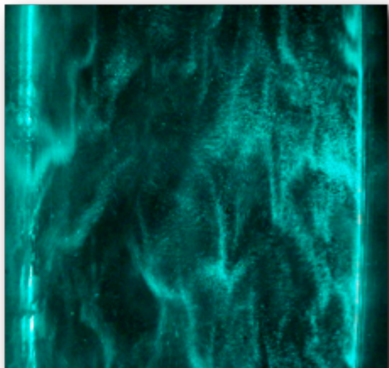
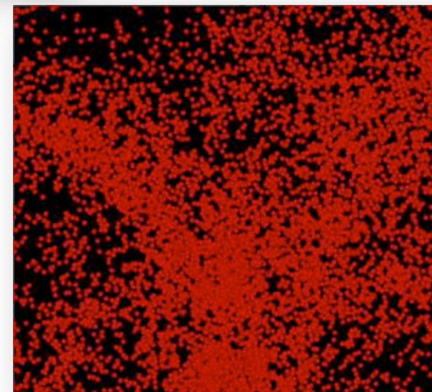
Clustering in macroscale two-phase flows





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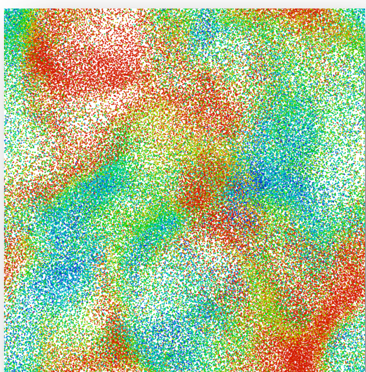
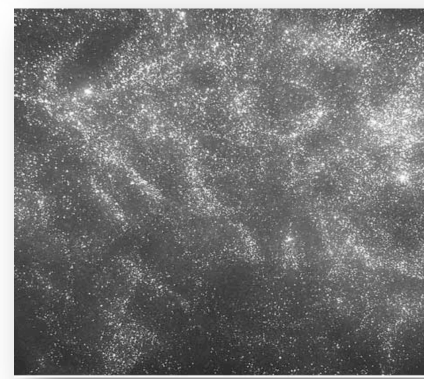




NETL 2010 Multiphase Flow Science Workshop
Coraopolis, PA

Overview of multiphase flow work in Pitsch Group (Stanford University)

Primary focus area: Gas-liquid flows

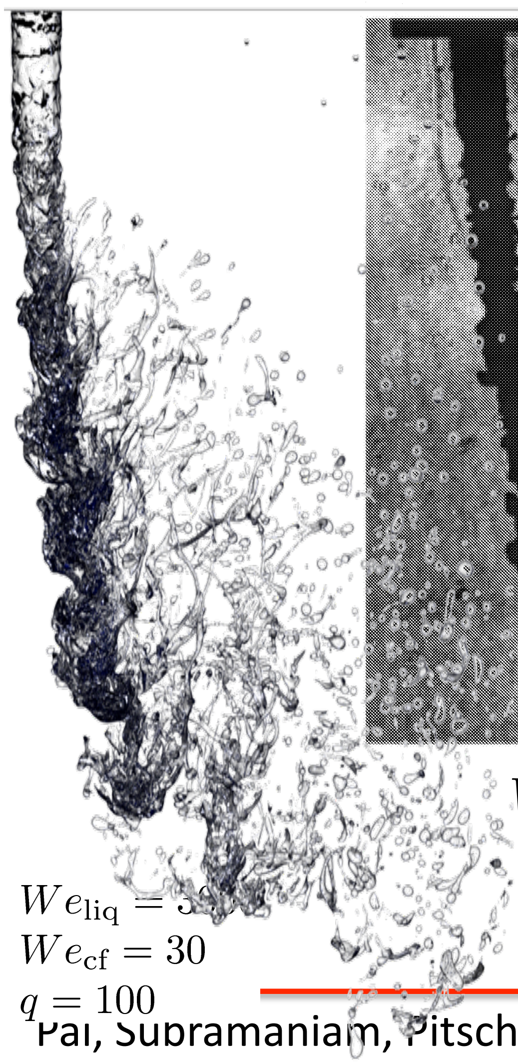
- Detailed simulations (DS) of primary breakup of liquid jets
  - Unsolved problem; predictive models for primary breakup unavailable
- Development of DS methodologies for large density ratio, evaporating sprays – *Dr. Mehdi Raessi, Vincent LeChenadec*
- Spray combustion – *Dr. Kun Luo*
  - Studies in a simplified gas turbine combustor configuration
  - Evaluate models

External collaboration:
Prof. Olivier Desjardins, U Colorado, Boulder

Simulations of primary breakup of liquid jets in crossflow

NUMERICAL SIMULATION

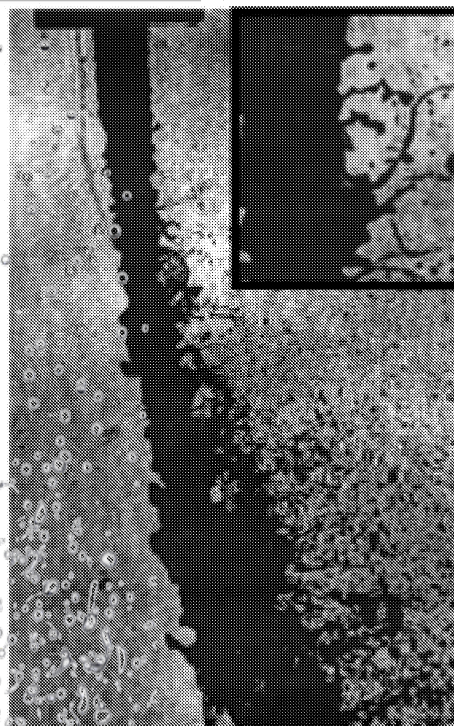
M. G. Pai et al. AIAA (2009)



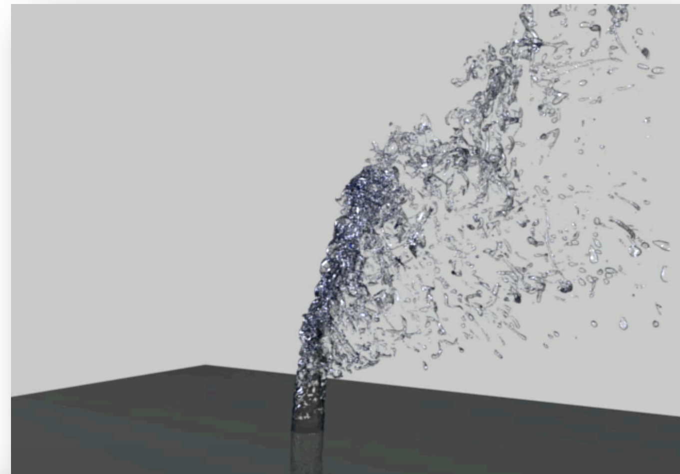
$We_{\mathrm{liq}} = 3$[illegible]
$We_{\mathrm{cf}} = 30$
$q = 100$

EXPERIMENT

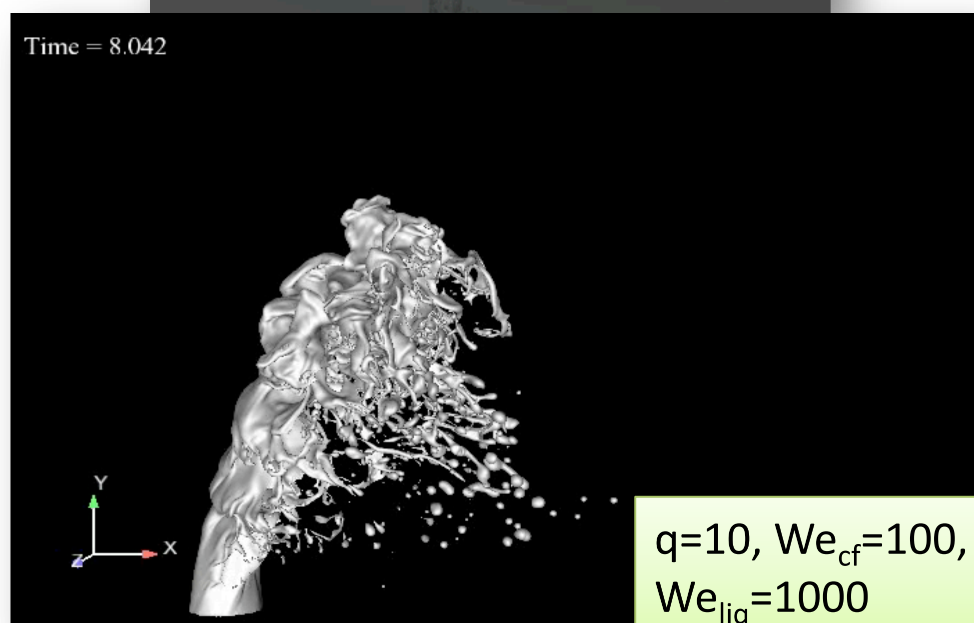
Lee et al. (2007)



$$We_{\mathrm{liq}} = 2547$$
$$We_{\mathrm{cf}} = 30$$
$$q = 68$$

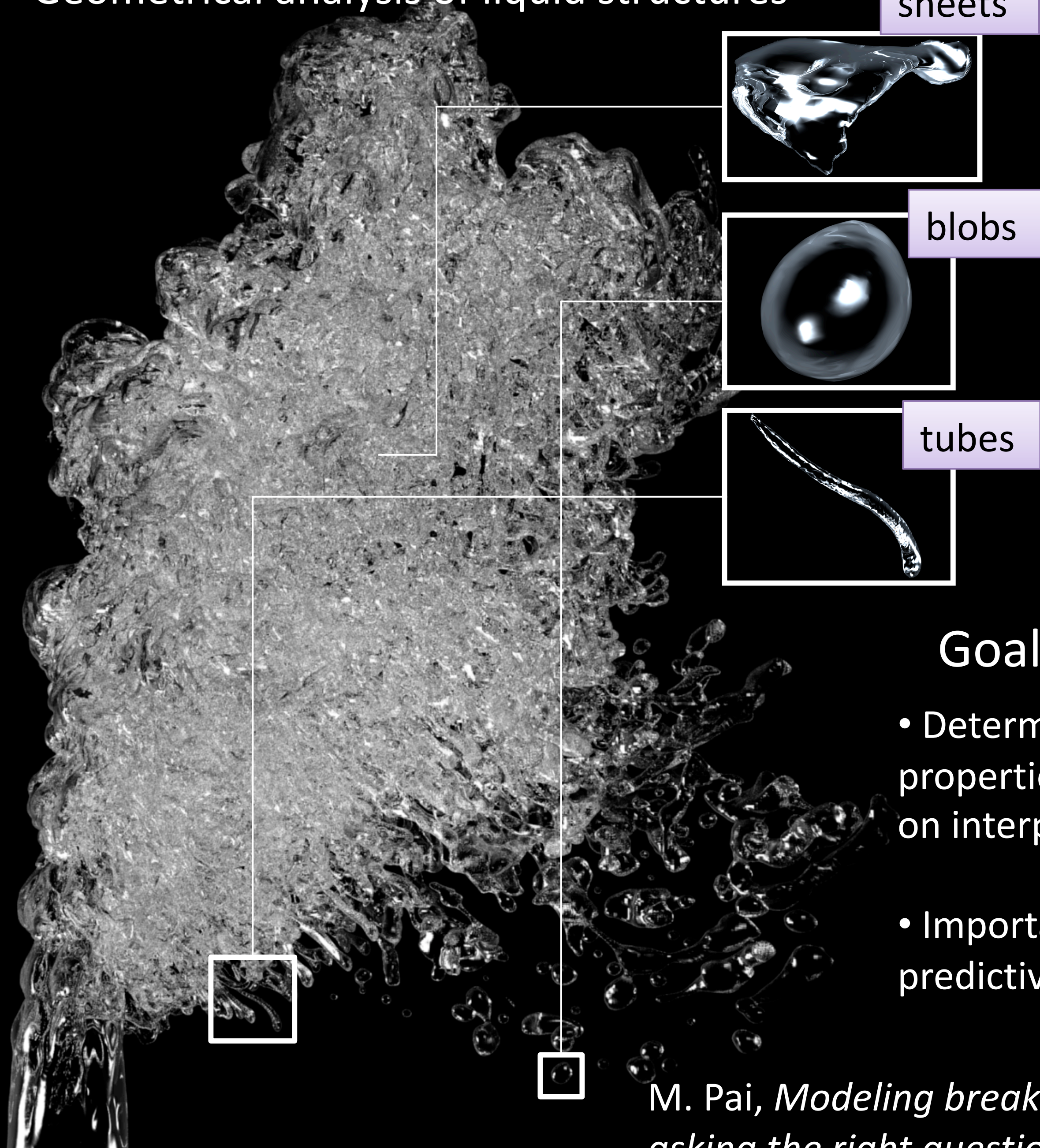


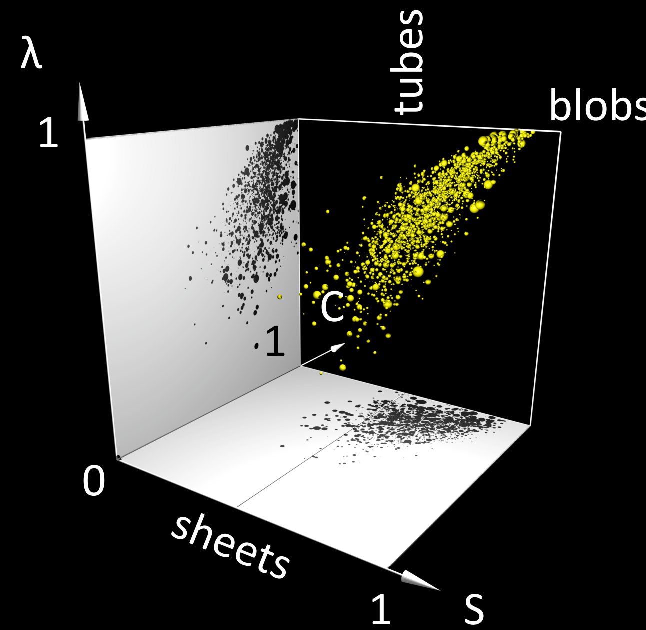
M. Pai et al. AIAA (2009, 2010)



q=10, We_{cf}=100, We_{liq}=1000

Geometrical analysis of liquid structures





Goal

- Determine dependence of geometrical properties of separated liquid structures on interphase transfer processes
- Important and significant step toward predictive primary breakup model

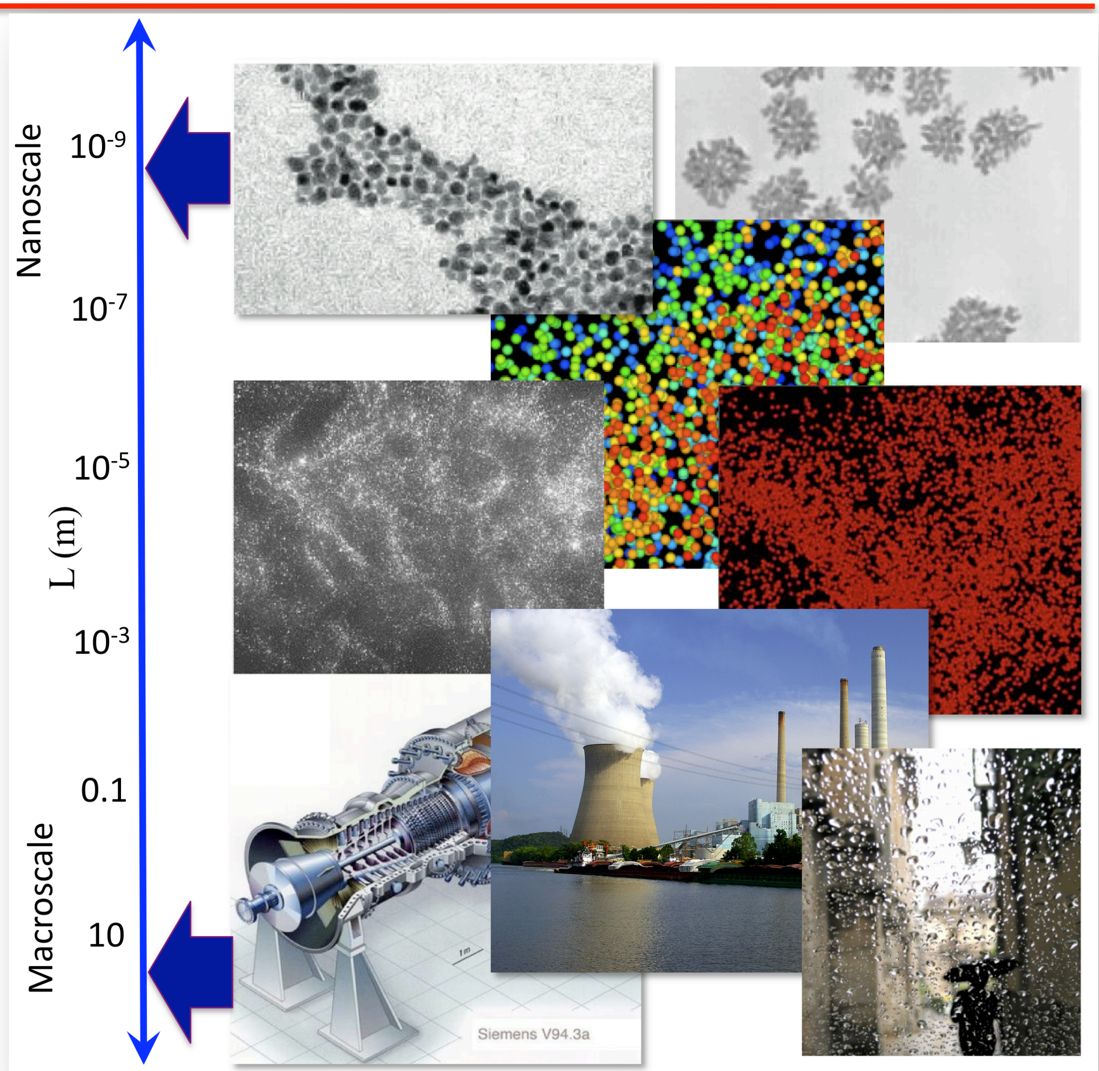
M. Pai, *Modeling breakup of turbulent liquid jets: Are we asking the right questions?* (In preparation)

Clustering across multiple scales

- Clustering observed in a variety of systems spanning the entire size spectrum

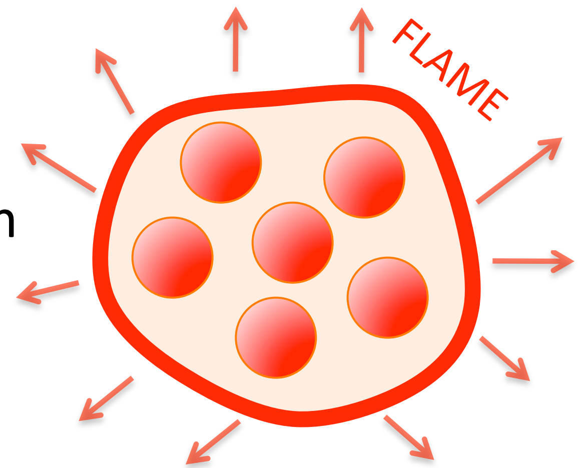
- Nanoparticle synthesis, nanomedicine, rain formation, gas turbine combustion, coal gasification, fluidized beds, …

- Clustering identified as a principal hurdle in our understanding of gas-solid flows (NETL report, 2006)

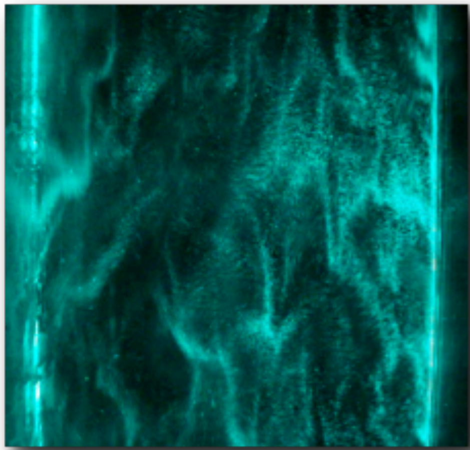


Motivation to study clustering

- Spray combustion
  - Even at low volume fractions, certain spatial configurations may lead to group combustion modes (Chiu and Liu, 1977)
  - Numerical models based on solitary droplets (no interactions with neighboring droplets) do not capture physics associated with such combustion modes
- Coal combustion: group combustion modes observed (Annamalai & Ryan, PECS, 1993)



Group combustion (schematic)



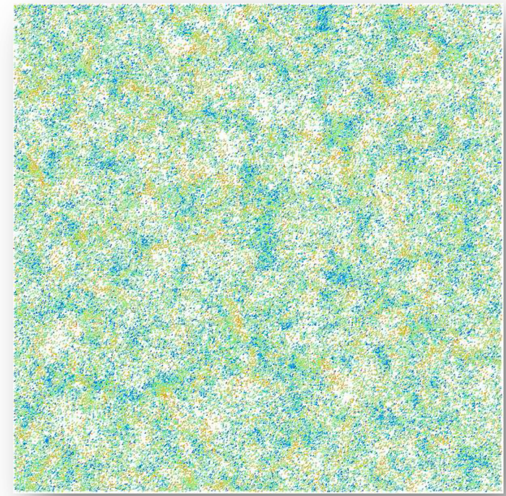
Taneka et al. (2002)

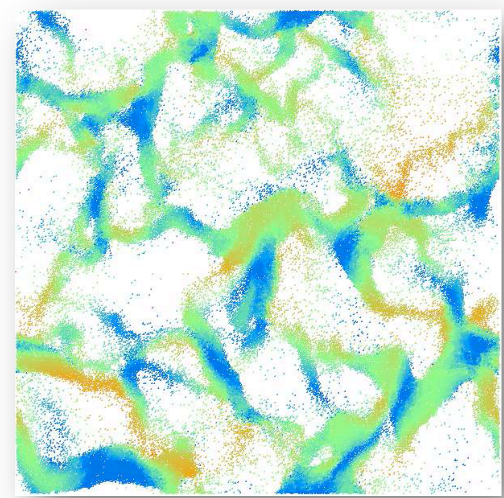
Need mathematical framework to capture the effect of spatial configuration of droplets or particles on physical processes

Outline of talk

Clustering has important implications, but …

- How does one characterize clustering?
  – Identify statistical measure(s)
- Test in example problem: Homogeneously cooling granular gas
- What determines the evolution of the statistical measure(s)?
- Outlook for future study



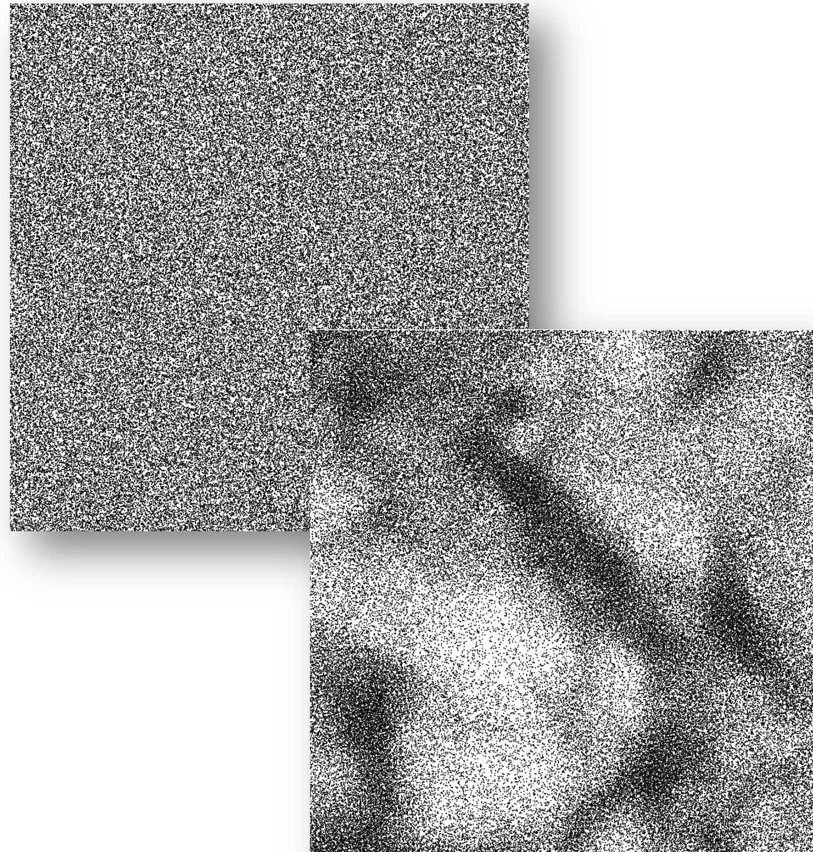


How does one characterize clustering?

Single-point averaged descriptions

- Can number density or volume fraction characterize clustering?

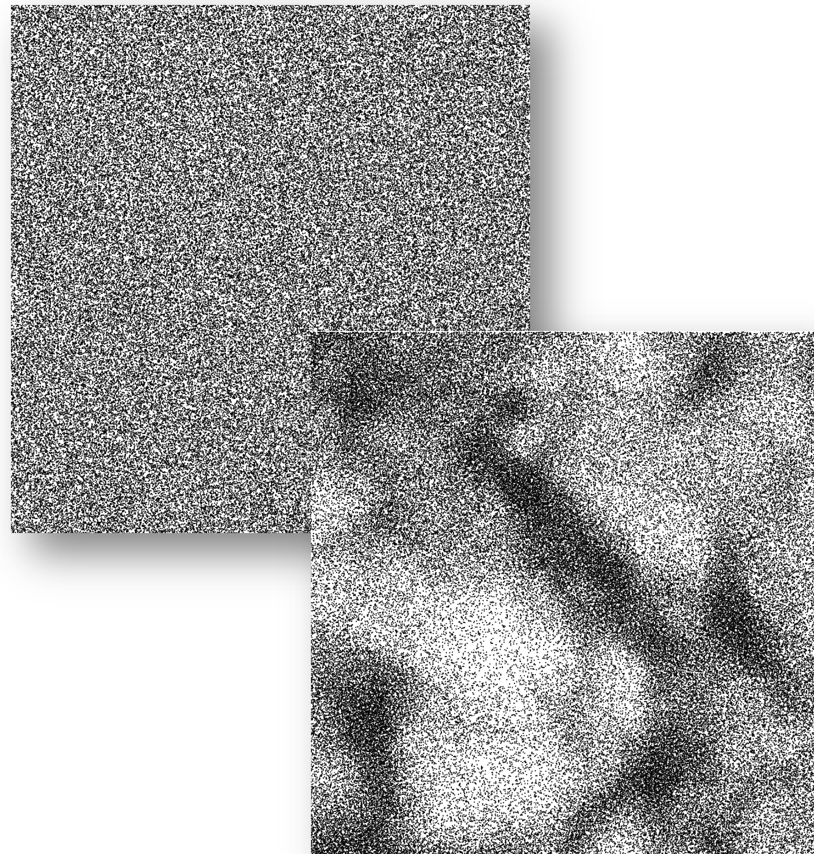
- Can generate two point fields with same homogeneous number density but different spatial configurations (Stoyan and Stoyan, 1994; Stoyan, Kendall and Mecke, 1995), also see example later



✓Single-point statistics **insufficient**

How does one characterize clustering?

Two-point descriptions



➢Popular two-point statistic: radial distribution function g(r)

➢Does radial distribution function characterize clustering?

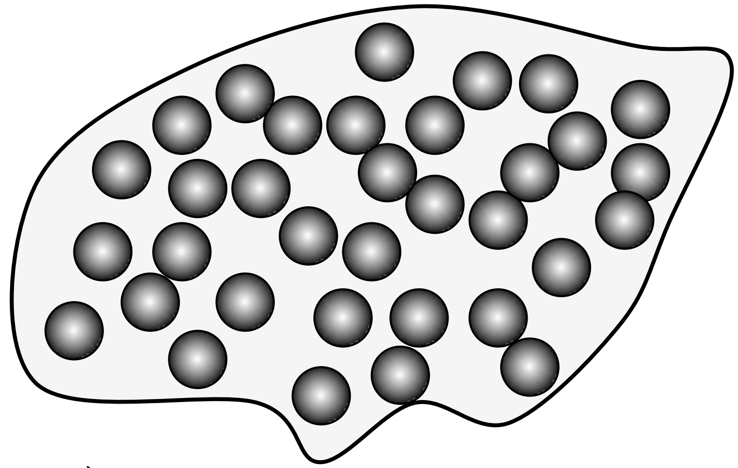
➢YES! Even in systems with same homogeneous number density, g(r) can distinguish spatial configuration of dispersed elements (see later)

✓ Need to understand quantities that determine evolution of g(r)

Single-point distribution function

- Single-point distribution function

$$f(\mathbf{x}, \mathbf{v}, t)$$



gives probable number of particles in

$$(\mathbf{x}, \mathbf{x} + d\mathbf{x})(\mathbf{v}, \mathbf{v} + d\mathbf{v})$$

- Can associate a number density $n(\mathbf{x}, t)$

$$n(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{v}, t)\ d\mathbf{v}$$

- Mean number associated with a certain volume

$$\langle N \rangle (V_M) = \int_{V_M} n(\mathbf{x}, t) d\mathbf{x}$$

Two-point distribution function

Two-point distribution function

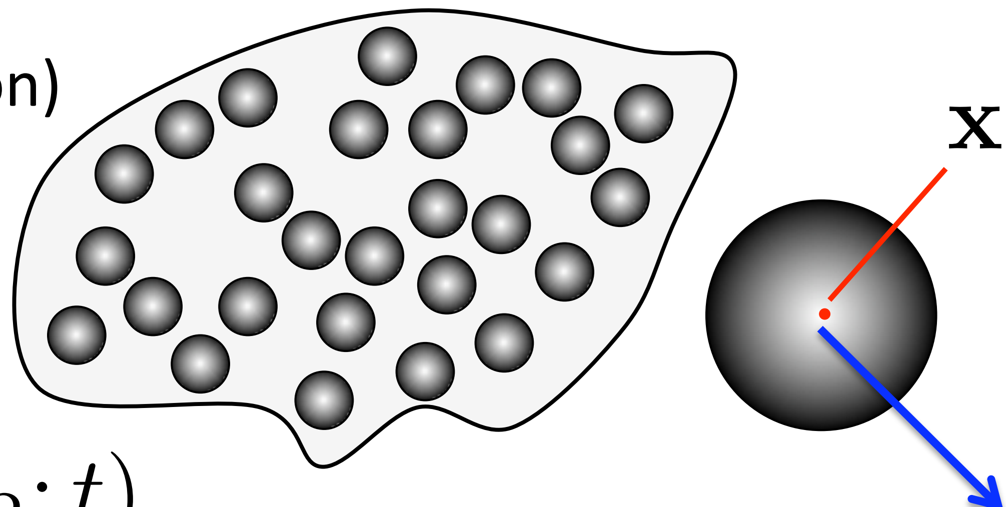
$$f^{(2)}(\mathbf{x}_1, \mathbf{v}_1, \mathbf{x}_2, \mathbf{v}_2, t)$$

- Determines collisions (cf. collisional integral in Boltzmann-Enskog equation)

(Slight change in notation)

Marked second-order density

$$\rho_m^{(2)}(\mathbf{x}_1, \mathbf{v}_1, \mathbf{x}_2, \mathbf{v}_2; t)$$



Particles can have **"marks"** such as **Velocity, Temperature,** etc.

(Stoyan and Stoyan, 1994; Stoyan, Kendall and Mecke, 1995)

Two-point distribution function

$$\rho_m^{(2)}(\mathbf{x}_1, \mathbf{v}_1, \mathbf{x}_2, \mathbf{v}_2) = \underbrace{\rho^{(2)}(\mathbf{x}_1, \mathbf{x}_2)}_{\text{Second-order density}} g_2^c(\mathbf{v}_1, \mathbf{v}_2 | \mathbf{x}_1, \mathbf{x}_2)$$

Second-order density

$$\rho^{(2)}(\mathbf{x}_1, \mathbf{x}_2) = n(\mathbf{x}_1) n(\mathbf{x}_2) g(\mathbf{x}_1, \mathbf{x}_2)$$

$$= n^2 g(\mathbf{r})$$ assuming spatial homogeneity

$$\rho_m^{(2)}(\mathbf{x}_1, \mathbf{v}_1, \mathbf{x}_2, \mathbf{x}_2) = n^2 g(\mathbf{r}) g_2^c(\mathbf{W}, \mathbf{w} | \mathbf{r})$$

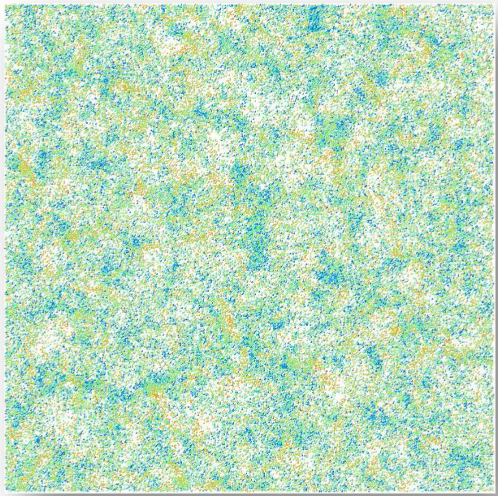
where
$$\mathbf{W} = \mathbf{v}_1 + \mathbf{v}_2$$
$$\mathbf{w} = \mathbf{v}_1 - \mathbf{v}_2$$

Upon further simplification

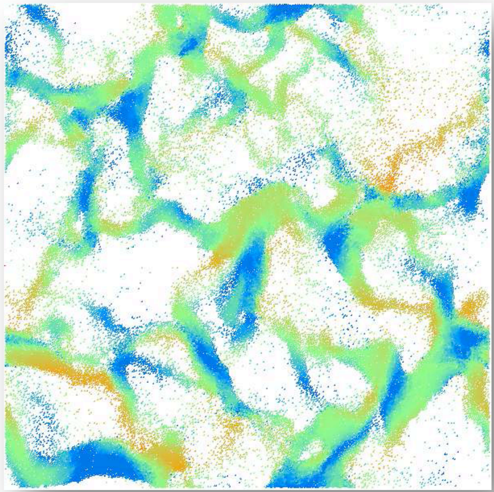
$$\rho^{(2)}(\mathbf{x}_1, \mathbf{x}_2) = n^2 g(r)$$ assuming isotropy

Outline of talk

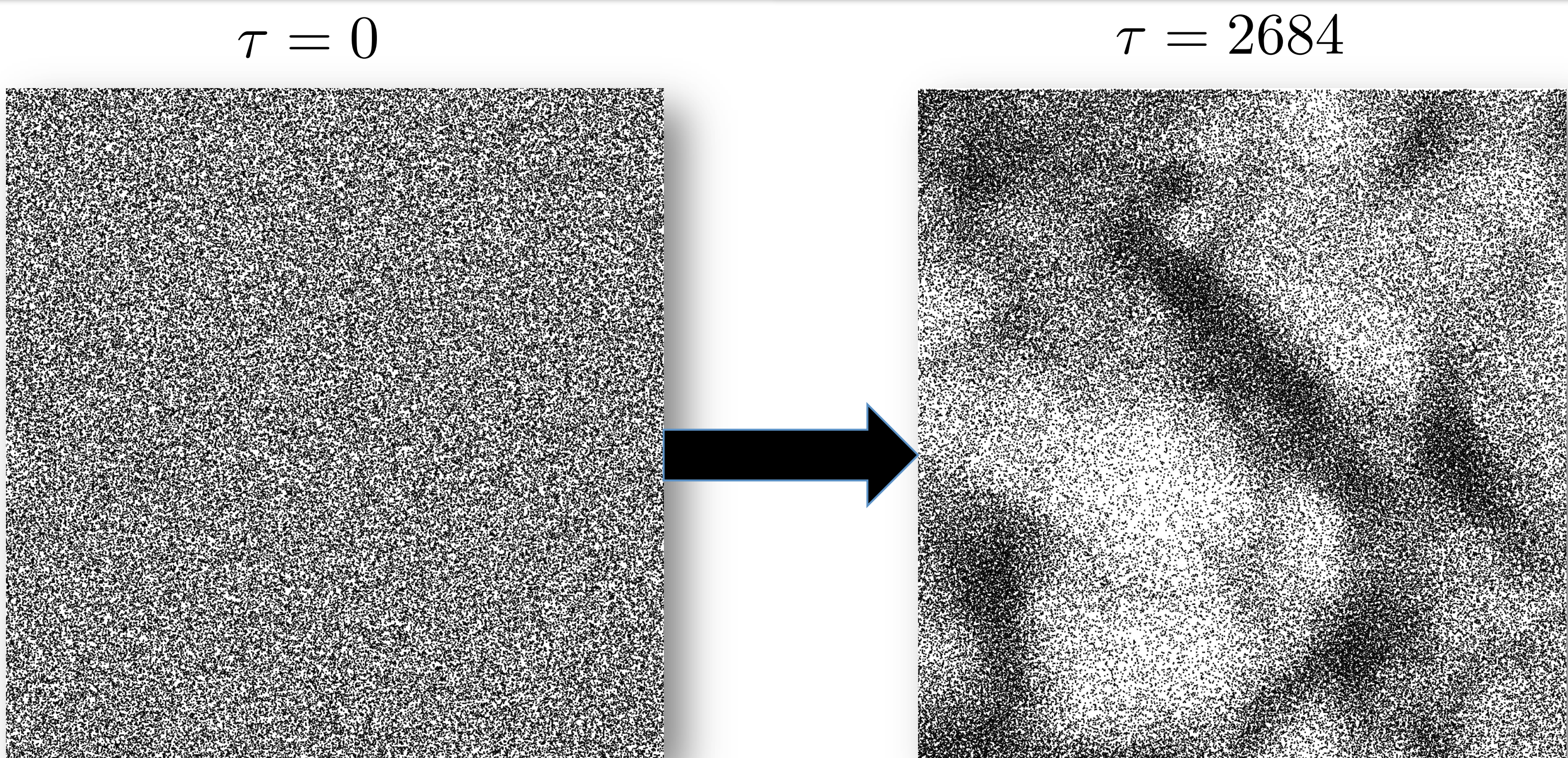
Clustering has important implications, but …



- How does one characterize clustering?
  - – Identify statistical measure(s)
- Test in example problem: Homogeneously cooling granular gas
- What determines the evolution of the statistical measure(s)?
- Outlook for future study



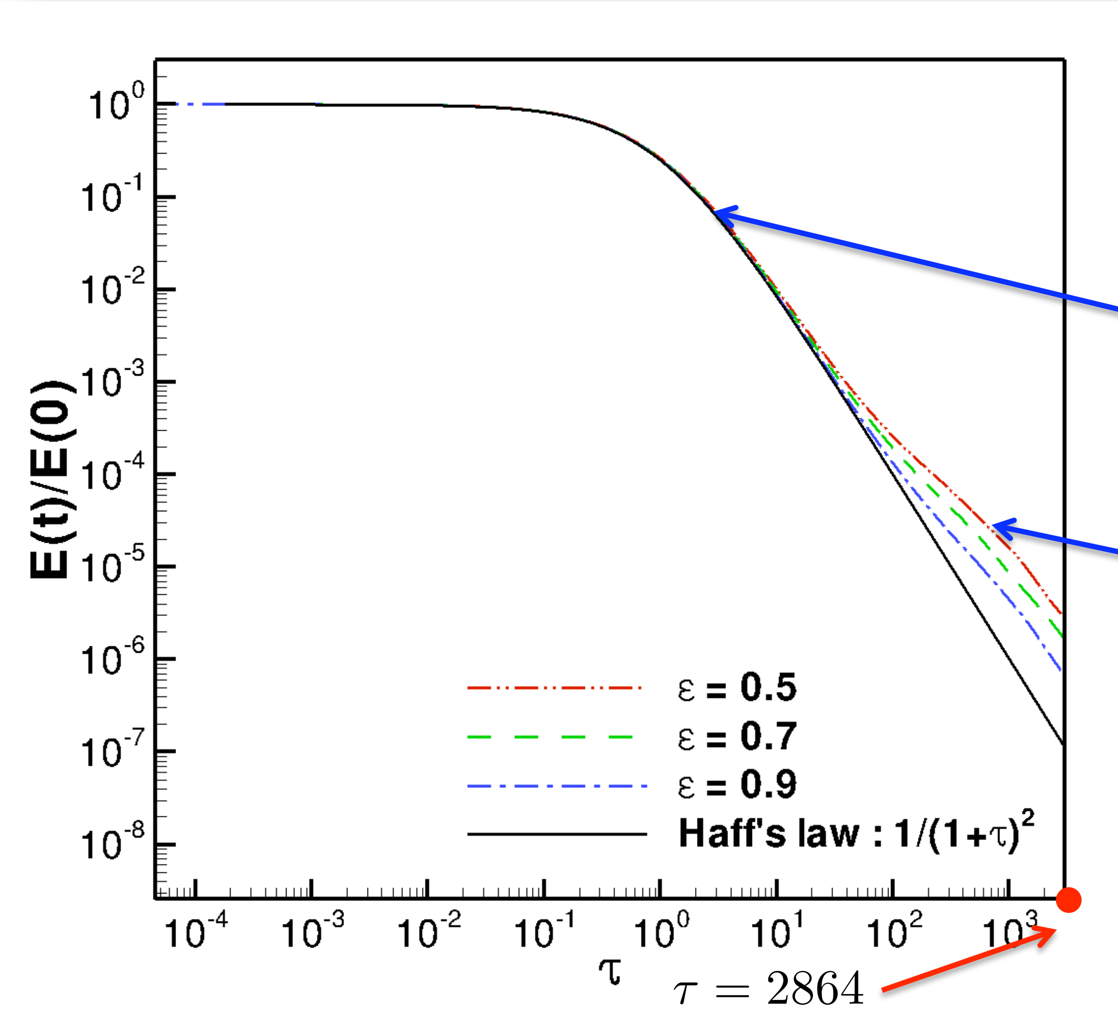
Example: Homogeneously cooling granular gas



- Volume fraction: ~0.08
- L/d : ~ 100
- N = 150000

- Hard sphere collisions
- Event-driven algorithm
- Restitution coefficient: 0.5, 0.7, 0.9

HCGG: Evolution of translational kinetic energy



Granular gas exhibits

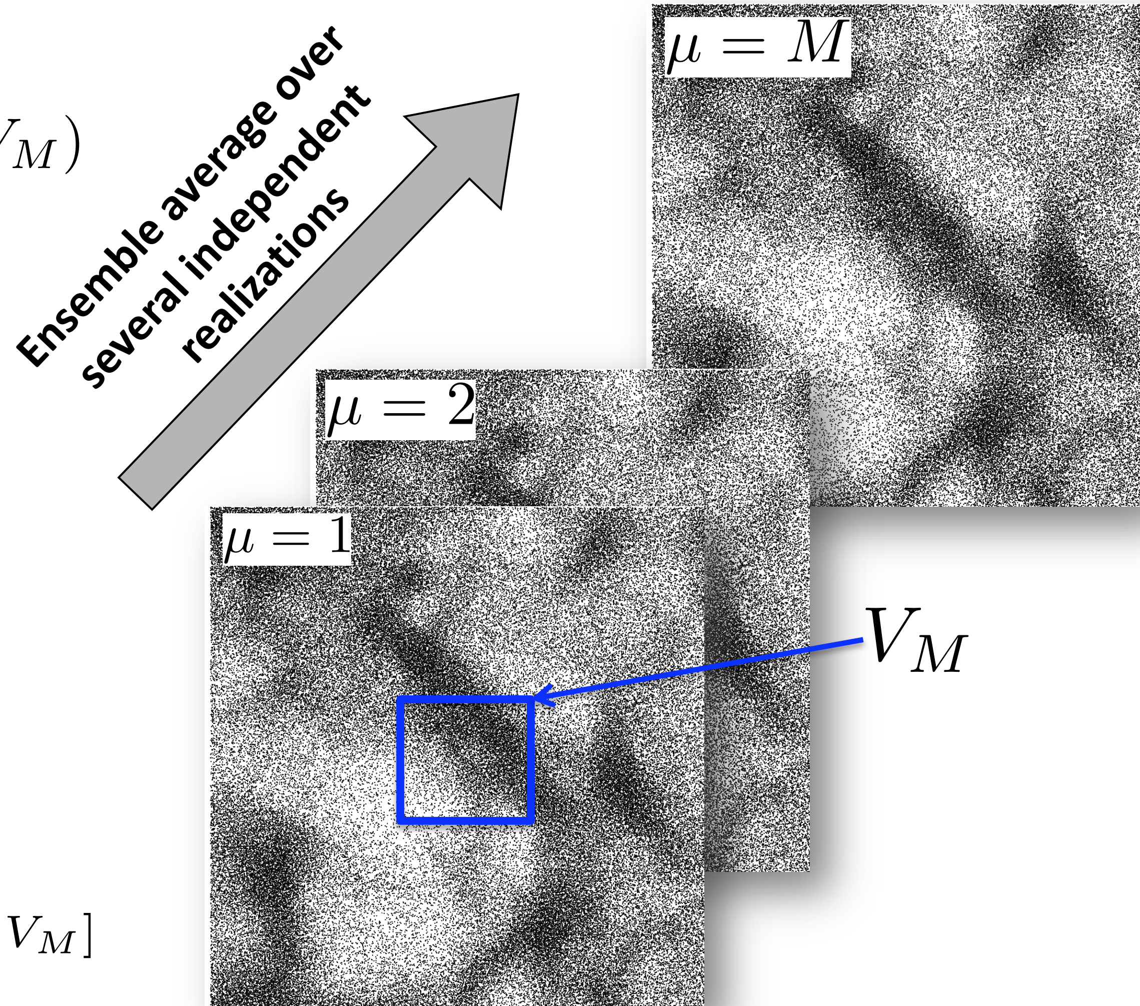
- Homogeneous cooling regime
- Clustering regime

HCGG: Mean number vs measurement volume

$$\langle N(V_M)\rangle_E = \frac{1}{M}\sum_{\mu=1}^{M} N(V_M)$$

M – Number of independent realizations

$$N(V_M) = \sum_{i=1}^{N} 1_{[\mathbf{X}^{(i)} \in V_M]}$$



HCGG: Mean number vs measurement volume

Mean number

$$\langle N \rangle (V_M) = \int_{V_M} n(\mathbf{x}, t) d\mathbf{x}$$

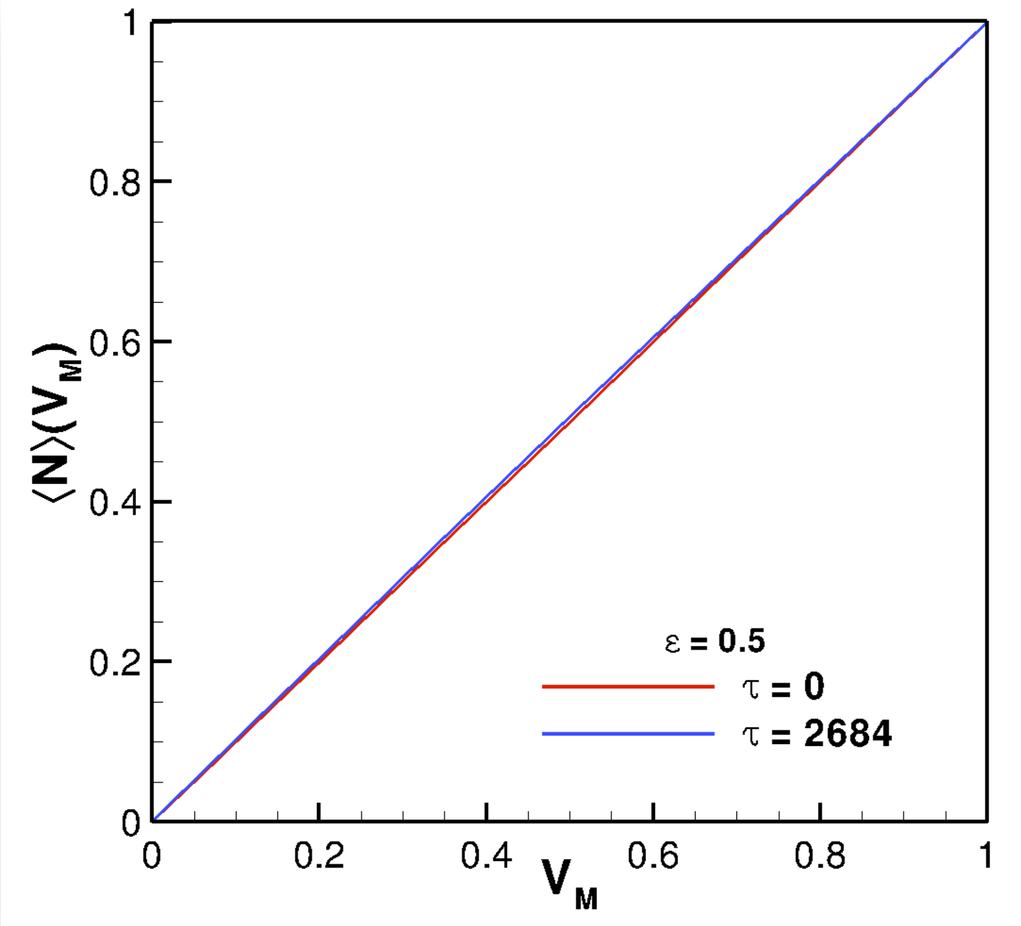
If number density is homogeneous

$$\langle N \rangle (V_M) = n \int_{V_M} d\mathbf{x}$$

$$\langle N \rangle (V_M) = n V_M$$

Mean number is linear in V_M

Number density is homogeneous !

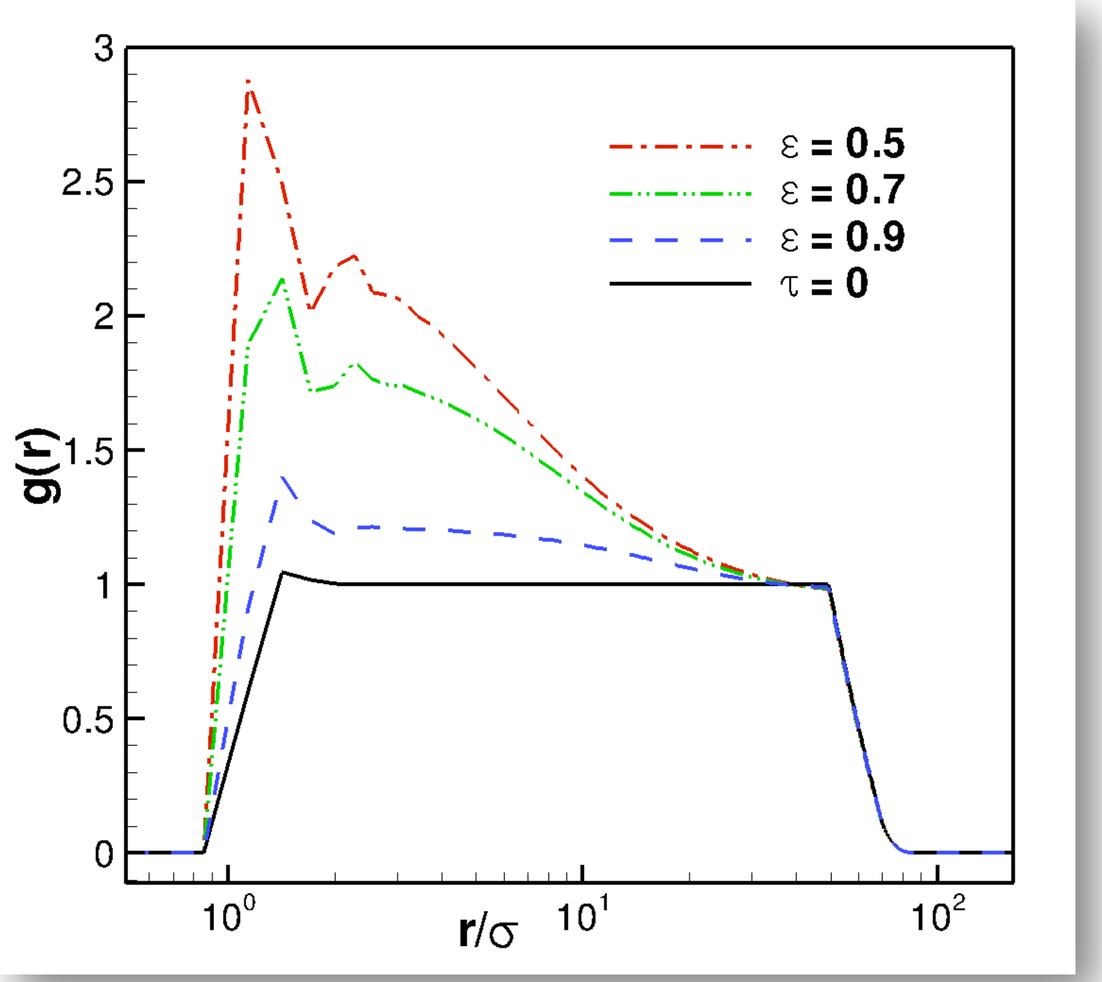


HCGG: Radial distribution function

- Increasing restitution increases g(r) at contact

- HCGG: an excellent example for homogeneous point field with clustering

- Spatial point processes provide more measures than just g(r)*



*Stoyan and Stoyan, 1994; Stoyan, Kendall and Mecke, 1995

HCGG: Fluctuations in number

Second Factorial Moment

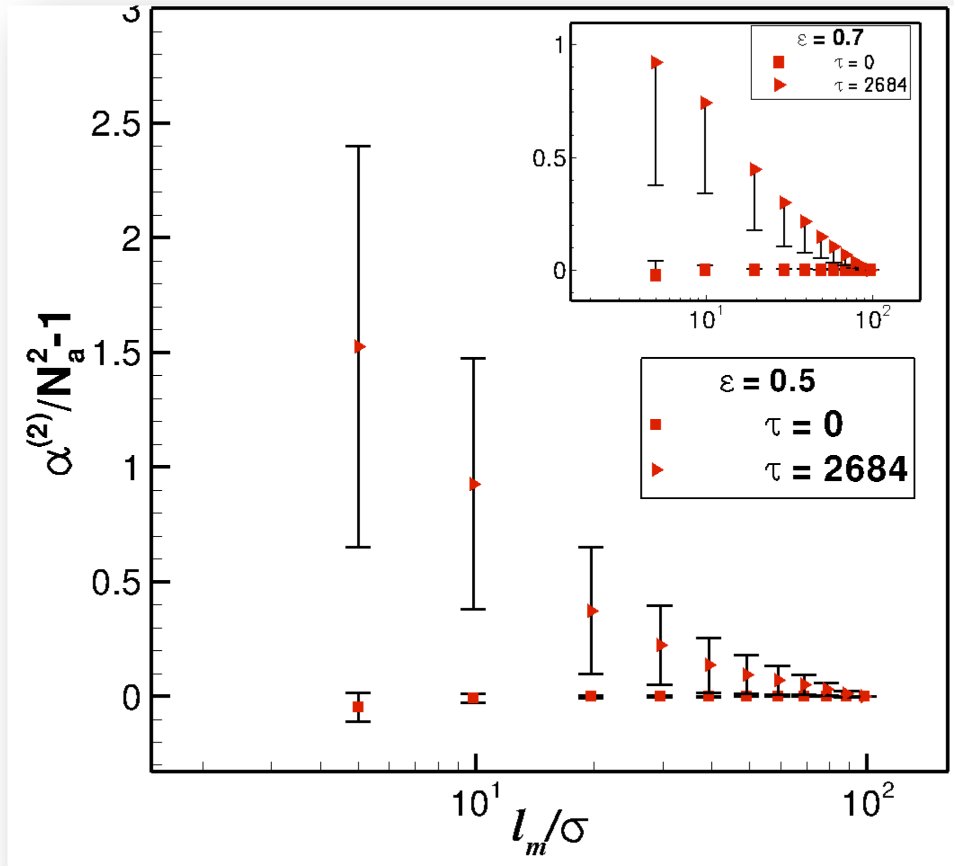
$$\alpha^{(2)}(\mathcal{B}\times\mathcal{B}) = \langle N(N-1)\rangle$$

$$= \int_{\mathcal{B}}\int_{\mathcal{B}} \rho^{(2)}(\mathbf{x}_1,\mathbf{x}_2)\, d\mathbf{x}_1\, d\mathbf{x}_2$$

$$= \langle N^2(\mathcal{B}\times\mathcal{B})\rangle - nV(\mathcal{B})$$

Scaled Second Factorial Moment

$$SSFM = \frac{\alpha^{(2)}(\mathcal{B}\times\mathcal{B})}{\langle N(\mathcal{B})\rangle^2}$$



$SSFM - 1$ characterizes clustering

Poisson point field: *SSFM* = 1

Stoyan and Stoyan, 1994; Stoyan, Kendall and Mecke, 1995

Outline of talk

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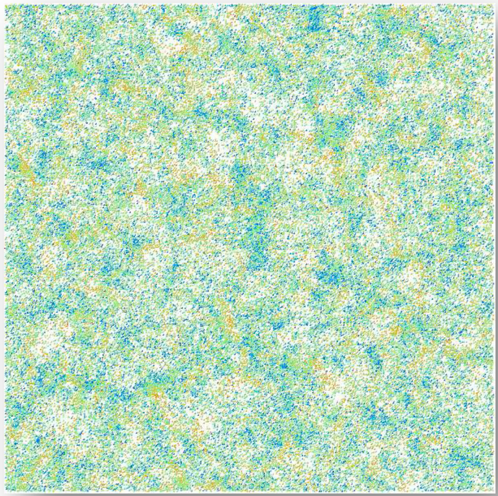
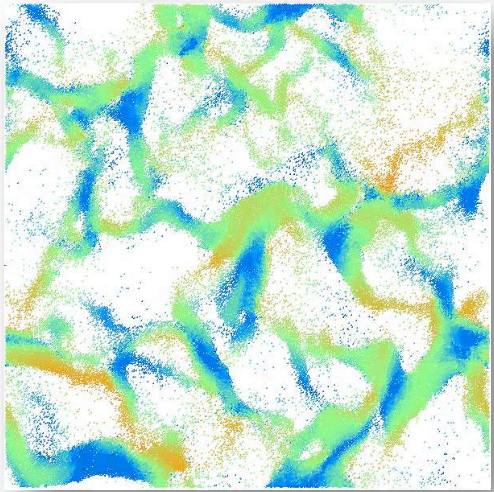
- What determines the evolution of the statistical measure(s)?
- Outlook for future study





Evolution of $\rho_m^{(2)}(\mathbf{r}, \mathbf{w}, t)$

Statistical homogeneity in position and velocity space

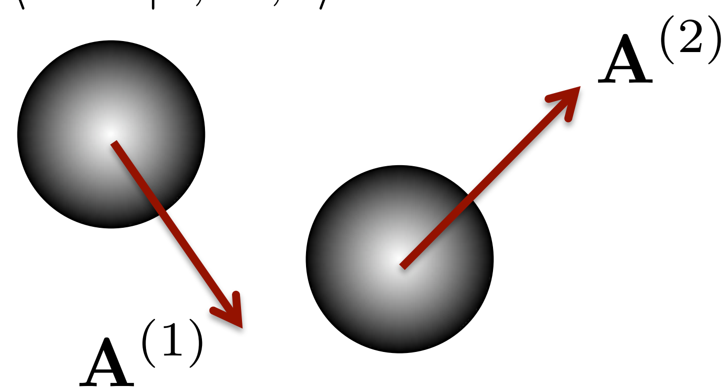
$$\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2 \qquad \mathbf{w} = \mathbf{v}_1 - \mathbf{v}_2$$

Evolution of marked second-order density

$$\frac{\partial}{\partial t}\rho_m^{(2)}(\mathbf{r}, \mathbf{w}, t) + \nabla_{\mathbf{r}} \cdot \left(\mathbf{w}\rho_m^{(2)}\right) + \nabla_{\mathbf{w}} \cdot \left(\langle \triangle \mathbf{A} | \mathbf{r}, \mathbf{w}, t\rangle \rho_m^{(2)}\right) = 0$$

Expected relative acceleration

$$\langle \triangle \mathbf{A} | \mathbf{r}, \mathbf{w}, t\rangle = \langle \mathbf{A}^{(1)} | \mathbf{r}, \mathbf{w}, t\rangle - \langle \mathbf{A}^{(2)} | \mathbf{r}, \mathbf{w}, t\rangle$$



Integrating over $\mathbf{w}$ space

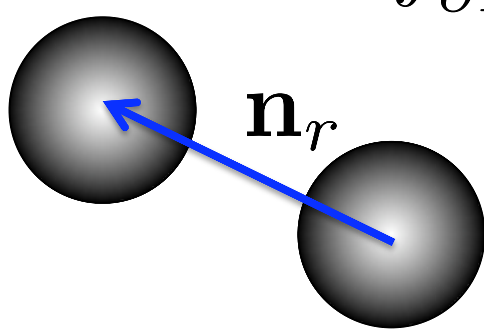
$$\frac{\partial}{\partial t}\rho^{(2)}(\mathbf{r}, t) + \nabla_{\mathbf{r}} \cdot \left(\langle \mathbf{w} | \mathbf{r}, t\rangle \rho^{(2)}\right) = 0$$

Krall and Trivelpiece, Principles of Plasma Physics; Pai and Subramaniam, APS, 2007; Markutsya and Subramaniam, 2010

Evolution of $\alpha^{(2)}$

Transforming $(\mathbf{x}_1, \mathbf{x}_2)$ to $(\mathbf{R}, \mathbf{r})$ where $\mathbf{R} = \mathbf{x}_1 + \mathbf{x}_2$, $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$

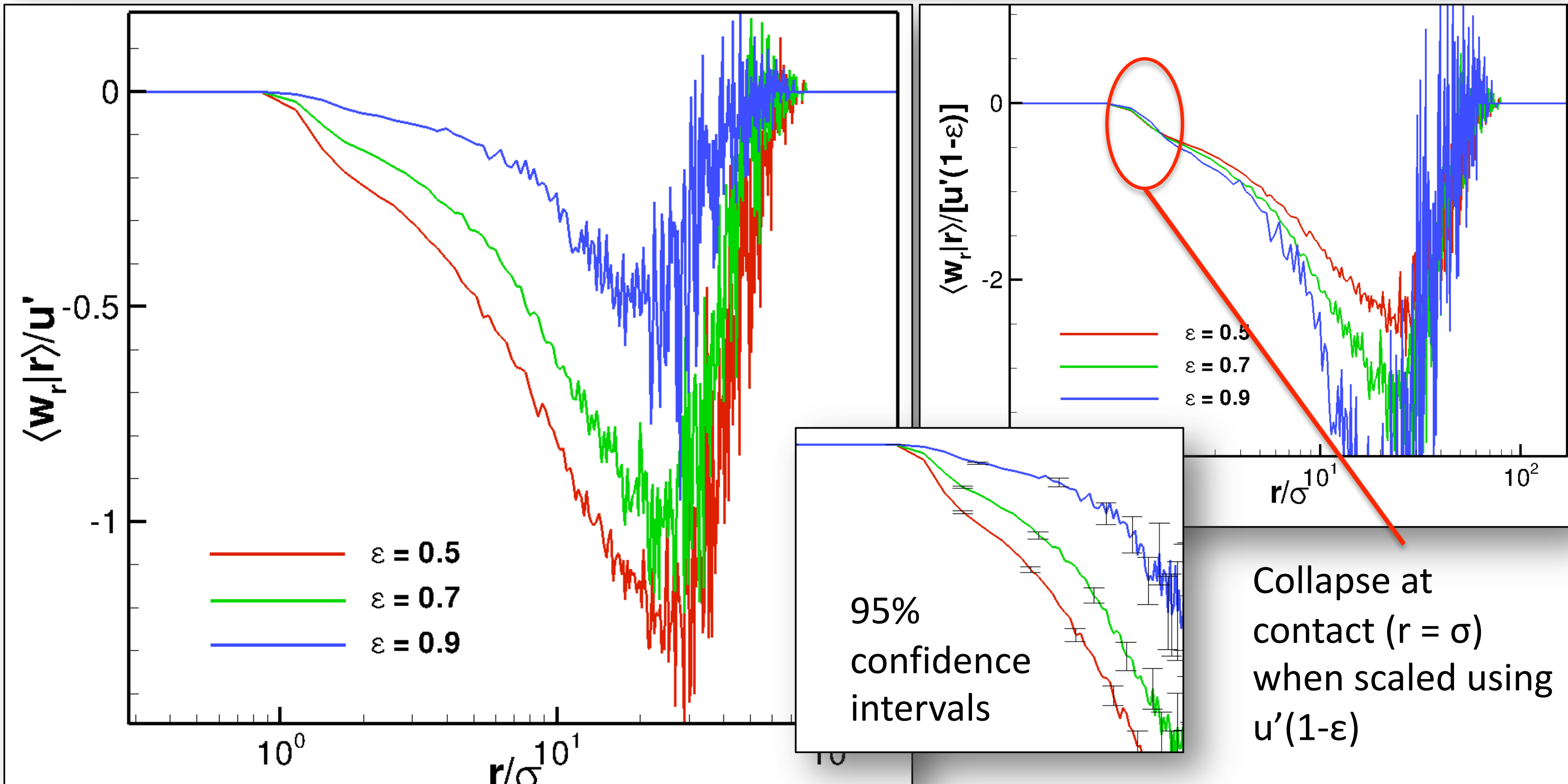
$$\frac{\partial}{\partial t}\alpha^{(2)} = -V(\mathcal{B}_R)\int_{\partial B_r} \rho^{(2)}(\mathbf{r}, t)\langle \mathbf{w} | \mathbf{r}, t\rangle \cdot \mathbf{n}_r \, d\mathbf{r}$$



Conditional relative velocity

✓A negative component of conditional relative velocity along line joining centers indicates a tendency to cluster

HCGG: Conditional relative velocity $\langle w_r | r \rangle$



✓ Negative component of conditional relative velocity (along line joining centers) → tendency to cluster

Outline of talk

Clustering has important implications, but …

- How does one characterize clustering?
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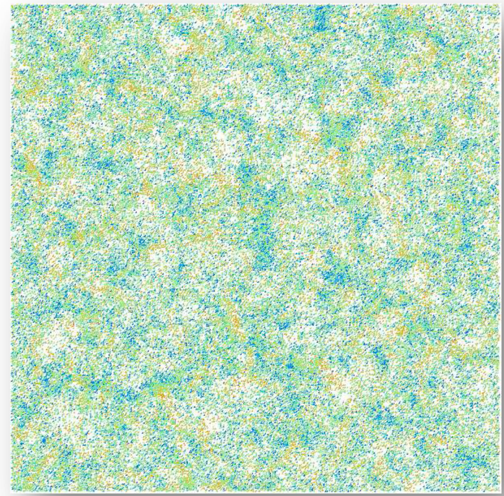
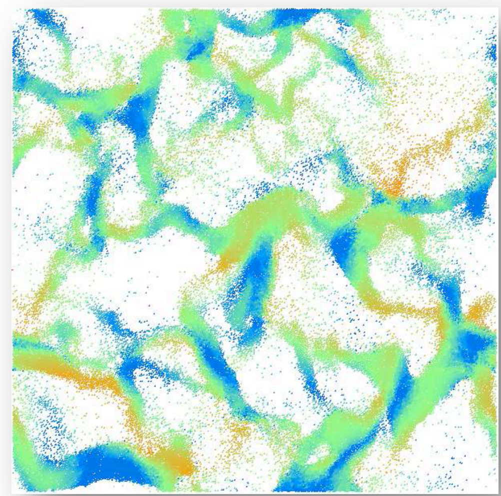
- What determines the evolution of the statistical measure(s)?
- Example problem: Homogeneously cooling granular gas
- Conclusions/ Outlook for future study





Characterization of clustering

✓ Under homogeneous conditions, number density cannot characterize clustering

✓ Under inhomogeneous conditions, number density is insufficient to characterize clustering

- ➢ Spatial structure in an inhomogeneous point field can arise due to:

∇n : gradients in the number density

$\rho^{(2)}, \langle N^2 \rangle, \; g(r)$: second-order effects

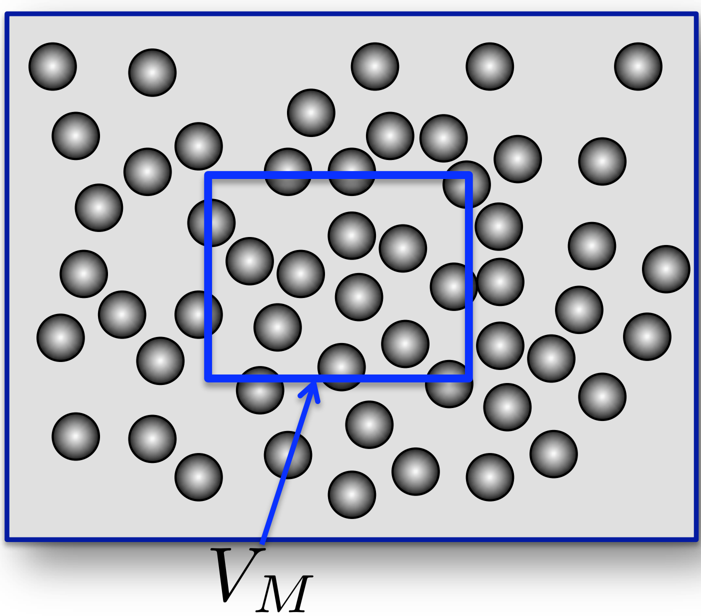
→ Need to distinguish the two contributions to accurately capture effect of spatial structure on interphase transfer processes

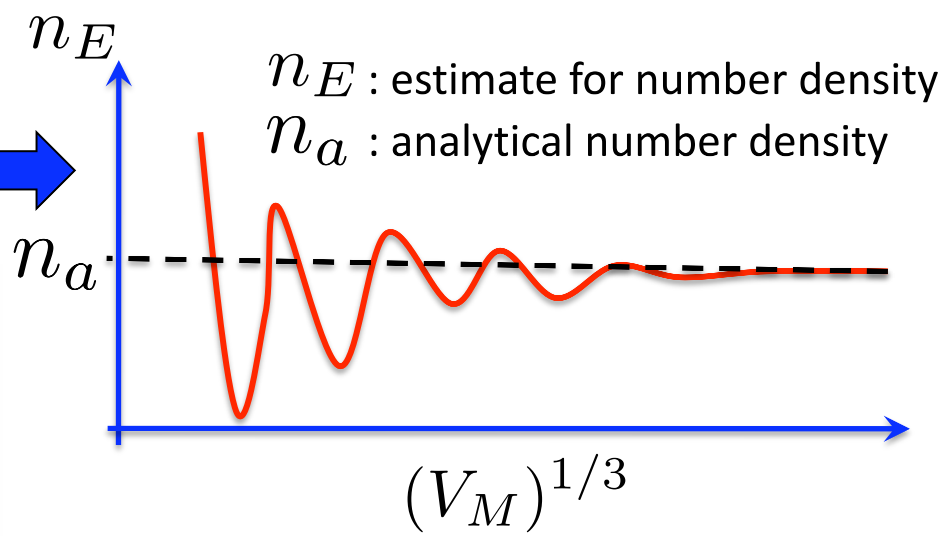
Estimate for number density

✓ Estimating number density/ volume fraction from a single snapshot may lead to erroneous results

→ A homogeneous number density field can be misconstrued to be inhomogeneous

If single snapshot is used to estimate number density…





➢ Reminiscent of dependence of measured thermodynamic density on microscopic length scales (ref: Batchelor); Implications in LES of gas-solid flows?

➢ No separation of scales → Principal issue in description of multiphase flows

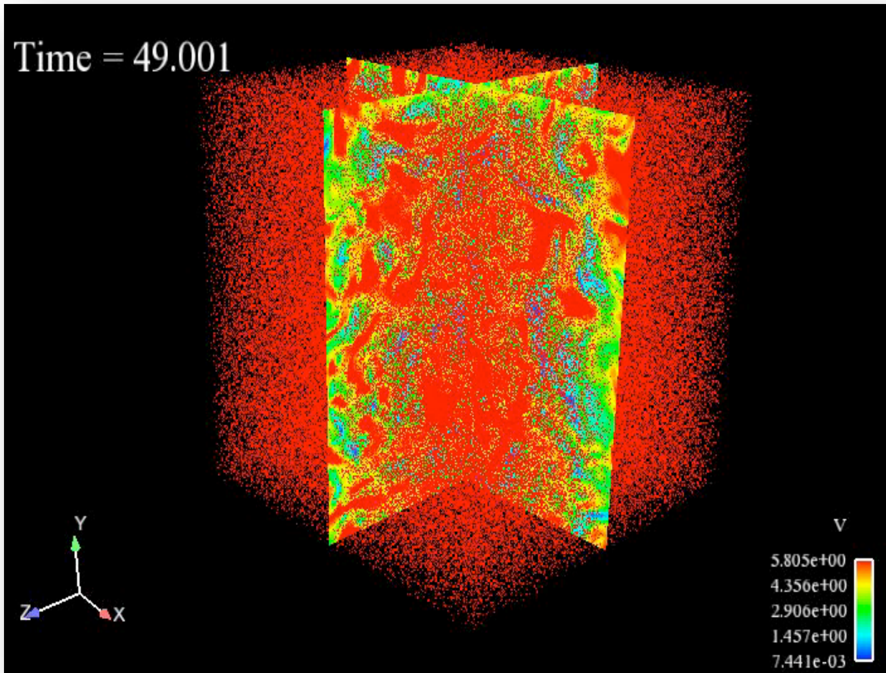
Conditional relative velocity $\langle w_r | r \rangle$

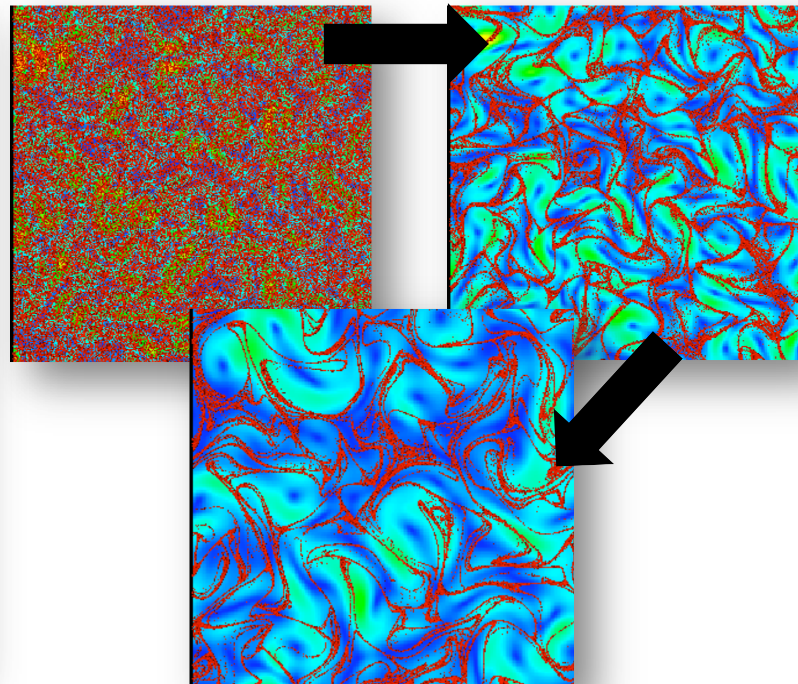
✓ Negative conditional relative velocity indicates tendency to cluster: key quantity to capture clustering (at level of second-order statistics)

✓ BE model for collisional integral employs a decomposition of the form $f^{(2)}(\mathbf{v}_1, \mathbf{v}_2, \mathbf{x}_1, \mathbf{x}_2) \propto g(r) f(\mathbf{v}_1) f(\mathbf{v}_2)$

✓Assumption of molecular chaos? Granular gas develops long range correlations in velocity as it cools; Poschel et al. (2002): modified model for $f^{(2)}$; Implications of model form on $\langle w_r | r \rangle$?

Dilute particle-laden turbulent flows





- Homogeneous particle-laden turbulent flow; decaying turbulence

✓Exhibits preferential concentration; dilute flow → collisions negligible; “clustering” due to particle motion in underlying gas phase. What is the signature of $\langle w_r | r \rangle$ in this system?

[redacted]