Temperature of dense granular systems

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with

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Main goals

Understand the dynamics of dense granular systems
Reconsider the concept of granular temperature
Work towards out-of-equilibrium statistical theory for these systems

Techniques

Discrete element simulations (mostly soft spheres in 2D)

Overview

- Velocity profiles for sheared granular systems: conditions for uniform shear
- Elasticity and generalized granular temperature
- Flow of energy and relation to generalized temperature

Simulations

Discrete element techniques

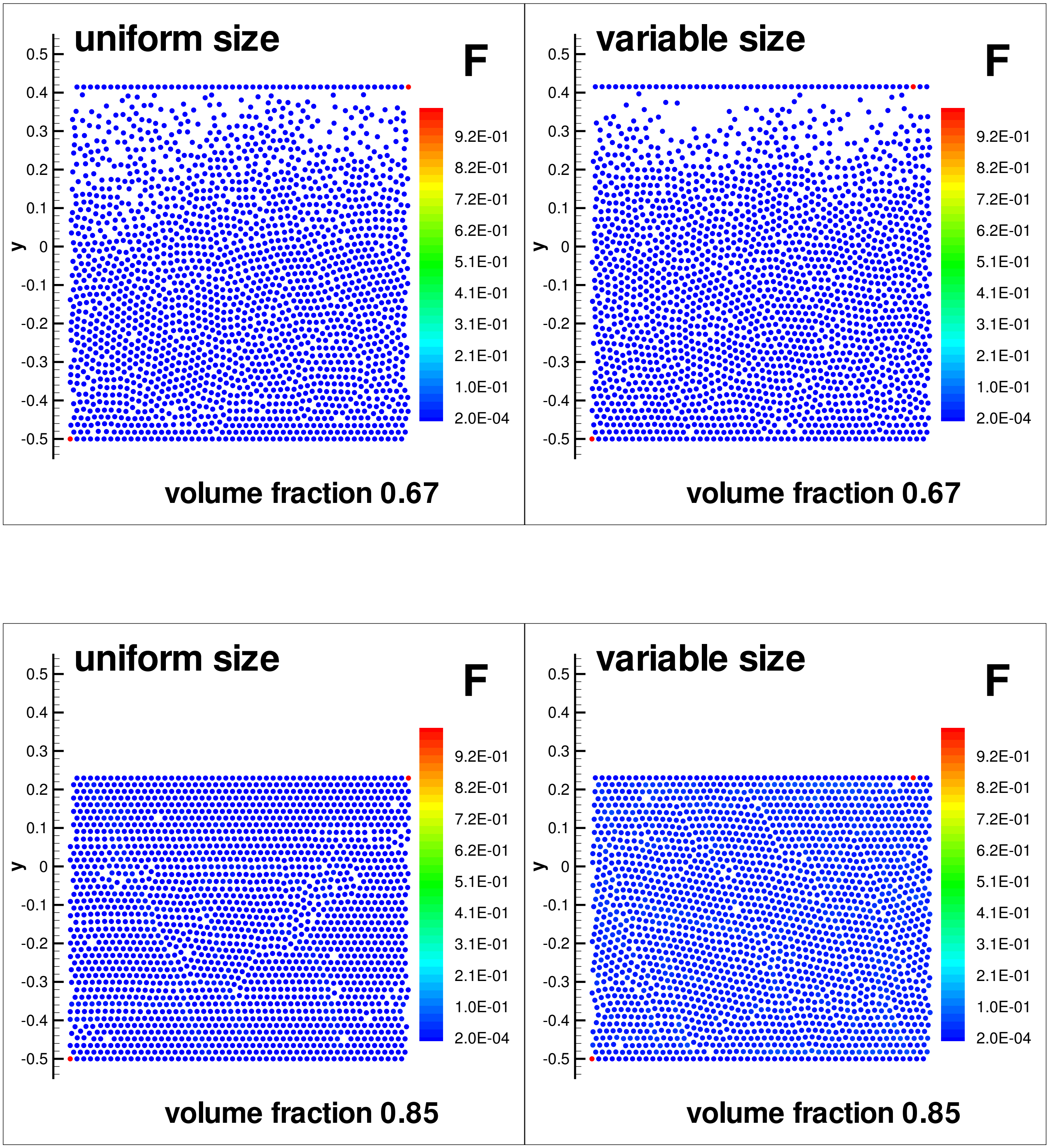
Linear force model with damping in normal and tangential directions - frictional particles, inelastic collisions, rotational degrees of freedom

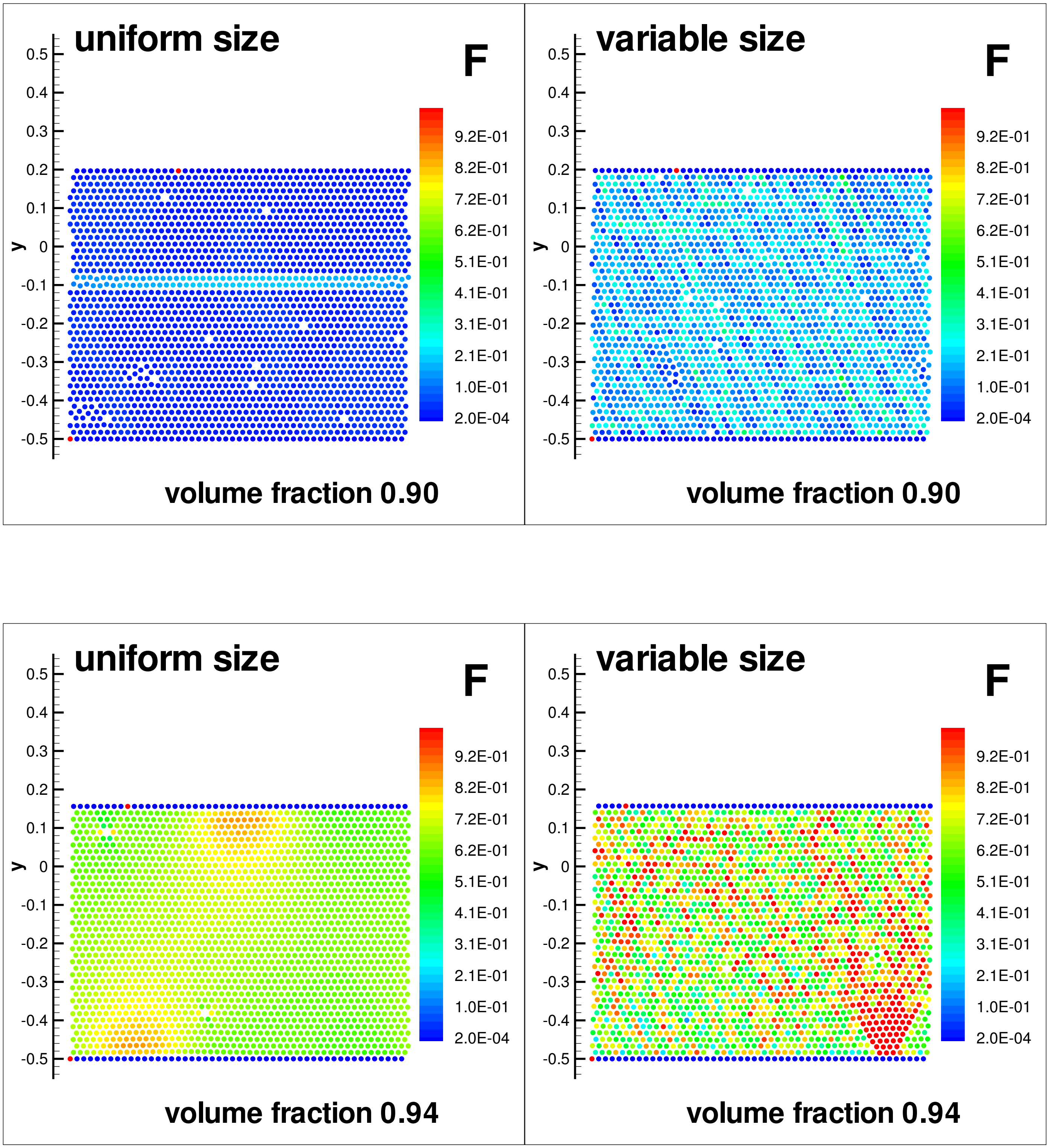
Rough shearing walls

Parameters chosen appropriately for (soft) photoelastic disks, (e.g. Howell and Behringer, PRL ('99))

Monodisperse and (10%) polydisperse particles

Consider first sheared systems with slowly varying volume fraction


uniform size
F
variable size
F
y
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
9.2E-01
8.2E-01
7.2E-01
6.2E-01
5.1E-01
4.1E-01
3.1E-01
2.1E-01
1.0E-01
2.0E-04
volume fraction 0.67
volume fraction 0.67
uniform size
F
variable size
F
volume fraction 0.85
volume fraction 0.85



uniform size
F
volume fraction 0.90
variable size
F
volume fraction 0.90
uniform size
F
volume fraction 0.94
variable size
F
volume fraction 0.94
y
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
9.2E-01
8.2E-01
7.2E-01
6.2E-01
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3.1E-01
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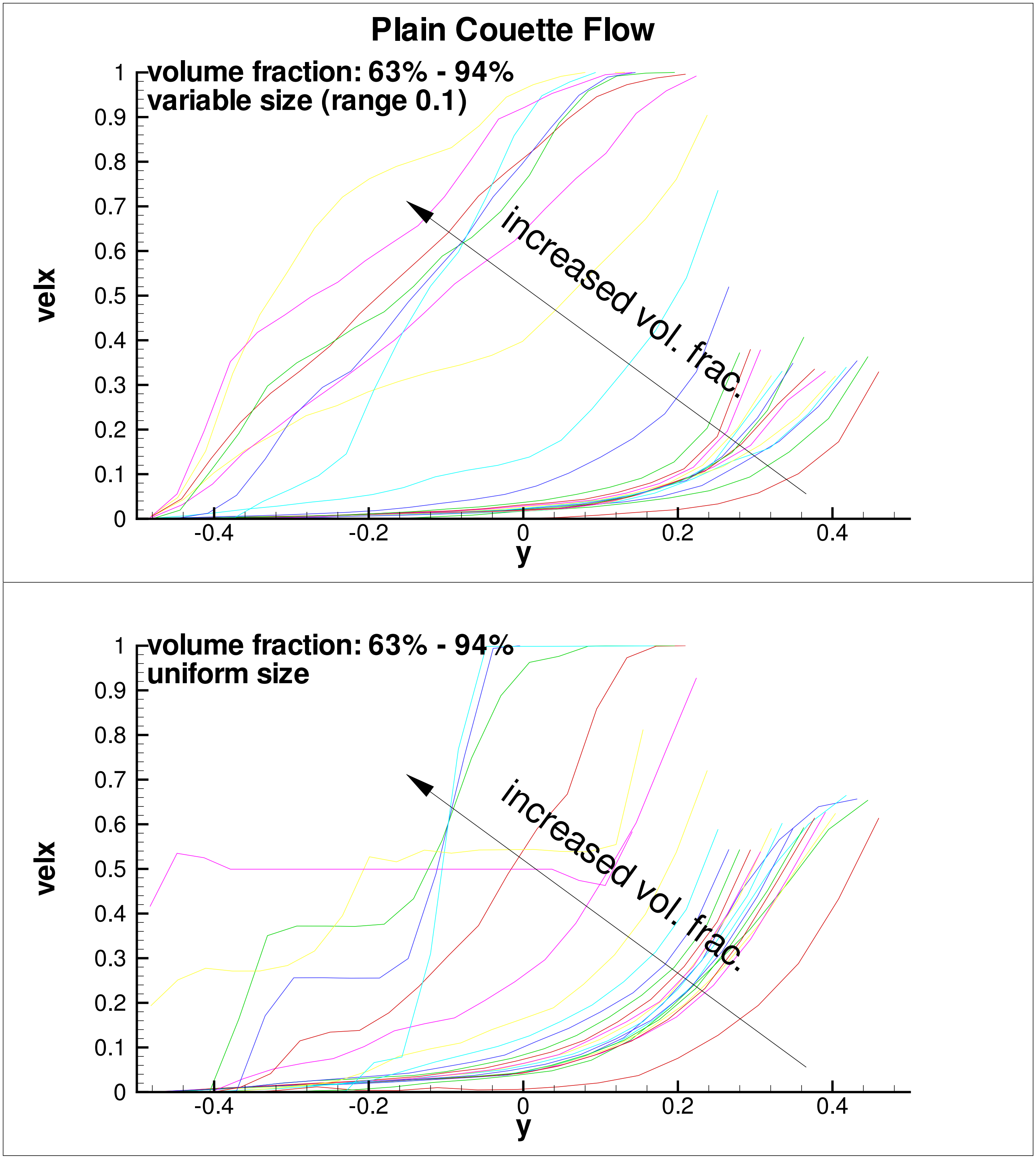


Plain Couette Flow
volume fraction: 63% - 94%
variable size (range 0.1)
increased vol. frac.
velx
y
volume fraction: 63% - 94%
uniform size
increased vol. frac.
velx
y

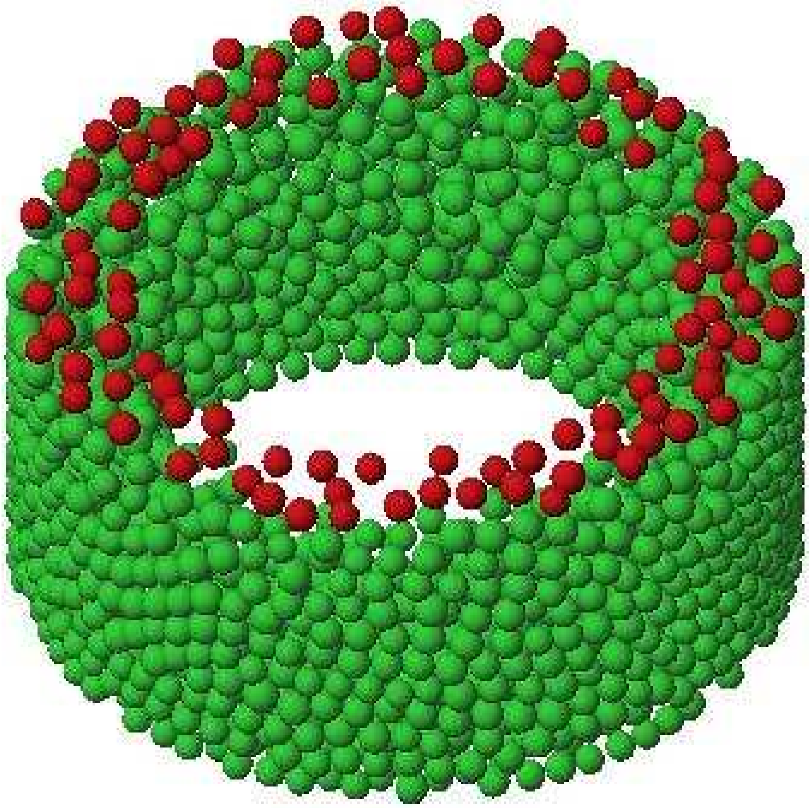
Low volume fractions: Gas-like regime

No significant difference between monodisperse and polydisperse materials
System dilated next to the shearing wall
Rate-independent system behavior
Shearing band formation similarly as in radial Couette geometry (Howell and Behringer, PRL '99)

Related works
Jenkins, Richman, Phys. Fluids '85
Walton, Braun, J. Rheol., '86
Campbell, Annu. Rev. Fluid Mech. '90
Hopkins, Louge, Phys. Fluids '91
Savage, JFM '98
Moon etal PRE '01 ...

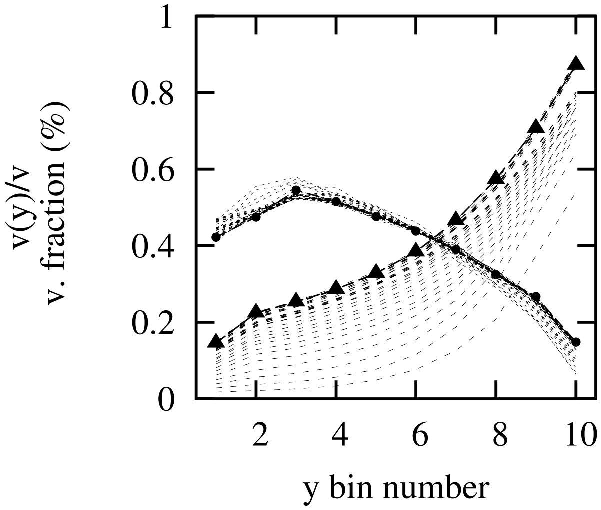
Digression: intermediate volume fractions simulations in 3D: work with Oleh Baran

3D simulations of polydisperse, frictional, spherical particles including rotations
intermediate volume fractions 40 – 50 %

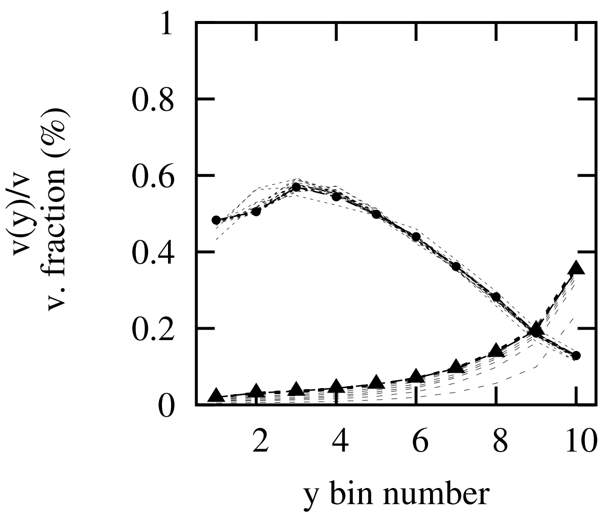


Concentrate on influence of boundaries

rough shearing wall, inelastic, frictional side walls



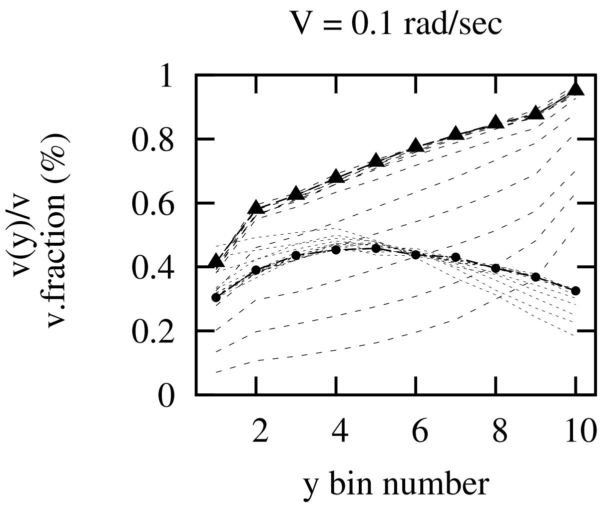
smooth, but inelastic, frictional shearing wall, inelastic, frictional side walls



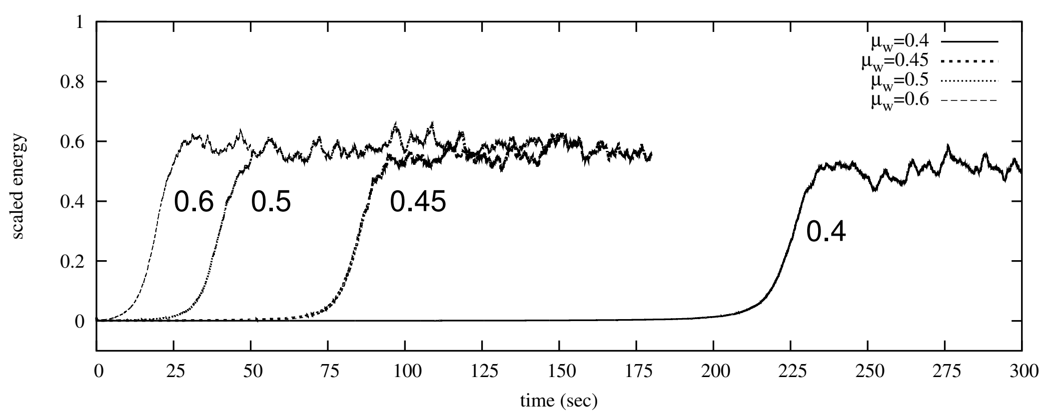
Conclude: Rough (glued particles) shearing wall necessary to induce significant shear, except if...

Side walls are smooth:

Elastic, frictionless side walls, no glued particles

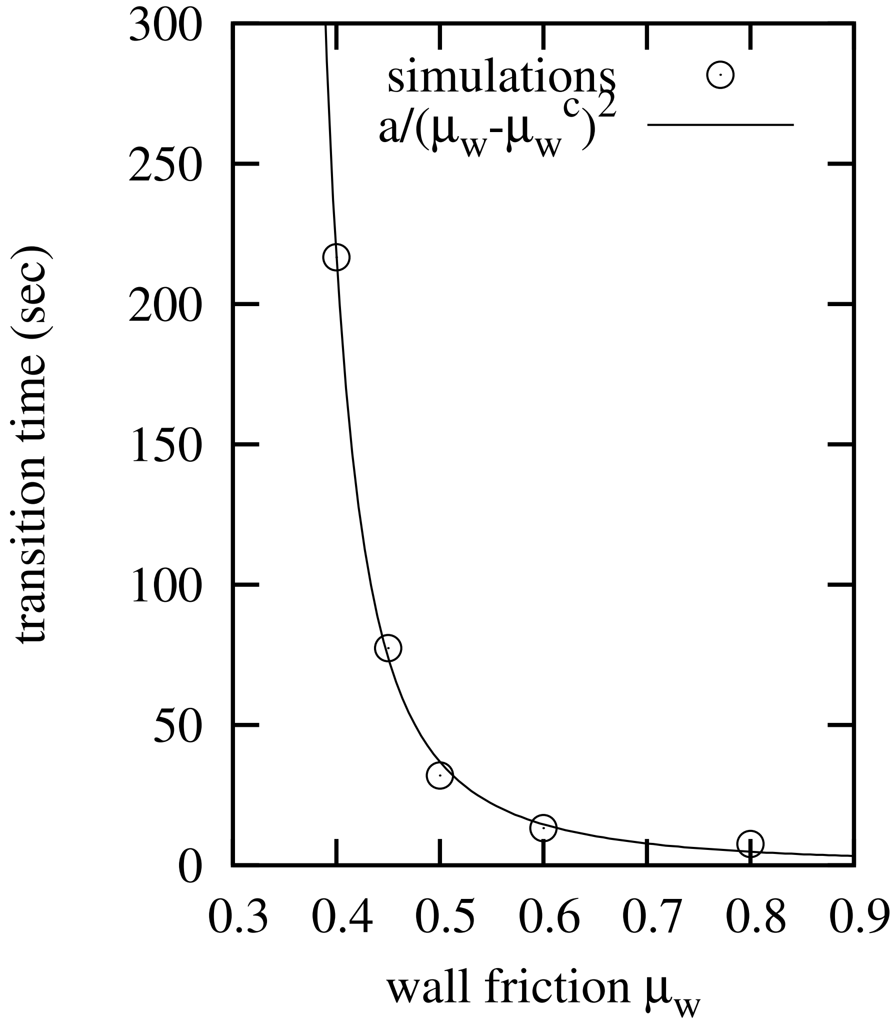


Shear can be induced without mechanically rough walls if side walls are not an obstacle, and driving wall is sufficiently frictional



However, one may need to wait for very long time!

Waiting time depends on the how close one is to ‘critical’ friction



More details, including effects of vibrations and the stresses in this system in Baran & Kondic, Phys. Fluids, to appear July’05.

High volume fractions

From gas-like to solid-like behavior: jamming
Formation of force chains
Large stress fluctuations both in space and time

Rate-dependent behavior for large volume fractions (stress does not scale with square of the shear rate)

Significant differences between monodisperse and polydisperse systems:
Fracture occurs for monodisperse systems
Monodisperse systems are compressed easier (crystallization) $\rightarrow$ large difference in the stored elastic energy compared to polydisperse systems

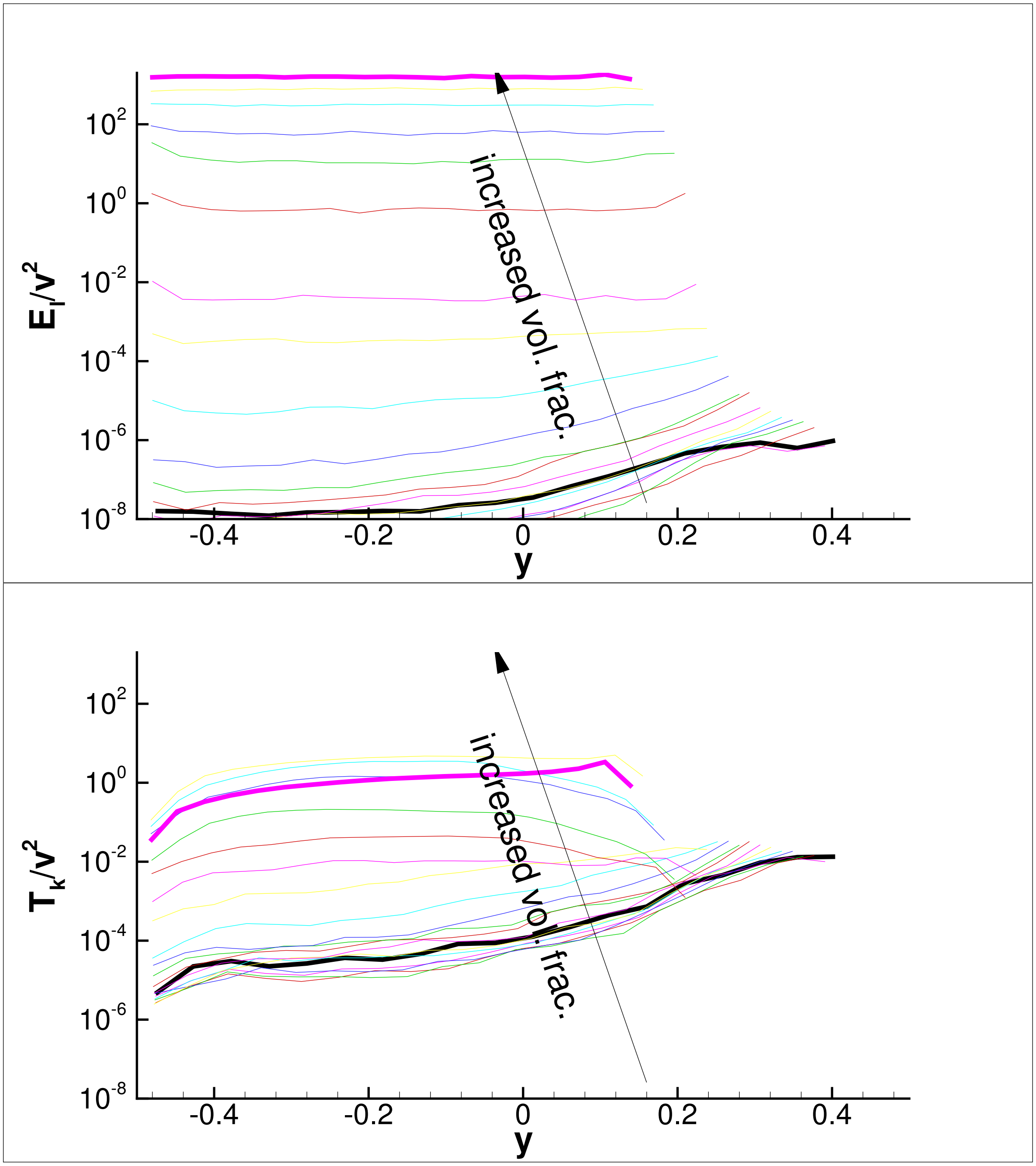
Concentrate on polydisperse systems next

High volume fractions - Velocity profiles:

From exponential to linear velocity profiles as volume fraction is increased

However, this is not the whole story...
Even for high vol. fractions, both linear and shear-banding velocity profiles can be found
Main result: As shearing velocity increases and becomes comparable to the speed of shear waves in the system, transition from linear to shear-banded velocity profiles occurs
(Xu, O'Hern & Kondic, PRL '05)
Important issues:
influence of dissipation, in particular friction on the dynamics
Stability of the nonlinear profiles
Concentrate next on relevant energies in slowly sheared systems (approx. linear velocity profiles)

Energy balance for sheared granular systems



Elastic energy for dense slowly sheared granular systems is much larger than kinetic energy

Kinetic granular temperature T_k does not seem to be energetically relevant for dense, slowly sheared granular systems

Can we formulate a relevant temperature based on the involved energies?

Can we relate this ‘relevant’ temperature to:

- ‘effective’ temperature used in supercooled glass-forming liquids, colloids, foams (mostly based on mode-coupling theory)
Berthier and Barrat, J. Chem. Phys. ’02
- fluctuation-dissipation temperatures
Ono et al PRL ’02
- Edwards temperature resulting from the entropy associated with the number of jammed configurations
Blumenfeld and Edwards, PRL ’03
Edwards and Grinev, Gran. Matter ’03

Consider this temperature

$$T_g = T_k + T_e = \frac{m}{2} < v >^2 + \frac{k}{2} < x >^2$$

- x is compression of a particle
- k is the force constant

$< ... >$ stands for the space and time average over *fluctuating* component

Note analogy to harmonic oscillator

Definitions

$$T_k = \frac{1}{2}\left[\langle m(u')^2\rangle + \langle m(v')^2\rangle + \frac{\beta}{4}\langle m(d_p\omega')^2\rangle\right]$$

with

$$\langle u'v'\rangle = \langle uv\rangle - \langle u\rangle\langle v\rangle$$

Elastic energy and temperature require more care due to multiple collisions:

$$E_{e,l} = \frac{1}{N_t n_l} \frac{k_f}{2} \sum_{k=1}^{N_t} \sum_{j=1}^{n_l} \sum_{c=1}^{n_{c,j}} \left[x_{j,c} \right]^2$$

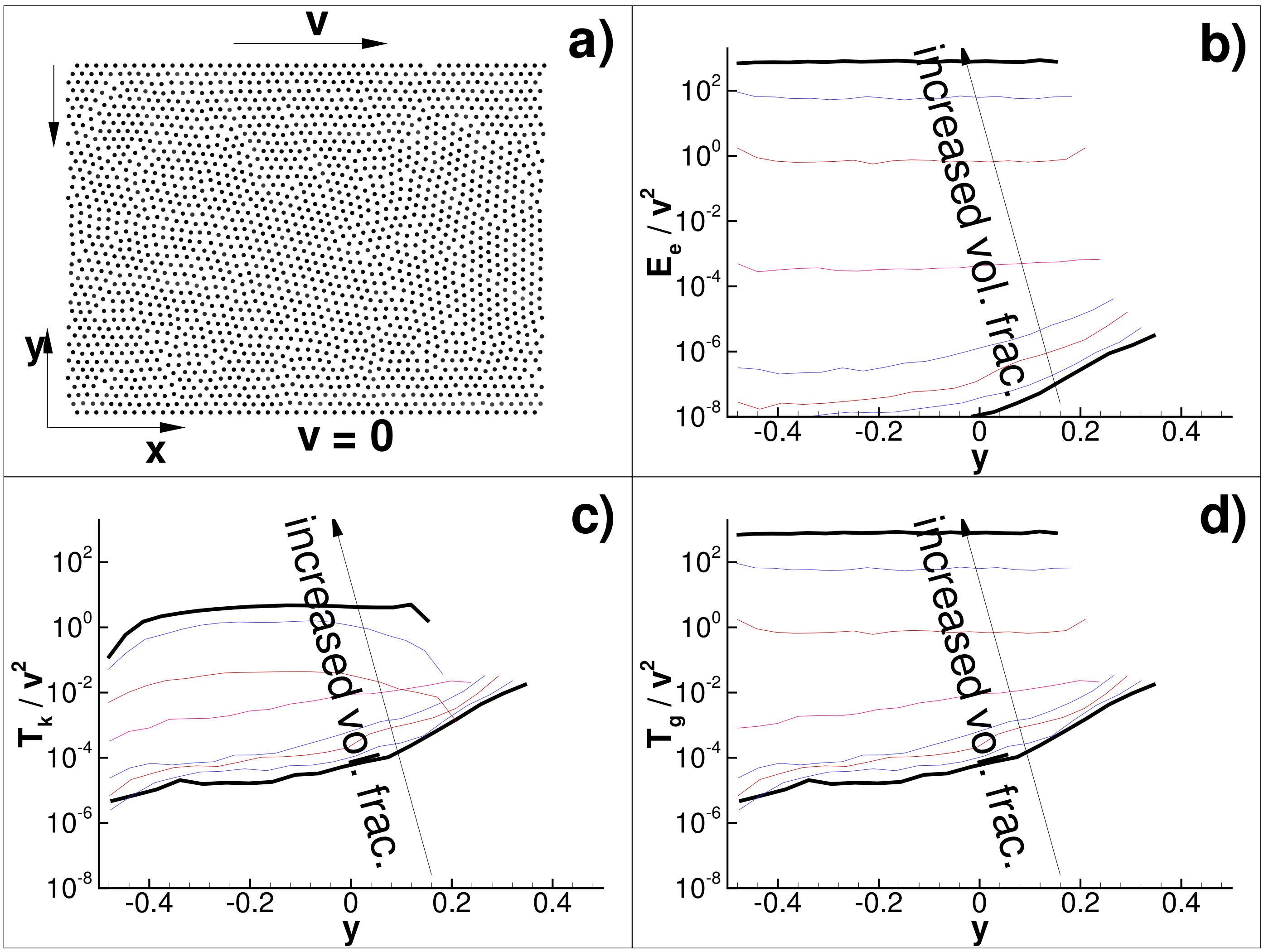
$$\langle E_{e,l} \rangle = \frac{k_f}{2} n_c \langle x_l \rangle^2 = \frac{k_f}{2} n_c \left[\frac{1}{N_t \bar{n}_l n_c} \sum_{k=1}^{N_t} \sum_{j=1}^{n_l} \sum_{c=1}^{n_{c,j}} x_{j,c} \right]^2$$

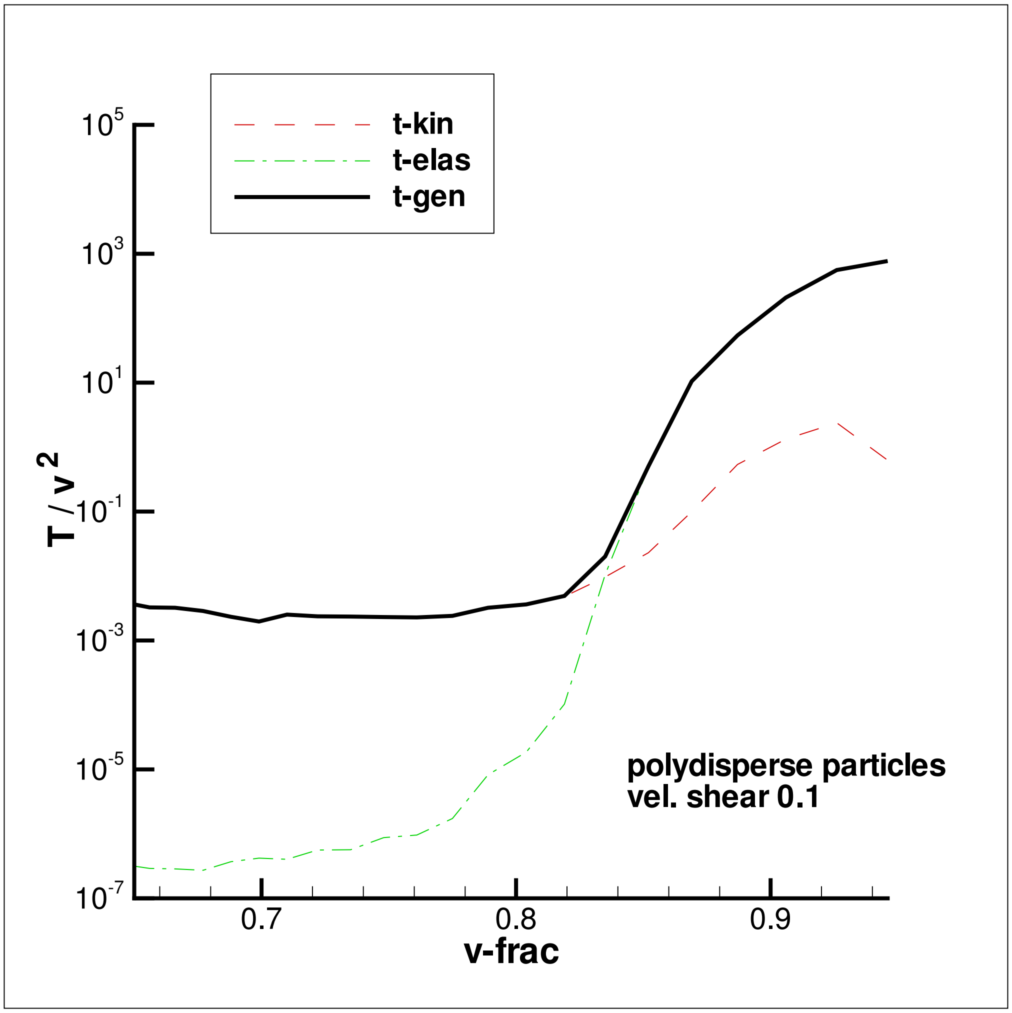
$$T_{e,l} = \frac{k_f}{2} n_c \langle \delta x^2 \rangle = \frac{k_f}{2} n_c \langle (x_{j,c} - \langle x_l \rangle)^2 \rangle = E_{e,l} - \langle E_{e,l} \rangle$$

x_l: average compression per particle

Note: all quantities are calculated locally

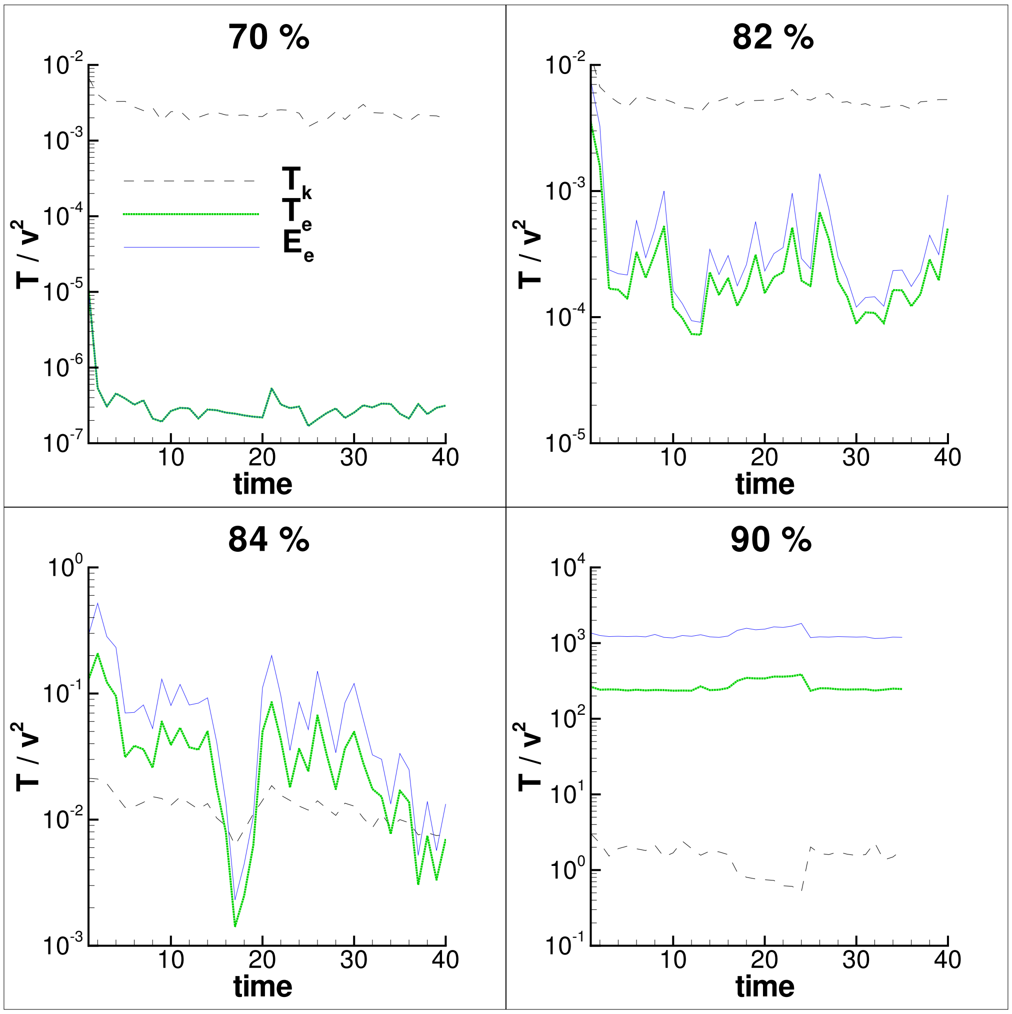
Comparison of various temperatures





Note smooth transition between kinetic dominated to elastic dominated regime as vol. fraction is increased

Temperature for fixed volume fractions



Large fluctuations at vol. frac. at which dominant energy changes from kinetic to elastic

Relation to Fluctuation-Dissipation Thm

Discuss how well T_g satisfies the following relation from equilibrium statistical mechanics (example of fluctuation-dissipation theorem)

$$\frac{dU}{dT} = \frac{\delta U^2}{T^2}$$

$\delta U^2 = < U^2 > - < U >^2$: energy fluctuations

Compute T_m defined by

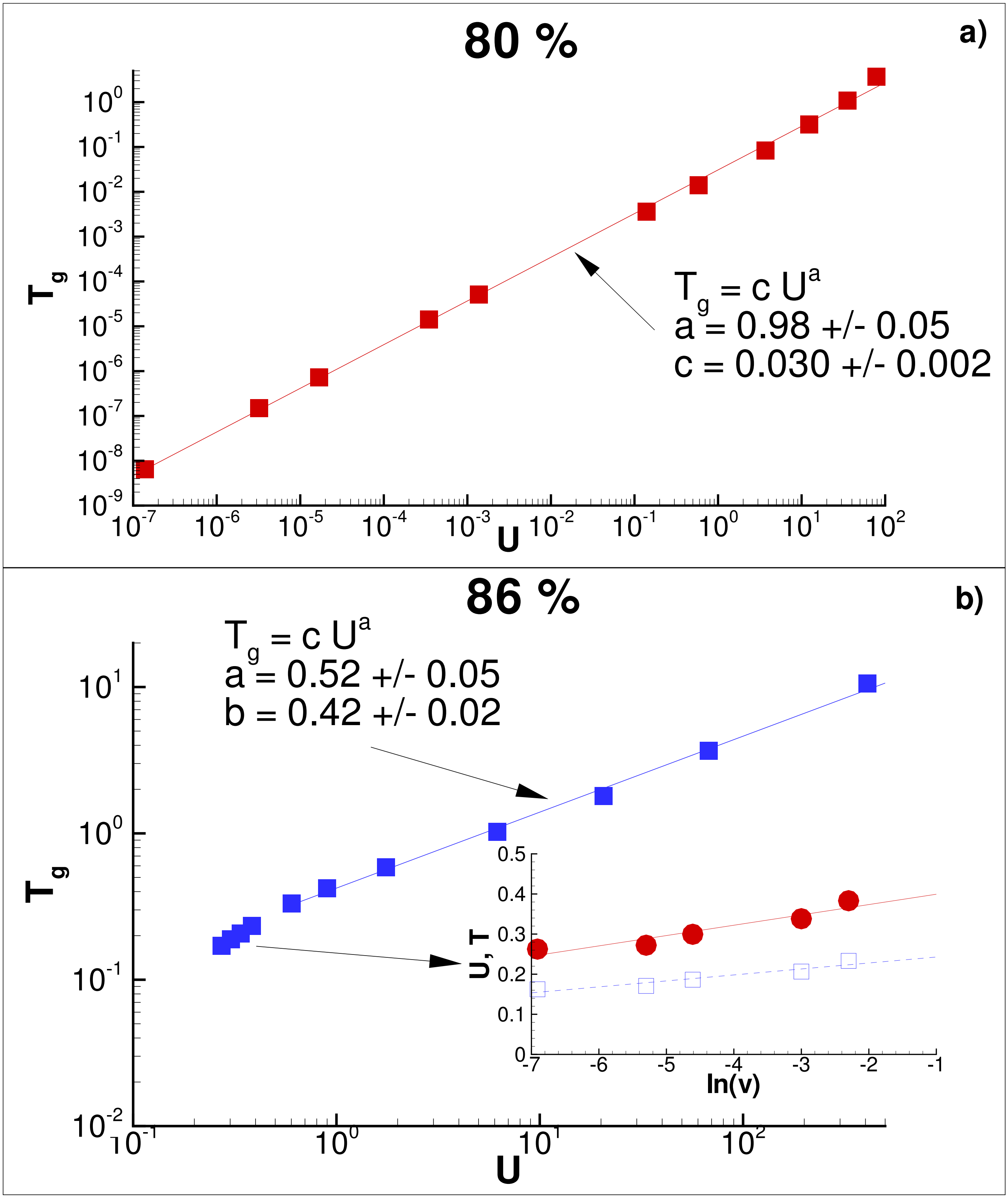
$$T_m^2 = \frac{\delta U^2}{dU/dT_g}$$

and check if $T_m \approx T_g$

First, find the analogy of heat capacity

$$c_v = dU/dT_g$$

To ensure that steady-state has been reached, the simulations are performed for fixed volume fractions



80 %
a)
T_g
U
$T_g = c\, U^a$
a = 0.98 +/- 0.05
c = 0.030 +/- 0.002
86 %
b)
$T_g = c\, U^a$
a = 0.52 +/- 0.05
b = 0.42 +/- 0.02
T_g
U
U, T
ln(v)

Heat capacity approximately constant for low volume fractions for many decades of relevant energies

Heat capacity not a constant for large volume fractions

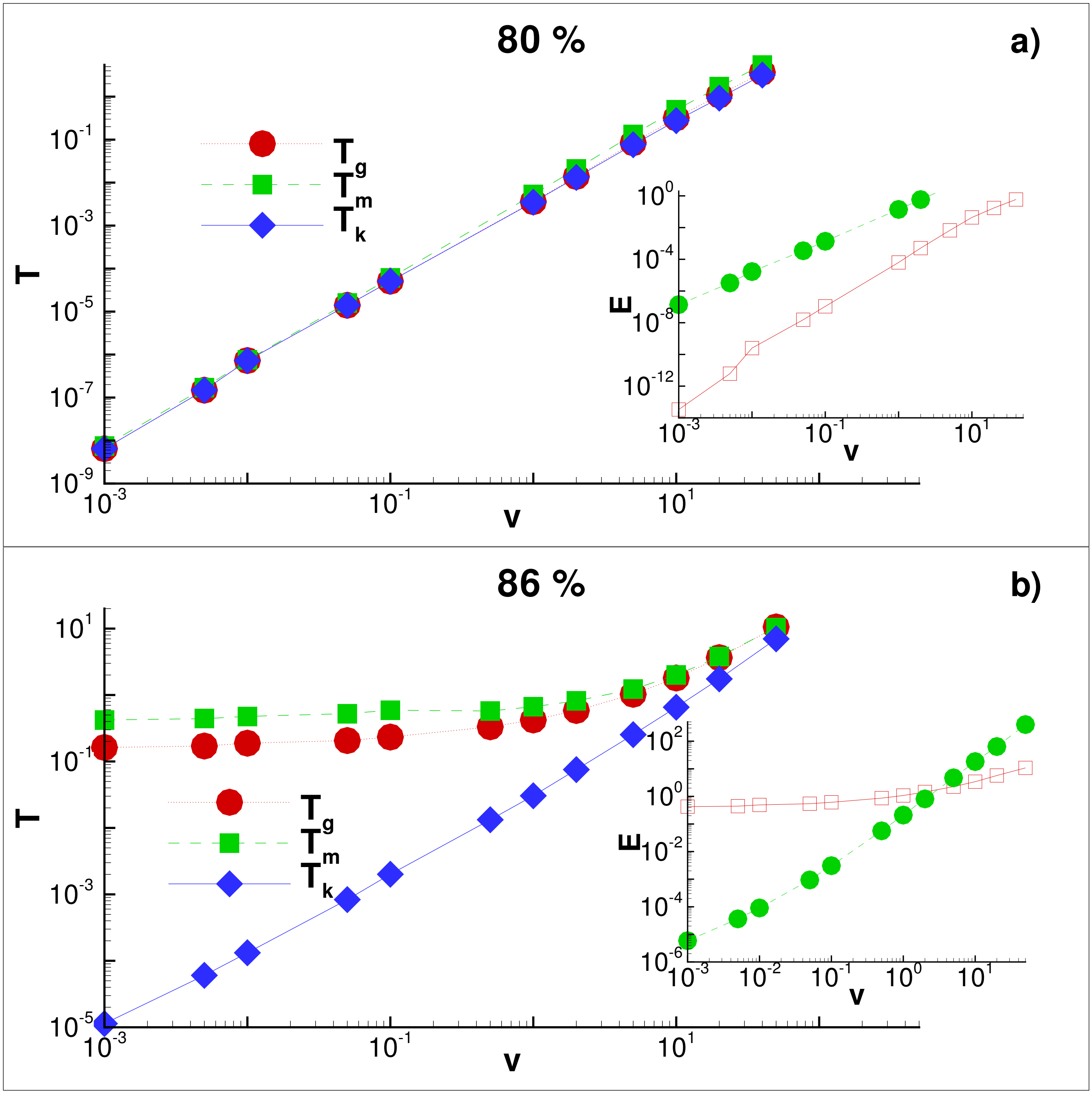
Instead, $c_v \sim T \sim \sqrt{U}$ for not too slow shearing (jamming?)

For slow shear, we observe logarithmic dependence of both U and T on v

(logarithmic dependence also seen in experiments by Behringer and Hartley, Nature '03)

($c_v \approx$ constant for slow shear)

Now we use this c_v to check for agreement with FDT


80 %
a)
T
v
T_g
T_m
T_k
E
86 %
b)

Comments

Generalized granular temperature satisfies surprisingly well an equilibrium FD relation
There is no equipartition of energy; ratio of relevant temperatures changes depending on volume fraction and on shearing rate
Although granular system is far from equilibrium, it appears to make sense to apply equilibrium concepts

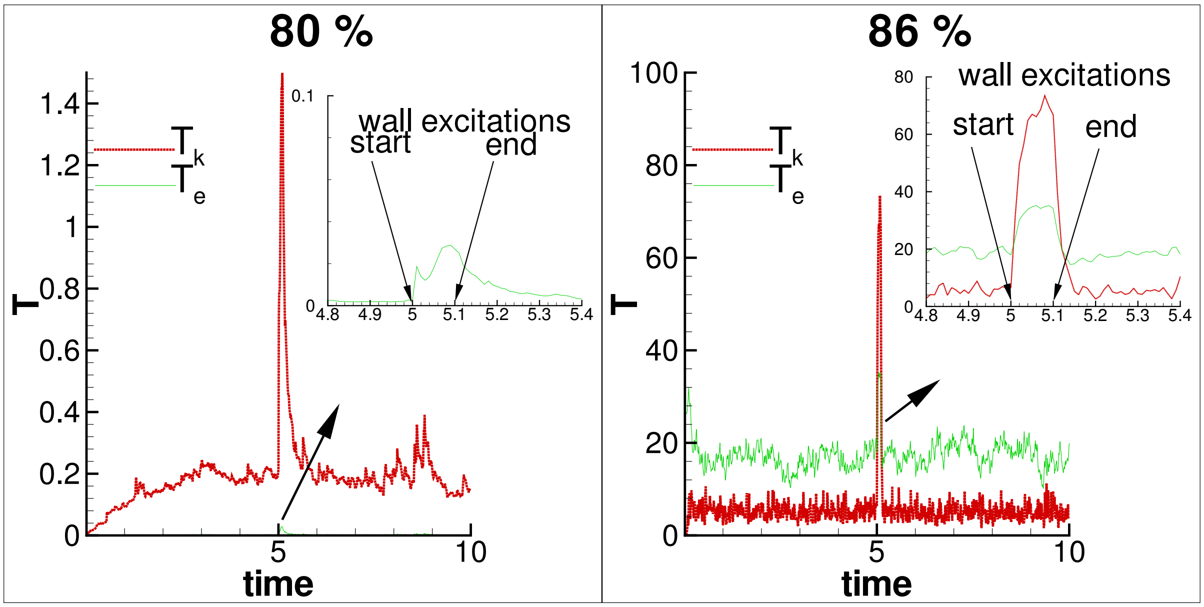
Kondic & Behringer, Europhys. Lett. (2004)

Does the generalized temperature govern the energy ('heat') flow?
Consider:

- Elastic system particles
- Symmetric shear
- (One) wall heated by a pulse of energy

Observe heat flow from hot to cold

Plot energy in the middle of the domain (far away from the sources and sinks of energy)

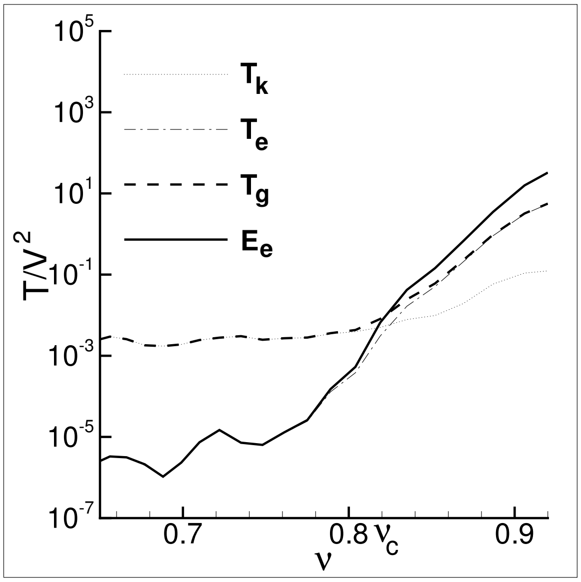


Heat flows from high to low temperatures

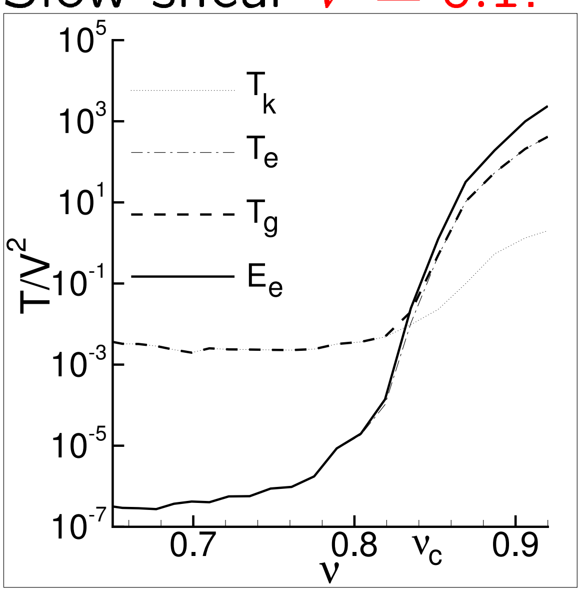
However, more work is needed to understand all relevant issues in particular regarding the nature of system response to excitations

Parametric dependence: Shearing velocity

Typical shear $V = 1$:



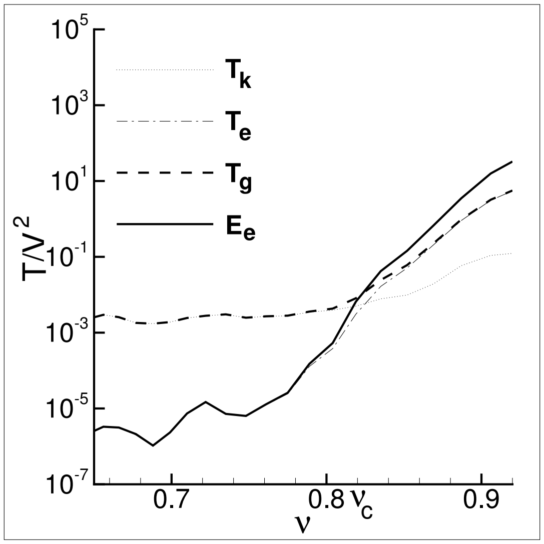
Slow shear $V = 0.1$:



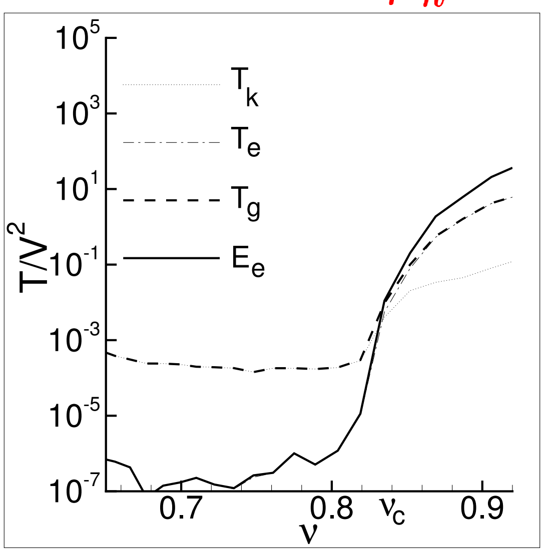
Note lack of scaling with V for high ν

Parametric dependence: Friction

Typical friction $\mu_k = 0.5$:



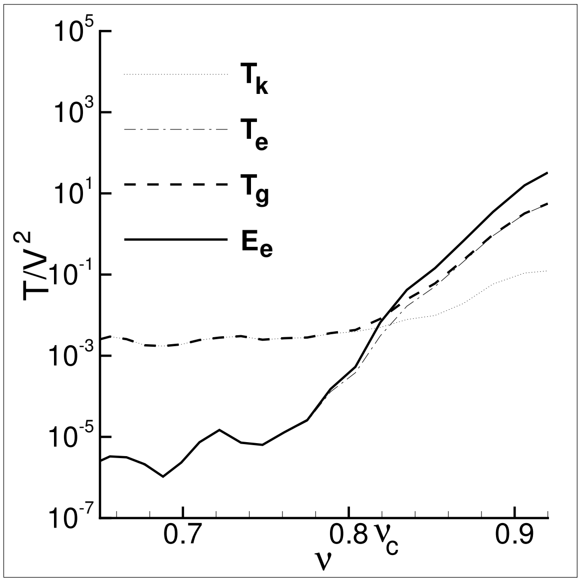
Small friction $\mu_k = 0.1$



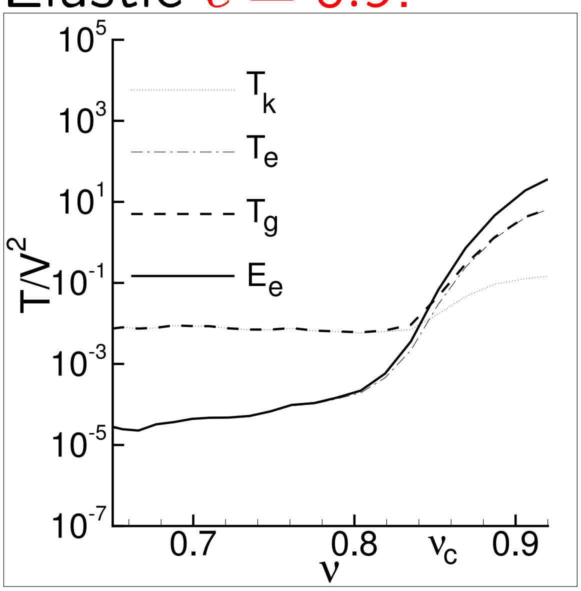
Faster transition to elastic regime for small μ_k

Parametric dependence: Elasticity

Typical $e = 0.5$:



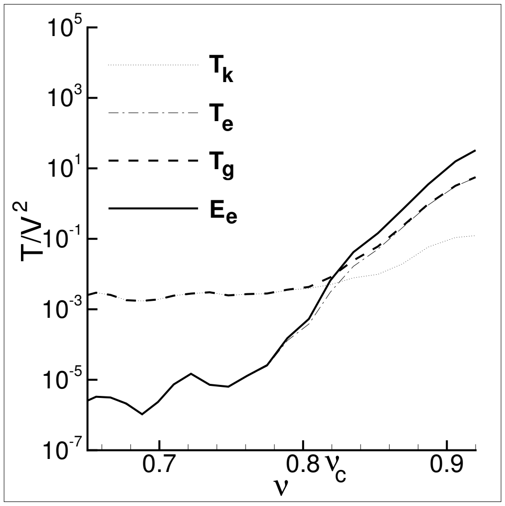
Elastic $e = 0.9$:



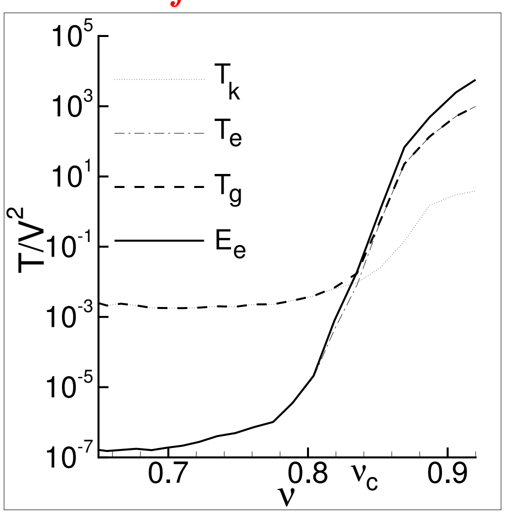
Weak effect

Parametric dependence: Stiffness

Typical $k_f = 4.0d3$:



Stiff $k_f = 1.024d6$:



Larger elastic temperature for stiff particles (more details in Kondic& Behringer, Powders & Grains '05).

Comments, questions and open issues

There is a well defined transition between kinetic and elastic - dominated regimes
Details of this transition depend only weakly on material parameters and imposed shear
Proposed generalized temperature satisfies reasonably well (equilibrium) FD theorem

TO DO list

Understand connection of generalized temperature to other temperature concepts

Verify/discuss other statistical relations

Understand importance of dissipation

Relevance of spatial inhomogeneities

Anisotropy

Time dependence of computed temperatures and energies

Discrete element techniques

Linear force model with damping in normal and tangential directions

$$\mathbf{F}^n_{i,j} = \left[k(d - r_{i,j}) - \gamma_n \bar{m}(\mathbf{v}_{i,j} \cdot \mathbf{n})\right]\mathbf{n}$$

Tangential force

$$\mathbf{F}^t_{i,j} = min\left(-\gamma_s \bar{m} v_{rel}, \mu|\mathbf{F}_{i,j} \cdot \mathbf{n}|\right)\mathbf{s}$$

$$\mathbf{F}^t_{i,j} = min\left(-\gamma_s \bar{m} v_{rel}, \mu|\mathbf{F}_{i,j} \cdot \mathbf{n}|\right)\mathbf{s}$$

$$v_{rel} = \mathbf{v}_{i,j} \cdot \mathbf{s} + (r_i\Omega_i + r_j\Omega_j)$$

$$\mathbf{s} : \mathbf{s} \perp \mathbf{n}$$

γ_s tangential damping

μ: Coulomb coefficient