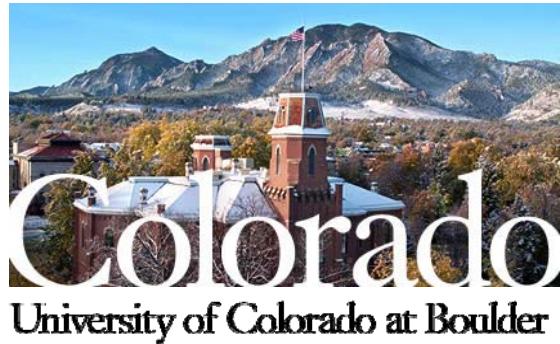


# Instabilities in Particle Flows: Assessing Hydrodynamics and Understanding Dominant Mechanisms

Peter P. Mitrano  
Christine M. Hrenya  
John R. Zenk



Xiaolong Yin

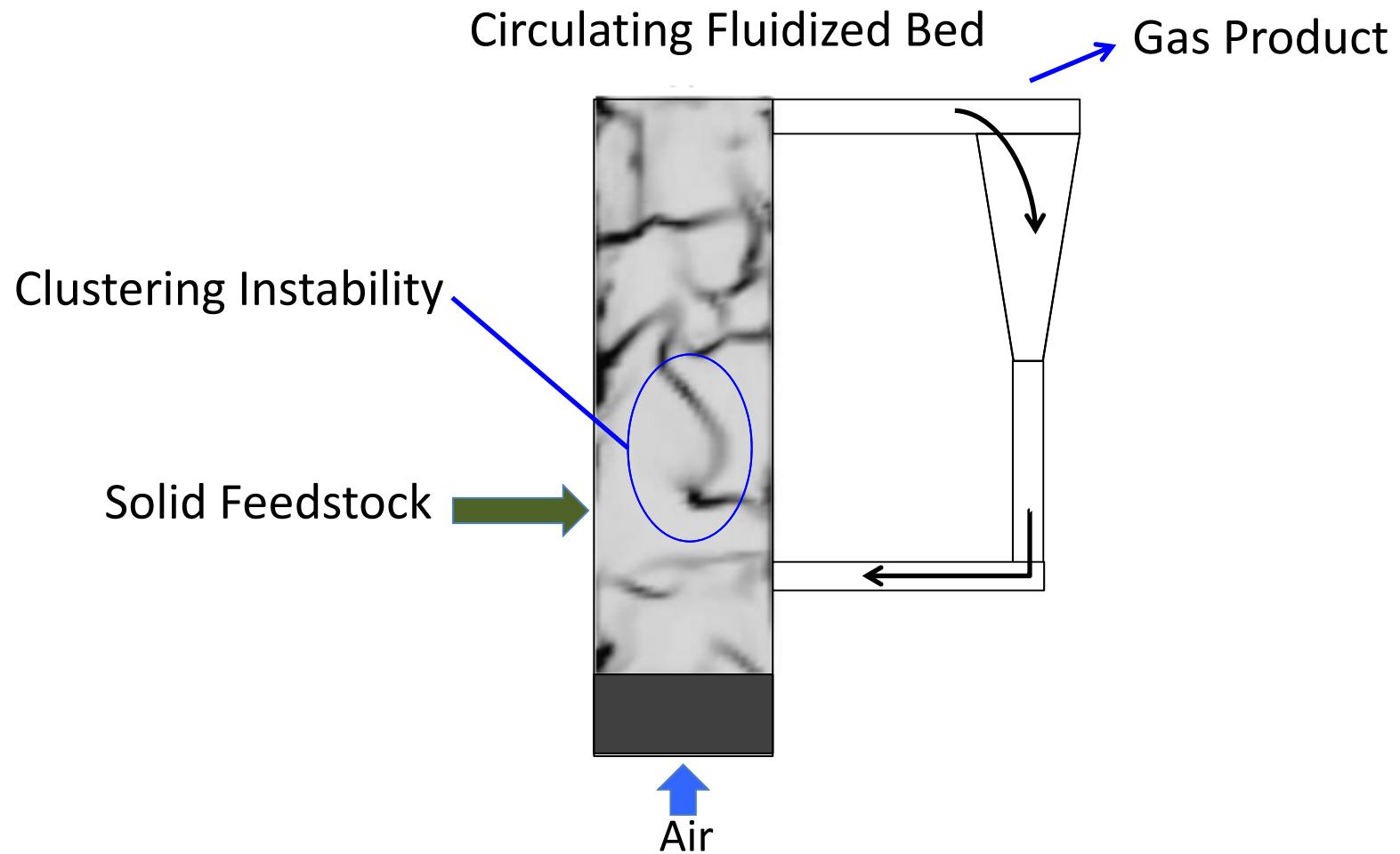


Sofiane Benyahia  
Janine E. Galvin



June 13th, 2013  
Pittsburgh  
UCR Conference

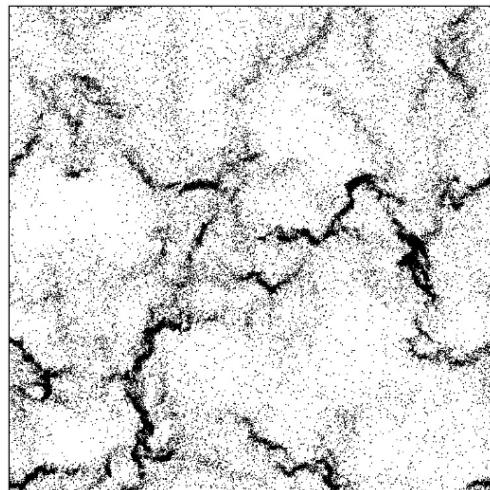
# Motivation: Instabilities in Particulate Flows



CFD simulation from Agrawal, Loezos, Syamlal, Sundareson, J. Fluid Mech. (2001)

# Particle Clustering Instability: Known Mechanisms

Homogeneous Cooling System



## Granular Work

Solid Effects  
(Dissipative Collisions)

Inelasticity

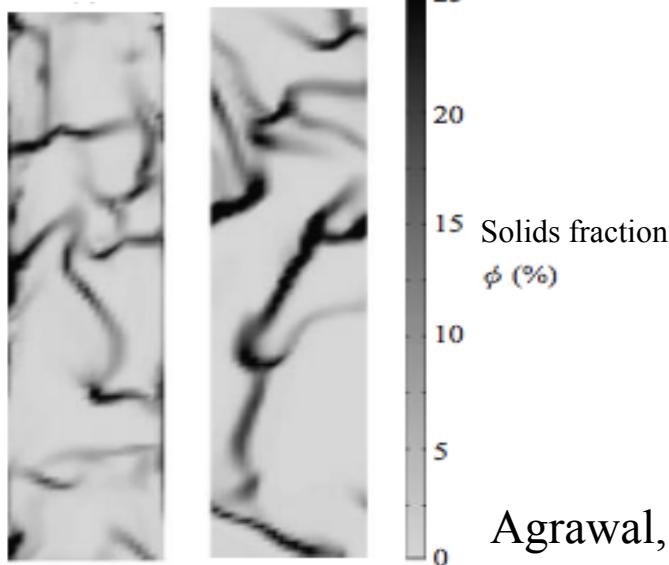
- Hopkins & Louge 1991
- Goldhirsch et al. 1993

Friction

- Mitrano et al.

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

Fluidized Flow



## Fluidization Work

Fluid Effects

Mean Drag

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

Viscous Damping

- Wylie & Koch 2000

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

# Objectives

- Relative importance of mechanisms in gas-solid flow instabilities
  - DNS, MD simulations, hydrodynamics
- Hydrodynamic description for developed gradients and correlated particle velocities
  - MD simulations, hydrodynamics
- Hydrodynamic description of binary mixture of particles
  - MD simulations, linear hydrodynamics

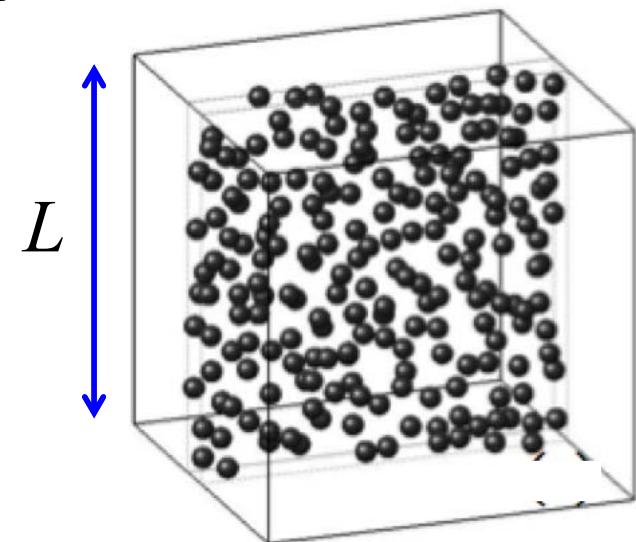
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# Input: Typical CFB Conditions

- Restitution coefficient:  $0.8 \leq e \leq 1.0$
- Solids fraction:  $0.1 \leq \phi \leq 0.4$
- Density ratio:  $800 \leq \frac{\rho_{solid}}{\rho_{fluid}} \leq 1500$
- System length scale  $L/d = 30 \times 30 \times 4$
- Reynolds Number:  $3 \leq \text{Re}_T \leq 30$

$$\begin{aligned}\text{Re}_T &\propto \rho_{fluid} \sqrt{T_0} \\ &\propto \frac{\text{Particle inertial forces}}{\text{Fluid viscous forces}}\end{aligned}$$



# System

## Homogeneous Cooling System (HCS)

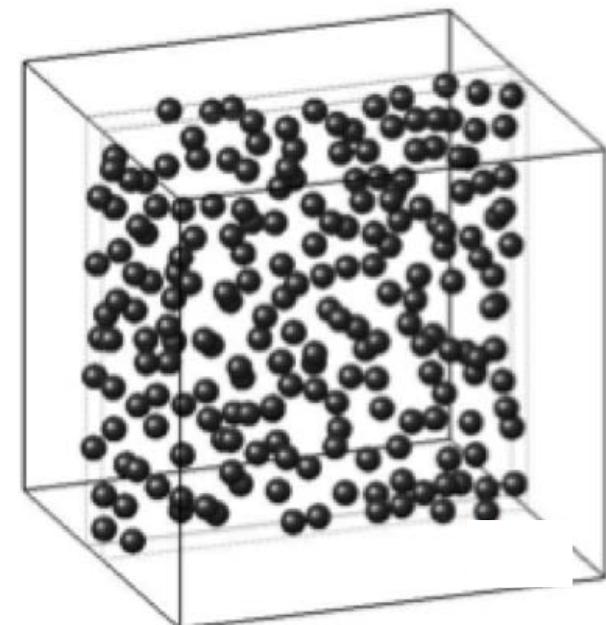
- No external forces
- Periodic boundaries
- 3-D domain
- Random initial configuration
- No net momentum

}

Kinetic energy  
decays over time

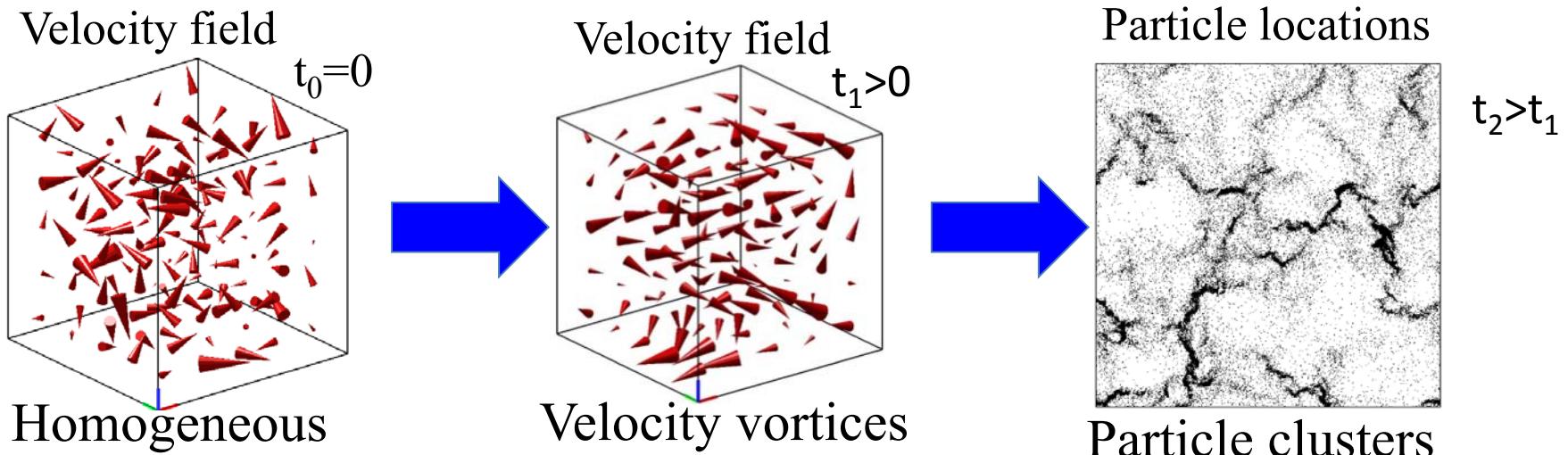
## Particle properties

- Coefficient of normal restitution ( $e$ )
- Monodisperse, frictionless spheres



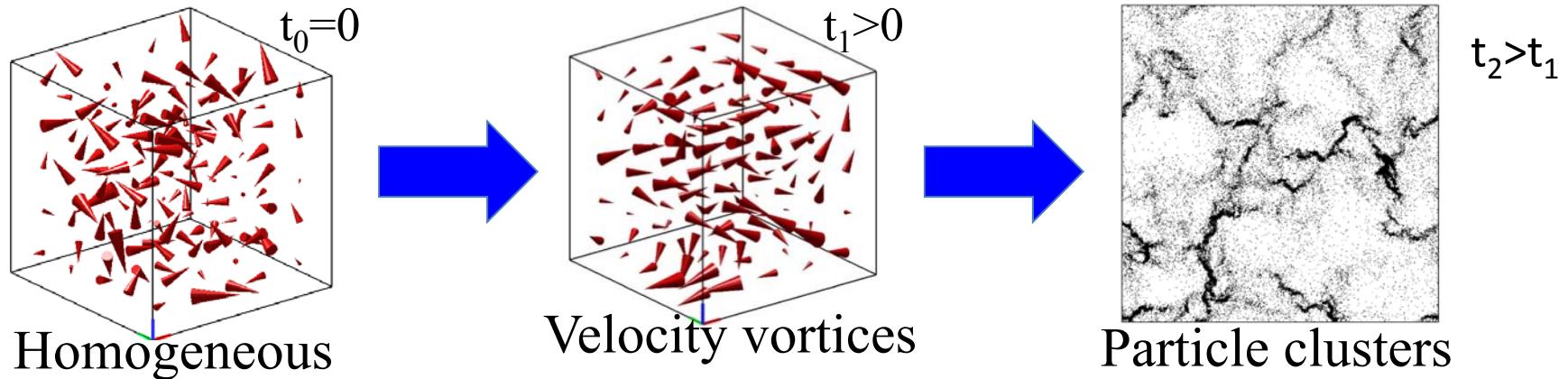
# Previous HCS work

Granular flow: *inelastic* solids; no gas (Goldhirsch 1993)



# Previous HCS work

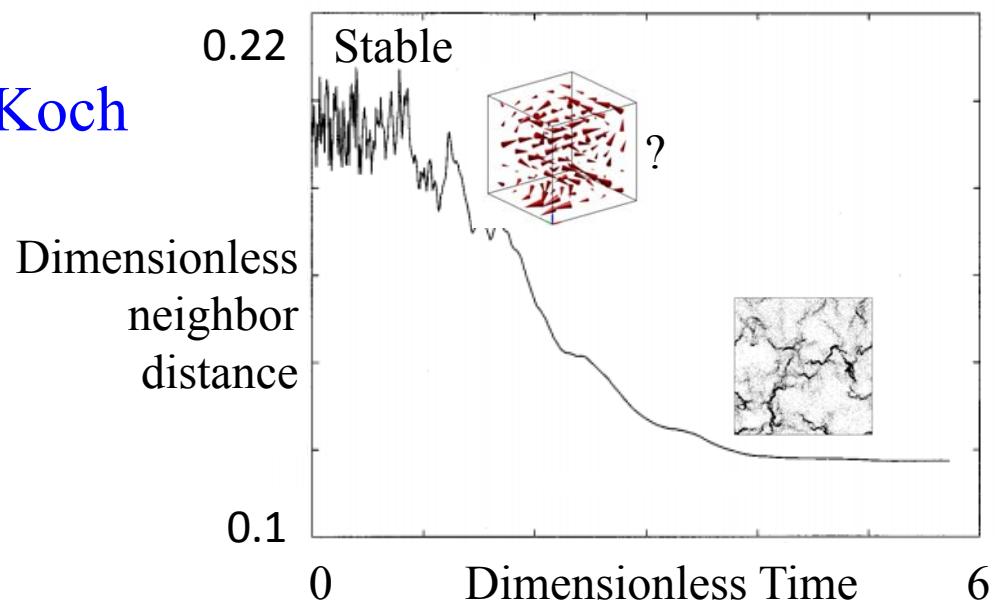
Granular flow: *inelastic* solids; no gas (Goldhirsch 1993)



Gas-solid flow (Wylie & Koch 2000)

- *elastic* particles in viscous fluid flow

Focus: viscous effects



# Kinetic Theory

$$\frac{dT}{dt} = -\zeta T - \frac{2T}{m}\gamma$$

$\zeta$  cooling rate due to collisions  
 $\gamma$  cooling rate due to viscous forces  
 $T$  granular temperature

Energy balance for stable, homogeneous cooling

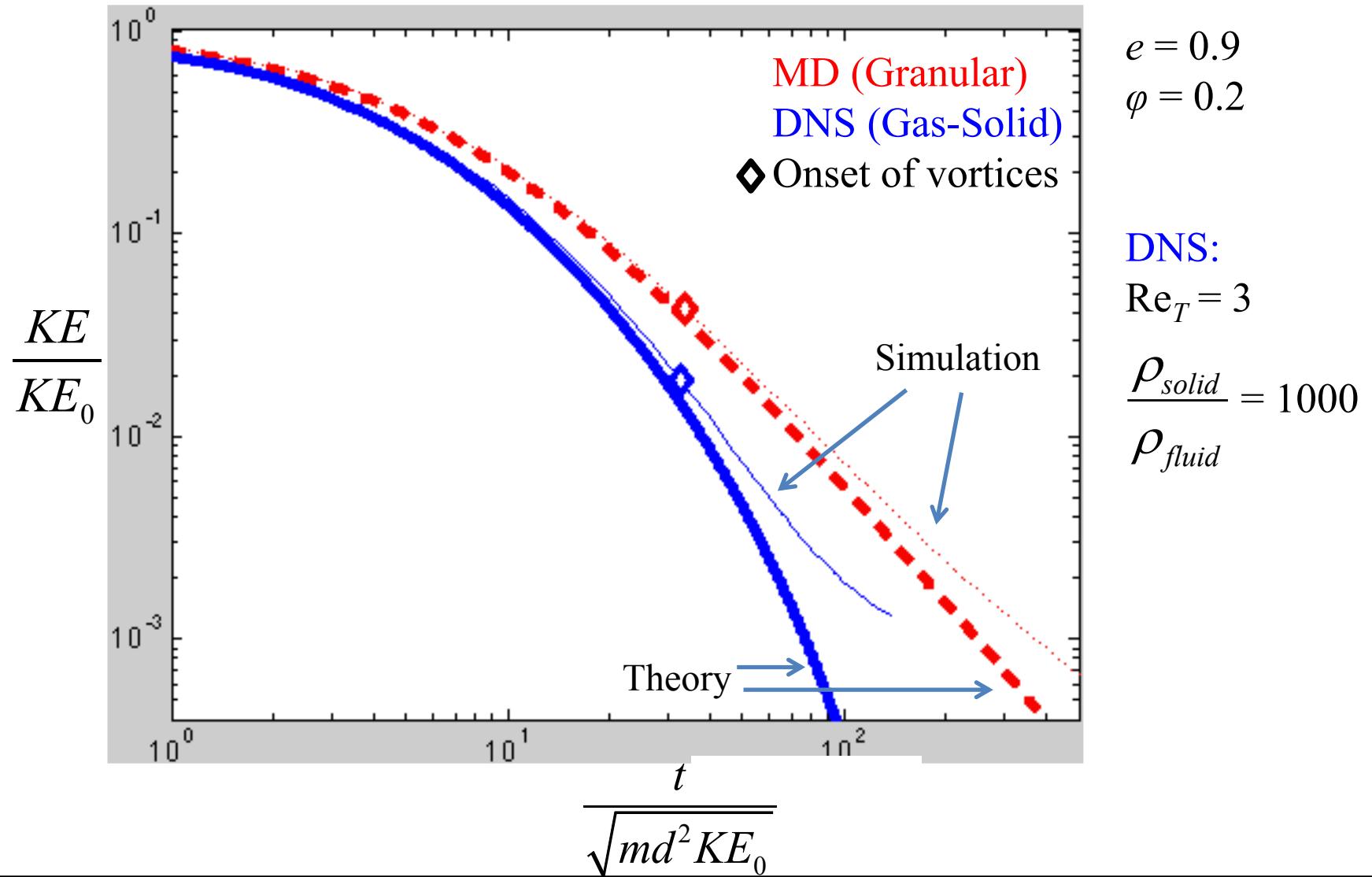
1. Verification of instability-detection method
2. Preliminary validation for new theory\*

$$(\bar{\mathbf{U}}_s - \bar{\mathbf{U}}_f) \rightarrow (\mathbf{U}_s - \mathbf{U}_f)$$

New theory: rigorous incorporation of *instantaneous* viscous force in starting kinetic (Enskog) equation

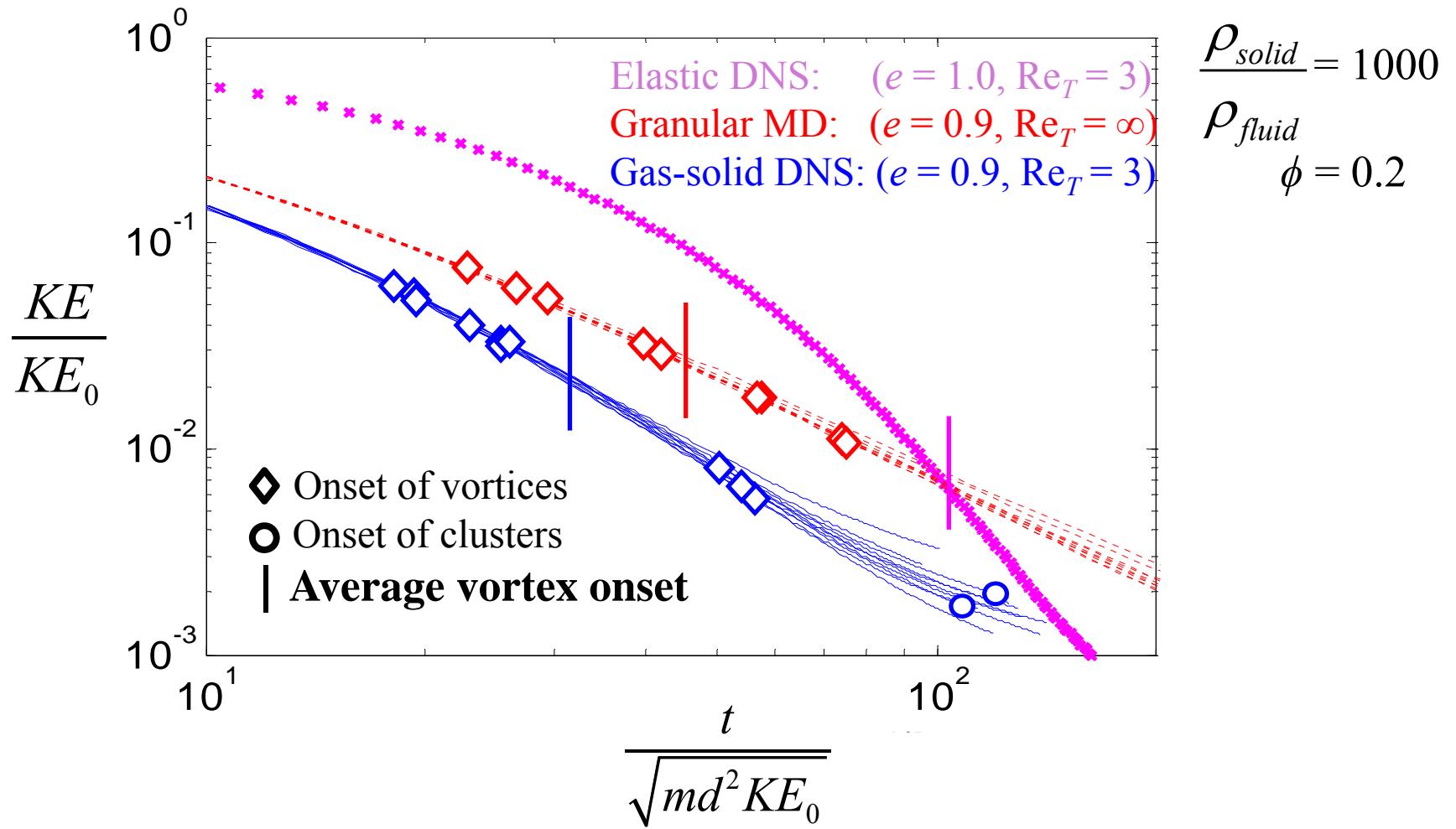
\*Garzó, Tenneti, Subramaniam, Hrenya, *J. Fluid Mech.* (2012)

# Simulation vs. Kinetic Theory



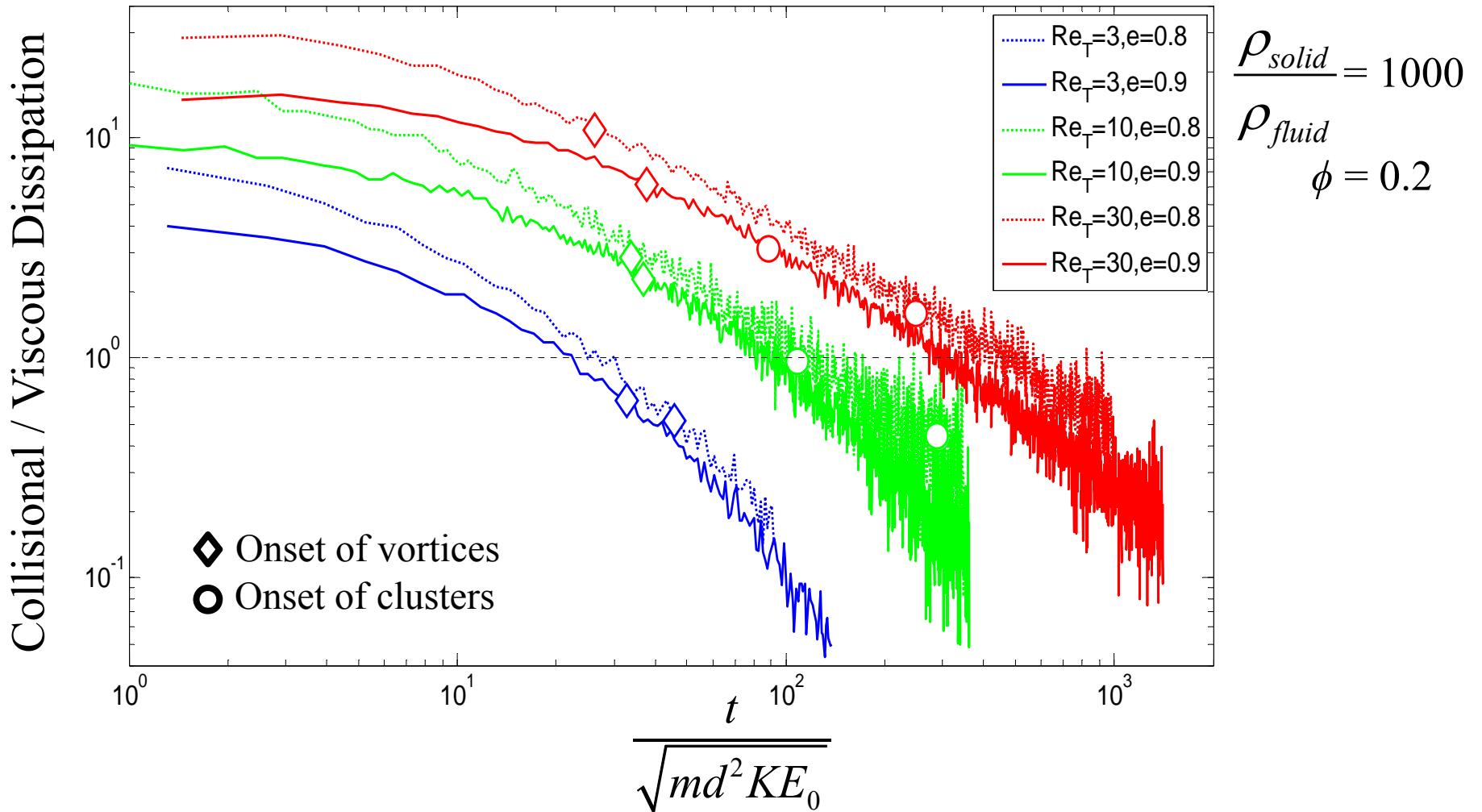
Theory agrees with simulation *before onset of instability* (as expected)

# Influence of Dissipative Mechanisms



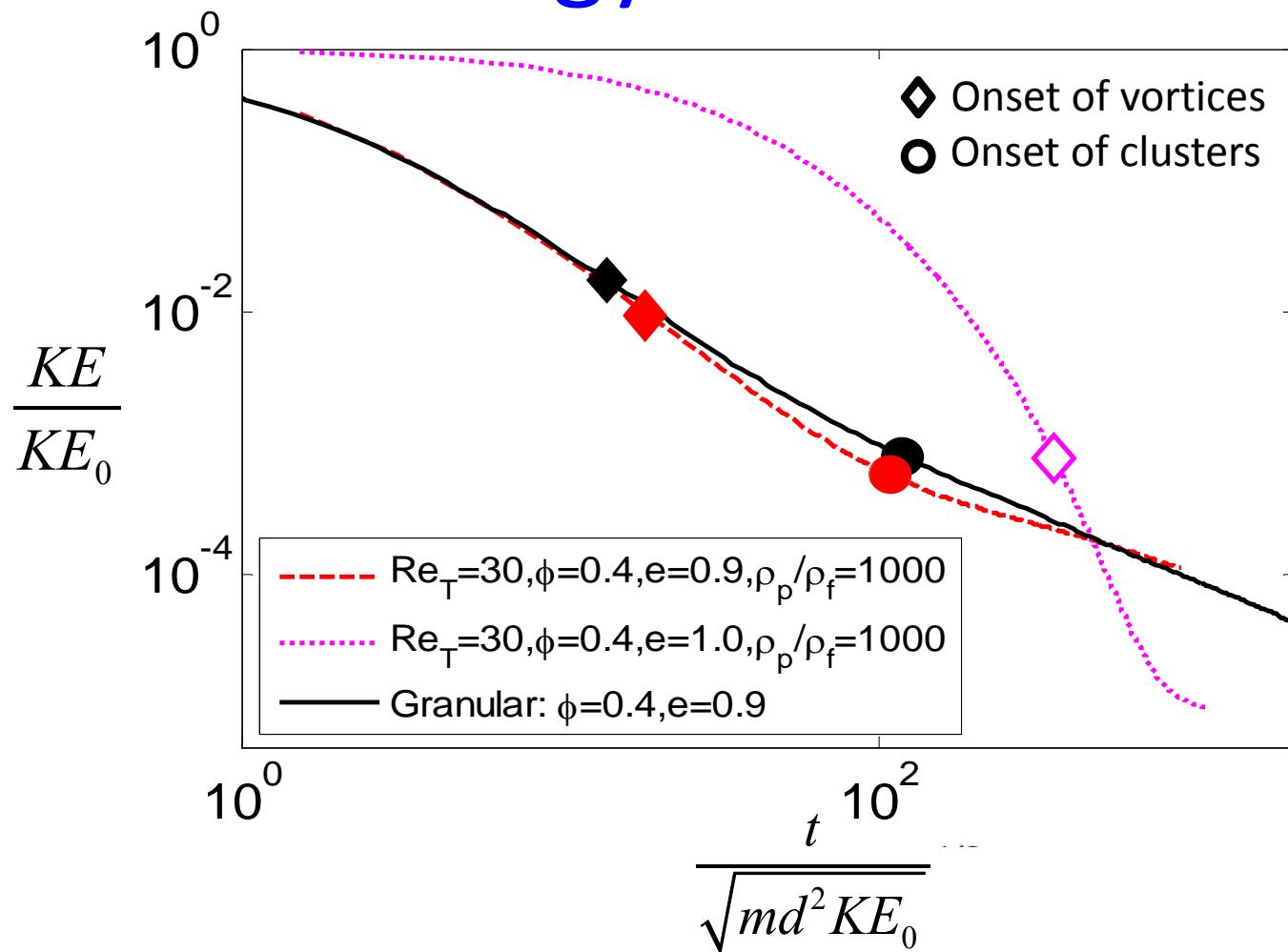
Increased dissipation promotes instability, regardless of mechanism

# Relative Importance of Dissipative Mechanisms



Collisional dissipation dominates for high  $Re_T$

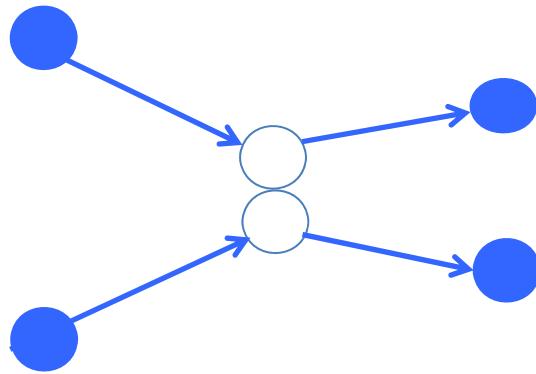
# Energy Crossover



More dissipative systems may actually possess  
higher energy levels due to velocity vortices

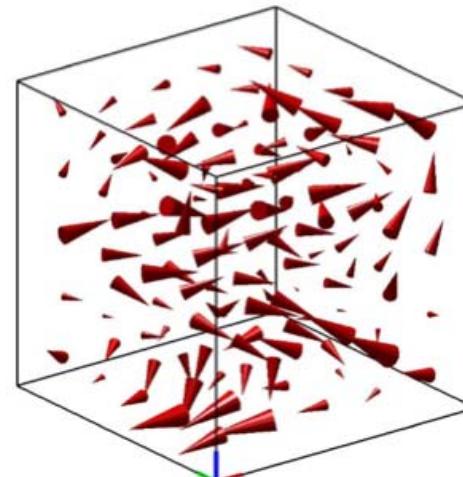
# Energy Crossover: Physical Mechanism

- Dissipation promotes velocity vortex instability
- Collisions reduce normal relative velocity to greater extent than tangential relative velocity



- Both collisional and viscous losses align particle motion
- Dissipation decreases with normal relative velocity

1. Velocity vortices
2. Glancing collisions
3. Smaller relative normal velocity
4. Reduced dissipation

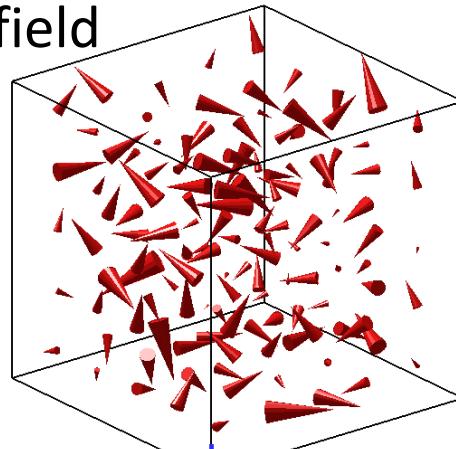


# Outline

- Relative importance of mechanisms in gas-solid flow instabilities
  - DNS, MD simulations, hydrodynamics
- Hydrodynamic description in spite of developed gradients and correlated particle velocities
  - MD simulations, hydrodynamics
- Hydrodynamic description of binary mixture of particles
  - MD simulations, linear hydrodynamics

# Critical Length Scales for Instability

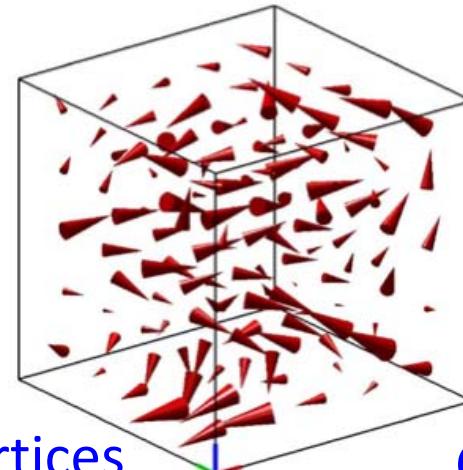
Velocity  
field



- Dissipative collisions
- Sufficiently large system domain

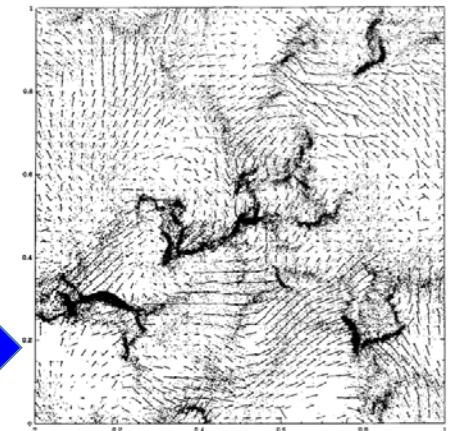
Molecular dynamics (MD)  
simulations of the HCS

Velocity field



Vortices

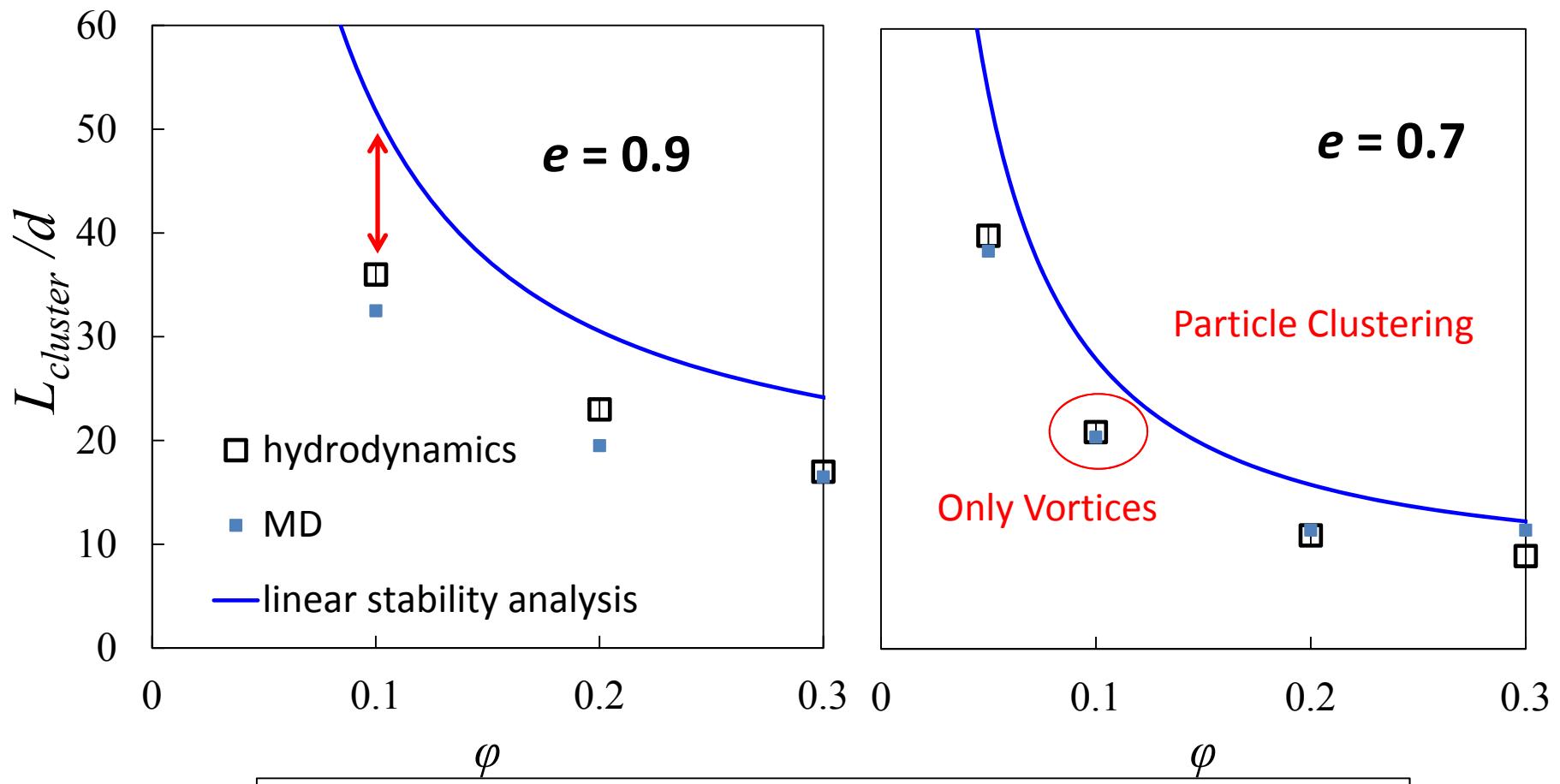
Particle locations



Clusters

Goldhirsch, Tan, Zanetti, J. Sci. Comput. (1993)

# Hydrodynamics vs. MD



Non-linear mechanisms (e.g. viscous heating) are important to cluster formation

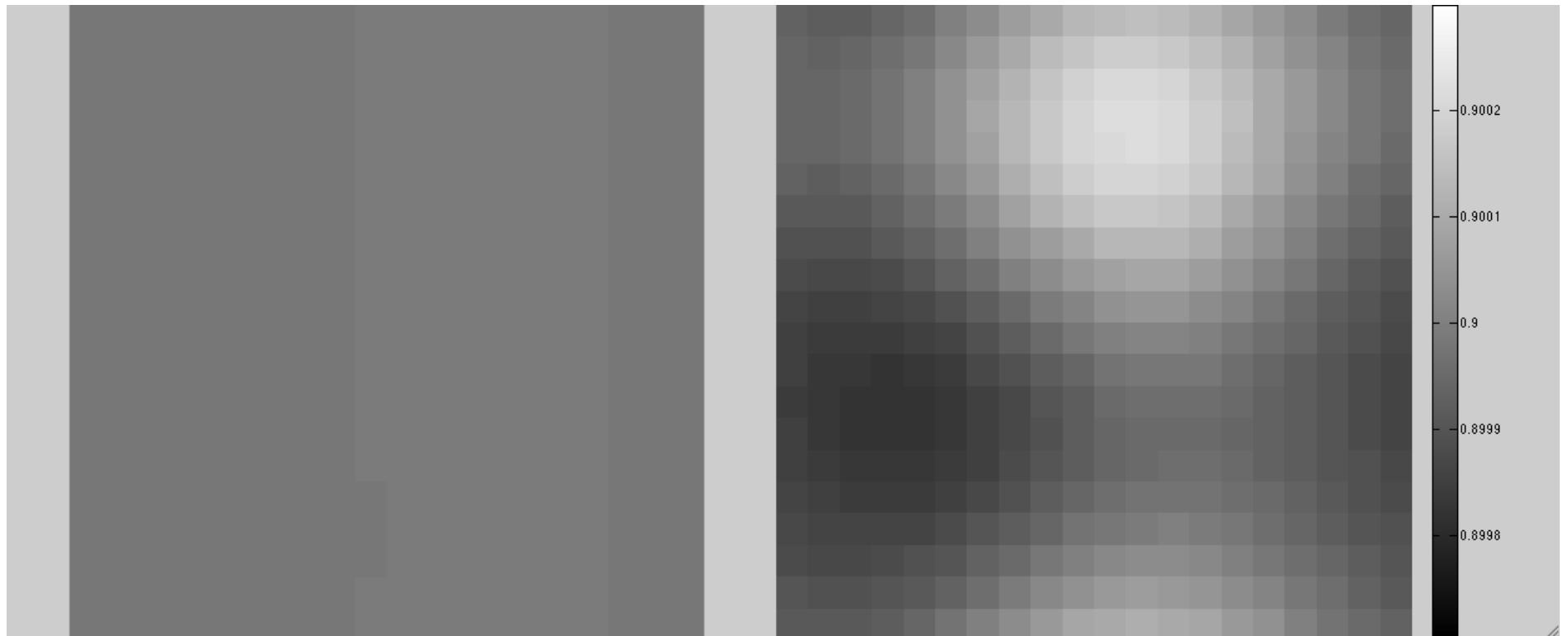
# Hydrodynamics: Onset of Instability

$L/d = 18$

$t = 100s$

$L/d = 20$

$1-\varphi = 0.9003$

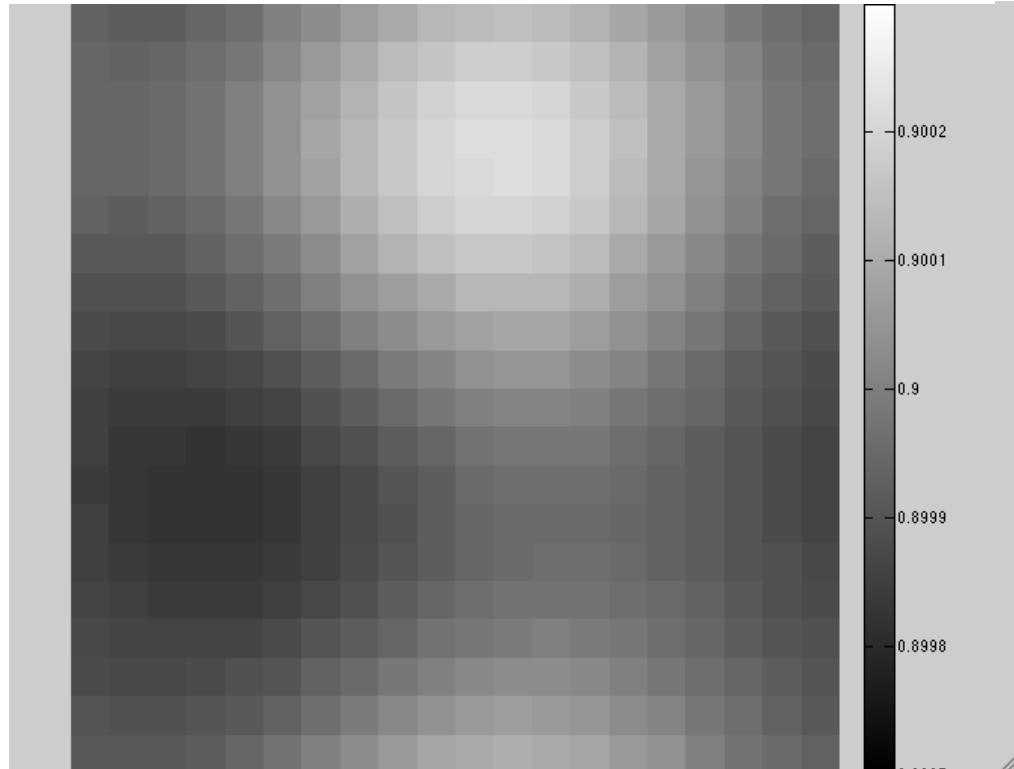


Voidage ( $1-\varphi$ ) in slice of 3D domain

$1-\varphi = 0.8997$

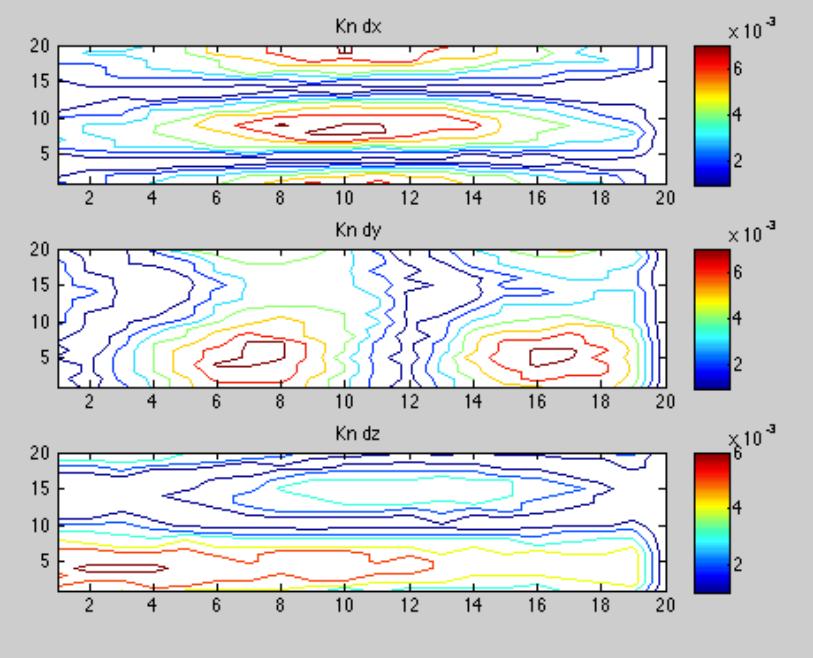
# Hydrodynamics: Onset of Instability

Voidage ( $1-\varphi$ )



$1-\varphi = 0.9003$

Concentration Kn map



$1-\varphi = 0.8997$

$L/d = 20, t=100s$

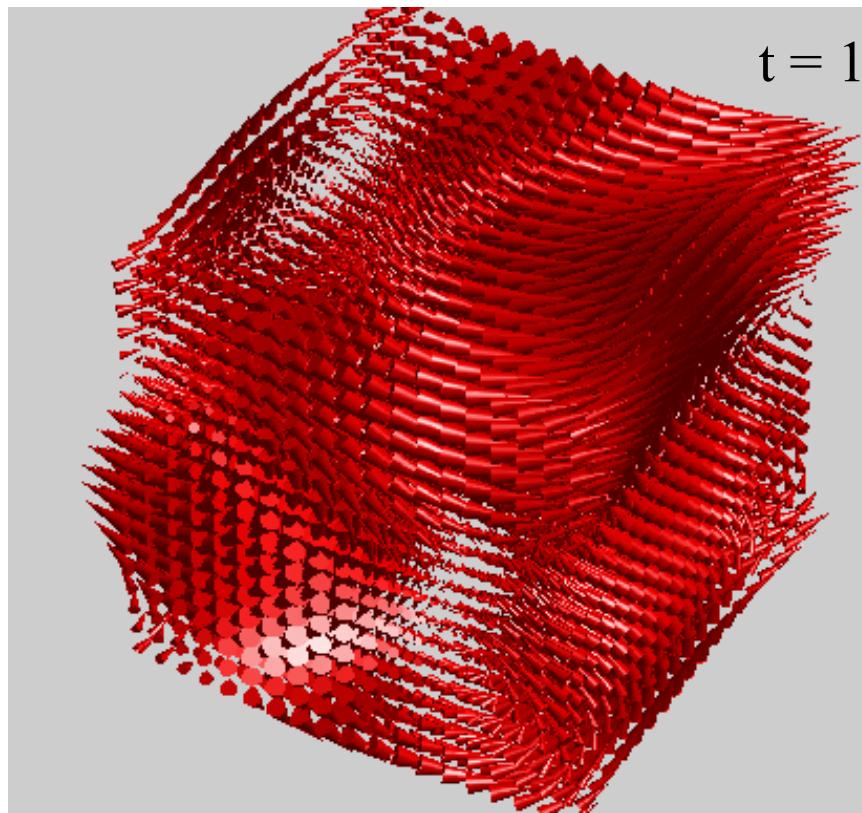
Concentration Kn  $\sim 10^{-3}$

# Hydrodynamics: Onset of Instability

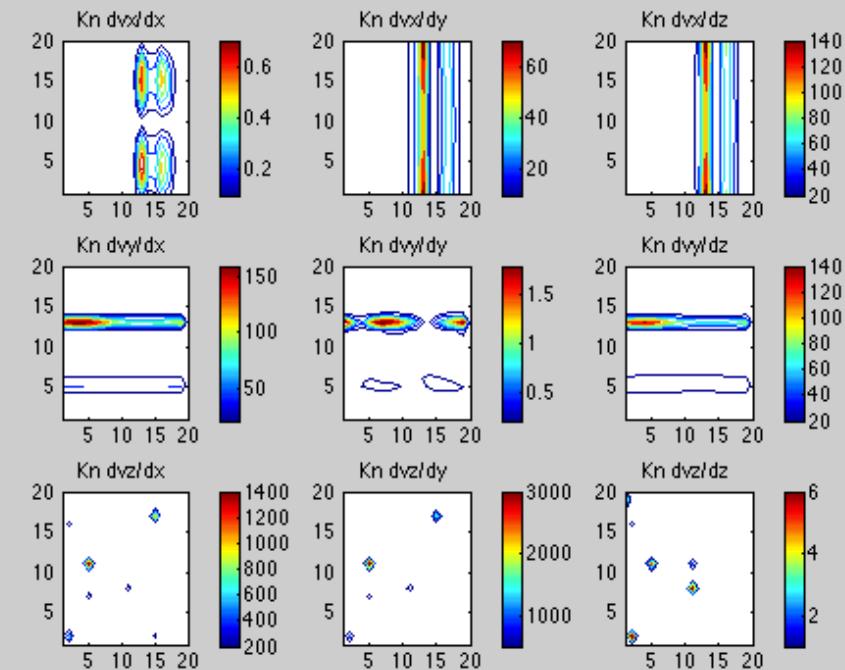
Velocity field

$L/d = 20$

$t = 100s$



Velocity Kn maps (2D slice)



$\text{Velocity Kn} < \mathcal{O}(10^3)$

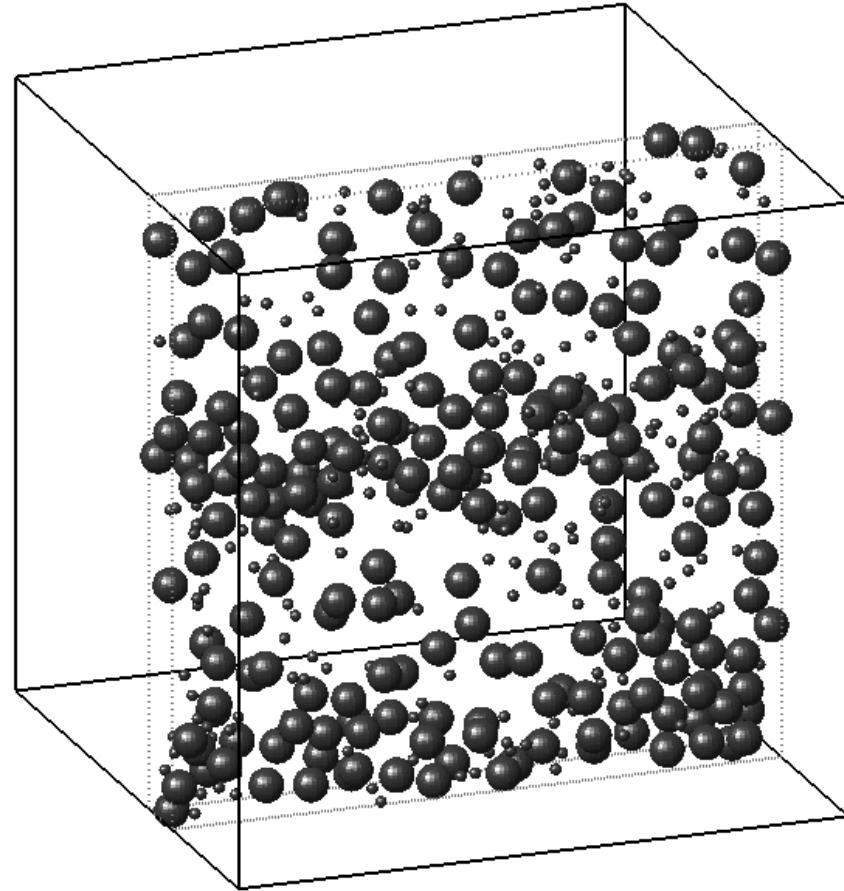
Small-Kn and molecular chaos assumptions not so  
restrictive to hydrodynamics

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- **Hydrodynamic description of binary mixture of particles**
  - MD simulations, *linear* hydrodynamics

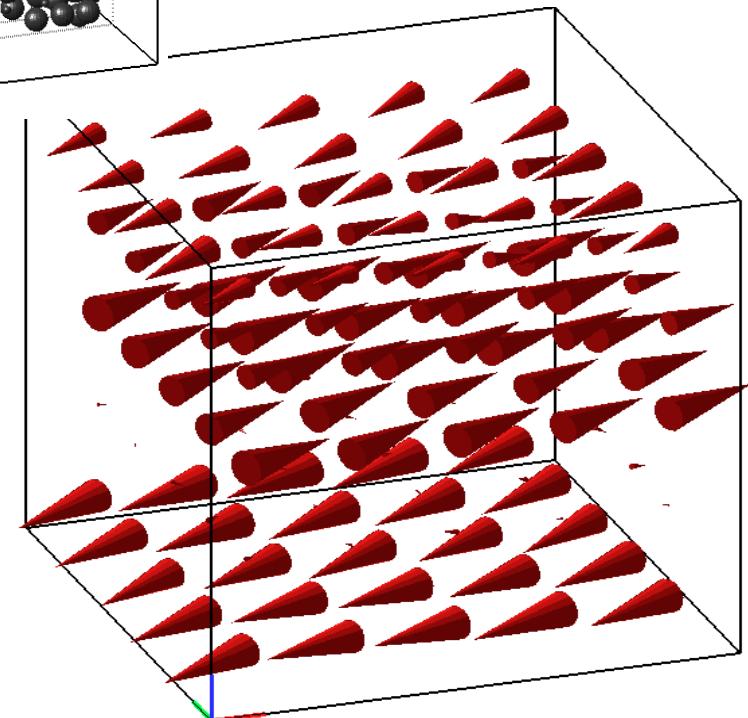
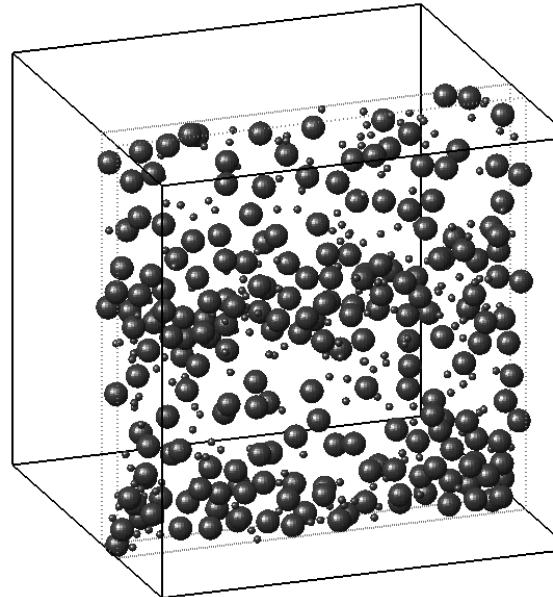
# Binary Systems: Extra Input

- Diameter ratio
  - $d_1/d_2$
- Mass ratio
  - $\gamma = m_1/m_2$
- Number fraction
  - $x_1 = n_1/N$
  - $n_1$  = number of type 1 particles
  - $N$  = total number of particles



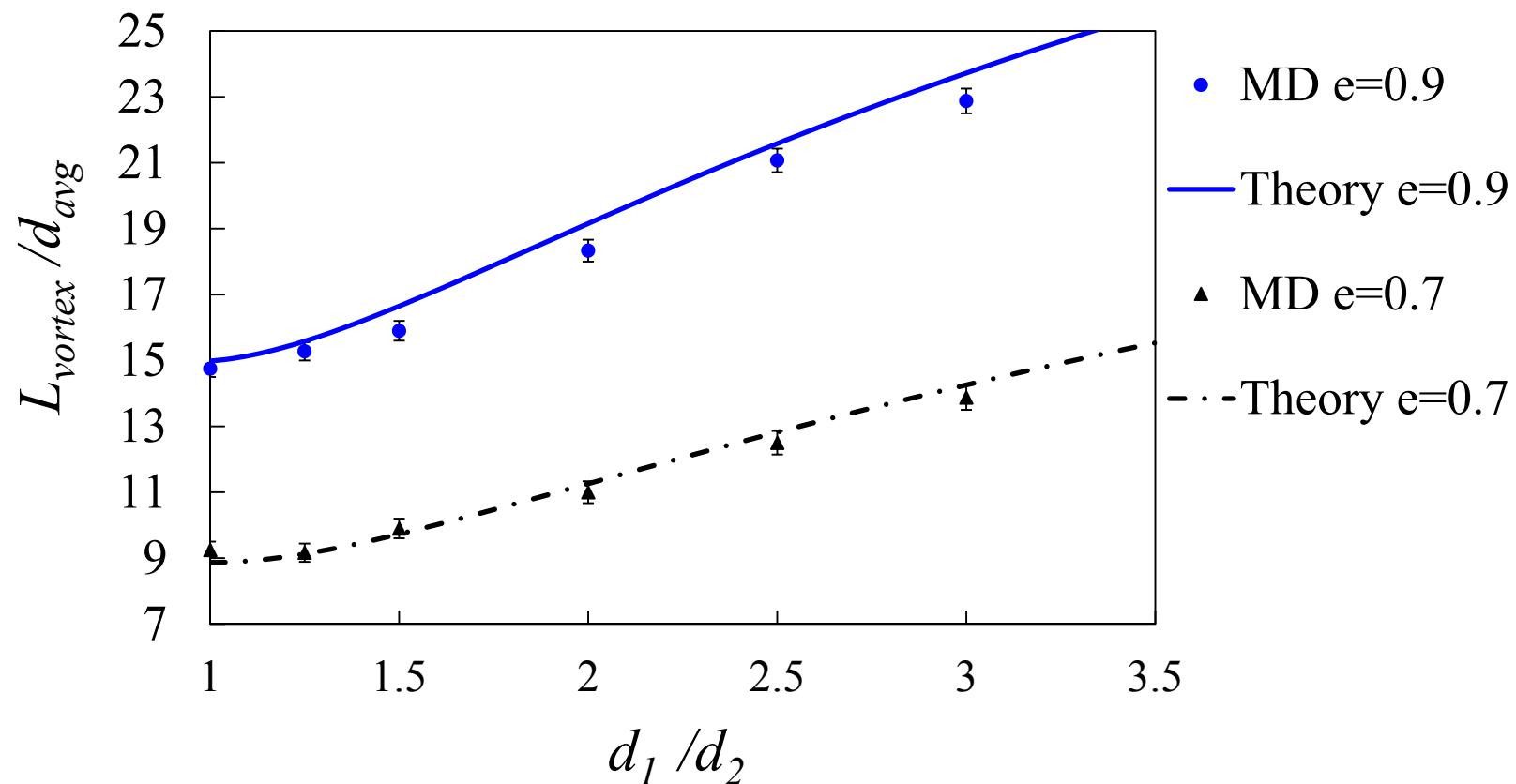
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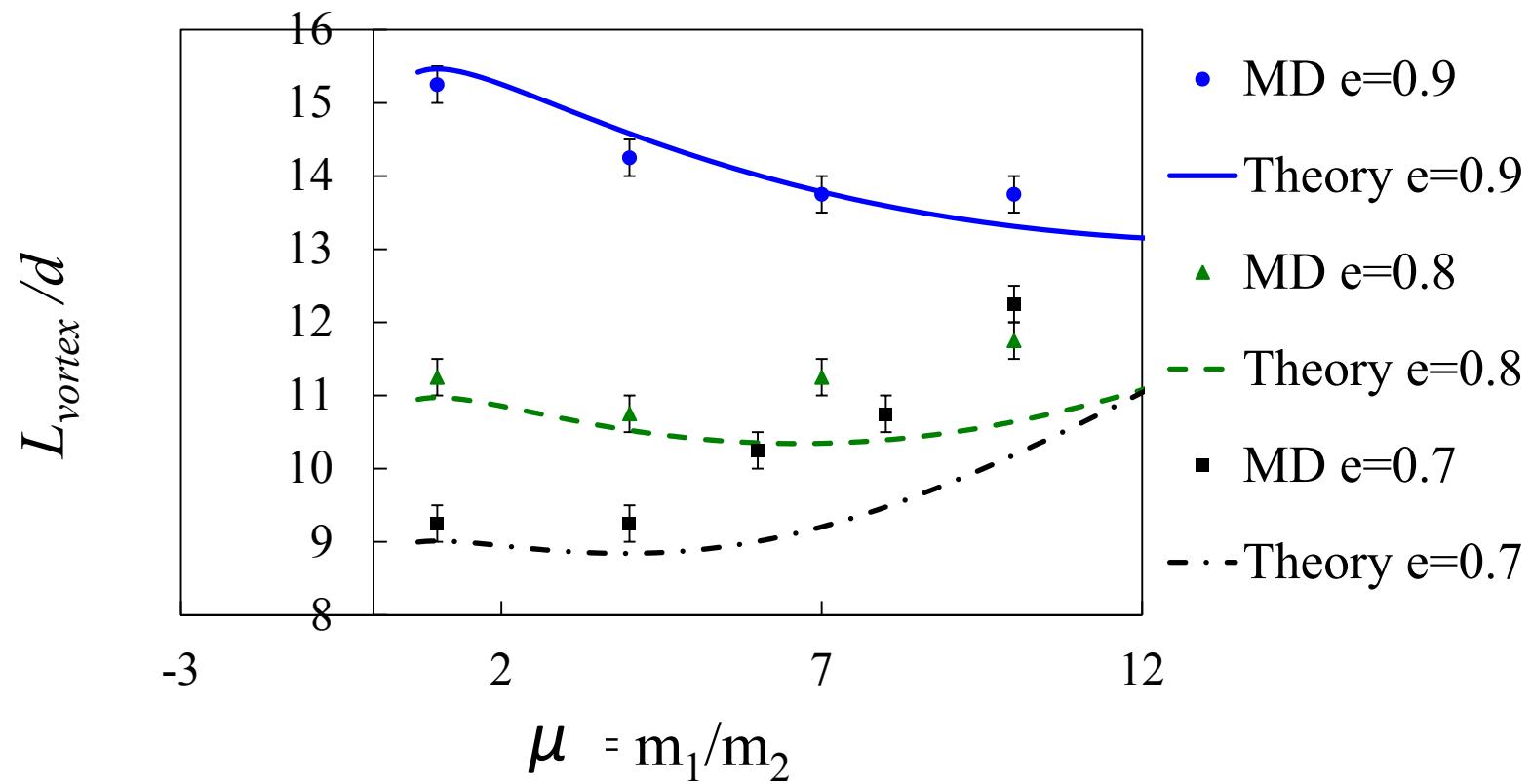
# Diameter Ratio

$$x_1 = n_1/N = 0.5, \mu = m1/m2 = 2, \phi = 0.2$$



# Mass Ratio

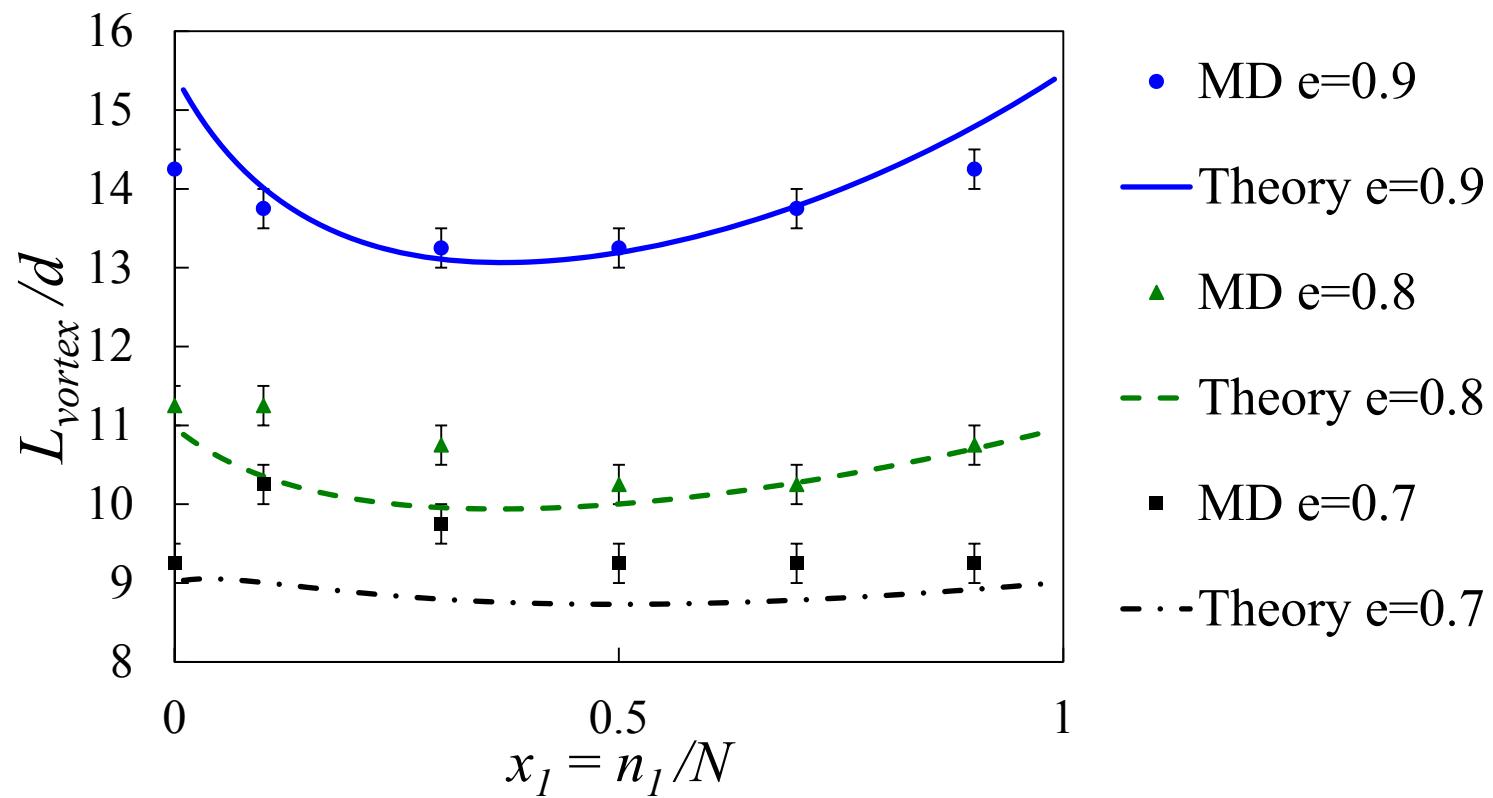
$$d_1/d_2 = 1, \quad x_1 = n_1/N = 0.1, \quad \phi = 0.2$$



Theory does quite well until moderate dissipation  
is combined with disparate particle species

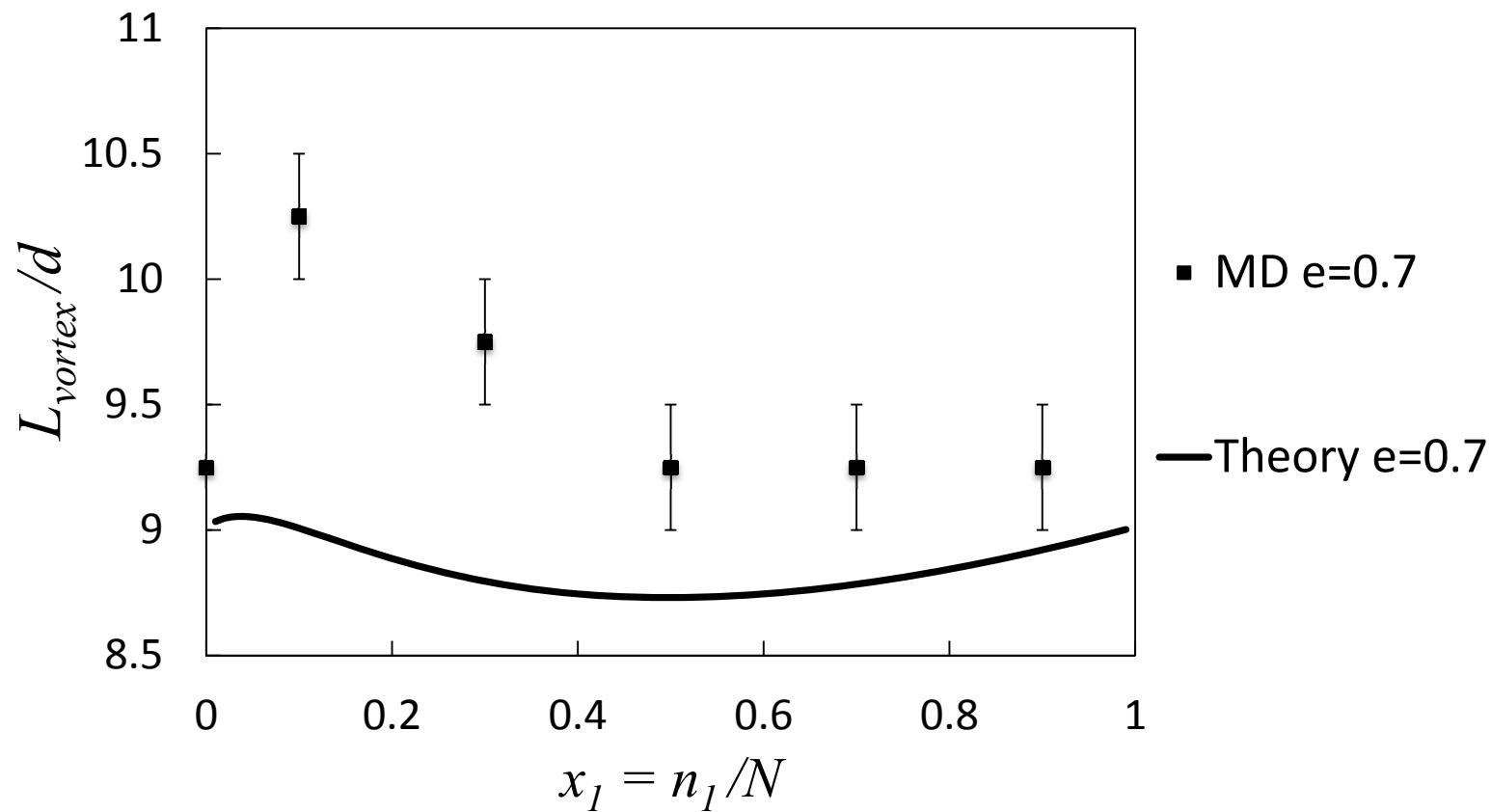
# Number Fraction

$$d_1/d_2 = 1, \quad \mu = m_1/m_2 = 6, \quad \phi = 0.2$$



# Number Fraction: Zoomed In

$$d_1/d_2 = 1, \quad \mu = m_1/m_2 = 6, \quad \phi = 0.2$$



# Concluding Remarks

- Both dissipative collisions and viscous losses are important for conditions studied

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- Both dissipative collisions and viscous losses are important for conditions studied
- More dissipative systems may actually possess highly levels energy due to vortices
- Molecular chaos and small Knudsen number assumptions not so restrictive
- Binary mixture hydrodynamics do well until moderate dissipation is combined with disparate species parameters

# Outline

- Relative importance of mechanisms in gas-solid flow instabilities
- Hydrodynamic description in spite of developed gradients and correlated particle velocities
- Hydrodynamic description of binary mixture of particles

# Instabilities in Particle Flows: Assessing Hydrodynamics and Understanding Dominant Mechanisms

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# Lattice Boltzmann Information

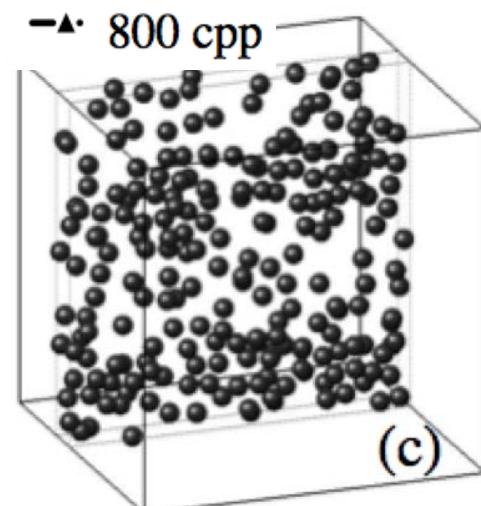
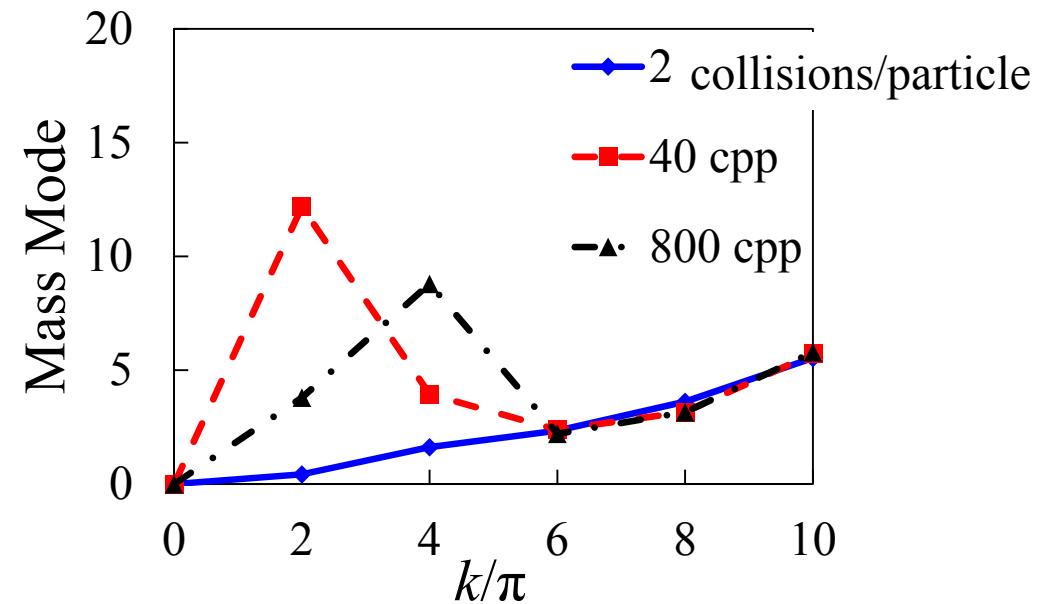
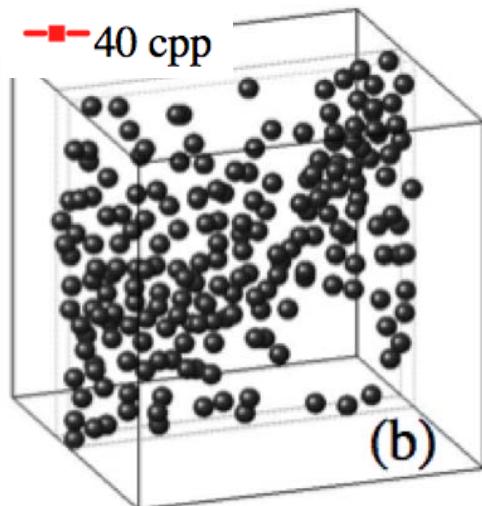
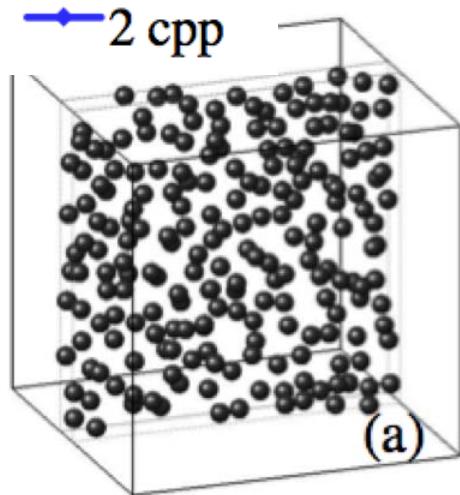
- Susp3D – A 3D particulate flow solver<sup>1, 2</sup>
  - Fluid flow is solved by a D3Q19 lattice Boltzmann model
  - Fluid-particle interaction is fully resolved
  - Particle motion is based on Newton's equation
- Particle-particle short-range interaction models
  - Lubrication interaction is implemented analytically<sup>3</sup>
  - Particle-particle collisions are treated as normal dissipative collisions between hard spheres (i.e. normal restitution, no friction)
- Simulation parameters
  - Domain size:  $300(dx) \times 300 (dx) \times 40 (dx)$  where  $dx$  is the lattice spacing
  - Particle size:  $\sim 10(dx)$
  - Fluid kinematic viscosity:  $1/6 (dx^2/dt)$  at low Re and  $1/100 (dx^2/dt)$  at high Re
- System parameters
  - Re: 1-30
  - Solid fraction: 0.1-0.4
  - Normal restitution coefficient: 0.8, 0.9, 1.0
  - Particle-fluid density ratio: 800, **1000**, 1500

<sup>1</sup>Ladd 1994a, 1994b, *J. Fluid Mech.*

<sup>2</sup>Ladd and Verberg 2001, *J. Stat. Phys.*

<sup>3</sup>Nguyen and Ladd 2002, *Phys. Rev. E*

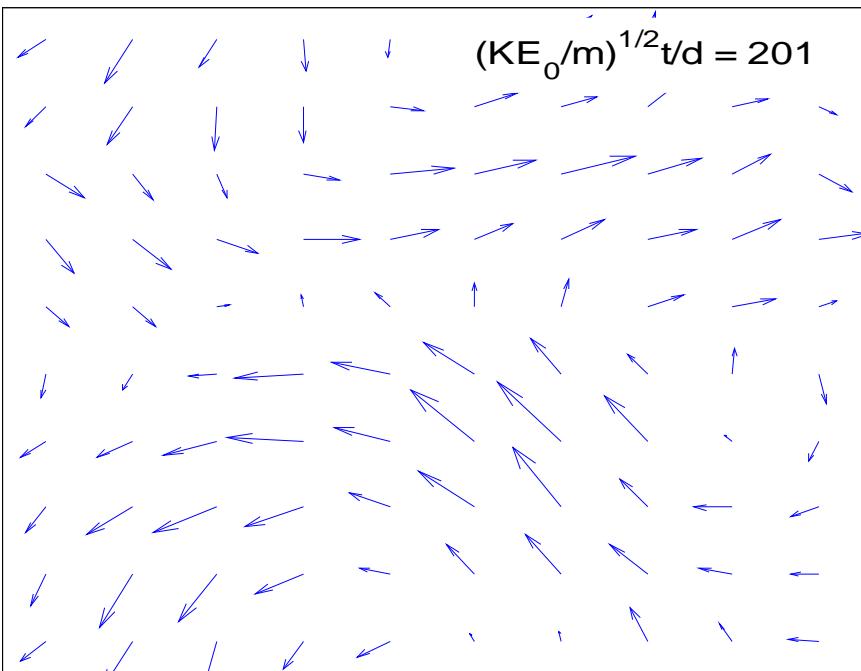
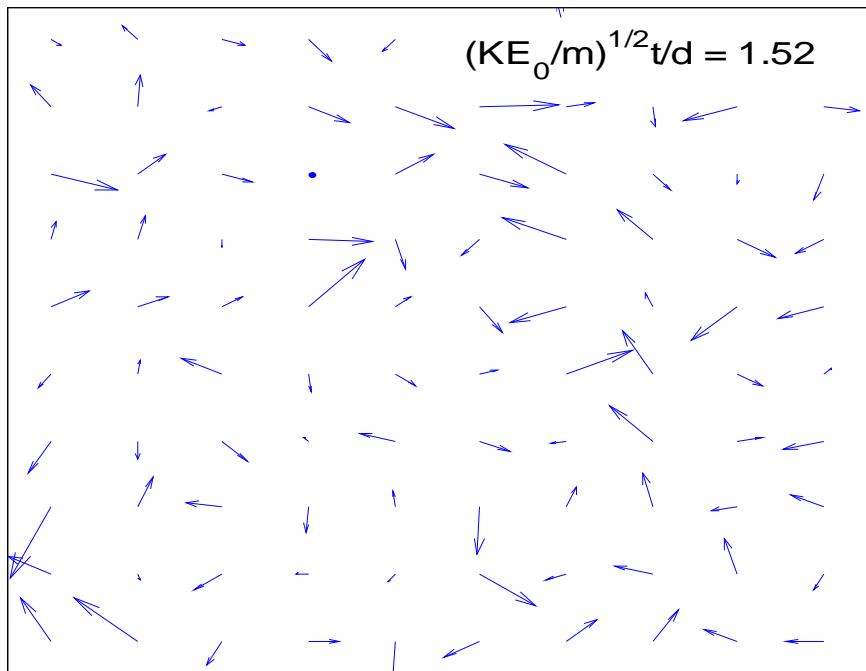
# MD: Fourier Analysis



$e=0.6, \phi=0.2$   
 $N=2000$

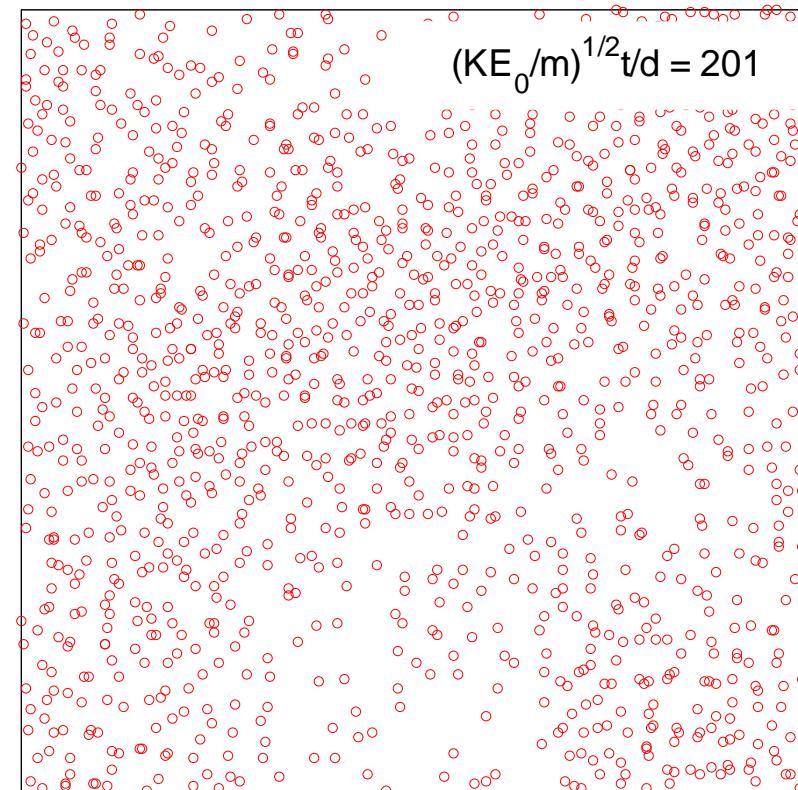
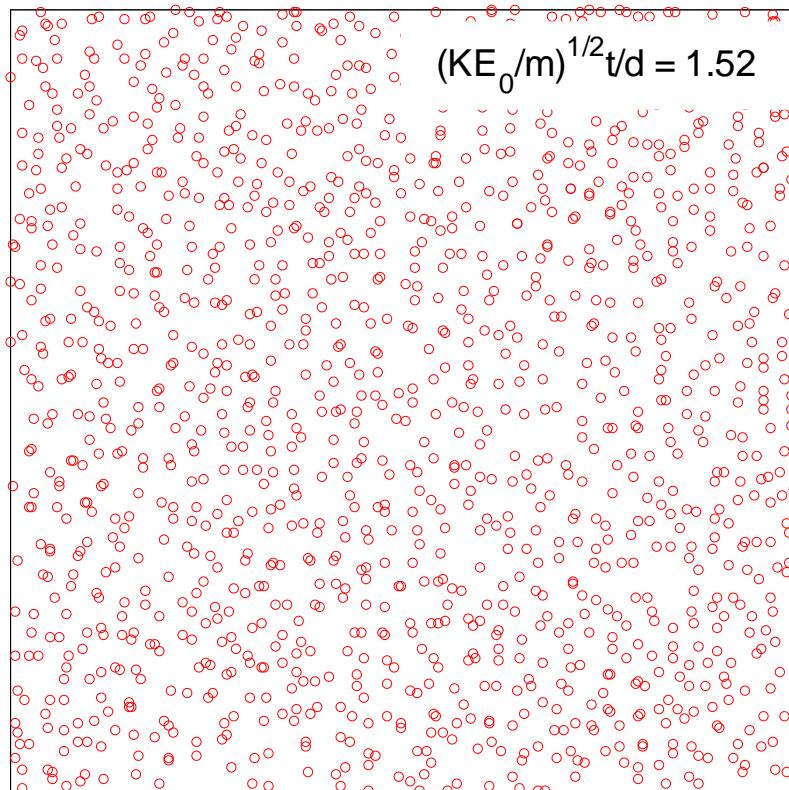
Mitrano et al.,  
PRE (2012)

# Velocity Vortices



Time →

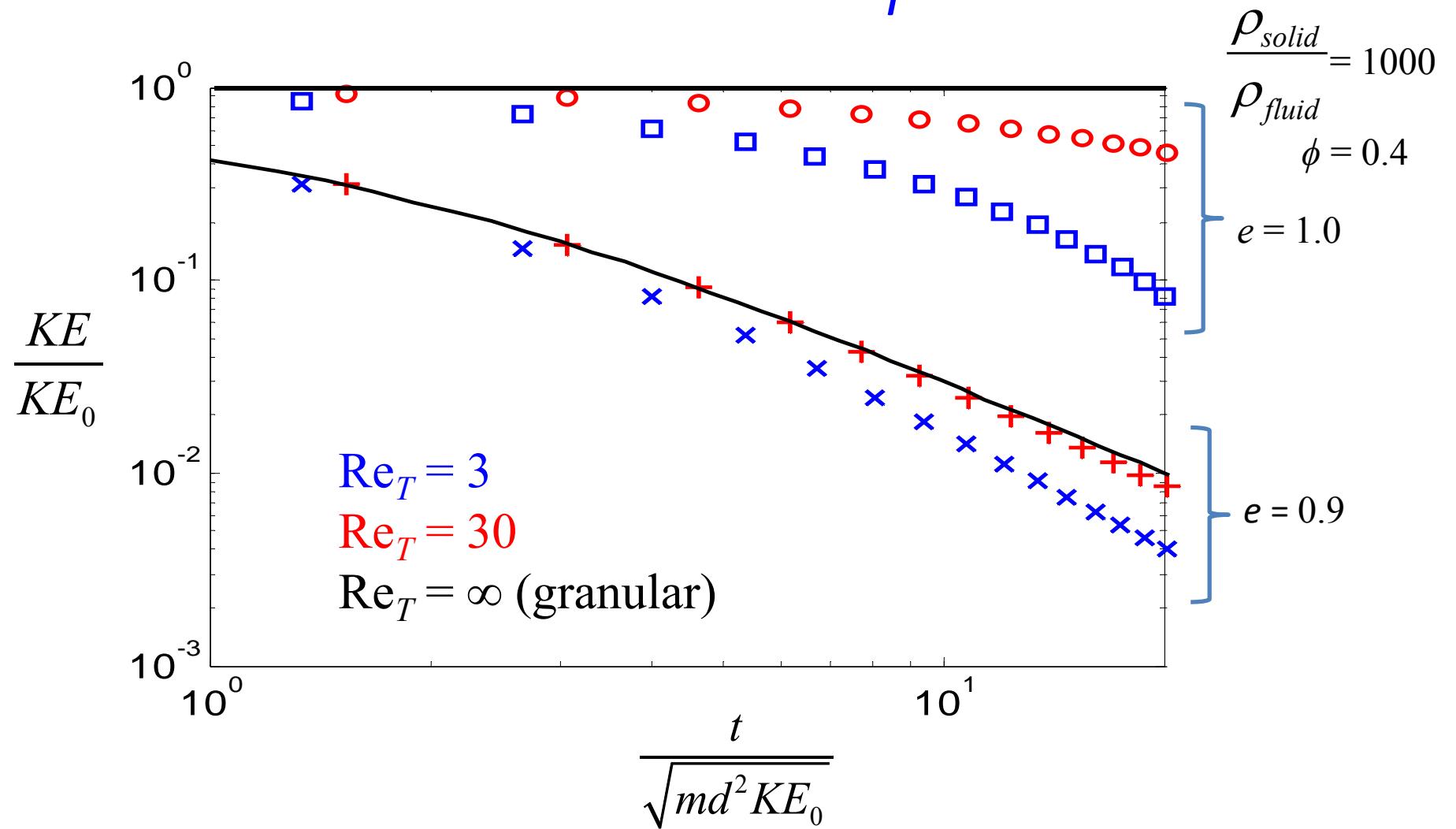
# Particle Clusters



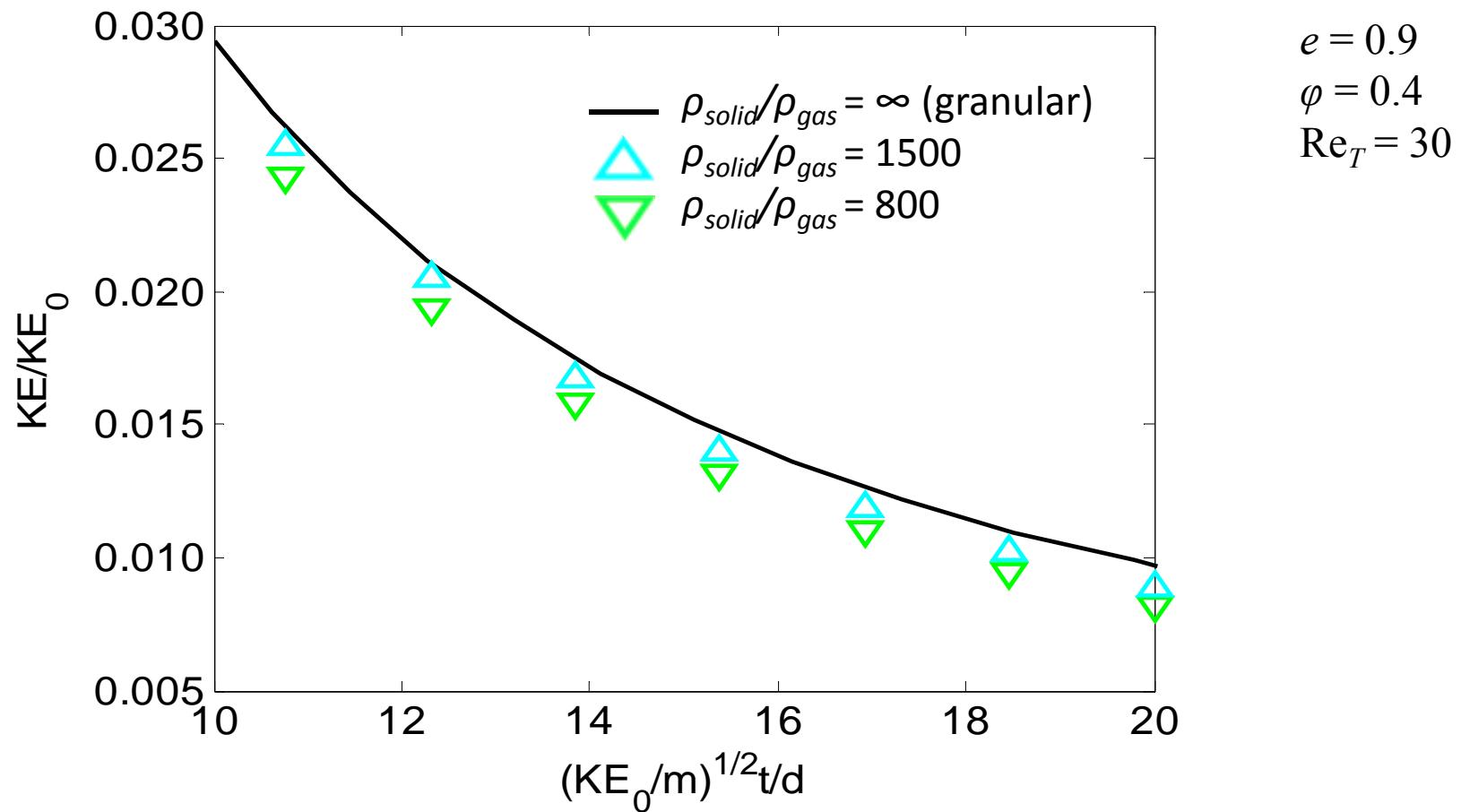
→

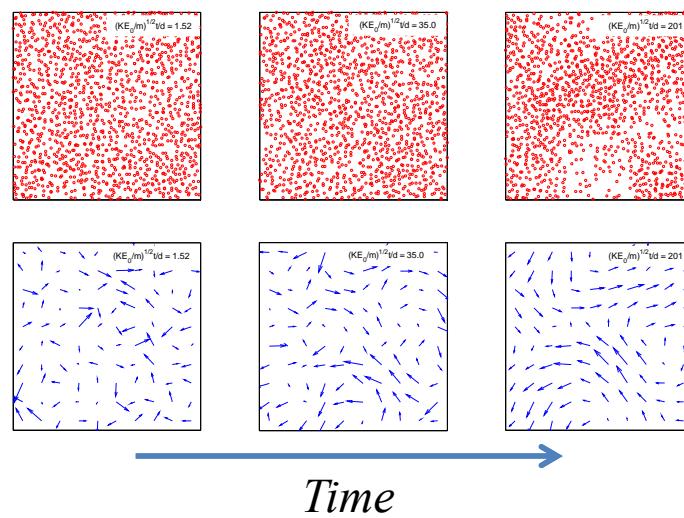
*Time*

# Influence of $Re_T$ and $e$



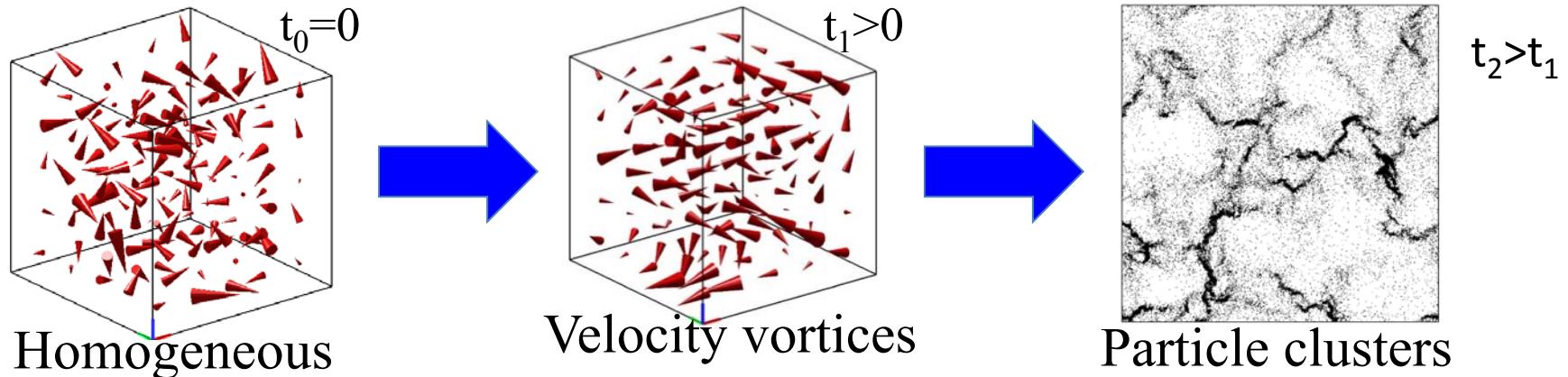
# Density Ratio





# Previous HCS work

Granular flow: *inelastic* solids; no gas (Goldhirsch 1993)



Gas-solid flow (Wylie & Koch 2000)

- *elastic* particles in viscous fluid flow

Focus: viscous effects

