University of Colorado at Boulder

Chemical and Biological Engineering

QUANTIFYING THE UNCERTAINTY OF KINETIC-THEORY PREDICTIONS OF CLUSTERING

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May 31st, 2012

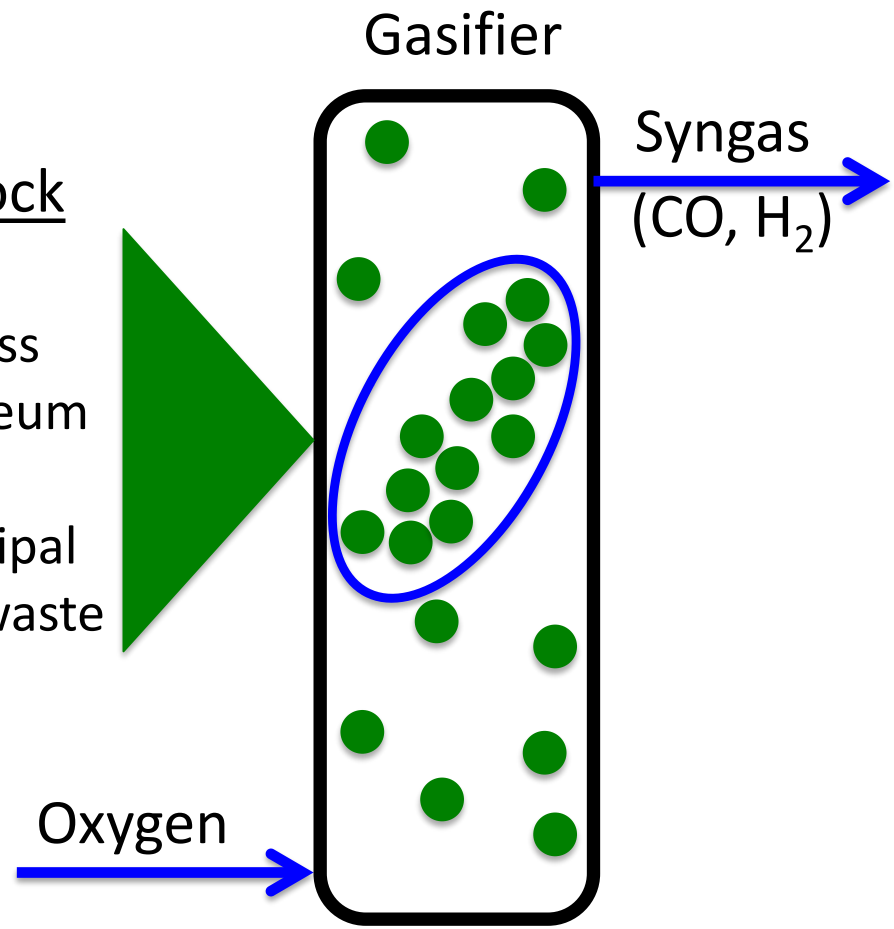
University Coal Research Conference

Pittsburgh, PA

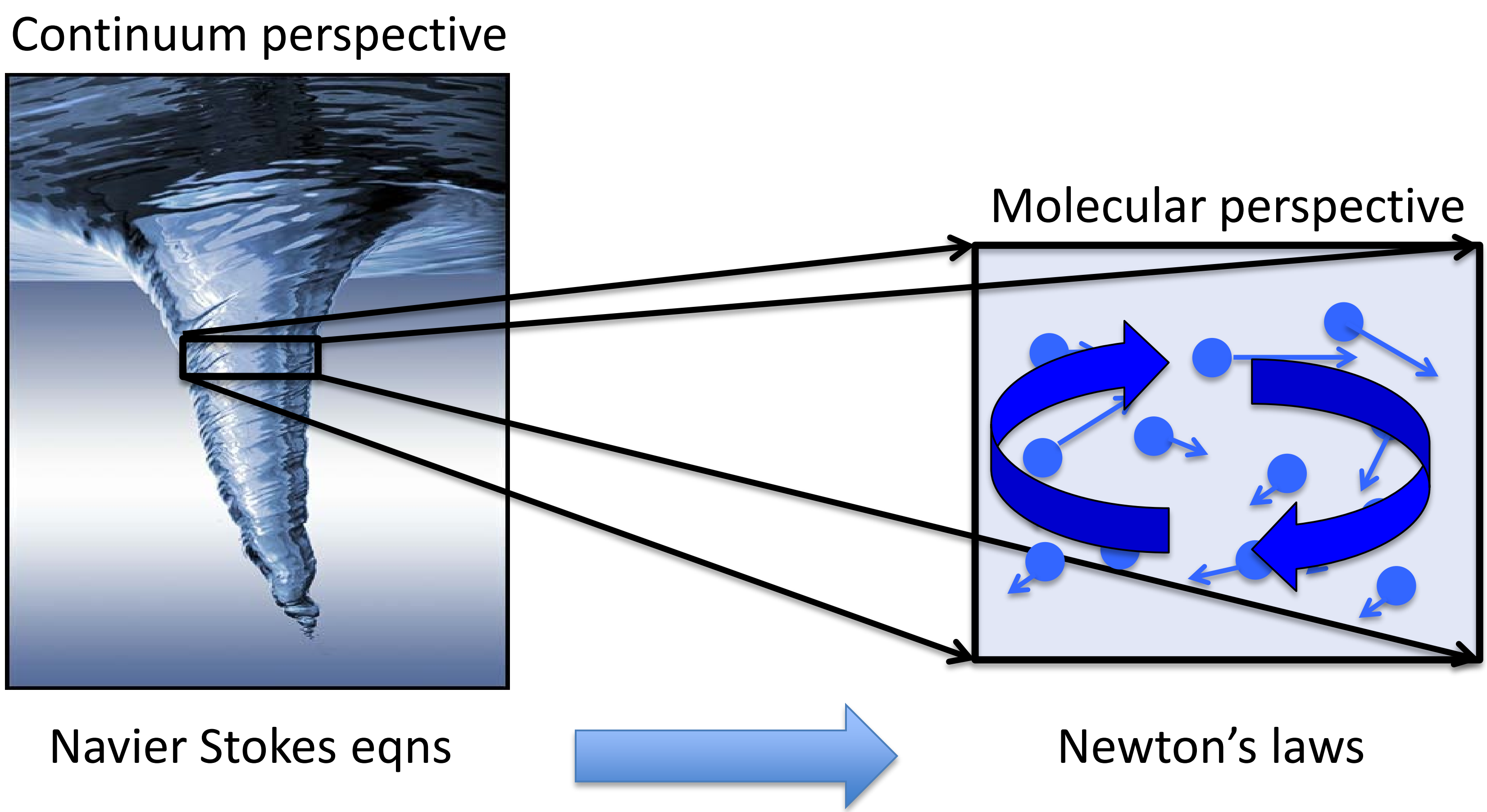
Motivation: Granular instabilities

<u>Feedstock</u>

- **Coal**
- Biomass
- Petroleum coke
- Municipal solid waste



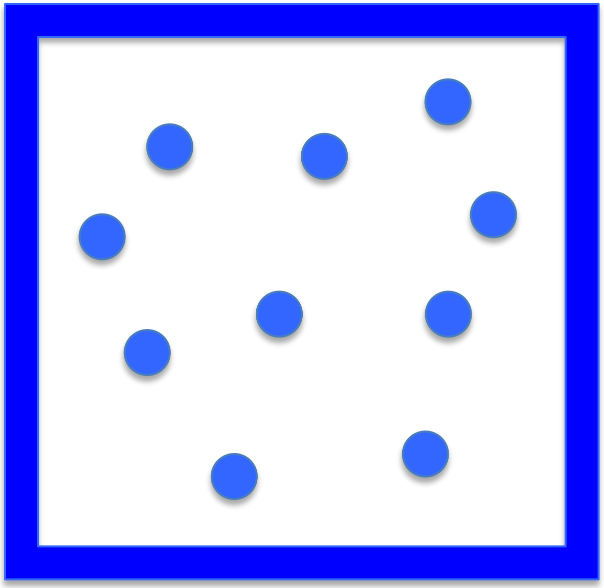
Fluid Analogy: Continuous vs. Discrete



System of Interest: Granular Flow

- The Homogeneous Cooling System (HCS)
  - No external forces
  - Periodic boundaries
  - No gradients in the hydrodynamic variables

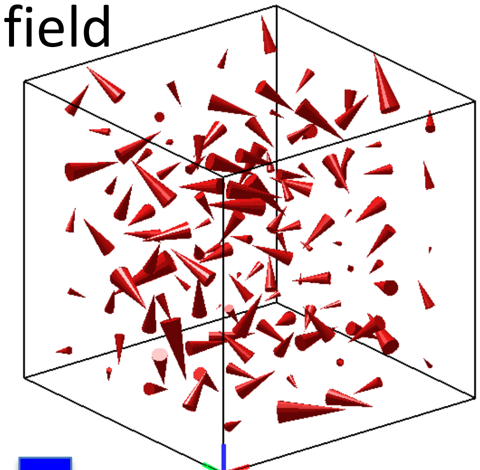
- Particle properties
  - Constant coefficient of restitution (e)
  - Monodisperse particles
  - No enduring contacts



Background

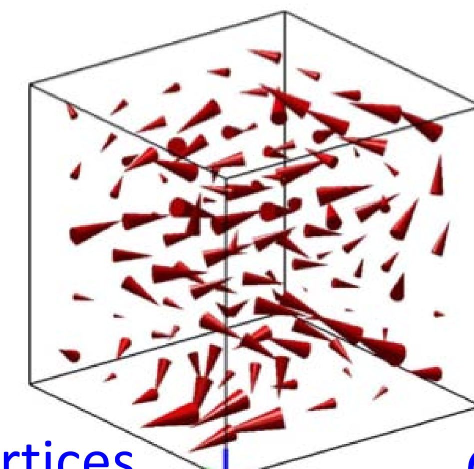
Molecular dynamics (MD) simulations of the HCS

Velocity field



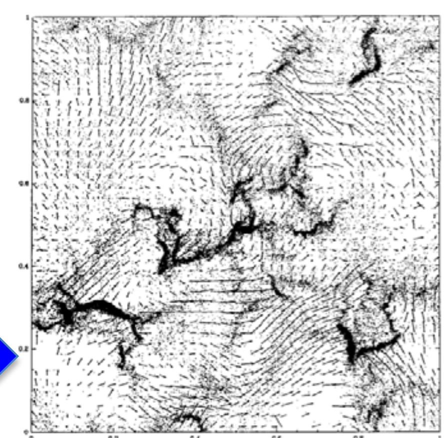
- Dissipative collisions
- Sufficiently large system domain

Velocity field



Vortices

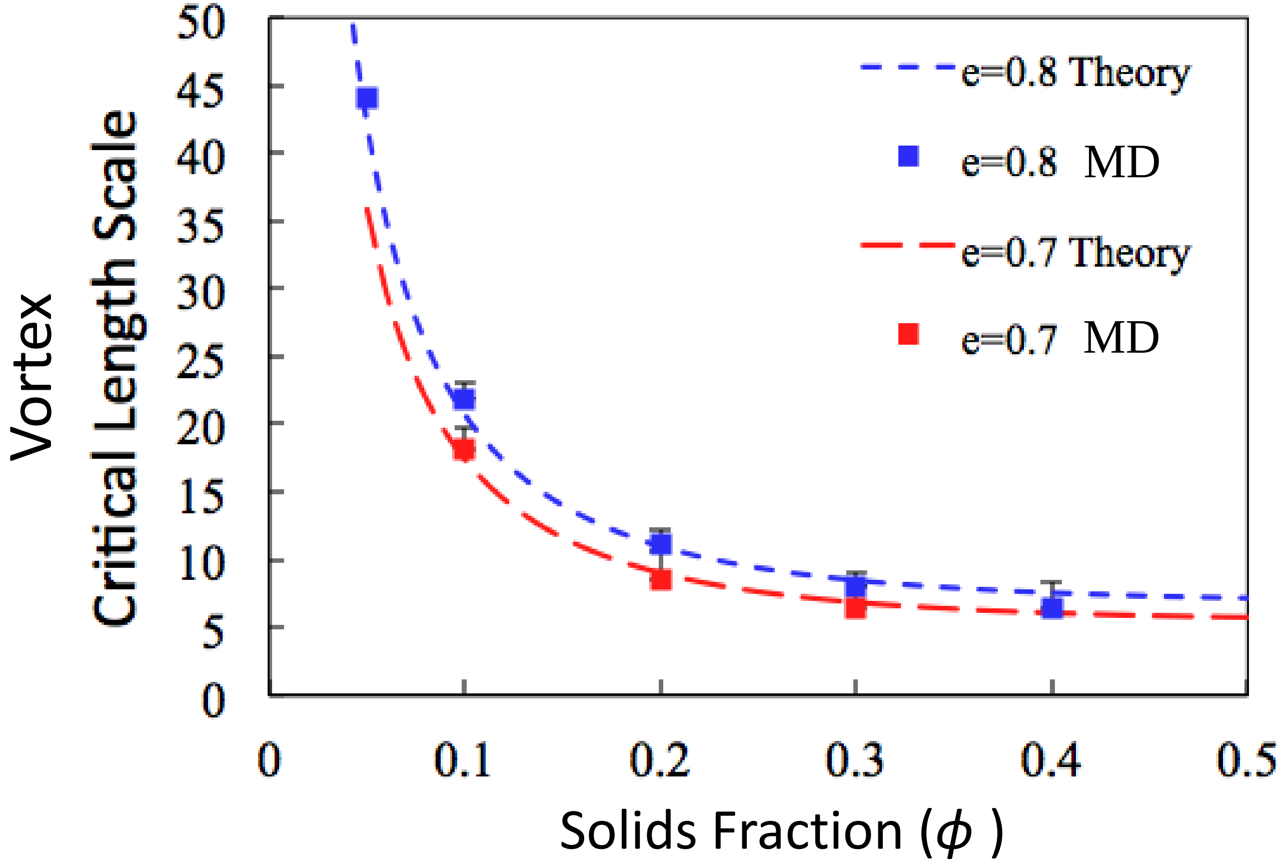
Particle locations



Clusters

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

Background



Mitrano et al., Phys. Fluids (2011)

Kinetic-Theory-based stability analysis: Garzó, 2005

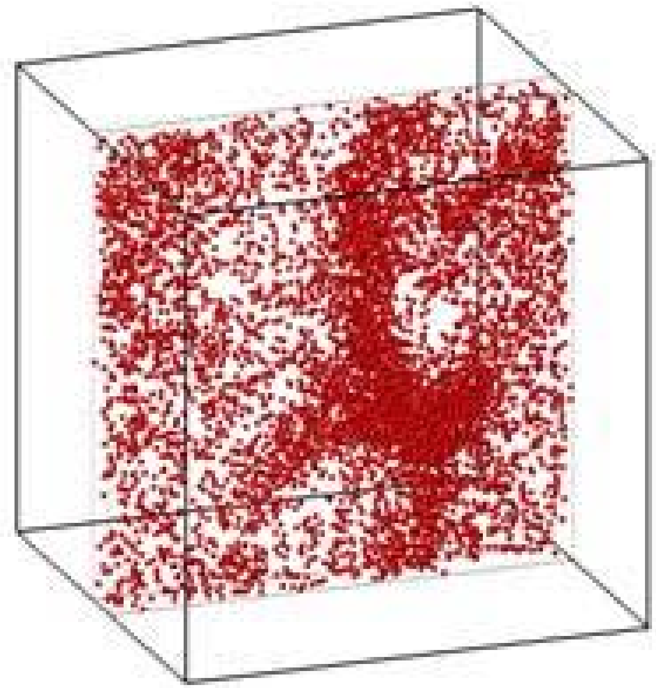
Objectives

Quantitatively assess Kinetic-theory-based predictions of instabilities via MD simulations

- Clustering instabilities
  - MD vs. CFD theory solution
- Effect of friction on instabilities
  - MD vs. *linear* stability analysis (LSA) of theory

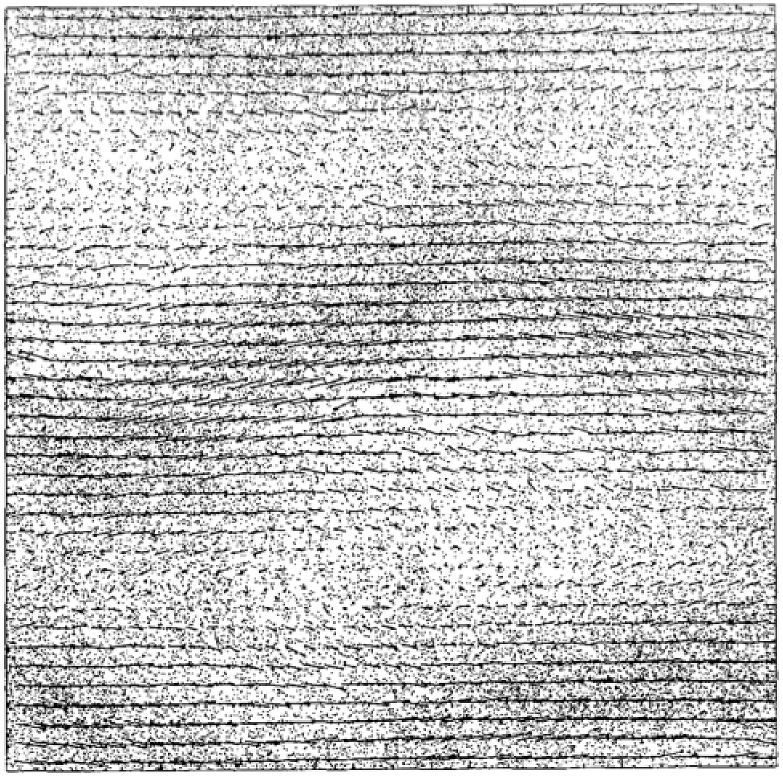
Molecular Dynamics

- Input
  - System length scale (*L/d*)
  - Restitution coefficient (*e*)
  - Volume fraction (ϕ)
- 3-dimensional domain
- Hard sphere collision model
  - Binary, instantaneous collisions
- Relevant Output
  - Particle positions & velocities

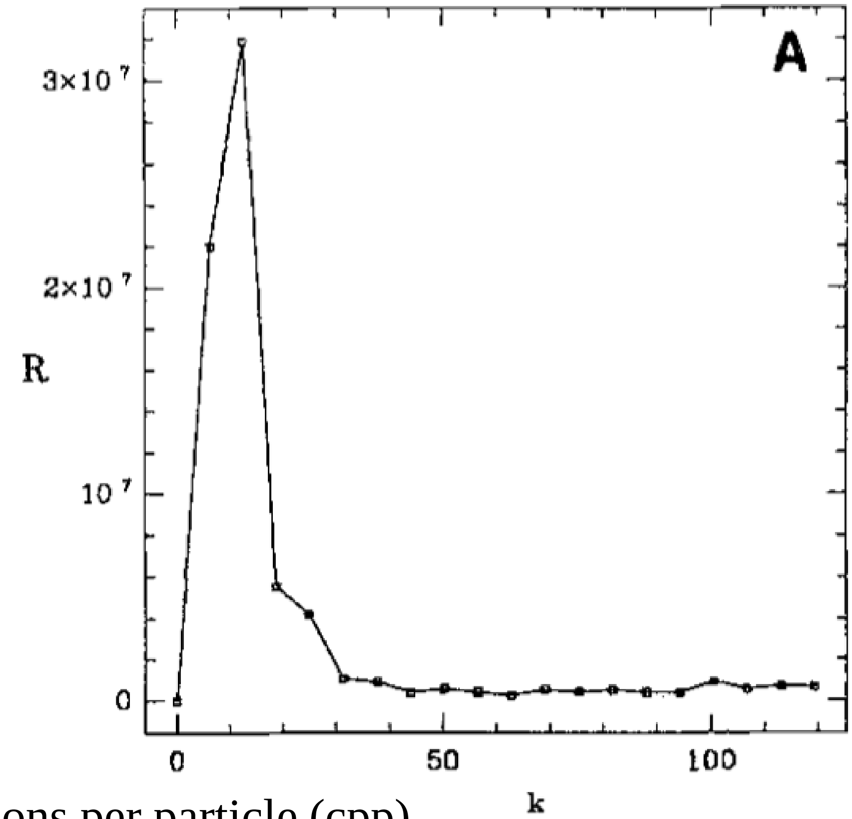


MD: Fourier Analysis

Particle positions (2D MD simulation)



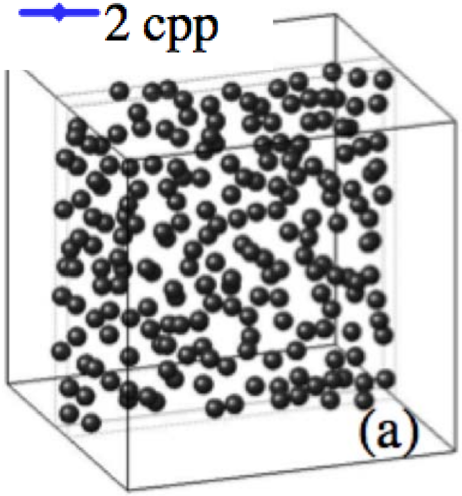
"Mass Mode" vs. wavenumber

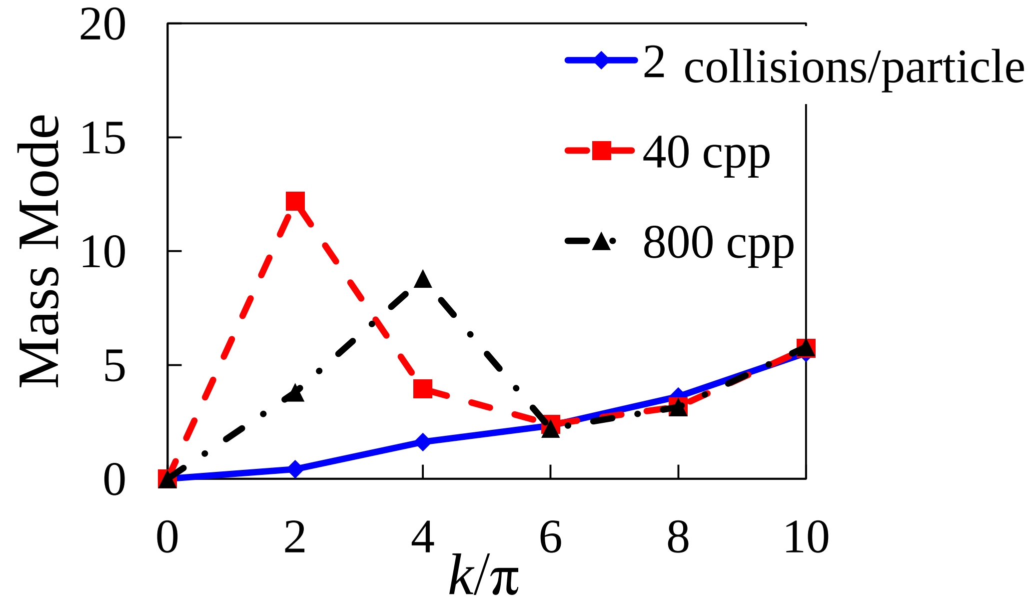


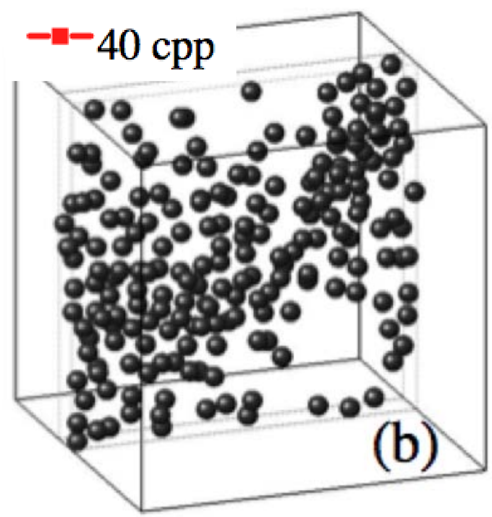
At 400 collisions per particle (cpp)

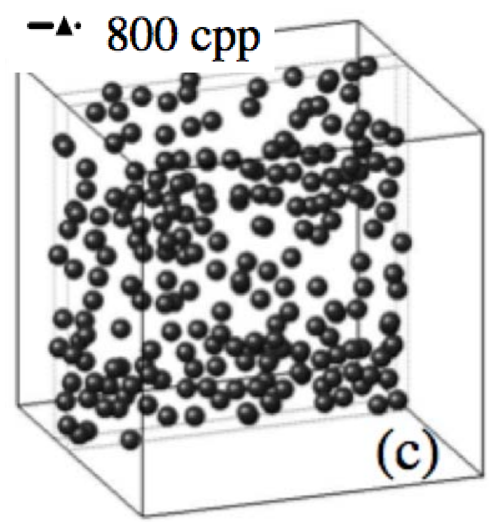
Goldhirsch, Tan, Zanetti, J. Sci. Comput. (1993)

MD: Fourier Analysis





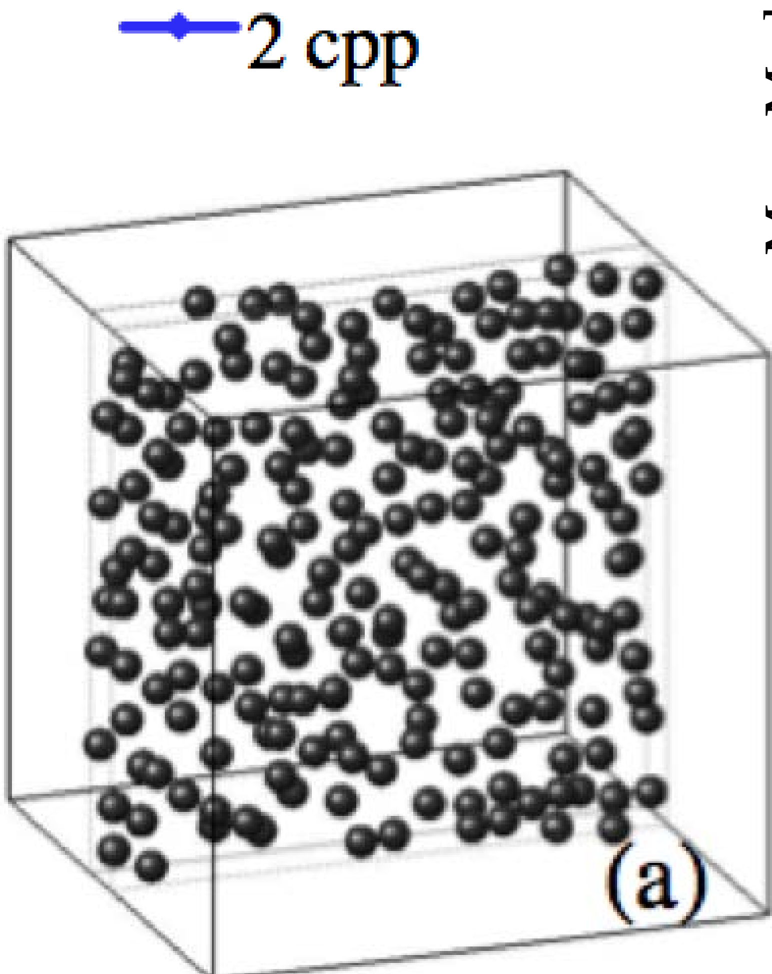


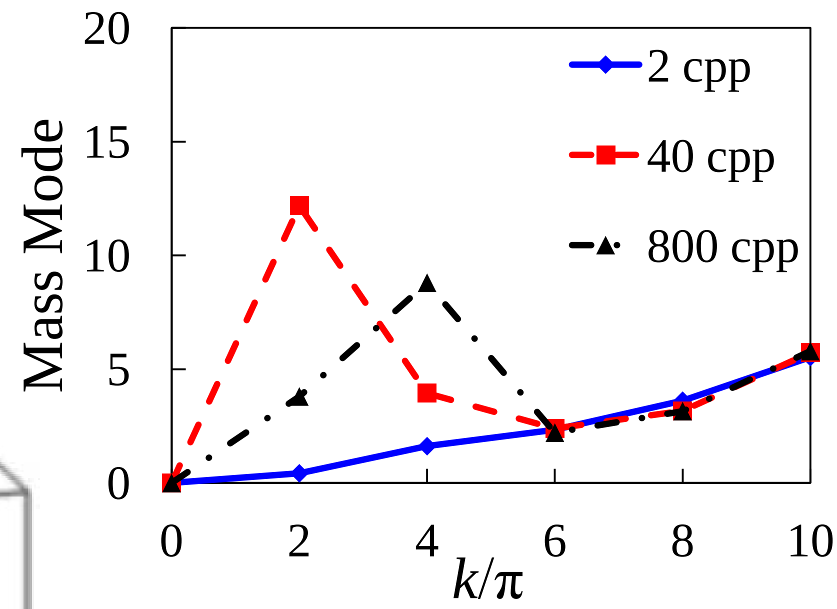


e=0.6, ϕ=0.2
N=2000

Mitrano et al.,
PRE (2012)

MD: Fourier Analysis





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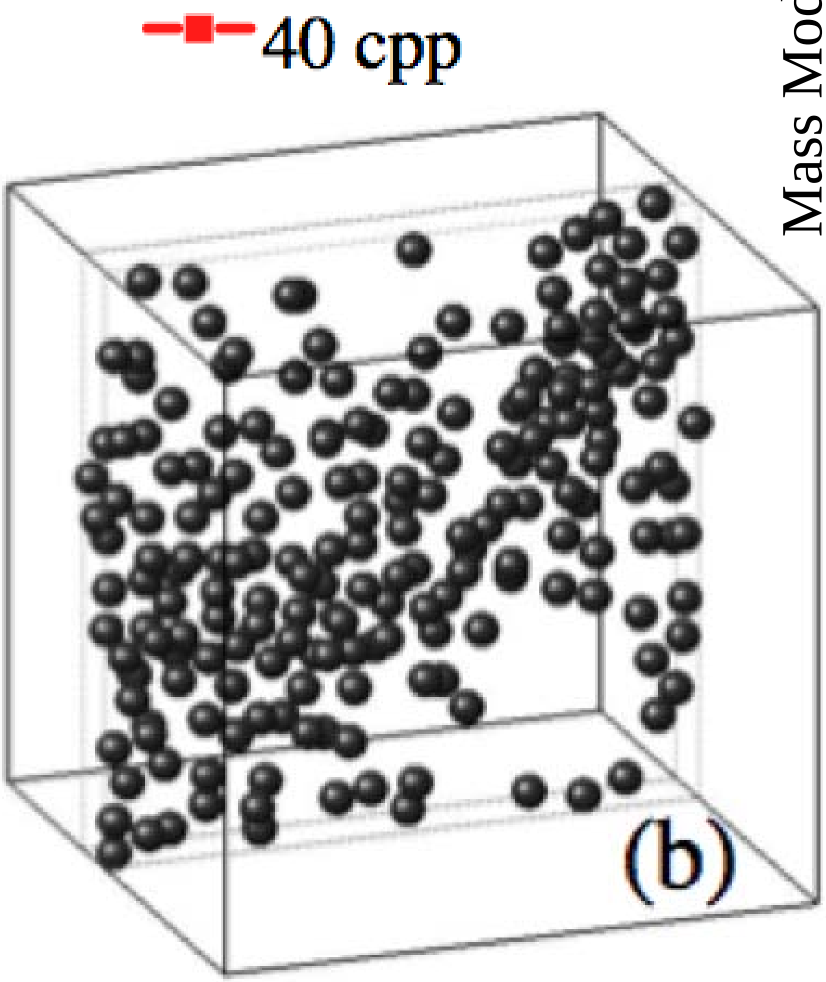

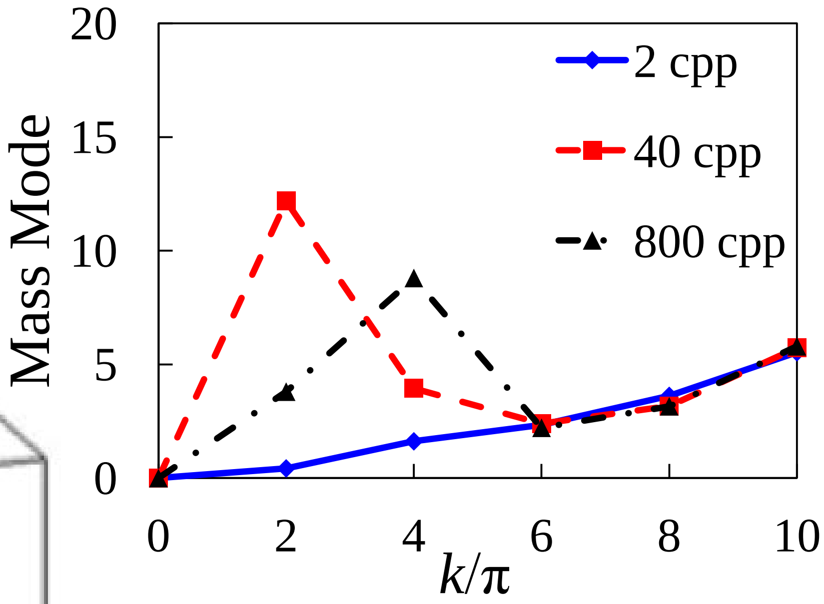

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Mitrano et al., PRE (2012)

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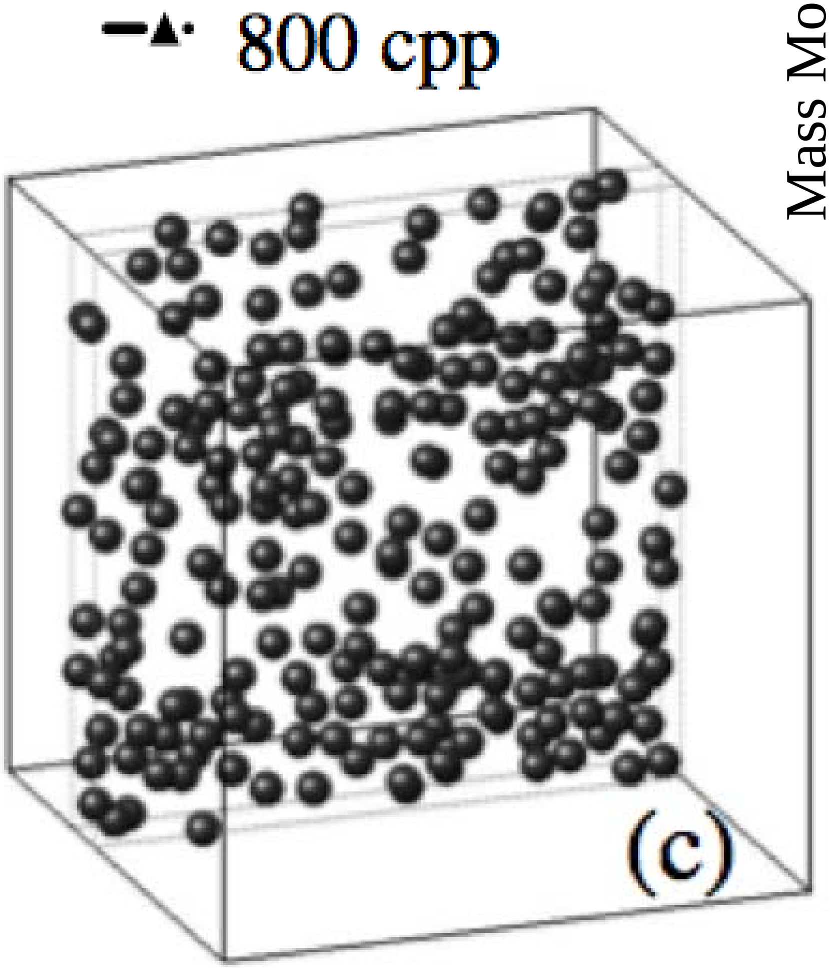

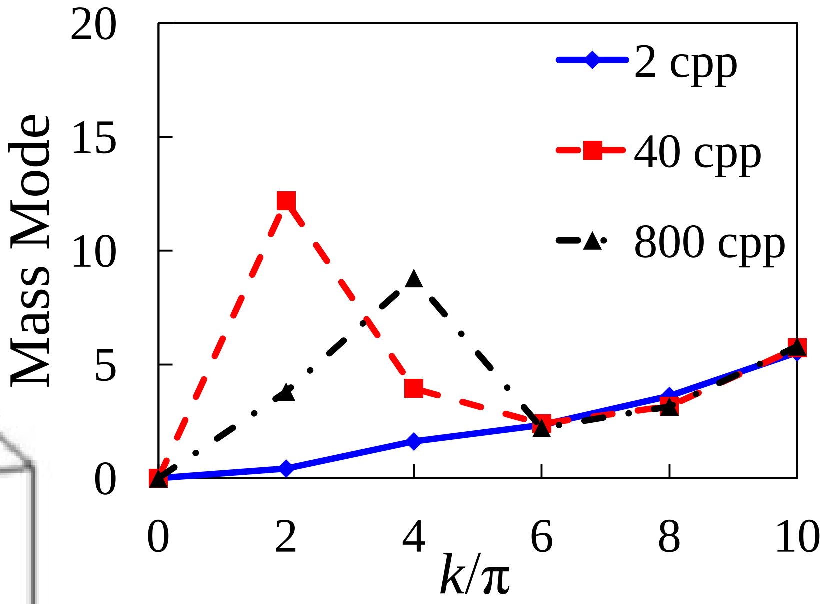

e=0.6, ϕ=0.2
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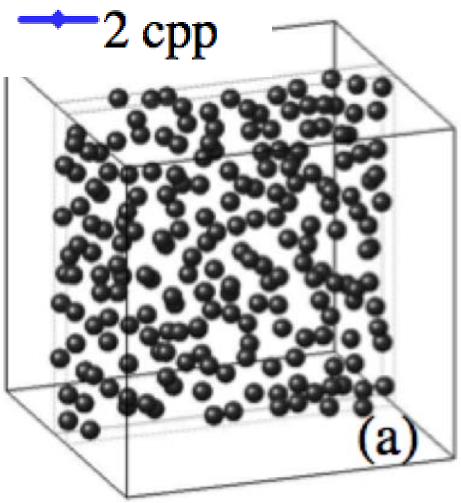
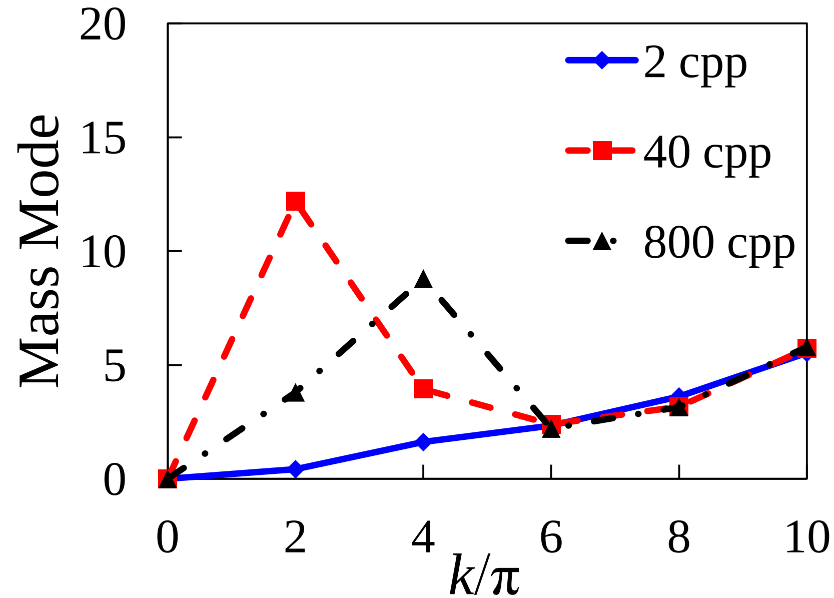
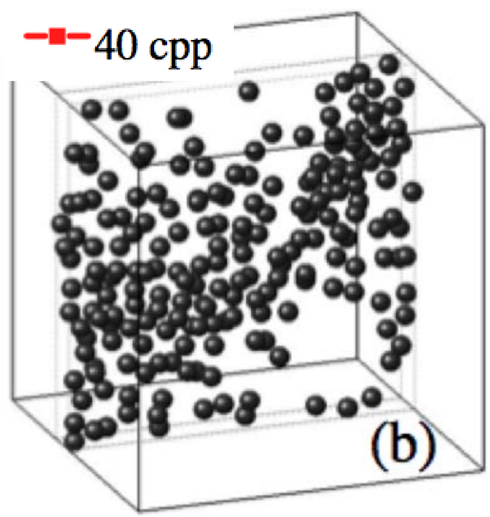
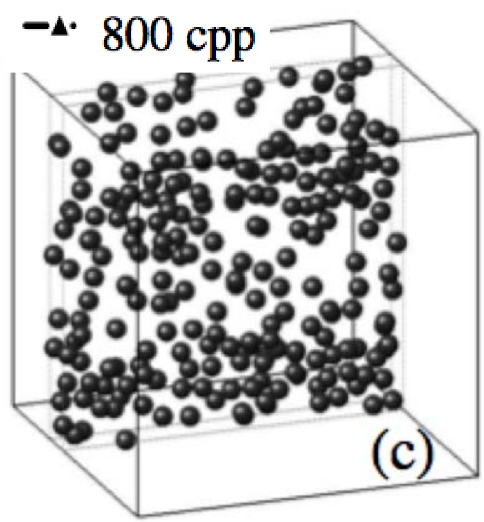
Mitrano et al., PRE (2012)

MD: Fourier Analysis









e=0.6, ϕ=0.2
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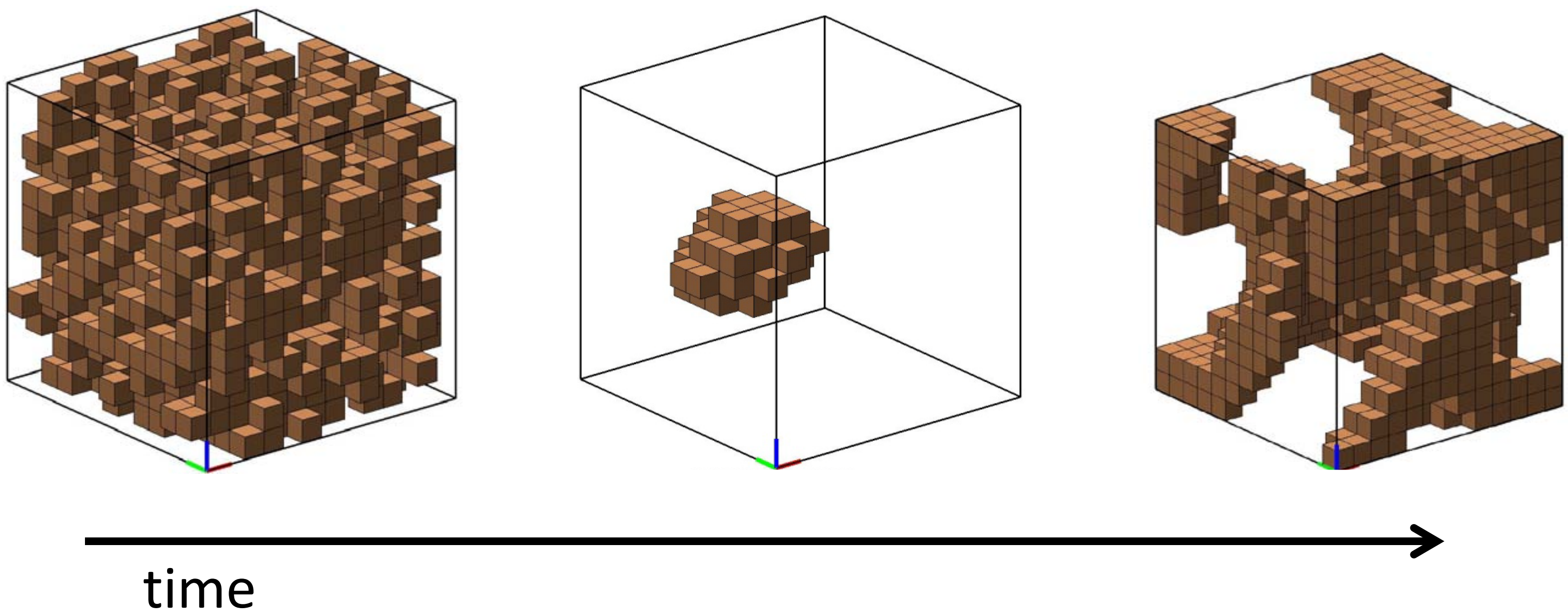
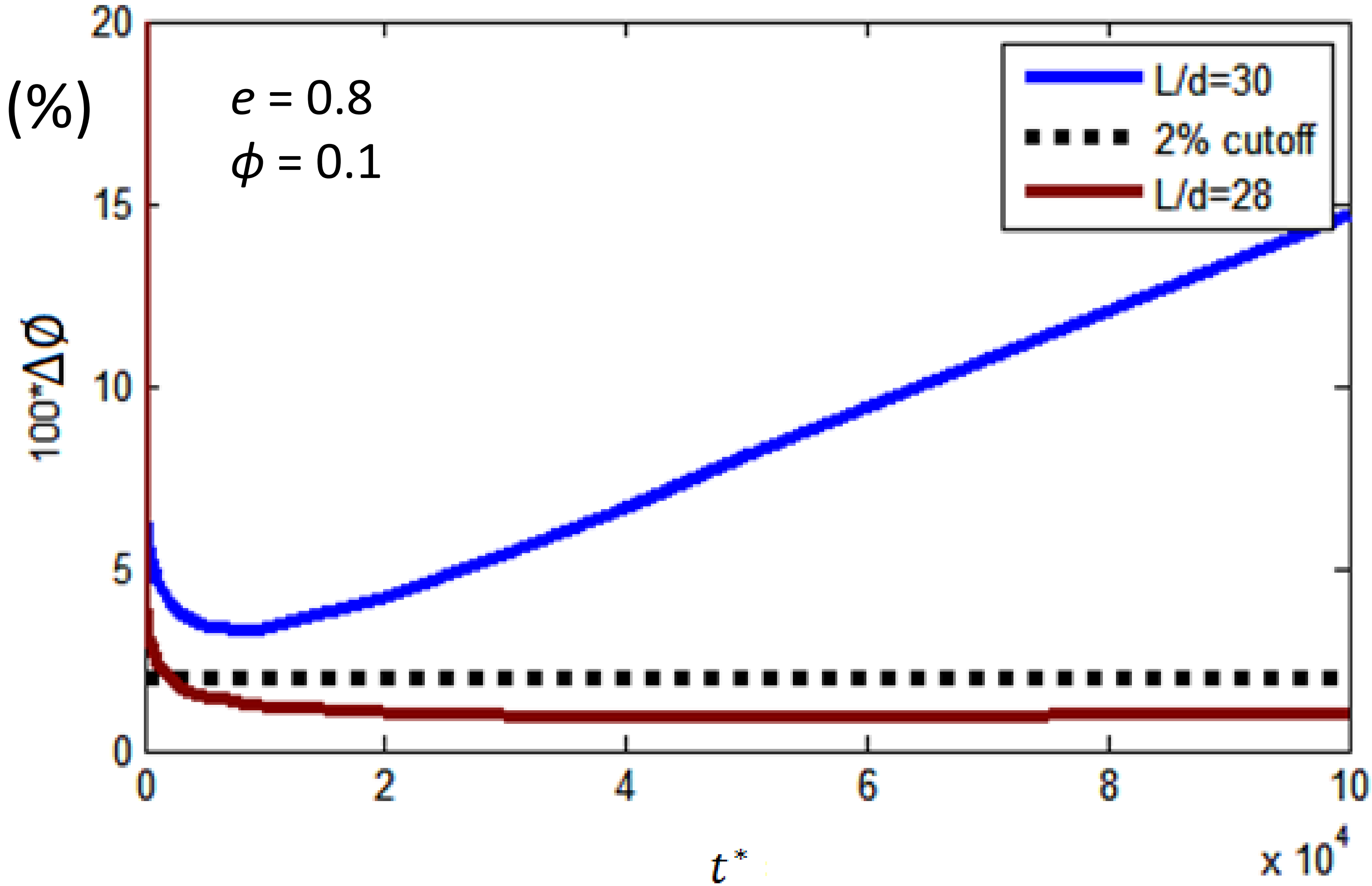
Mitrano et al.,
PRE (2012)

CFD: Cluster Detection

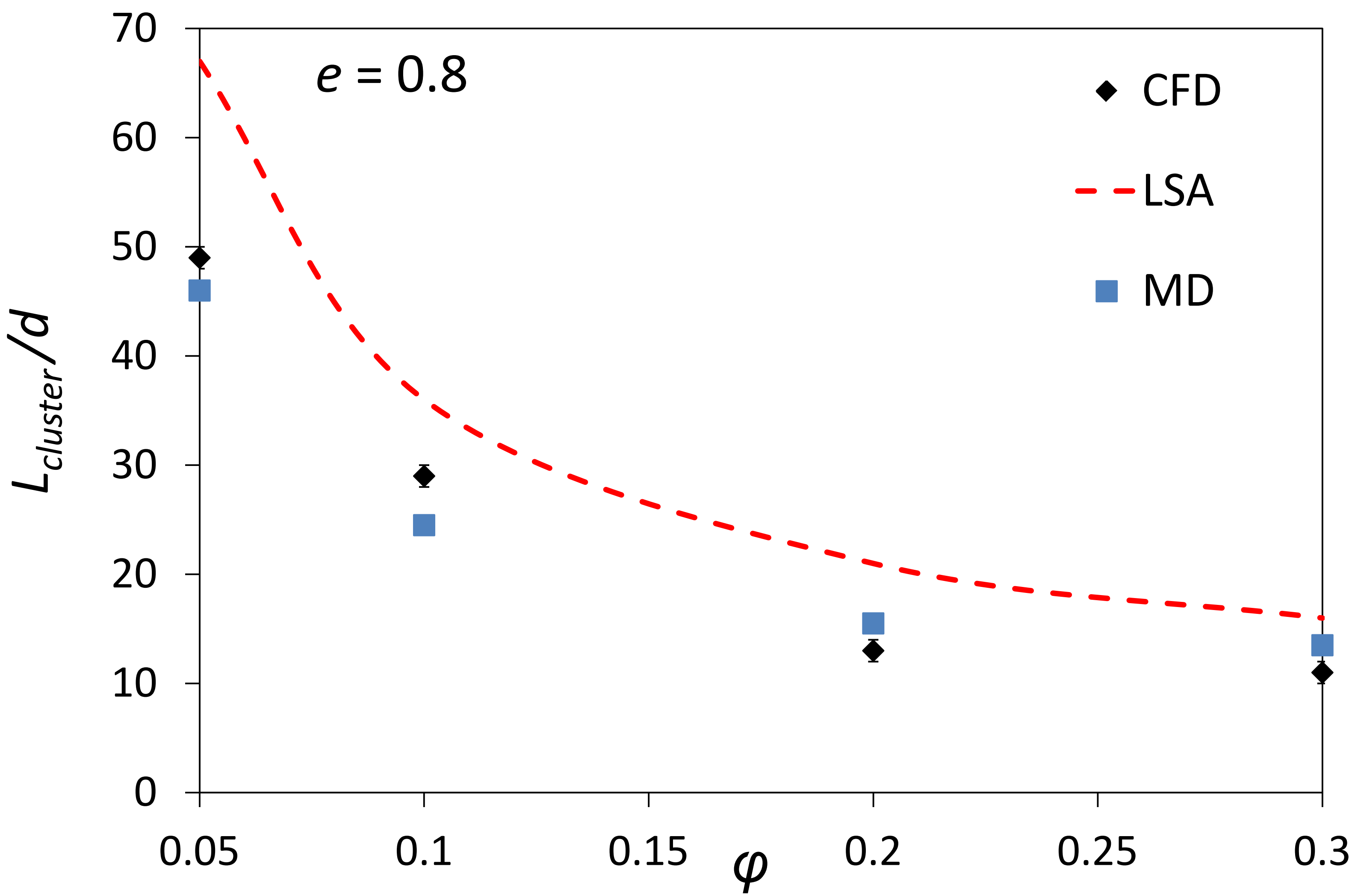


$$\Delta\varnothing = \frac{\varnothing_{cell,max} - \varnothing_{cell,min}}{\varnothing}$$

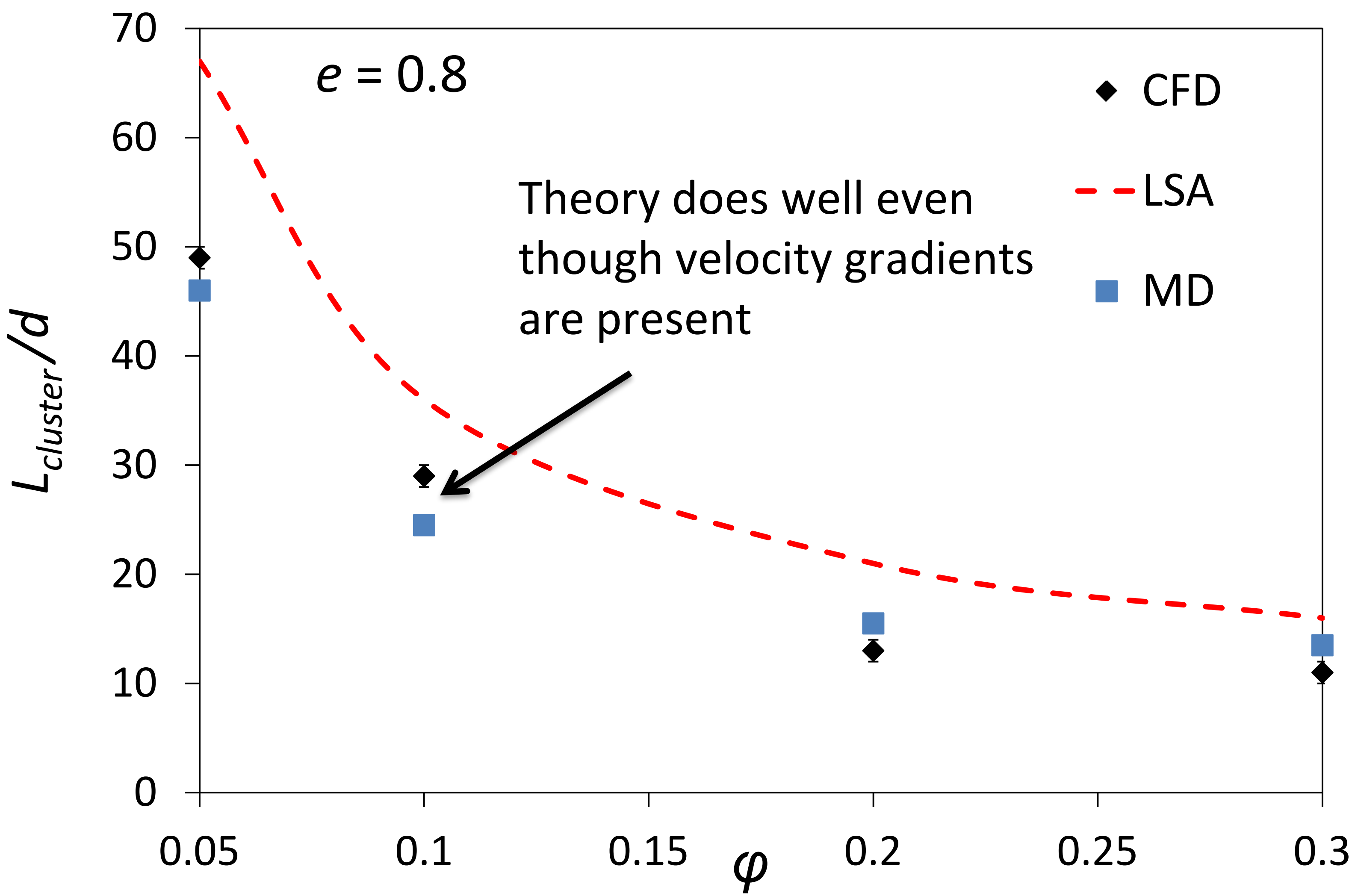
CFD: Cluster Detection



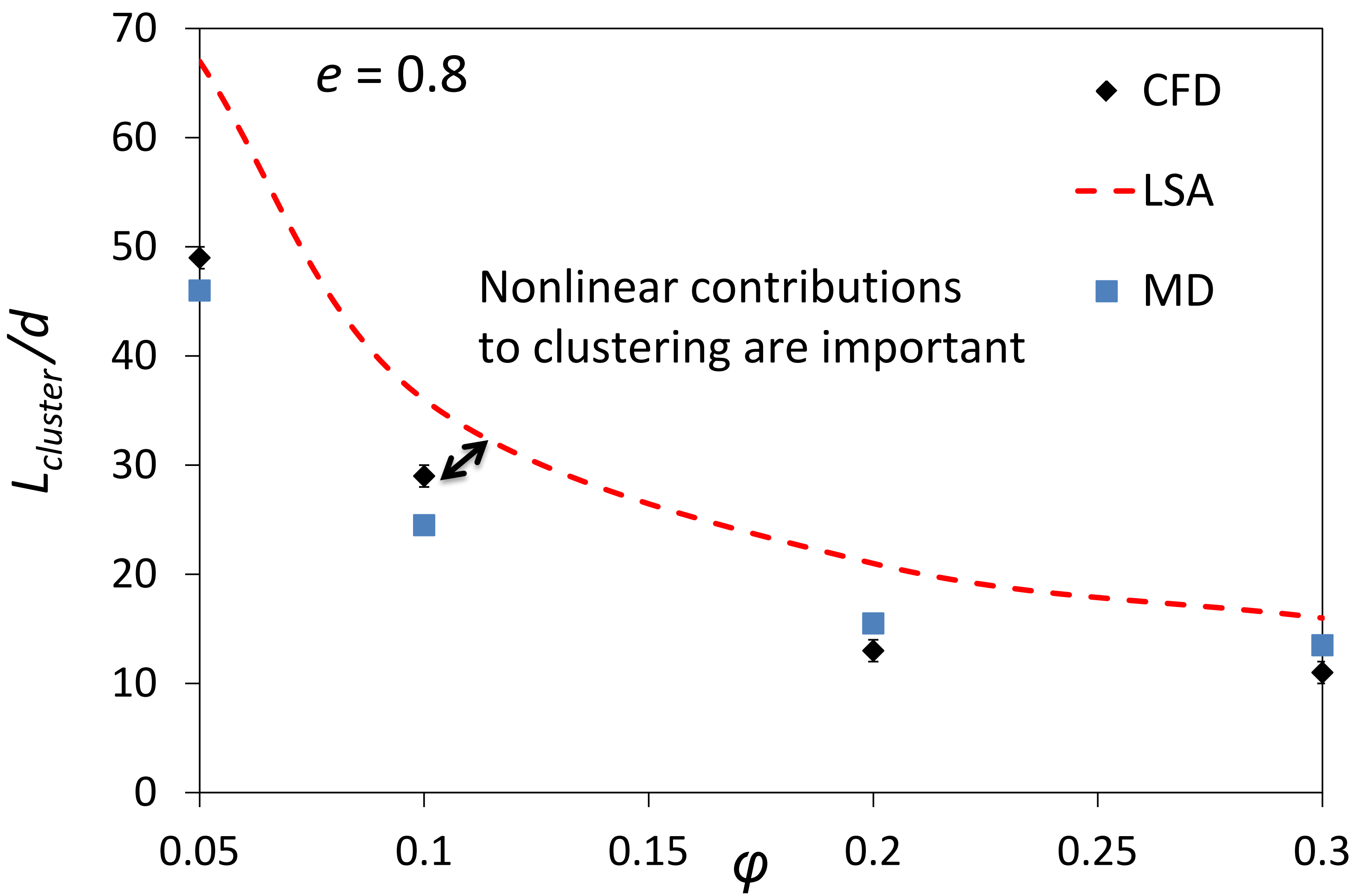
Clustering Onset: CFD-MD-LSA



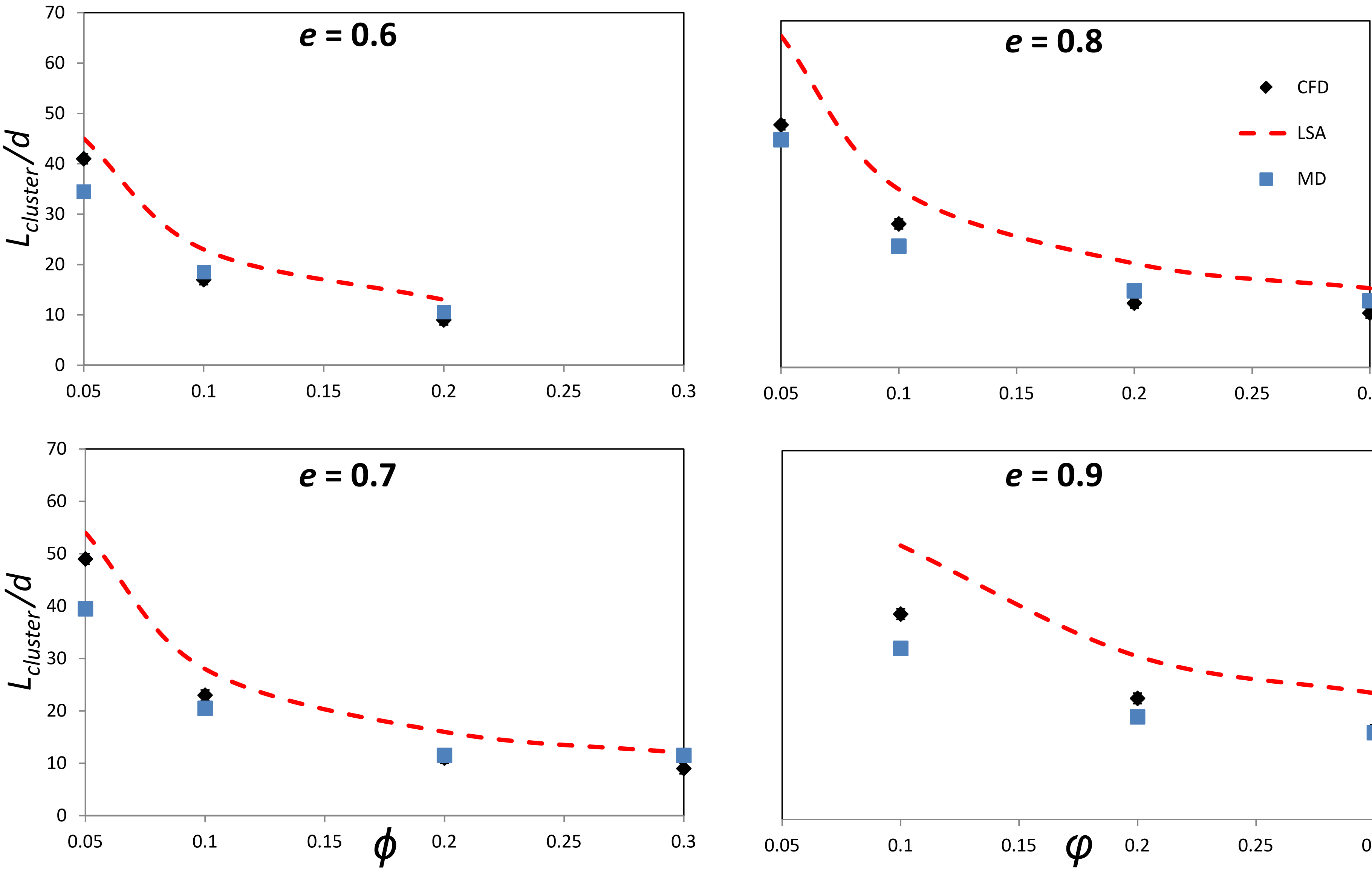
Clustering Onset: CFD-MD-LSA



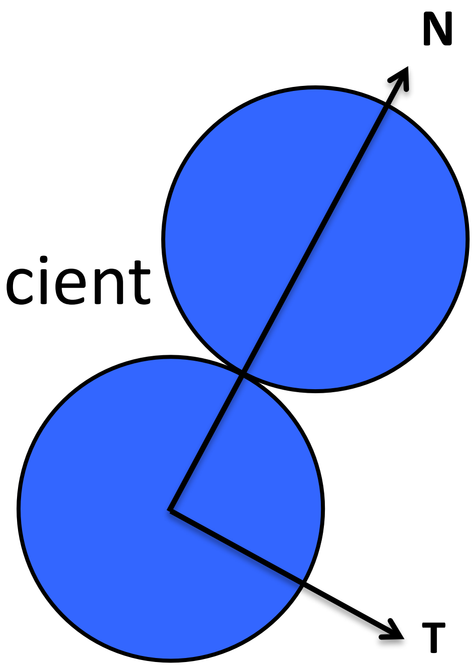
Clustering Onset: CFD-MD-LSA



Clustering Onset: CFD-MD-LSA



Types of Dissipation



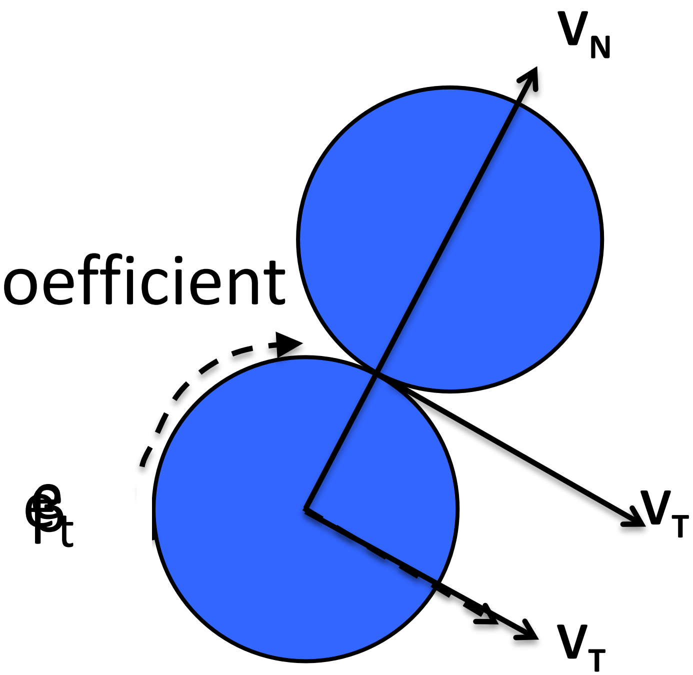
- Normal dissipation
  - Constant normal restitution coefficient

$$0 \leq e \leq 1$$

- Tangential dissipation
  - Constant tangential restitution coefficient

$$-1 \leq \beta \leq 1$$

Types of Dissipation



- Normal dissipation
  - Constant normal restitution coefficient

$$0 \leq e \leq 1$$

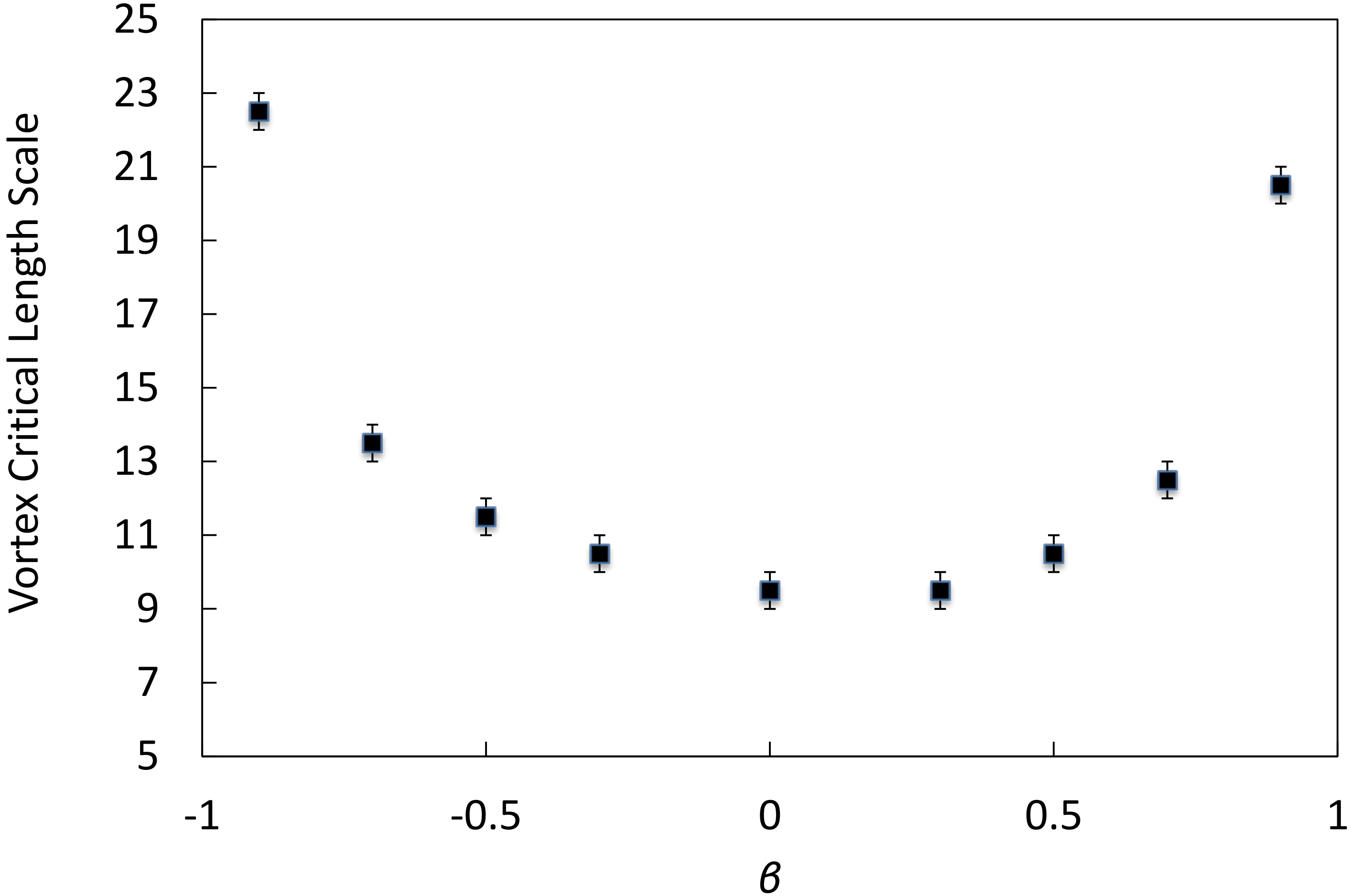
- Tangential dissipation
  - Constant tangential restitution coefficient

$$-1 \leq \beta \leq 1$$

No tangential impulse:
"perfectly smooth"

Elastic tang. Impulse:
"perfectly rough"

Elastic Results

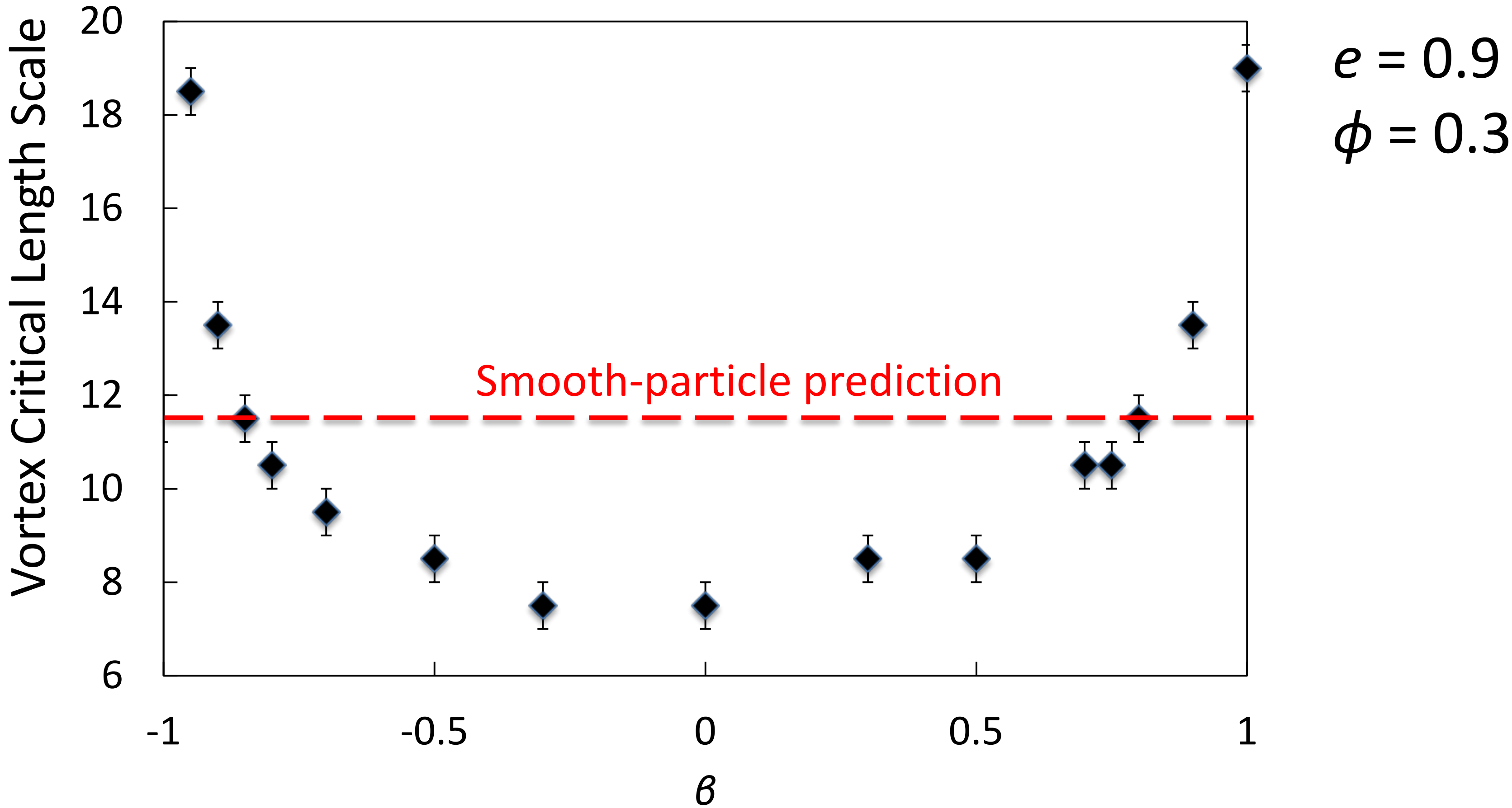


e = 1
ϕ = 0.3

(perfectly smooth)

(perfectly rough)

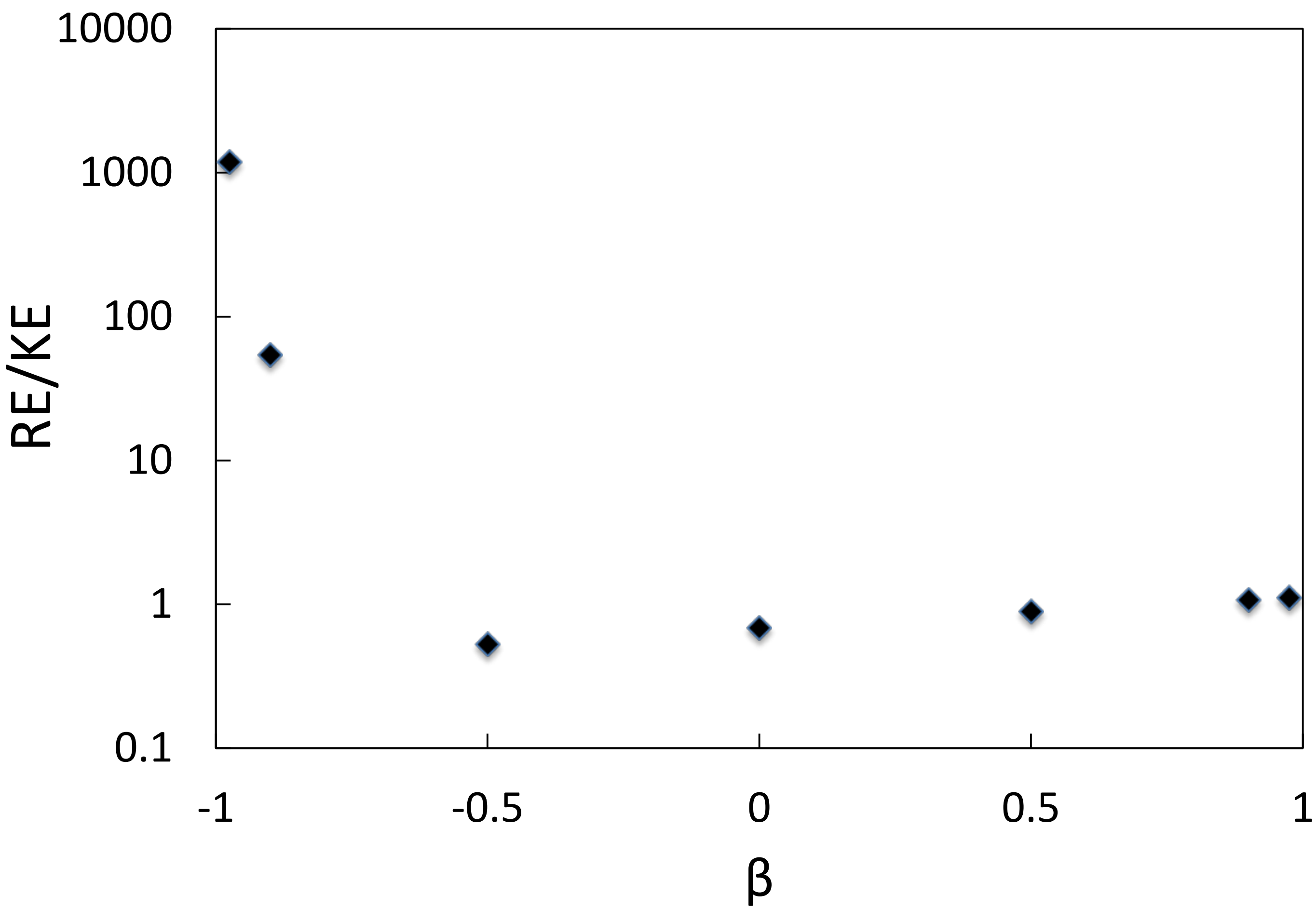
Frictional Results



Extra note (not in original presentation)

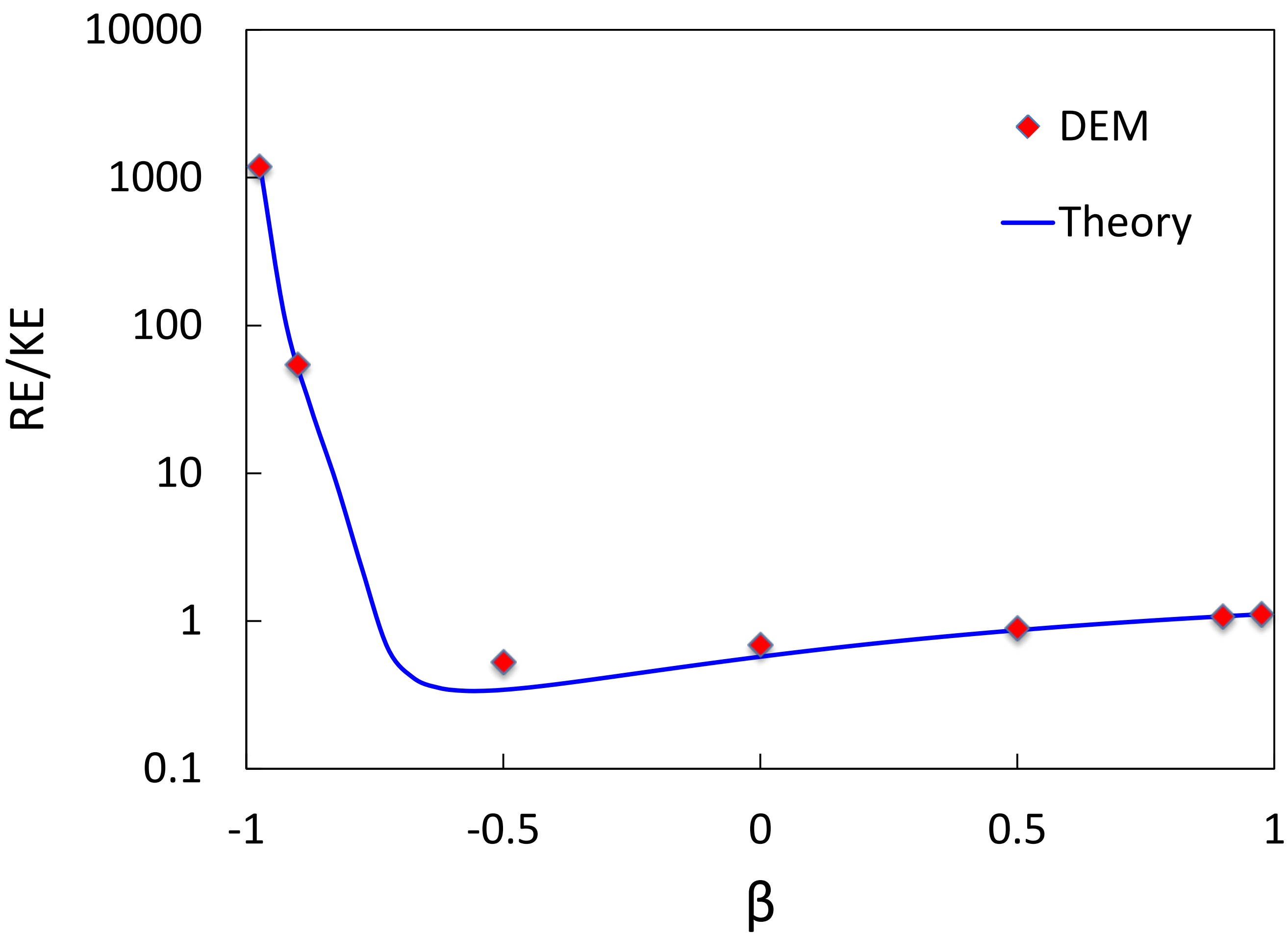
- Very strange behavior for nearly smooth and nearly perfectly (elastically) rough particles can be traced to the energy ratio and more directly the fact that we only allow for “sticking” collisions that depend on the relative tangential overall velocity. Highly rotating particle are caused to separate since the tangential component is so large giving to a large tangential impulse. (vortex motion is dependent on the tangential translation alignment). E_t is a tangential translational restitution coefficient that is well correlated to vortex motion- high et values hinder vortex formation. Next slide shows that the particle rotation is very high on the left side. As particle become more and more rough the tangential impulse is inherently larger. We briefly examine a friction model that allows for either sticking or coulomb-governed sliding collisions a few slides later.

Temperature Ratio (Rotation/Translation)



e = 0.9
ϕ = 0.3

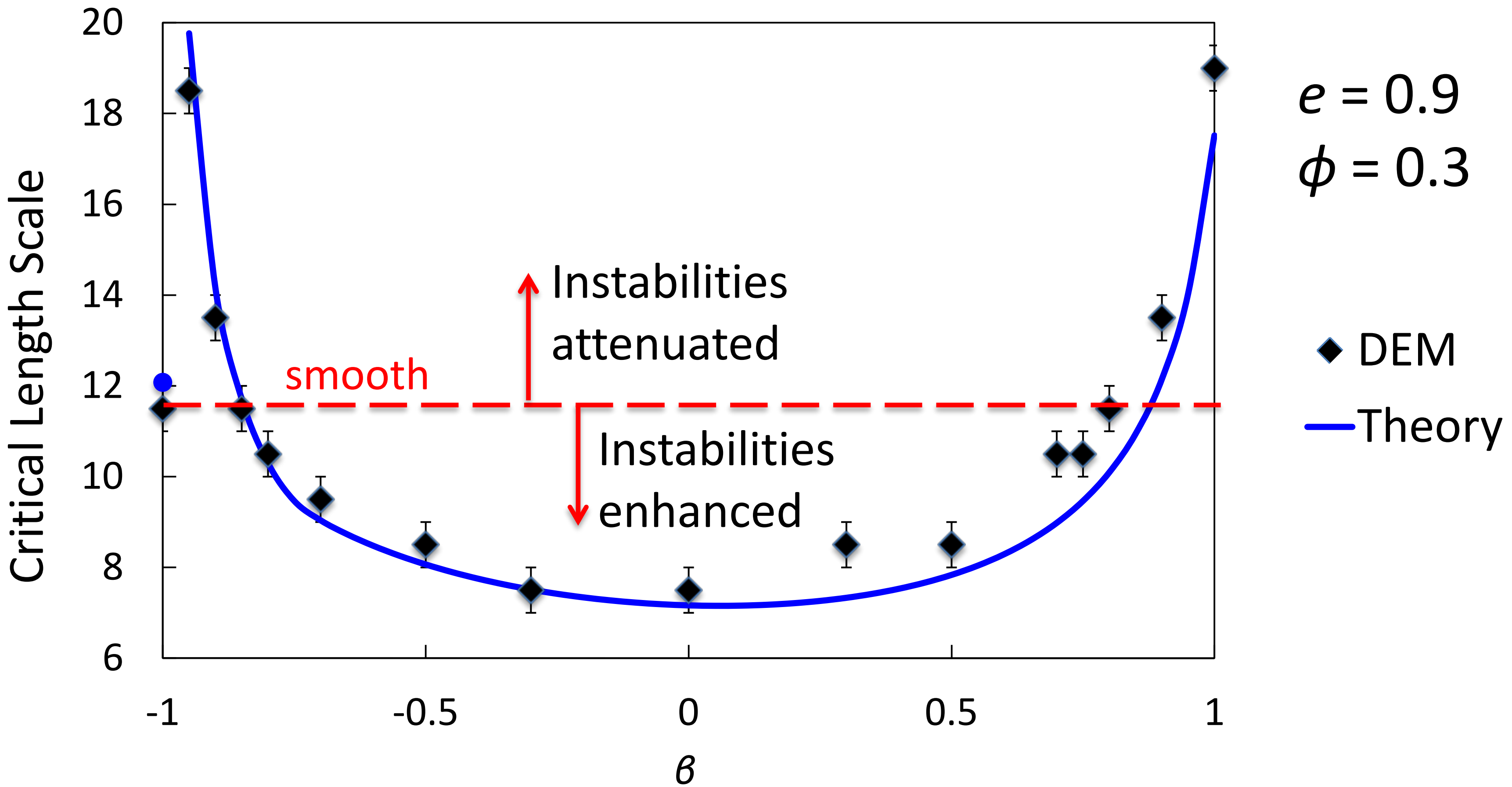
Temperature Ratio (DEM-theory comparison)



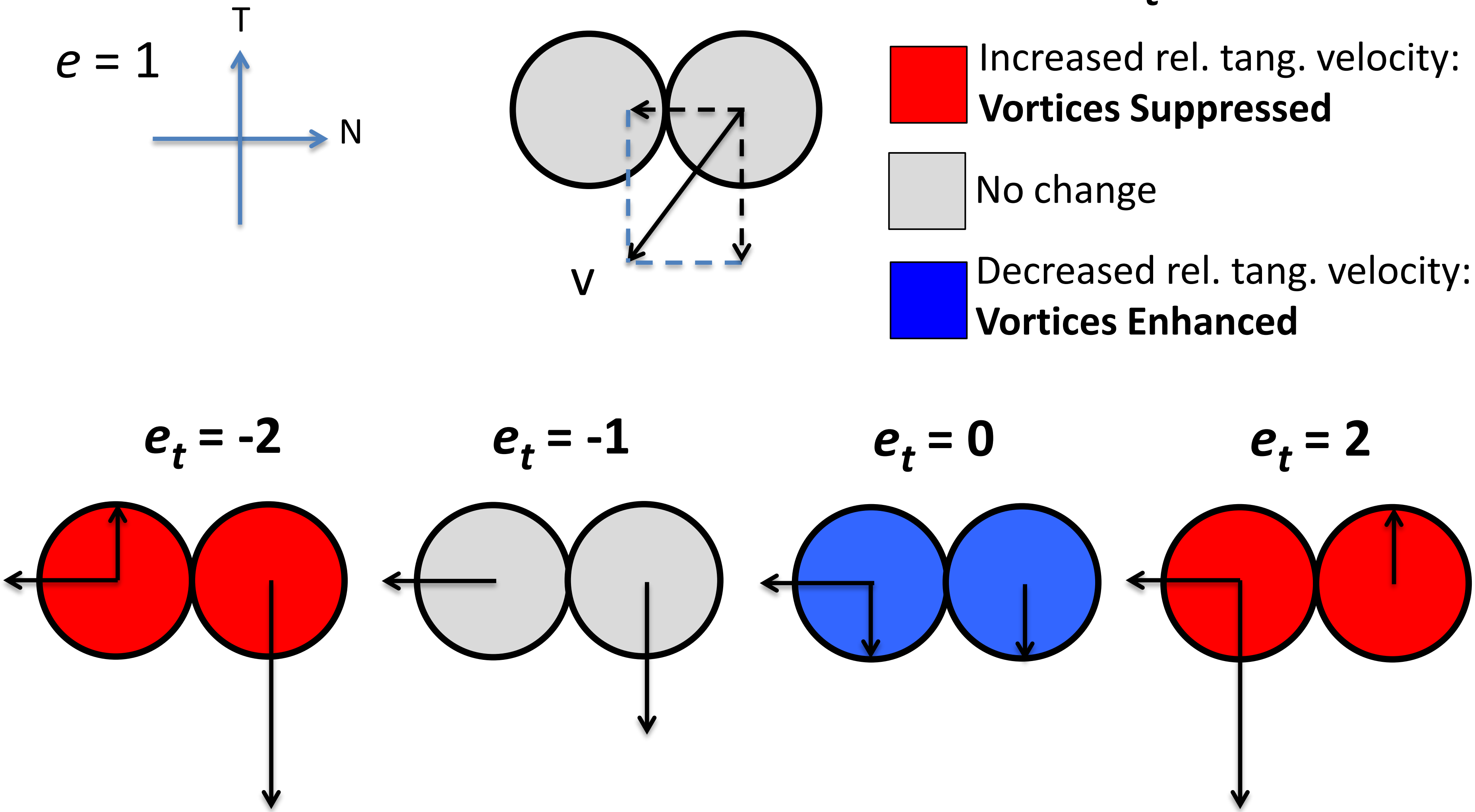
e = 0.9
ϕ = 0.3

Theory: Santos, Kremer, Garzó, *Prog Theor Phys, Suppl* (2010)

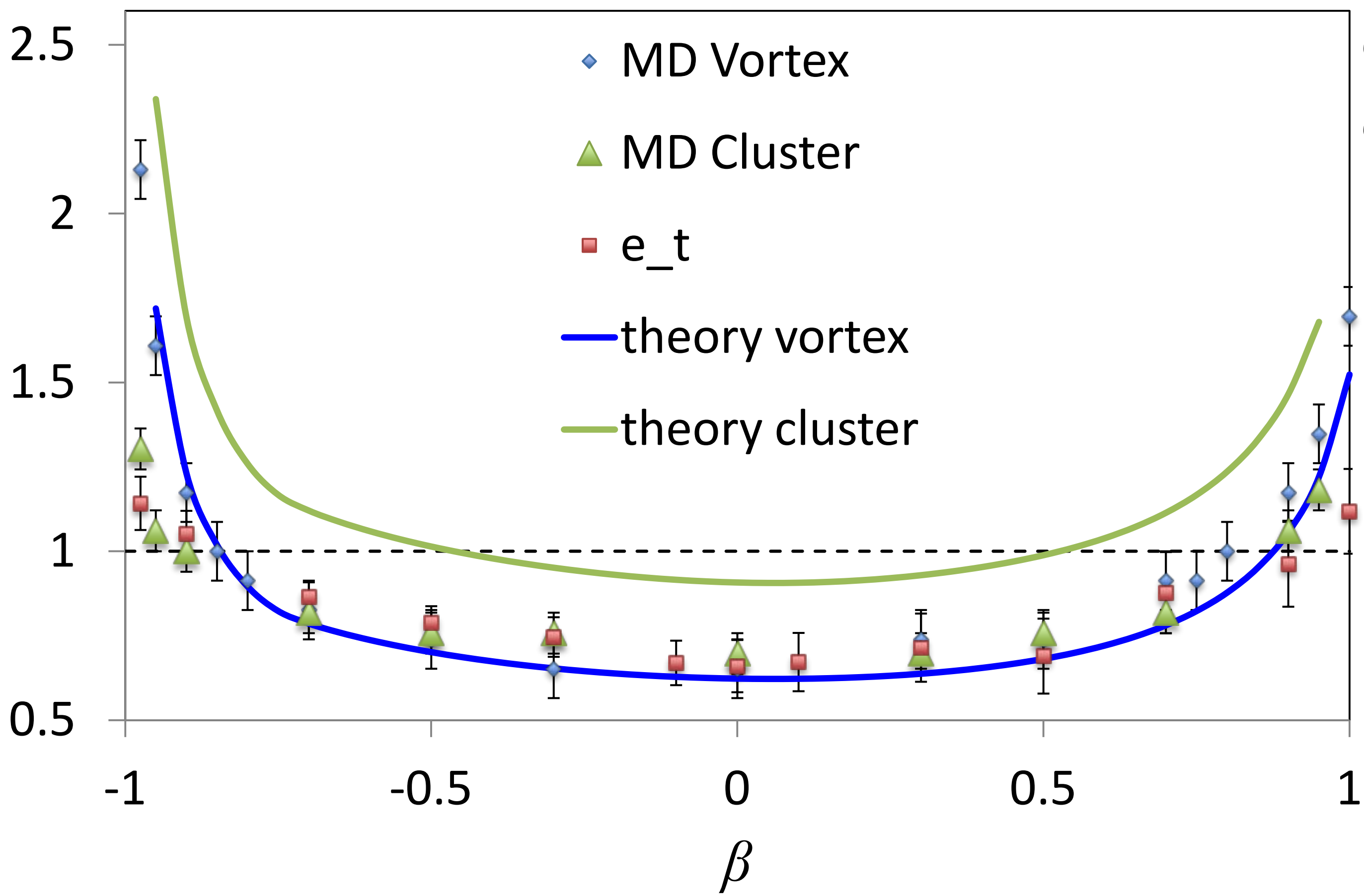
Frictional Results



Tangential *Translational* Restitution Coefficient (e_t)



Onsets normalized to smooth-particle value



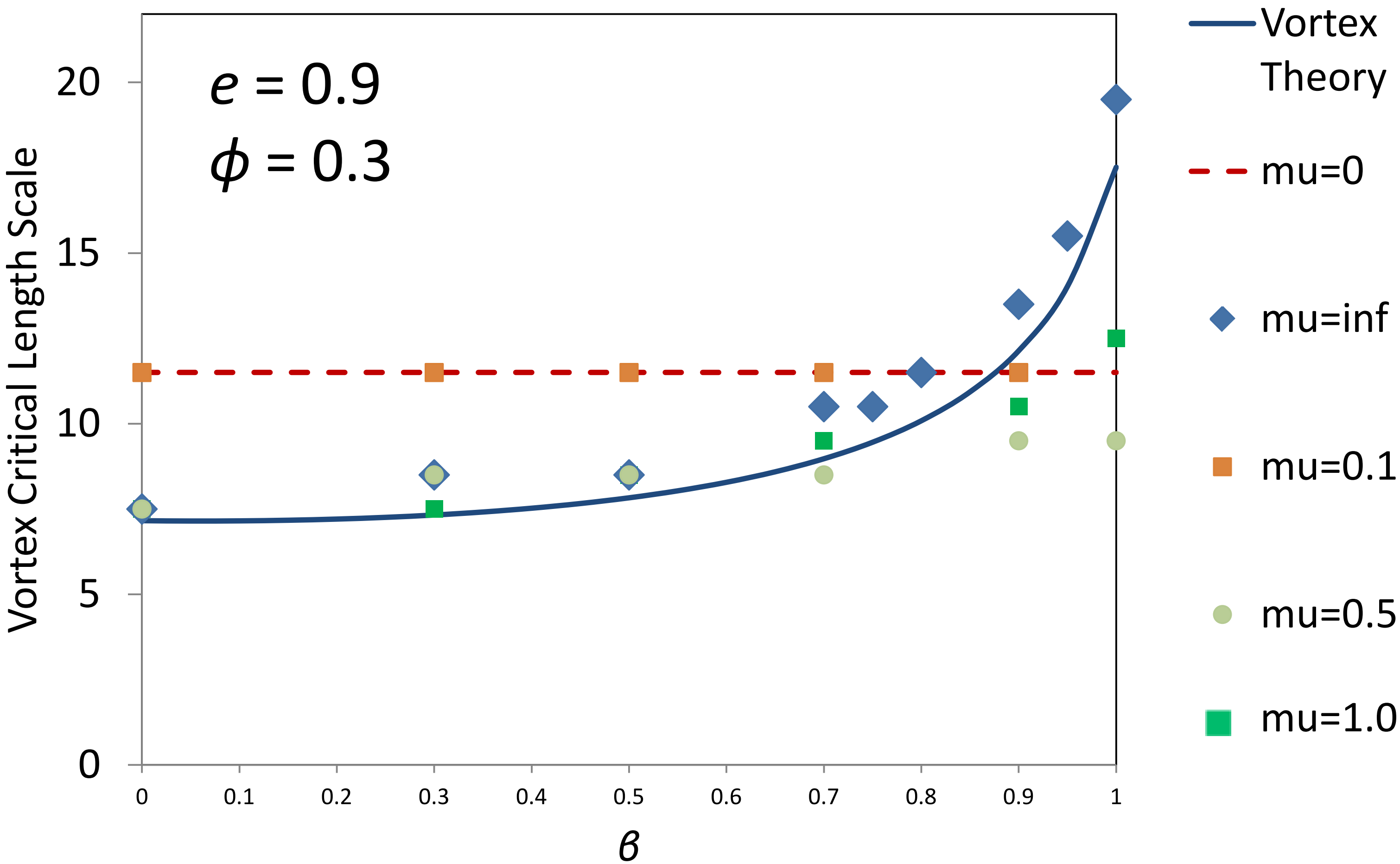
e = 0.9
ϕ = 0.3

Extra note 2

- The et shown is not just averaged

- First take absolute value of et
- Take log10
- Average
- Raise 10 to the average
- This is because we want et=0.1 and 10 to average to 1 not close to 5

A Coulomb-friction model: Onset of vortices



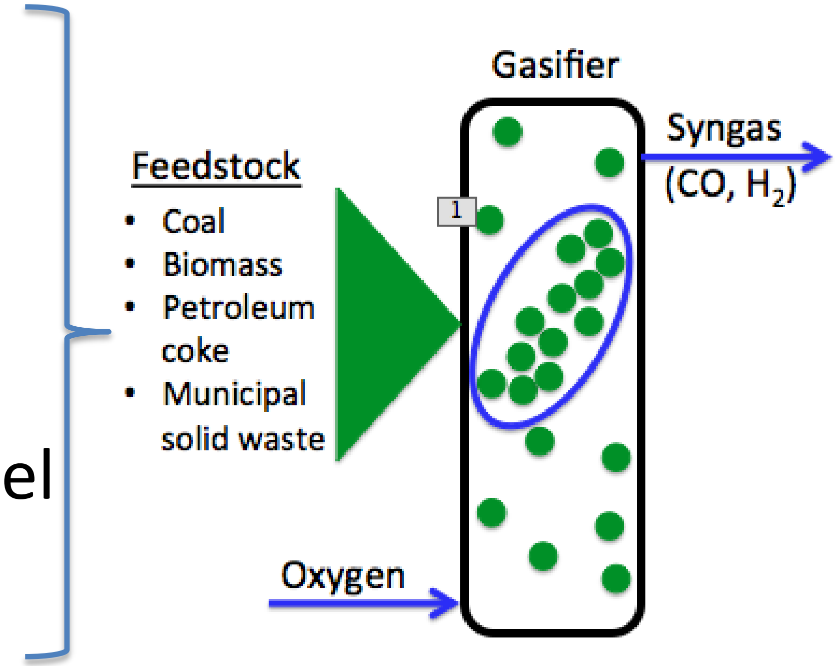
Concluding Remarks

- MD vs CFD vs LSA
  - Excellent agreement between kinetic theory and MD simulations
  - Small-gradient, molecular chaos assumptions of theory are not so restrictive
  - Nonlinear mechanisms are important for clusters
- Frictional dissipation
  - All dissipation is not created equal
  - A frictional cooling rate alone does well

    (other transport coef.'s neglect friction)

Future Work

- Increased system complexity
  - Polydisperse particles
  - Non-spherical particles
  - Fluid phase
  - Bulk flow
  - Improved dissipation model
  - Wall boundaries



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