RECENT PROGRESS IN SIMULATION AND MODELING OF GAS-PARTICLE FLOWS

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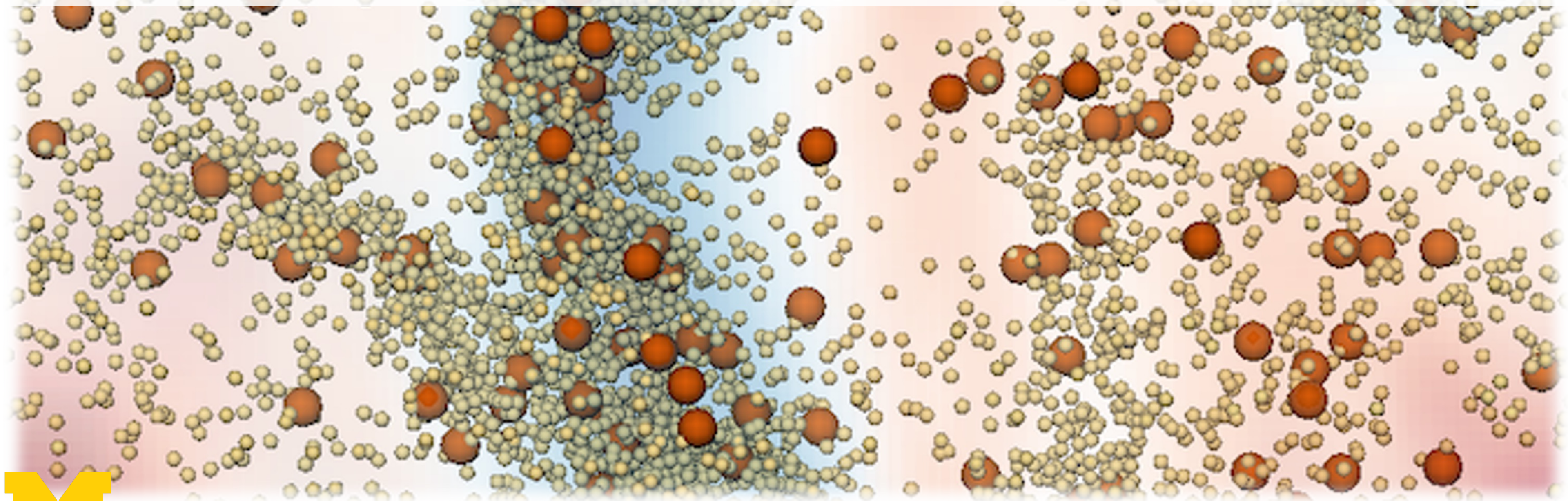
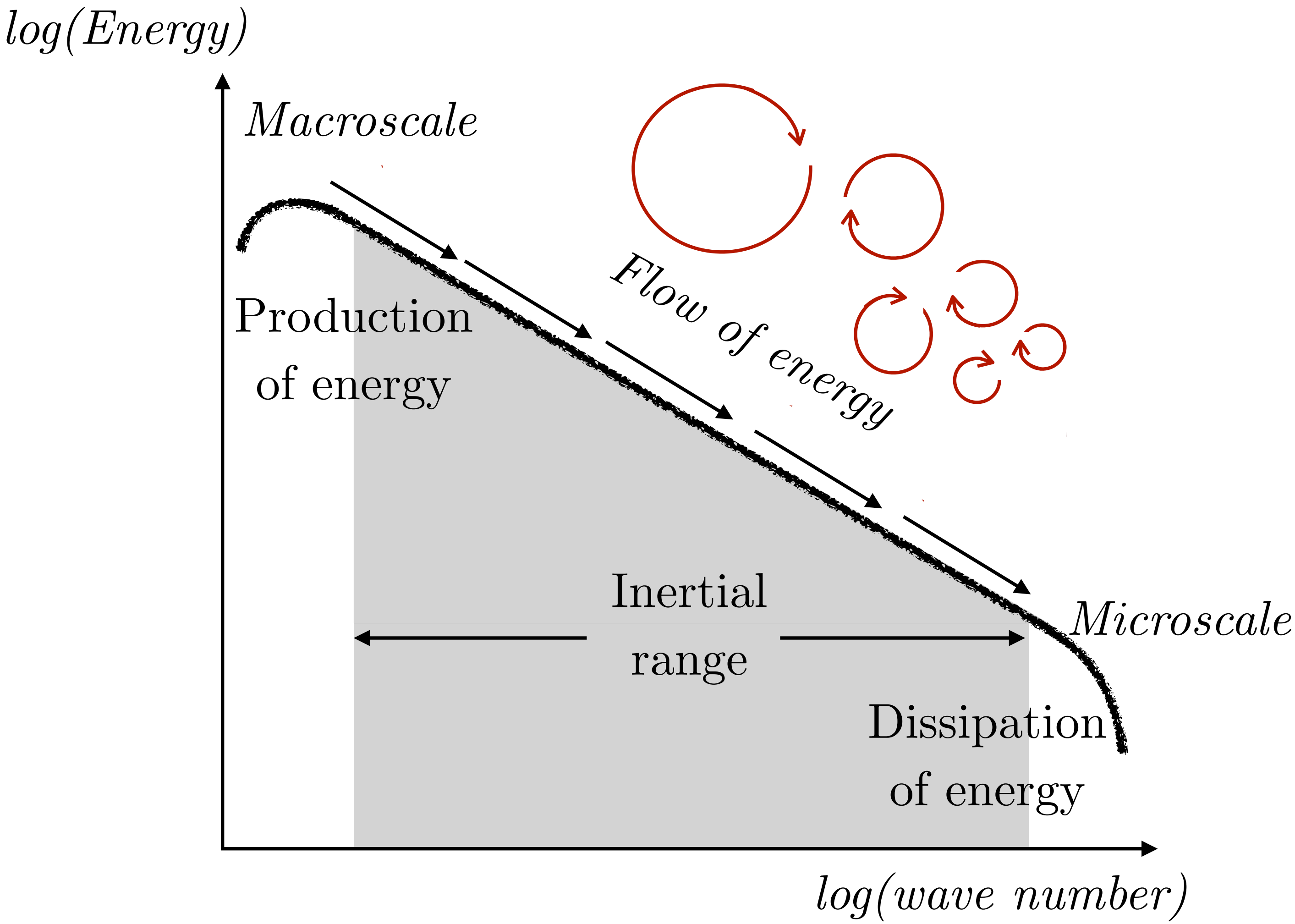
11th IFPRI Workshop on Particle Technology
Modelling of Powder Flow, June 9-10, 2023

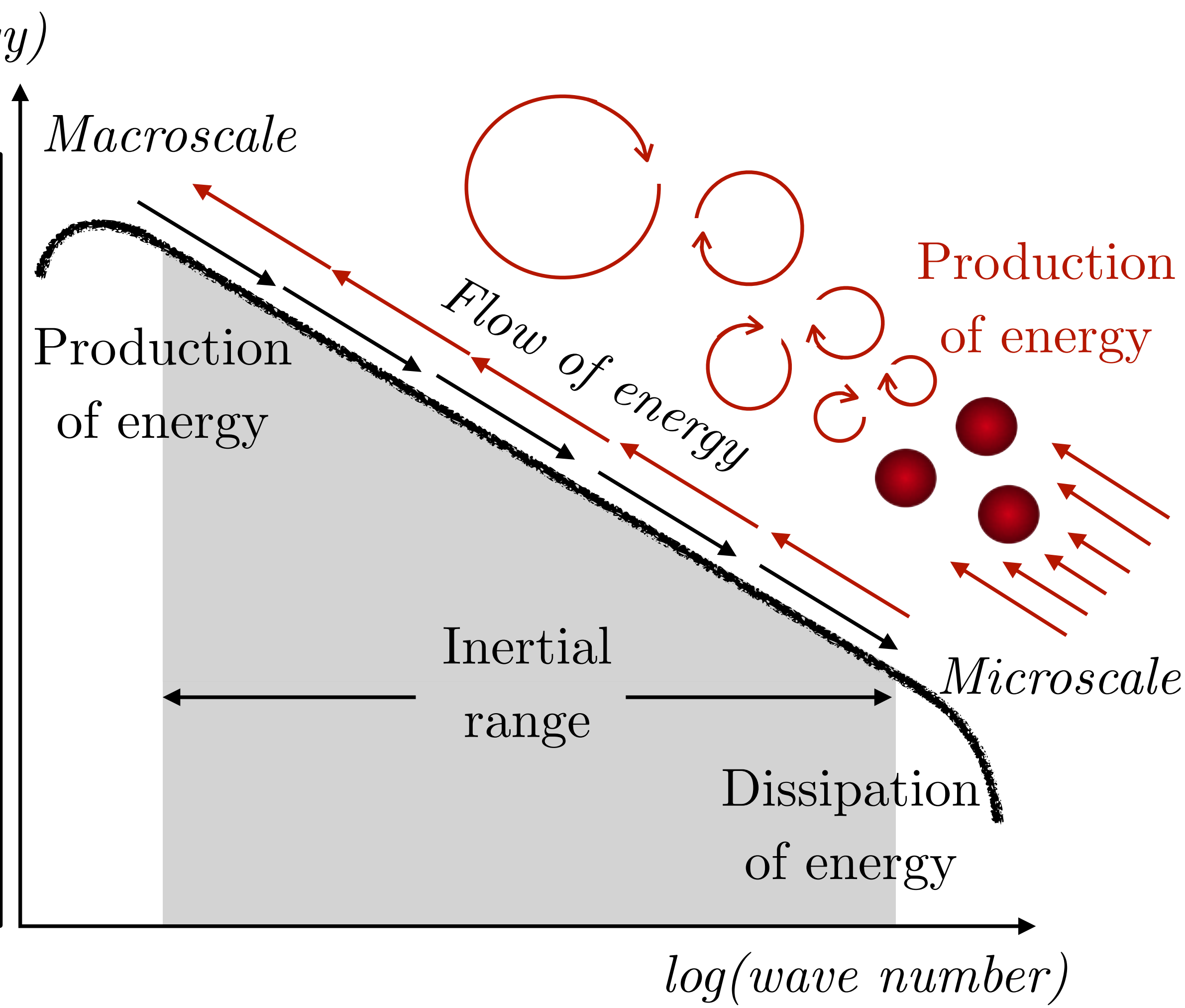


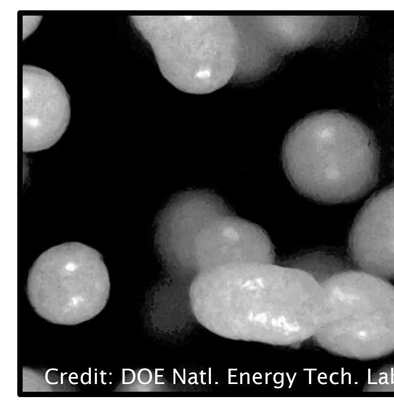
The National Energy Technology Laboratory’s chemical looping reactor

Challenge: how to bridge scales in turbulent particle-laden flows?



Challenge: how to bridge scales in turbulent particle-laden flows?

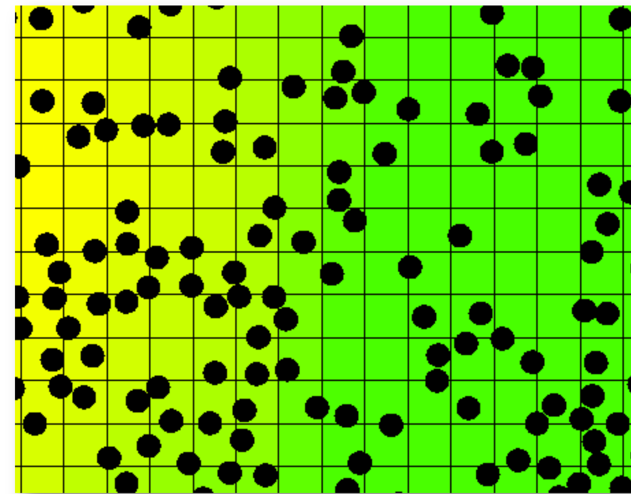




Outline for today's talk

1. New stochastic drag law for CFD-DEM
2. Role of clusters on heat and mass transport
3. Incorporating heterogeneity into coarse-grained models

CFD-DEM equations



- Fluid equations

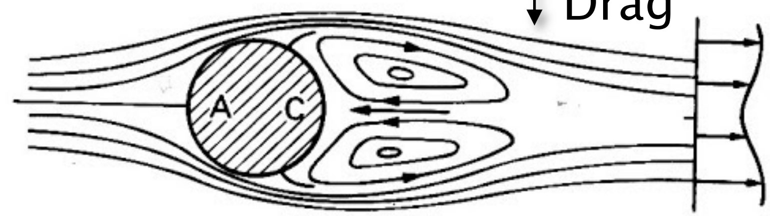
$$\frac{\partial}{\partial t}\left((1-\phi)\rho_f \boldsymbol{u}_f\right) + \nabla\cdot\left((1-\phi)\rho_f \boldsymbol{u}_f \otimes \boldsymbol{u}_f\right) = \nabla\cdot\boldsymbol{\tau} + (1-\phi)\rho_f \boldsymbol{g} - \boldsymbol{\mathcal{F}}_{\text{inter}}$$

- Lagrangian particle tracking

$$\frac{\mathrm{d}\boldsymbol{x}_p}{\mathrm{d}t} = \boldsymbol{v}_p, \quad m_p \frac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} = \boldsymbol{F}_{\text{col}} + m_p \boldsymbol{g} + \int \check{\boldsymbol{\tau}}\cdot\boldsymbol{n}\mathrm{d}S$$

Fluid-particle coupling: $\boldsymbol{F}_{f\to p} \equiv \int \check{\boldsymbol{\tau}}\cdot\boldsymbol{n}\mathrm{d}S = V_p \nabla\cdot\boldsymbol{\tau} + \boxed{\int \boldsymbol{\tau}'\cdot\boldsymbol{n}\mathrm{d}S}$

Drag



- Two-way coupling
(recall Berend van Wachem's talk)

$$\phi = \sum_{p=1}^{N_p} \mathcal{G}\left(|\boldsymbol{x}-\boldsymbol{x}_p|\right) V_p, \quad \mathcal{F}_{\text{inter}} = \sum_{p=1}^{N_p} \mathcal{G}\left(|\boldsymbol{x}-\boldsymbol{x}_p|\right) \boldsymbol{F}_{f\to p}$$

Developing drag laws from direct numerical simulations

Directly solve Navier—Stoke equation with appropriate boundary conditions at the surface of each particle

- Immersed boundary methods
- Lattice Boltzmann

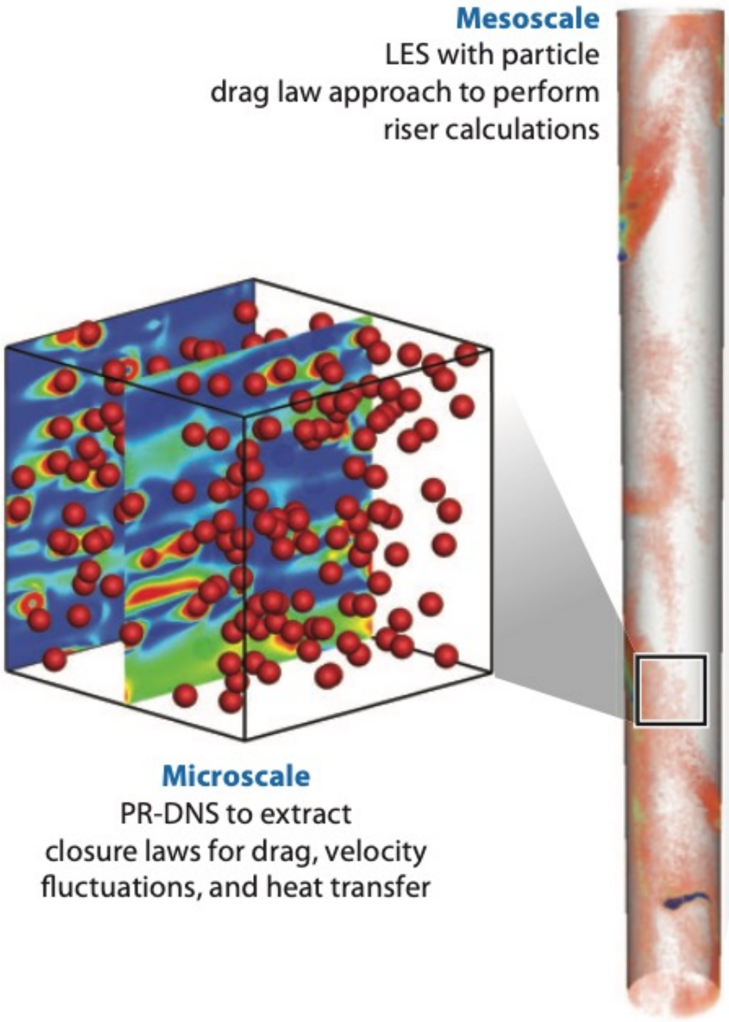
Drag → Output

Typical setup: homogeneous (triply-periodic) box of particles with applied mean velocity

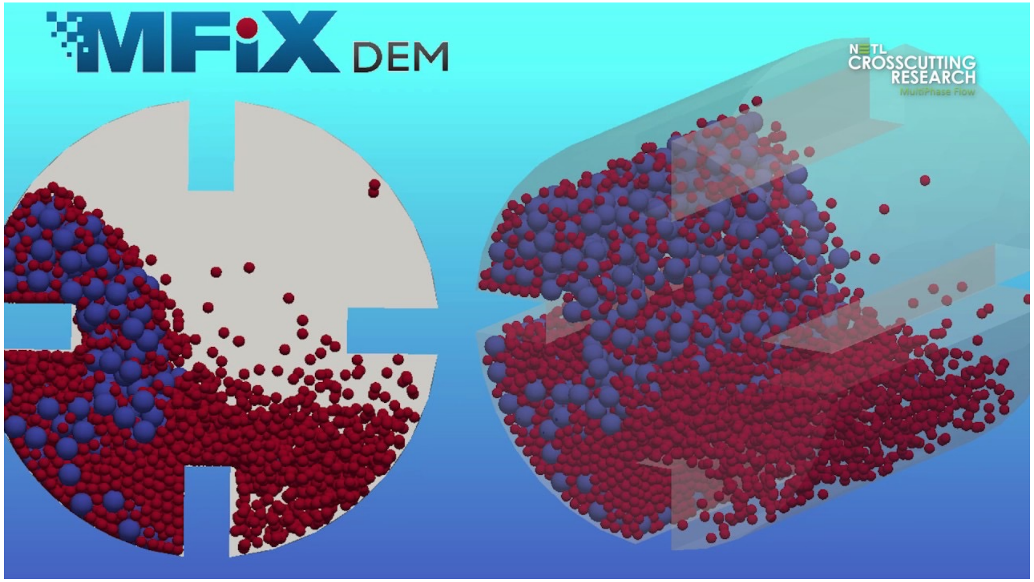
Ensemble average the drag force over multiple realizations and correlate to input parameters

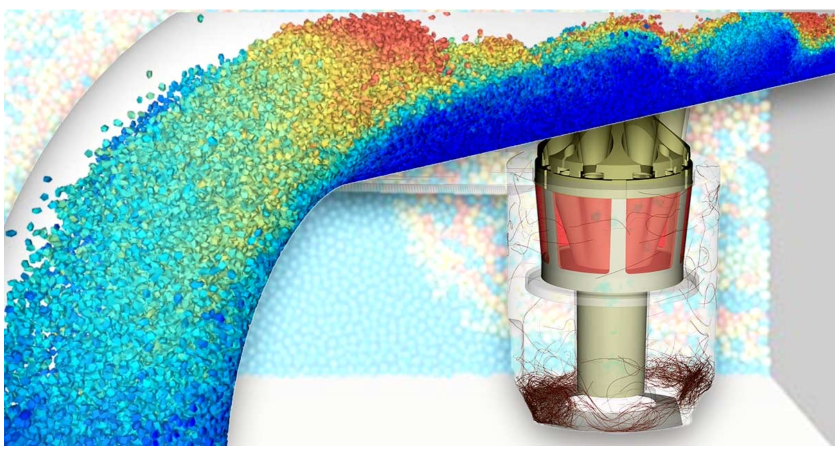
Example: Tenneti et al. (2011)

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



Standard practice in commercial CFD software





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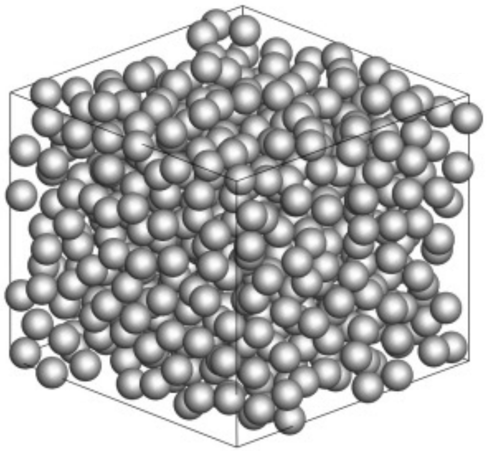
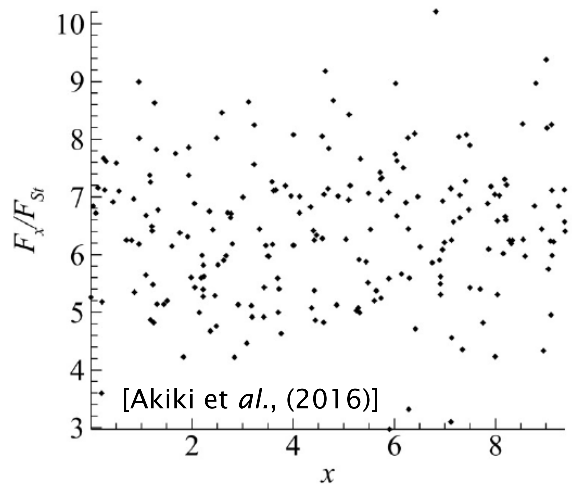
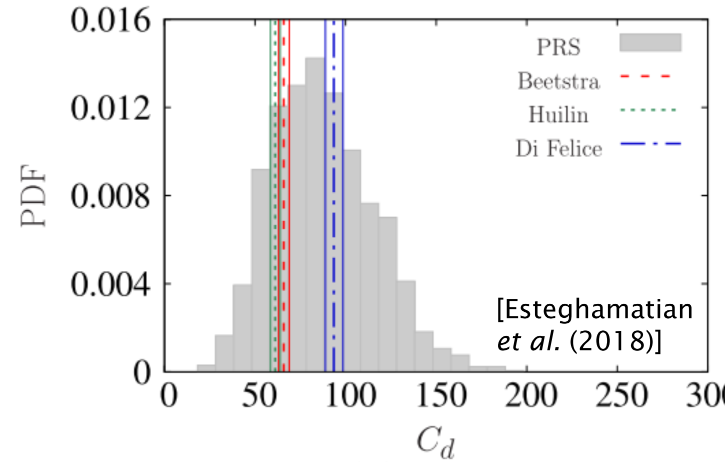
Drag in a dense assembly of particles

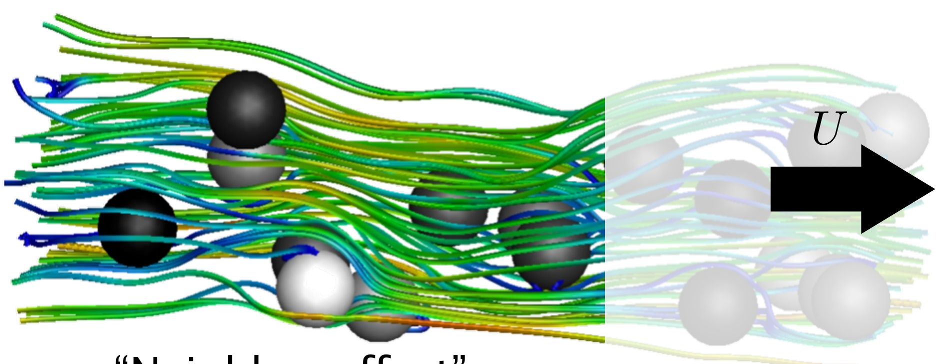
It is now well established that a collection of particles exhibit a significant *variation in drag about its mean*.



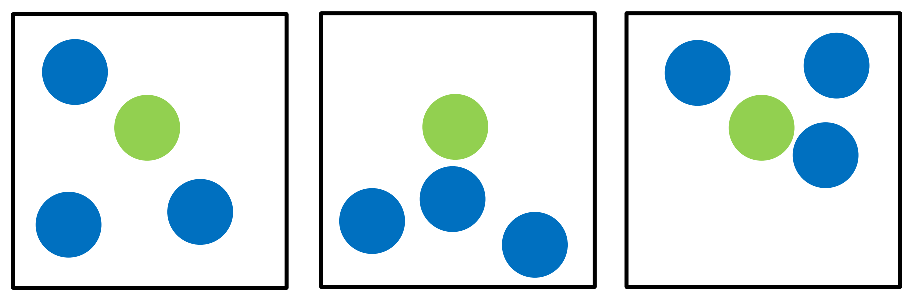




Existing drag laws fail to capture particle *velocity variance* and *dispersion*.



"Neighbor effect"



Each case has the same value of Re_m and ϕ

New stochastic drag force model

Equation of particle motion: $m_p \frac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} = \boldsymbol{F}_{\mathrm{col}} + m_p \boldsymbol{g} + \underbrace{\int \check{\boldsymbol{\tau}} \cdot \boldsymbol{n} \mathrm{d}S}_{\mathrm{Drag}}$

Split drag into mean and fluctuation components:

$$\int \boldsymbol{\tau} \cdot \boldsymbol{n} \mathrm{d}S = \langle \boldsymbol{F}_d \rangle + \boldsymbol{F}_d''$$

Mean drag modeled by adding Re_p and ϕ correction to drag for an isolated particle $\boldsymbol{F}_{iso}$ (Tenneti et al. 2011):

$$\langle \boldsymbol{F}_{\mathrm{drag}} \rangle = f(\mathrm{Re}_p, \phi, \dots)$$ ✔

Treat fluctuating component *stochastically* as an Ornstein-Uhlenbeck process:

$$\mathrm{d}\boldsymbol{F}''_{\mathrm{drag}} = -\frac{1}{\tau_F} \boldsymbol{F}''_{\mathrm{drag}} \mathrm{d}t + \frac{\sigma_F}{\sqrt{\tau_F}} \mathrm{d}\boldsymbol{W}$$

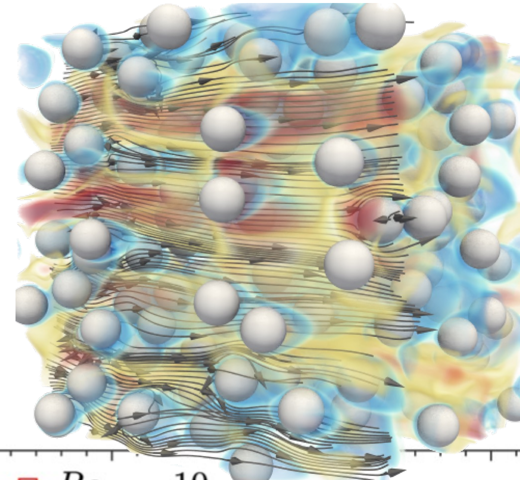
Time scale of fluctuating hydrodynamic drag force approximated by time between successive collisions[1] (Chapman et al. 1970):

$$\tau_F \approx \tau_{\mathrm{col}} = \frac{d_p}{24\phi\chi}\sqrt{\frac{\pi}{\Theta}}$$ ✔

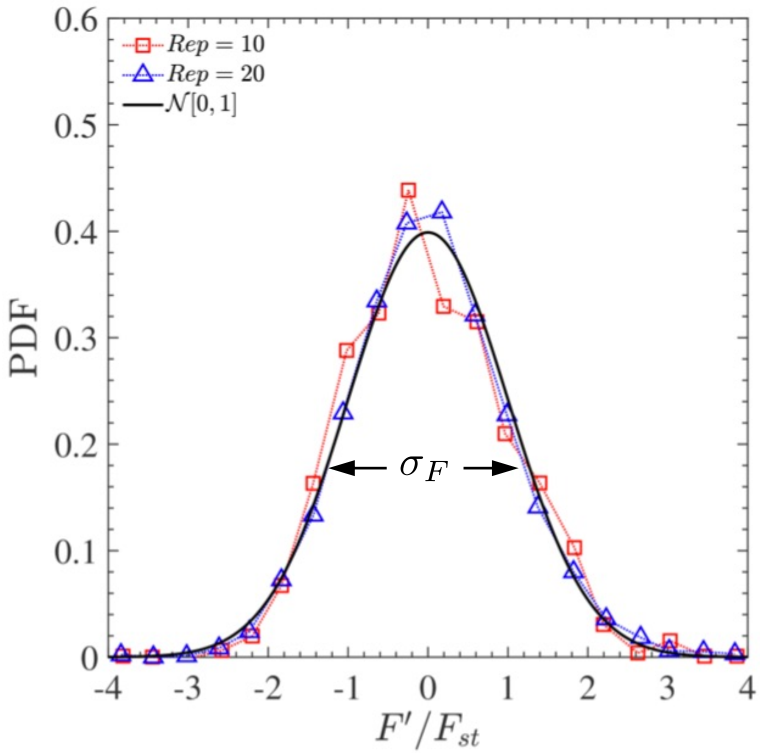
Need a model for the standard deviation in drag force!

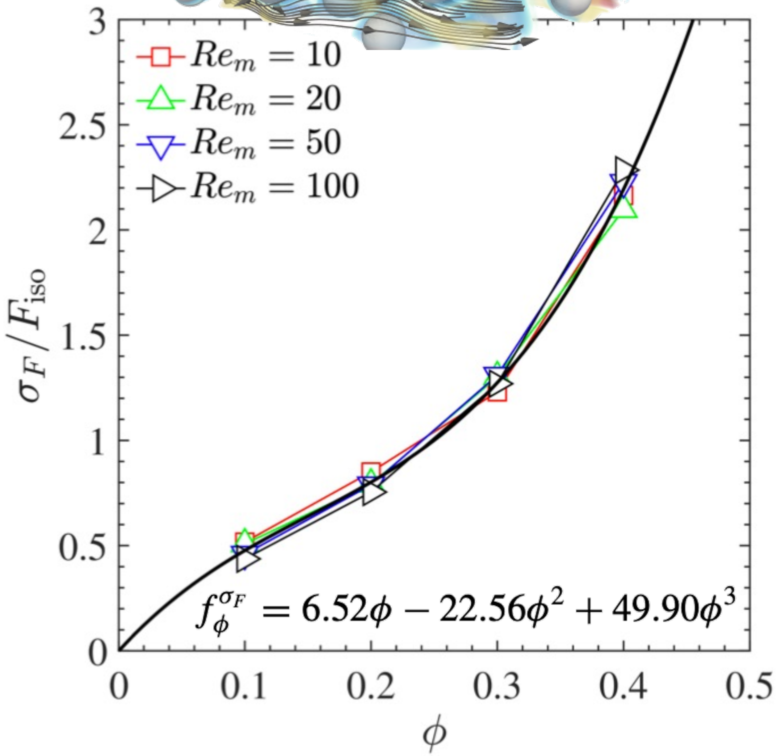
New stochastic drag force model

- Particle-resolved simulations reveal the distribution of drag forces is **Gaussian**
- Like the mean drag, the standard deviation collapses when normalizing by $\boldsymbol{F}_{\text{iso}}$!



$$\frac{\sigma_F}{m_p^{(i)}} \equiv f_\phi^{\sigma_F} \frac{F_{\text{single}}}{m_p^{(i)}} = f_\phi^{\sigma_F} f_{\text{iso}} \frac{(1-\phi)\left\|\boldsymbol{u}_f[\boldsymbol{X}_p^{(i)}] - \boldsymbol{U}_p^{(i)}\right\|}{\tau_p}$$

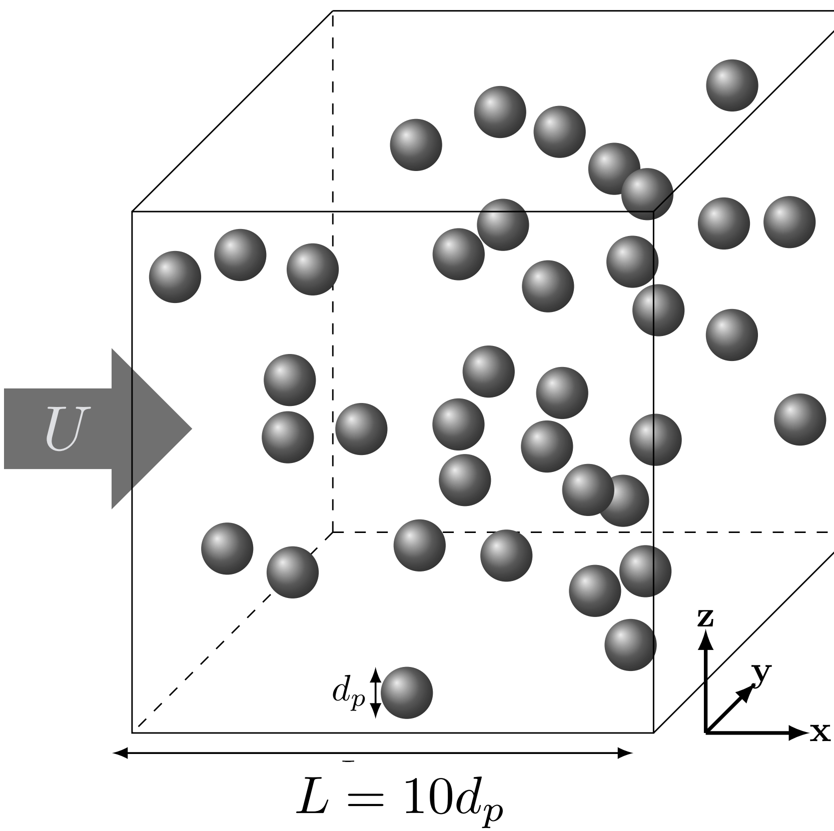


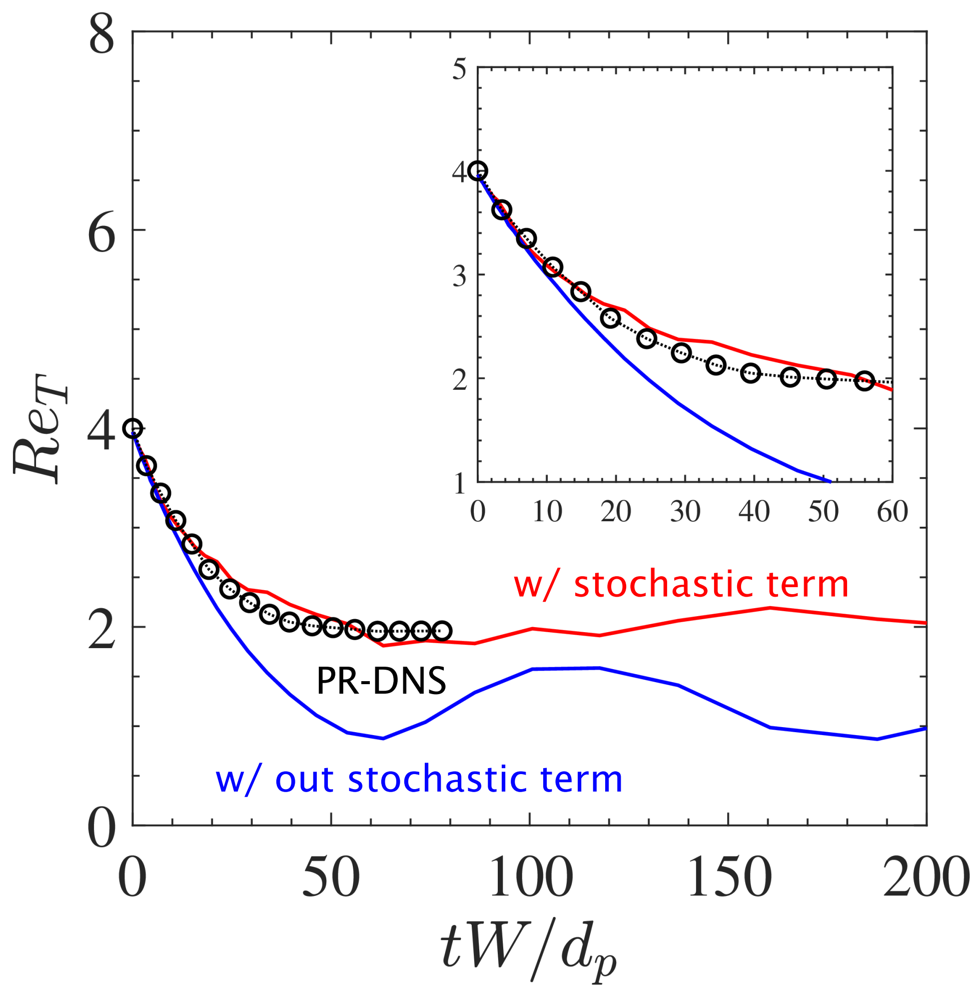


Evaluation of granular temperature (Re_m=20, ϕ=0.1, ρ_p/ρ_f=100)

Homogeneous cooling / heating $T = \frac{1}{3}\langle \boldsymbol{v}'_p \cdot \boldsymbol{v}'_p \rangle$

- *Cooling:* $T(t=0) > T(t=\infty)$





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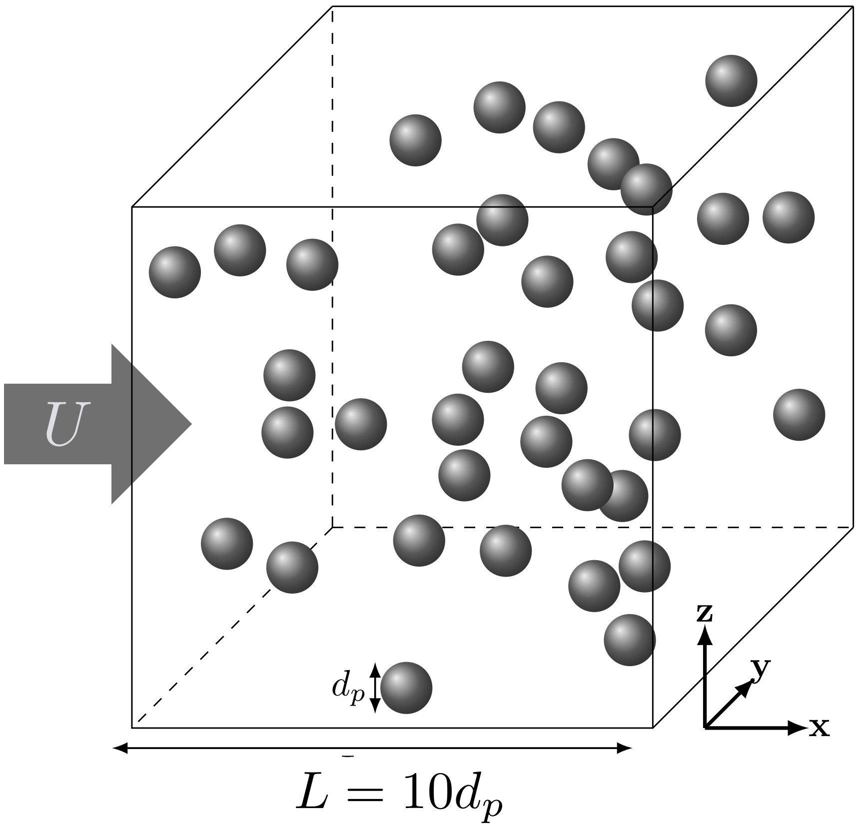

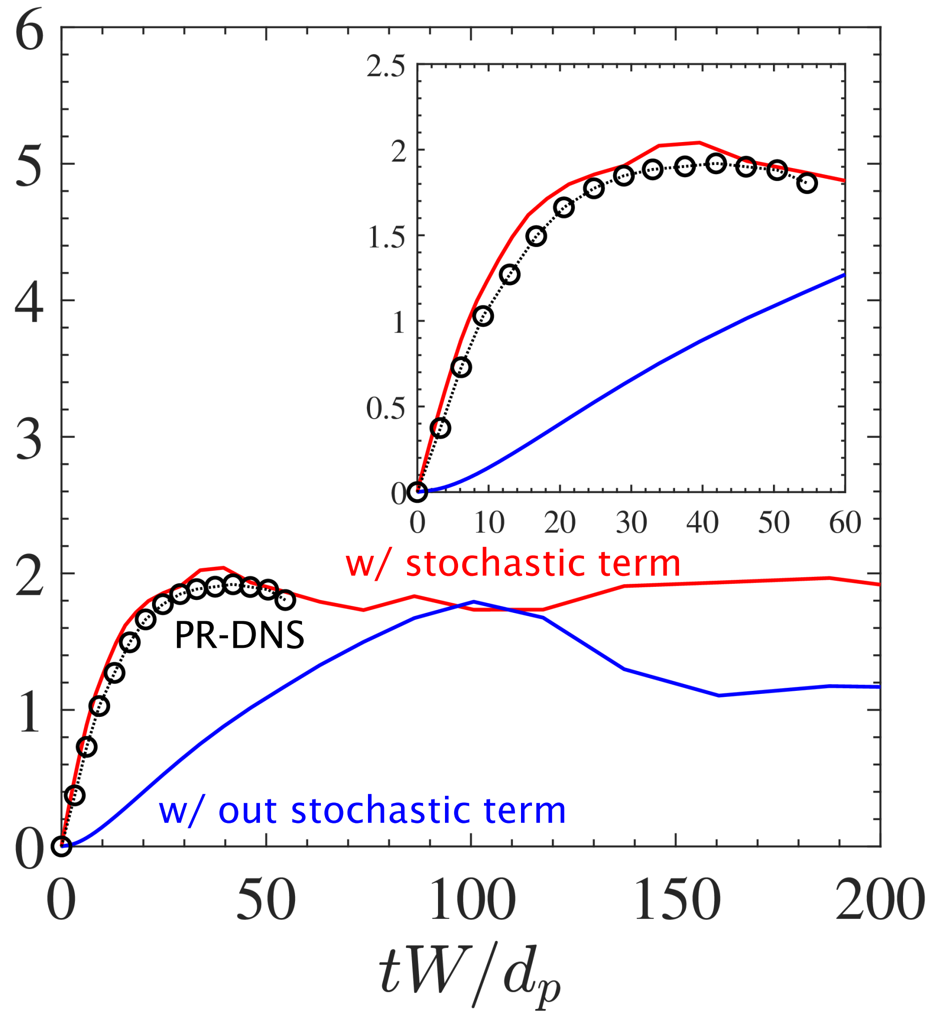

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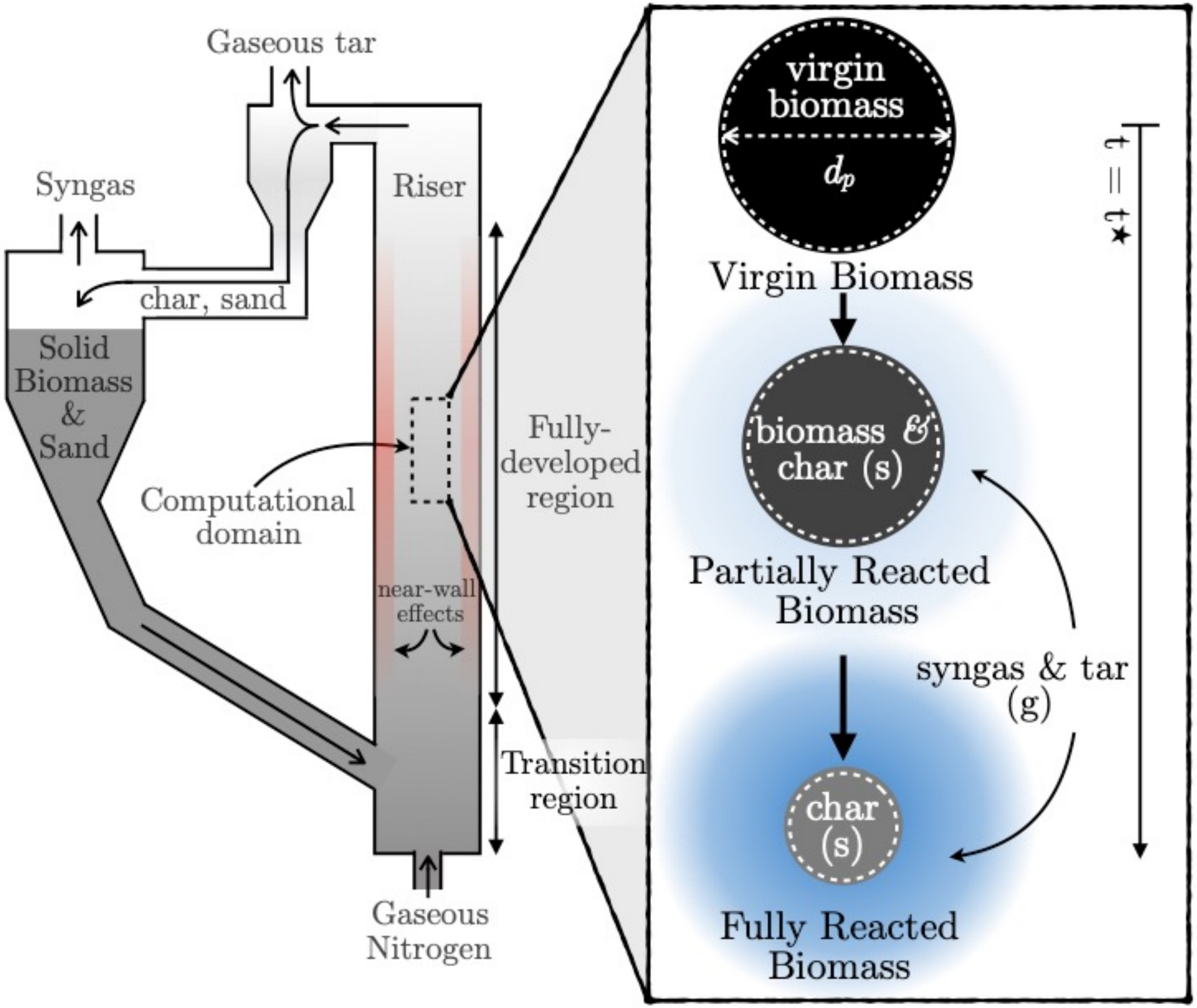
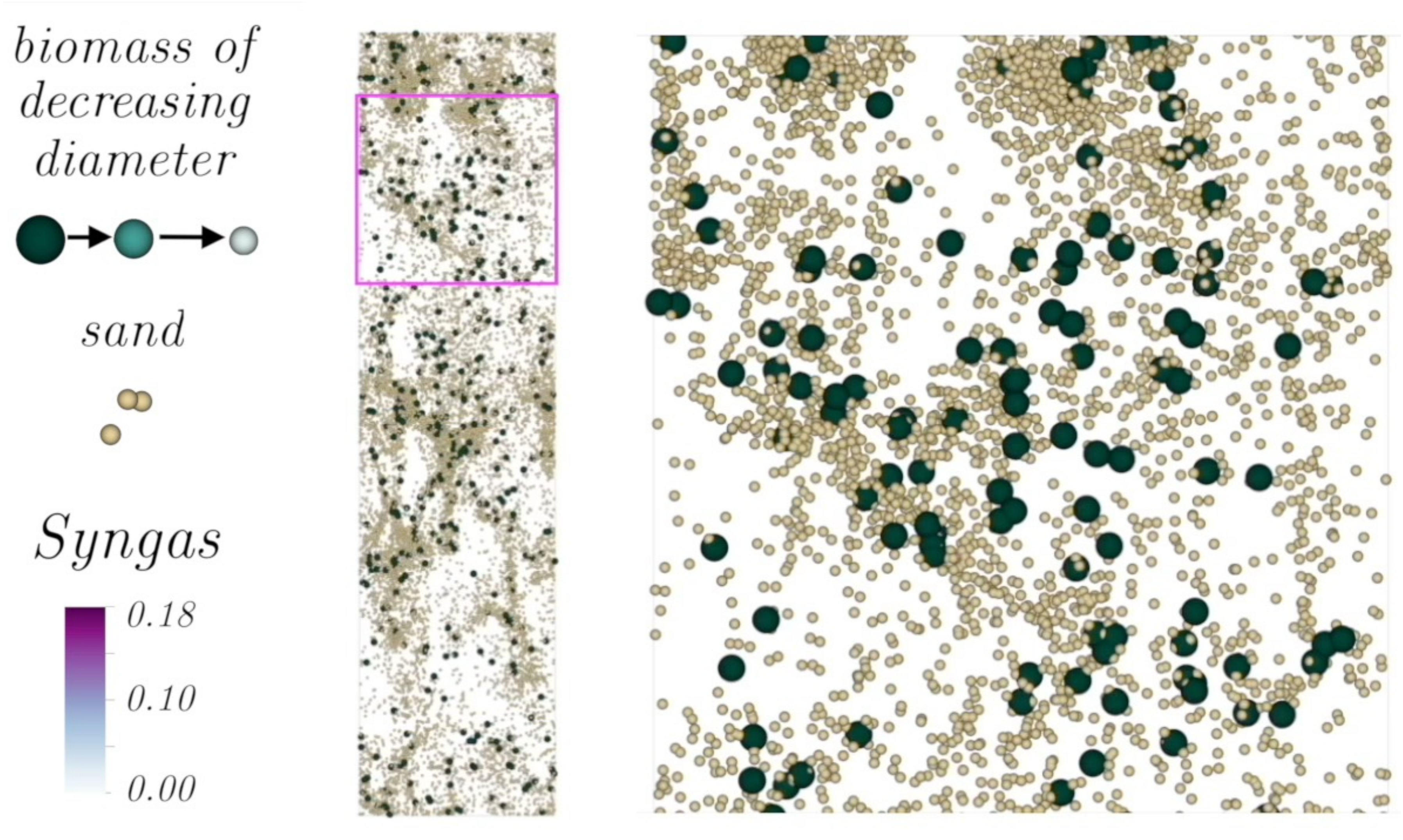
Biomass pyrolysis in fully-developed riser flow

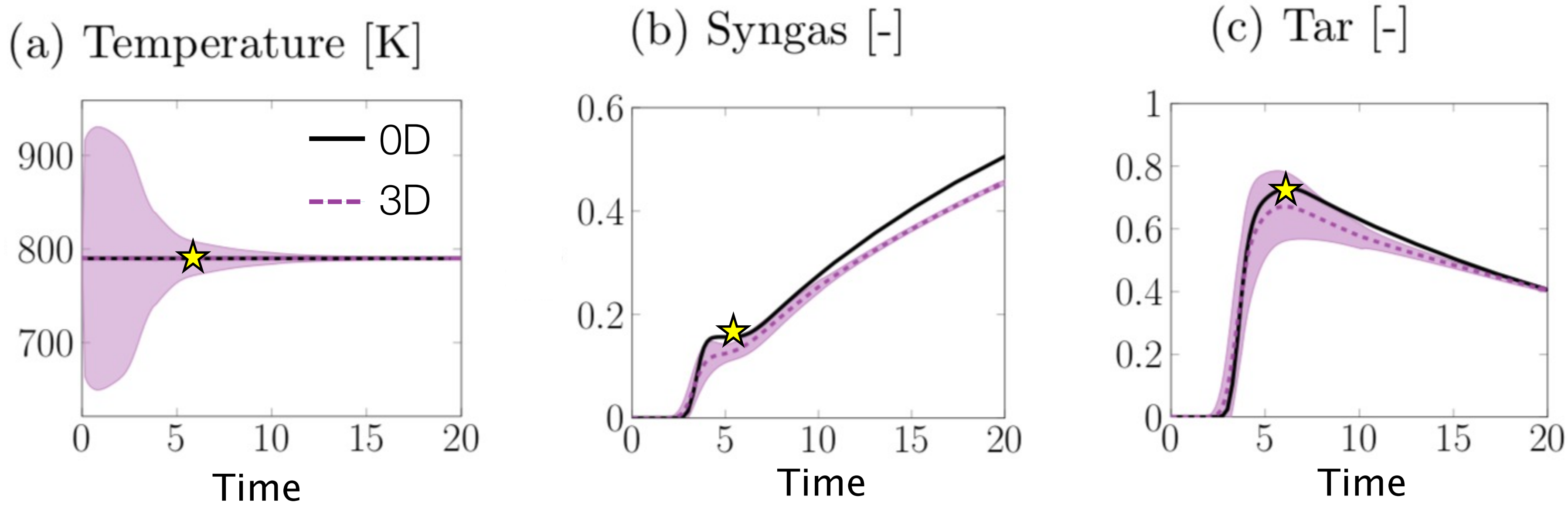


Biomass: bagasse, the woody pulp bi-product from the commercial processing of sugarcane

Biomass pyrolysis in fully-developed riser flow

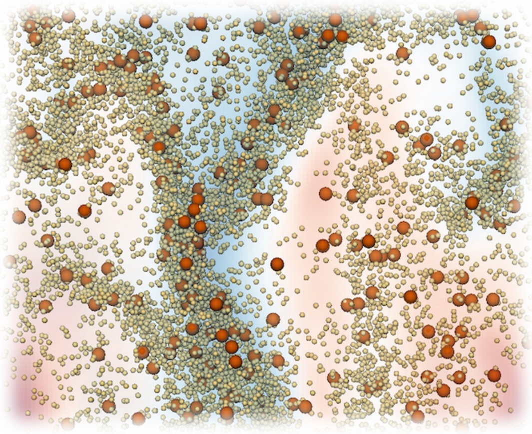


Comparison with a perfectly mixed (0D) model

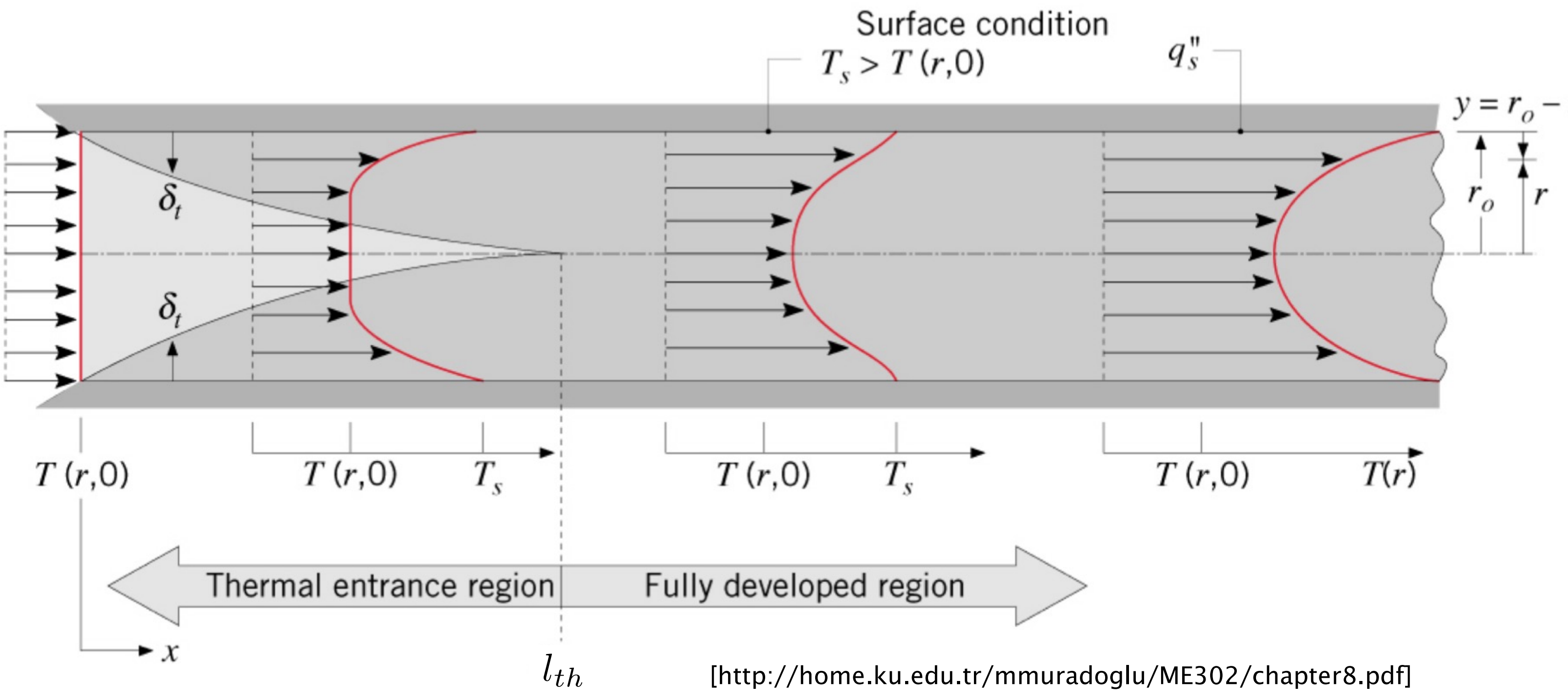


Ignoring multiphase effects results in a maximum over-prediction of 33% for syngas and 9% for tar during standard residence times.

Clusters restrict contact between phases → lower yield!



Effect of particles on the thermal entrance length



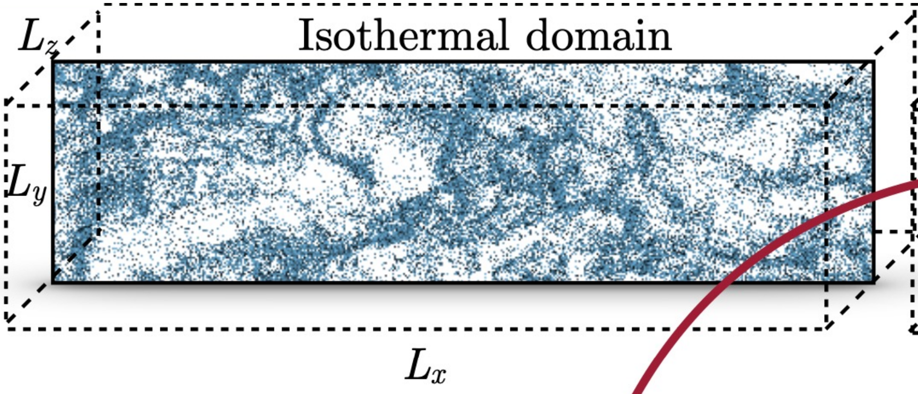
[http://home.ku.edu.tr/mmuradoglu/ME302/chapter8.pdf]

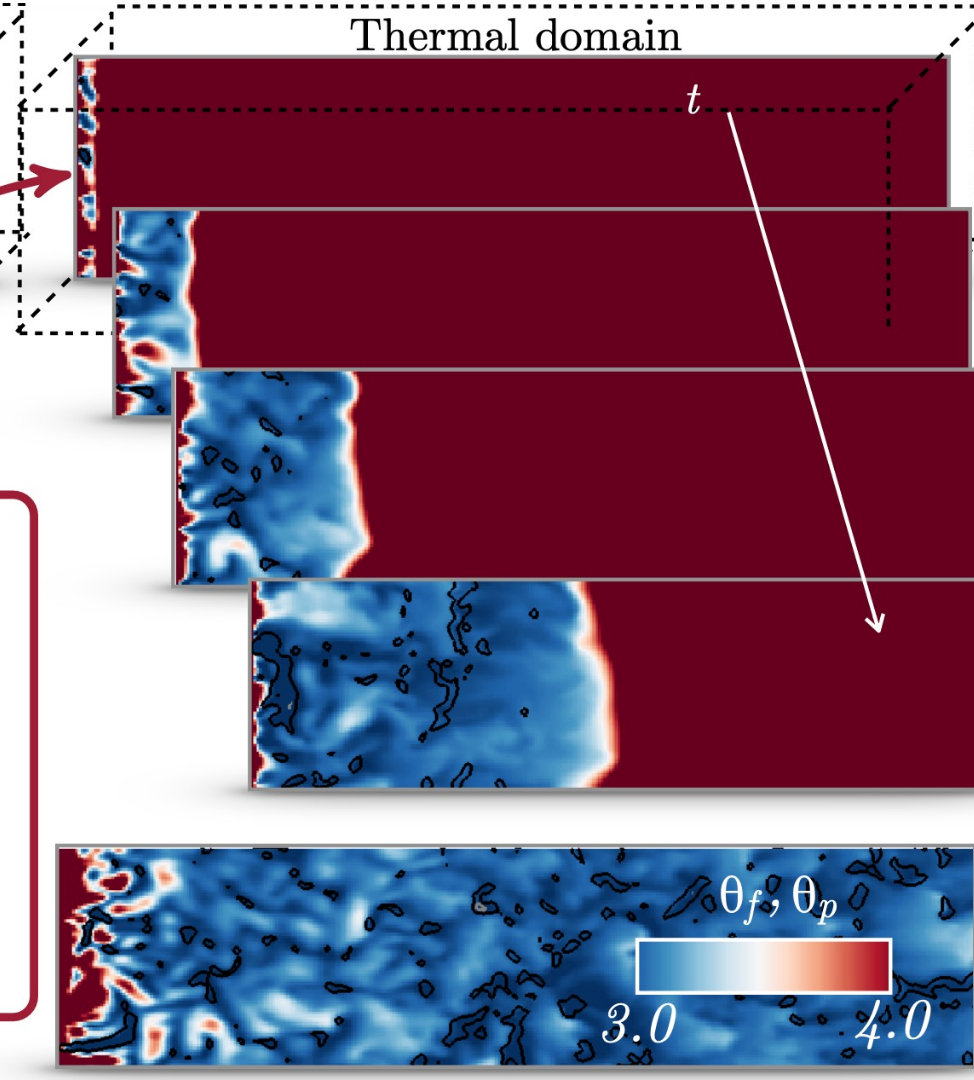
Thermal entrance length is a critical parameter in the design of industrial reactors

For single-phase laminar flow: $l_{th}/D = 0.05\mathrm{Re}_D\mathrm{Pr}$

How is this modified for turbulent particle-laden flows?

Effect of particles on the thermal entrance length



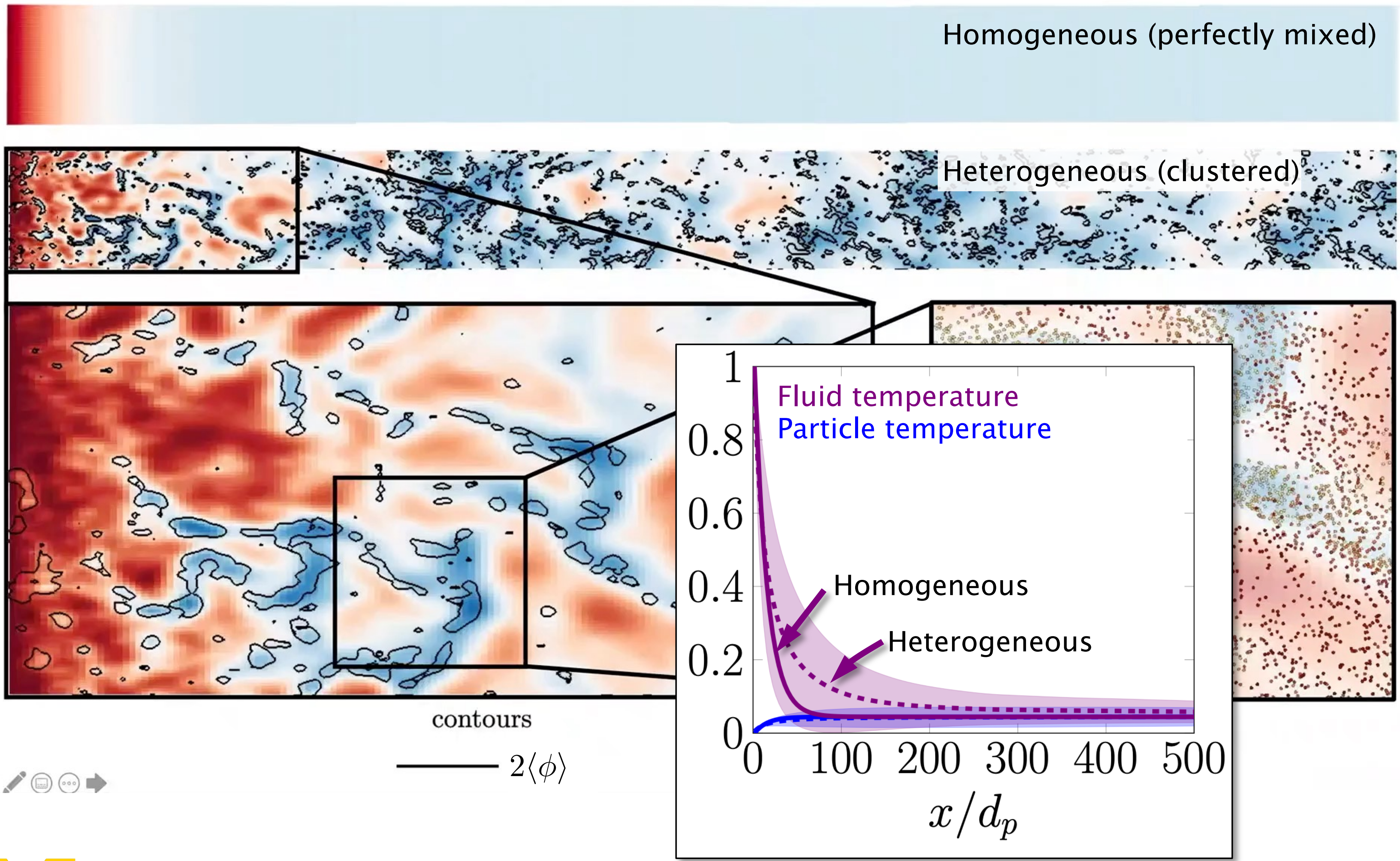


Fully developed

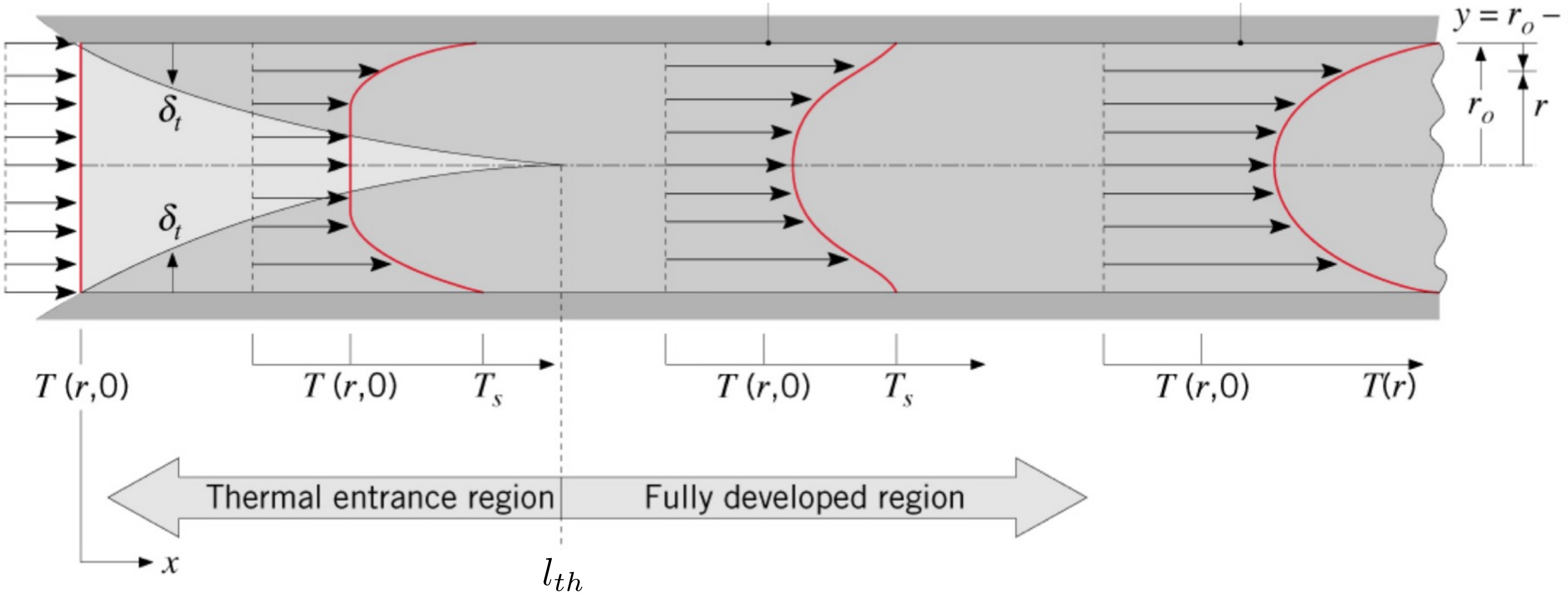
After a stationary state is reached:

- ΔT between the phases is imposed.
- $y - z$ planes of gas and particle data are injected into the thermal domain until a thermally steady state is reached.

Effect of particles on the thermal entrance length



CFD-DEM derived empirical correlations



- For single-phase pipe flow: $l_{th} = 0.05\mathrm{Re}_D\mathrm{Pr}$
- For a homogeneous (well-mixed) particle distribution: $l^0_{th} = 0.1\mathrm{RePr}/\langle\phi\rangle$
- For a heterogeneous (clustered) particle distribution:

$$l_{th} = 0.1\mathrm{RePr}/\langle\phi\rangle + 0.64\frac{\sqrt{\langle\phi'^2\rangle}}{\langle\phi\rangle}\left(0.1\frac{\mathrm{Re}}{\langle\phi\rangle} + 0.02\mathrm{Re}^3\right)$$

  - Model for volume fraction variance: $\langle\phi'^2\rangle = 1.48\langle\phi\rangle\left(0.55 - \langle\phi\rangle\right)$

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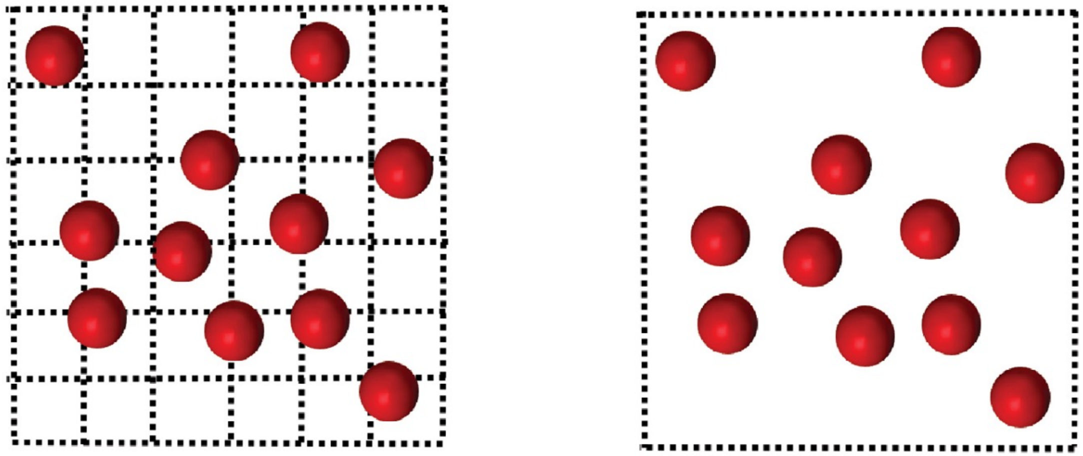
What models should be used at industrial scales?

We just showed that heterogeneity (clustering) plays a significant role

Challenge: *how to model subgrid-scale heterogeneity in industrial-scale simulations?*

- Filtered two-fluid model?
- MP-PIC?
- Random walk?
- EMMS (CFD-DEM or TFM)?



Random walk models coupled w/ RANS are among the most popular:

- Particle equations: $\frac{\mathrm{d}\boldsymbol{x}_p}{\mathrm{d}t} = \boldsymbol{v}_p, \quad \frac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} = \boldsymbol{F}_{\mathrm{col}} + m_p\boldsymbol{g} + \frac{F(\mathrm{Re},\phi)}{\tau_p}(\boldsymbol{u} - \boldsymbol{v}_p)$
- Fluid velocity *seen* decomposed into resolves/unresolved: $\boldsymbol{u} = \overline{\boldsymbol{u}} + \boldsymbol{u}'$
- Model unresolved velocity stochastically: $\mathrm{d}\boldsymbol{u}' = -\frac{\boldsymbol{u}'}{\tau_L} + \sqrt{\frac{2\sigma_{\mathrm{SGS}}^2}{\tau_L}}\mathrm{d}\boldsymbol{W}$

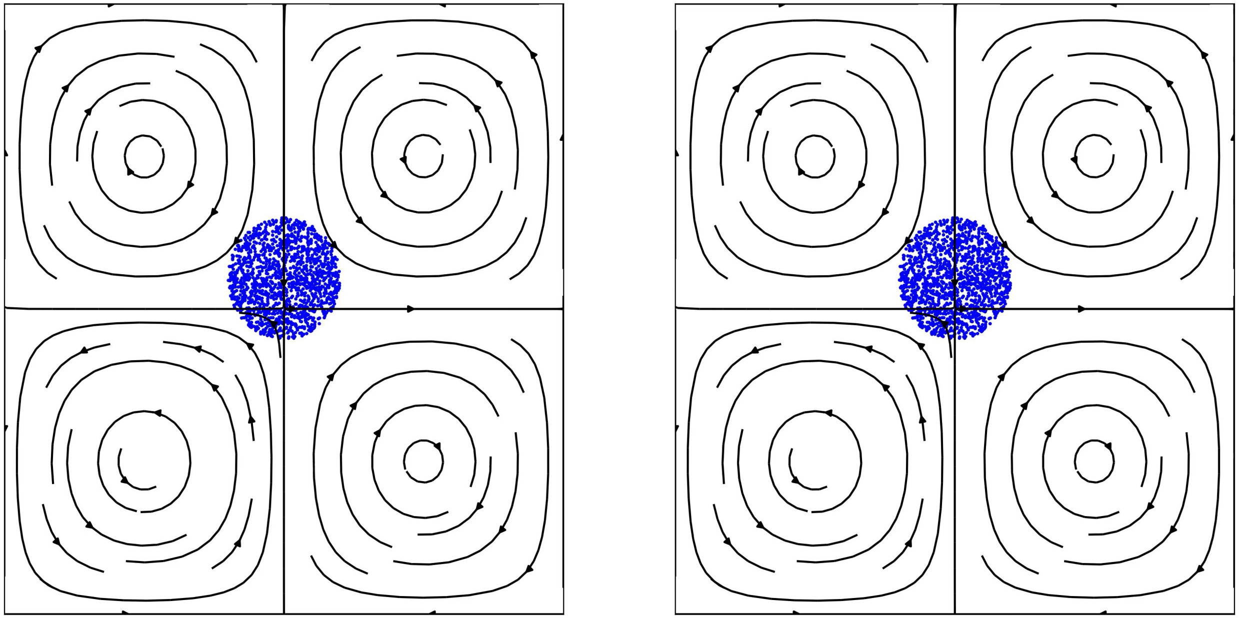
Continuous random walk (CRW)

- **Pros:** Random walk models reproduce with accuracy one-point statistical moments (such as dispersion coefficients and particle kinetic energy)
- **Cons:** Fail to capture instantaneous spatial distributions (clustering)
- Consider a Taylor—Green vortex as a model for an LES/RANS grid cell

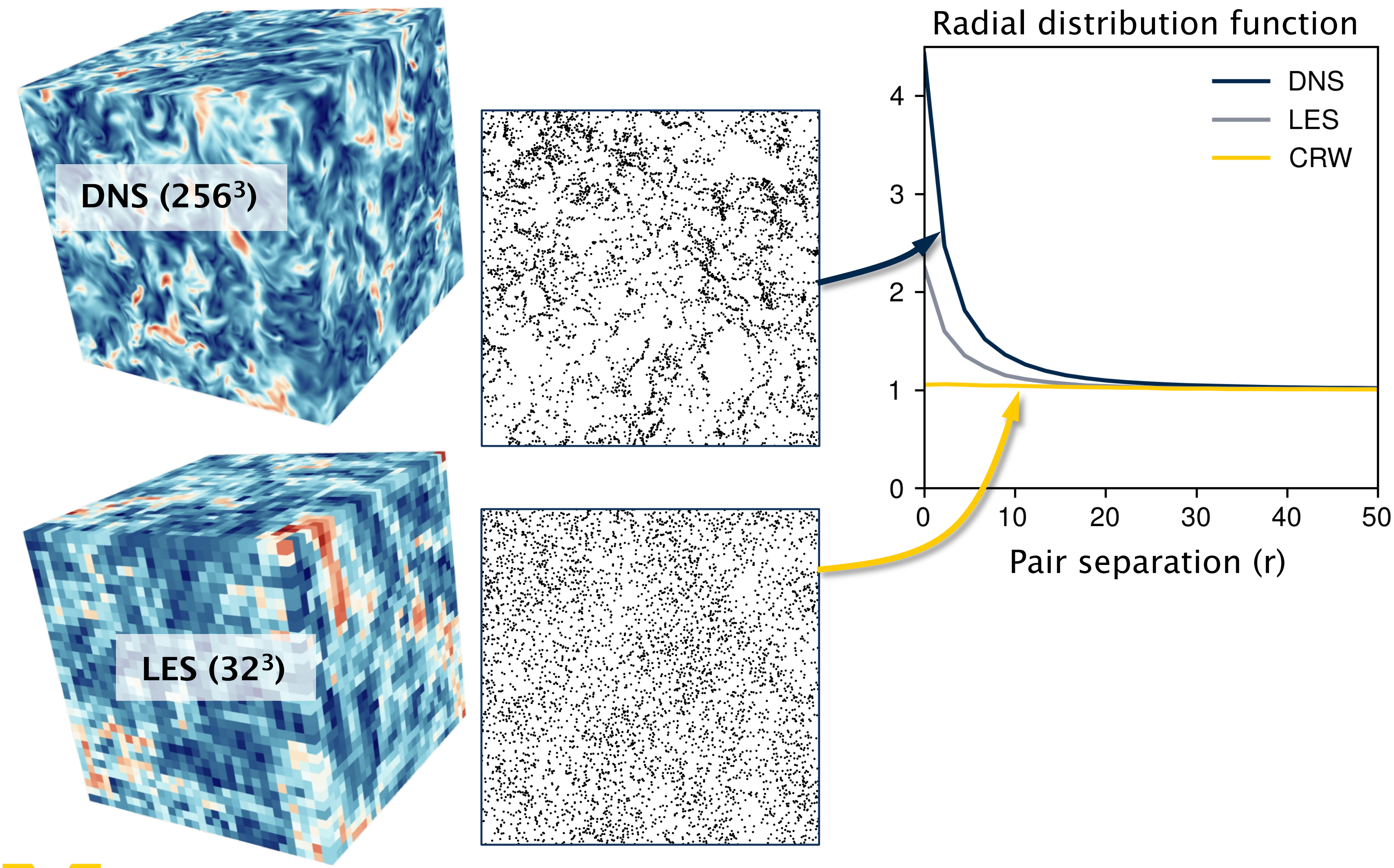
$$\mathrm{d}\boldsymbol{u}' = -\frac{\boldsymbol{u}'}{\tau_L} + \sqrt{\frac{2\sigma_{\mathrm{SGS}}^2}{\tau_L}}\mathrm{d}\boldsymbol{W}$$

Culprit: white noise destroys spatial correlation

Exact solution   Random walk

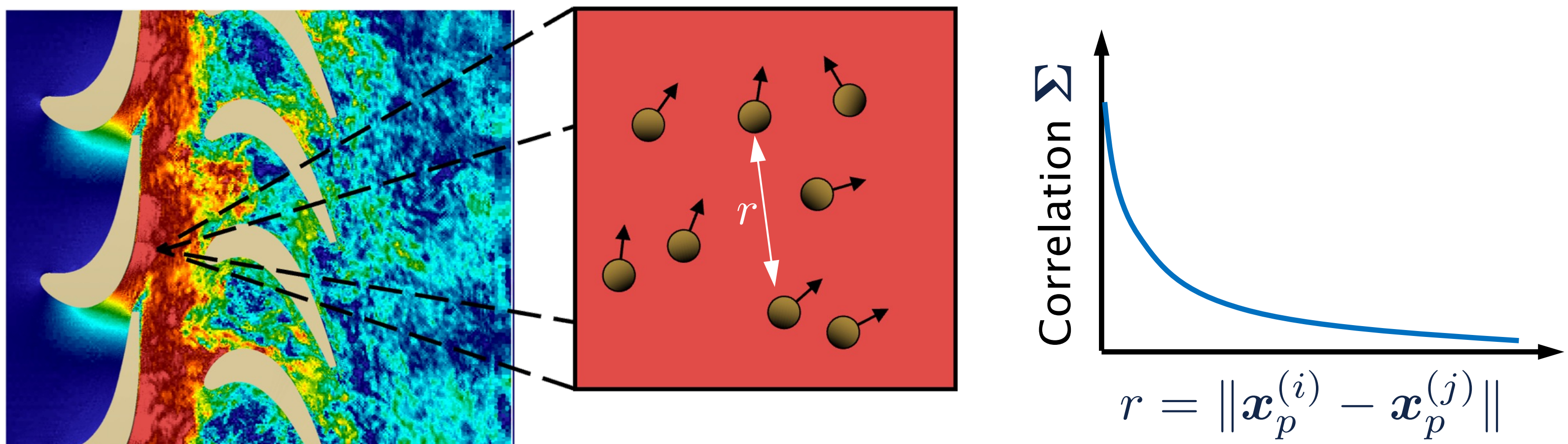


Particle clustering in homogeneous turbulence



Embedding spatial information

- How to capture instantaneous spatial distribution in LES/RANS?



$$\mathrm{d}\boldsymbol{u}' = -\boldsymbol{A}\mathrm{d}t + \boldsymbol{B} \cdot \mathrm{d}\boldsymbol{W} \quad \boldsymbol{\Sigma} = \boldsymbol{B}\boldsymbol{B}^T$$

- Key idea: leverage what is available. In each grid cell we know:
  - One-point fluid information (turbulent kinetic energy, dissipation, etc.)
  - Two-point particle information (relative particle positions)

- Introduce covariance matrix **Σ** in the diffusion term
  (replace white noise with spatially correlated noise)

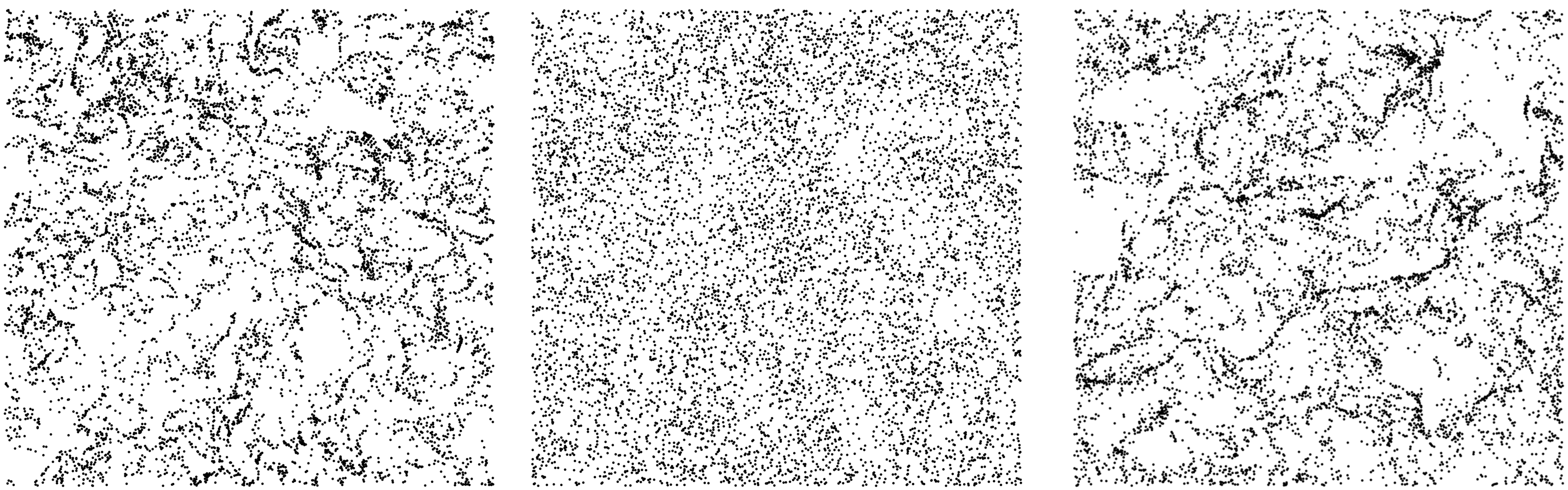
Spatially-correlated random walk

- We propose a model of the form:

$$\boldsymbol{B}^{(i)}\,\mathrm{d}\boldsymbol{W} \approx \widetilde{\boldsymbol{B}\,\mathrm{d}\boldsymbol{W}}^{(i)} = \frac{\sum_{j=1}^{N} b(\boldsymbol{x}^{(j)})\rho(|\boldsymbol{x}^{(j)} - \boldsymbol{x}^{(i)}|)\,\mathrm{d}\boldsymbol{W}^{(j)}}{\sqrt{\sum_{j=1}^{N} \rho(|\boldsymbol{x}^{(j)} - \boldsymbol{x}^{(i)}|)^2}}$$

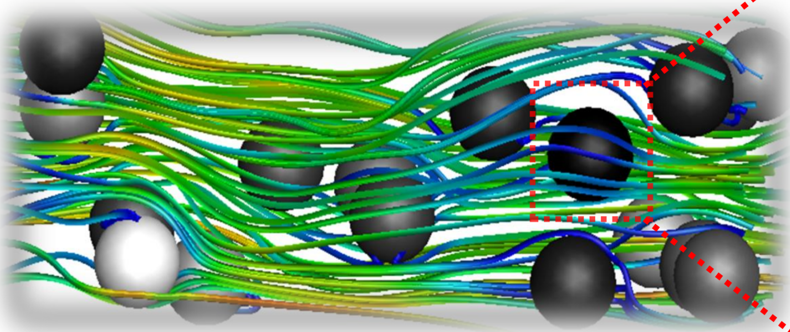
- SGS model that captures one-point *and* two-point statistics!

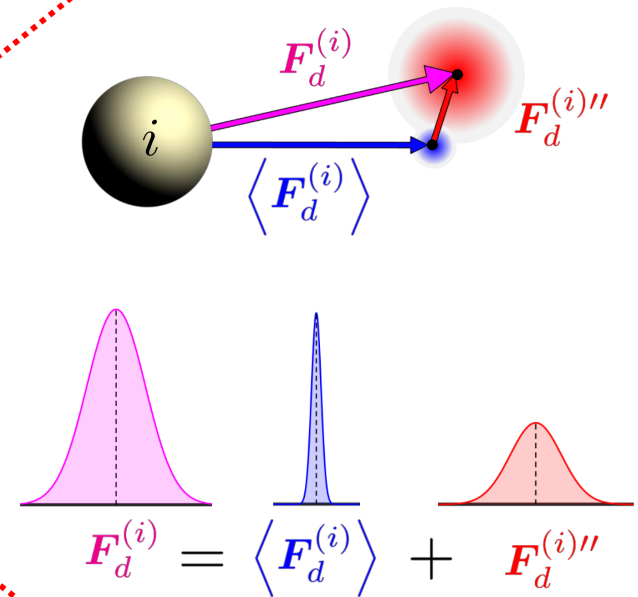
DNS **LES+CRW** **LES+SCRW**



Concluding remarks

1. Introduced a stochastic approach for neighbor-induced drag fluctuations
   - Time scale closure from kinetic theory
   - Proposed model for force variance



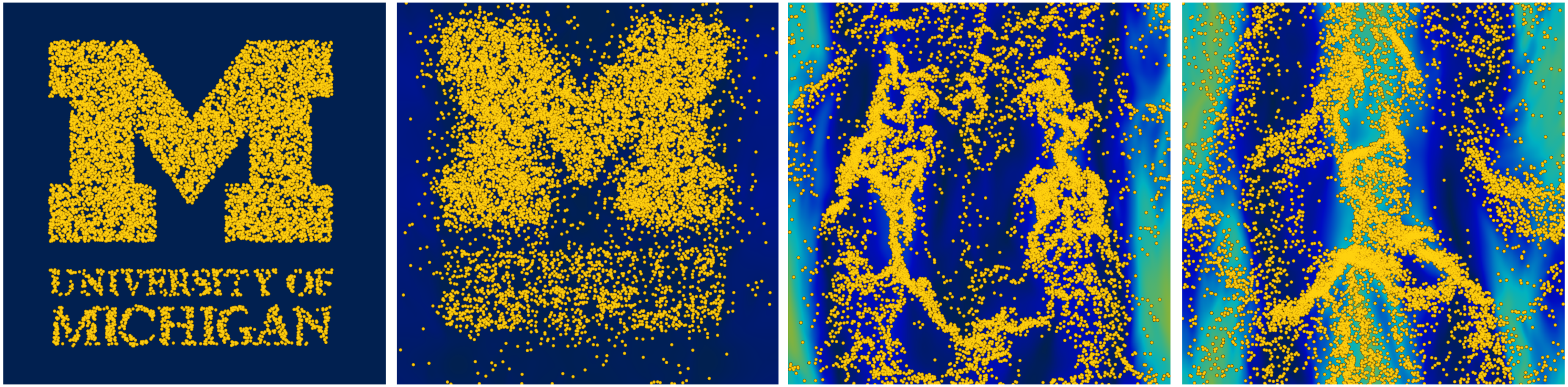


2. Force Langevin framework yields accurate statistics for *homogeneous* suspensions

3. Industrial-scale simulations remain challenging. Need models that can capture subgrid-scale heterogeneity!

4. Proposed a framework based on spatially-correlated random walks

Questions?



Related publications

1. Capecelatro, J., Desjardins, O. (2013) An Euler-Lagrange strategy for simulating particle-laden flows, *Journal of Computational Physics*. **238**, 1 - 31.
2. Guo, L., Capecelatro, J. (2019) The role of clusters on heat transfer in sedimenting gas-solid flows, *International Journal of Heat and Mass Transfer*. **132**, 1217-1230.
3. Beetham, S., Capecelatro, J. (2019) Biomass pyrolysis in fully-developed turbulent riser flow, *Renewable Energy*. **140**, 751-760.
4. Beetham, S., Lattanzi, A., Capecelatro, J. (2022) On the thermal entrance length of moderately dense gas-particle flows. *International Journal of Heat and Mass Transfer.* **182**, 121985.
5. Lattanzi, A.M., Tavanashad, V., Subramaniam, S., Capecelatro, J., (2022) Stochastic model for the hydrodynamic force in Euler-Lagrange simulations of particle-laden flows. *Physical Review Fluids*. **7**, 014301.
6. Pakseresht, P., Yao, Y., Fan, L., Theuerkauf, J., Capecelatro, J. (2023) A critical assessment of the Energy Minimization Multi-Scale (EMMS) model. *Powder Technology*. **425**, 118569.

New book: Subramaniam, S., & Balachandar, S. (Eds). (2022). Modeling Approaches and Computational Methods for Particle-laden Turbulent Flows. *Academic Press*.