Developing drag models for non-spherical particles through machine learning

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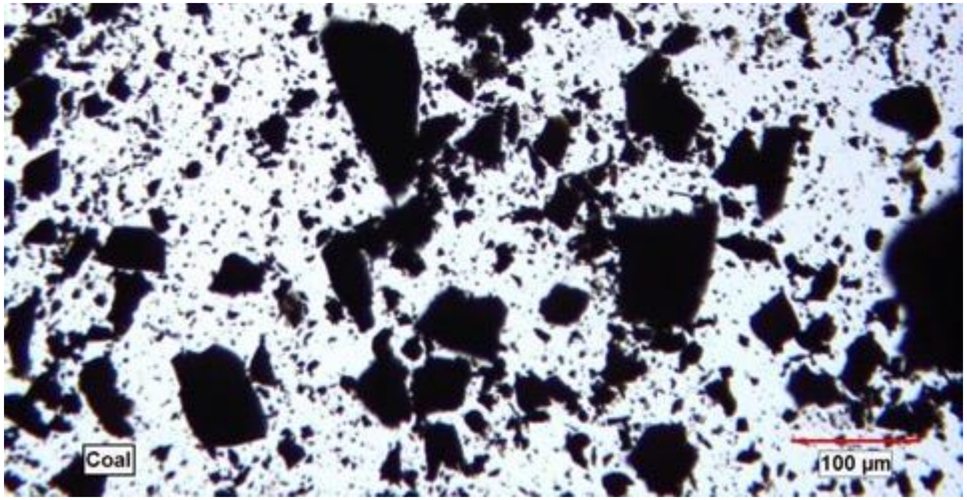
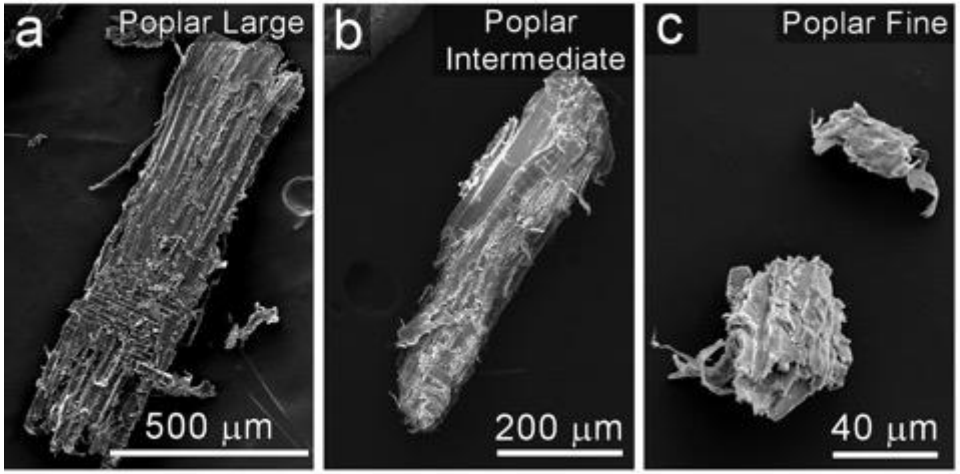
Motivation: coal and biomass gasification

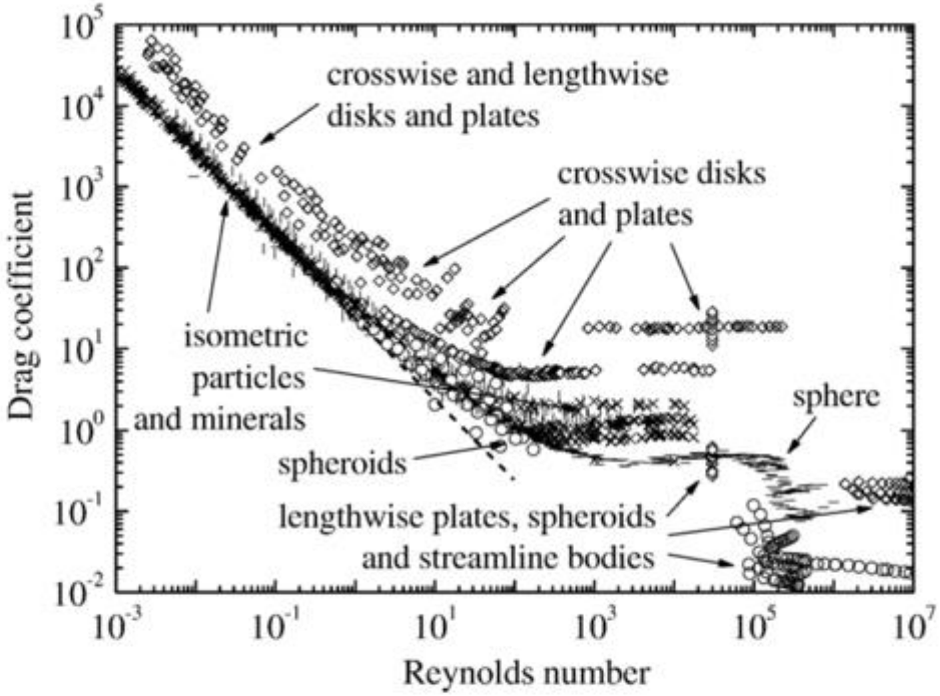
- Thermal conversion systems are very challenging to model:
  - Particles have complex shapes, a broad range of sizes, shapes and density.
  - Non-spherical particle interact with other particles.
  - Force closures are needed for non-spherical particles, i.e. drag and lift (maybe even other unsteady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



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

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

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 ($Re < 10^5$):

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

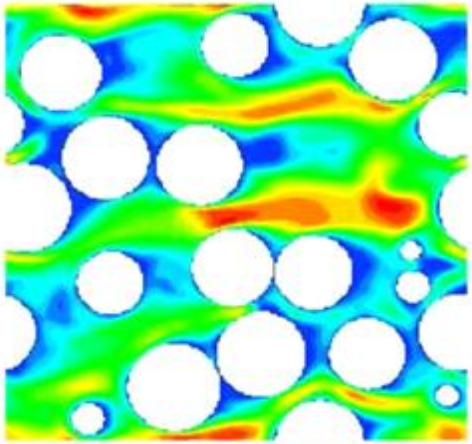
$$K_2 = 10^{1.8148(-\log\phi)^{0.5743}}$$ (Newton factor)

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



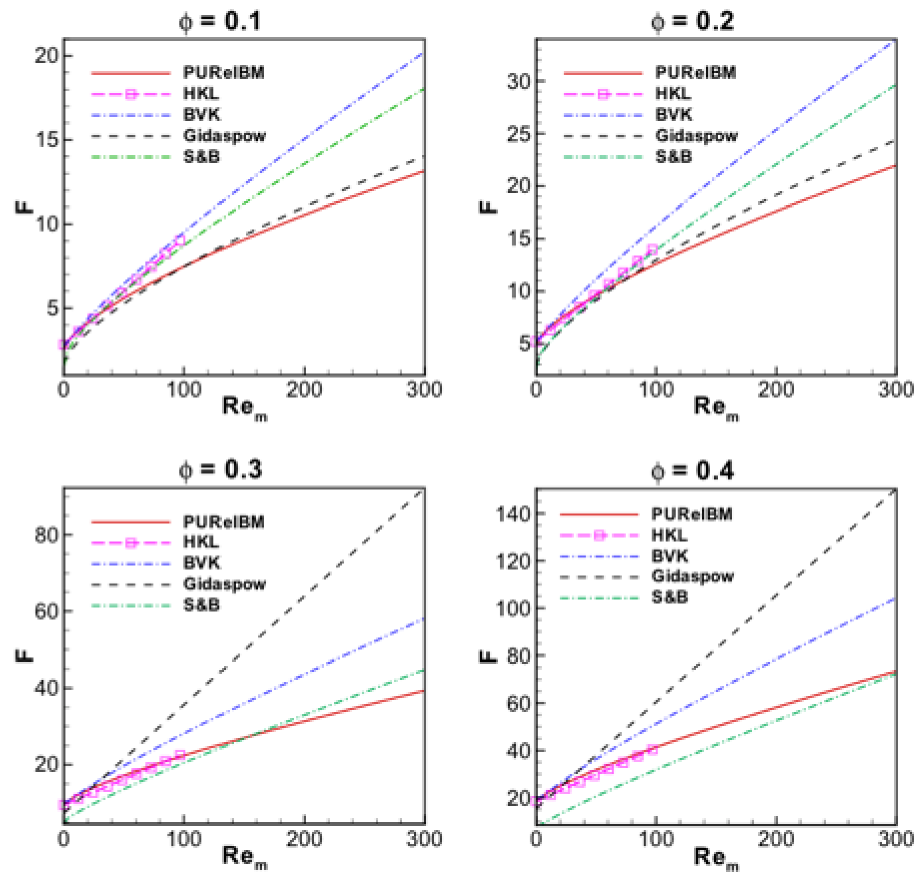
Tenneti et al. (2011)

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

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

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

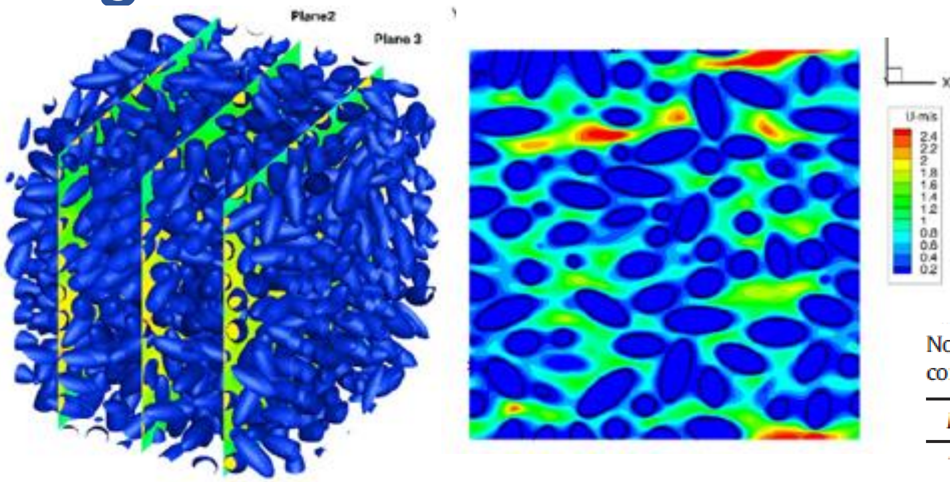
Wen & Yu (1966) for dilute suspensions and Ergun's equation (Ergun 1952) for denser systems are the earliest experimental efforts.



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

Tenneti et al. (2011)

Drag Coefficient on Packed Non-spherical Particle



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

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

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

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

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%

$$\boxed{c_D=\frac{8}{\mathrm{Re}}\frac{1}{\sqrt{\Phi_{\parallel}}}+\frac{16}{\mathrm{Re}}\frac{1}{\sqrt{\Phi}}+\frac{3}{\sqrt{\mathrm{Re}}}\frac{1}{\Phi^{\frac{3}{4}}}+0.42 10^{0.4(-\log\Phi)^{0.2}}\frac{1}{\Phi_{\perp}}}$$

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

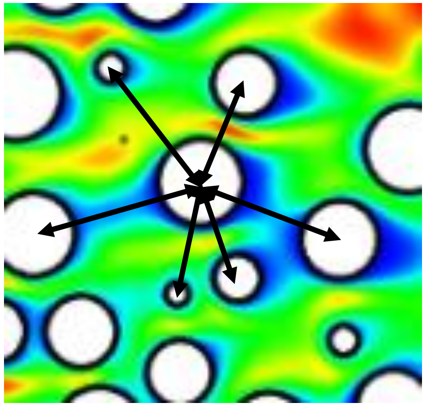
$$\boldsymbol{F}_i = \langle \boldsymbol{F}_i \rangle (Re, \phi) + \Delta \boldsymbol{F}_i(Re, \phi, \{\boldsymbol{r}_{j=1}, \ldots, \boldsymbol{r}_{j=M}\}),$$
$$\boldsymbol{T}_i = \Delta \boldsymbol{T}_i(Re, \phi, \{\boldsymbol{r}_{j=1}, \ldots, \boldsymbol{r}_{j=M}\}),$$

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.

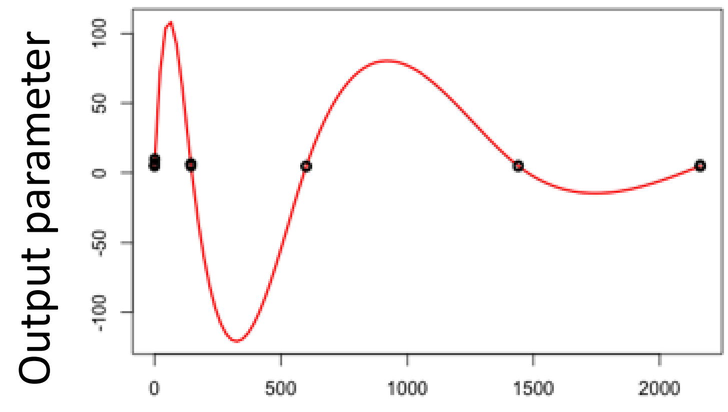
Number of particles (N)	$\boldsymbol{\phi = 0.1}$	191
	$\boldsymbol{\phi = 0.2}$	382
	$\boldsymbol{\phi = 0.3}$	573
	$\boldsymbol{\phi = 0.35}$	669

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

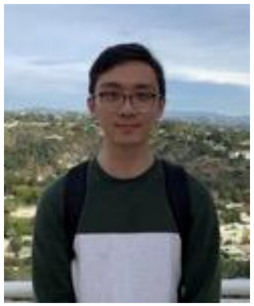


1. Reduce the number of dimensions
2. Increase the sample size

Introduce our team and methodology

Subteam 1: Experiment

Rui Ni

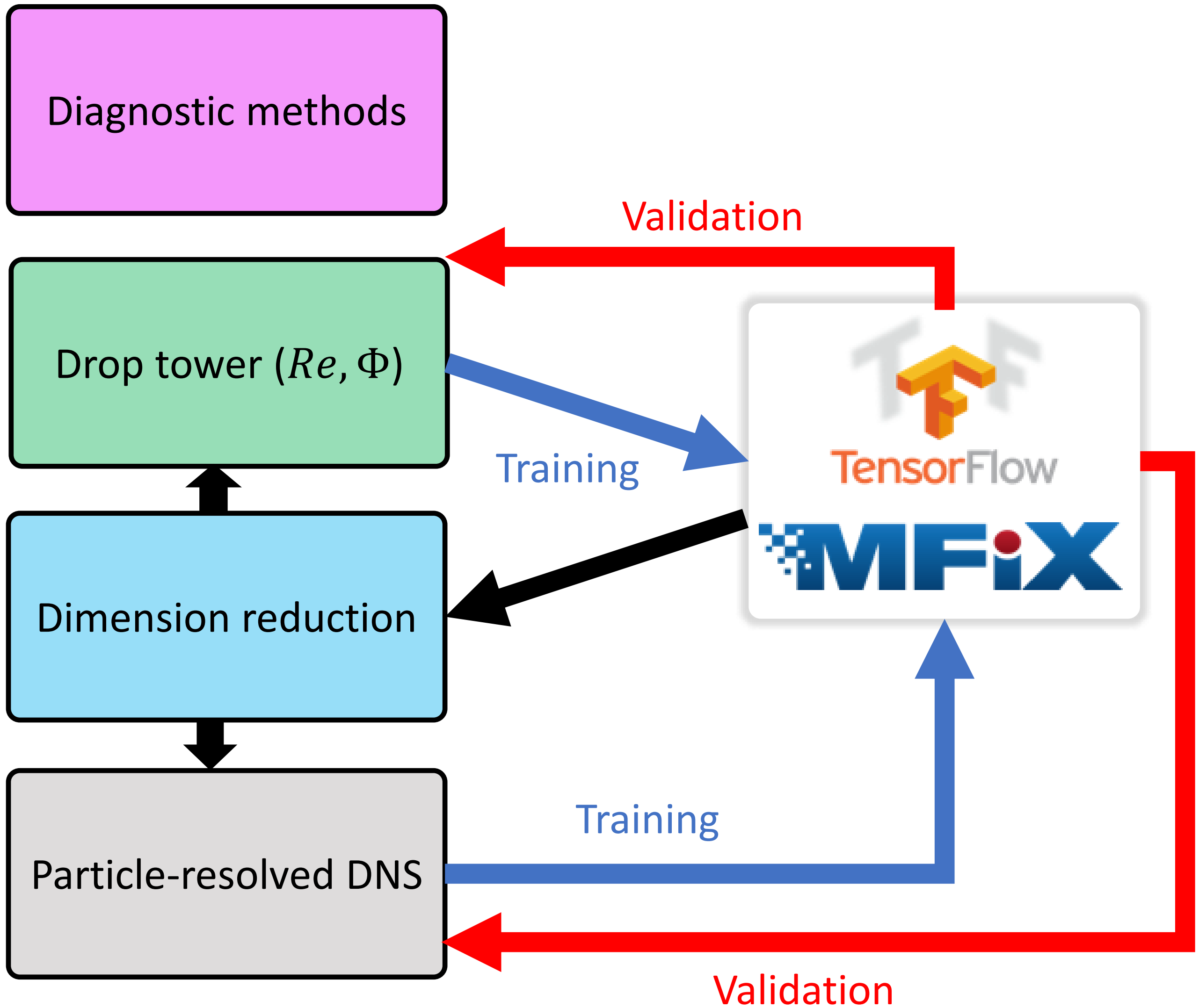


Xu Xu

Subteam 2: Simulation

Gretar Tryggvason

Jiacai Lu



Computational Method & Setup

The Navier-Stokes equations are solved on a fixed uniform staggered grid

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \rho \mathbf{u}\mathbf{u} = -\nabla p + (\rho - \rho_{av})\mathbf{g} + \nabla \cdot \mathbf{D} + \mathbf{f}_c$$

$$\mathbf{D} = \begin{cases} \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T) & \text{in the fluid} \\ 0 & \text{in the solid.} \end{cases}$$

We compute the centroid velocity and the solid body rate of rotation by

$$M_S \mathbf{U}_{SC}^{n+1} = \int_S (1-\xi)\rho \mathbf{u} dv \qquad \mathbf{I}_S \mathbf{\Omega}_S^{n+1} = \int_S (1-\xi) + \mathbf{r} \times \rho \mathbf{u} dv$$

The velocity inside the solid is then updated

$$\mathbf{U}_S^{n+1} = \mathbf{U}_{SC}^{n+1} + \mathbf{r} \times \mathbf{\Omega}_S^{n+1}$$

Since the stress inside the particles is not included, a collision force is added to prevent the particles from overlapping

Computational Setup

For ellipsoids of a given shape, the flow is governed by the Galilei number, the density ratio and the volume fraction

$$N = \frac{\Delta\rho g \rho_f d_e^3}{\mu_f^2} \qquad r = \frac{\rho_s}{\rho_f}$$

Here, $N = 1,751 \quad r = 10$

Giving a Reynolds number $Re_s = \dfrac{\rho_f u_s d_e}{\mu_f}$

of around 20, depending on the volume fraction

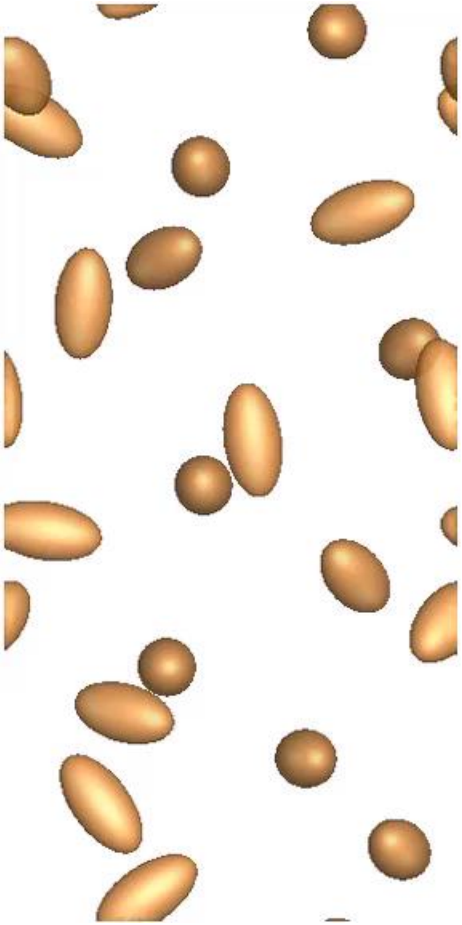
This system can be approximately realized by copper particles of effective diameter 1.4 cm in olive oil at 20 centigrade

The computations are done in a domain 1.25 by 1.25 by 2.5

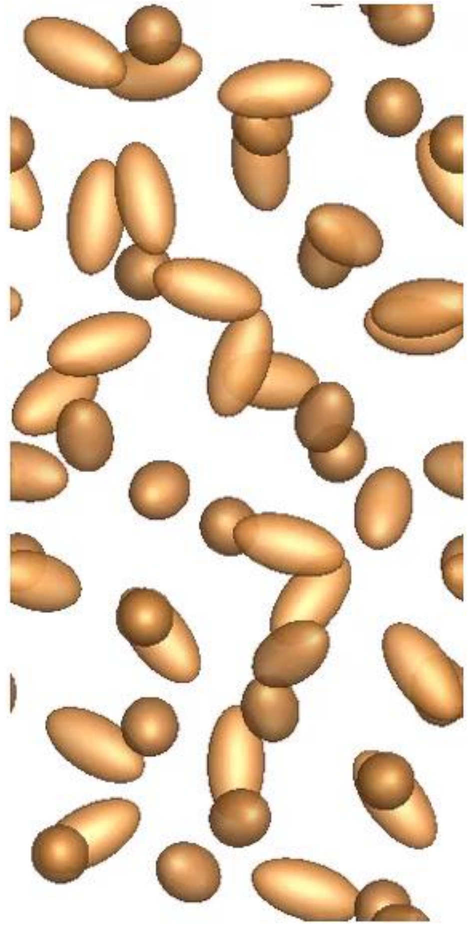
The particles are ellipsoids with an “effective” diameter of 0.2

Falling Ellipsoids

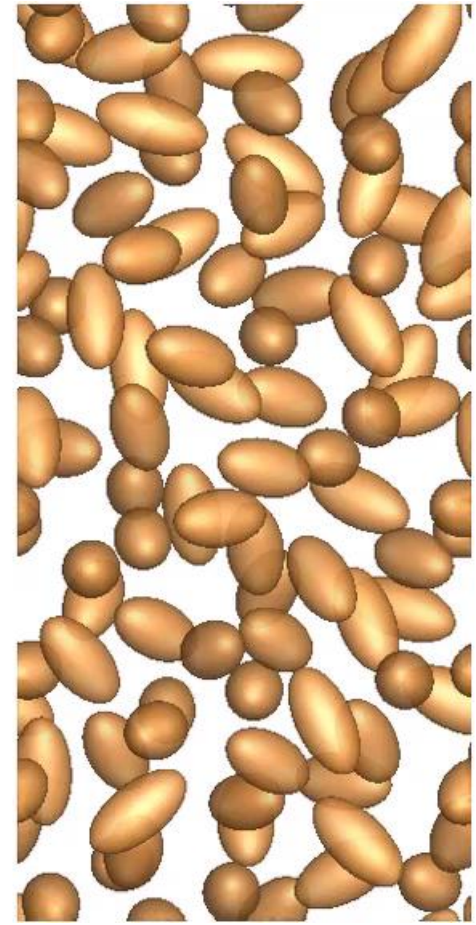
N=20; α=2.2%



N=50; α=5.5%

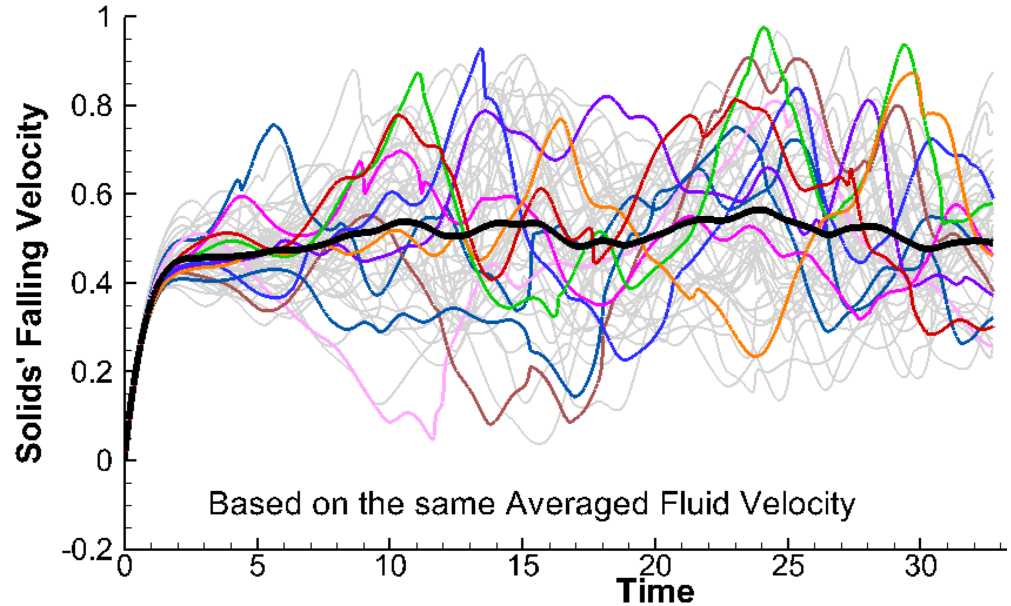


N=90; α=9.9%

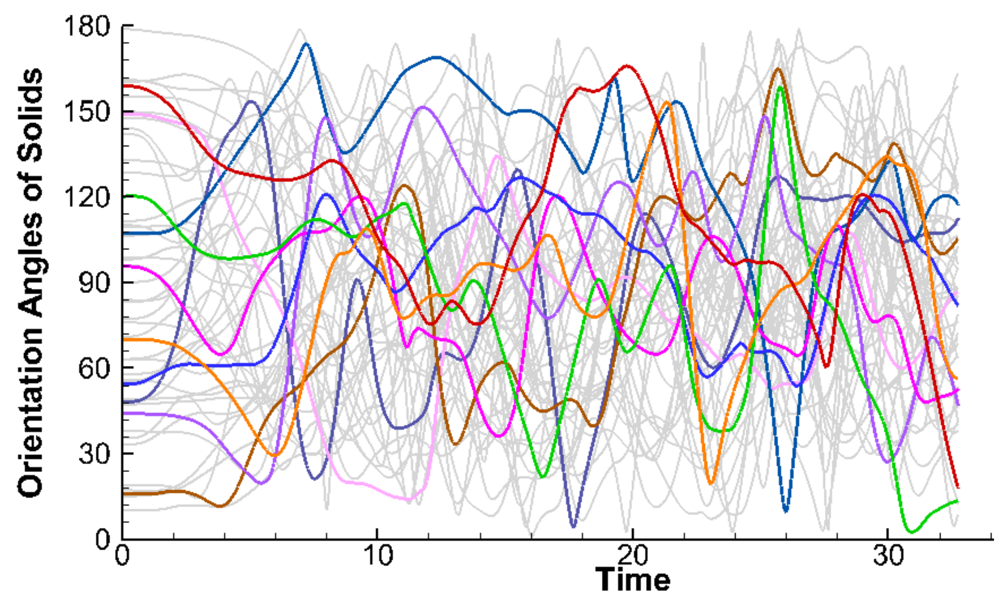


Falling Ellipsoids

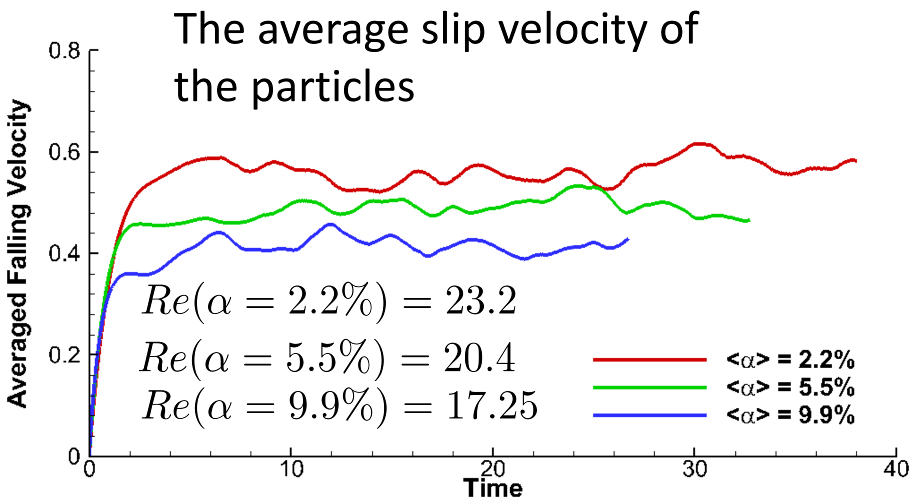
The slip velocity for each particle, computed as the velocity of the particle minus the average fluid velocity in the entire domain, versus time for 50 particles. 10 trajectories are shown in color, the rest in gray. The thick line is the average velocity for all the particles

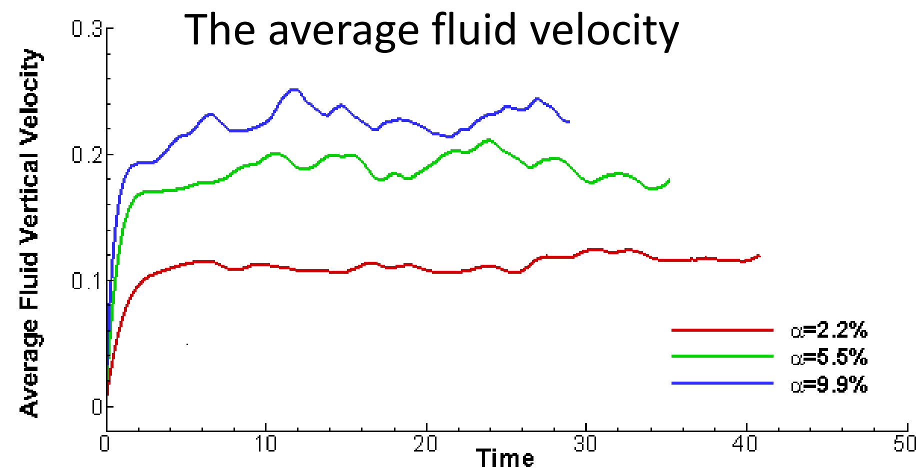


The orientation of each particle, as measured by the angle the long axis makes with the direction of gravity (vertical axis), is versus time for 50 particles. The plot is for 180 degrees to include particles that pass through a horizontal orientation



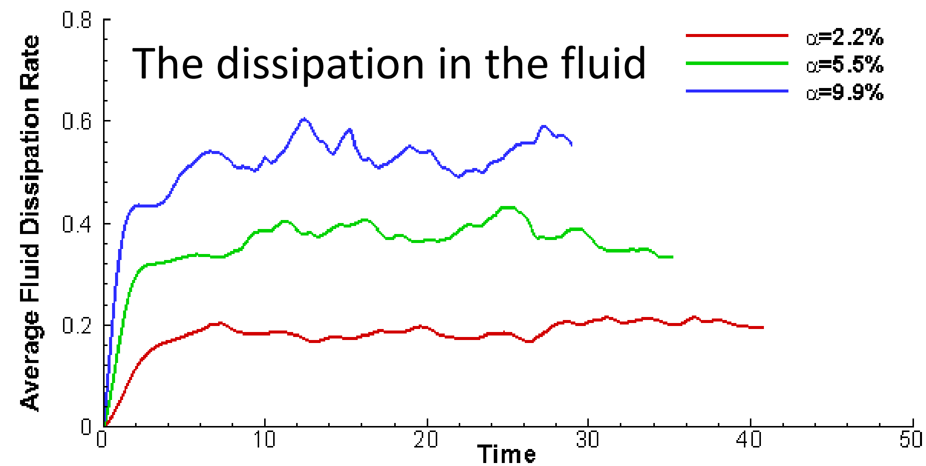
Falling Ellipsoids





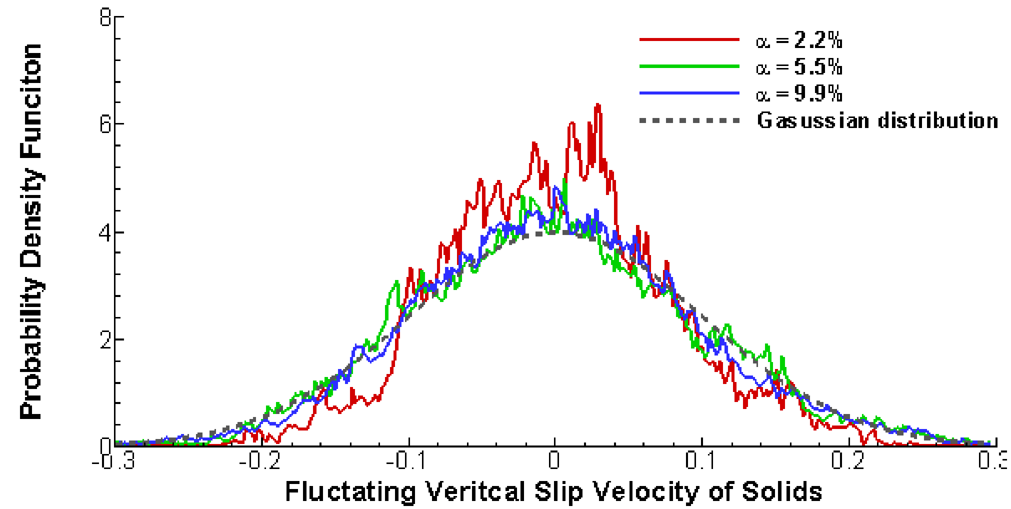
Average quantities versus time for three different volume fractions.

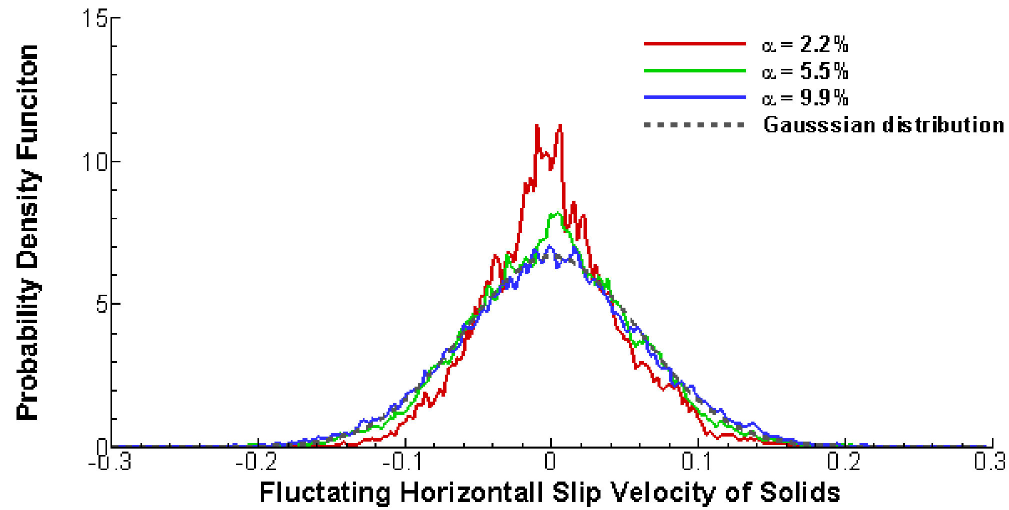
The averages converge relatively quickly in time but the fluctuations in reflect the relatively small size of the domain



Falling Ellipsoids

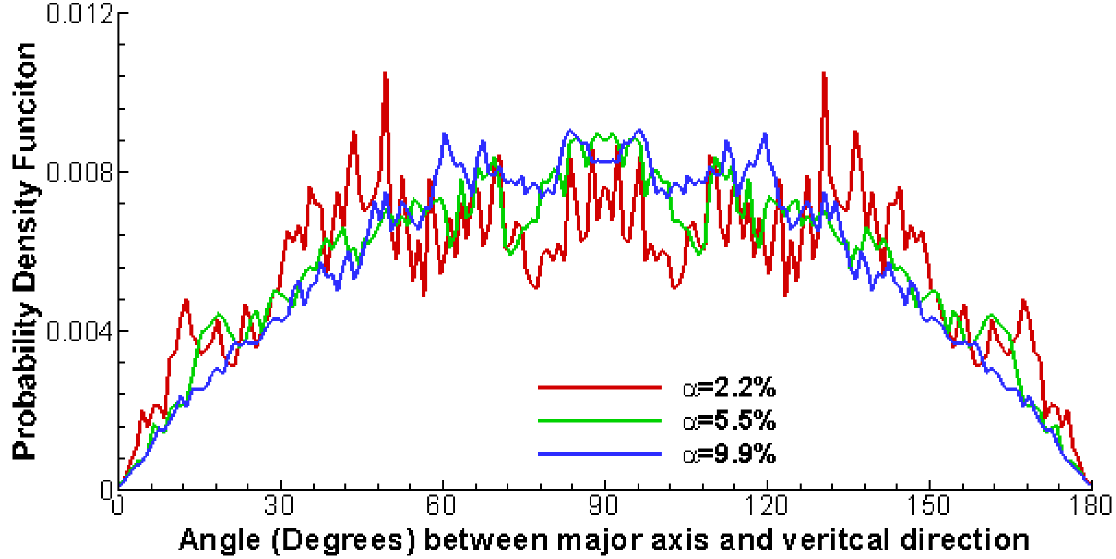
The probability distribution of the velocity fluctuations for the three volume fractions. The top frame is the fluctuations in the vertical component and the bottom one is the the horizontal probability is the average value of the probabilities is the horizontal velocity. The dashed black line is a Gaussian distribution with the same standard deviation



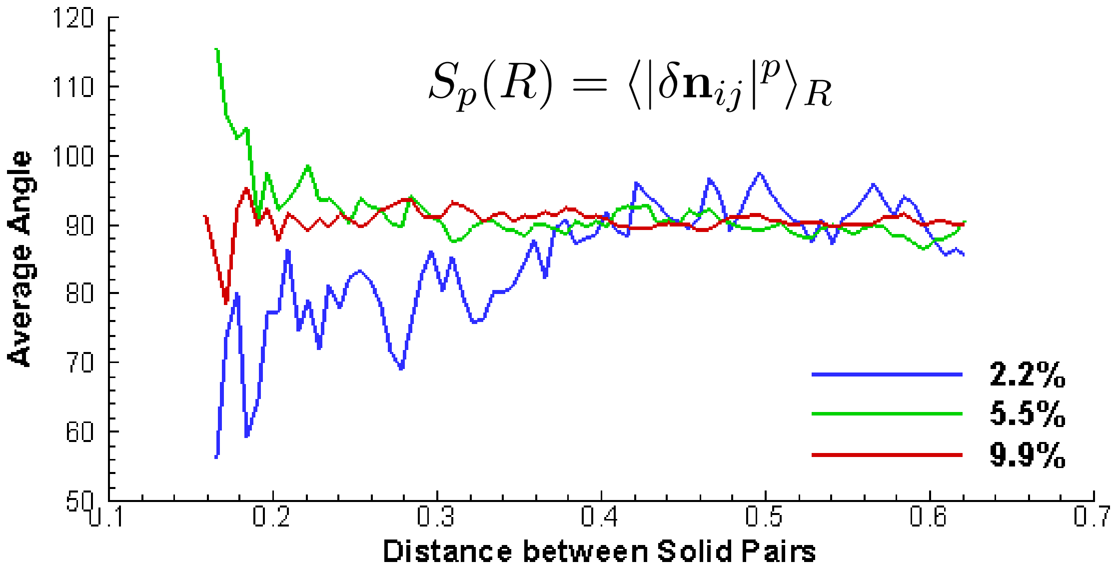


Falling Ellipsoids

The distribution of orientations for the particles, measure as the angle between the longest axis and the horizontal direction. For 90 degrees the longest axis is horizontal.

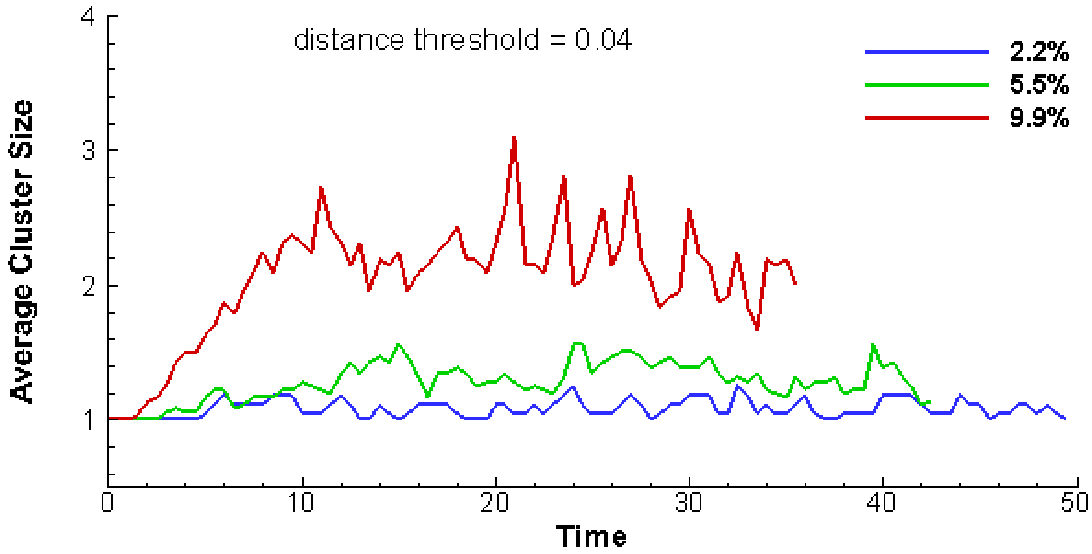


The average angle between the longest axes of different particles, versus the distance between the particle pair.

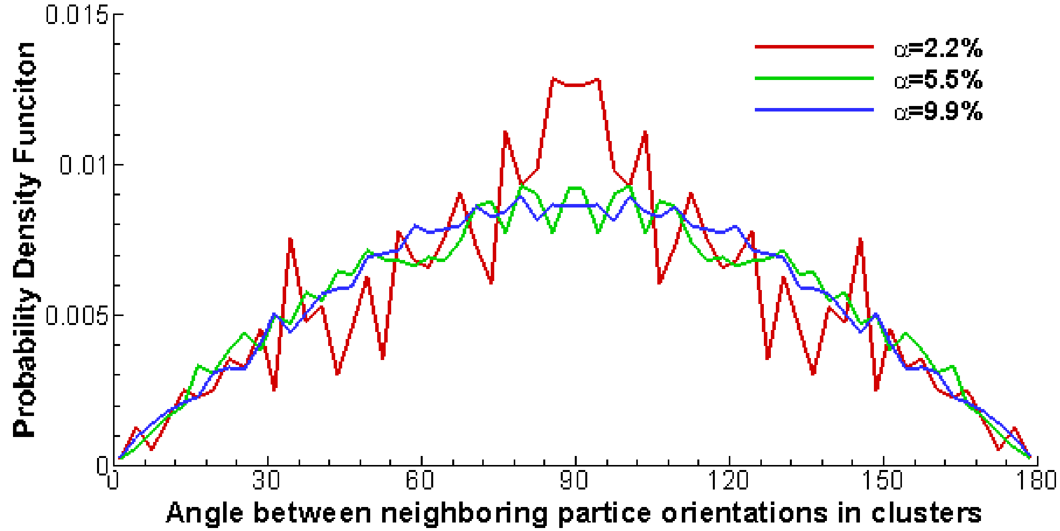


Falling Spheroids

Average cluster size versus time for the three different volume fractions. Cluster size is computed by assuming that the shortest distance between the surfaces of two particles falls below a threshold.



The angle between neighboring particles in the cluster, identified as particles that are almost touching each other



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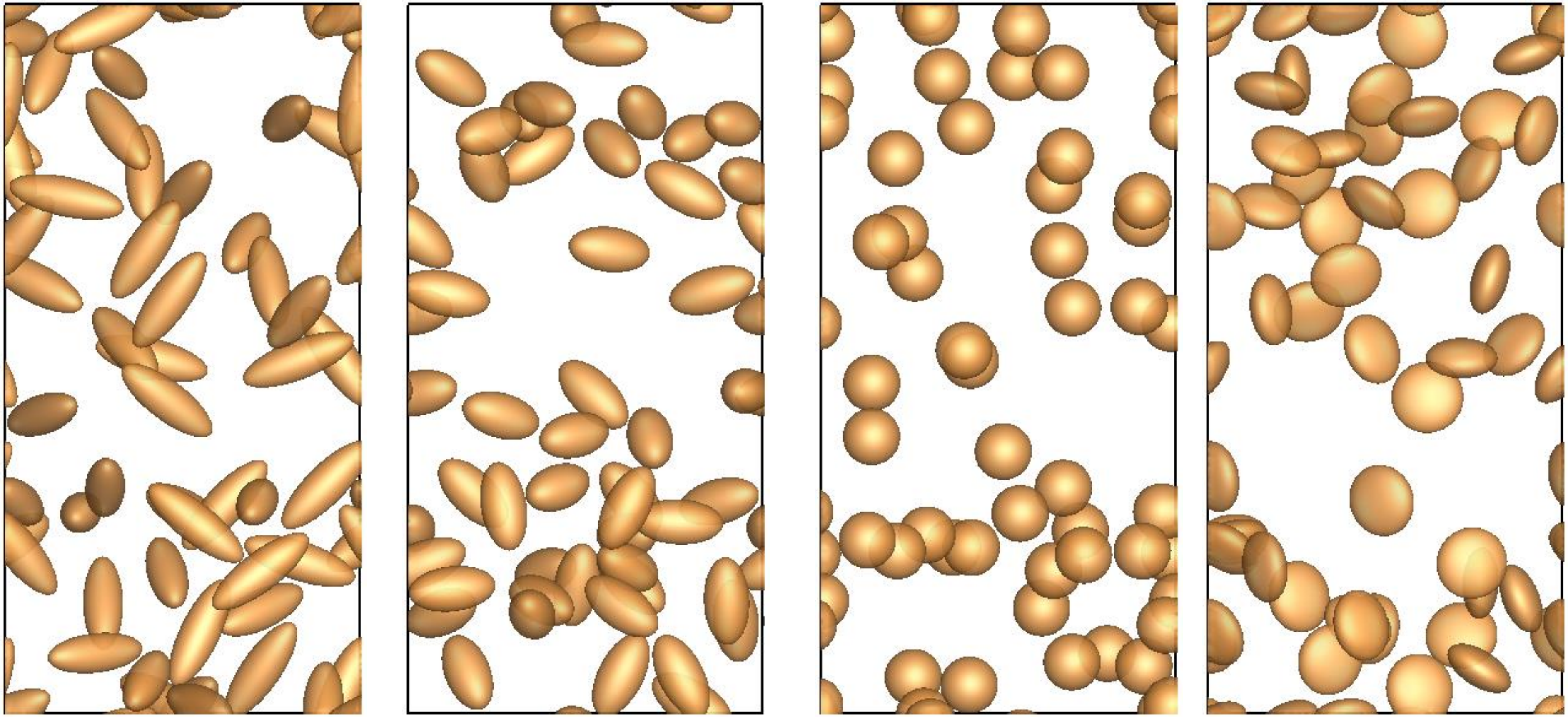
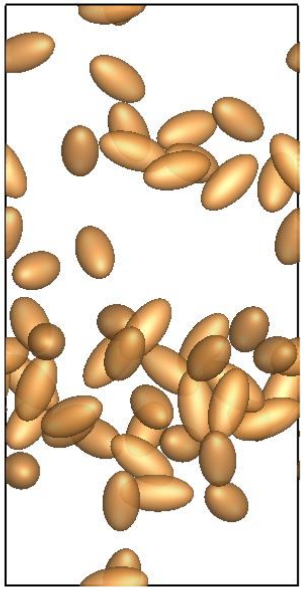
Falling Spheroids



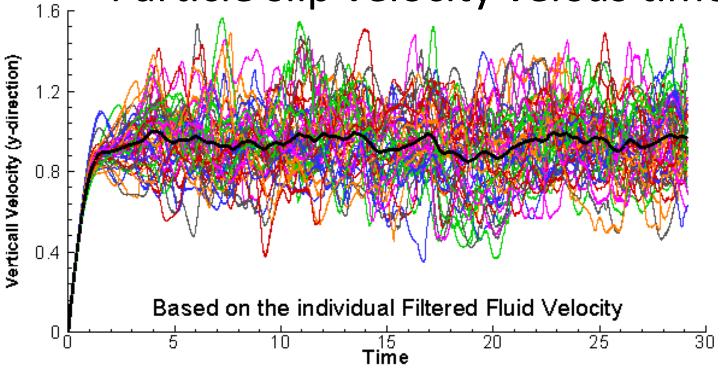
The distribution of ellipsoidal particles at time = 30 for different “aspect ratios”

Falling Spheroids

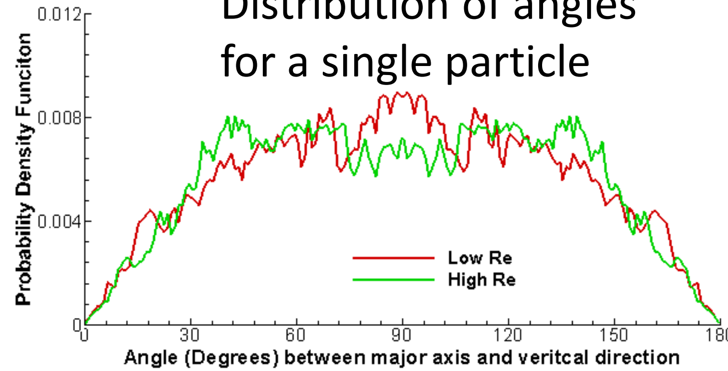
Higher Reynolds numbers



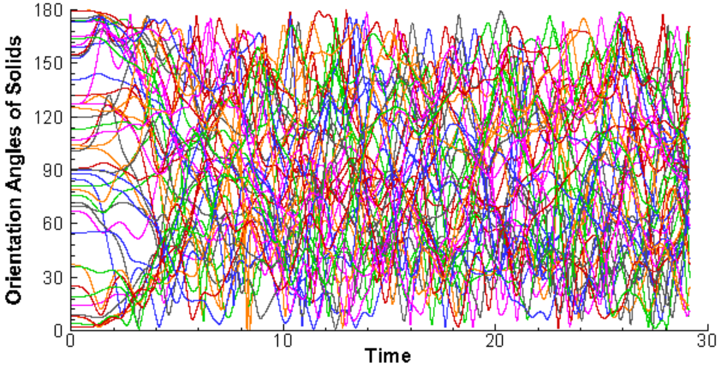
Particle slip velocity versus time



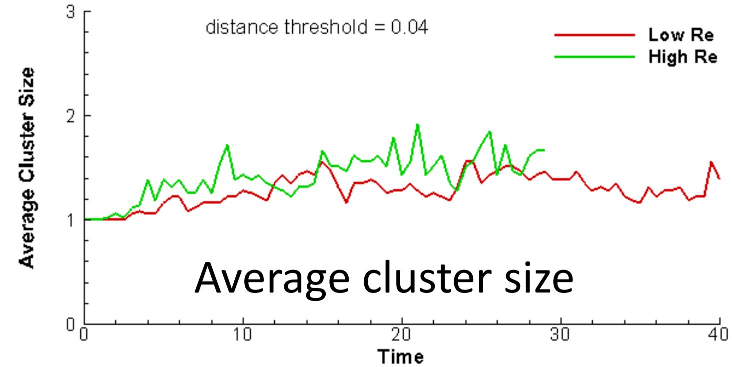
Distribution of angles for a single particle



At higher Reynolds numbers the particles interact more violently



The particle angle versus time



Average cluster size

$$Re_s = \frac{\rho_f u_s d_e}{\mu_f} = 187.6$$

Forces by Machine Learning

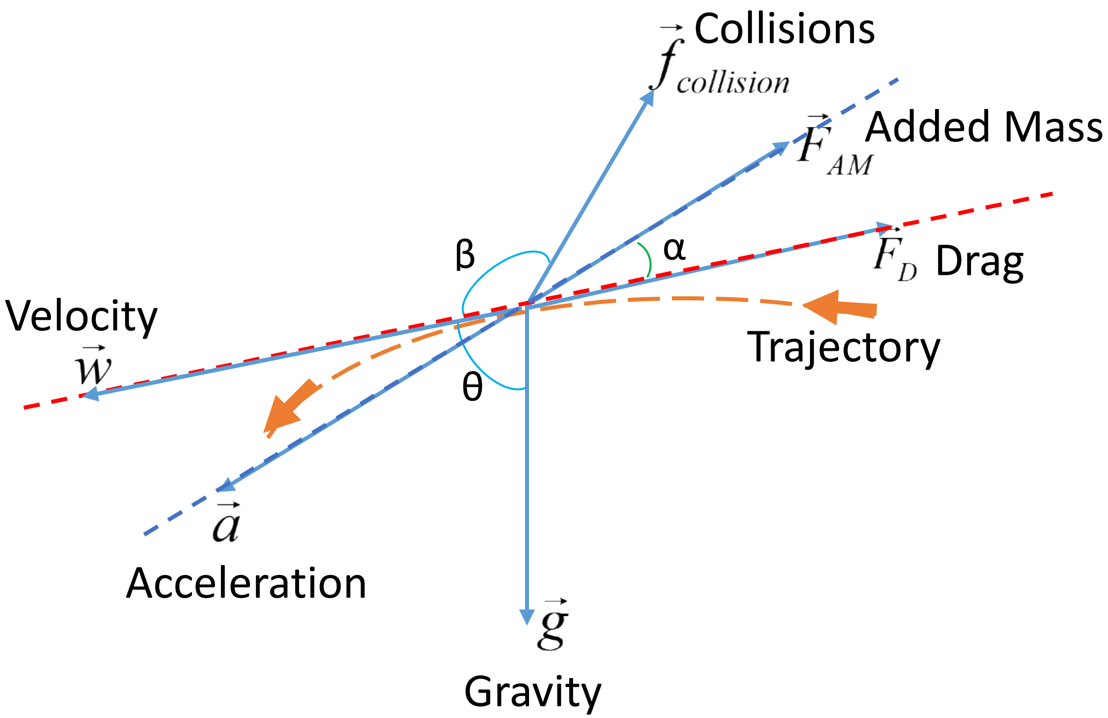
The motion of a particle is given by

$$M_p \frac{d\mathbf{U}_p}{dt} = \mathbf{F}_p + (\rho_s - \rho_f) V_p \mathbf{g}$$

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{U}_p$$

The force on the particle in unsteady motion has many parts, but the simplest assumption is that it is dominated by the steady drag

$$\mathbf{F}_p \approx \mathbf{F}_D = \frac{C_D}{\frac{1}{2}\rho U_p^2 A_p}$$



The drag coefficient depends the fluid, the slip velocity and the "neighborhood"

$$C_D = C_D(Re_p, \text{Orientation}, \text{Flow Configuration}, \text{Volume Fraction}, \text{Neighbors}, ...)$$

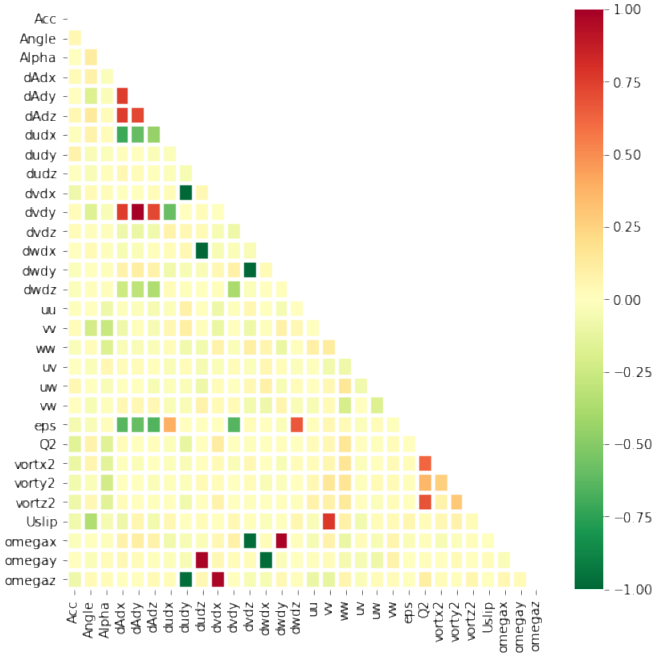
Forces by Machine Learning

Finding total force by machine learning: The total dataset is collected from 50 ellipsoids at 647 different times, and the data where the collision force is not zero are removed. The total input matrix size is 28548 x 30, and the target matrix size is 28548 x 1.

Deep Learning Steps:

1) Split the dataset into a training set (80%) and a test set (20%). The training set is used to train the model, and the test set is used in the final evaluation of the model.
2) Standardize the dataset by removing the mean and scaling to unit variance for each input/feature.
3) Build a model. Use Tensorflow 2 to build a sequential model, which consists of 4 dense hidden layers with 200, 100, 50 and 25 nodes (neurons), and 1 out layer.
4) Compile and train the model. During the training, 20% of the training data is used to validate the model.
5) Evaluate the model's predication with the testing data.

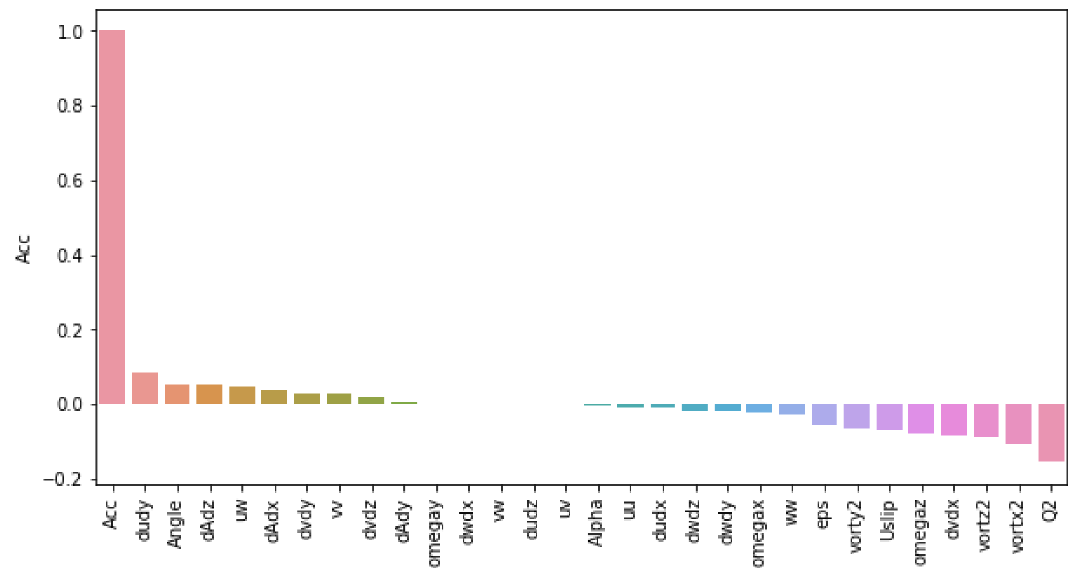
Forces by Machine Learning



Pearson's correlation coefficients between all features.

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

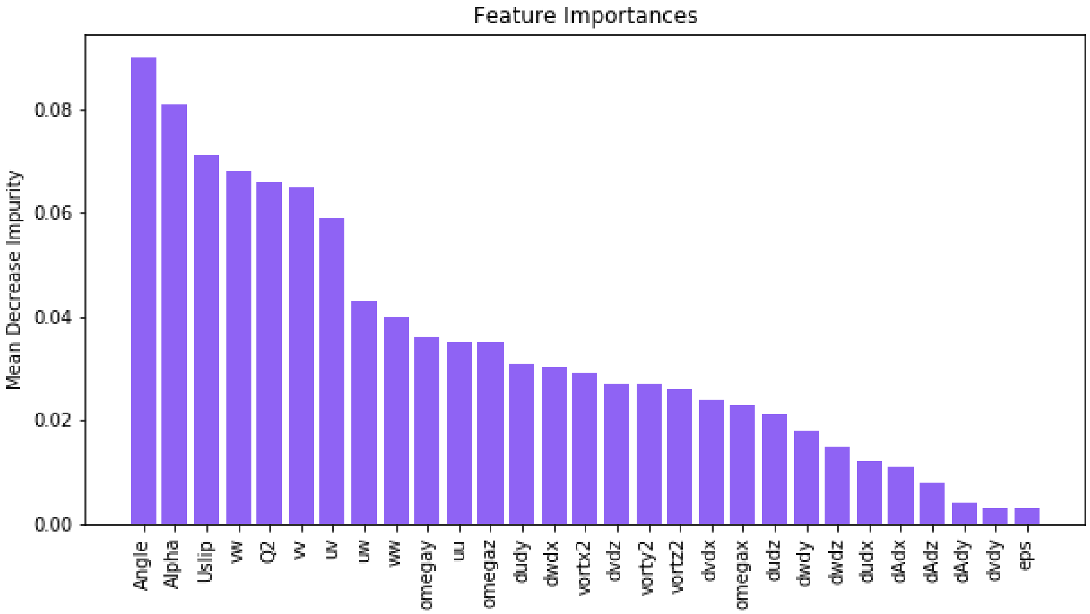
Finding the optimum independent variable. We have explored several ways to do so.



Sorted correlation coefficients between the target acceleration and other input features

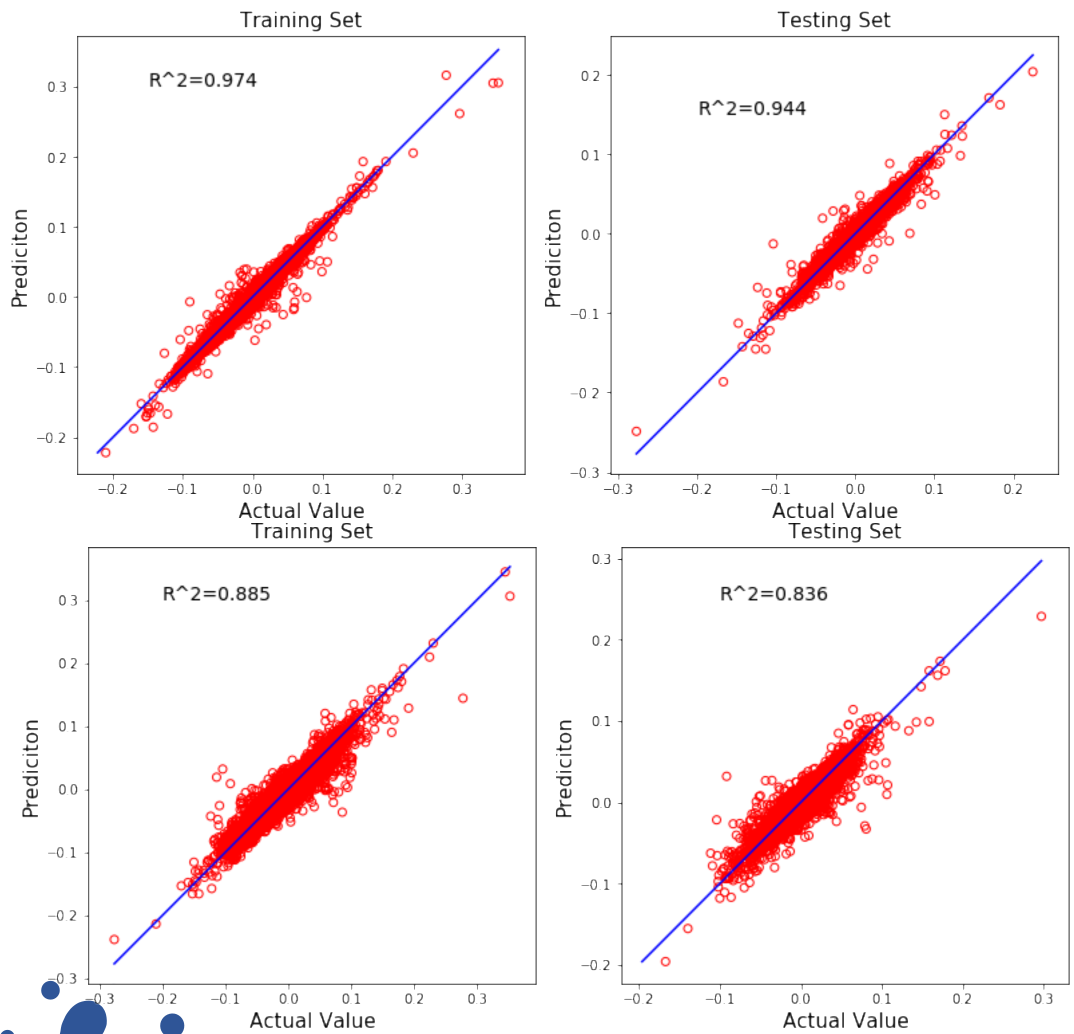
Forces by Machine Learning

Another way to determine the most important independent variables



Feature importance are ranked according to the mean decrease impurity from Random Forest method. Random forest consists of multiple single decision trees. Every nodes in the decision trees is a condition on a single variable, and the measure based on which the locally optimal condition is chosen is called impurity. When training a tree, it can be computed how much each variable decreases the weighted impurity in a tree. For a forest, the impurity decrease from each variable can be averaged and the variables are ranked according to this measure.

Forces by Machine Learning

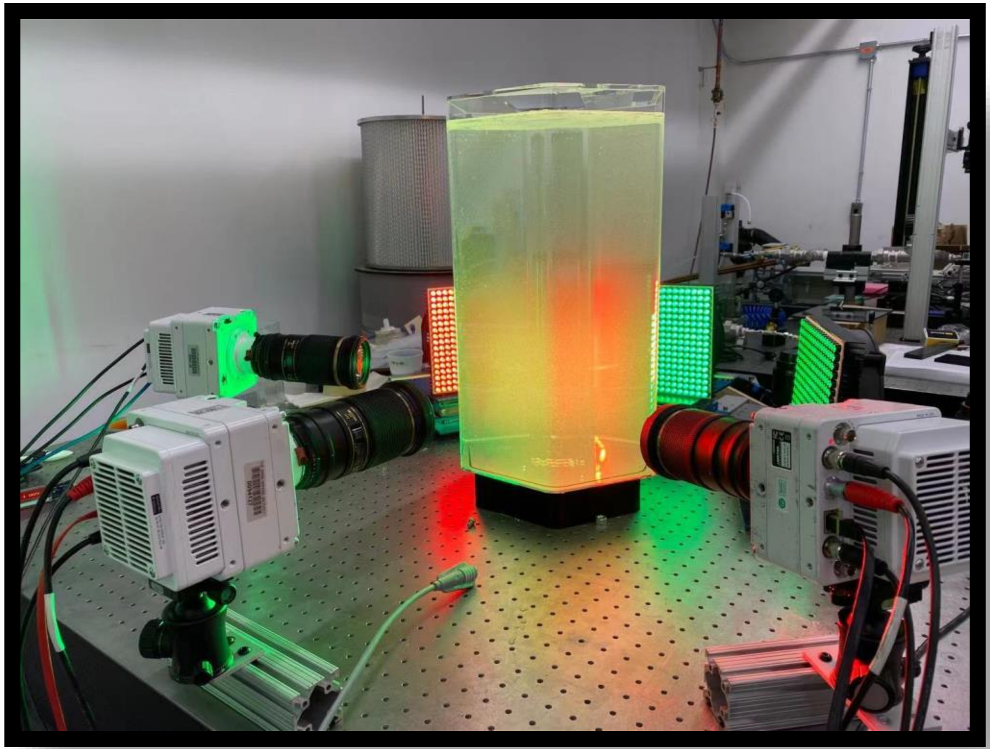


Total force values versus the predicted values for full set of input features. (Left for Training dataset, and Right for the Testing dataset). R squared (coefficient of determination) as a regression score function is also shown on each figure.

Total force versus the predicted values with a reduced set of input features. While the correlation is not as good as for the full set, it remains reasonably high

Experimental Setup

- We utilize three Phantom cameras with LED backlight.
- We kept a 60-degree angle between each cameras.
- All cameras are facing downward with roughly 5-degree angle.
- The test tank is hexagonal, 30 cm wide, and 80 cm tall.



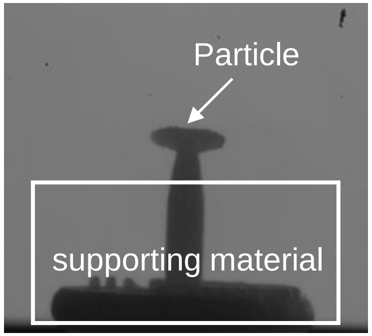
Camera frame rate	Exposure time	Tracer diameter	Fluid	Fluid initial condition
4000 fps	150 μs	60 μm	Water	Stagnant

Goal: simultaneously measure particle and fluid flow.

Non-spherical Particles

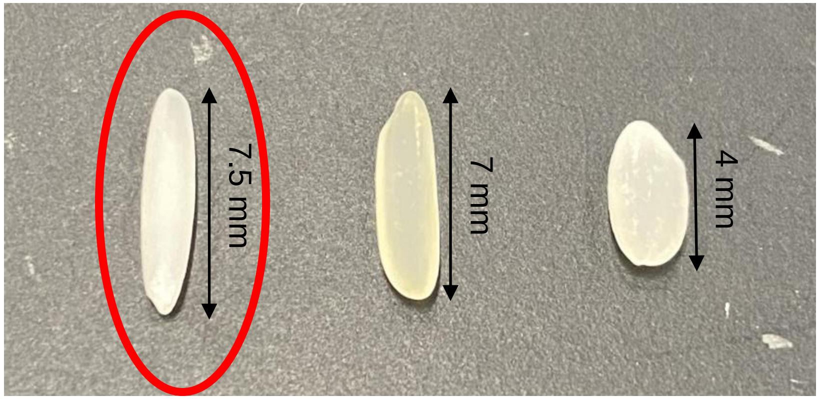
Formlabs Form2 3D printer

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



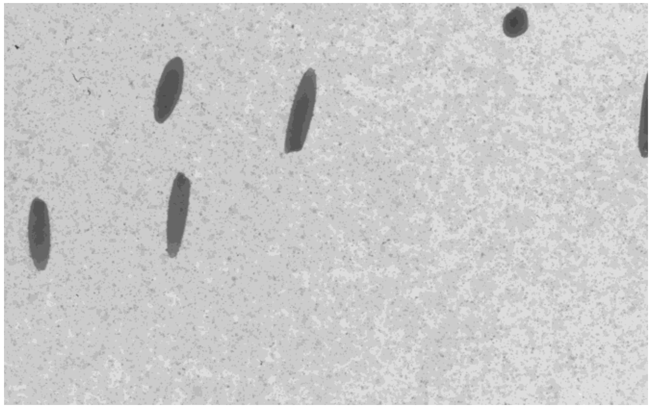
This is a 3D printed particle with supporting material. It has a 2.5 mm major diameter and 0.5 mm minor diameter.

Non-spherical particles also exist in nature



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

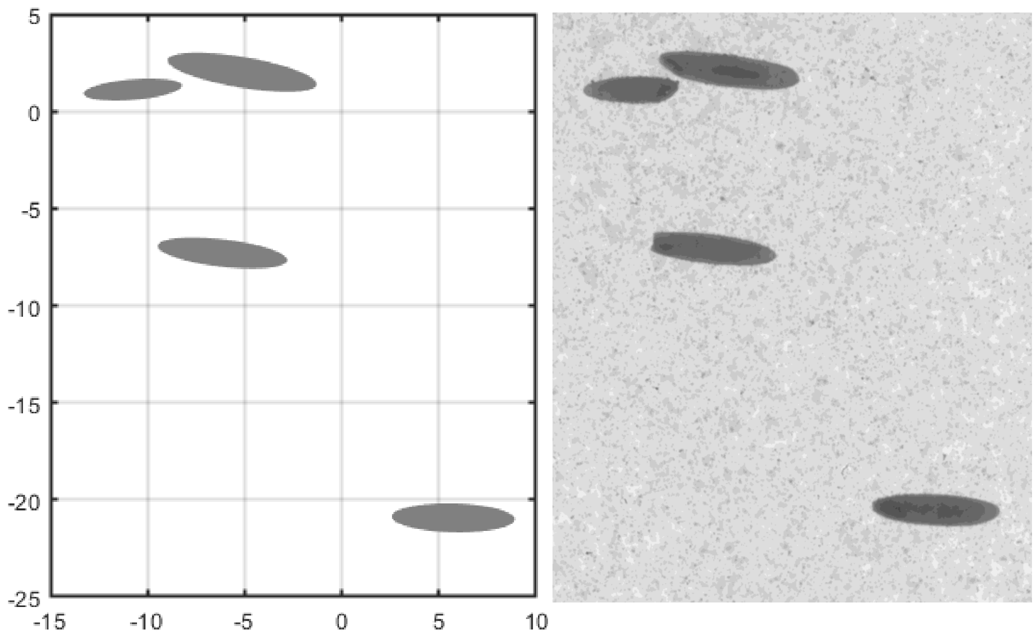
Phase Separation

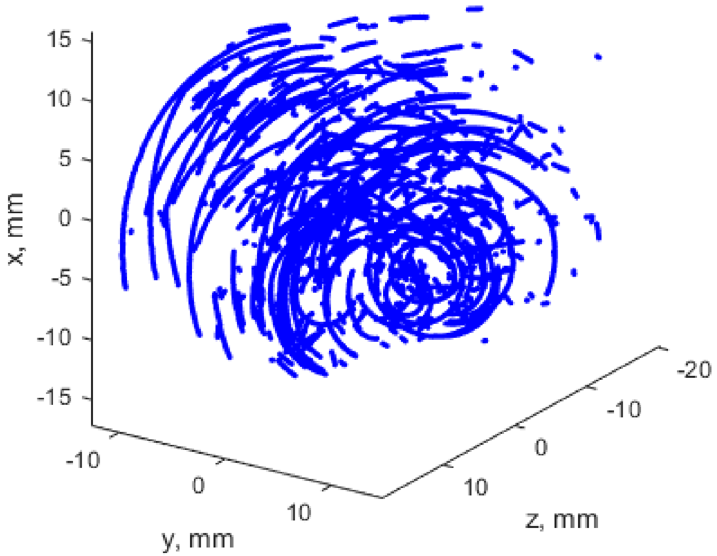


A.U.M. Masuk et. al. 2019, “Virtual-Camera Reconstruction”

Tan et. al. 2020, “OpenLPT (Shake-The-Box)”

Two Phase Measurements

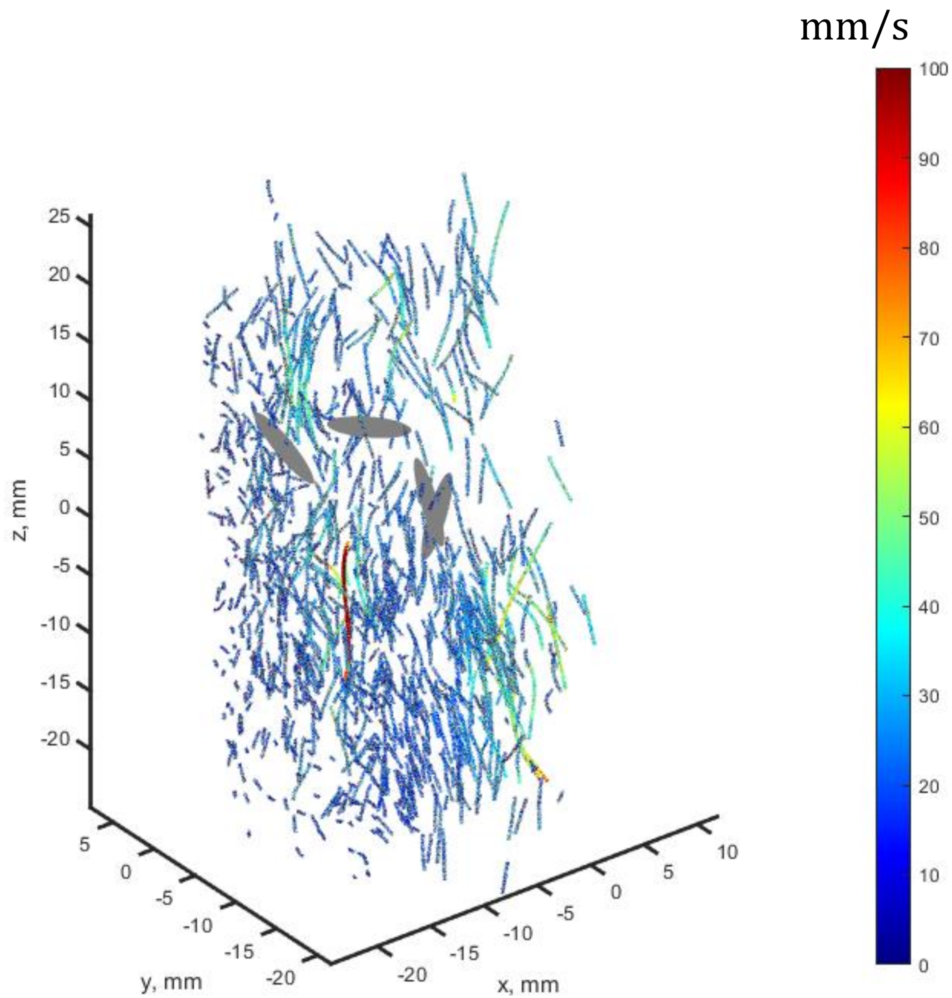




- Left panel show reconstructed particles.
- Right panel show raw image at the same frame.

- This is a single-phase test case where a vortex structure is created by stirring the tank.
- The vortex structure is captured

Reconstructed Rice Particles



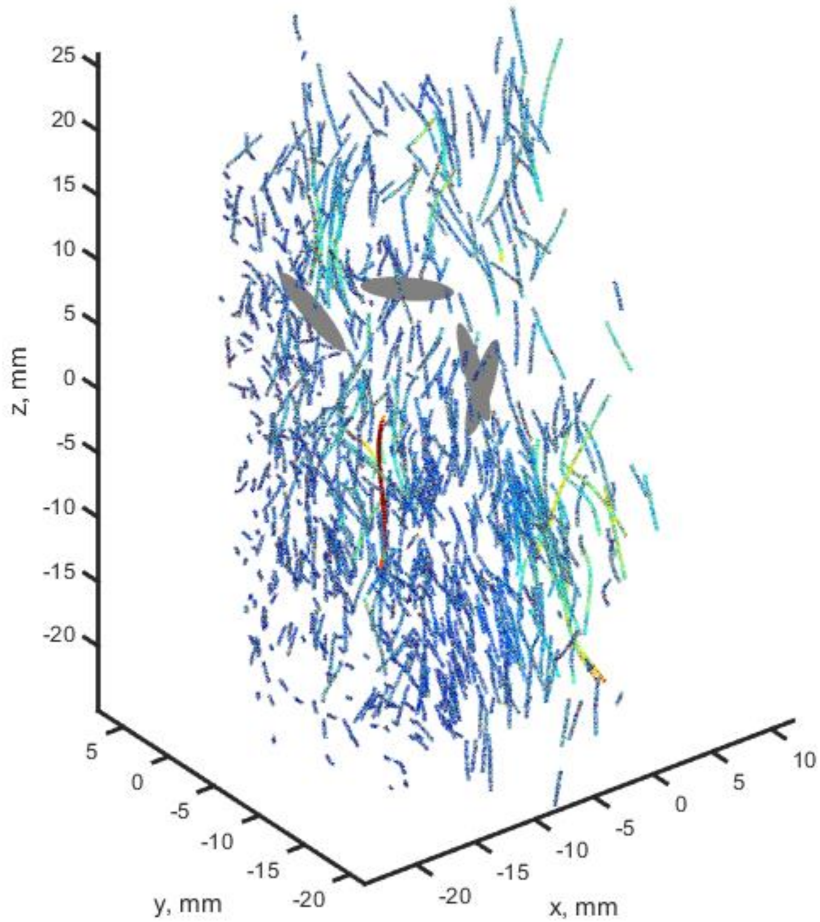
How does particle interaction affect drag coefficient?

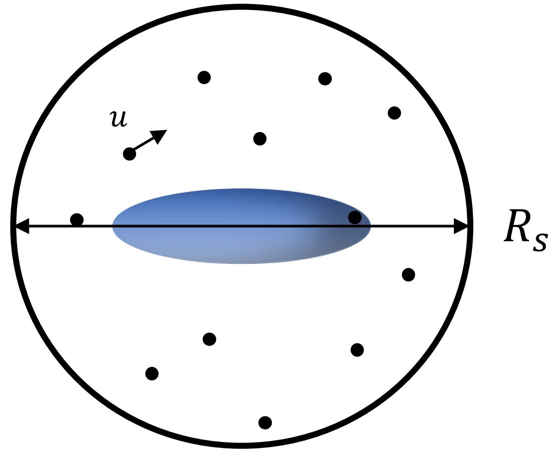
Maybe through wake interaction.

Particles in others wake can have smaller Reynolds number.

How does the drag coefficient experienced by a group of particles compare with an isolated particle?

Results





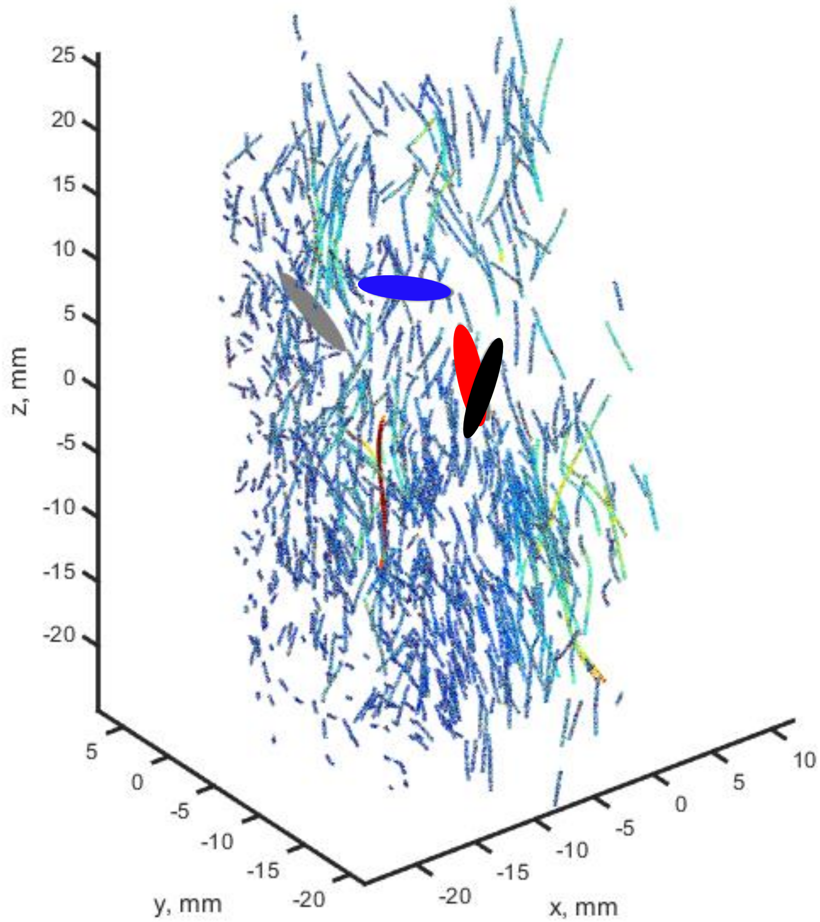
Slip velocity:

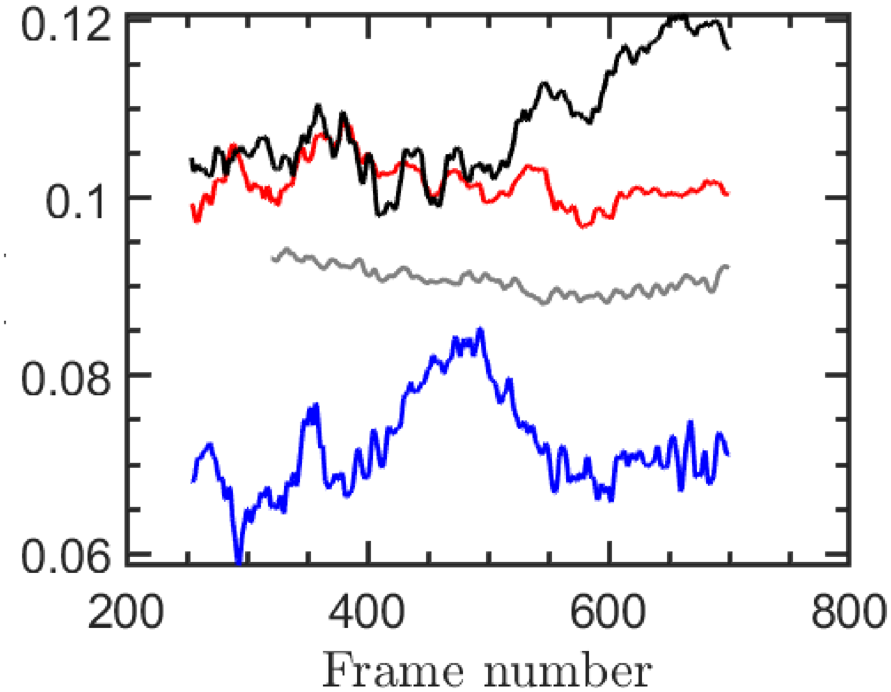
$$\boldsymbol{u}_{\mathrm{s}} = \boldsymbol{u}_{\mathrm{p}} - \boldsymbol{u}_{\mathrm{f}}$$

$$R_s = 2d_{\mathrm{p}}$$

- R_s is the search radius.
- d_{p} is the equivalent radius of a sphere with the same volume.
- $\boldsymbol{u}_{\mathrm{p}}$ is the particle velocity
- $\boldsymbol{u}_{\mathrm{f}}$ is the fluid velocity

Results



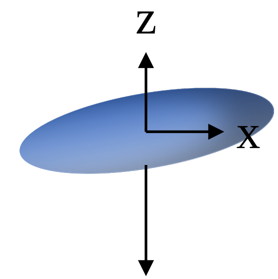


$$\boldsymbol{u}_{\mathrm{s}} = \boldsymbol{u}_{\mathrm{r}} - \boldsymbol{u}_{\mathrm{f}}$$

The gray line is the slip velocity of the isolated particle.
The colored lines correspond to particles of the same color in the 3D plot.

Comparison with drag coefficient model

Model for non-spherical particle ($\boldsymbol{Re} < \mathbf{10^5}$):



$\boldsymbol{u}_{\mathbf{s}}, \boldsymbol{a}_{\mathbf{p}}, \boldsymbol{g}$

$$C_D = \frac{8}{Re}\frac{1}{\sqrt{\Phi_\parallel}} + \frac{16}{Re}\frac{1}{\sqrt{\Phi}} + \frac{3}{\sqrt{Re}}\frac{1}{\Phi^{\frac{3}{4}}} + 0.421 * 10^{0.4(-log\Phi)^{0.2}}\frac{1}{\Phi_\perp}$$

Estimation from experimental measurements:

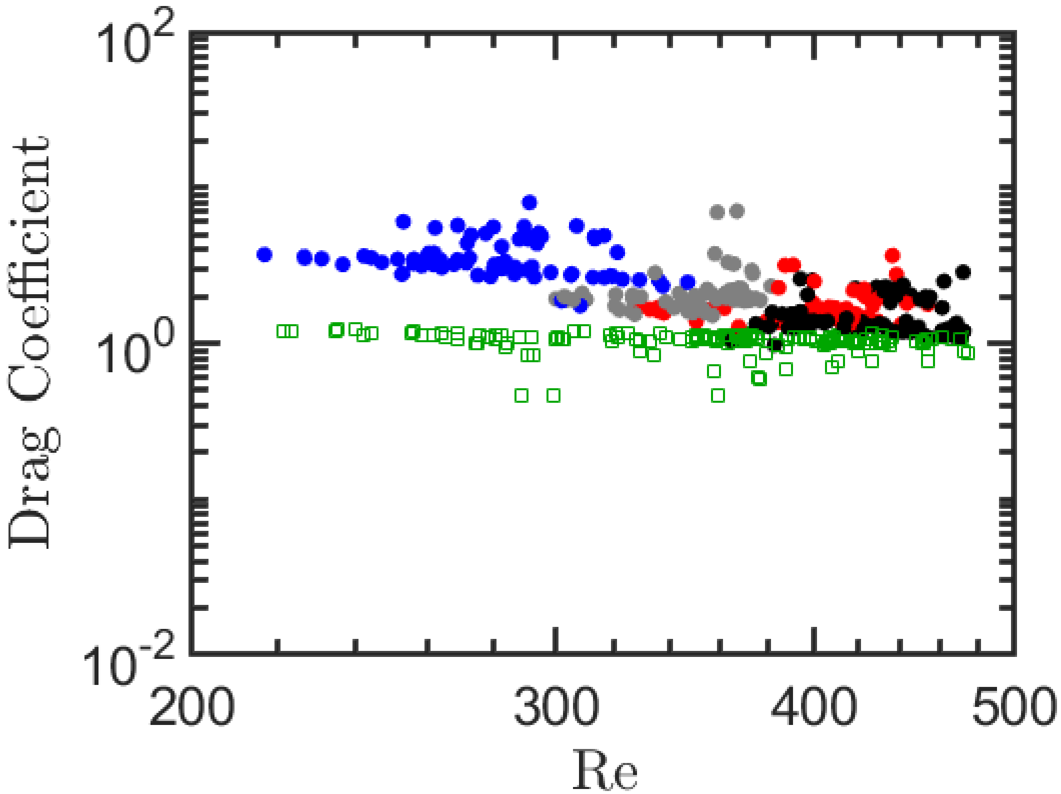
$$\boldsymbol{F}_{\mathrm{D}} = \rho_{\mathrm{p}} V \boldsymbol{a}_{\mathbf{p}} + (\rho_{\mathrm{p}} - \rho_{\mathrm{f}}) V \boldsymbol{g}$$

$$C_{\mathrm{D}} = 2\frac{|\boldsymbol{F}_{\mathrm{D}}|}{A\rho_{\mathrm{f}}|\boldsymbol{u}_{\mathrm{s}}|^2}$$

- $\boldsymbol{a}_{\mathbf{p}}$ is the particle acceleration
- $\boldsymbol{g}$ is the gravitational acceleration
- V is the particle volume
- ρ_{p} is the particle density
- ρ_{f} is the fluid density

- Re is particle Reynolds number.
- Φ is the sphericity defined as ratio between sphere equivalent surface area and actual surface area.
- $\Phi_\parallel$ is the lengthwise sphericity.
- $\Phi_\perp$ is the crosswise sphericity.
- A is the cross-sectional area.

Comparison with drag coefficient model

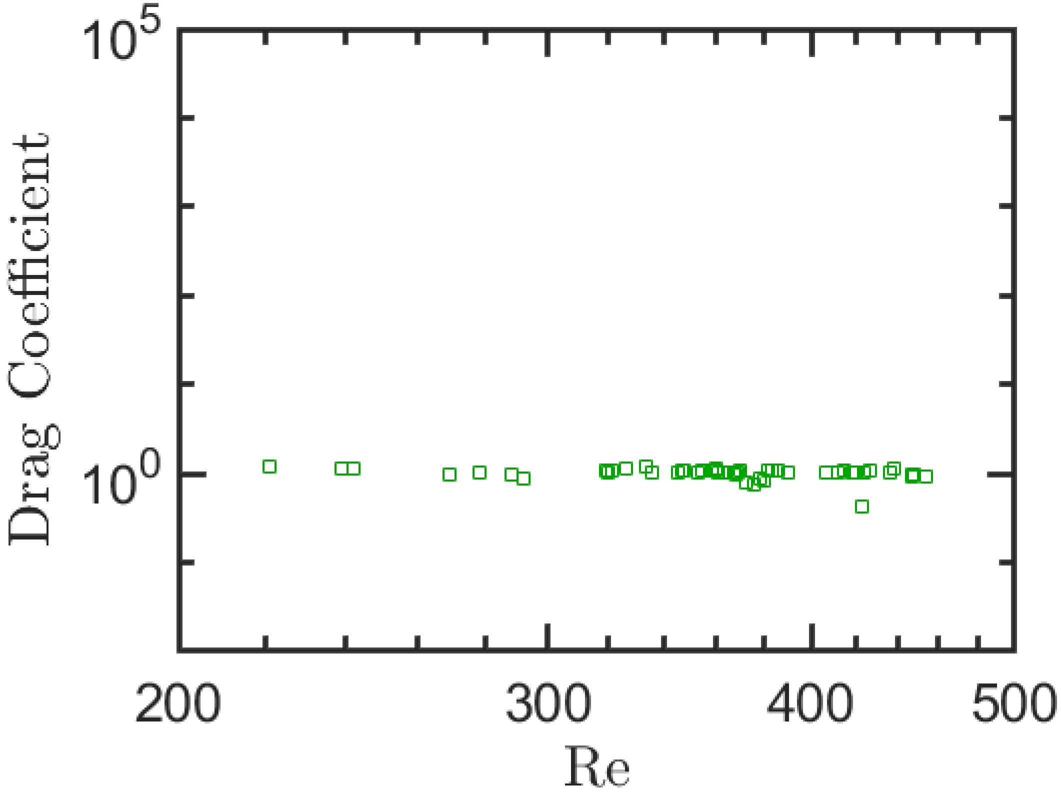


- The colored circle symbols represent the particles adjacent to each other
- The gray circle symbols represent the isolated particle.
- The green square symbols are results calculated with the drag coefficient model

What about added mass force?

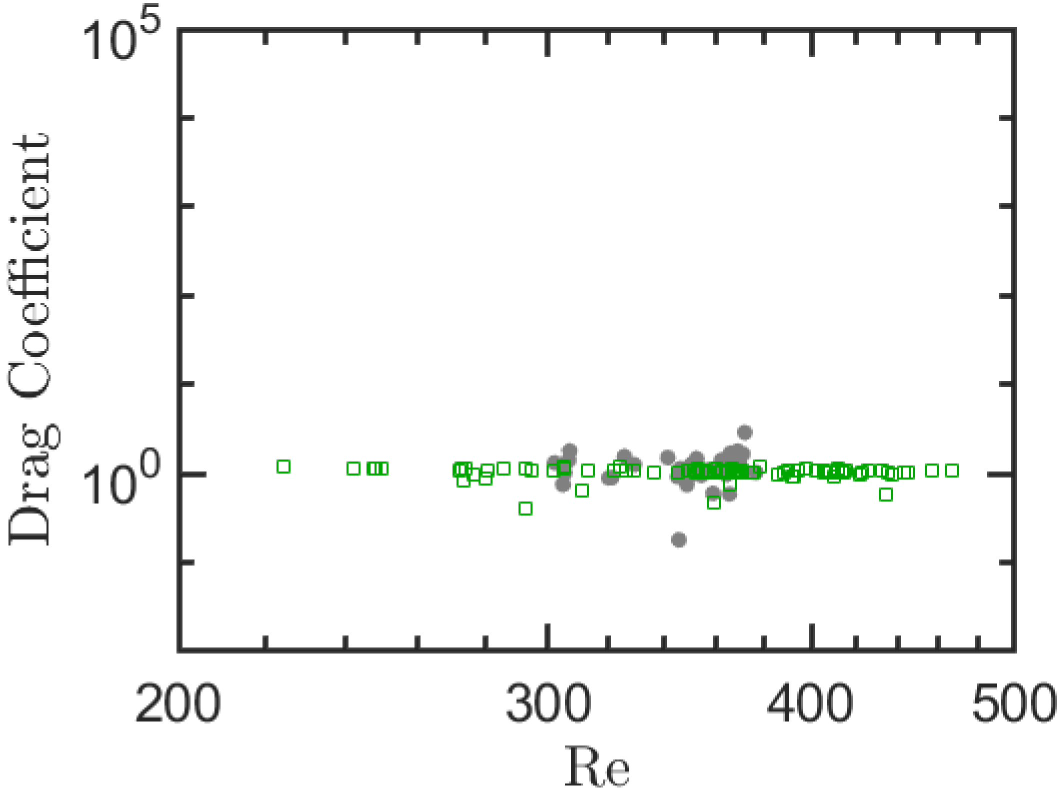
Comparison with drag coefficient model

$$\boldsymbol{F}_{\mathrm{D}} = \rho_{\mathrm{p}} V \boldsymbol{a}_{\mathbf{p}} + (\rho_{\mathrm{p}} - \rho_{\mathrm{f}}) V \boldsymbol{g} - \frac{1}{2} \rho_{\mathrm{f}} V (\boldsymbol{a}_{\mathrm{f}} - \boldsymbol{a}_{\mathbf{p}})$$



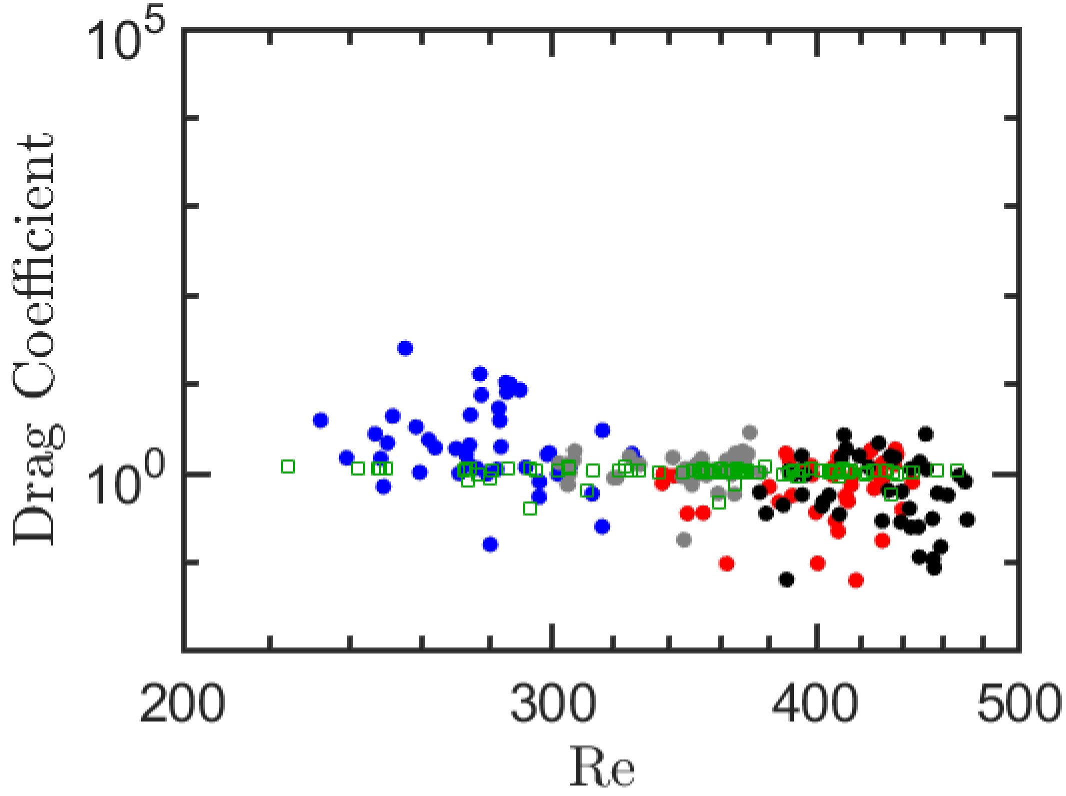
- The added mass coefficient utilized here is for spherical particles, a more accurate added mass coefficient for spheroid will be used in the future.

Comparison with drag coefficient model



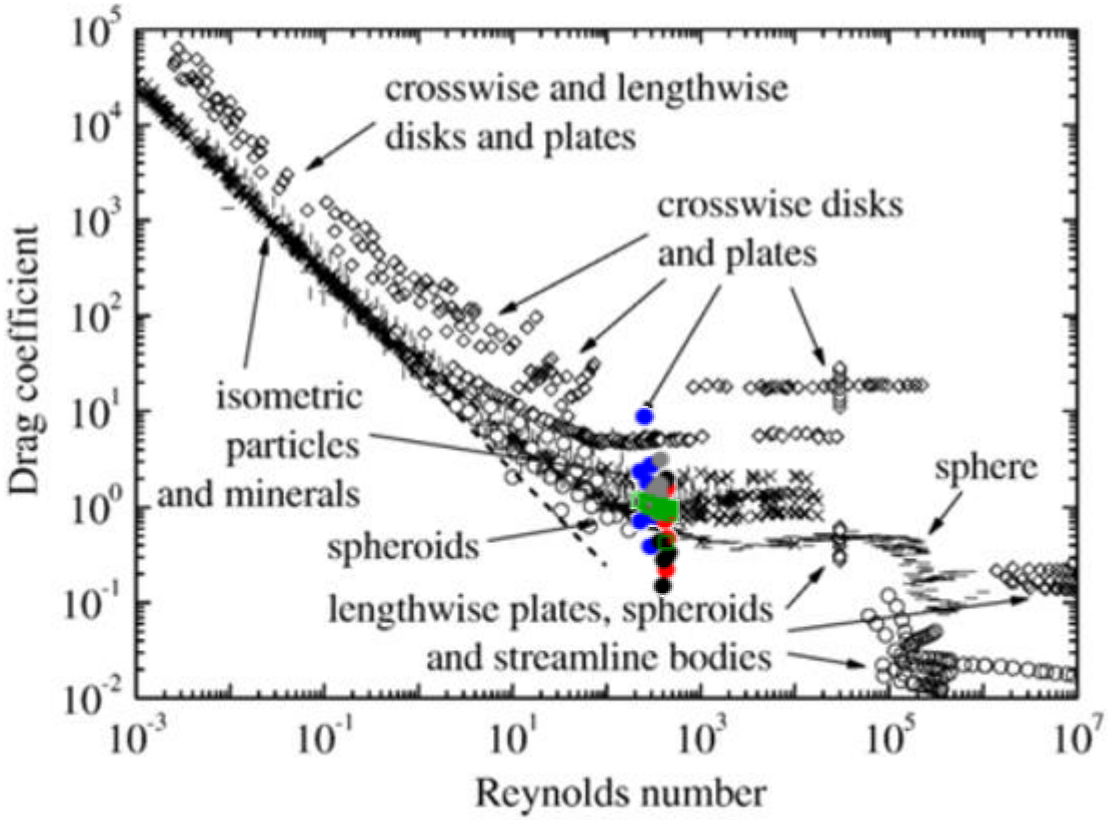
- When accounting for the added mass force, isolated particle agrees with the steady drag model
- Does particle-particle interaction influence the results?

Comparison with drag coefficient model



- Particle-particle interaction cause the instantaneous drag coefficient to deviate away from the green symbols.

Comparison with drag coefficient model

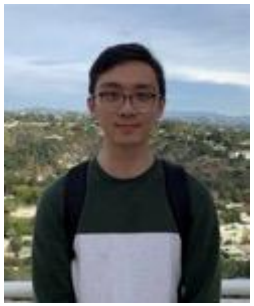


- Our instantaneous drag coefficient results generally agree with the previous efforts.
- Particle-particle interaction may change the instantaneous drag coefficient by one order of magnitude.

Plan

Subteam 1: Experiment

Rui Ni

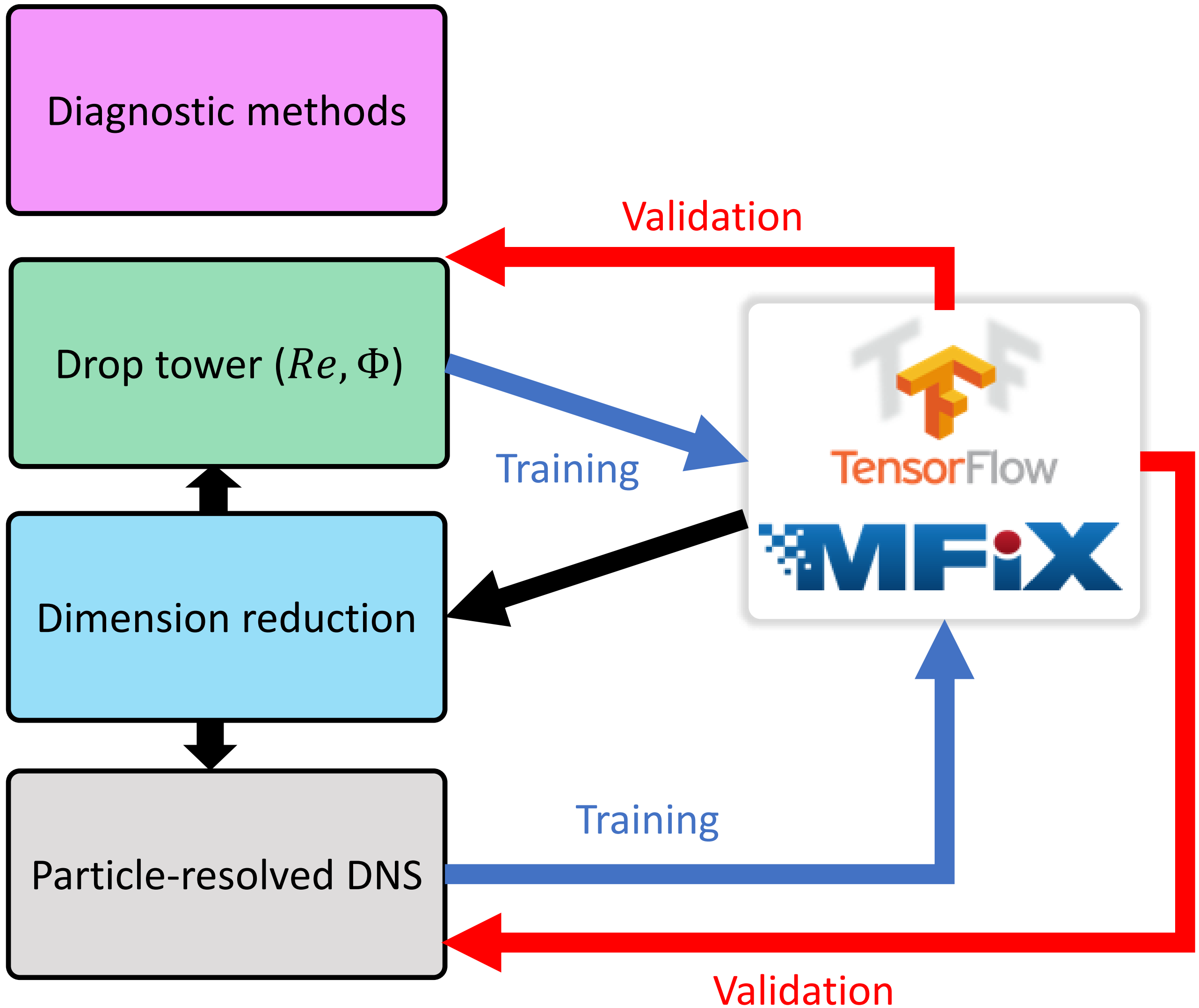


Xu Xu

Subteam 2: Simulation

Gretar Tryggvason

Jiacai Lu



Acknowledgment

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