Quantifying the Uncertainty of Kinetic Theory Predictions of Clustering

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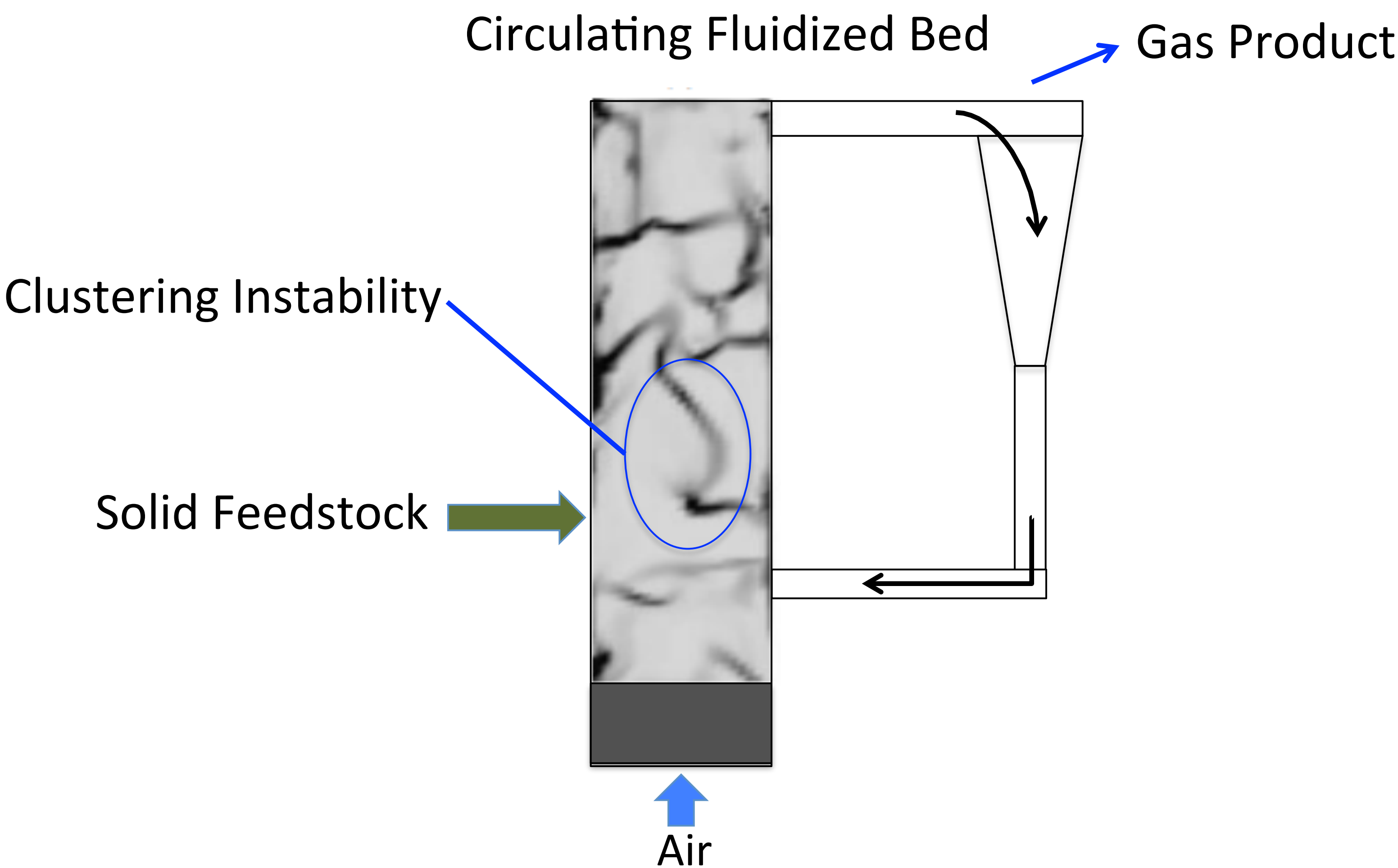
Motivation: Instabilities in Particulate Flows

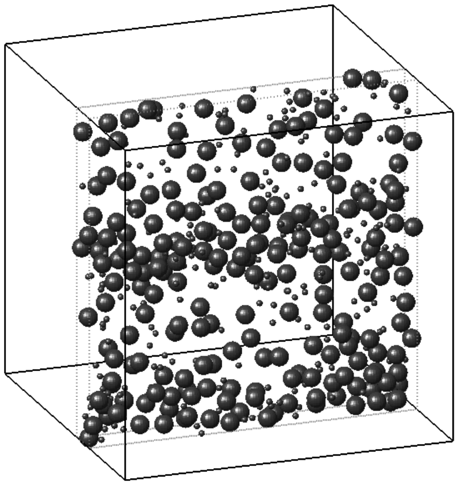


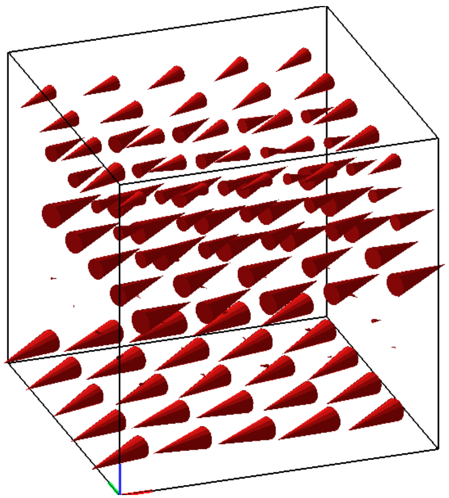
CFD simulation from Agrawal *et al. J. Fluid Mech.* (2001)

Overall Goal

(i) Assess kinetic-theory-based continuum models via ability to quantitatively predict instabilities

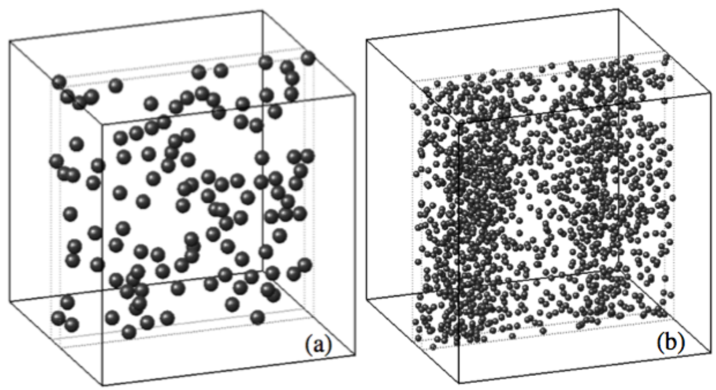
(ii) Understand relative importance of clustering mechanisms



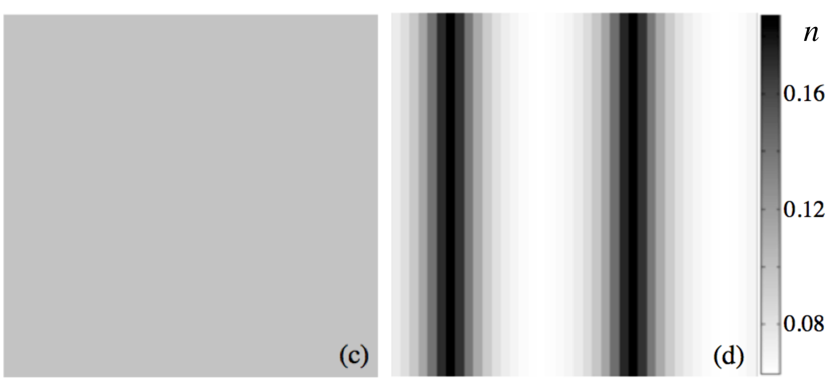


Approach

- Discrete particle simulations (free of kinetic theory)
  - Molecular dynamics (MD)
  - Direct numerical simulation (DNS)

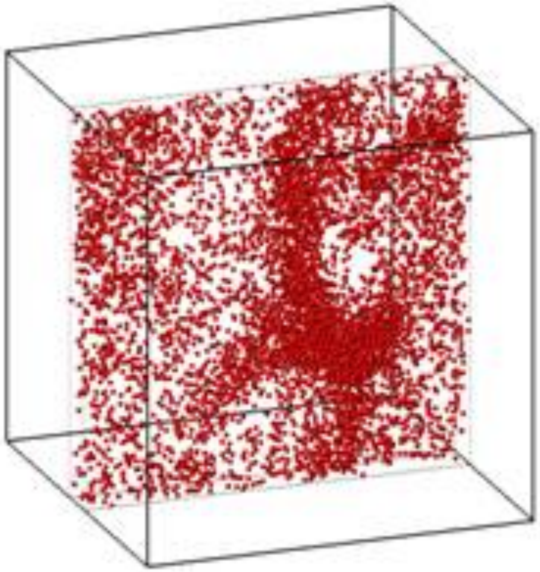


- Continuum model (based on kinetic theory)
  - Linear stability analysis
  - Transient continuum simulations



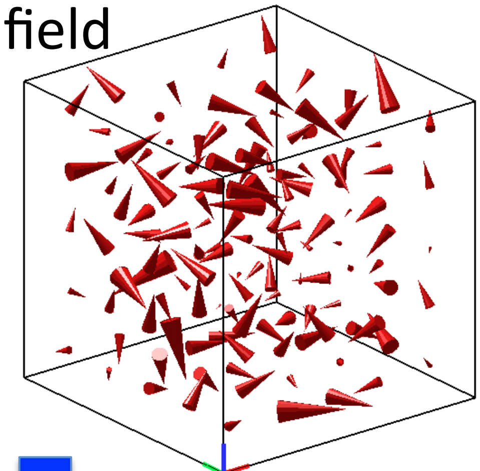
Homogeneous cooling system (HCS)

- System properties
  - No external forces
  - Periodic boundaries in all 3 directions
  - No gradients in the hydrodynamic variables
- Particle properties
  - Constant coefficient of restitution (e)
  - Spherical particles of concentration ϕ
  - Monodisperse, frictionless



Background

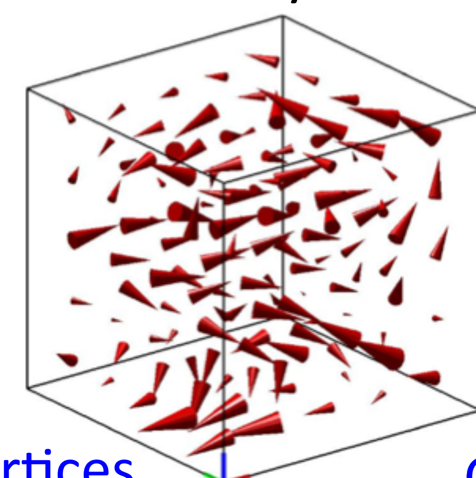
Velocity field



- Dissipative collisions
- Sufficiently large system domain

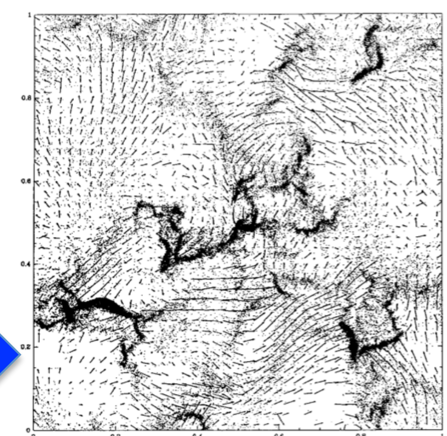
Molecular dynamics (MD) simulations of the HCS

Velocity field



Vortices

Particle locations



Clusters

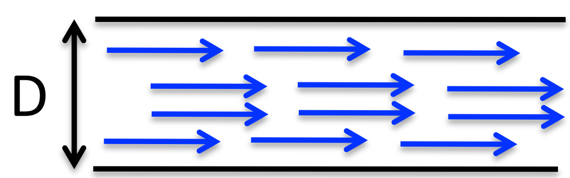
Goldhirsch *et al*., *J. Sci. Comput*. (1993)

Onset of Instability: A Dimensionless Length Scale

Fluid Flow

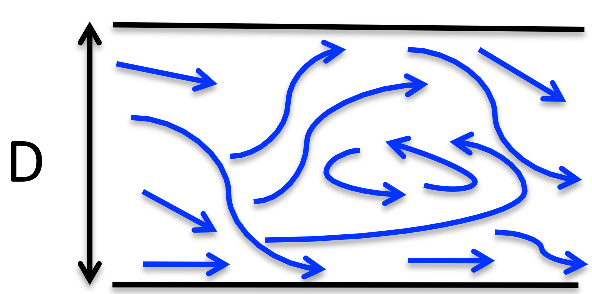
$$\mathrm{Re} = \frac{\rho v D}{\mu}$$

Stable (laminar)



$\mathrm{Re} < \mathrm{Re}_C$

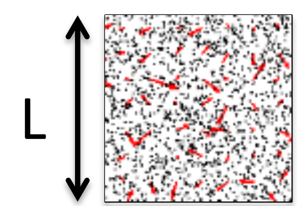
Unstable (turbulent)



$\mathrm{Re} > \mathrm{Re}_C$

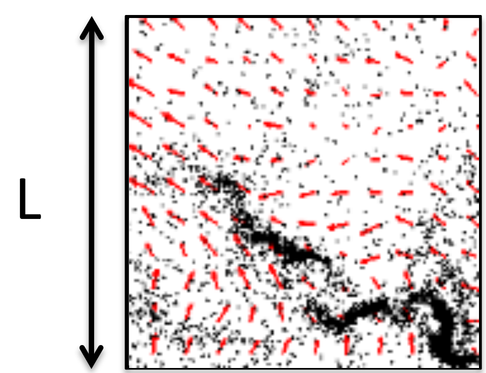
Granular Flow

$$\frac{L}{d} \equiv \frac{\text{Linear domain size}}{\text{particle diameter}}$$



Stable

$L/d < (L/d)_C$

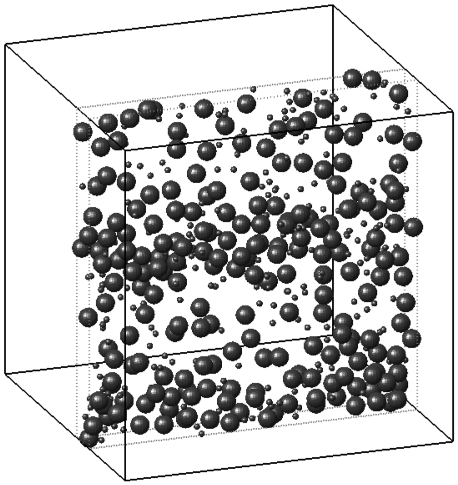


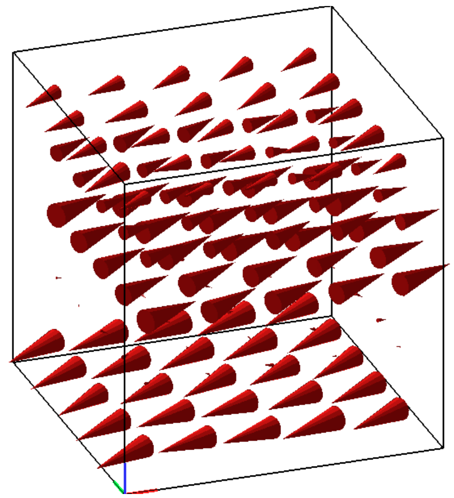
Unstable

$L/d > (L/d)_C$

Overall Goal

(i) Assess kinetic-theory-based continuum models via ability to quantitatively predict instabilities





The continuum model

Mass balance

$$\frac{\partial n}{\partial t} + \underline{u} \cdot \nabla n + n \nabla \cdot \underline{u} = 0$$

(Granular) Pressure tensor

Heat flux

Momentum balance

$$\rho \left[\frac{\partial \underline{u}}{\partial t} + \underline{u} \cdot \nabla \underline{u} \right] = -\nabla \underline{\underline{P}}$$

Cooling rate

Energy balance

$$\frac{\partial T}{\partial t} + \underline{u} \cdot \nabla T = -\frac{2}{3n} \left(\nabla \cdot \underline{q} + \underline{\underline{P}} : \nabla \underline{u} \right) - \zeta T$$

Chapman-Enskog expansion for heat flux

$$\underline{q} = -\kappa \nabla T - \mu \nabla n - \kappa_2 \nabla T^2 - \mu_2 \nabla n^2 + \ldots$$

Thermal conductivity

New coefficient for solids flow

Second-order coef.

Truncate at first order in gradients (Navier-Stokes-order)

Implies small gradients (small Knudsen number)

The continuum model

Mass balance

$$\frac{\partial n}{\partial t} + \underline{u} \cdot \nabla n + n \nabla \cdot \underline{u} = 0$$

Momentum balance

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Energy balance

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(Granular) Pressure tensor

Heat flux

Cooling rate

Truncate at first order in gradients (Navier-Stokes-order)

Implies small gradients (small Knudsen number)

$$\underline{q} = -\kappa \nabla T - \mu \nabla n$$

$$\zeta = \zeta_0 + \zeta \nabla \cdot \underline{u}$$

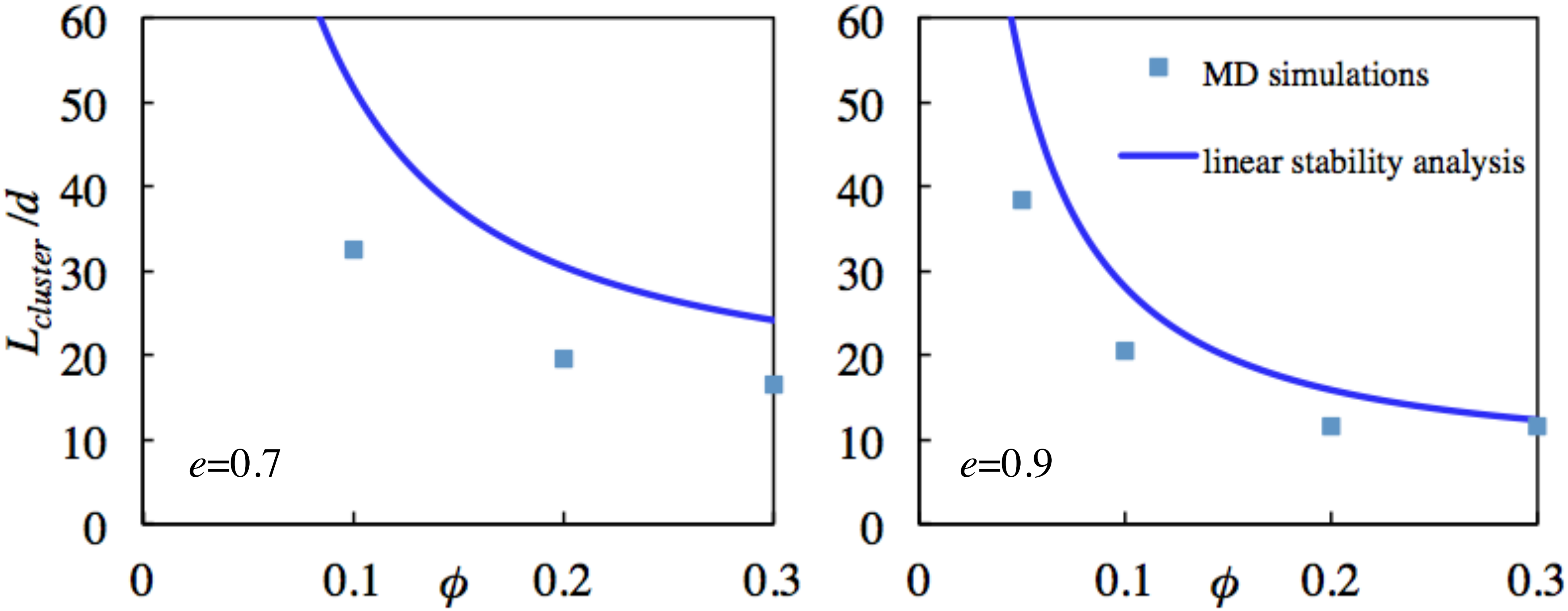
$$P_{ij} = p\delta_{ij} - \eta \left(\nabla_j u_i + \nabla_i u_j - \frac{2}{3} \delta_{ij} \nabla \cdot \underline{u} \right) - \gamma \delta_{ij} \nabla \cdot \underline{u}$$

Hydrostatic pressure

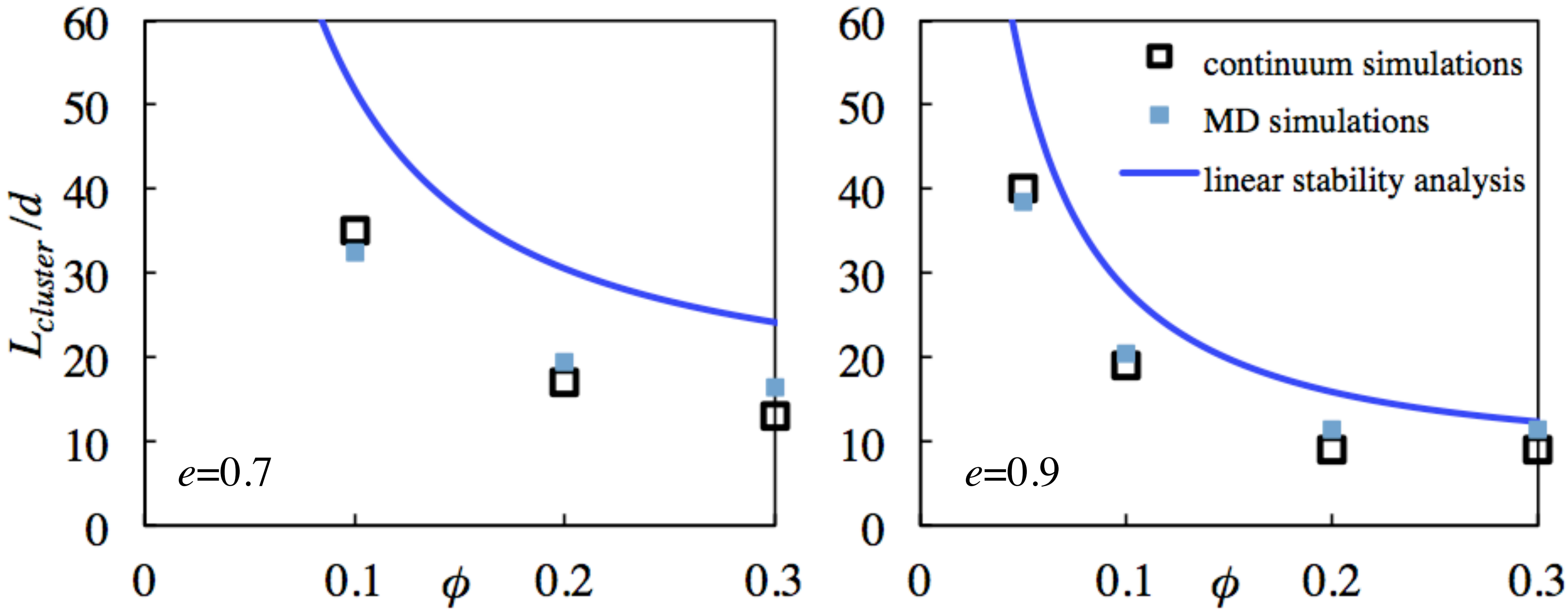
Shear viscosity

Bulk viscosity

High-gradient flows



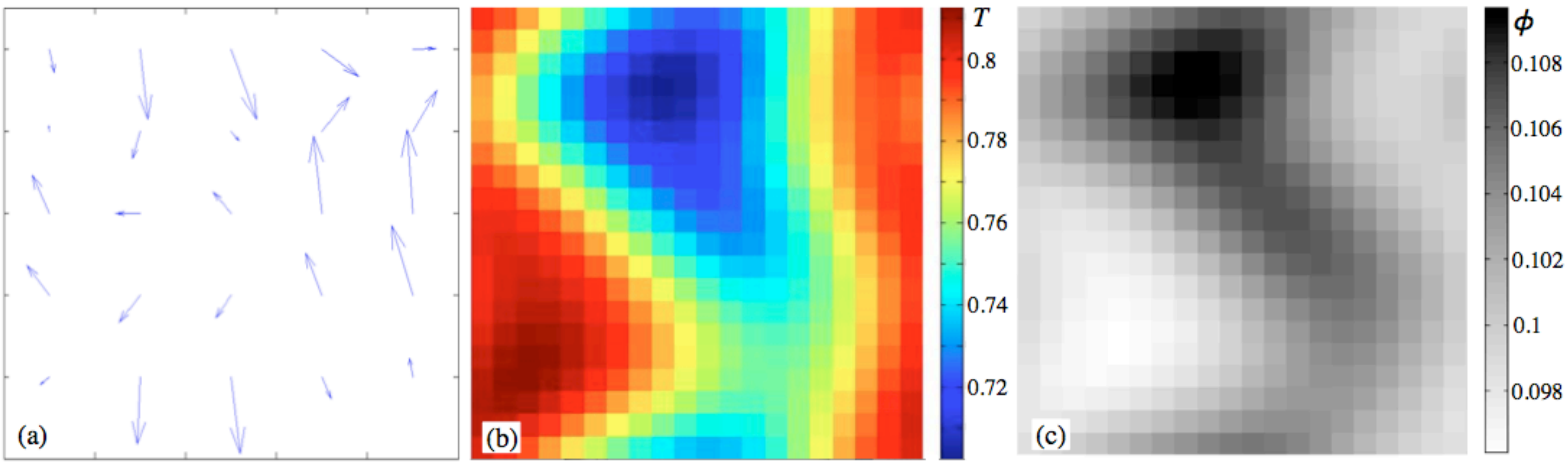
High-gradient flows



Excellent agreement when nonlinearity is considered

High-gradient flows

Coarse-grained hydrodynamic fields at the time of cluster onset



Velocity Granular temperature Concentration

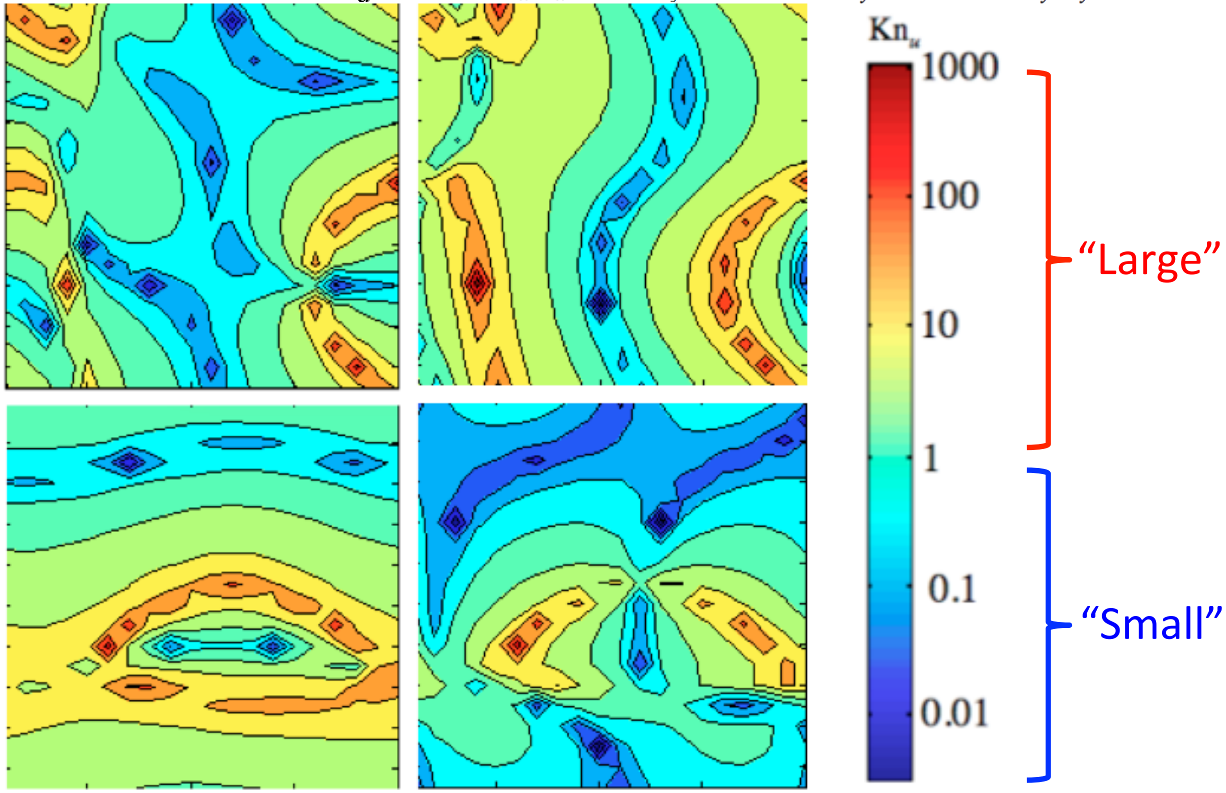
Qualitative evidence of velocity gradients

High-gradient flows

Measure of gradients in **velocity field** at the time of cluster onset

Velocity Knudsen number $\mathrm{Kn_u}$ for (a) $\partial_x U_x$, (b) $\partial_y U_x$, (c) $\partial_x U_y$, and (d) $\partial_y U_y$

$$Kn_u = \frac{MFP}{L_{gradient}}$$



High-gradient flows

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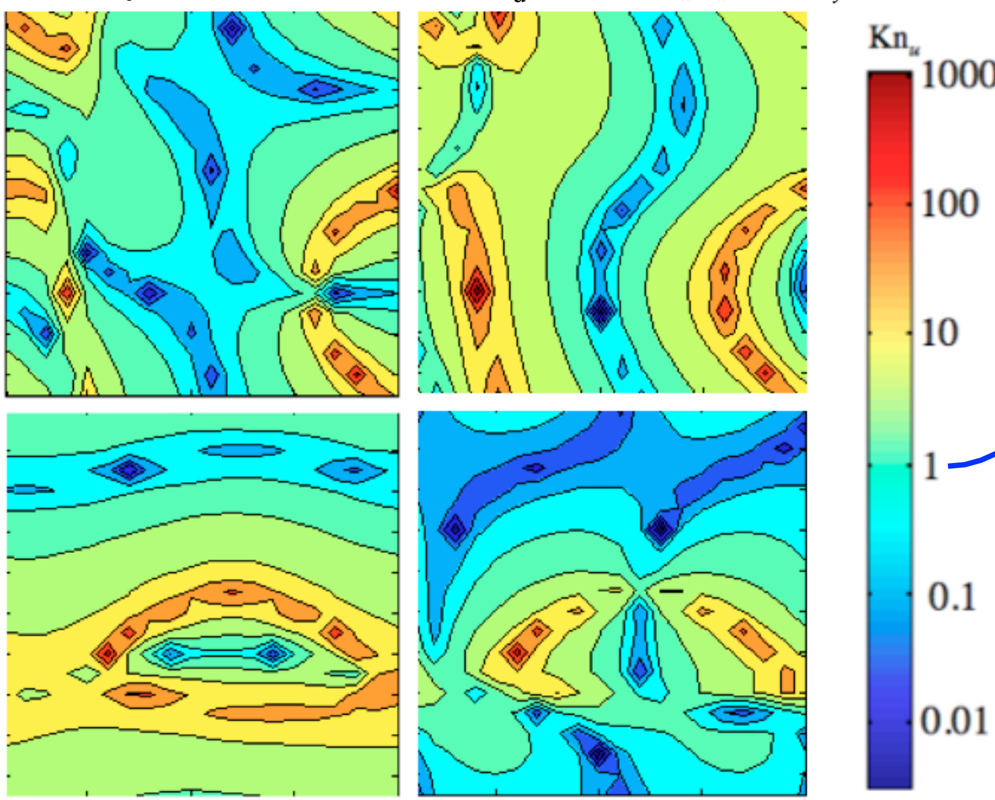


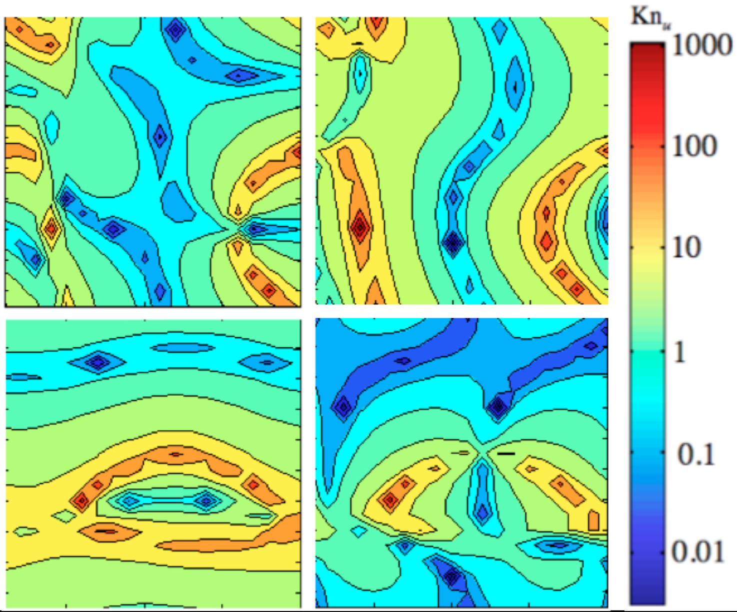
First-order truncation implies $\mathrm{Kn} < \mathrm{Kn}^2$ however $\mathrm{Kn_u} > O(1)$

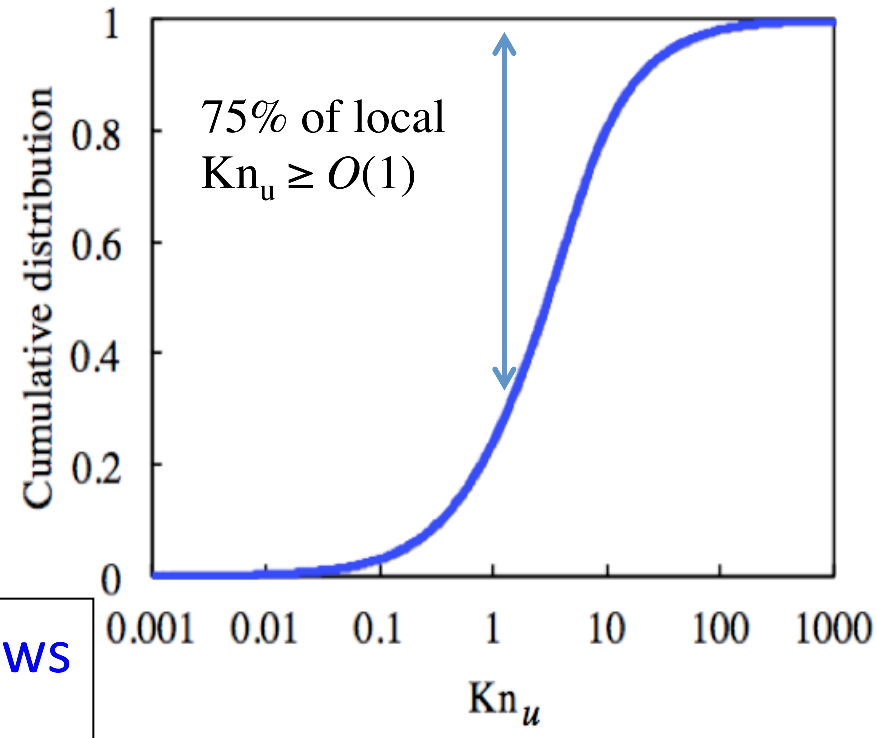
$$\underline{q} = -\kappa\nabla T - \mu\nabla n - \kappa_2\nabla T^2 - \mu_2\nabla n^2 + \ldots$$

High-gradient flows

Measure of gradients in **velocity field** at the time of cluster onset

Velocity Knudsen number Kn_u for (a) $\partial_x U_x$, (b) $\partial_y U_x$, (c) $\partial_x U_y$, and (d) $\partial_y U_y$

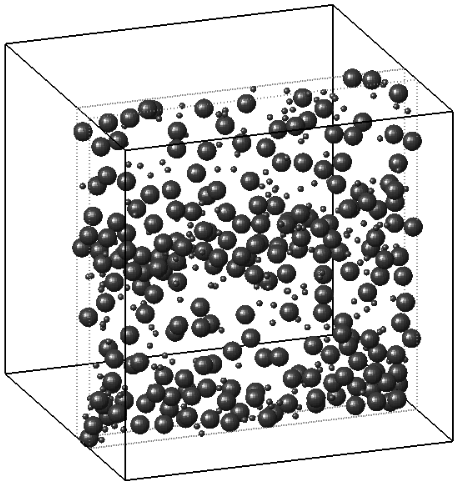


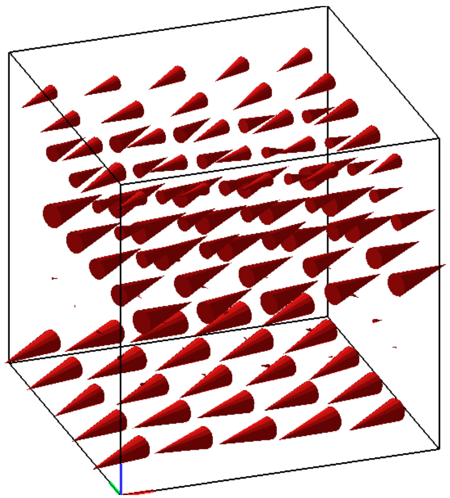


Theory does well in high-gradient flows despite small-Kn assumption

Overall Goal

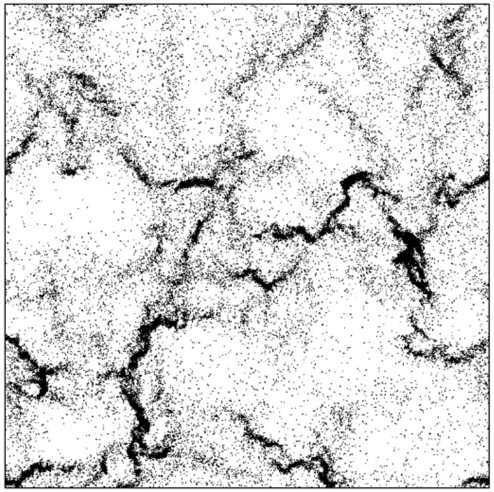
(i) Understand relative importance of clustering mechanisms





Particle Clustering Instability: Known Mechanisms

Homogeneous Cooling System



Granular Work

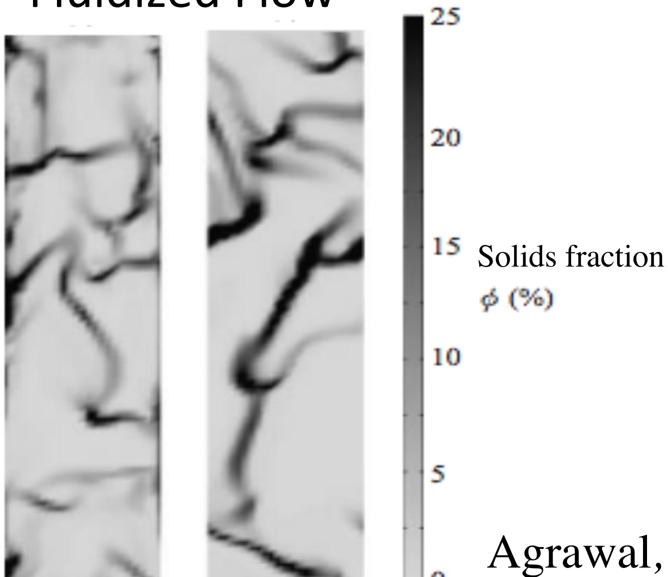
Solid Effects
(Dissipative Collisions)

Inelasticity
- Hopkins & Louge 1991
- Goldhirsch et al. 1993

Friction
- Mitrano et al. 2013

Goldhirsch, *et al.*, *J. Sci. Comput.* (1993)

Fluidized Flow



Fluidization Work

Fluid Effects

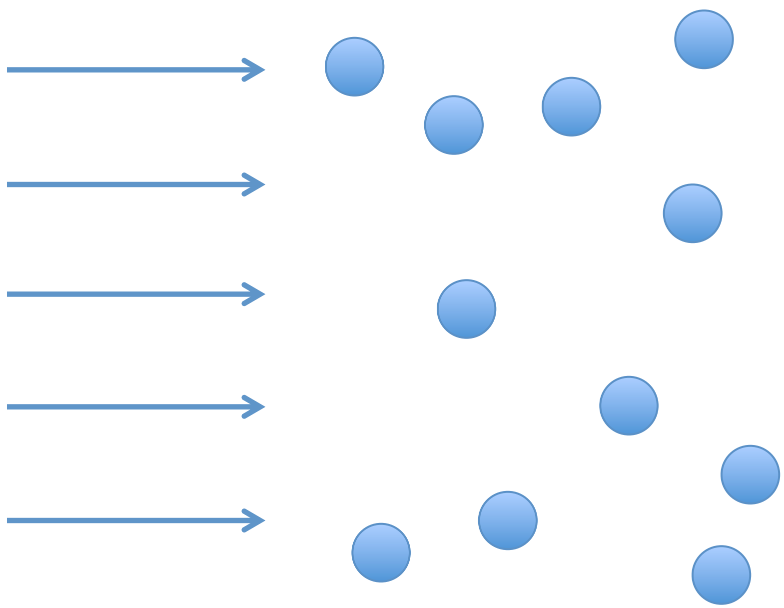
Mean Drag
- Glasser et al. 1998
- Agrawal et al. 2001

"Viscous Losses"
- Wylie & Koch 2000

Agrawal, *et al.*, *J. Fluid Mech.* (2001)

Mean Drag v. Viscous Losses

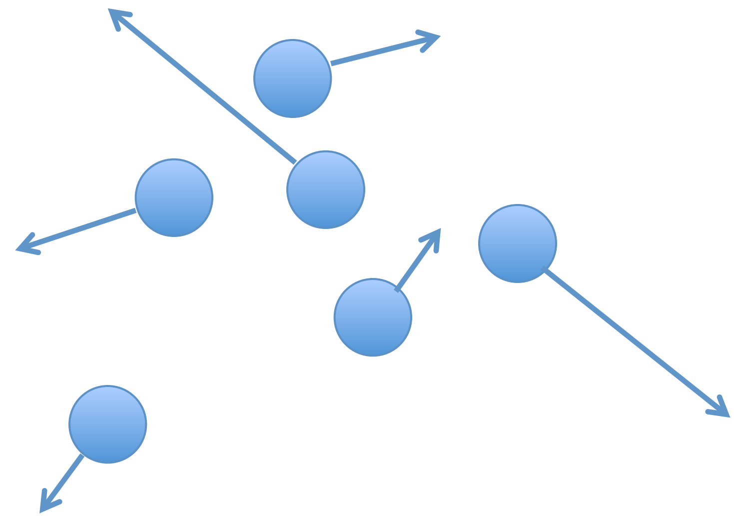
Gas flow fixed particles



Mean relative velocity decreases

When $\overline{U}_g - \overline{U}_s = 0$, $\boldsymbol{F}_{fluid} = 0$

Particle flow in gas with $\overline{U}_g - \overline{U}_s = 0$



Clearly $\boldsymbol{F}_{fluid} \neq 0$

Granular temperature decreases

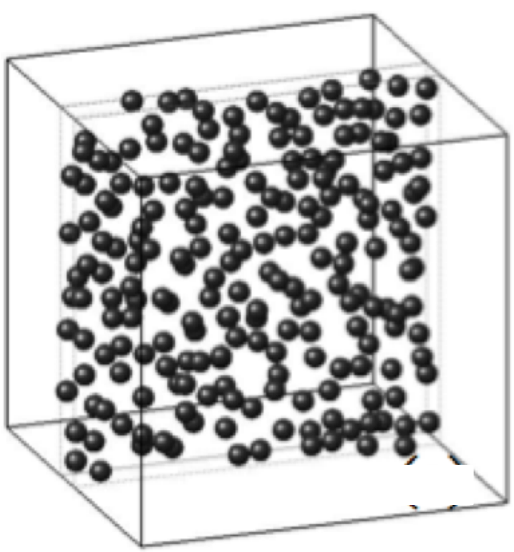
When $T = 0$, $\boldsymbol{F}_{fluid} = 0$

Conditions

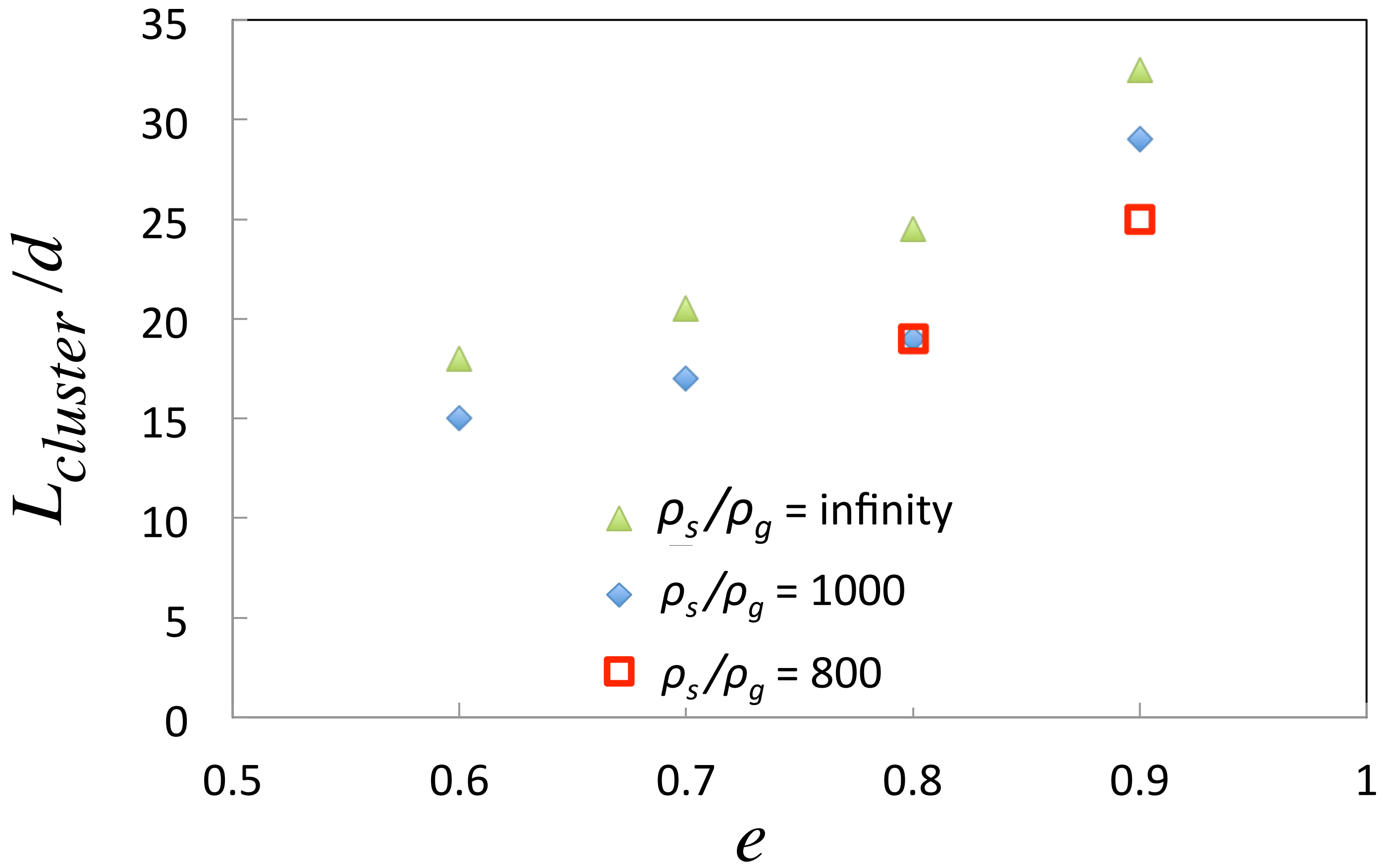
- Restitution coefficient: $0.8 \le e \le 1.0$
- Solids fraction: $0.1 \le \phi \le 0.4$
- Density ratio: $800 \le \dfrac{\rho_{solid}}{\rho_{fluid}} \le 1500$

$$\mathrm{Re}_T \propto \sqrt{T_0}$$

$$\mathrm{Re}_M \propto V_{rel} \propto \frac{\text{Particle inertial forces}}{\text{Fluid viscous forces}}$$



Gas-solid Continuum Model of HCS

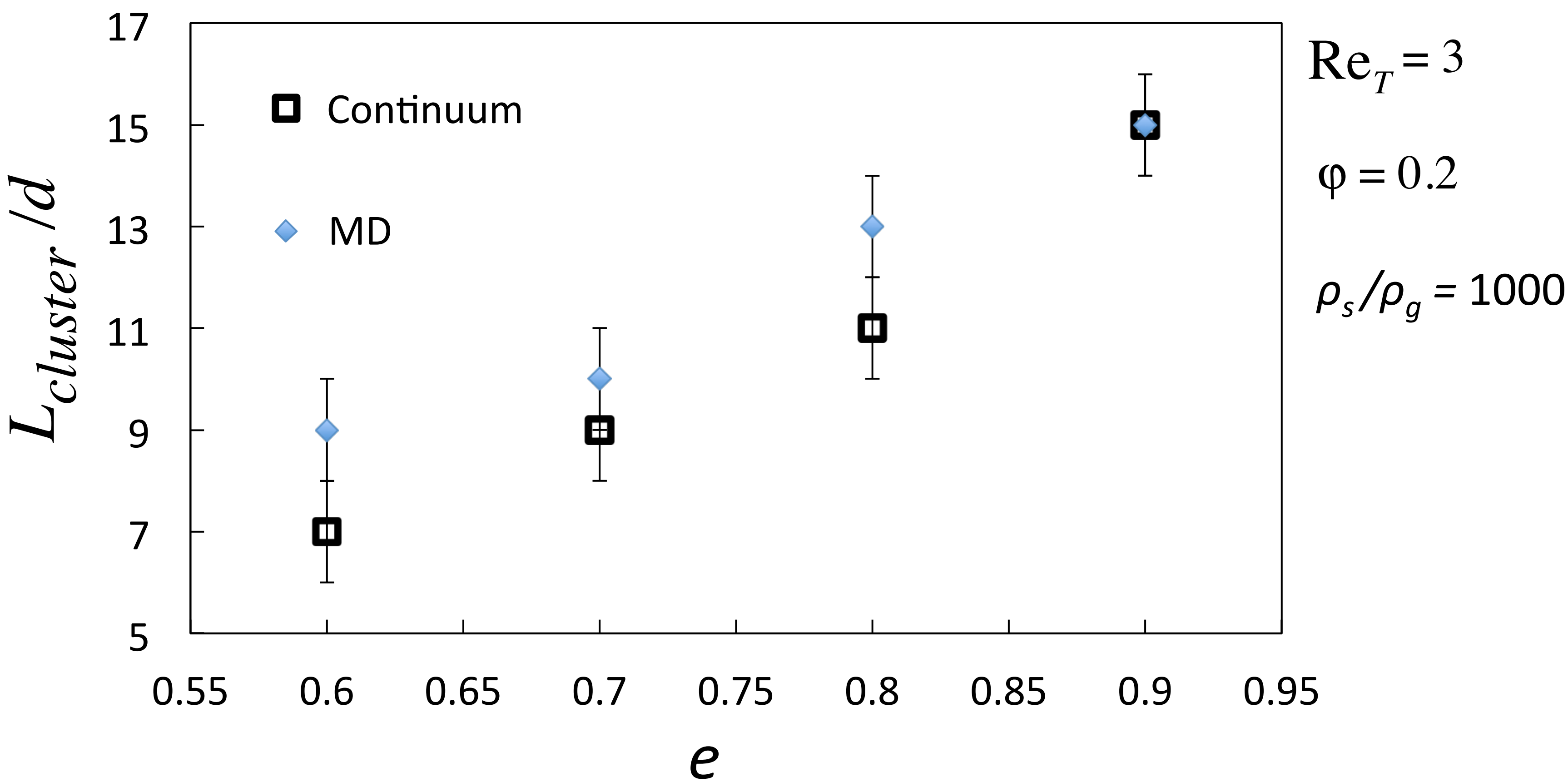


$\mathrm{Re}_T = 3$

$\varphi = 0.1$

Both viscous losses and collisional dissipation important

Gas-solid HCS: Continuum v. MD



Strong Agreement between continuum model and MD

Particle Clustering Instability: Known Mechanisms

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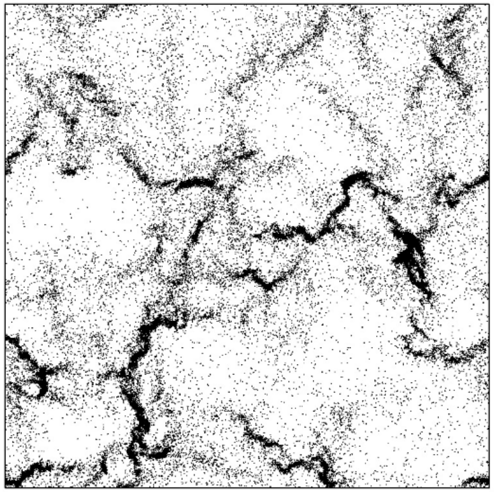

Granular Work

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(Dissipative Collisions)

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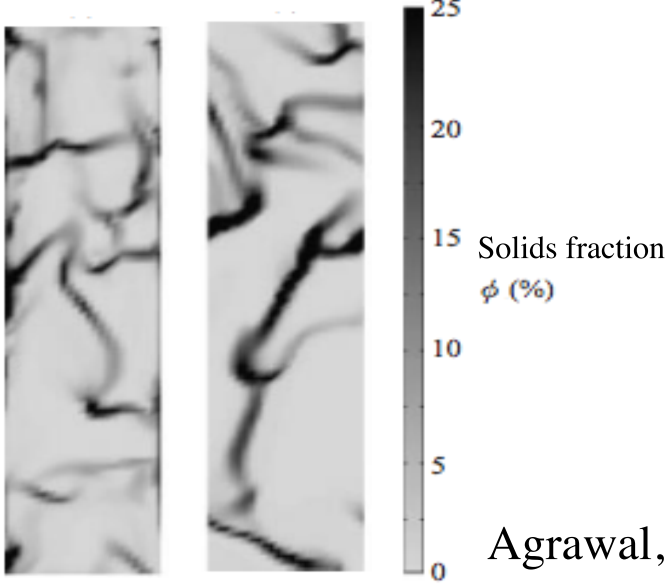
Fluidized Flow



Fluidization Work

Fluid Effects

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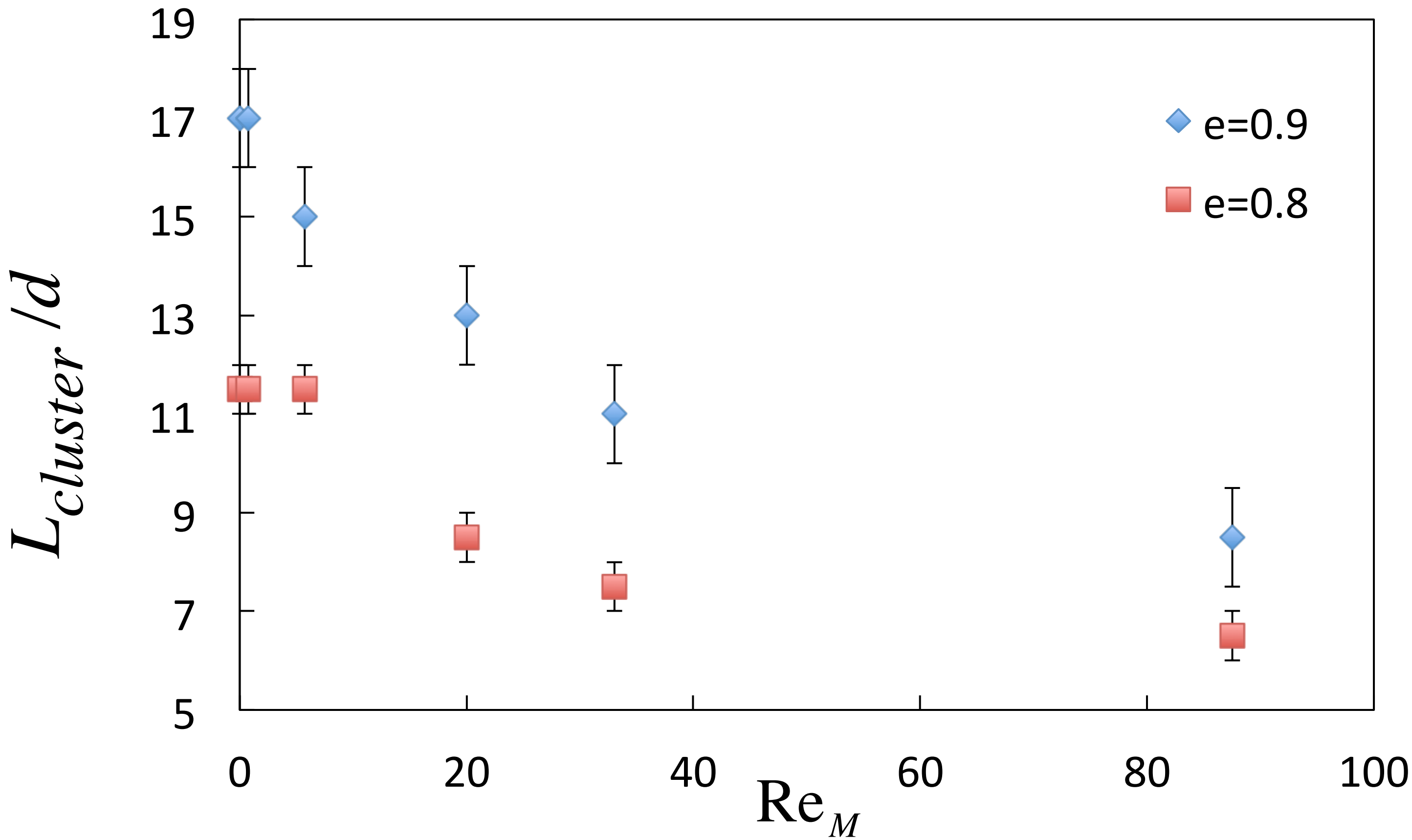
- Glasser et al. 1998
- Agrawal et al. 2001

Viscous Losses
- Wylie & Koch 2000

Agrawal, *et al.*, *J. Fluid Mech.* (2001)

Gas-solid Continuum Model of Settling Flow



$\mathrm{Re}_T = 5$

$\varphi = 0.2$

$\rho_s/\rho_g = 1000$

Both mean drag and collisional dissipation important

Concluding Remarks

- Small Knudsen number assumption not so restrictive
- Collisional dissipation, mean drag, and viscous losses all important in conditions studied
- Strong agreement between continuum model and discrete particle simulations

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