BES/Materials Sciences
Center Synthesis Processing

Center of Excellence for Synthesis and Processing

Granular Flow and Kinetics

Shankar Subramaniam
Ames Lab
Iowa State University

Principal Labs and Investigators

Eli Ben-Naim, Los Alamos
Alan J. Hurd, Los Alamos
Gary S. Grest, Sandia/NM
Igor Aronson, Argonne
Rodney O. Fox, Ames Lab/ISU
David K. Hoffman, Ames Lab

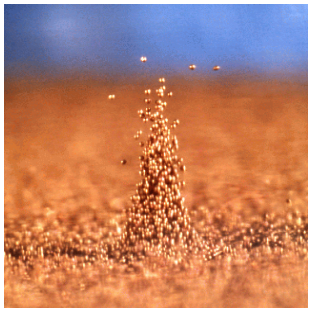
Plan

- Flow of granular materials: introduction, issues, project objectives
- Goals and organization
- Accomplishments: progress report
- Ongoing research projects and future work

Granular Flow

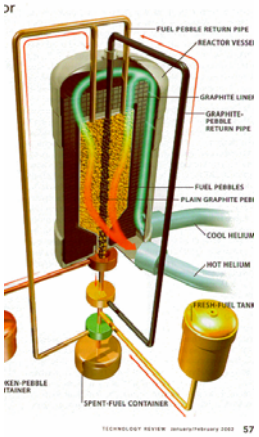
Definition of granular material: ensembles of

- Macroscopic particles (10^{-5}-10^{-2}m), but…
- Hard particles (~1% deformation)
- Dissipative collisions



Multiphase flows: ubiquitous in industry … and in nature

- Industry:
  - packed/fluidized beds
  - pebble bed reactors
  - slurries
  - chemical process industry
  - particle transport: powders, grains, explosives



Geophysics:

- sand dune motion, landslides, snow avalanches
- flow in porous media, volcanic flows

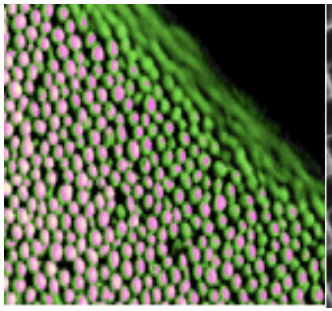
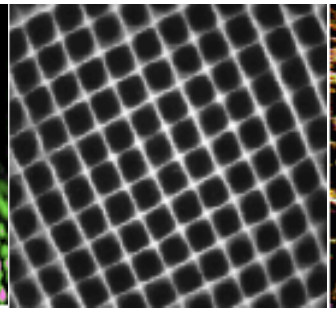
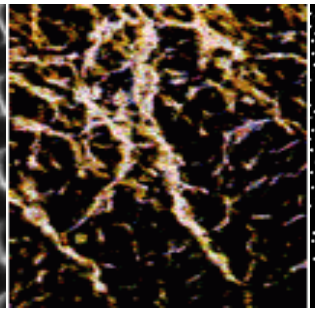
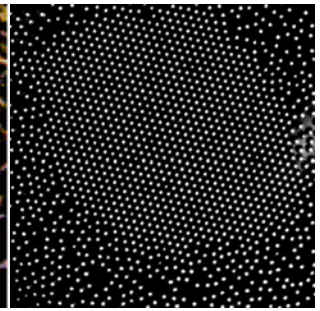
Simple system, complex collective phenomena

Dynamics

- Shearing
- Clustering
- Jamming
- Fluid interaction

Statics

- Granular packs
- Size segregation
- Cohesion effects
- Force transmission

Basic science issues

Stretching the boundaries of mechanics, thermodynamics…

Common Themes	Issues
Extract meso or macroscale behavior from detailed description at particle-level	Flow equations Constitutive relations
Small-scale inhomogeneities in particle field: can they affect macroscale behavior ? Transitional regimes, polydispersity, influence of fluid	Statistical description Pattern characterization (disorder function formalism) Bridging regimes, fluid-particle interactions

- **Constitutive relations?**
- **Physical mechanisms**
- **Predictive models?**

Project Objectives

- **Seek a fundamental understanding of granular and multiphase flows**
- **Experiments and simulation to discover new phenomena; theory and simulation to explain and guide new questions**
- **Identify physical mechanisms and build predictive models**

Experiment

- Understand collisional relaxation mechanism in granular gases
- Study shearing in granular systems; avalanching

Theory

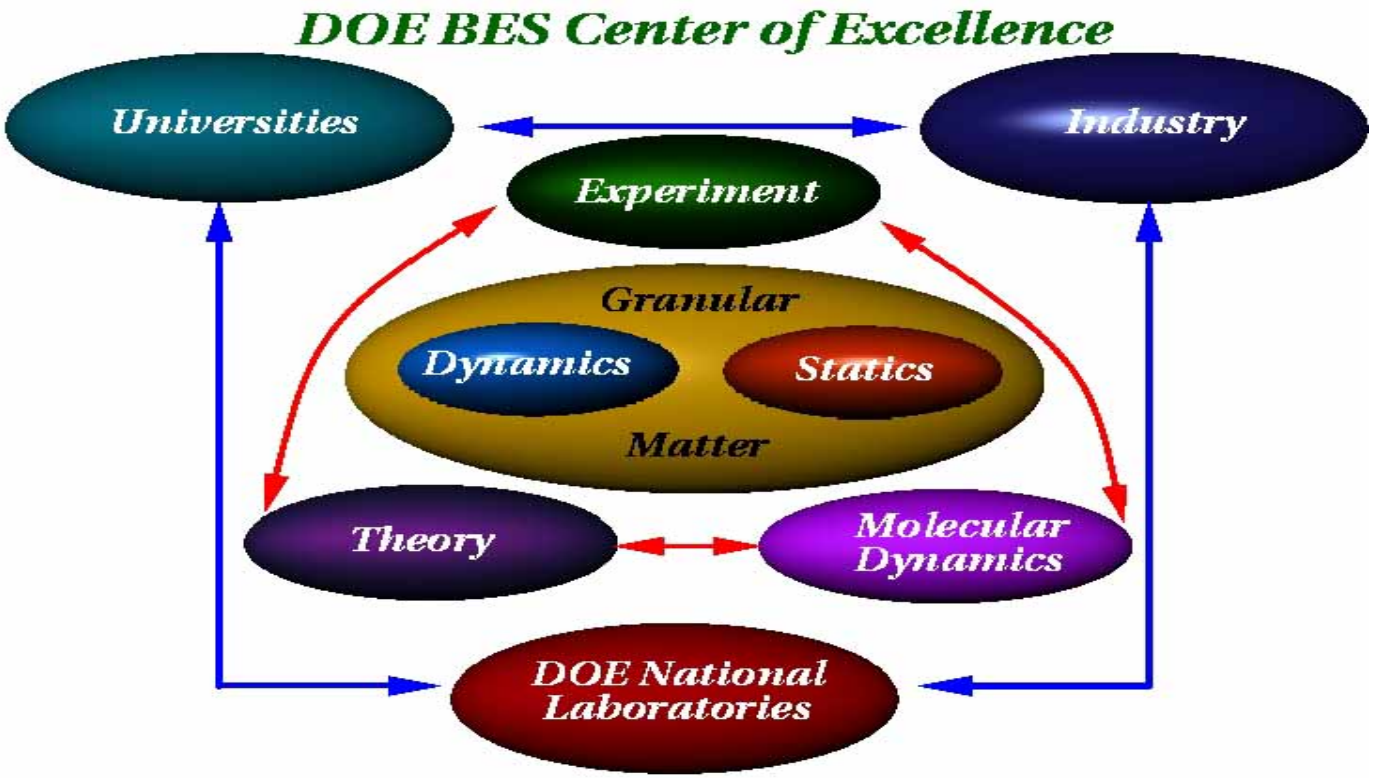
- Further develop kinetic theory for granular gases
- Continuum theory for transition from "solid" to "fluid"

Simulation

- Use Molecular Dynamics to study granular flow (hopper, shear)
- Couple spectral iBM (particle-fluid) to MD: study P-F interactions

Argonne National Laboratory University of Chicago
Los Alamos National Laboratory
Ames Laboratory
Sandia National Laboratories

DOE center of excellence



BES/Materials Sciences
Center Synthesis Processing

DOE labs:
Leaders in simulation & modeling

Simulation

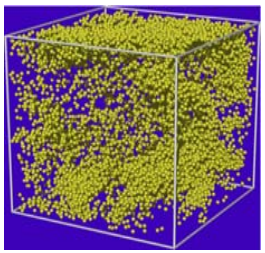
- Molecular Dynamics **(soft, hard, parallel)** (SNL, LANL, Ames)
- Monte Carlo (LANL, Ames)

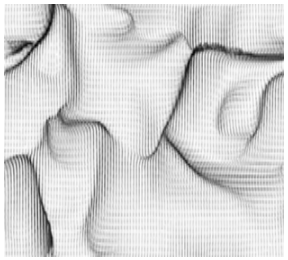
Theory

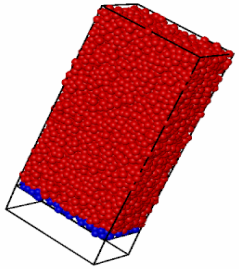
- Continuum mechanics, probabilistic approach (Ames, LANL)
- Kinetic theory, statistical physics (LANL, Ames, Argonne)

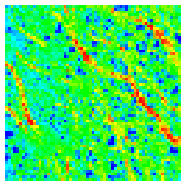
Experiment

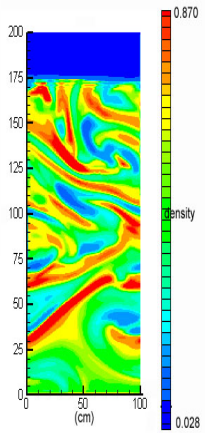
- Vibration, Shaking, Imaging (Argonne, LANL)
- Electrostatic driving (Argonne), Compaction (Sandia, LANL)











Center Administration

Executive committee:

Chair: Rodney Fox (Ames)

I Aronson (ANL), E Ben-Naim (LANL), G Grest (SNL)

D Hoffman (ex-officio, Ames)

- Oversees center operation
- Apportions resources
  - Travel
  - Workshops/Meetings
  - Evaluates outreach research proposals
  - Personnel (students, postdocs, visitors)

Goals & Methods

Goals

- Close the gap between physics and engineering approaches to granular matter
- Develop integrated long-term experimental and computational capabilities at DOE labs

Methods

- **Collaborations:** Lab-Lab and Lab-partner via personnel exchange, visits:
  - Kevin Kohlstedt (U. Kansas summer intern at ANL)
  - 14 Visits of GLUE participants and collaborators
- **Outreach:** Workshops, visits

Granular Flow and Kinetics Meetings

- Third Granular Flow and Kinetics Workshop: Jan 15, 2004 at Sandia, Albuquerque
  - 13 participants, 5 from universities, 8 from national labs
- Talks:
  - Granular gases
  - Chute and Hopper flows
  - Dense granular flows
  - Segregation and multiphase flows
- Coordinate projects between research groups; progress update
- Eurosummer School on Pattern Formation, Granular Physics and Soft Condensed Matter, Spain 2003 (Igor Aronson organizer, attended by several GLUE participants)

Focus Areas

- **Granular gases:** dilute, collision dominated
  - Velocity statistics, correlations, kinetic theory
  - Flow equations, equation of state
- **Granular fluids:** dense, contact dominated
  - Constitutive relations, force propagation
  - Flow equations: shear, avalanches
- **Granular mixtures:** dilute and dense
  - Multiphase flow, fluid-particle coupling
  - Chains, rods

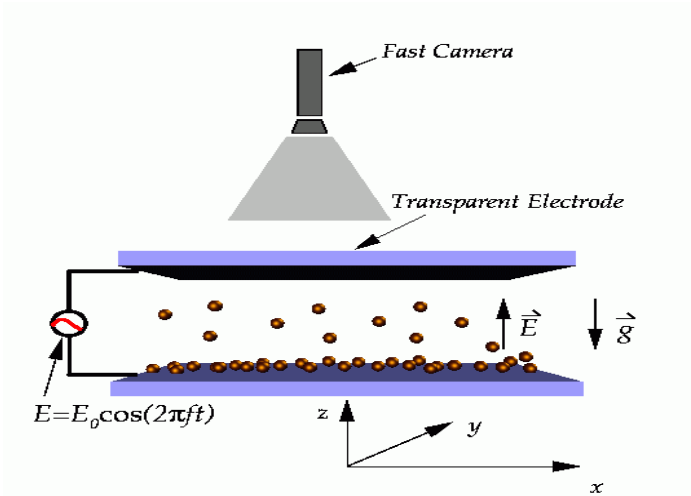
Selected Center research projects

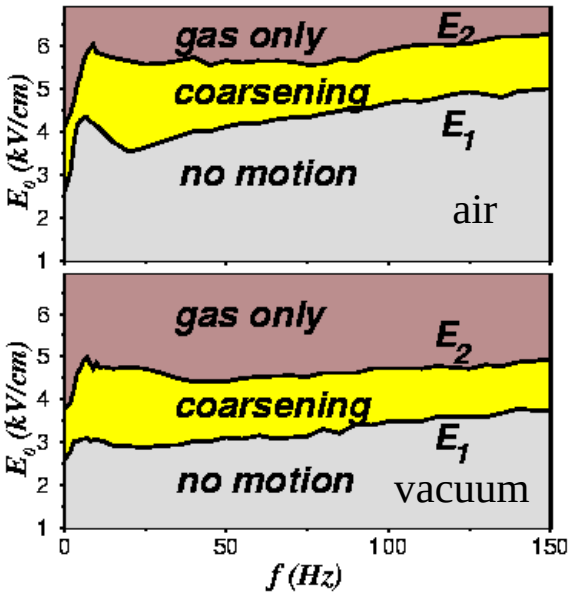
- **Granular gases**
  - Electrostatically driven granular matter (U. Kansas, LANL, ANL)
  - Kinetic Theory for granular flow with friction (LANL, UCSD, ANL)
- **Granular fluids**
  - Couette flow: experiment (Chicago), MD (SNL)
  - Hopper flow (Clark, MIT, SNL)
  - Theory of partially fluidized granular flow (UCSD, ANL)
- **Granular mixtures**
  - Fluid-particle interaction simulations (Ames, SNL)

Electrostatically driven granular matter

Experiment: electrostatically-driven granular layers (ANL)

Aranson, Blair, Kalatsky, Kwok, Crabtree, Vinokur, Welp, *Phys. Rev. Lett.* **84**, (2000)



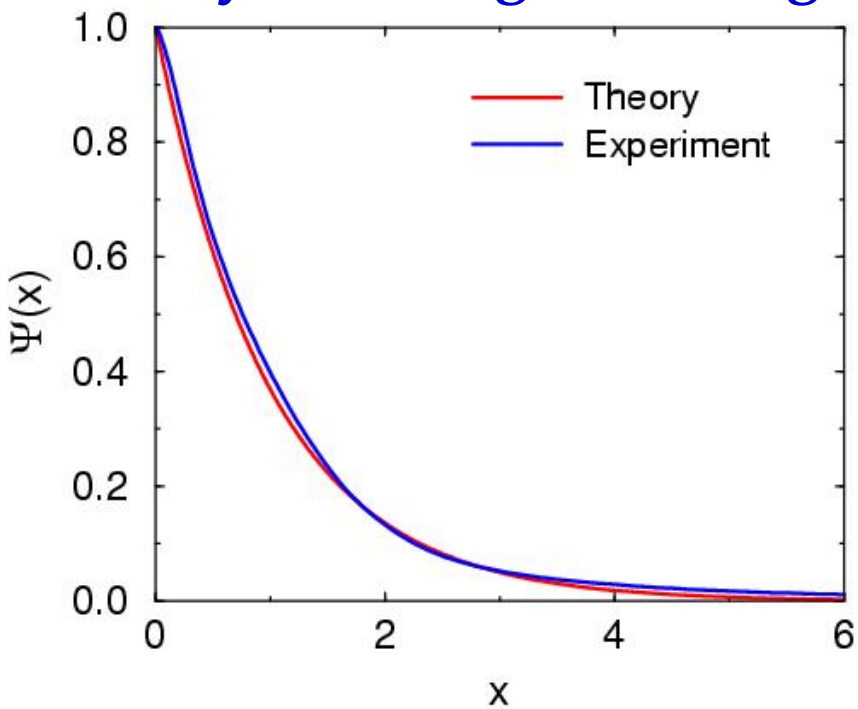


Size: 15x15 cm, spacing 1.5 mm
Field: 0-15 kV/cm, frequency 0-600 Hz
Particles: 35 mm or 150 mm Bronze spheres
Number of particles >10^6

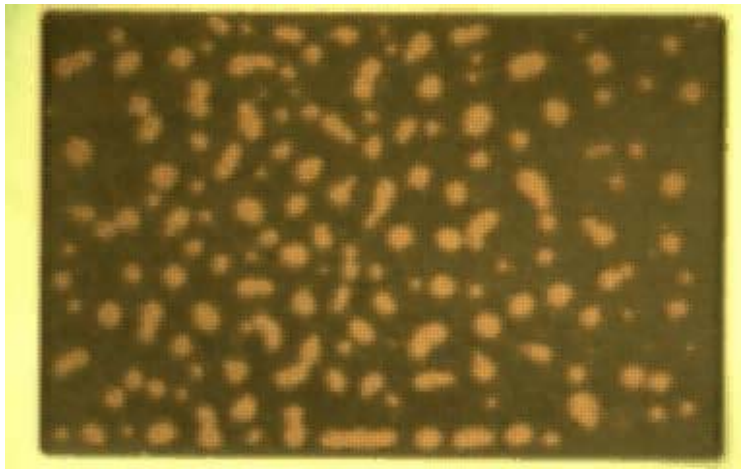
BES/Materials Sciences
Center Synthesis Processing

Coarsening in driven granular media

Experiment: electrostatically-driven granular layers (ANL)
Theory: Exchange driven growth (LANL)



In air



- Self-similar cluster distribution
- Exponential size distribution

Kinetic Theory: non-Maxwellian distributions

1. **Velocity distribution is isotropic**

$$P(\mathrm{v}_x, \mathrm{v}_y, \mathrm{v}_z) = P(|\mathrm{v}|)$$

2. **No correlations between velocity components**

$$P(\mathrm{v}_x, \mathrm{v}_y, \mathrm{v}_z) = P(\mathrm{v}_x)P(\mathrm{v}_y)P(\mathrm{v}_z)$$

?

Only possibility is Maxwellian

$$\boxed{P(\mathrm{v}) \propto \exp[-\mathrm{v}^2/2T]}$$

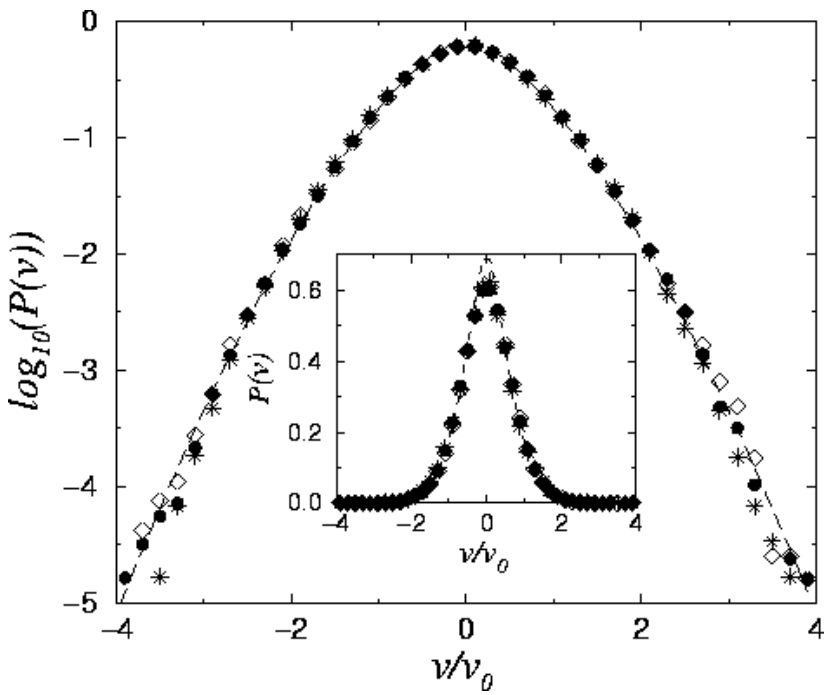
Granular gases: collisions create correlations

New Physics

Granular Gases: velocity distributions

In Air

Aranson & Olafsen, PRE (2003)

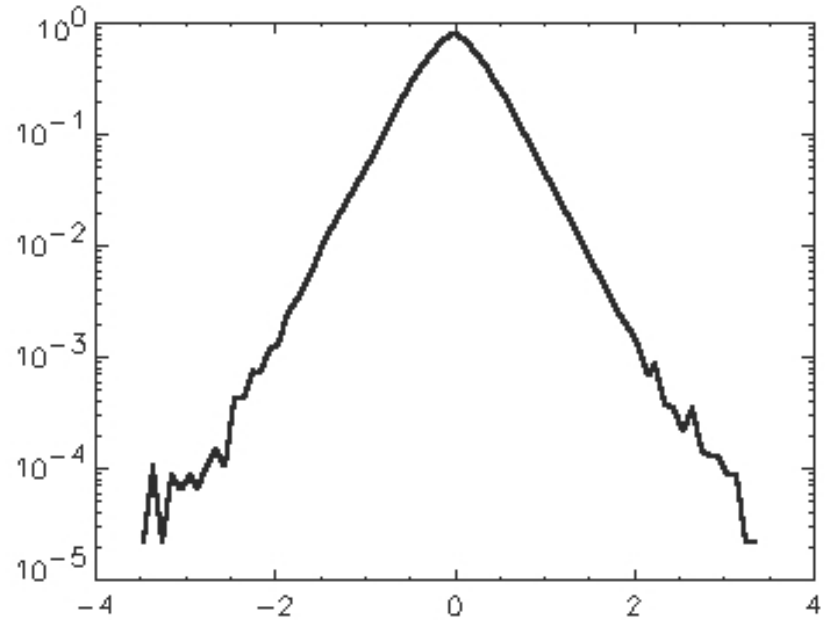


Best fit: P(v)~ exp[*-const* · |*v*|$^{3/2}$]

Theory: van Noije & Ernst, Granular Matter (1998)

In Toluene

Aranson, Olafsen & Ben-Naim, in progress



Best fit: P(v)~ exp[*-const* · |*v*|]

Kinetic Theory: long range interactions

Theory: LANL, experiment: ANL

- **Central interaction**

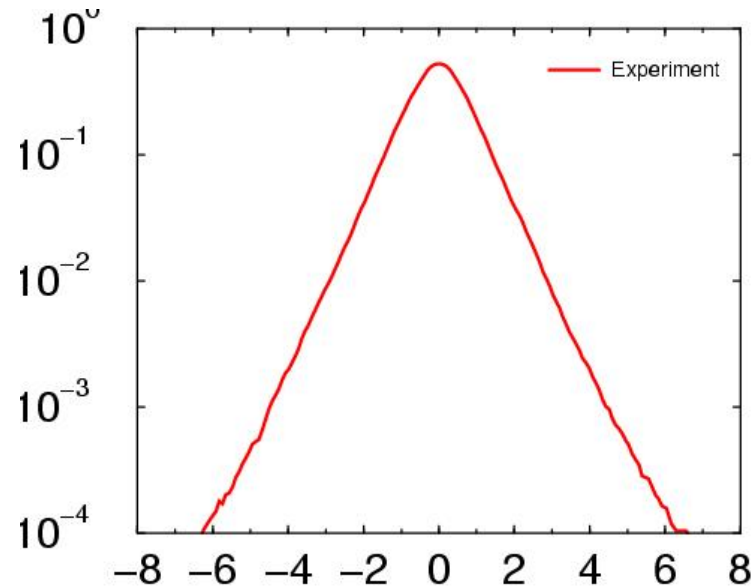
$$V(r) \sim r^{-\sigma}$$

- **Collision rate**

$$K(\mathrm{v}_1, \mathrm{v}_2) \propto \left|\mathrm{v}_1 - \mathrm{v}_2\right|^{1-2(d-1)/\sigma}$$

- **Over-populated velocity tail**

$$P(\mathrm{v}) \propto \exp\left(-\mathrm{v}^{\alpha}\right) \qquad \alpha = \frac{3}{2} - \frac{d-1}{\sigma}$$



- **Electrostatic driving in fluid**

$$d = 2 \qquad \sigma = 2 \qquad \Rightarrow \qquad \alpha = 1$$

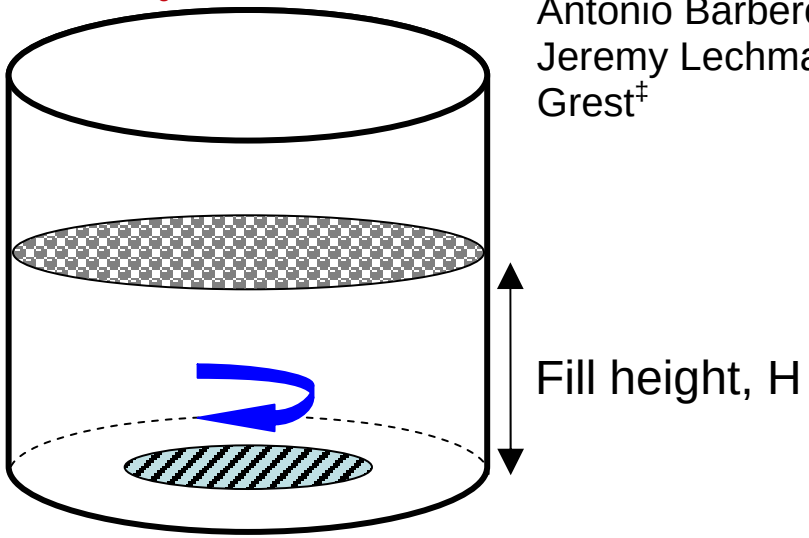
High energy tail probes particle interactions!

BES/Materials Sciences
Center Synthesis Processing

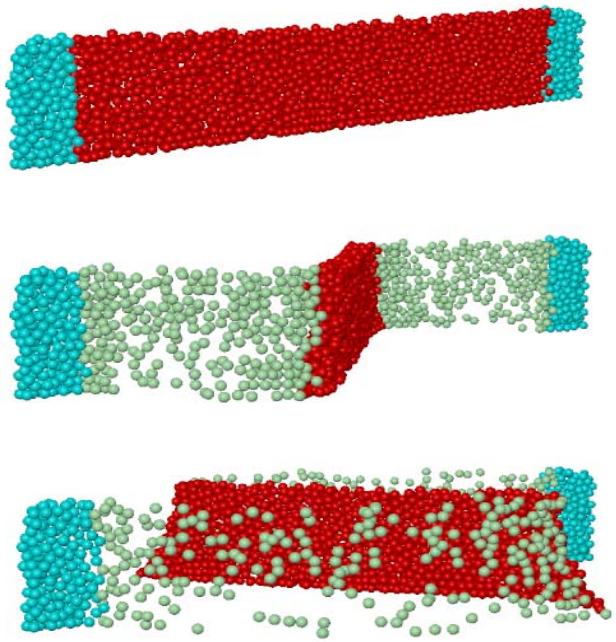
Granular Flows: Split-Bottom Couette Cell

University of Chicago and Sandia NL Collaboration

Antonio Barbero*, Sid Nagel†,
Jeremy Lechman‡, James Landry‡, and Gary Grest‡



Example Simulation system:
60k particles, H = 12.6d
Note inner, 'quasi-solid' (red) core.



Experimental setup:

D_{outer} = 75.7 d

D_{inner} = 59.8 d

d particle diameter

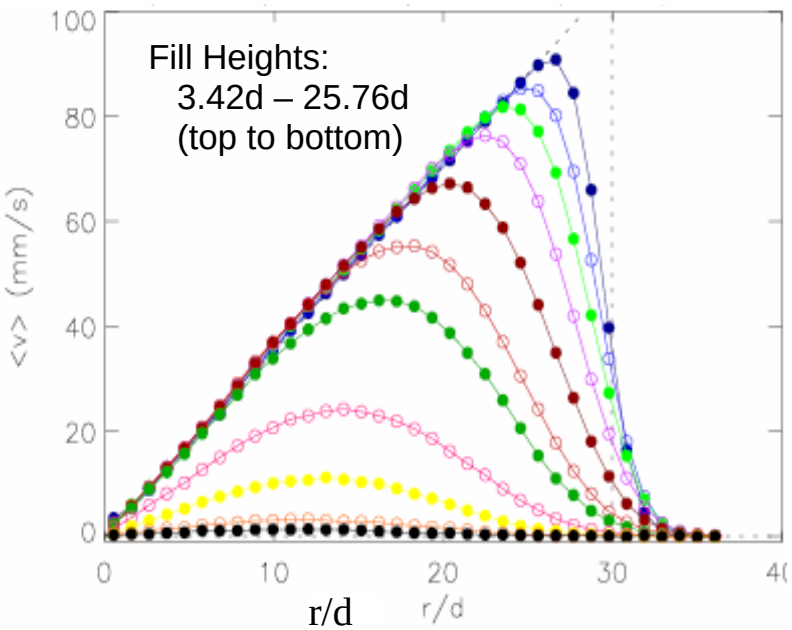
*- visiting professor James Franck Institute;
† - James Franck Institute; ‡ - Sandia NL

LABORATORY
Sandia National Laboratories

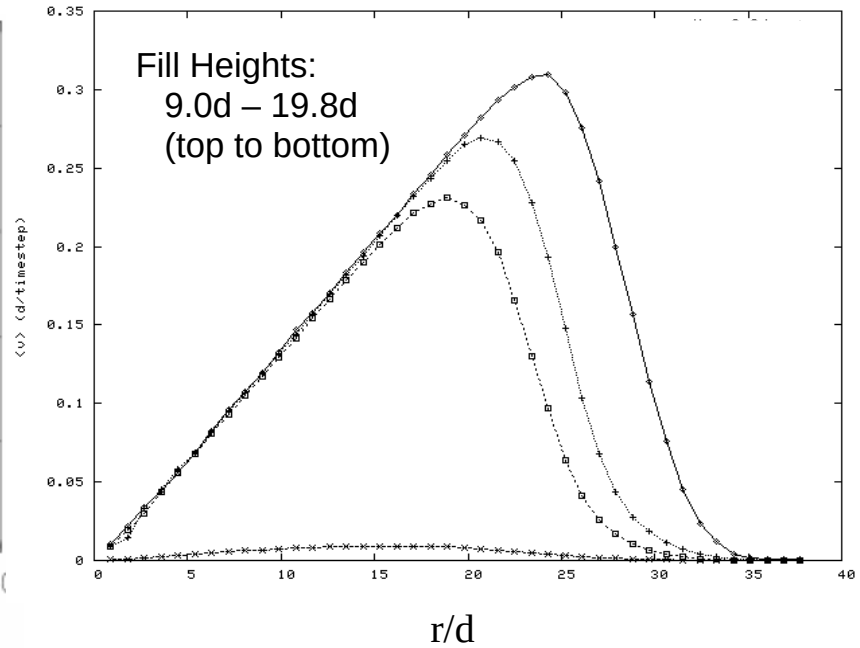
BES/Materials Sciences
Center Synthesis Processing

Split-Bottom Couette Cell
Comparison of Experiment and Simulation

Average surface azimuthal velocity as a function of radius



Experimental results, glass beads



Simulation results: 40k, 60k, 80k and 100k particles, H = 9.0d – 19.8d

- Experiments and Simulations both show the existence of well defined shear bands

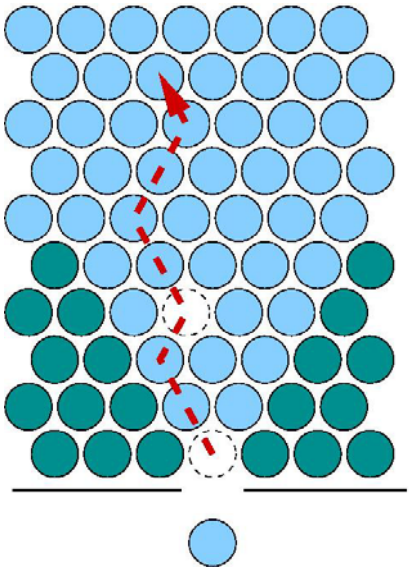
BES/Materials Sciences
Center Synthesis Processing

Hopper Flow: Granular Flow Model Validation

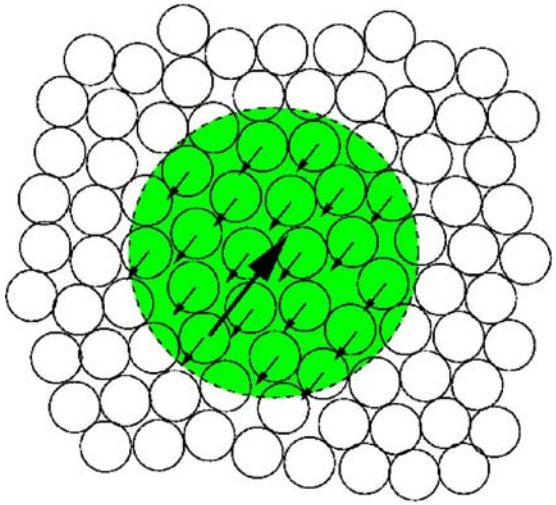
Clark University, MIT and Sandia NL Collaboration

James Landry‡ (SNL), Martin Bazant* (MIT),
Arshad Kudrolli† (Clark), and Gary Grest‡ (SNL)

- Develop and validate a robust model for flow in granular drainage
  - Previous models based on diffusion of particle size voids overestimates amount of horizontal mixing
  - MIT spot model considers collective motion of larger regions
- Study the feasibility of pebble bed nuclear reactors



Void model



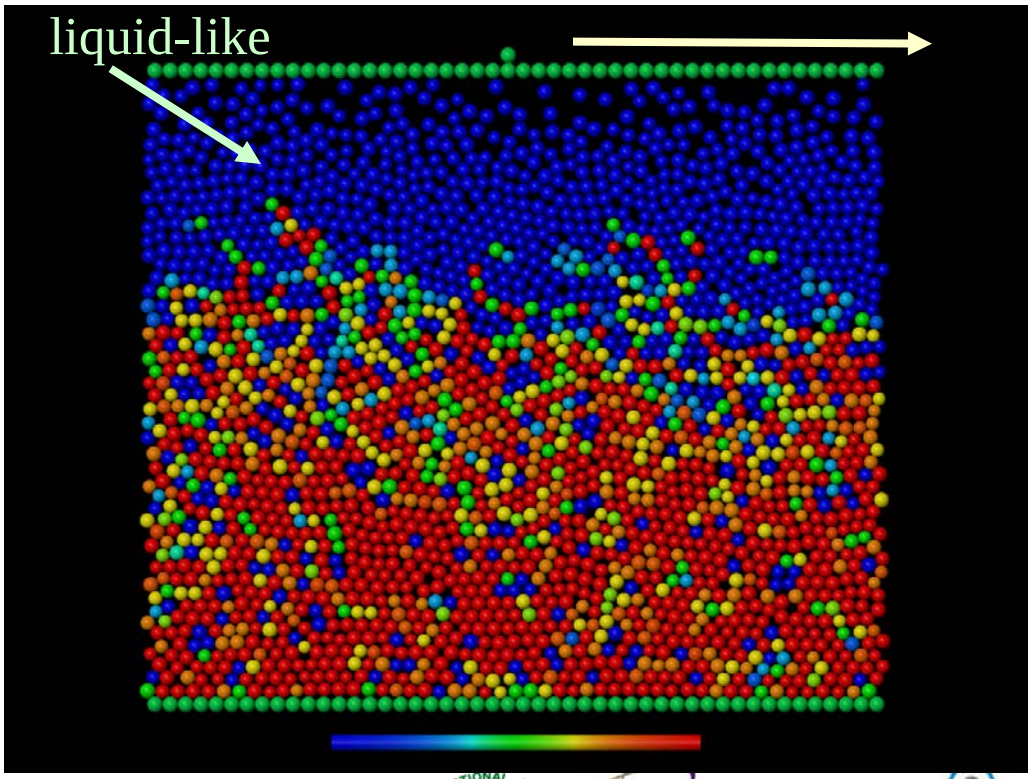
Spot Model

Order parameter for fluidization: "shear melting" of granular material

BES/Ma
Center Sy

$$\rho = \frac{Z_{st}}{Z}$$

- Z -total number of contacts per particle (coarse-grained)
- Z_{st} -number of persistent contacts



OP characterizes the phase state of granular matter:

solid: $\rho = 1$

liquid: $\rho = 0$

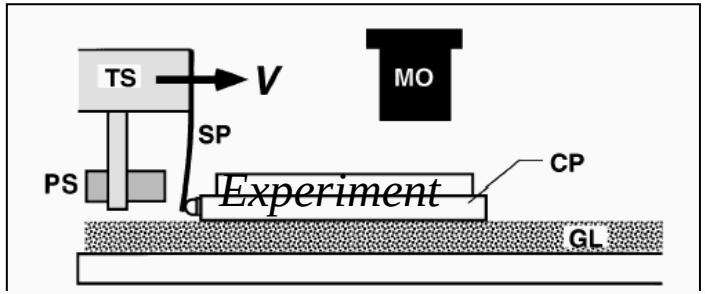
2D simulations of granular shear flow between 2 plates. OP is shown by color

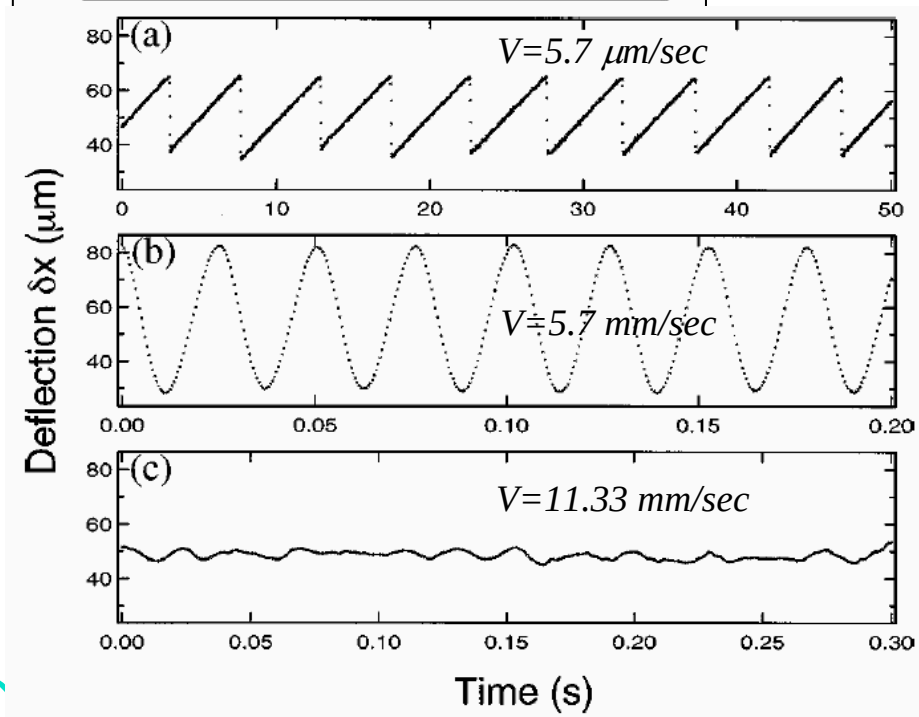
Volfson, Tsimring & Aronson, PRL 2003

Application to Non-Stationary Problem

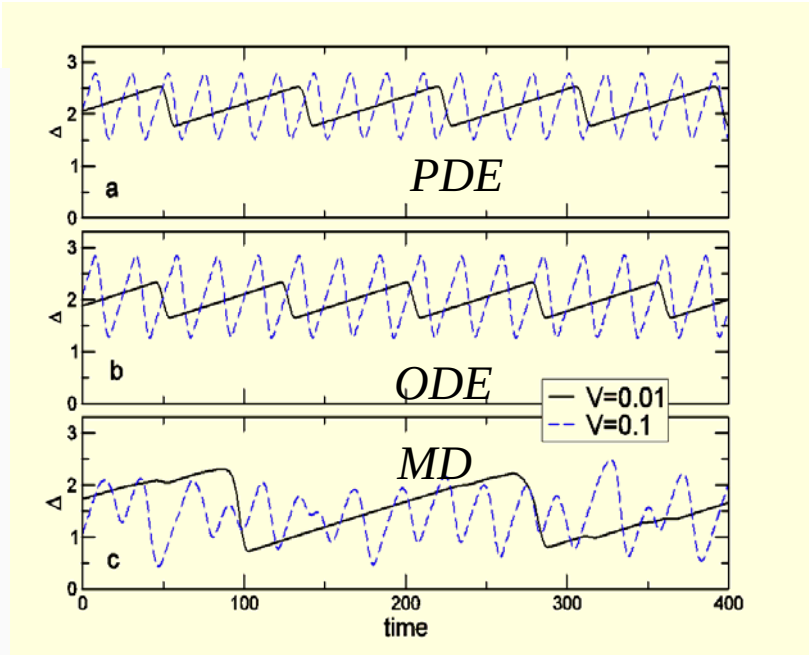
BES/Materials Sciences
Center Synthesis Processing

Experiment: Nasuno, Kudrolli, Bak and Gollub, *PRE*, **58**, 2161 (1998).
Theory: Volfson, Tsimring, Aronson, PRE (2004)





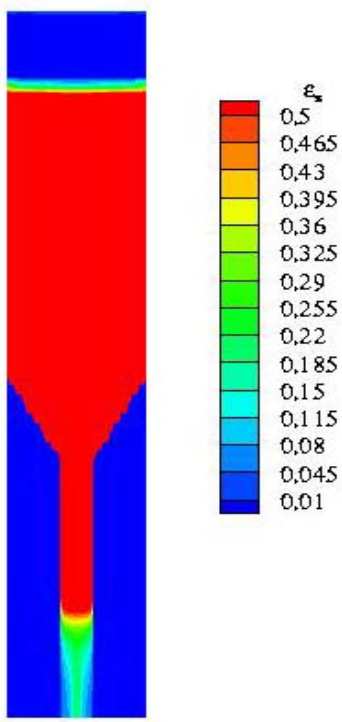
Theory/MD



Granular Flows: Constitutive Models

Engineering devices: Hopper Simulation using MFIX (NETL)

- Regime: transition from collisional to frictional
  - Collisional regime (1-30%): kinetic theory
  - High solids volume fraction: enduring contacts with multiple neighbors
- Additive stress models:
  - Sundaresan (frictional+kinetic; gas-particle mixture)
  - Louge (impulsive rate-dependent + enduring rate-independent)
  - Aronson-Tsimring (AT): "fluid" stress (strain rate dependent) + solid stress



General Objective Model

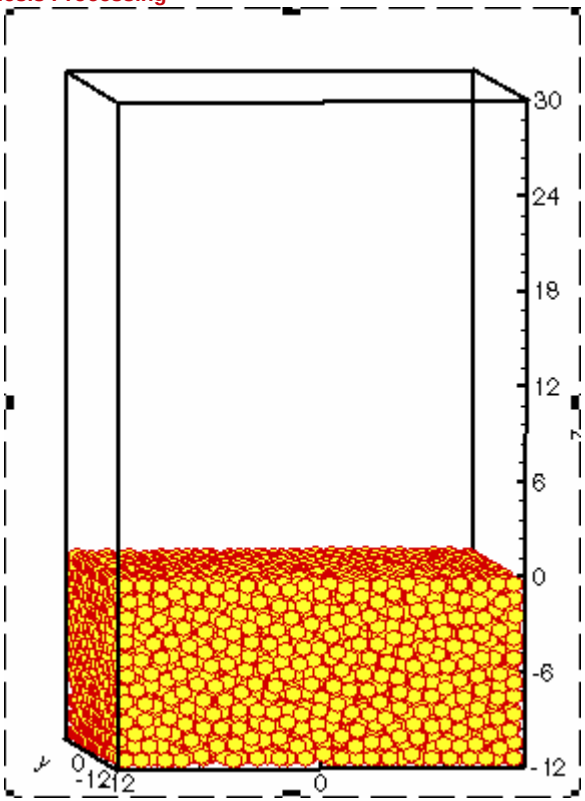
- **AL/ISU contribution:**
  - **generalized AT model using representation theorems for tensor functions, and relaxed assumptions**
  - *Objective decomposition of the stress tensor in granular mixtures*, Gao, Subramaniam, Fox & Hoffman, PRE submitted
- **Express "fluid" stress in terms of isotropic and anisotropic parts of total granular stress**

$$\sigma_{ij}^{f} = \sigma_0 \left\{ \alpha\delta_{ij} + \beta b_{ij} + \gamma \left[(\mathbf{b}^2)_{ij} - \frac{1}{3}(\mathbf{b}^2)_{ll}\delta_{ij} \right] \right\}$$

α, β, γ: model coefficients that are functions of the invariants of b_{ij} (anisotropic part of stress tensor) and the order parameter ρ.

Particle-Fluid Interaction using GranFlow

BES/Materials Sciences
Center Synthesis Processing



Fluid inlet velocity=7×10^{-3} m/s

Properties (in SI units):

Fluid:

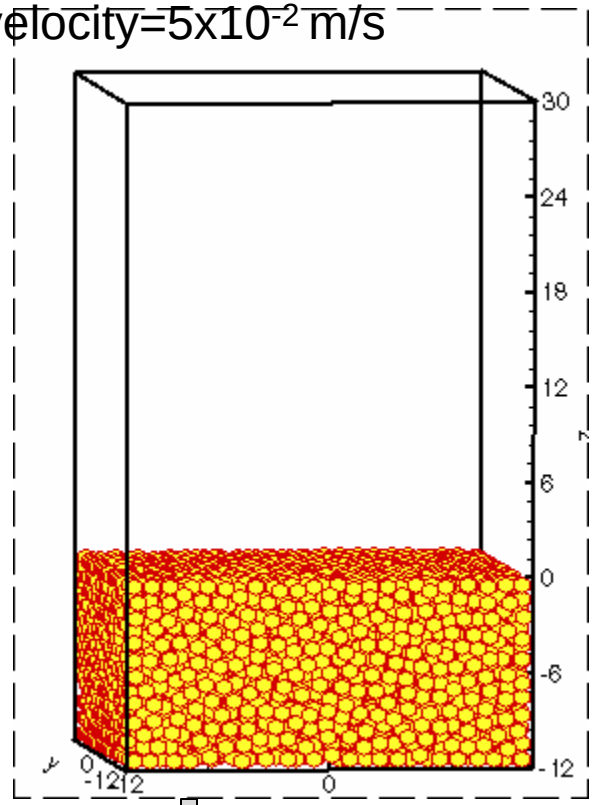
Viscosity= 2×10^{-5}
Density=1

Particle:

Diameter=1×10^{-4}

Density=1×10^{3}

Fluid inlet velocity=5×10^{-2} m/s



Lift-height~12

Gao, Subramaniam, Fox, Hoffman (AL/ISU) and Grest (Sandia)

Summary

- <u>Goal:</u> Improve understanding of behavior of granular materials
  - Obj 1: Close the gap between continuum & discrete descriptions; develop constitutive models
  - Obj 2: Roadmapping and outreach
- <u>Strategy</u>: Multidisciplinary approach to flow and kinetics of granular materials, theory, high-performance computing, and experiment.
- <u>Technical tasks</u>:
  - Granular Gases: velocity statistics & kinetic theory
  - Granular Fluids: constitutive relations & continuum theory
  - Granular Mixtures: multiphase flows
- <u>Method</u>: collaborations via personnel exchange & yearly workshops

Past Year Accomplishments

- Experiments: revealed interesting new phenomena
  - coarsening and effect of ambient fluid in granular gases
  - shear bands in Couette cells
- Theory:
  - kinetic theory has been developed to explain velocity tails
  - exchange-driven growth explains coarsening
  - order-parameter model for transition from fluid to solid constitutive behavior
- Simulations:
  - revealed fluid-solid transition
  - explain shear banding in Couette cell
  - effect of wall friction in hopper simulations
- Collaborations are successful via personnel exchange & yearly workshops

Future Work

- Electrostatic driving experiments to be extended to micron and sub-micron particles
- Further develop fluid-particle simulation
- Effects of polydisperse particles
- Effects of cohesion
- Pebble-bed reactor modeling using GranFlow
- Theoretical study of shear bands

BES/Materials Sciences
Center Synthesis Processing

Publications

1. **Confined granular packings: Structure, stress, and forces,** J. W. Landry, G. S. Grest, L. E. Silbert, and S. J. Plimpton, Phys. Rev. E **67**, 041303 (2003)
2. **Exchange Driven Growth**, E. Ben-Naim and P.L. Krapivsky. *Phys. Rev. E*, submitted (2003)
3. **Spontaneous spirals in vibrated granular chains**, R. Ecke, Z. A. Daya, M. K. Rivera, and E. Ben-Naim. *Proc. Of MRS 02 Fall Meeting*, accepted (2002).
4. **The Inelastic Maxwell Model**, E. Ben-Naim and P.L. Krapivsky. *Lecture Notes in Physics*, accepted (2003)
5. **Dynamics of Freely Cooling Granular Gases**, X. Nie, E. Ben-Naim and S.Y. Chen. *Phys. Rev. Lett.*, **89**, 204301, (2002)
6. **Impurity in a Maxwellian Unforced Granular Fluid**, E. Ben-Naim and P.L. Krapivsky. *Eur. Phys. Jour. E 8*, **507** (2002)
7. **Inontrivial velocity distributions in Inelastic Gases**, E. Ben-Naim and P.L. Krapivsky. *Phys. Rev. E*, **66**, 025102 (2002)

Publications

8. **Molecular dynamics simulations and continuum theory of partially fluidized shear granular flows**, Dmitri Volfson, Lev S. Tsimring, and Igor S. Aranson, *Phys. Rev. Lett.*, to appear (2003)

9. **Model of coarsening and vortex formation in vibrated granular rods**, Igor S. Aranson and Lev S. Tsimring, *Phys. Rev. E* (Statistical, Nonlinear, and Soft Matter Physics), Volume 67, Issue 2, Article 021305

10. **Velocity fluctuations in electrostatically driven granular media**, I. S. Aranson and J. S. Olafsen Physical Review E (Statistical, Nonlinear, and Soft Matter Physics), Volume 66, Issue 6, Article 061302

11. **Coarsening of granular clusters: Two types of scaling behaviors**, M. V. Sapozhnikov, I. S. Aranson, and J. S. Olafsen, *Phys. Rev. E* (Statistical, Nonlinear, and Soft Matter Physics), Volume 67, Issue 1, Article 010302

12. **Vortices in vibrated granular rods**, Daniel L. Blair, T. Neicu, and A. Kudrolli Physical Review E (Statistical, Nonlinear, and Soft Matter Physics) *Phys. Rev. E*, **67**, 031303 (2003)