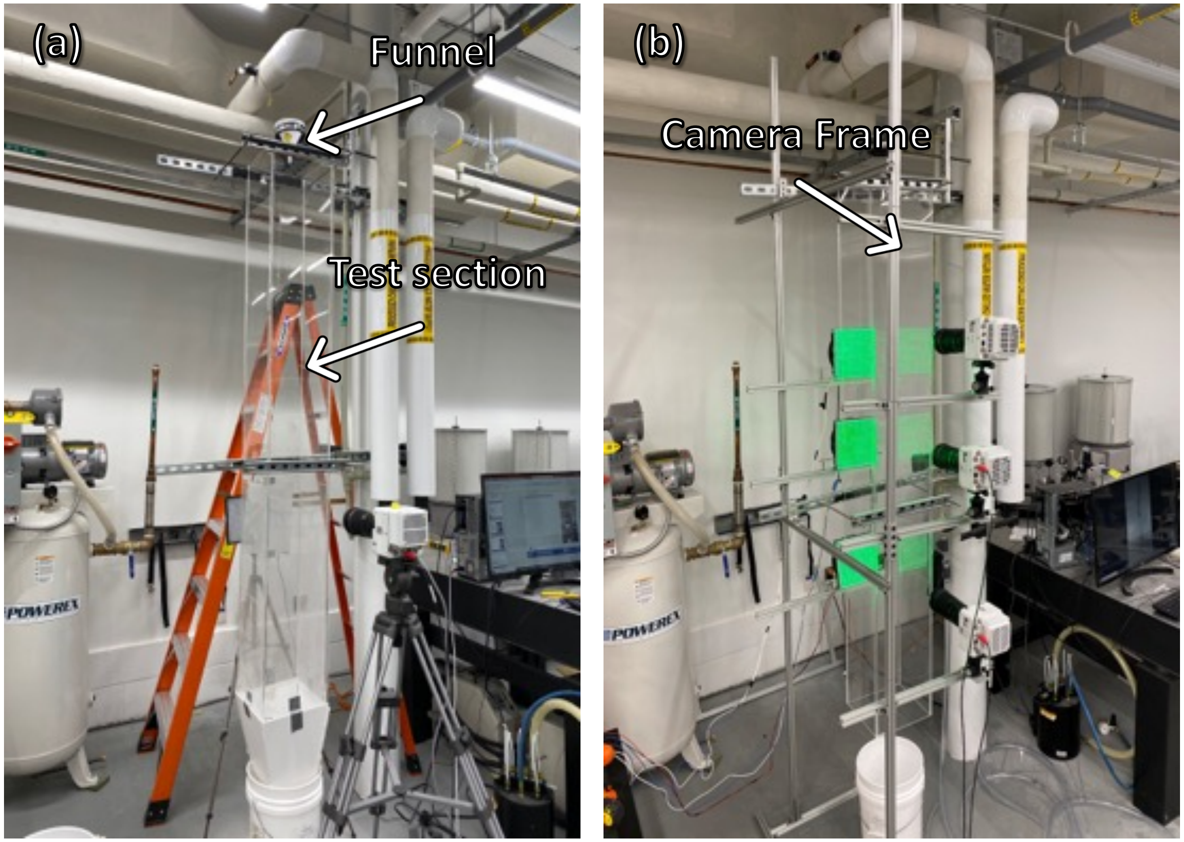


The aspect ratios from left to right are roughly 5, 3.5 and 1.5.



This is a 3D printed particle with supporting material. It has a 2.5 mm major diameter and 0.5 mm minor diameter.

Preliminary drop tower



The goals of preliminary setup:

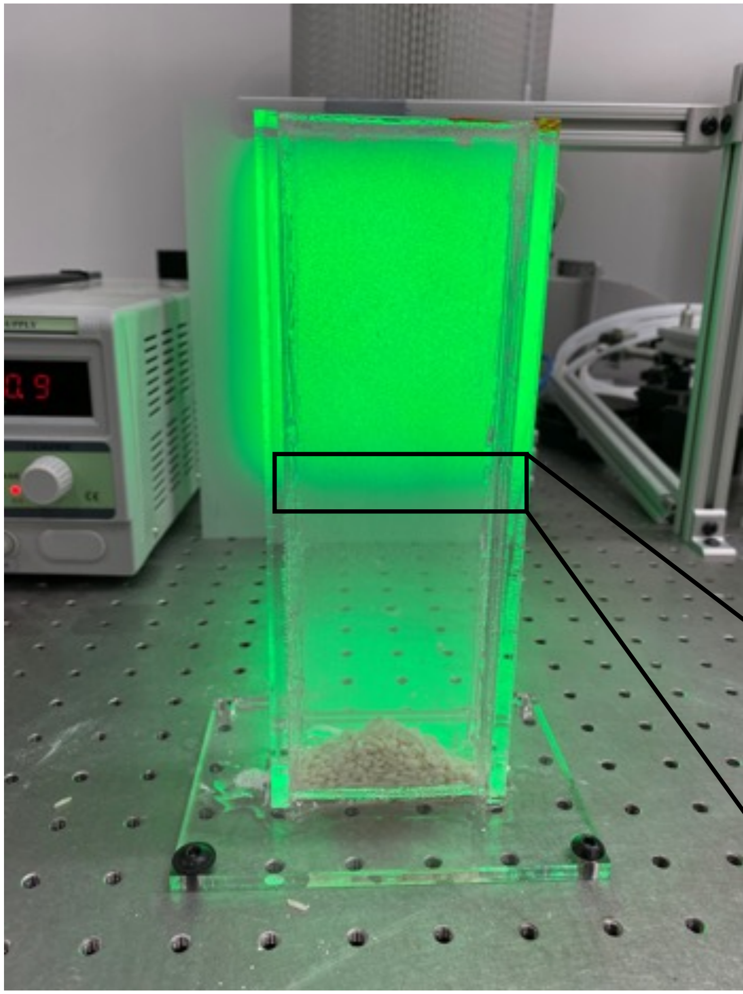
- Automated experiment procedure
- Data acquisition system
- Post-processing algorithm

Control Parameters:

- Particle shape
- Particle size
- Particle material density
- Particle number density

Test section dimension	Funnel volume	Total number of cameras rack
0.25×0.25×3 m	350 ml	4

Water channel



The goals of this setup:

- Use tracer and LED backlighting to obtain fluid phase data.
- Experimentally investigate pair particle interaction with controlled initial conditions.
- Experimentally investigate fluid flow within a free-falling anisotropic particle swarm.
  - Fluid phase is quiescent water
  - Anisotropic particle is rice

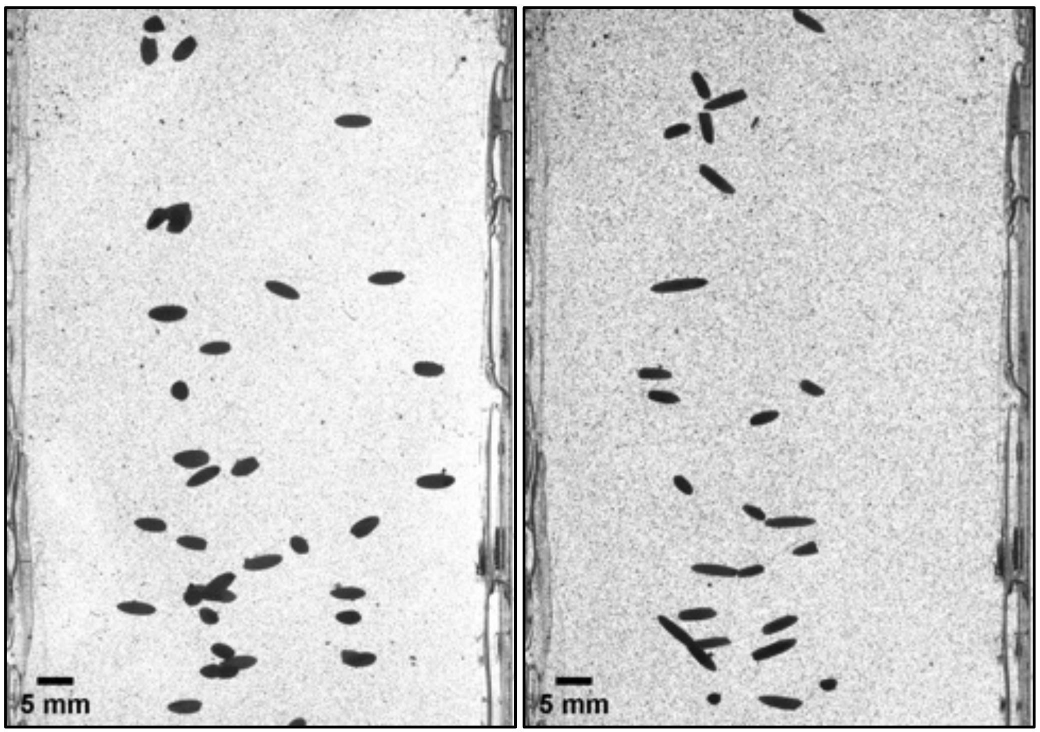
Preliminary experimental tests

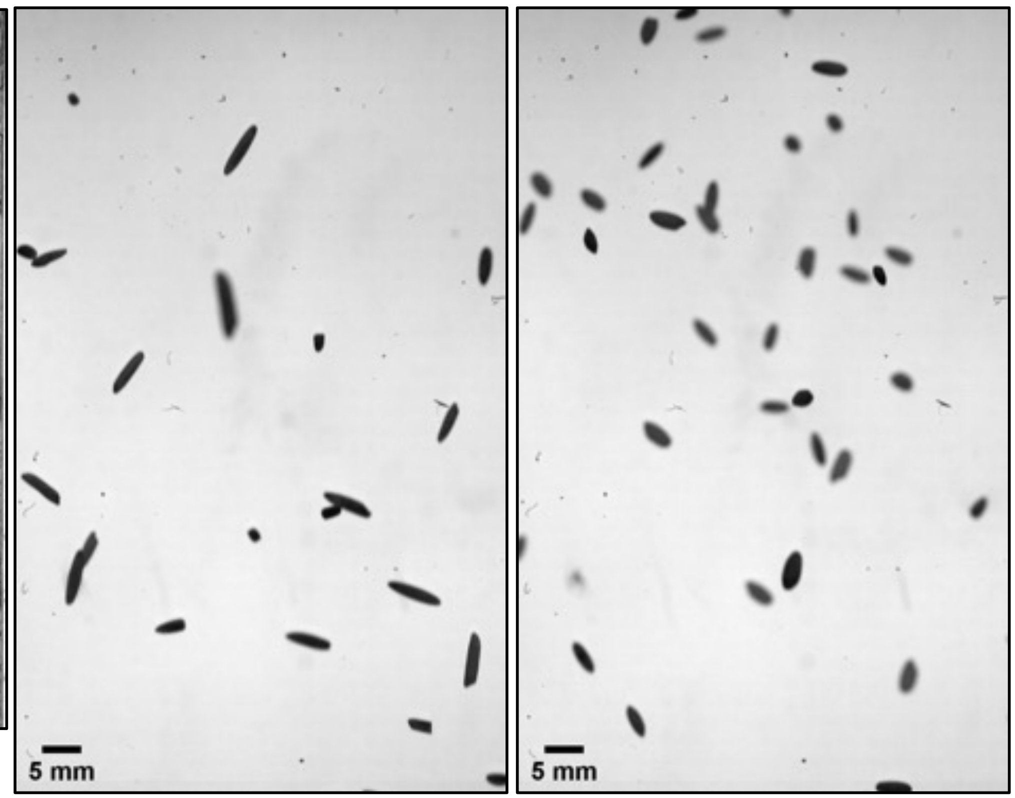
Water channel:
Left panel: 4 mm rice
Right panel: 7.5 mm rice

Images taken at ~5cm below particle release location

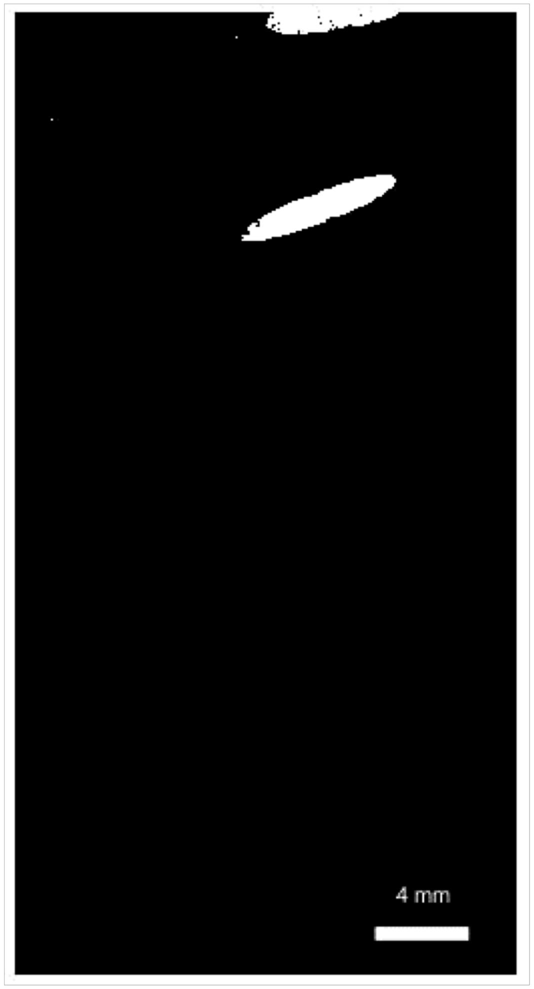
Preliminary drop tower:
Left panel: 4 mm rice
Right panel: 7.5 mm rice

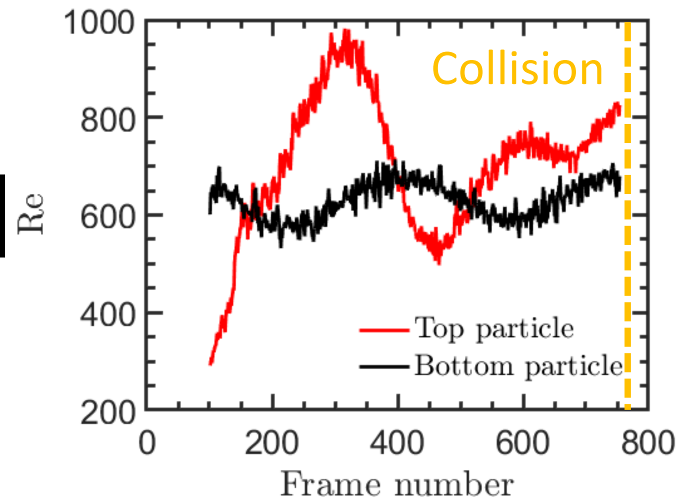
Images taken at ~1m below particle release location

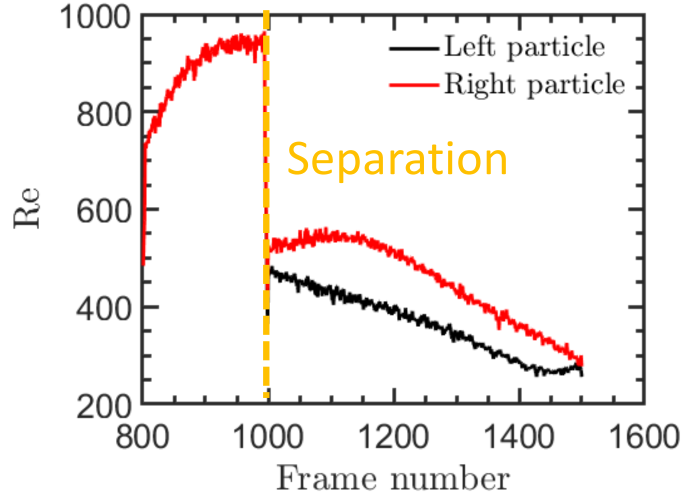


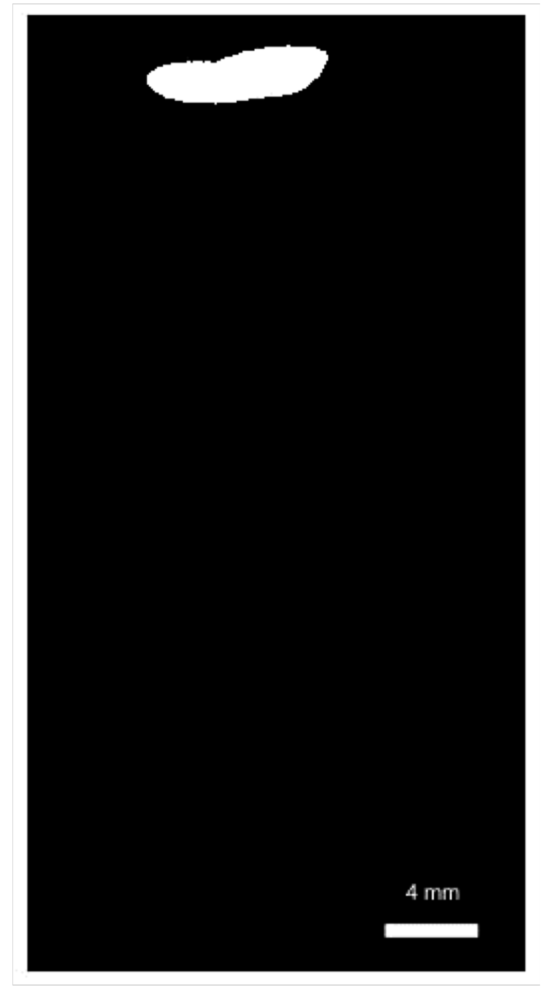


2D particle tracking velocimetry





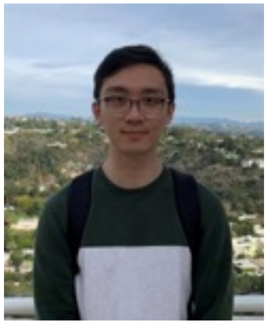




Plan

Subteam 1: Experiment

Rui Ni



Xu Xu

Subteam 2: Simulation

Gretar Tryggvason

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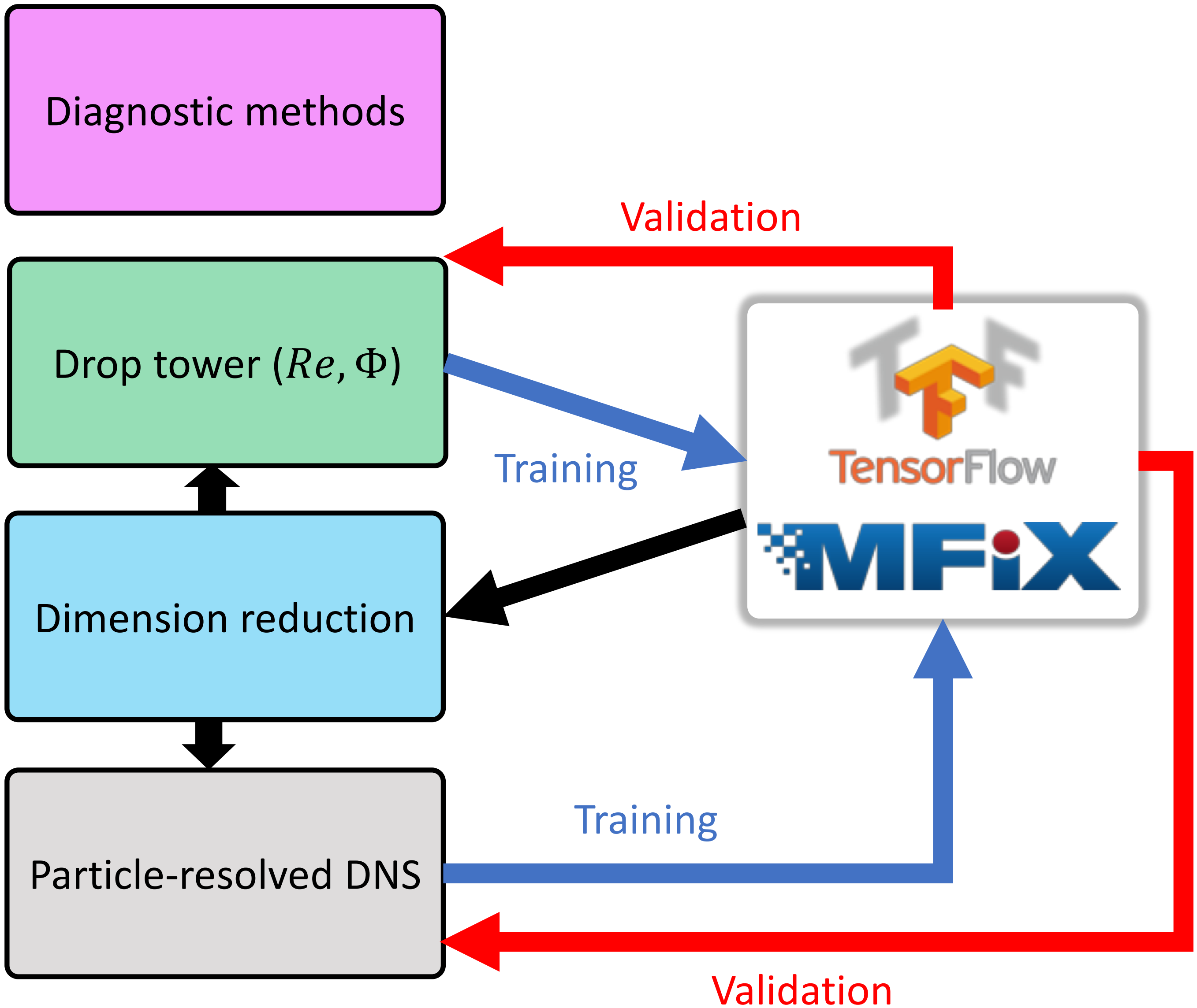

Acknowledgment

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