Stochastic Lagrangian subgrid-scale models for turbulent particle-laden flows

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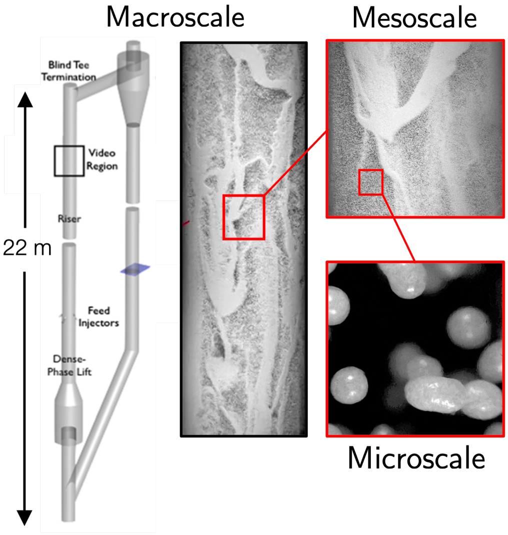
Motivation - The complexity of scales



Microscale interactions induce macroscale heterogeneity

Individual particles cannot be tracked at the macroscale

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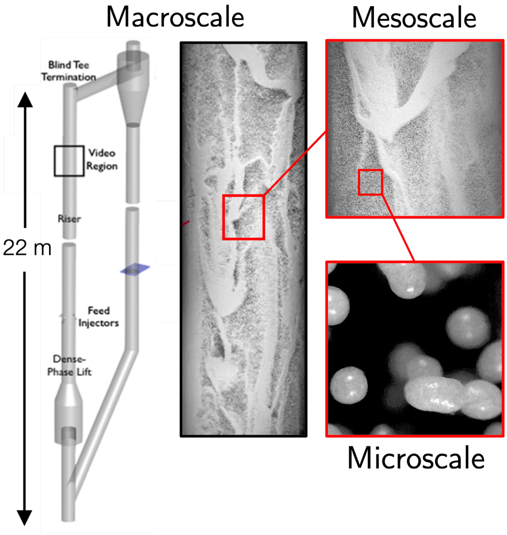
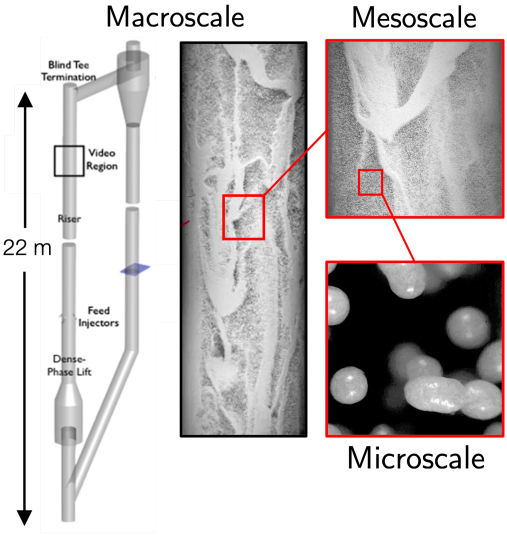


How can microscale effects be **accurately** and **efficiently** captured at the macroscale?

- EMMS
  - Drag correction via heterogeneous index
  - Needs meso/microscale correlations as an input
- Filtered two-fluid models
- Parcel approach*
- Structural methods
- **Stochastic models**



How can microscale effects be **accurately** and **efficiently** captured at the macroscale?

- EMMS
- Filtered two-fluid models
  - Disperse phase stresses, size, shapes, etc.
  - Filtered non-linear/unclosed terms (non-linear drag)
- Parcel approach*
- Structural methods
- **Stochastic models**

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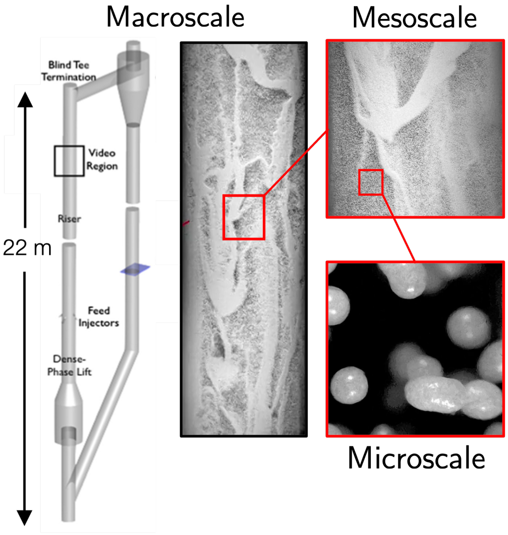

How can microscale effects be **accurately** and **efficiently** captured at the macroscale?

- EMMS
- Filtered two-fluid models
- Parcel approach*
  - Not grounded in first principles
  - Questions remain on grid size, parcel size, etc.
- Structural methods
- **Stochastic models**

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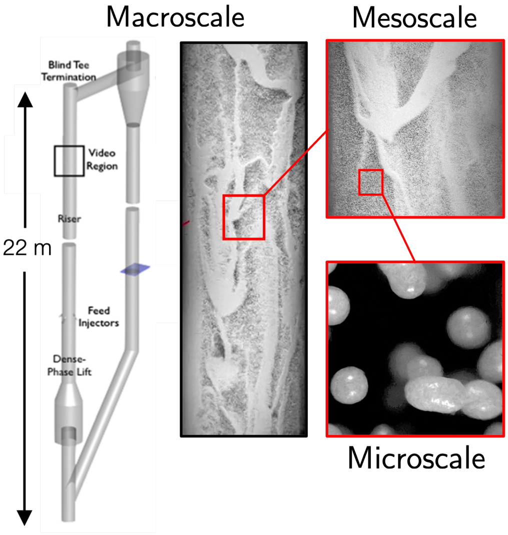
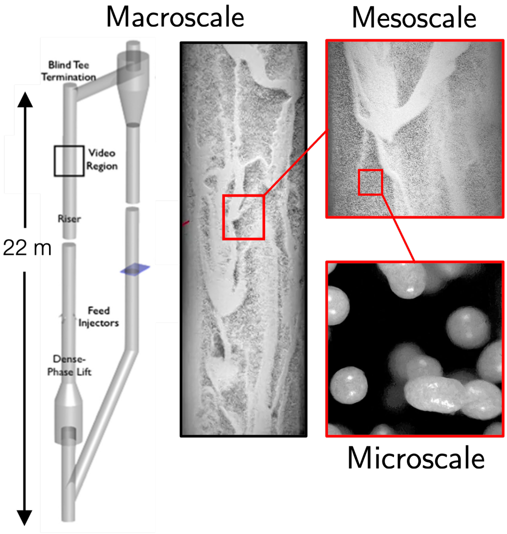


How can microscale effects be **accurately** and **efficiently** captured at the macroscale?

- EMMS
- Filtered two-fluid models
- Parcel approach*
- Structural methods
  - Reconstructs SGS flow field
  - Inherent heterogeneity
- **Stochastic models**

Motivation - The complexity of scales



How can microscale effects be **accurately** and **efficiently** captured at the macroscale?

- EMMS
- Filtered two-fluid models
- Parcel approach*
- Structural methods
- **Stochastic models**
  - Widely used
  - Embedded statistics
  - Resists degradation with grid coarsening
  - No heterogeneity?

Two stochastic approaches

1. **A stochastic description of drag**
   - Lattanzi, Aaron, *et al*. 2022. "Stochastic Model for the Hydrodynamic Force in Euler–Lagrange Simulations of Particle-Laden Flows." Physical Review Fluids 7 (1).
2. Towards two-point statistics and SGS heterogeneity

The stochastic hierarchy

Position Langevin

$$\mathrm{d}\boldsymbol{X}_p = \boldsymbol{U}_p \,\mathrm{d}t + \overline{\boldsymbol{b}}\,\mathrm{d}\boldsymbol{W}_t$$

- Direct control over dispersion statistics
- No control over granular temperature

Velocity Langevin

$$\mathrm{d}\boldsymbol{X}_p = \boldsymbol{U}_p \,\mathrm{d}t$$

$$\mathrm{d}\boldsymbol{U}_p = \frac{\boldsymbol{u}_f - \boldsymbol{U}_p}{\tau_p}\,\mathrm{d}t + \overline{\boldsymbol{b}}\,\mathrm{d}\boldsymbol{W}_t$$

- Direct control of granular temperature*
- Dispersion depends on drag timescale
- No time correlation in fluctuating force

Force Langevin

$$\mathrm{d}\boldsymbol{X}_p = \boldsymbol{U}_p \,\mathrm{d}t$$

$$\mathrm{d}\boldsymbol{U}_p = -\frac{1}{\tau_p}\boldsymbol{U}_p\,\mathrm{d}t + \frac{\boldsymbol{F}_d}{m_p}\,\mathrm{d}t$$

$$\mathrm{d}\boldsymbol{F}_d = -\frac{1}{\tau_F}\boldsymbol{F}_d\,\mathrm{d}t + \overline{\boldsymbol{b}}\,\mathrm{d}\boldsymbol{W}_t$$

- Direct control over granular temperature and dispersion
- Timescale and variance of drag fluctuation must be closed

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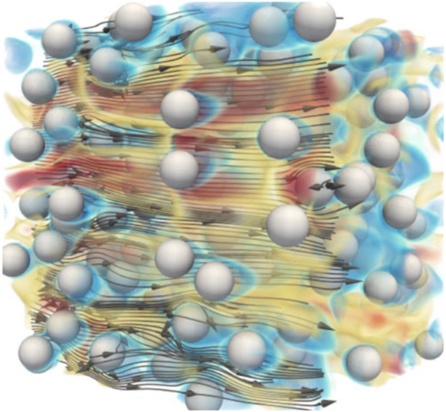
Towards a stochastic description of drag

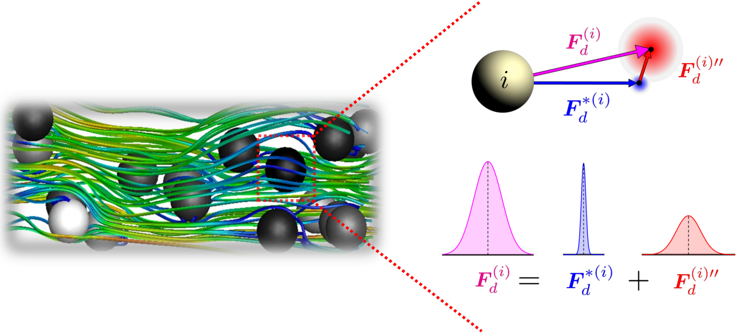
$$m_p \frac{\mathrm{d}\boldsymbol{U}_p}{\mathrm{d}t} = \boldsymbol{F}_{col} + m_p \boldsymbol{g} + \int_{\delta S} \boldsymbol{\tau} \cdot \boldsymbol{n} \, \mathrm{d}S$$



- Collisions
- Gravity
- **Stress**

Towards a stochastic description of drag

$$m_p \frac{\mathrm{d}\boldsymbol{U}_p}{\mathrm{d}t} = \boldsymbol{F}_{col} + m_p \boldsymbol{g} + \boxed{\int_{\delta S} \boldsymbol{\tau} \cdot \boldsymbol{n} \, \mathrm{d}S}$$



Drag decomposition:

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

The $\boldsymbol{\tau}$ decomposition

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

Pick and choose a mean drag model (Tenetti *et al.*, 2011):

$$\langle \boldsymbol{F}_d \rangle = f(\mathrm{Re}_p, \phi, \ldots) \tag{1}$$

Ornstein-Uhlenbeck (OU) process for what's left:

$$\mathrm{d}\boldsymbol{F}_d'' = -\frac{1}{\tau_F} \boldsymbol{F}_d'' \, \mathrm{d}t + \frac{\sigma_F}{\sqrt{\tau_F}} \, \mathrm{d}\boldsymbol{W}_t \tag{2}$$

Constructing the force Langevin

$$\mathrm{d}\boldsymbol{F}_d'' = -\frac{1}{\tau_F}\boldsymbol{F}_d''\,\mathrm{d}t + \frac{\sigma_F}{\sqrt{\tau_F}}\,\mathrm{d}\boldsymbol{W}_t \qquad (2)$$

Force timescale τ_F:

- Approximated by time between successive collisions (Chapman *et al.*, 1970)

$$\tau_F \approx \tau_{col} = \frac{d_p}{24\phi\chi}\sqrt{\frac{\pi}{\Theta}} \qquad (3)$$

- Implicit dependence on granular temperature – evaluate locally (Capecelatro *et al.*, 2015)

Standard deviation of drag force σ_F:

- F_d'' known to be Gaussian (PR-DNS[1])

Constructing the force Langevin

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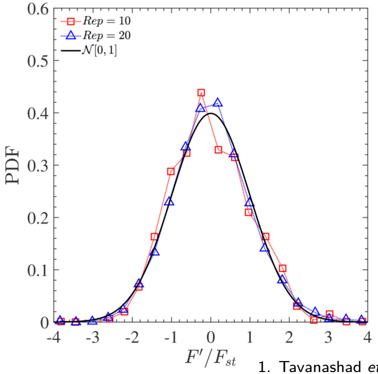
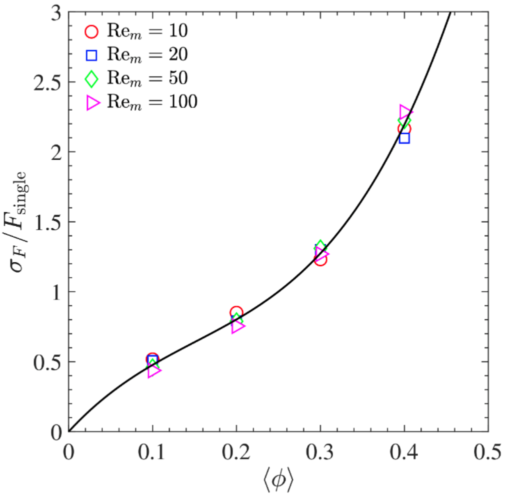


1. Tavanashad *et al.*, 2021

Constructing the force Langevin

$$\frac{\sigma_F}{m_p^{(i)}} \equiv f_\phi^{\sigma_F} f_{\rm iso} \frac{(1-\phi)||\boldsymbol{u}[\boldsymbol{x}_p^{(i)}] - \boldsymbol{U}_p^{(i)}||}{\tau_p}$$
$$f_\phi^{\sigma_F} = 6.52\phi - 22.56\phi^2 + 49.90\phi^3$$
$$f_{\rm iso} = 1 + 0.15\mathrm{Re}_p^{0.687} \tag{4}$$

- Ready for use in Euler-Lagrange simulations
- Isotropic!



Evaluating granular temperature

Granular temperature: $\Theta = \frac{1}{3}\langle \boldsymbol{U}_p' \cdot \boldsymbol{U}_p' \rangle$

Homogeneous heating

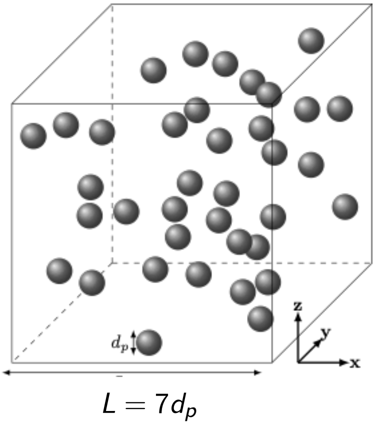
$\Theta(t=0) < \Theta(t \to \infty)$

Homogeneous cooling

$\Theta(t=0) > \Theta(t \to \infty)$

Numerics:

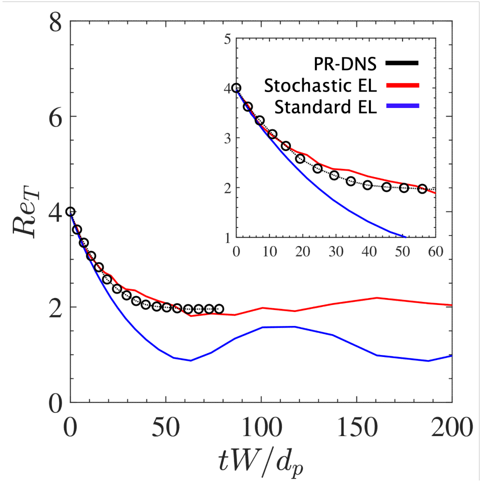
- NGA (Desjardins *et al.*, 2008)
- Lagrangian particle tracking (Capecelatro & Desjardins, 2013)
- Soft-sphere collisions (elastic)
- RK2/Euler-Maruyama method (Lattanzi *et al.*, 2022)



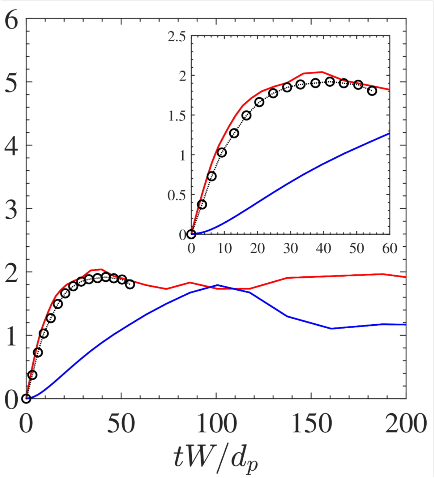
Simulation results

$Re_m = 20, \ \phi = 0.1, \ \rho_p/\rho_f = 100$

Cooling



Heating



Two stochastic approaches - from homogeneous to heterogeneous

1. A stochastic description of drag
   - Captures evolution of granular temperature
   - See Lattanzi *et al.*, 2022
2. **Towards two-point statistics and SGS heterogeneity**

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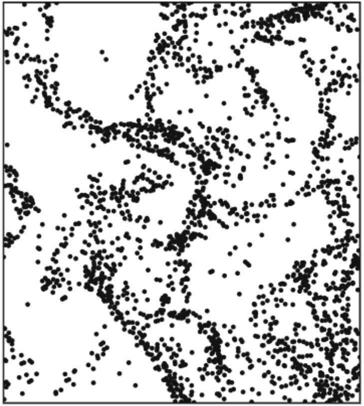
Subgrid-scale heterogeneity

Spatial segregation

- Significant for Stk $= \mathcal{O}(1)$
- One-point $\rightarrow$ homogeneous
- Two-point information must be used to capture preferential concentration



Pozorski & Apte 2009

Subgrid-scale heterogeneity

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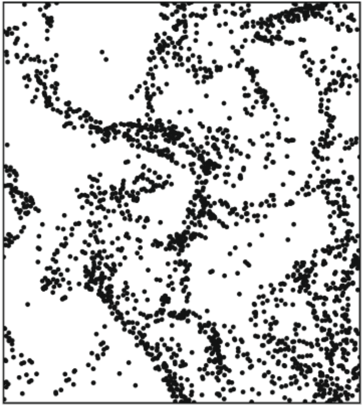
Preliminary work:

- Dilute suspensions
- Stokes drag
- Point particles



Pozorski & Apte 2009

Continous random walk (CRW)

Pozorski & Apte (2009)

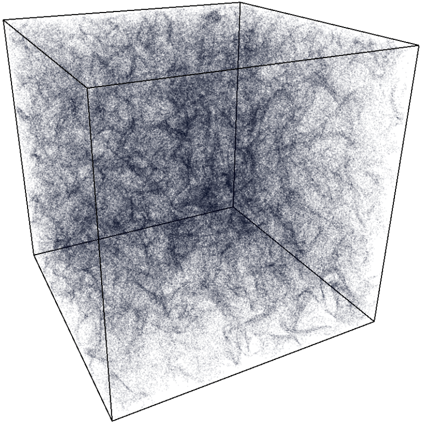
$$\mathrm{d}\boldsymbol{u} = -\frac{\boldsymbol{u}}{\tau_L}\,\mathrm{d}t + \sigma_{sg}\sqrt{\frac{2}{\tau_L}}\,\mathrm{d}\boldsymbol{W} \quad (5)$$

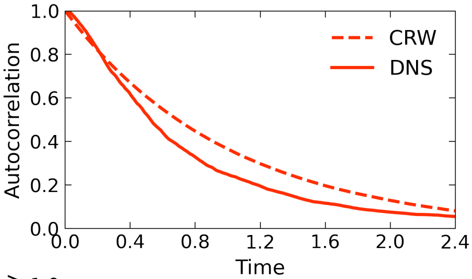
$$\mathrm{d}\boldsymbol{v} = \frac{\boldsymbol{u}-\boldsymbol{v}}{\tau_p}\,\mathrm{d}t \quad (6)$$

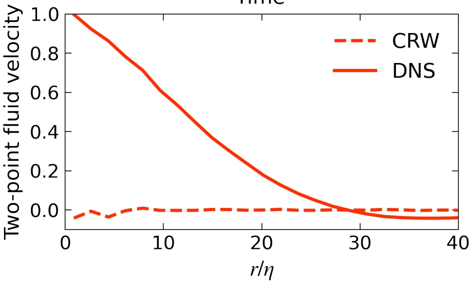
$$\mathrm{d}\boldsymbol{x} = \boldsymbol{v}\,\mathrm{d}t \quad (7)$$

- Particles evolve **independently**
- Embedded one-point statistics
  - $\overline{C} = \sigma_{sg}^2 = \frac{2}{3}k_{sg}$
- Two-time correlation
  - $\overline{\kappa}(s) = \sigma_{sg}^2 \exp\left\{-\frac{|s|}{\tau_L}\right\}$
- $\tau_L^{-1} = \left(\frac{1}{2} + \frac{3}{4}C_0\right)\frac{\epsilon}{k_{sg}}$
- Csanady corrections to τ_L not considered here (low Stokes!)

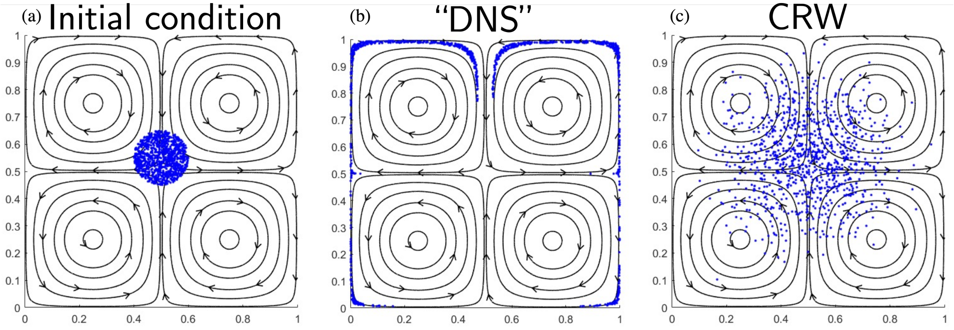
CRW - Two-point and two-time statistics







CRW - Taylor-Green vortex as a RANS cell



CRW $\rightarrow$ homogeneous dispersion!

Spatial correlation – Multivariate distributions

$$f_{\boldsymbol{u}^{(p)}}(\boldsymbol{u}^{(1)}, \ldots, \boldsymbol{u}^{(N)}) = \frac{1}{\sqrt{(2\pi)^{3N}|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\boldsymbol{u}^{(p)} - \boldsymbol{\mu})^\intercal \boldsymbol{\Sigma}^{-1} (\boldsymbol{u}^{(p)} - \boldsymbol{\mu})\right\}$$

The Ornstein-Uhlenbeck (OU) process

$$\mathrm{d}\boldsymbol{u}^{(p)} = \boldsymbol{A}\,\mathrm{d}t + \boldsymbol{B}\,\mathrm{d}\boldsymbol{W}\,, \qquad \boldsymbol{B}\boldsymbol{B}^\intercal = \boldsymbol{\Sigma}$$

- Choleskey decomposition of $\boldsymbol{\Sigma}$ allows for direct implementation into OU process
- Particle states correlated through $\boldsymbol{B}$
- CRW: $\sigma_{ij,i\neq j} = 0$
  - No correlation between particle states!

Spatial correlation – Particles as a high-dimensional system

$9N$-dimensional stochastic system

$$\mathrm{d}\boldsymbol{u}^{(p)} = -\frac{\boldsymbol{u}^{(p)}}{\tau_L}\,\mathrm{d}t + \boldsymbol{B}\,\mathrm{d}\boldsymbol{W} \tag{8}$$

$$\mathrm{d}\boldsymbol{v}^{(p)} = \frac{\boldsymbol{u}^{(p)} - \boldsymbol{v}^{(p)}}{\tau_p}\,\mathrm{d}t \tag{9}$$

$$\mathrm{d}\boldsymbol{x}^{(p)} = \boldsymbol{v}^{(p)}\,\mathrm{d}t \tag{10}$$

- $\boldsymbol{u}^{(p)} = \begin{bmatrix}\boldsymbol{u}^{(1)} & \boldsymbol{u}^{(2)} & \dots & \boldsymbol{u}^{(N)}\end{bmatrix}^\mathsf{T}$
- $\boldsymbol{v}^{(p)} = \begin{bmatrix}\boldsymbol{v}^{(1)} & \boldsymbol{v}^{(2)} & \dots & \boldsymbol{v}^{(N)}\end{bmatrix}^\mathsf{T}$
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What is the form of Σ that manifests SGS heterogeneity?

Spatial correlation – Starting from the OU process

We construct $\boldsymbol{\Sigma}$ starting from the OU process

$$\mathrm{d}\boldsymbol{u}^{(p)} = -\frac{\boldsymbol{u}^{(p)}}{\tau_L}\,\mathrm{d}t + \boldsymbol{B}\,\mathrm{d}\boldsymbol{W}$$
$$\boldsymbol{B}\,\mathrm{d}\boldsymbol{W}\,\mathrm{d}\boldsymbol{W}^{\intercal}\,\boldsymbol{B}^{\intercal} = \left(\mathrm{d}\boldsymbol{u}^{(p)} + \frac{\boldsymbol{u}^{(p)}}{\tau_L}\,\mathrm{d}t\right)\left(\mathrm{d}\boldsymbol{u}^{(p)} + \frac{\boldsymbol{u}^{(p)}}{\tau_L}\,\mathrm{d}t\right)^{\intercal}$$

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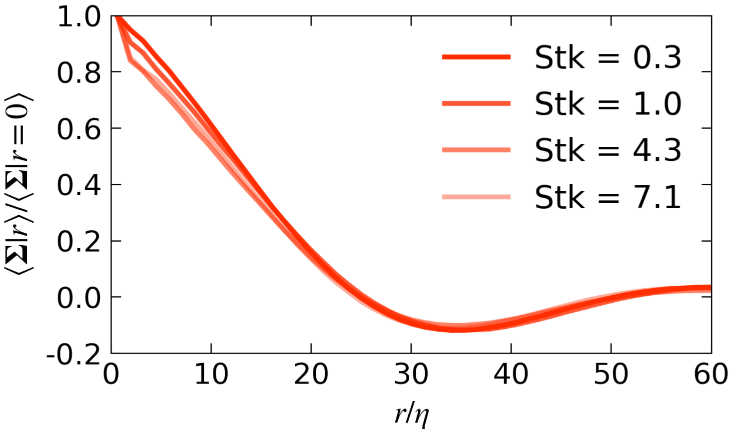
$$\langle \boldsymbol{B}\boldsymbol{B}^{\mathsf{T}} \rangle = \boldsymbol{\Sigma} = \frac{1}{\Delta t}\left\langle \left(\Delta\boldsymbol{u}^{(p)} + \frac{\boldsymbol{u}^{(p)}}{\tau_L}\Delta t\right)\left(\Delta\boldsymbol{u}^{(p)} + \frac{\boldsymbol{u}^{(p)}}{\tau_L}\Delta t\right)^{\mathsf{T}} \right\rangle \tag{11}$$

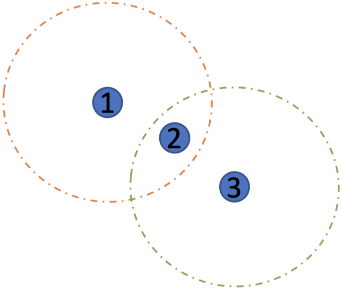
Spatial correlation – Σ as a function of r



Particles are correlated within a cutoff radius

Spatial correlation – Implementation

- A globally-correlated system of N particles is not computationally tractable
  - $\mathbf{\Sigma} \in \mathbb{R}^{3N \times 3N}$
  - Decay of $\langle \mathbf{\Sigma} | r \rangle$ leads to sparsity
  - Sparsity of $\mathbf{\Sigma}$ is ordering dependent
- Local correlation is not feasible via a cutoff radius
- Paths forward:
  - Local construction of $\mathbf{\Sigma}$
  - Particle based methods/local smoothing
  - Embed one- and two-point statistics



Summary

Stochastic models allow for direct control over evolution statistics

- Force Langevin
  - SGS particle-fluid-particle interactions
  - Correct evolution of granular temperature
  - Scalable
- Spatially-correlated random walk (SCRW)
  - Two-point statistics as variance $\rightarrow$ heterogeneity
  - Correlations expected!
  - Preferential concentration

Questions?

Email: maxzog@umich.edu
Lab: www.jessecaps.com

Extra slides

Direct numerical simulations

All DNS of homogeneous isotropic turbulence (HIT) carried out using NGA

- Second-order finite volume
- 128^3 grid
- Forced stochastically as in Eswaran & Pope (1988)
- $\mathrm{Re}_\lambda \approx 37$
- $\mathrm{Re}_L \approx 210$
- $\Delta x/\eta = 2.04$

Spatial correlation - Particle pairs

Reduction of the system to two particles permits numerical study (i.e. $p \in \{1, 2\}$)

$$\mathrm{d}\boldsymbol{u}^{(p)} = -\frac{\boldsymbol{u}^{(p)}}{\tau_L}\,\mathrm{d}t + \boldsymbol{B}\,\mathrm{d}\boldsymbol{W} \tag{12}$$

$$\mathrm{d}\boldsymbol{v}^{(p)} = -\frac{\boldsymbol{u}^{(p)} - \boldsymbol{v}^{(p)}}{\tau_p}\,\mathrm{d}t \tag{13}$$

$$\mathrm{d}\boldsymbol{x}^{(p)} = \boldsymbol{v}^{(p)}\,\mathrm{d}t \tag{14}$$

$$\frac{1}{2}\boldsymbol{B}\boldsymbol{B}^{\intercal} = \frac{1}{2}\boldsymbol{\Sigma} = \frac{\sigma_{sg}^2}{\tau_L}\begin{bmatrix} \boldsymbol{I} & \rho(r)\boldsymbol{I} \\ \rho(r)\boldsymbol{I} & \boldsymbol{I} \end{bmatrix} \tag{15}$$

- $\rho(r)$ obtained from degree-14 polynomial fit of $\langle\boldsymbol{\Sigma}|r\rangle / \langle\boldsymbol{\Sigma}|r = 0\rangle$
- τ_L is treated as a constant
- Possible to move up the stochastic hierarchy to $\boldsymbol{v}^{(p)}$, $\boldsymbol{x}^{(p)}$

Spatial correlation – Relevant work

Rani *et al.* (2014), Dharwiwal *et al.* (2017)

$$\frac{\partial \Omega}{\partial t} + \nabla_{\boldsymbol{r}} \cdot (\boldsymbol{U}\Omega) - \frac{1}{\tau_p}\nabla_{\boldsymbol{U}} \cdot (\boldsymbol{U}\Omega) - \nabla_{\boldsymbol{U}} \cdot (\boldsymbol{D}_{\boldsymbol{UU}} \cdot \nabla_{\boldsymbol{U}}\Omega) = 0 \tag{16}$$

$$\boldsymbol{D}_{UU} = \frac{1}{\tau_p^2}\int_{-\infty}^{0} \langle \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}_{cm}, 0) \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}_{cm}, t) \rangle \, \mathrm{d}t \tag{17}$$

- Particle-pair relative motion
  - $\boldsymbol{U} = \boldsymbol{v}^{(q)} - \boldsymbol{v}^{(p)}$
  - $\boldsymbol{r} = \boldsymbol{x}^{(q)} - \boldsymbol{x}^{(p)}$
- Diffusion matrix found via perturbation analysis of Fokker-Planck equation
- Captures particle-pair statistics (e.g. separation, radial velocity)

Spatial correlation – Fokker-Planck

Fokker-Planck equivalent to the system shown previously

$$\frac{\partial f}{\partial t} - \frac{1}{\tau_L}\nabla_{\boldsymbol{u}^{(p)}}(\boldsymbol{u}^{(p)} f) + \frac{1}{\tau_p}\nabla_{\boldsymbol{v}^{(p)}}(\boldsymbol{u}^{(p)} f) - \frac{1}{\tau_p}\nabla_{\boldsymbol{v}^{(p)}}(\boldsymbol{v}^{(p)} f) = \frac{1}{2}\frac{\partial^2(\Sigma_{ij} f)}{\partial u_i^{(p)} \partial u_j^{(p)}} \tag{18}$$

- $f(\boldsymbol{u}^{(p)}, \boldsymbol{v}^{(p)}, \boldsymbol{x}^{(p)}; t | \boldsymbol{u}_0^{(p)}, \boldsymbol{v}_0^{(p)}, \boldsymbol{x}_0^{(p)}; t_0)$
- High dimensionality makes analysis non-trivial
- Numerical solutions quickly become intractable