Validation of a Multiphase Turbulence Model Using Mesoscale DNS of Gravity-Driven Gas-Particle Flow

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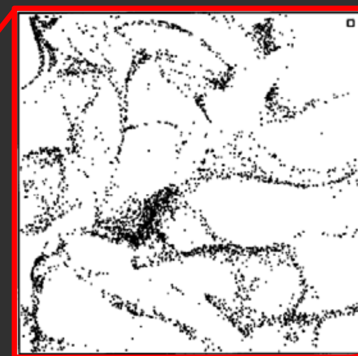
Moderately-dilute fluid-particle flows

Preferential concentration of cloud droplets by turbulence

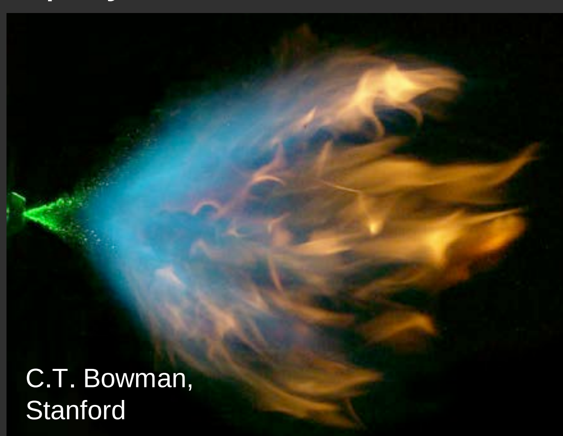


Shaw et al. (1998)

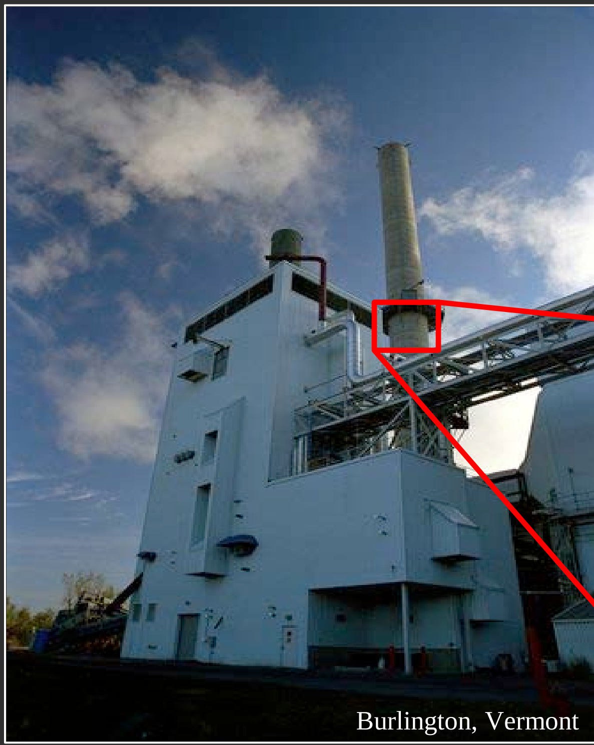
Atmospheric dispersion

Gasification of coal and biomass

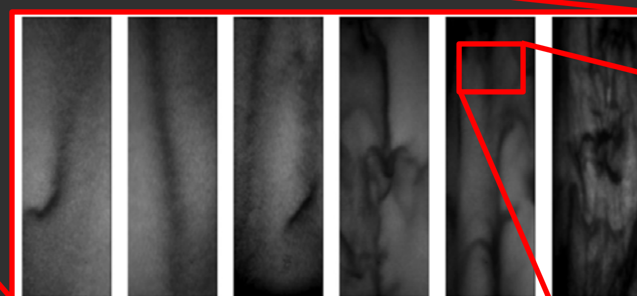
Spray flames



The multi-scale issue

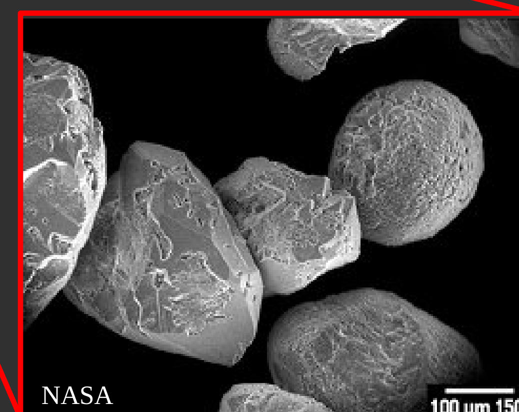

Burlington, Vermont

Macroscale
- Large number of particles $\mathcal{O}(10)$
- Length scales: m


Xu & Zhu, 2011

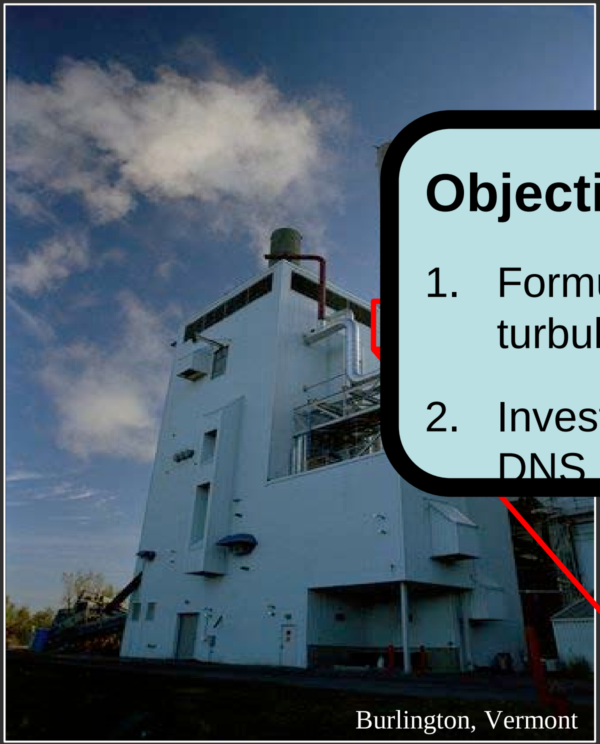
Mesoscale
- Clustering
- Bubbling
- Particle size segregation
- Turbulence modulation

Microscale
- Wakes
- Particle collisions
- Phase change



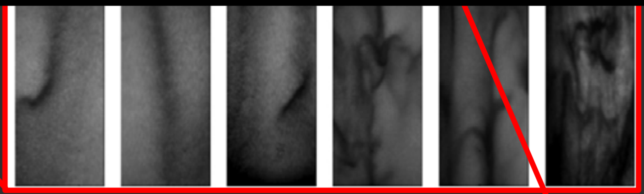
NASA

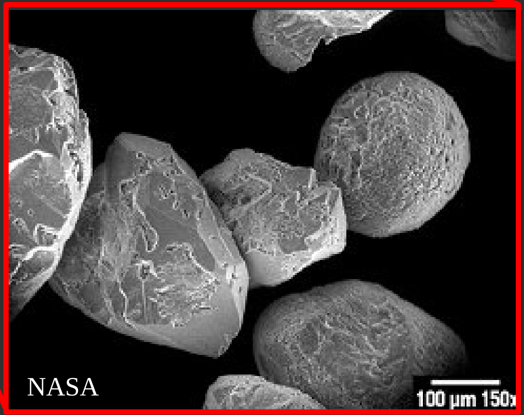
The multi-scale issue



Objectives:

1. Formulate from first-principles a macroscopic turbulence model
2. Investigate the unclosed terms using mesoscale DNS





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- Large number of particles $\mathcal{O}(10)$
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Mesoscale

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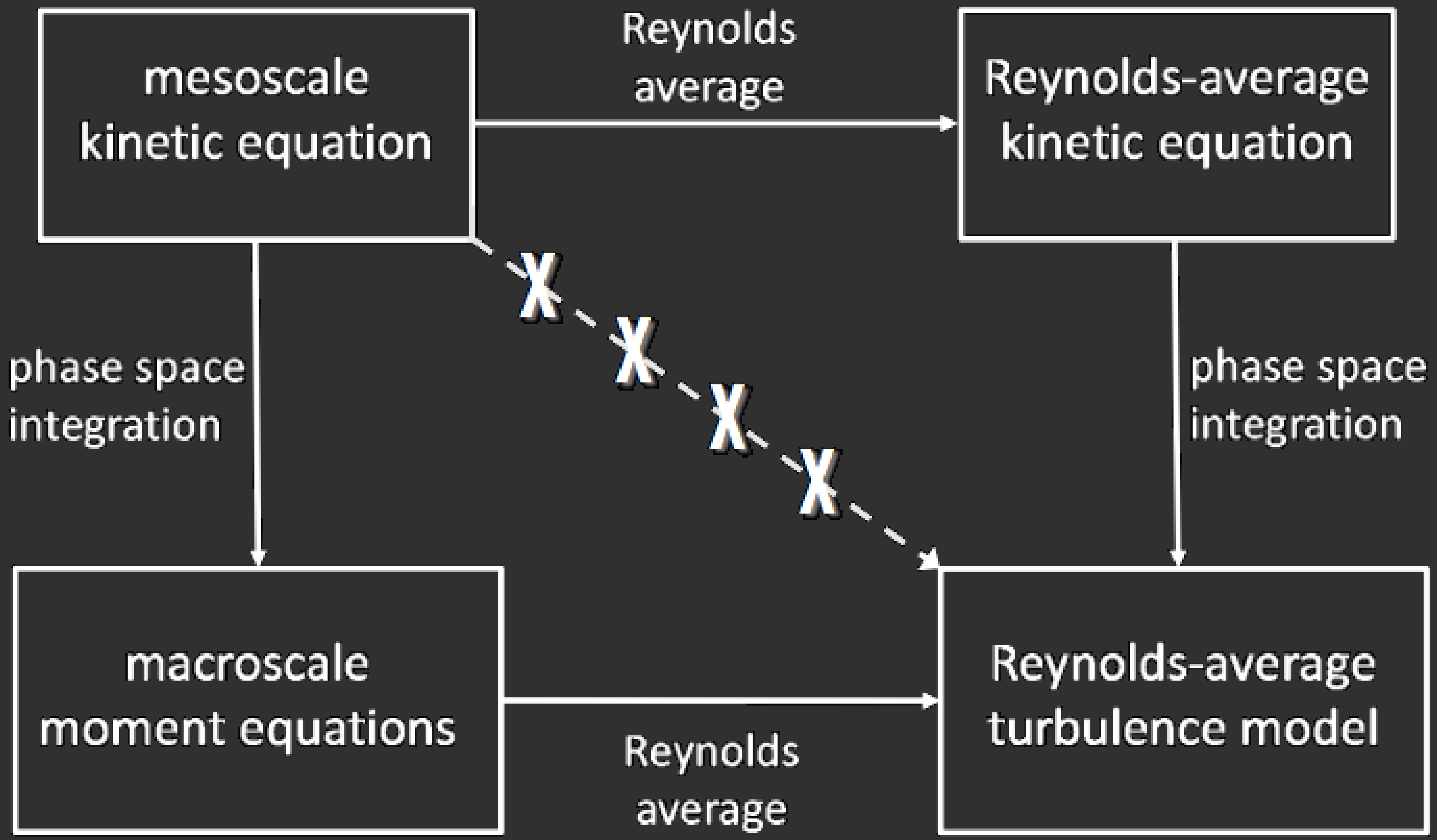
- ...se change

Outline

- Arriving at a macroscopic description of fluid-particle flows
  - Mesoscale description
  - Reynolds-averaged equations
  - Closure models
- Evaluating the unclosed terms using mesoscale DNS
  - Simulation configuration
  - Extracting the statistics
  - Preliminary results
- Conclusions

Multiscale turbulence modeling approach[1]



1. Fox, R.O., On multiphase turbulence models for collisional fluid-particle flows, *In preparation for JFM*, 2013

Starting from a mesoscale description

Kinetic theory model for monodisperse granular flow in the presence of a fluid

$$\frac{\partial \alpha}{\partial t} + \boldsymbol{\nabla}\cdot\alpha\boldsymbol{u} = 0$$

$$\frac{\partial \alpha\boldsymbol{u}}{\partial t} + \boldsymbol{\nabla}\cdot\alpha\left(\boldsymbol{u}\otimes\boldsymbol{u} + P\right) = \alpha\left(\boldsymbol{\mathcal{A}} + \boldsymbol{g}\right)$$

$$\boldsymbol{\mathcal{A}} = \frac{1}{\tau_D}\left(\boldsymbol{u}_f - \boldsymbol{u}\right)$$

$$\frac{\partial \alpha\Theta}{\partial t} + \boldsymbol{\nabla}\cdot\alpha\left(\Theta\boldsymbol{u} + \frac{2}{3}\boldsymbol{q}\right) = -\frac{2}{3}\alpha P\boldsymbol{:}\boldsymbol{\nabla}\boldsymbol{u} - \frac{2}{\tau_D}\Theta - \frac{8\left(1-\mathrm{e}^2\right)g_0}{\sqrt{\pi}d_p}\alpha^2\Theta^{3/2}$$

$$\frac{\partial \alpha e}{\partial t} + \boldsymbol{\nabla}\cdot\alpha\left(\boldsymbol{u}e + P\cdot\boldsymbol{u} + \boldsymbol{q}\right) = \alpha\left(\boldsymbol{\mathcal{E}} + \boldsymbol{u}\cdot\boldsymbol{g}\right) - \frac{12\left(1-\mathrm{e}^2\right)g_0}{\sqrt{\pi}d_p}\alpha^2\Theta^{3/2}$$

$$e = \frac{1}{2}\left(\boldsymbol{u}\cdot\boldsymbol{u} + 3\Theta\right)$$

$$\boldsymbol{\mathcal{E}} = \frac{1}{\tau_D}\boldsymbol{u}\cdot\left(\boldsymbol{u}_f - \boldsymbol{u}\right) - \frac{3}{\tau_D}\Theta$$

Starting from a mesoscale description

Fluid-phase transport equations

$$\frac{\partial (1-\alpha)}{\partial t} + \nabla\cdot (1-\alpha)\, \boldsymbol{u}_f = 0$$

$$\boldsymbol{F}_b = \frac{\rho_p}{\rho_f} \langle \alpha \rangle \langle \boldsymbol{\mathcal{A}} \rangle_p - \langle 1-\alpha \rangle \boldsymbol{g}$$

$$\frac{\partial (1-\alpha)\, \boldsymbol{u}_f}{\partial t} + \nabla\cdot (1-\alpha) \left(\boldsymbol{u}_f \otimes \boldsymbol{u}_f + P_f\right) = -\frac{\rho_p}{\rho_f} \alpha \boldsymbol{\mathcal{A}} + (1-\alpha)\boldsymbol{g} + \boldsymbol{F}_b$$

$$P_f = \frac{1}{\rho_f (1-\alpha)} \left(p_f \boldsymbol{I} - \boldsymbol{\sigma}_f\right) \longrightarrow \boldsymbol{\sigma}_f = \rho_f (1-\alpha) \left(\nu_f + \nu_f^*\right) \left[\nabla \boldsymbol{u}_f + \left(\nabla \boldsymbol{u}_f\right)^{\mathsf{T}} - \frac{2}{3} \nabla\cdot \boldsymbol{u}_f \boldsymbol{I}\right]$$

$$\frac{\partial (1-\alpha)\, e_f}{\partial t} + \nabla\cdot (1-\alpha)\, e_f \otimes \boldsymbol{u}_f + \boldsymbol{u}_f \cdot \nabla\cdot (1-\alpha)\, P_f = -\frac{\rho_p}{\rho_f} \alpha \boldsymbol{u}_f \cdot \boldsymbol{\mathcal{A}} + (1-\alpha) \boldsymbol{u}_f \cdot \boldsymbol{g} + \boldsymbol{u}_f \cdot \boldsymbol{F}_b$$

Towards a macroscopic model

- Reynolds-averaged definitions

$$A' = A - \langle A \rangle \qquad \langle A' \rangle = 0$$

- Phase-averaged definitions

$$\langle A \rangle_p = \frac{\langle \alpha A \rangle}{\langle \alpha \rangle} \qquad A'' = A - \langle A \rangle_p \qquad \langle A'' \rangle_p = 0$$

$$\langle A \rangle_f = \frac{\langle (1-\alpha) A \rangle}{\langle 1-\alpha \rangle} \qquad A''' = A - \langle A \rangle_f \qquad \langle A''' \rangle_f = 0$$

- Solve for:
  - Particle-phase: $\langle \alpha \rangle \qquad \langle \boldsymbol{u} \rangle_p \qquad k_p = \frac{1}{2}\langle \boldsymbol{u}'' \cdot \boldsymbol{u}'' \rangle_p \qquad \langle \Theta \rangle_p \qquad \kappa_p = k_p + \frac{3}{2}\langle \Theta \rangle_p$
  - Fluid-phase: $\langle \boldsymbol{u}_f \rangle_f \qquad k_f = \frac{1}{2}\langle \boldsymbol{u}_f'' \cdot \boldsymbol{u}_f'' \rangle_f$

Reynolds-average equations

Particle-phase equations

$$\frac{\partial\langle\alpha\rangle}{\partial t} + \boldsymbol{\nabla}\cdot\langle\alpha\rangle\langle\boldsymbol{u}\rangle_p = 0$$

$$\langle\boldsymbol{\mathcal{A}}\rangle_p = \frac{1}{\tau_D}\left(\langle\boldsymbol{u}_f\rangle_f - \langle\boldsymbol{u}\rangle_p + \frac{\langle\alpha'\boldsymbol{u}_f'''\rangle}{\langle\alpha\rangle\langle 1-\alpha\rangle}\right)$$

$$\frac{\partial\langle\alpha\rangle\langle\boldsymbol{u}\rangle_p}{\partial t} + \boldsymbol{\nabla}\cdot\langle\alpha\rangle(\langle\boldsymbol{u}\otimes\langle\boldsymbol{u}\rangle_p + \langle\boldsymbol{\mathcal{P}}\rangle_p) = \langle\alpha\rangle(\langle\boldsymbol{\mathcal{A}}\rangle_p + \boldsymbol{g})$$

$$\frac{\partial\langle\alpha\rangle k_p}{\partial t} + \boldsymbol{\nabla}\cdot\langle\alpha\rangle\left(k_p\langle\boldsymbol{u}\rangle_p + \frac{1}{2}\langle\boldsymbol{u}''\otimes\boldsymbol{u}''\cdot\boldsymbol{u}''\rangle_p + \langle P\cdot\boldsymbol{u}''\rangle_p\right)$$
$$= -\langle\alpha\rangle\langle\boldsymbol{u}''\otimes\boldsymbol{u}''\rangle_p\boldsymbol{:}\boldsymbol{\nabla}\langle\boldsymbol{u}\rangle_p + \langle\alpha\rangle\langle P\boldsymbol{:}\boldsymbol{\nabla}\boldsymbol{u}''\rangle_p + \frac{\langle\alpha\rangle}{\tau_D}\left(\langle\boldsymbol{u}''\cdot\boldsymbol{u}_f'''\rangle_p - 2k_p\right)$$

$$\frac{\partial\langle\alpha\rangle\langle\Theta\rangle_p}{\partial t} + \boldsymbol{\nabla}\cdot\langle\alpha\rangle\left(\langle\Theta\rangle_p\langle\boldsymbol{u}\rangle_p + \langle\boldsymbol{u}''\Theta\rangle_p + \frac{2}{3}\langle\boldsymbol{q}\rangle_p\right)$$
$$= -\frac{2}{3}\left(\langle\alpha\rangle\langle P\rangle_p\boldsymbol{:}\boldsymbol{\nabla}\langle\boldsymbol{u}\rangle_p - \langle\alpha\rangle\langle P\boldsymbol{:}\boldsymbol{\nabla}\boldsymbol{u}''\rangle_p\right) - \frac{2\langle\alpha\rangle}{\tau_D}\langle\Theta\rangle_p - \frac{8\left(1-\mathrm{e}^2\right)}{\sqrt{\pi}d_p}\langle g_o\alpha^2\Theta^{3/2}\rangle$$

Reynolds-average equations

Fluid-phase equations

$$\frac{\partial\langle 1-\alpha\rangle}{\partial t} + \nabla\cdot\langle 1-\alpha\rangle\langle \boldsymbol{u}_f\rangle_f = 0$$

$$\frac{\partial\langle 1-\alpha\rangle\langle \boldsymbol{u}_f\rangle_f}{\partial t} + \nabla\cdot\left(\langle 1-\alpha\rangle\langle \boldsymbol{u}_f\rangle_f \otimes \langle \boldsymbol{u}_f\rangle_f + \langle 1-\alpha\rangle\langle \boldsymbol{u}_f''' \otimes \boldsymbol{u}_f'''\rangle_f - \frac{1}{\rho_f}\langle \boldsymbol{\sigma}_f\rangle\right)$$
$$= -\frac{1}{\rho_f}\nabla\langle p_f\rangle + \frac{\rho_p\langle\alpha\rangle}{\rho_f\tau_D}\left(\langle \boldsymbol{u}\rangle_p - \langle \boldsymbol{u}_f\rangle_f - \frac{\langle \alpha' \boldsymbol{u}_f'''\rangle}{\langle\alpha\rangle\langle 1-\alpha\rangle}\right) + \langle 1-\alpha\rangle \boldsymbol{g} + \boldsymbol{F}_b$$

$$\frac{\partial\langle 1-\alpha\rangle k_f}{\partial t} + \nabla\cdot\left(\langle 1-\alpha\rangle k_f\langle \boldsymbol{u}_f\rangle_f + \langle 1-\alpha\rangle\frac{1}{2}\langle \boldsymbol{u}_f''' \otimes \boldsymbol{u}_f'''\cdot\boldsymbol{u}_f'''\rangle_f\right) = \frac{1}{\rho_f}\nabla\cdot\left(\langle \boldsymbol{\sigma}_f\cdot\boldsymbol{u}_f'''\rangle - \langle p_f' \boldsymbol{u}_f'''\rangle - \langle p_f\rangle\frac{\langle \alpha' \boldsymbol{u}_f'''\rangle}{\langle 1-\alpha\rangle}\right)$$
$$-\langle 1-\alpha\rangle\langle \boldsymbol{u}_f''' \otimes \boldsymbol{u}_f'''\rangle_f : \nabla\langle \boldsymbol{u}_f\rangle_f - \frac{1}{\rho_f}\left(\langle \boldsymbol{\sigma}_f : \nabla \boldsymbol{u}_f'''\rangle - \langle p_f\rangle\nabla\cdot\frac{\langle \alpha' \boldsymbol{u}_f'''\rangle}{\langle 1-\alpha\rangle} - \langle p_f' \nabla\cdot\boldsymbol{u}_f'''\rangle\right)$$
$$+\frac{\rho_p\langle\alpha\rangle}{\rho_f\tau_D}\left[\langle \boldsymbol{u}''\cdot\boldsymbol{u}_f'''\rangle_p - 2k_f + \frac{\langle \alpha' \boldsymbol{u}_f'''\rangle}{\langle\alpha\rangle\langle 1-\alpha\rangle}\cdot(\langle \boldsymbol{u}\rangle_p - \langle \boldsymbol{u}_f\rangle_f) - \frac{\langle \alpha' \boldsymbol{u}_f'''\cdot\boldsymbol{u}_f'''\rangle}{\langle\alpha\rangle\langle 1-\alpha\rangle}\right]$$

Application to homogeneous gravity-driven flow

- Single-phase unclosed terms (models exist in literature)
- Interphase coupling unclosed terms (new closures needed)

Particle-phase equations

$$\frac{\partial \langle \alpha \rangle}{\partial t} = 0$$

$$\frac{\partial \langle \boldsymbol{u} \rangle_p}{\partial t} = \frac{1}{\tau_D} \left(\langle \boldsymbol{u}_f \rangle_f - \langle \boldsymbol{u} \rangle_p + \frac{\langle \alpha' \boldsymbol{u}_f''' \rangle}{\langle \alpha \rangle \langle 1 - \alpha \rangle} \right) + \boldsymbol{g}$$

$$\frac{\partial k_p}{\partial t} = \langle P : \nabla \boldsymbol{u}'' \rangle_p + \frac{1}{\tau_D} \left(\langle \boldsymbol{u}'' \cdot \boldsymbol{u}_f''' \rangle_p - \langle \boldsymbol{u}'' \cdot \boldsymbol{u}'' \rangle_p \right)$$

$$\frac{\partial \langle \Theta \rangle_p}{\partial t} = - \langle P : \nabla \boldsymbol{u}'' \rangle_p - \frac{2}{\tau_D} \langle \Theta \rangle_p - \frac{8 \left(1 - \mathrm{e}^2 \right)}{\sqrt{\pi} d_p} \langle g_o \alpha^2 \Theta^{3/2} \rangle$$

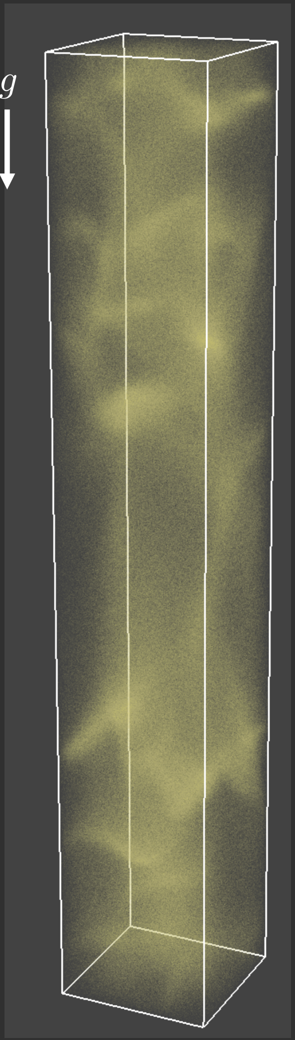
Fluid-phase equations

$$\frac{\partial \langle 1 - \alpha \rangle}{\partial t} = 0$$

$$\frac{\partial \langle \boldsymbol{u}_f \rangle_f}{\partial t} = 0$$

$$\varphi = \frac{\rho_p \langle \alpha \rangle}{\rho_f \langle 1 - \alpha \rangle}$$

$$\frac{\partial k_f}{\partial t} = \frac{1}{\rho_f \langle 1 - \alpha \rangle} \left(\langle p_f' \nabla \cdot \boldsymbol{u}_f''' \rangle - \langle \boldsymbol{\sigma}_f : \nabla \boldsymbol{u}_f''' \rangle \right) = + \frac{\varphi}{\tau_D} \left[\langle \boldsymbol{u}_f''' \cdot \boldsymbol{u}'' \rangle_p - k_f + \frac{\langle \alpha' \boldsymbol{u}_f''' \rangle}{\langle \alpha \rangle \langle 1 - \alpha \rangle} \cdot \left(\langle \boldsymbol{u} \rangle_p - \langle \boldsymbol{u}_f \rangle_f \right) - \frac{\langle \alpha' \boldsymbol{u}_f''' \cdot \boldsymbol{u}_f''' \rangle}{\langle \alpha \rangle \langle 1 - \alpha \rangle} \right]$$



A proposed model for drift velocity

- *Most important term – accounts for flow agitation due to clustering*

$$\langle \alpha' \boldsymbol{u}_f''' \rangle = C_g^* \langle (\alpha')^2 \rangle^{1/2} \left(\langle \boldsymbol{u} \rangle_p - \langle \boldsymbol{u}_f \rangle_f \right)$$

$$C_g^* = \frac{C_g \langle \alpha \rangle \langle 1 - \alpha \rangle}{\langle (\alpha')^2 \rangle^{1/2}}$$

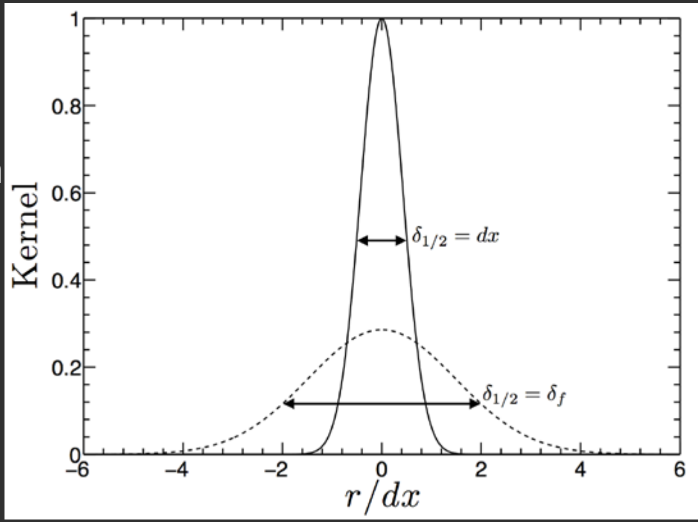
- Modeling constant C_g can be determined using mesoscale DNS

- In statistically homogeneous flow, this model increases terminal velocity:

$$\langle \boldsymbol{u} \rangle_p - \langle \boldsymbol{u}_f \rangle_f = \frac{\tau_D \boldsymbol{g}}{1 - C_g}$$

Mesoscale DNS framework

- NGA[2]
  - Arbitrarily high-order DNS/LES code
  - Massively parallel
  - Conservation of mass, momentum, and kinetic energy
  - Effective viscosity of Gibilaro et al. (2007) $\nu_f^* = \nu_f \left[(1-\alpha)^{-2.8} - 1 \right]$
- Lagrangian particle tracking[3]
  - 2nd-order Runge-Kutta for particle ODEs
  - Soft-sphere collision model
  - Linear drag: $\boldsymbol{\mathcal{A}} = \frac{1}{\tau_D} \left(\boldsymbol{u}_f - \boldsymbol{u} \right)$
- Interphase exchange[3]
  - Filter based on the convolution of mollification and diffusion
    1. Mollification: transfer particle data to neighboring cells
    2. Diffusion: smooth data with specified width δ_f
  - Fully conservative, implicit treatment
  - Transferred data converges under mesh refinement!



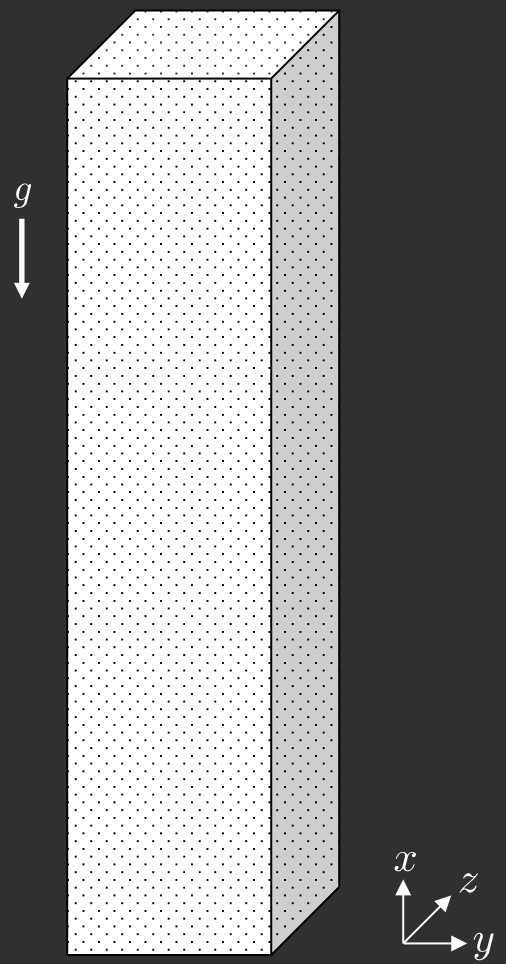
2. Desjardins et al., High order conservative finite difference scheme for variable density low Mach turbulent flow, *JCP*, 2008.
3. Capecelatro, J., Desjardins, O., An Euler-Lagrange strategy for simulating particle-laden flows, *JCP*, 2012.

Simulation configuration

- 3D triply-periodic domain
- Mass flow rate forced $\langle(1-\alpha)u_f\rangle = 0$
- Domain: $1920d_p \times 320d_p \times 320d_p$
- Mesh: $960 \times 160 \times 160$
- Case parameters

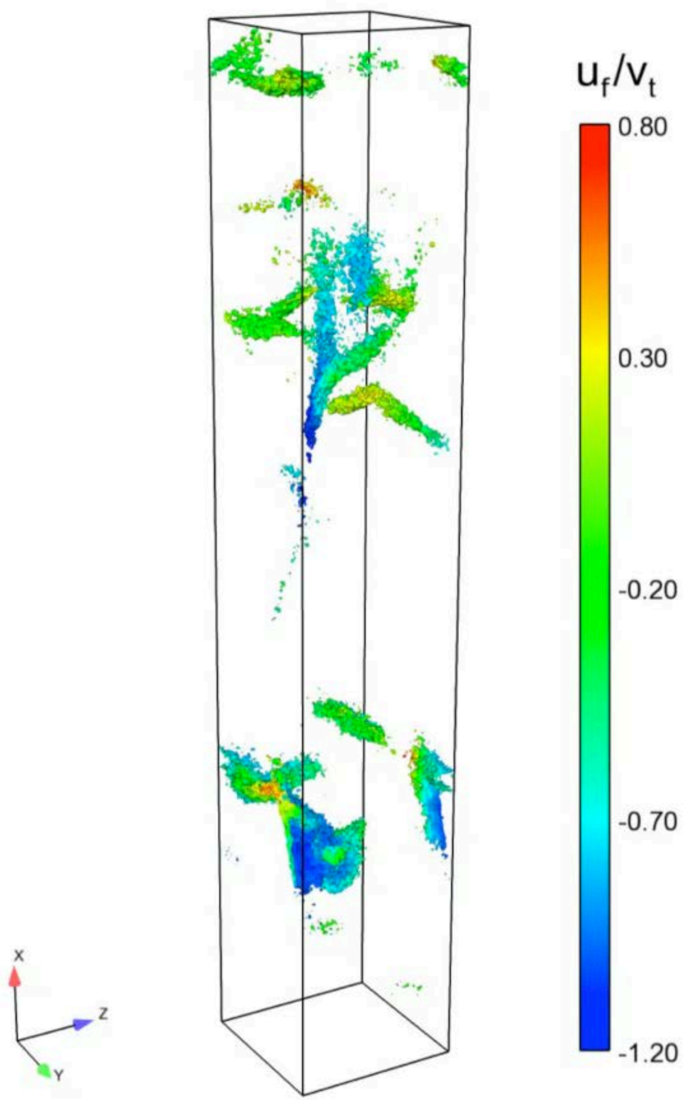
$$\mathrm{Re} = \frac{\rho_f \tau_D g d_p}{\mu} \qquad \tau_D = \frac{\rho_p d_p^2}{18\mu} \qquad \phi = \frac{\rho_p}{\rho_f}\frac{\alpha}{1-\alpha}$$

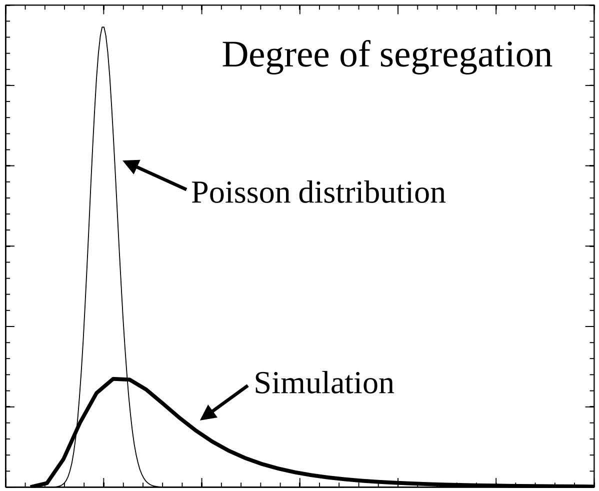
Name	Re	ϕ	ρ_p/ρ_f	$\langle\alpha\rangle$	n_p
Base	20	20	2000	0.01	3.71×10^6
A1	10	20	2000	0.01	3.71×10^6
A2	40	20	2000	0.01	3.71×10^6
A3	80	20	2000	0.01	3.71×10^6
B1	20	0.1	10	0.01	3.71×10^6
B2	20	1	100	0.01	3.71×10^6
B3	20	10	1000	0.01	3.71×10^6
C1	20	20	2000	0.005	1.85×10^6
C2	20	20	2000	0.05	18.55×10^6
C3	20	20	2000	0.1	37.14×10^6

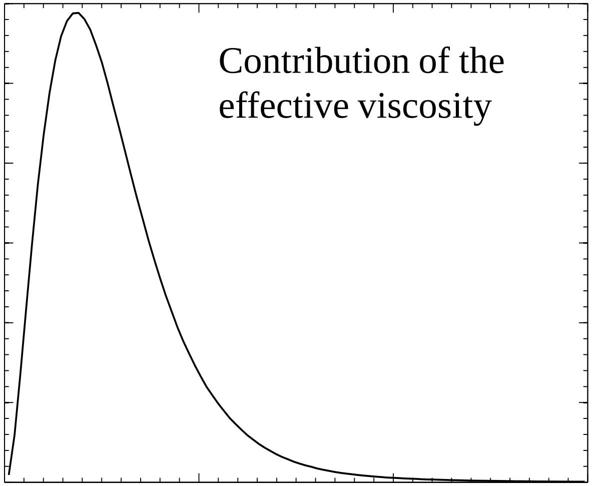


Base case simulation

Iso-surfaces of $\alpha = 3\langle(\alpha')^2\rangle^{1/2}$







Extracting multiphase statistics

- Separation of length scales much be established
- Any Lagrangian property A_p is filtered to the mesh by: $\alpha A = \sum_{i=1}^{n_p} A_p g\left(|\boldsymbol{x} - \boldsymbol{x}_p|\right) \mathcal{V}_p$
- Use 2-step filter with characteristic size δ_f

α

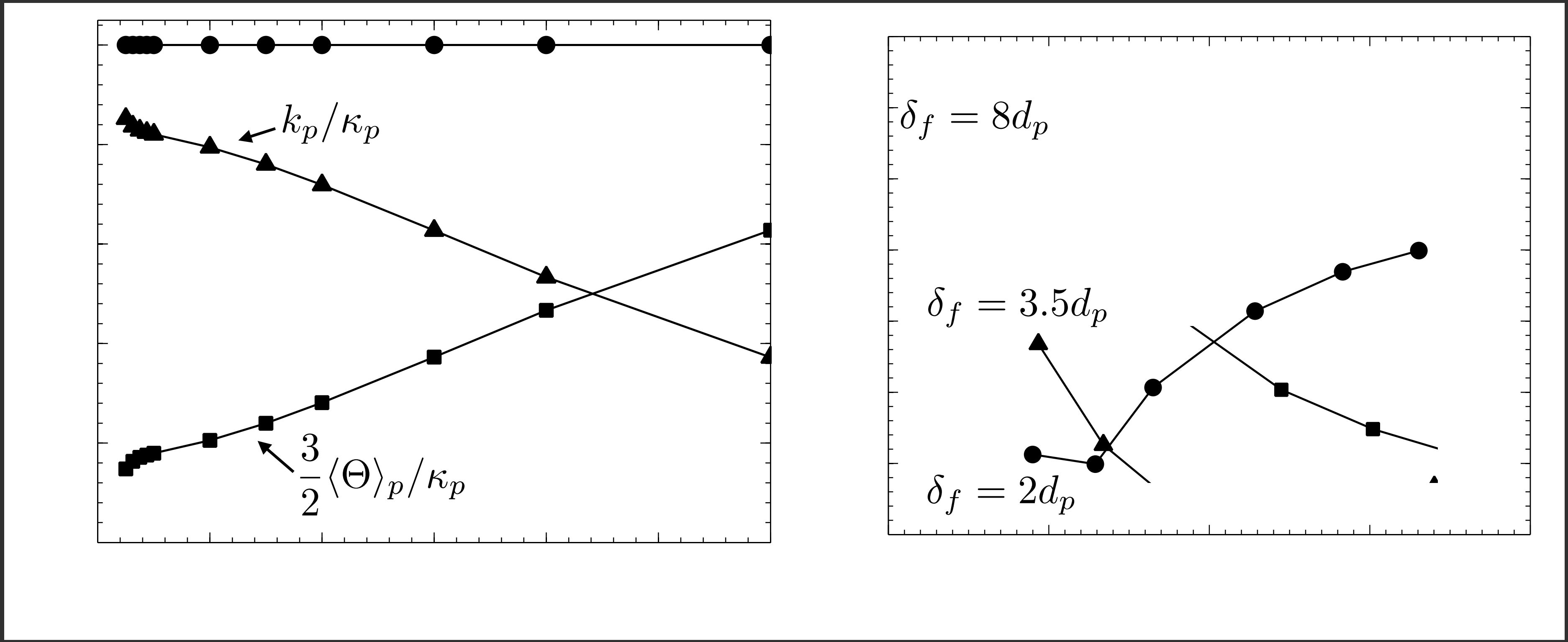
Particle velocity vectors

δ_f

- Total fluctuating energy: $\kappa_p = k_p + \frac{3}{2}\langle\Theta\rangle_p$
- If $\delta_f/d_p \ll 1$: $\boldsymbol{u} \approx \boldsymbol{u}_p \;\therefore\; \langle\Theta\rangle_p \approx 0$
- If $\delta_f/d_p \gg 1$: $\boldsymbol{u} \approx \langle\boldsymbol{u}\rangle_p \;\therefore\; k_p \approx 0$

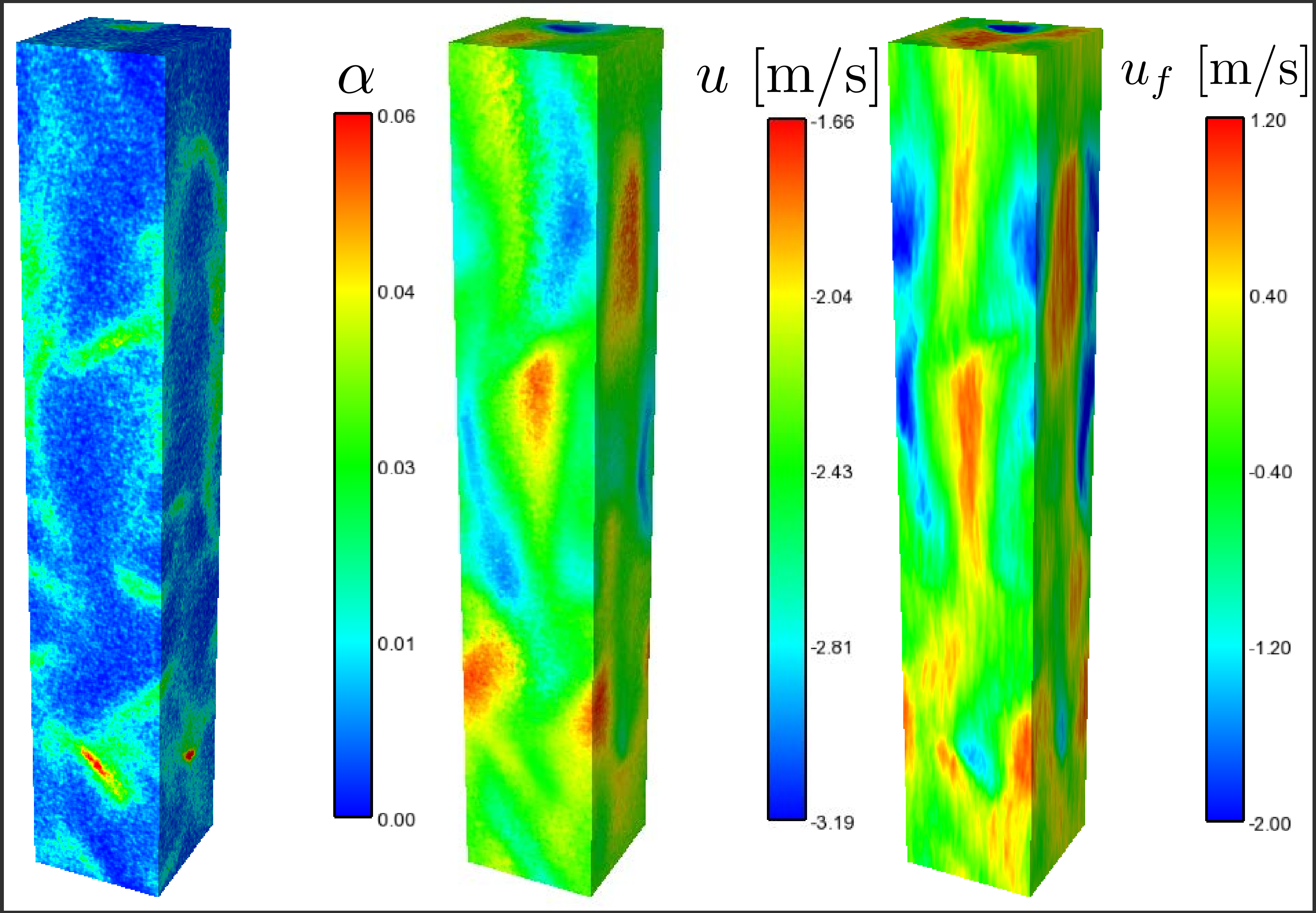
Choosing the correct filter size

- Use particle field from base case
- Assign each particle a random Gaussian velocity with
  - Mean set to local filtered velocity $\boldsymbol{u}$
  - Variance set to a prescribed granular temperature Θ^*

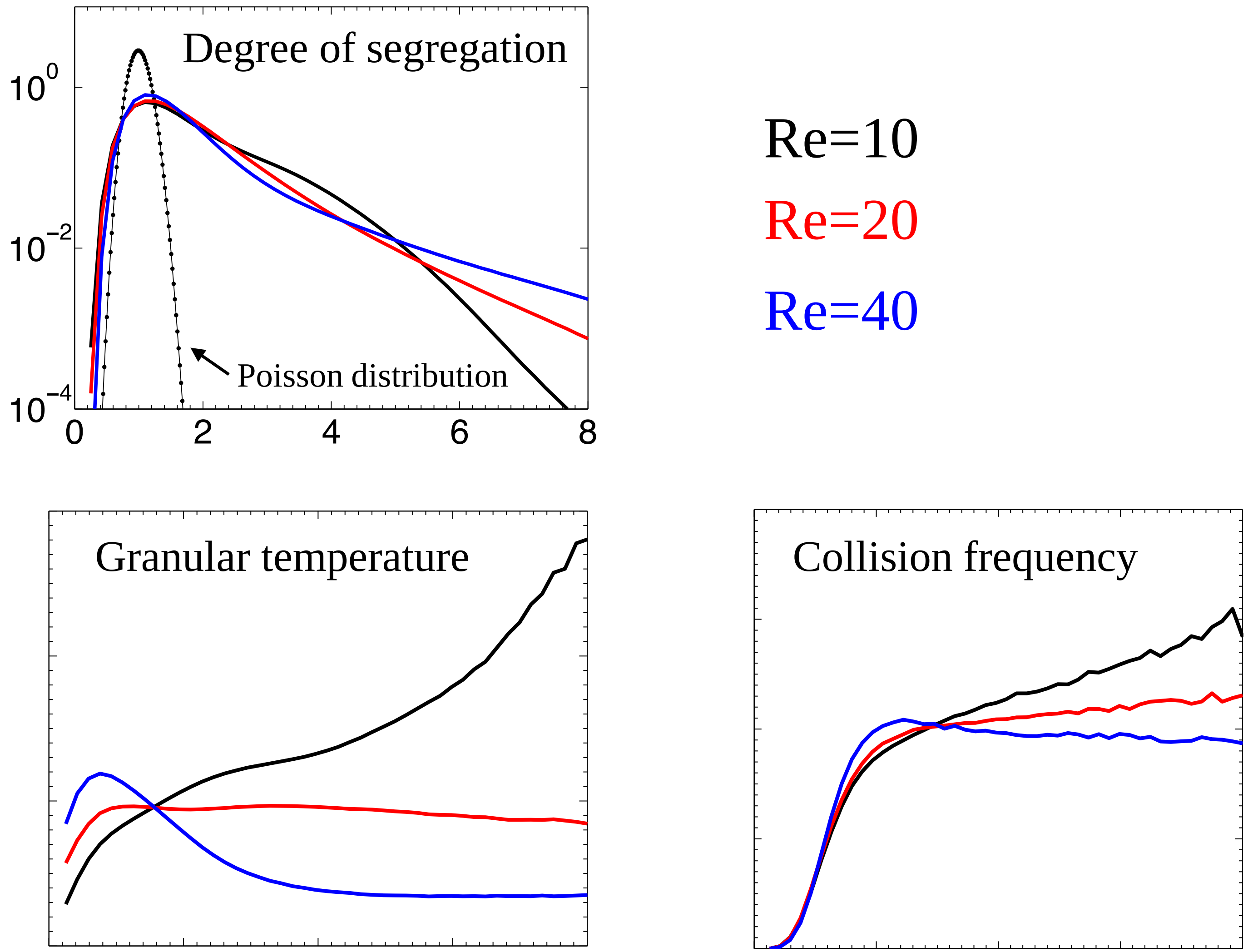


- Use filter size $\delta_f = 3.5d_p$

Instantaneous results (base case)



Reynolds number effect



Conclusions

In summary

- The exact Reynolds-averaged equations for fluid-particle flows have been derived
- Must distinguish between particle-phase TKE and granular temperature
- 2-step filter can be used to extract meaningful statistics

Looking forward

- Effect of mass loading and concentration on turbulence statistics
- Study wall-bounded risers
- Use RANS ideas in LES framework