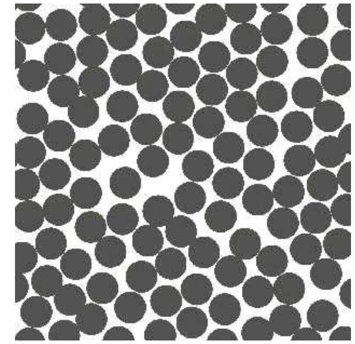
Problems in Granular Materials



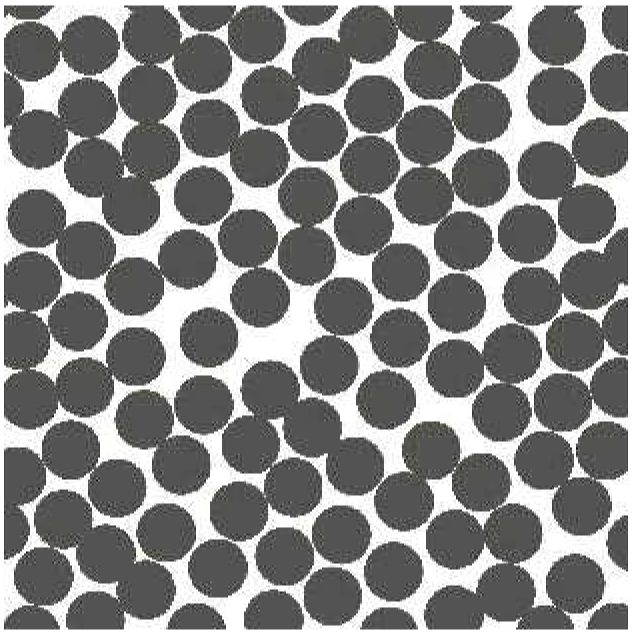
Abstract:

Granular materials, collections of particles which dissipate energy through inter-particle interactions, are important in a wide variety of industries such as energy production, food processing, and pharmaceuticals. A fundamental understanding of granular systems, comparable to our current understanding of fluids and solids, does not exist today but would have far reaching implications across many industries.

Like ordinary materials, granular systems can act like a fluid or solid depending on the granular temperature, defined as the average kinetic energy of the particles. Unlike ordinary materials, granular systems can change between solid to fluid (freeze/melt) over small intervals of space or time, due to granular temperature that often vary by 4 orders of magnitude or more in the same system. Further, granular system can be melted by small strains and often flow like supersonic fluids.

These properties explain many of the fascinating flow structures seen in granular systems. One of the most intriguing and beautiful is the patterns formed in vertically vibrated thin layers. Squares, stripes, hexagons, kinks, phase domains, and solitary structures can form, depending on the frequency and strength of shaking. These patterns states allow us to test microscopic law of granular interactions using molecular dynamics. Because granular systems often flow like supersonic fluids, shocks can easily be form when a granular stream hits a stationary obstacle. This type of system allows us to test continuum theories of granular flows like Navier-Stokes for ordinary fluids. Finally, rotating drum flows elucidates the difficulties that lie ahead for a unified granular continuum theory, displaying in one flow, solid, fluid, melting, freezing, super- and sub-sonic behavior.

Problems in Granular Materials



Mark D. Shattuck
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Benjamin Levich Institute
City College of New York
NSF-DMR

Hands On 2009

Granular Applications

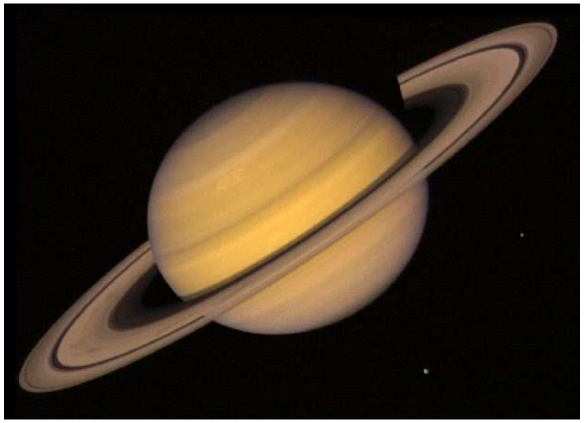
Sand dune formation

Food grains

Pharmaceutical Industry

Chemical Industry

Granular Applications



Planetary rings

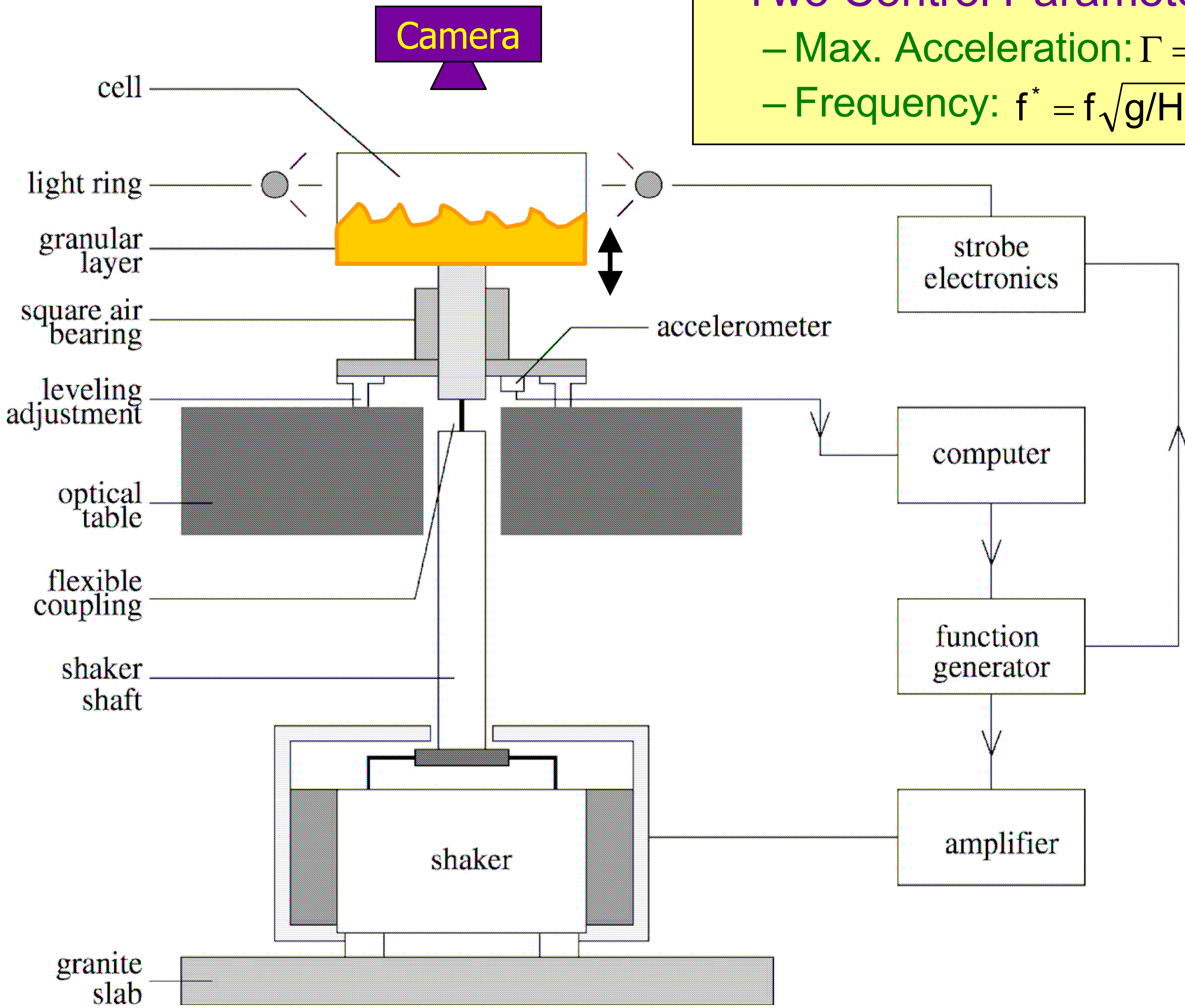
Space Exploration

NASA

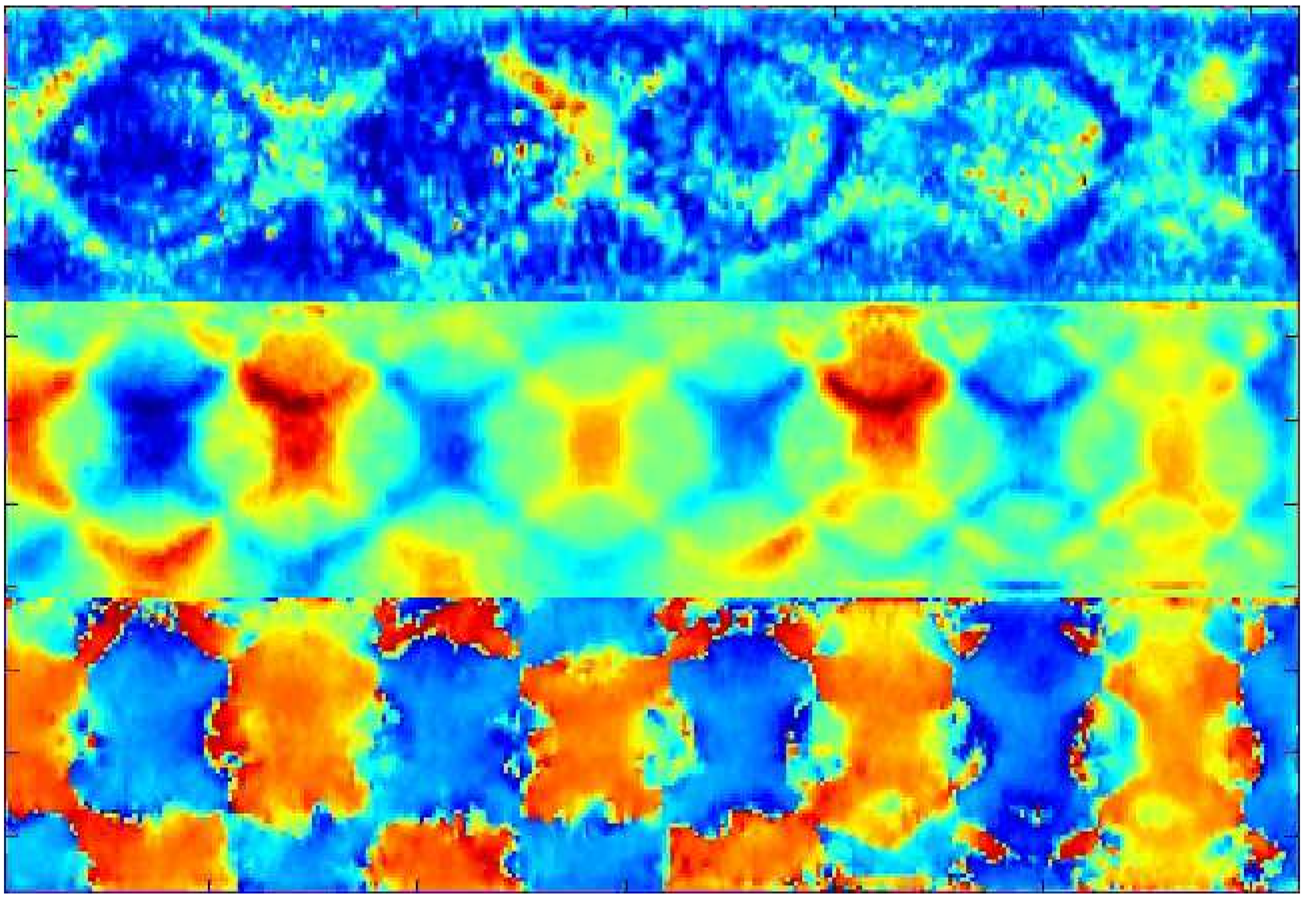
Mars Rover

Experimental Setup

- Oscillates Sinusoidally
  - $y(t) = A\sin(2\pi f t)$
- Two Control Parameters
  - Max. Acceleration: $\Gamma = A(2\pi f)^2 / g$
  - Frequency: $f^* = f\sqrt{g/H}$



Square Patterns in Vibrated Granular Media



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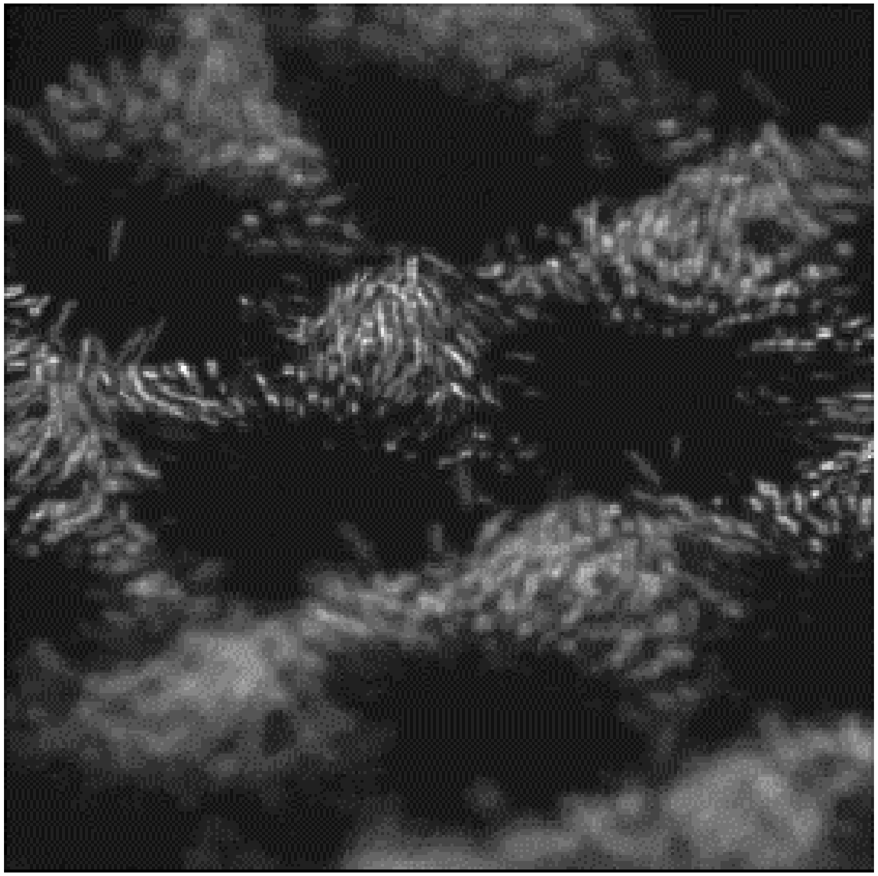
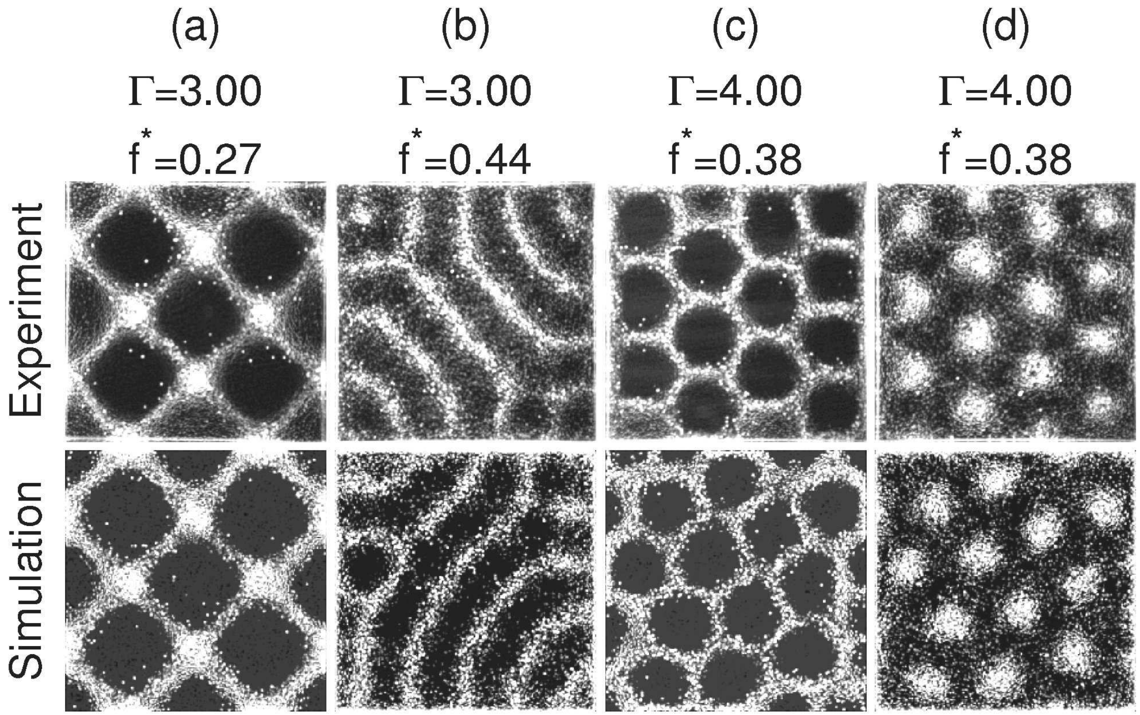
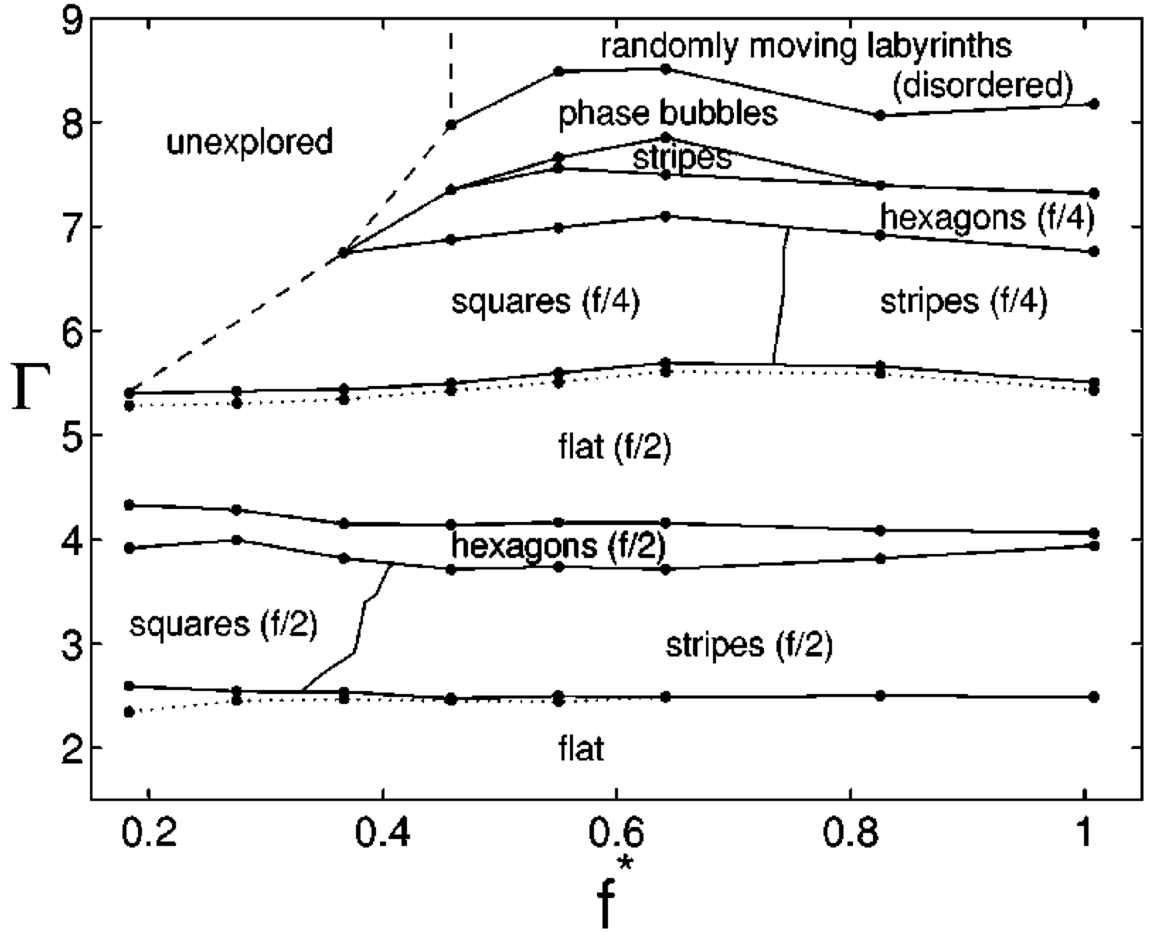


Squares, Stripes, Hexagons



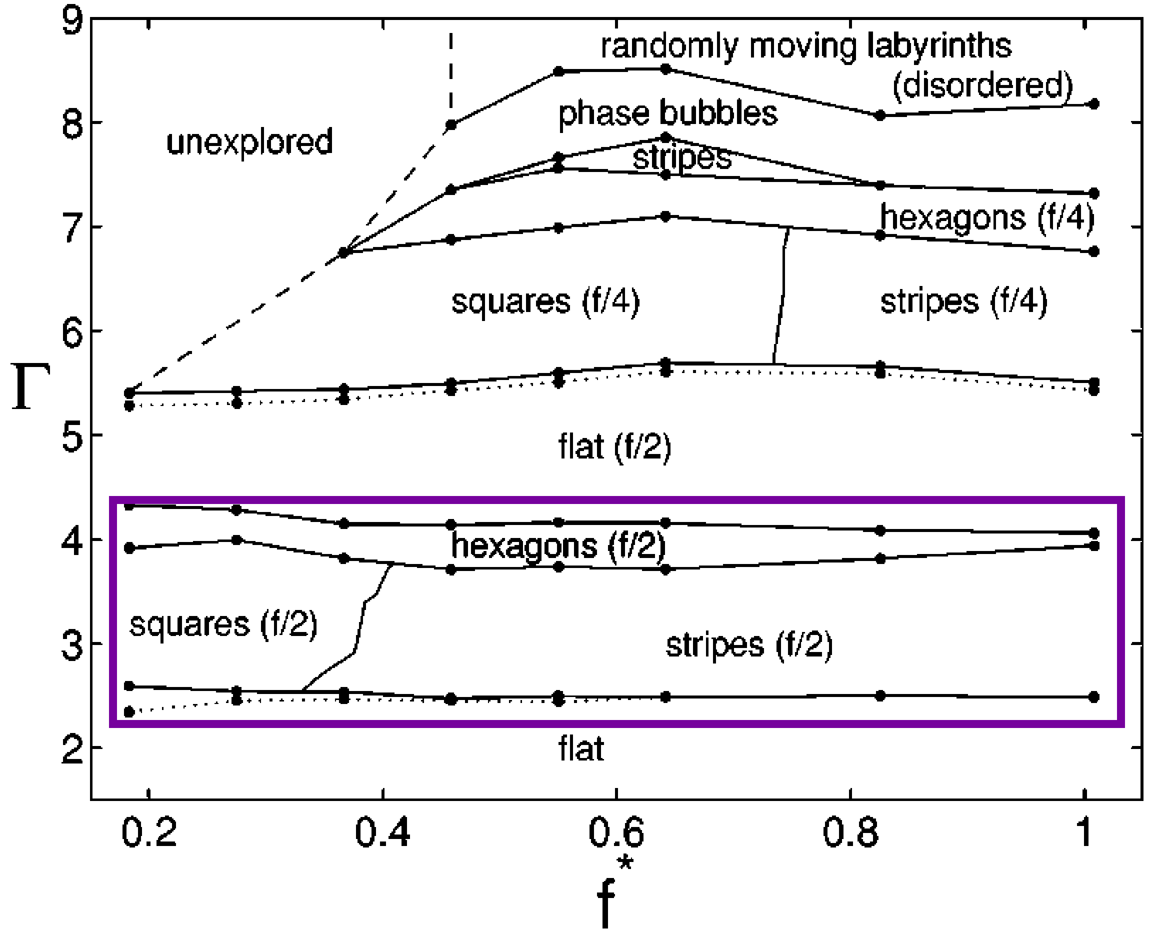
Bizon, MDS, McCormick, Swift, Swinney
PRL 1998

Phase Diagram for Vibrated Granular Media



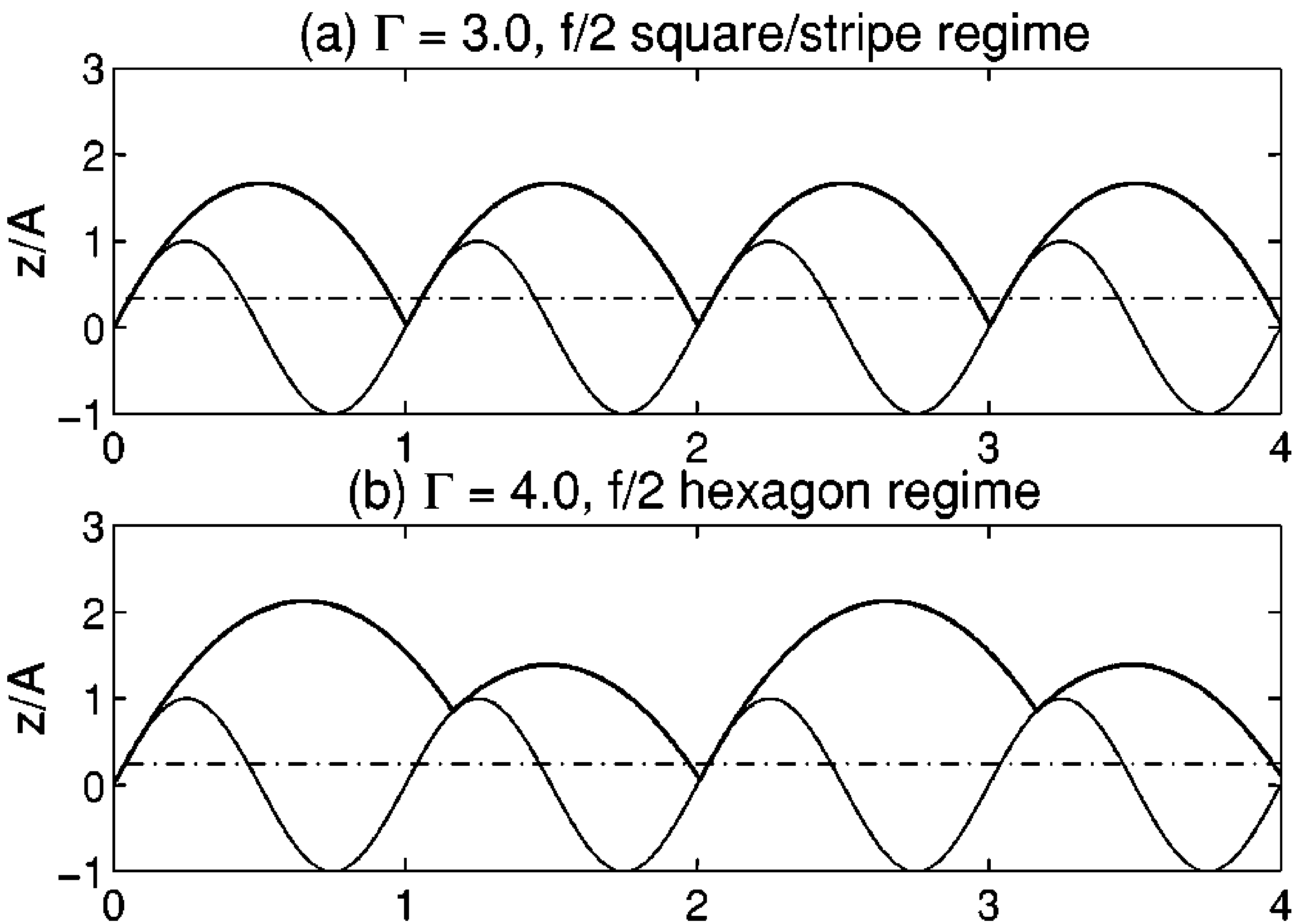
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Phase Diagram for Vibrated Granular Media



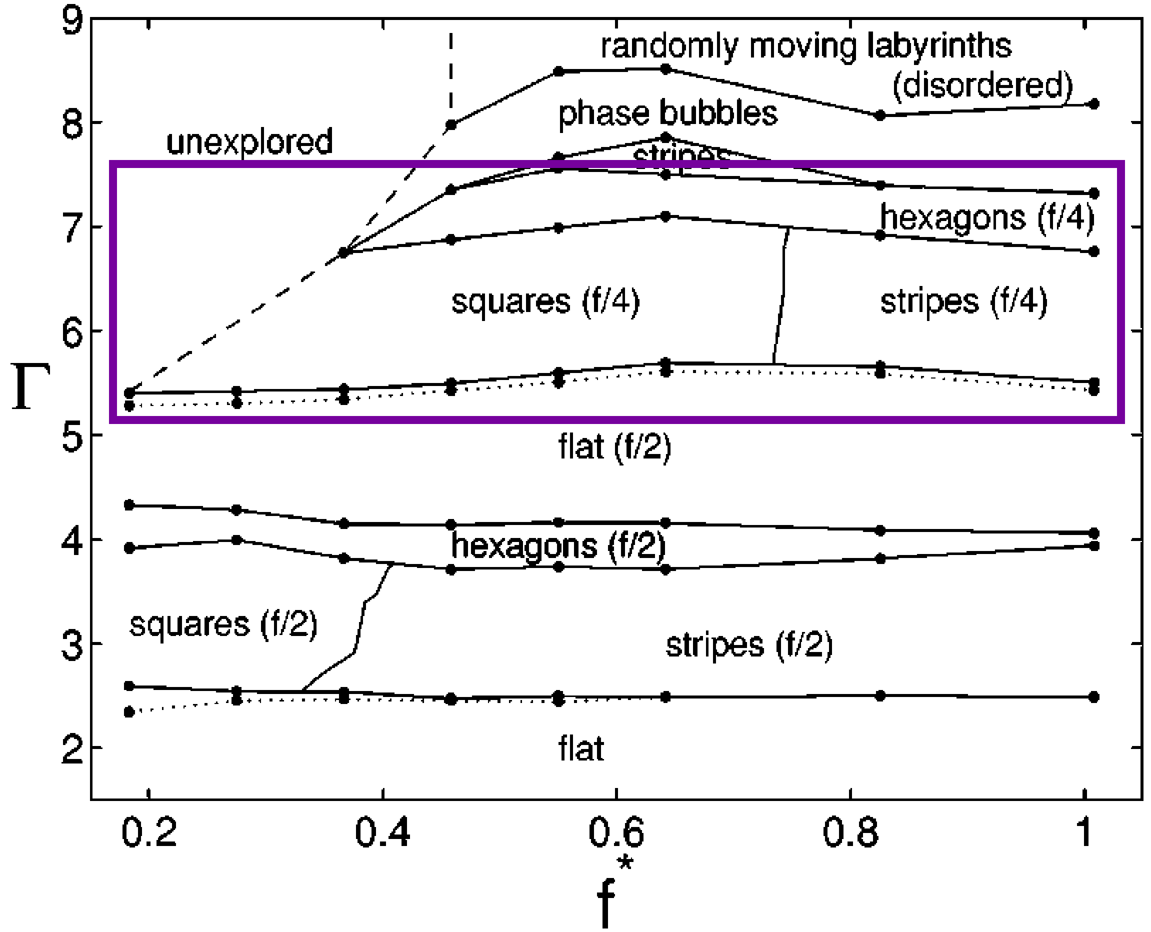
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Temporal Behavior



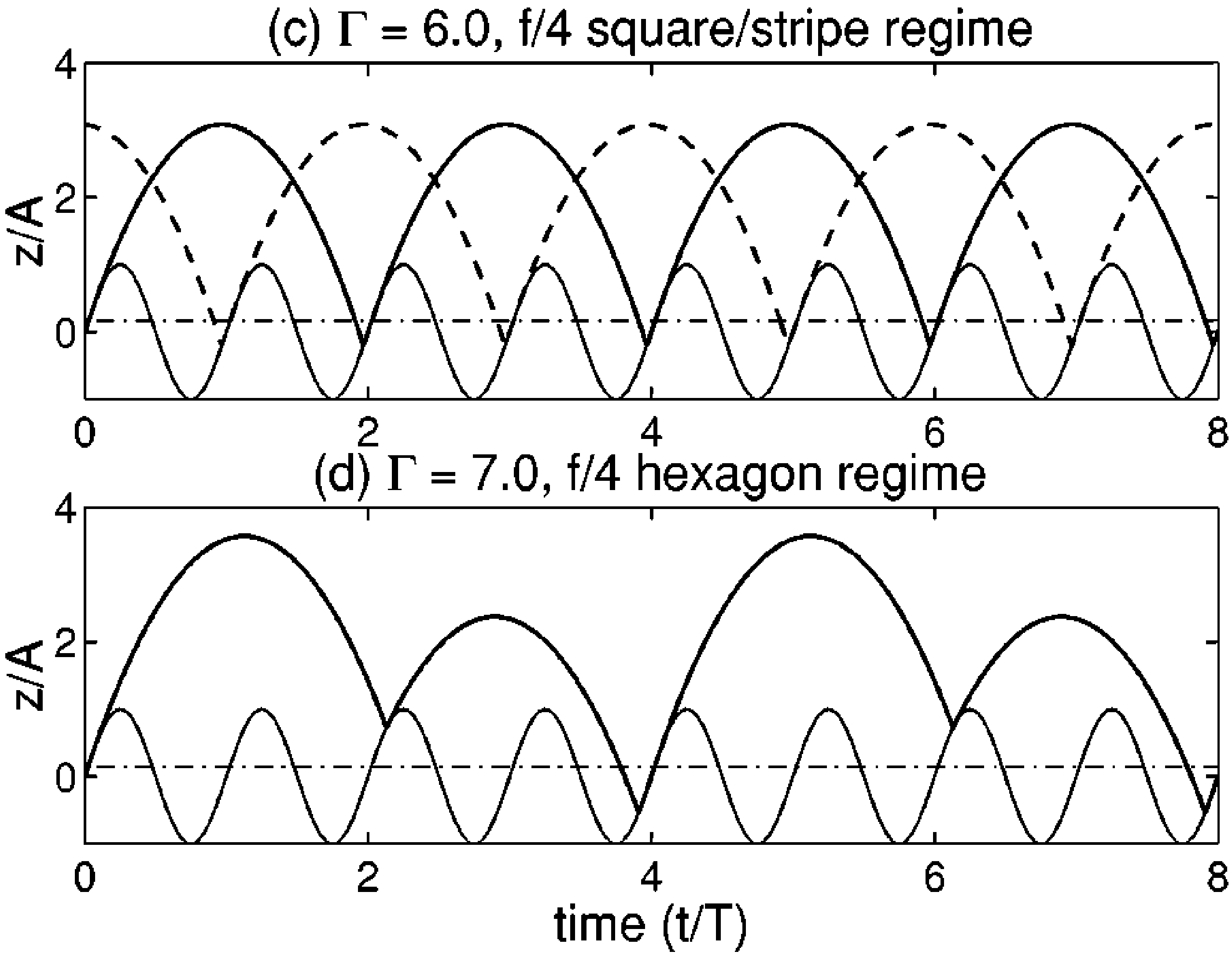
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Phase Diagram for Vibrated Granular Media



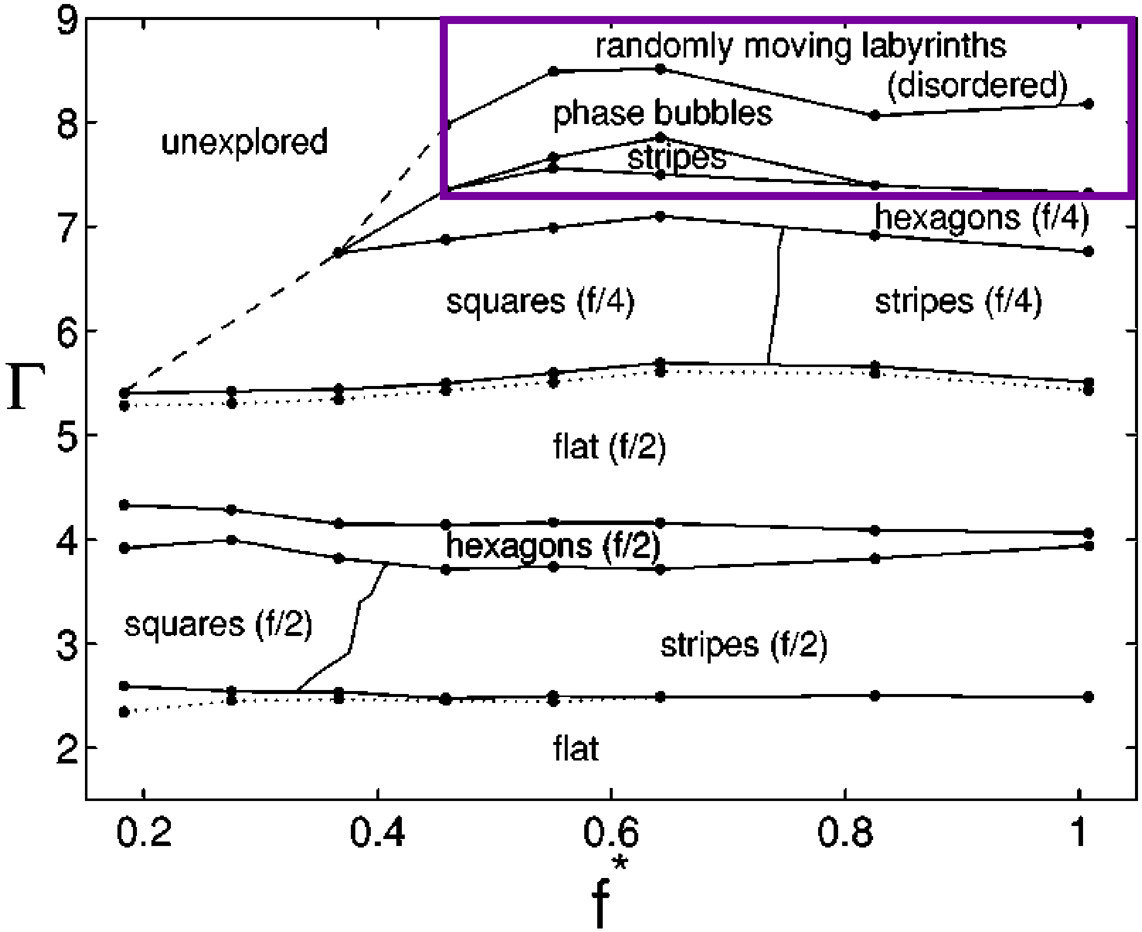
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Temporal Behavior



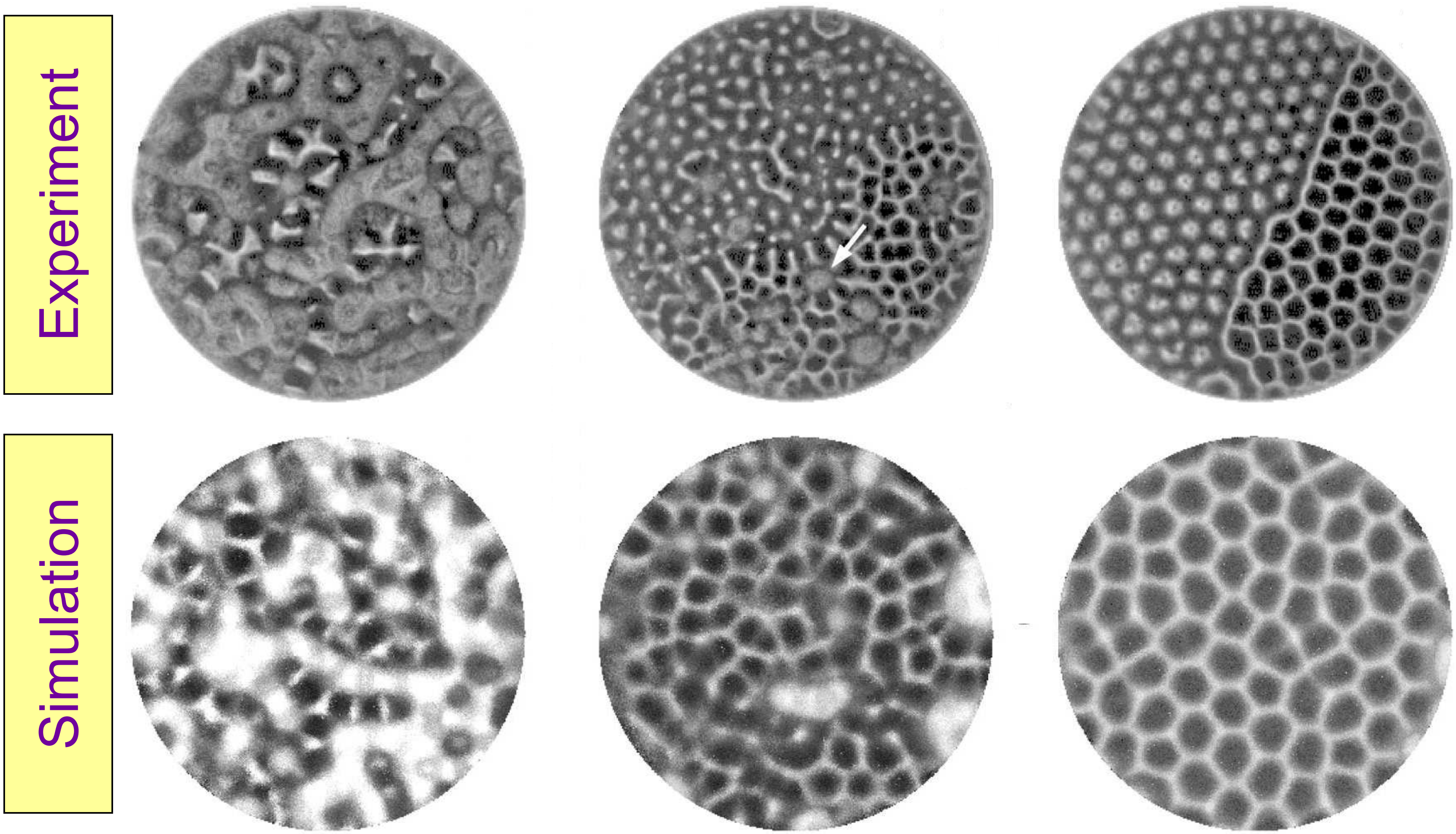
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Phase Diagram for Vibrated Granular Media



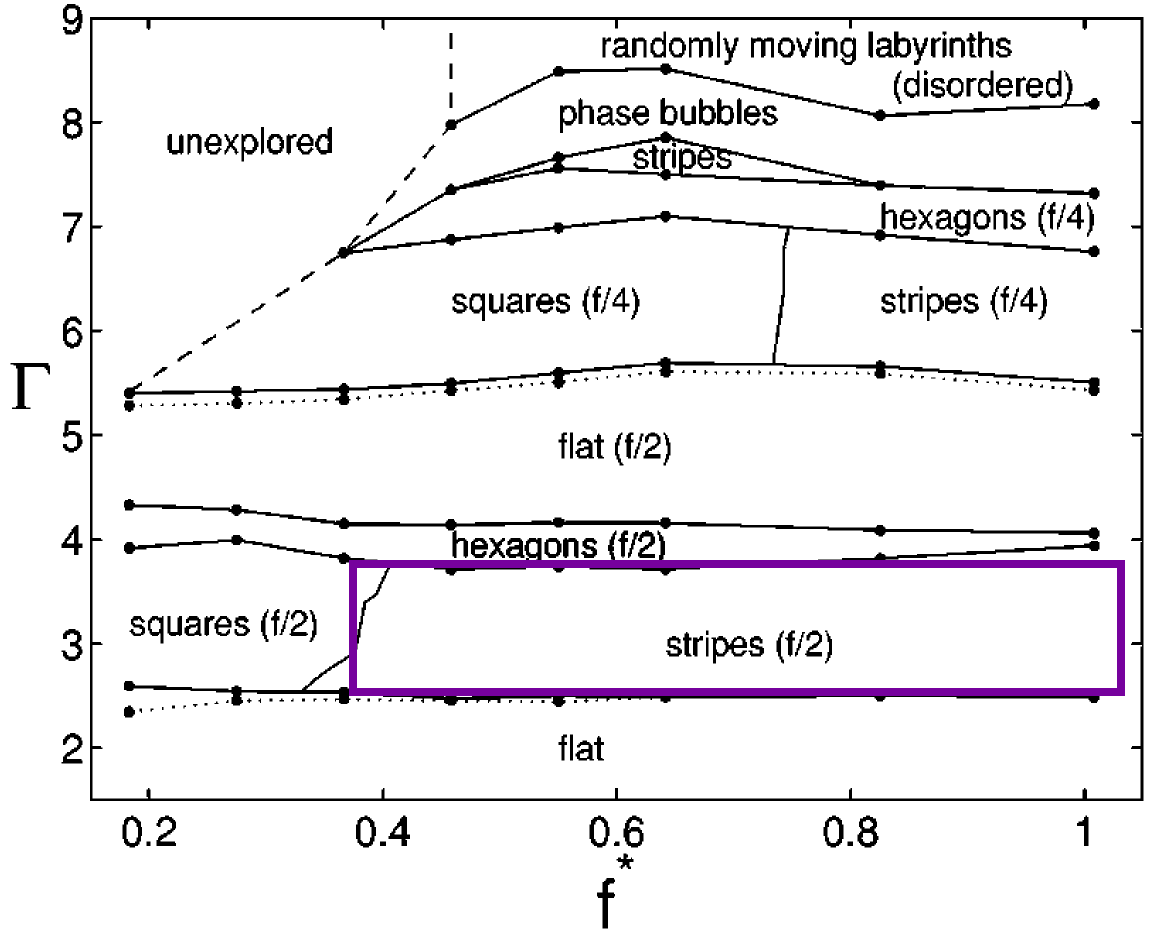
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Phase Bubbles



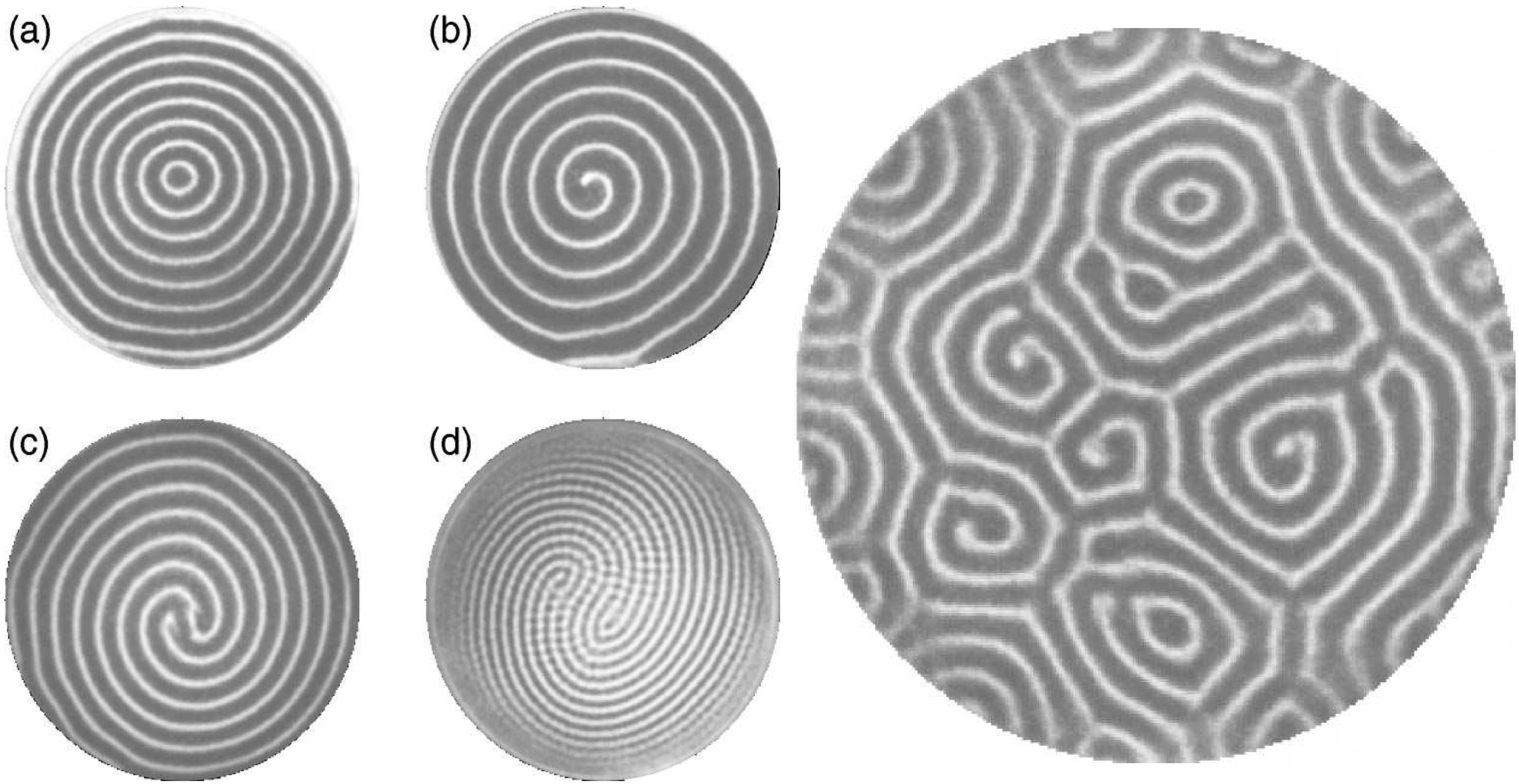
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Phase Diagram for Vibrated Granular Media



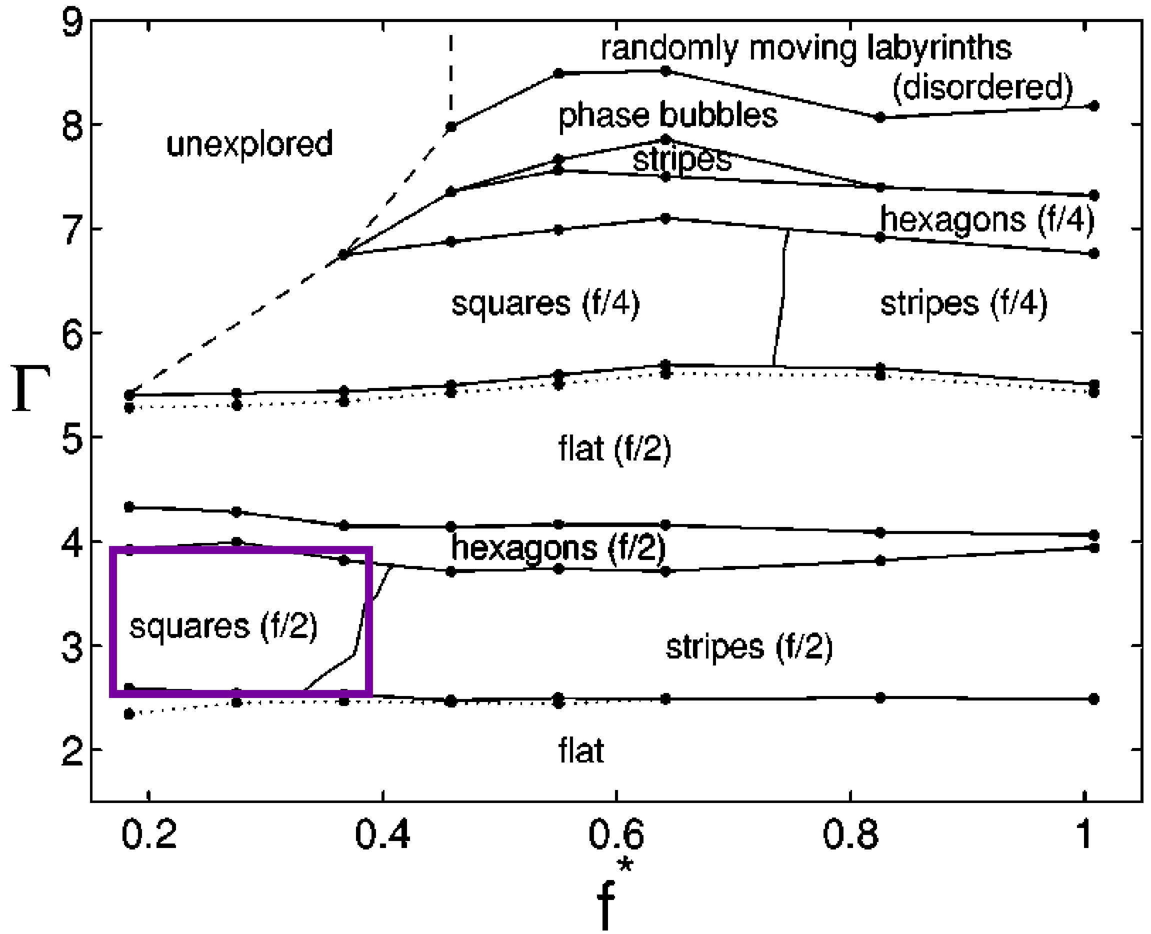
Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

Stripe Patterns in Vibrated Granular Media
Targets, Spirals, and Chaos



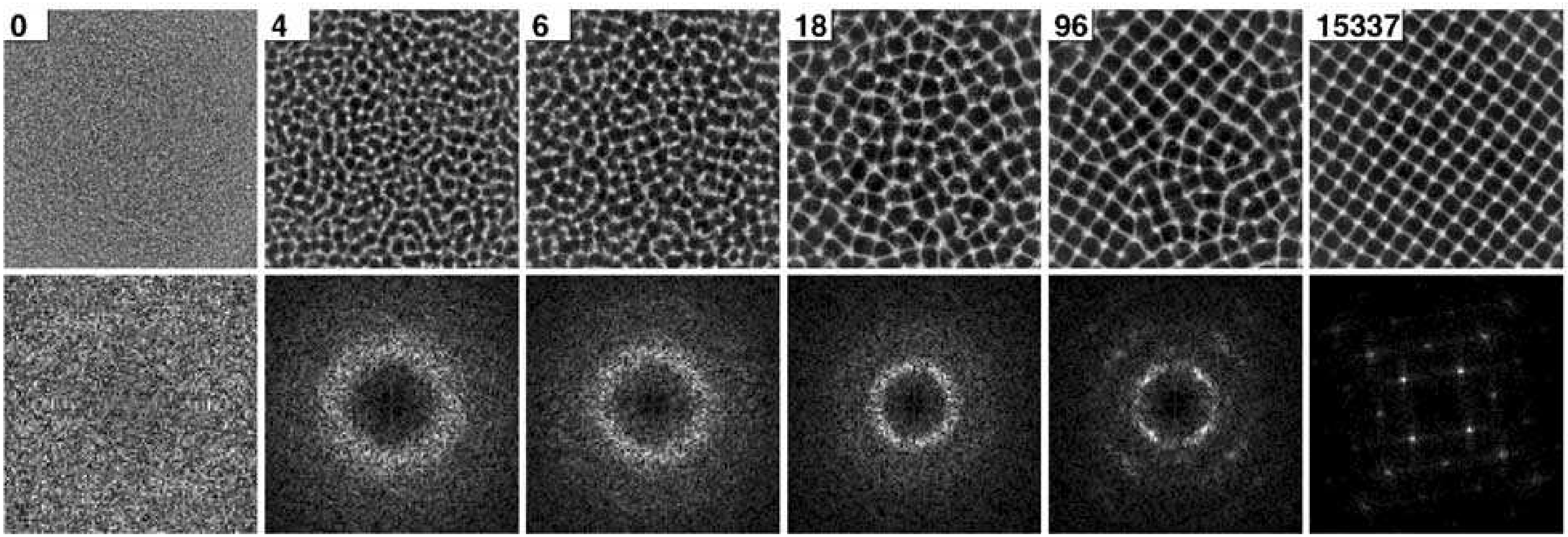
de Bruyn, Lewis, MDS, Swinney PRE 2001

Phase Diagram for Vibrated Granular Media



Moon, MDS, Bizon, Goldman, Swift, Swinney PRE 2002

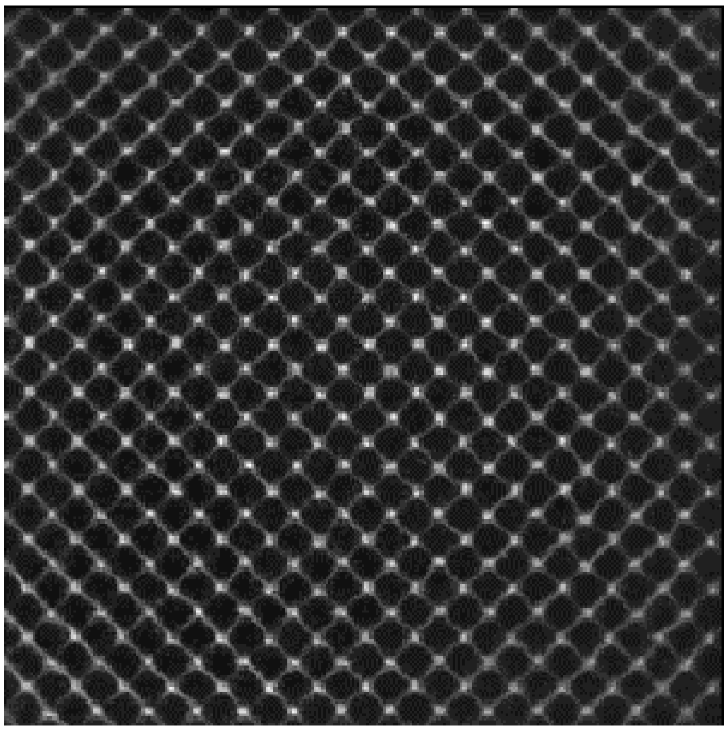
Emergence of Order and Pattern Coarsening

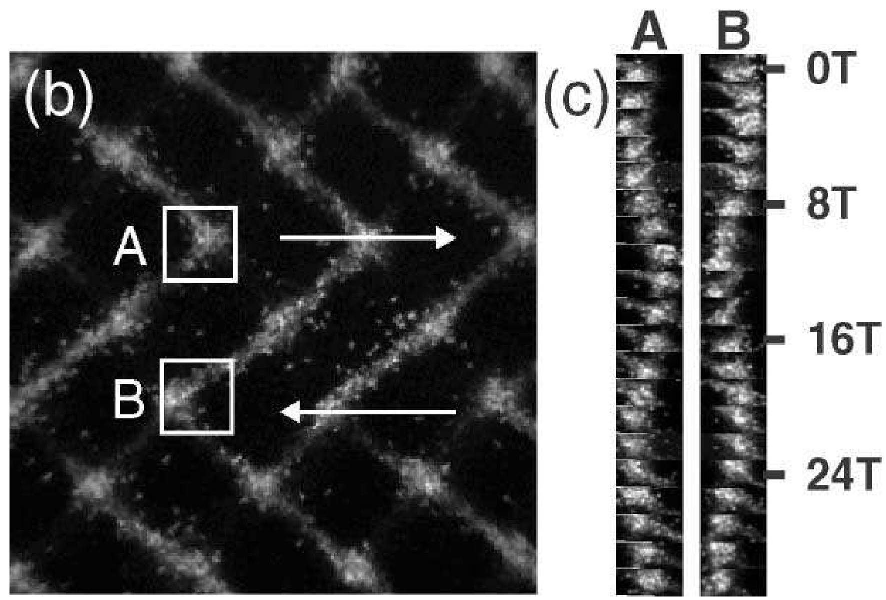


Goldman, MDS, Swinney, Gunaratne Physica A 2002

Square Lattice Dynamics

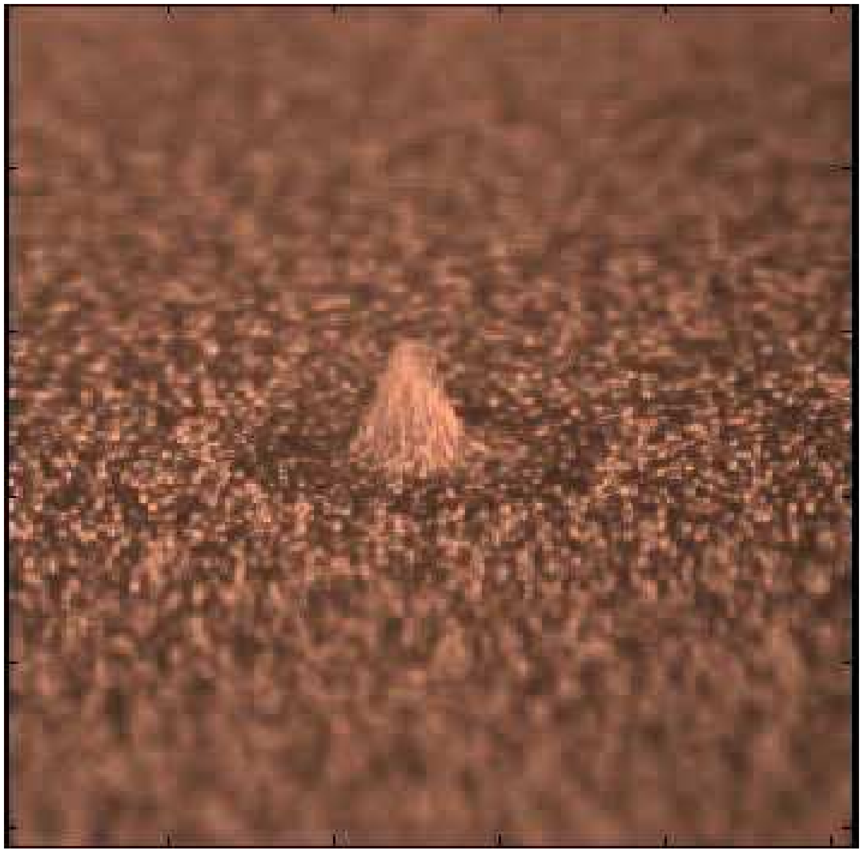
Pattern Crystal with "Phonons"

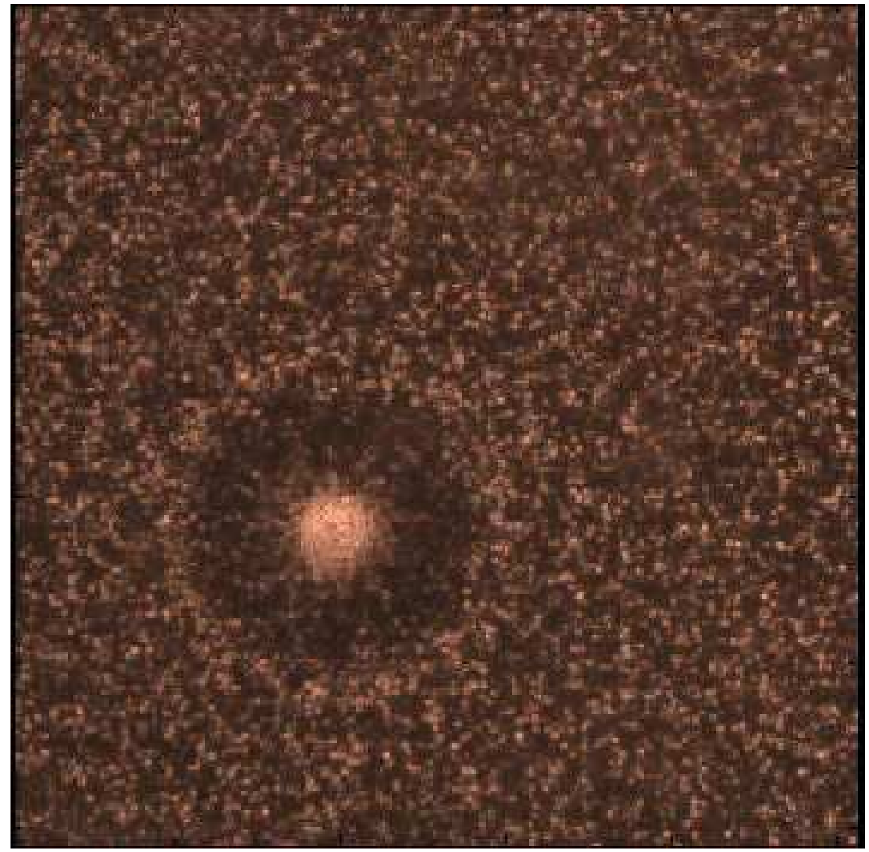




Goldman, MDS,Moon, Swift, Swinney PRL 2003

Localized Patterns in Vibrated Granular Media (Oscillons)





Granular Fluid Dynamics

Mass: $$\frac{\partial n}{\partial t} = \vec{\nabla} \cdot n\,\vec{\mathbf{u}}$$

Momentum: $$n\frac{D\vec{\mathbf{u}}}{Dt} = -\vec{\nabla} \cdot \underline{\mathbf{P}}$$

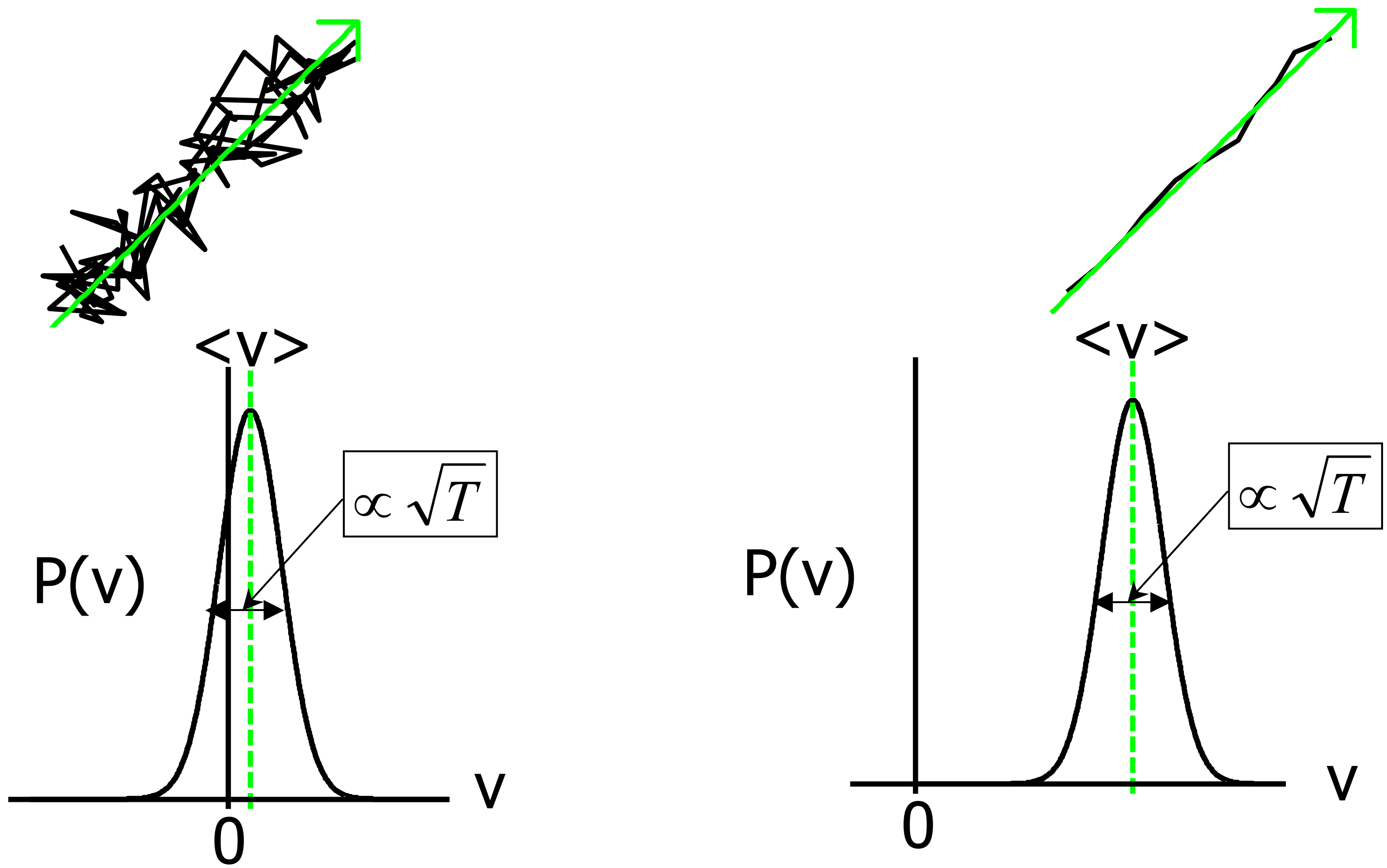
Newtonian Pressure Tensor

Fluctuational Energy Balance: $$n\frac{DT}{Dt} = -\kappa\vec{\nabla} T + \underline{\mathbf{P}} : \underline{\mathbf{E}} - \gamma$$

Temperature Loss Rate

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{\mathbf{u}} \cdot \vec{\nabla}$$

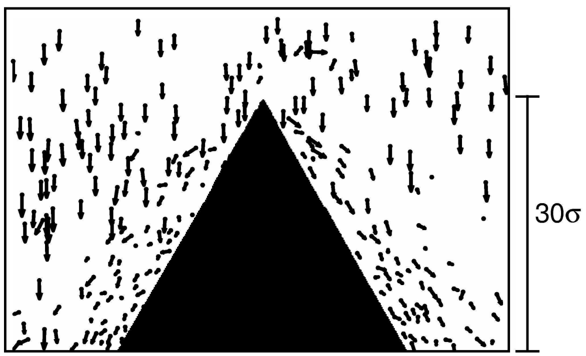
Microscopic Definition of Supersonic Flow

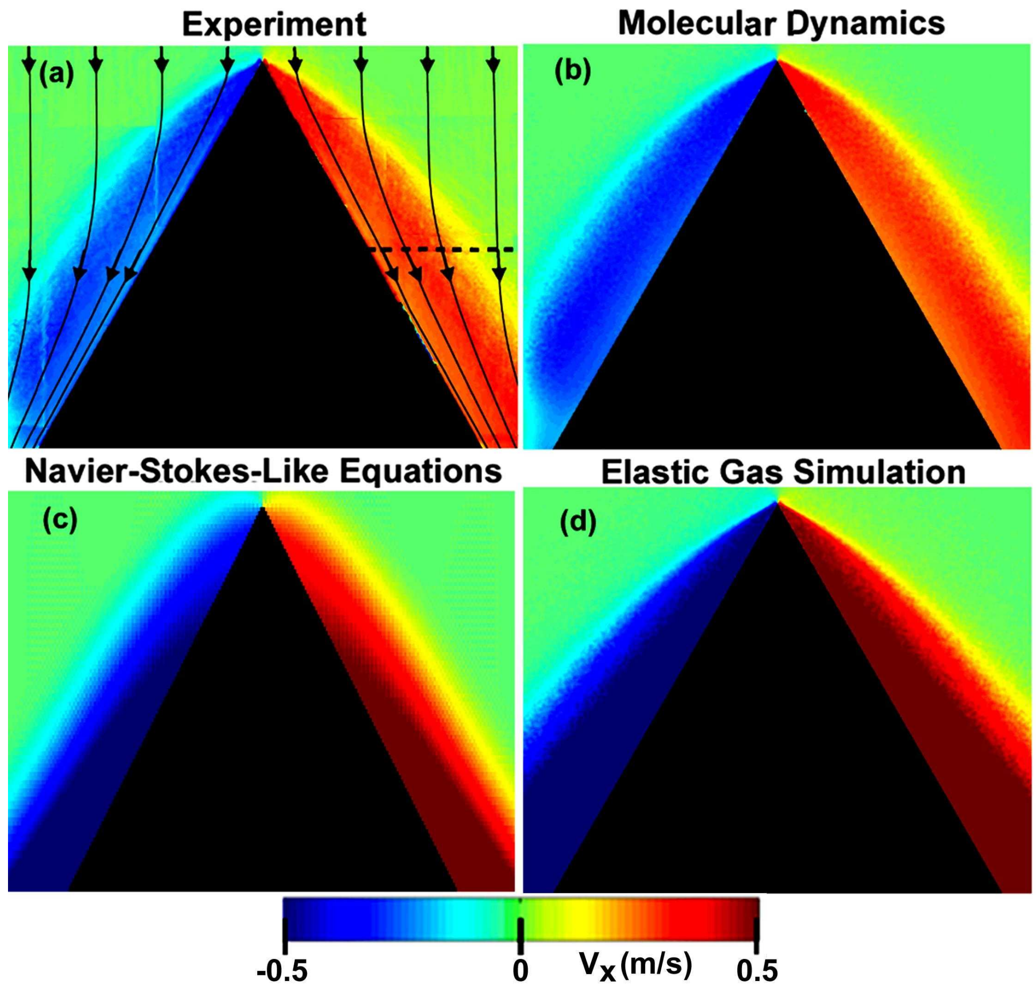


Ma<<1
Subsonic

Ma>>1
Supersonic

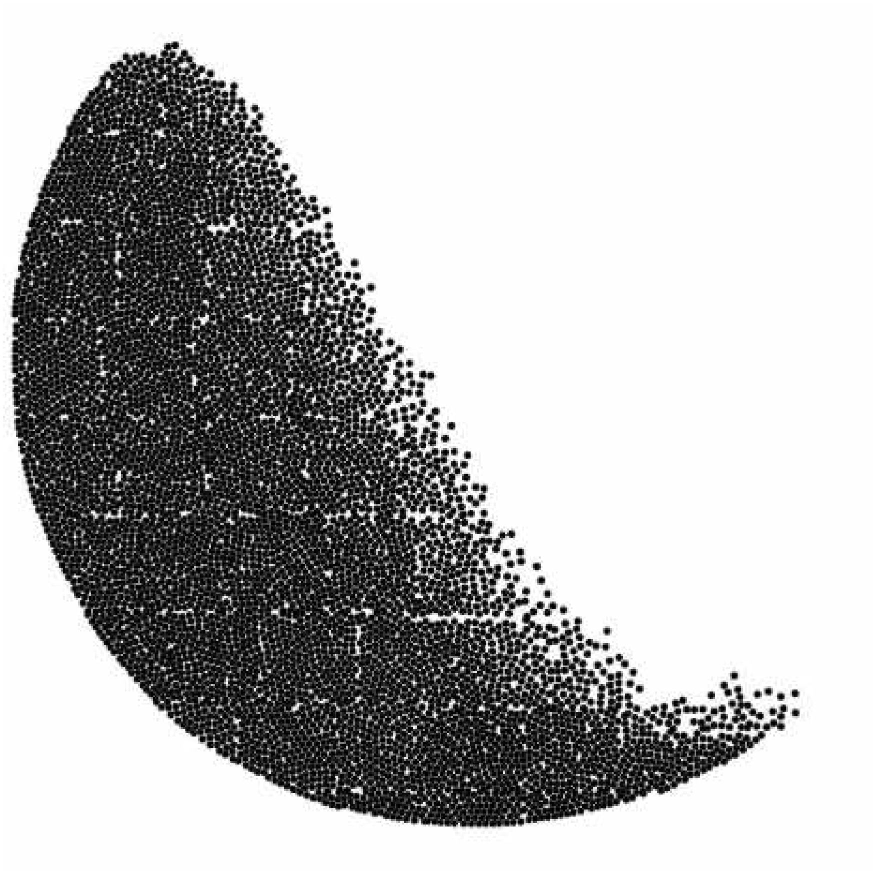
Supersonic flow past a wedge





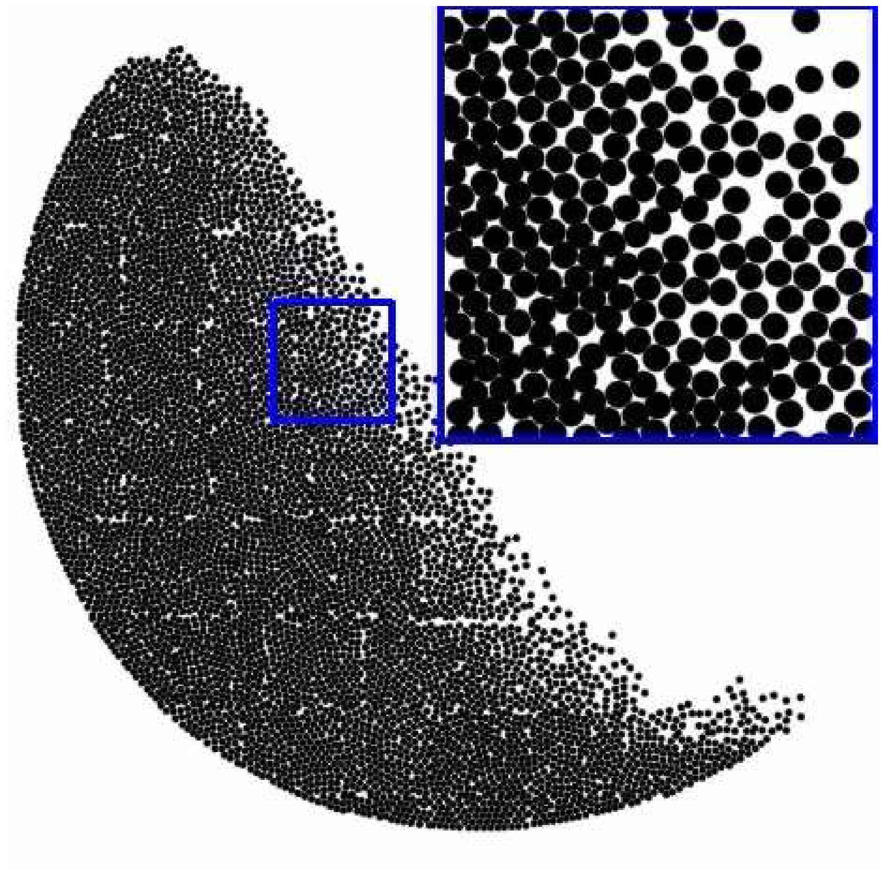
Rericha, Bizon, MDS, Swinney PRL 2002

Dense Granular Flow



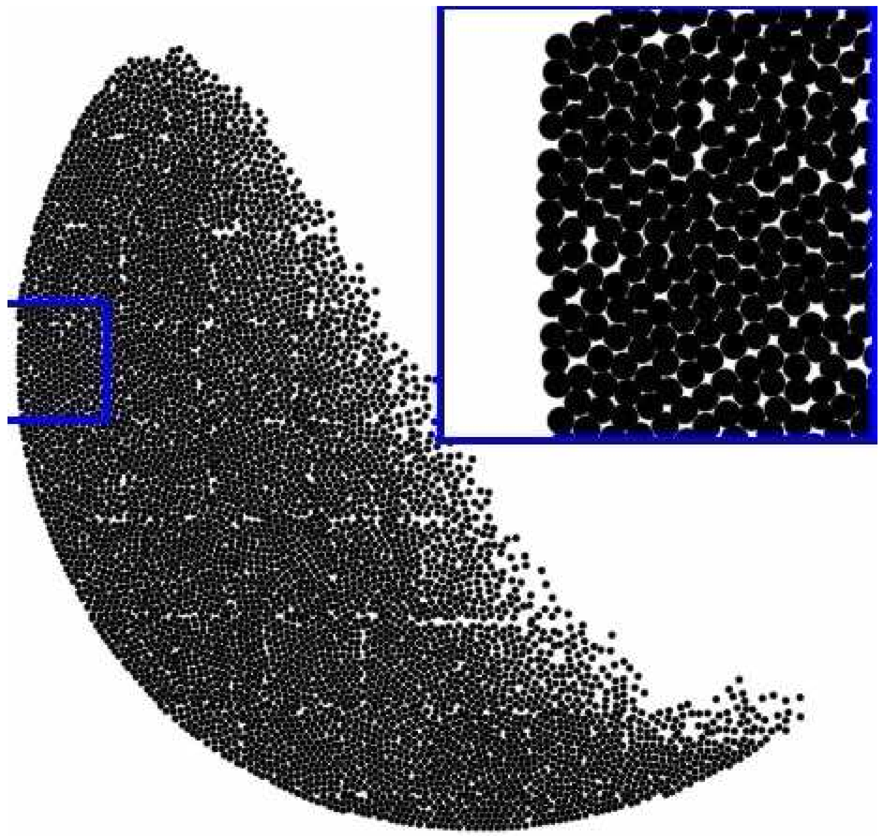
Dense Granular Flow

(gas)

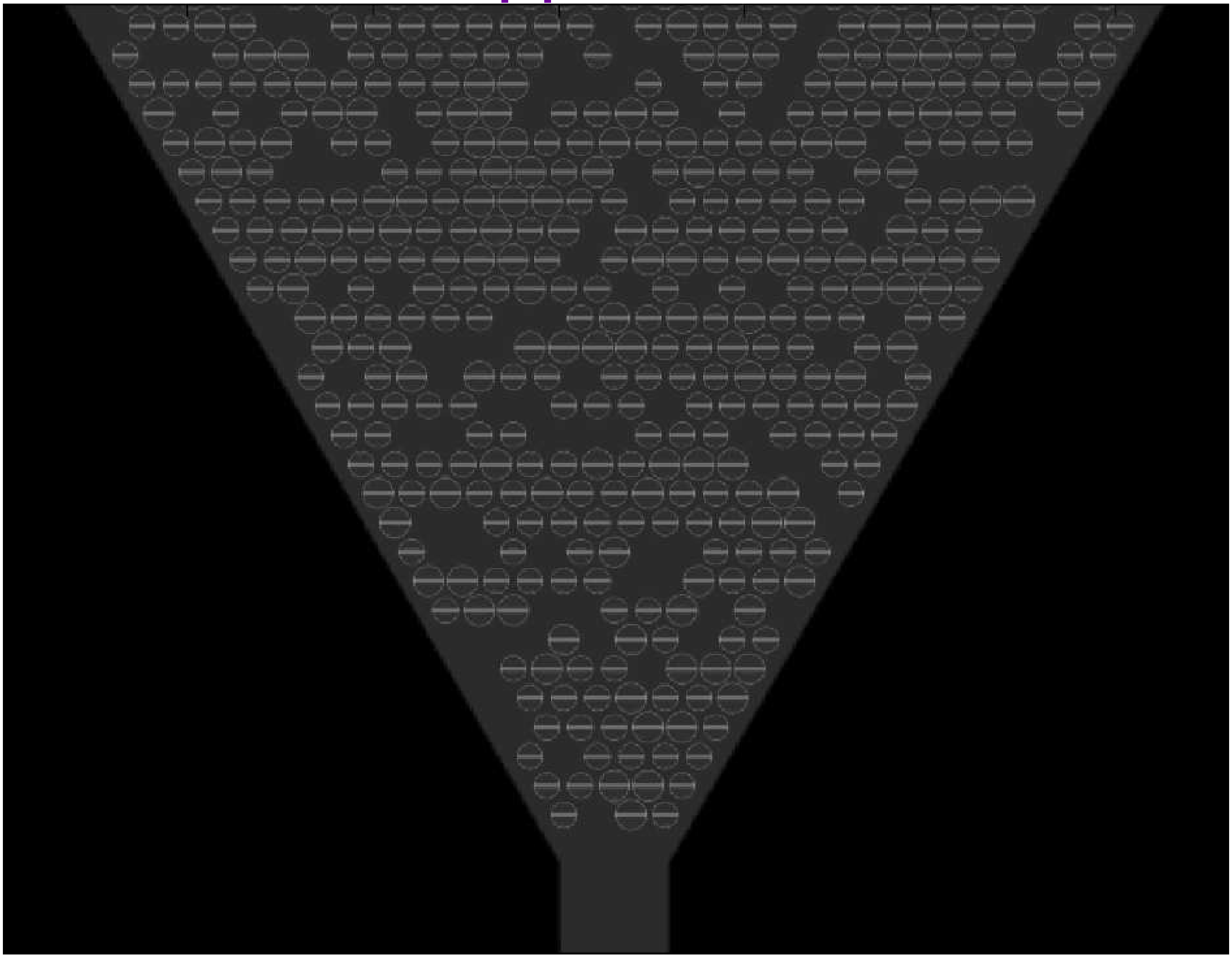


Dense Granular Flow

(Solid)



Hopper Flow



Introduction

Molecular Systems

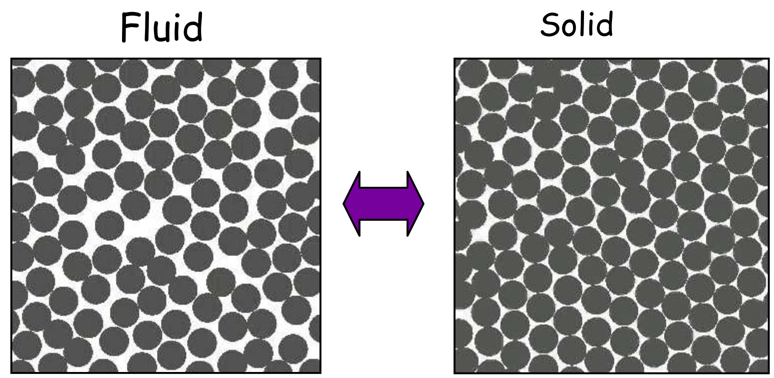
- Conserve energy
- Equilibrium steady state (Thermodynamics)
  - Unforced.
  - Time independent.
  - Uniform.
  - Fluid-Solid phase transition.
  - Extremum principle well established (e.g. entropy and free energy).
  - State depends only on small number of variables.

Granular Systems

- Dissipate energy
- Non-equilibrium steady state (NESS)
  - *Forcing required.*
  - Time independent.
  - Uniform.
  - *Fluid-Solid phase transition.*
  - *Can we explain NESS phase transitions using free energy arguments?*
  - *Can we predict State from small number of variables?*

Nonequilibrium phase transition

Constant Volume (isochoric)



Reis, Ingale, MDS PRL 96,258001 (2006)
- Structure identical to equilibrium.

Reis, Ingale, MDS PRL 98,188301 (2007)
- Caging dynamics.

Reis, Ingale, MDS PRE 75,051311 (2007)
- Velocity distribution.

Granular systems

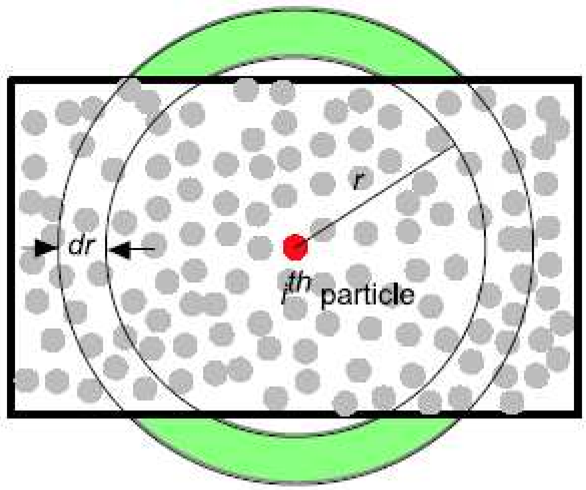
-Solid/Fluid phase transition

- Inelastic hard sphere system
- Energy dissipated
- Free energy/Entropy concepts not established

- Can we explain phase transition using thermodynamic ideas?
- Is there a functional form analogous to free energy?

Radial distribution function g(r)

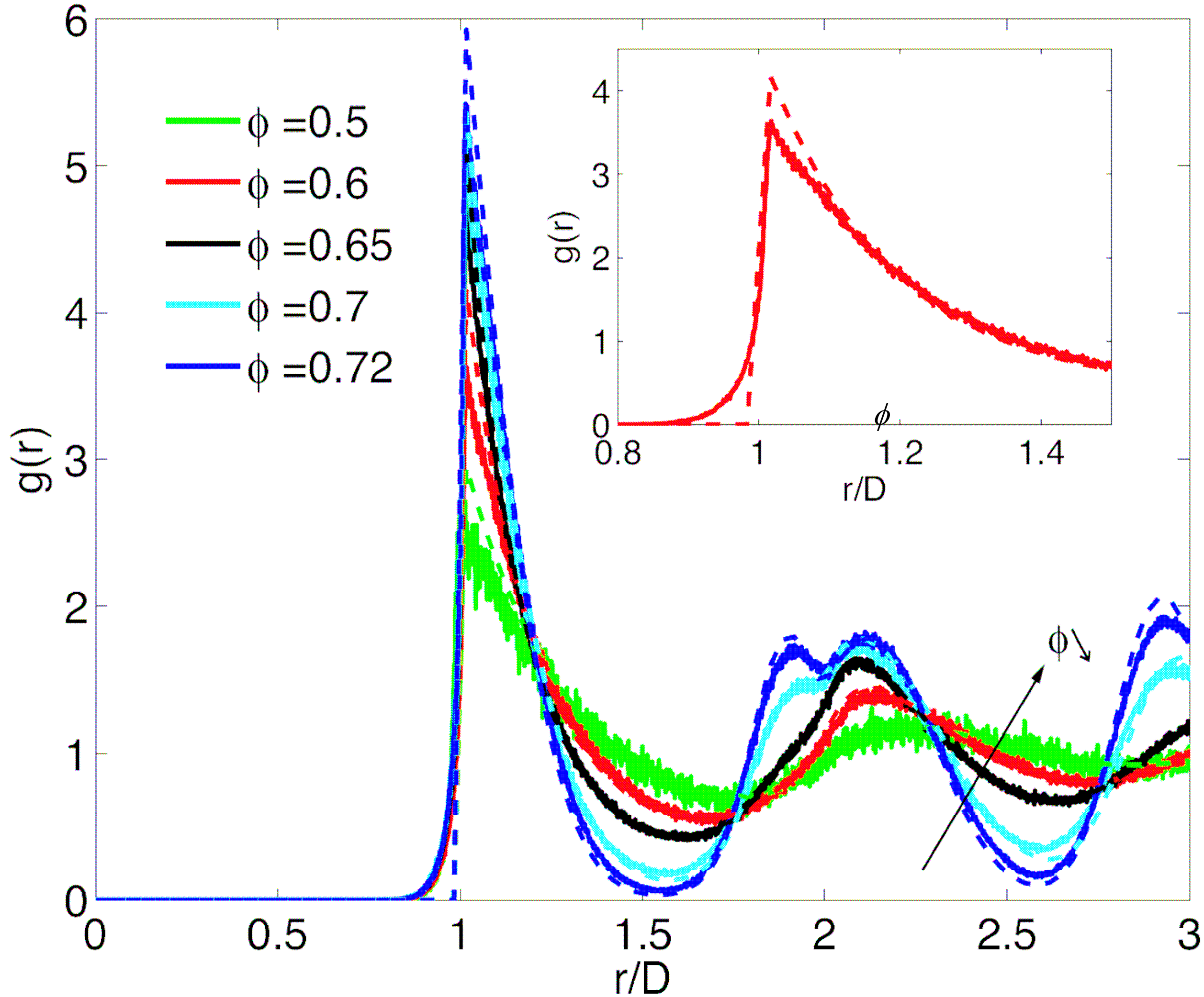
Most common way of describing the average structure of many particle systems.



$$g(r) = \frac{\text{no. particles found in shell between r and r+dr}}{\text{no. particles found in same shell for uniform distribution of points}}$$

$$g(r) = A(r)\langle \sum_i \sum_{j \neq i} \delta(r - r_{ij}) \rangle$$

Radial distribution function g(r)



- Excellent agreement with Monte Carlo Simulations (dashed lines).
- g(r) develops shoulder at ϕ=0.65
- Precursor of phase transition
- Distinct secondary peak at higher filling fractions ϕ=0.7 and ϕ=0.72.

Reis, Ingale, MDS PRL **96** (2006)

Nonequilibrium phase transition

Granular systems
-Solid/Fluid phase transition

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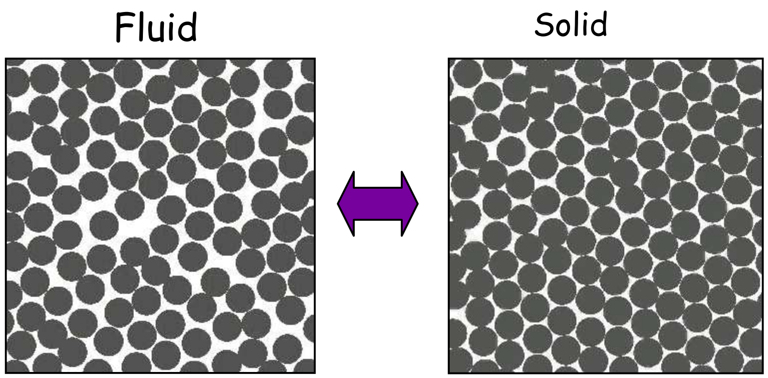

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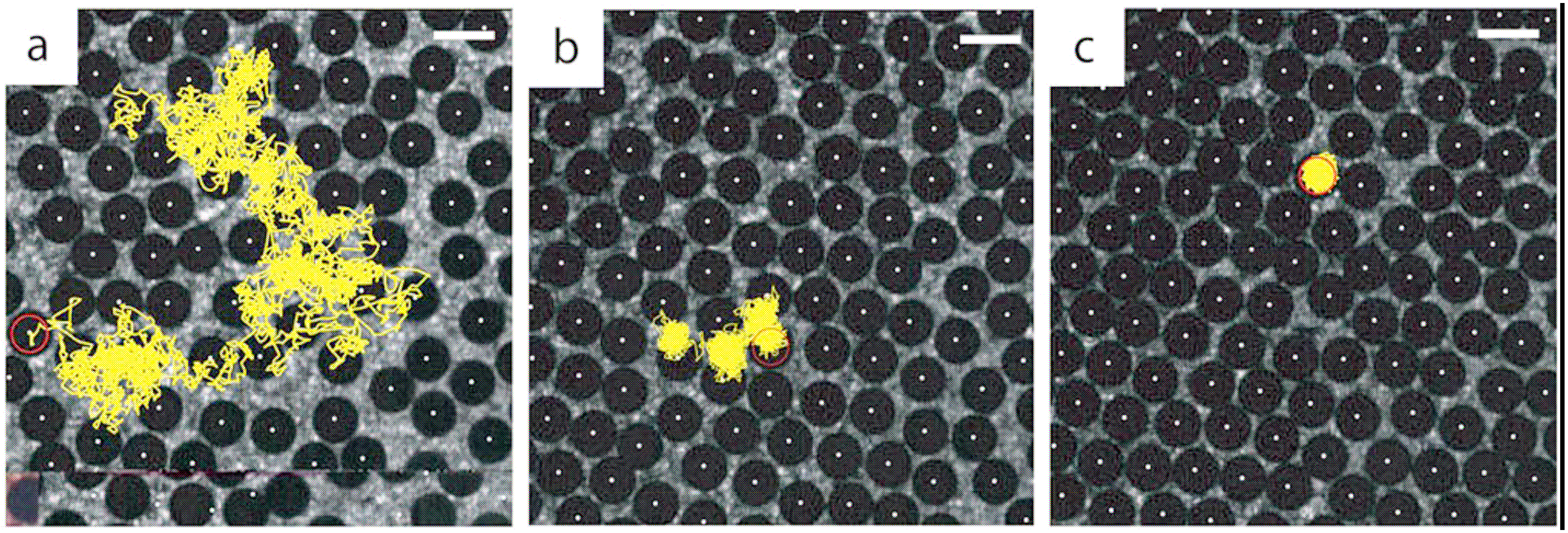
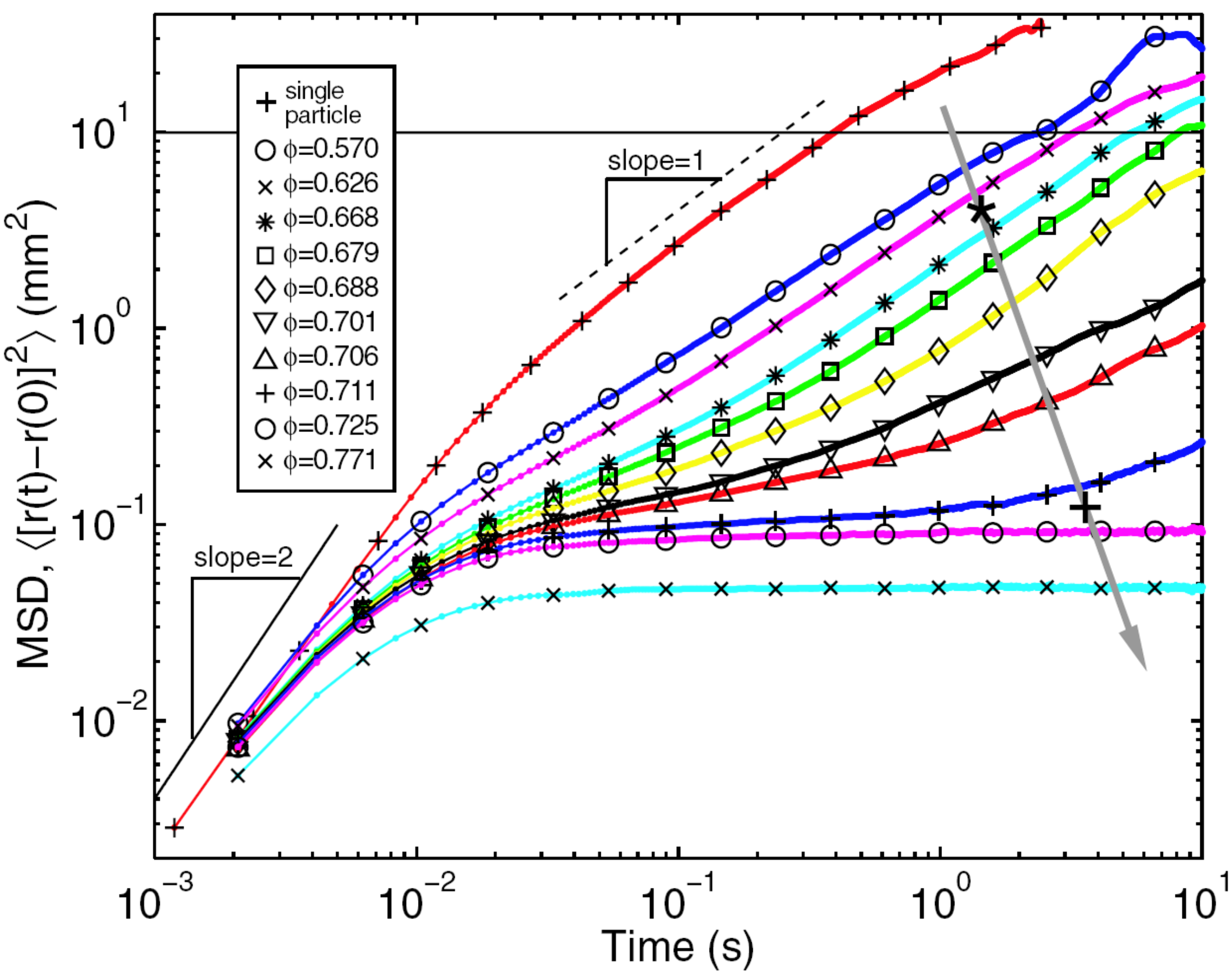
Caging Dynamics



- Diffusive behavior at low density.
  - Ballistic -> Diffusive
- Caging behavior at intermediate density.
  - Ballistic -> Sub-diffusive -> Diffusive
- Crystalline behavior at high densities
  - Ballistic -> No Diffusion (stuck)

Reis, Ingale, MDS PRL **98** (2007)

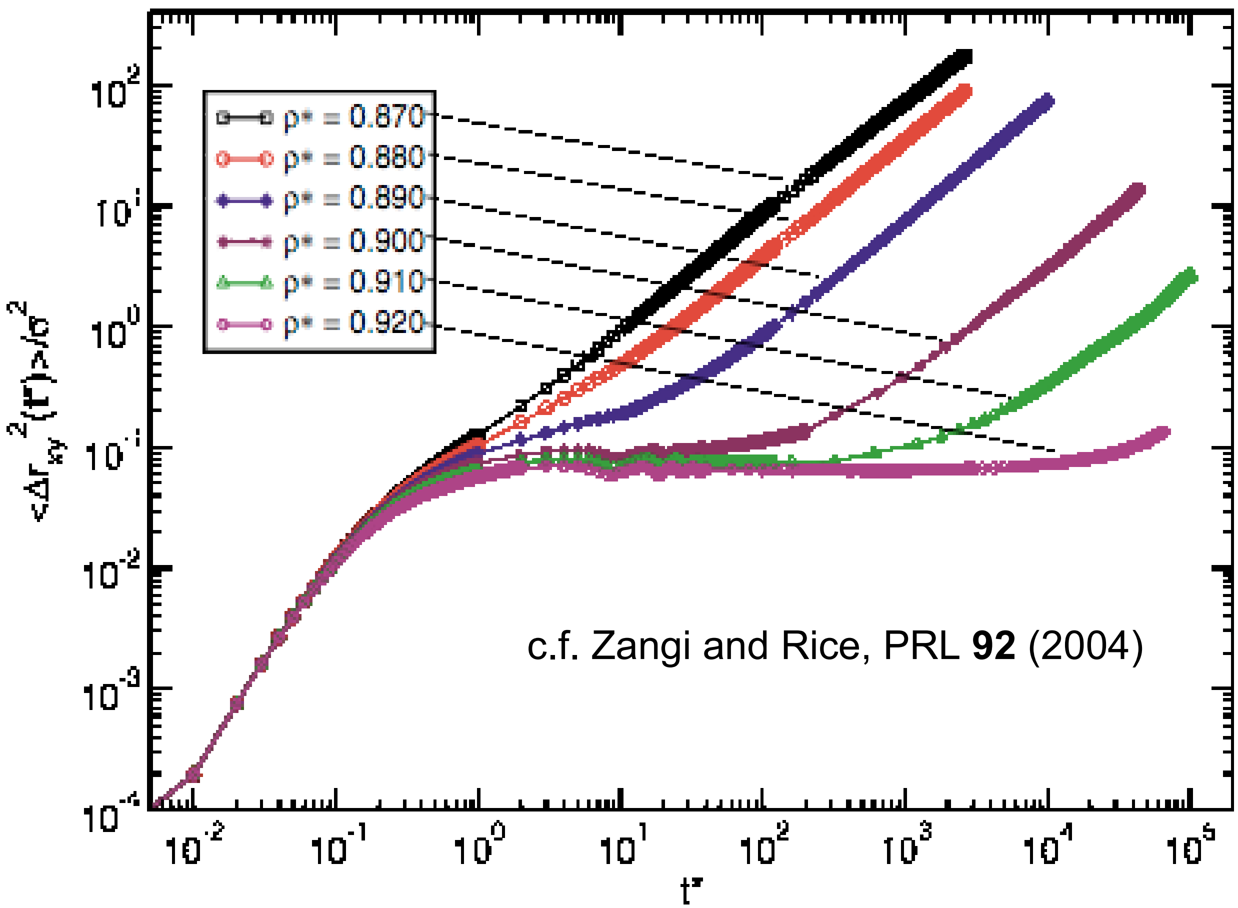
Caging Dynamics



- Diffusive (low density)
  - –Ballistic (short)
  - –Diffusive (long)
- Caging (intermediate density)
  - –Ballistic (short)
  - –Sub-diffusive
  - –Diffusive (long)
- Crystalline (high densities)
  - –Ballistic (short)
  - –No Diffusion (long)

Reis, Ingale, MDS PRL **98** (2007)

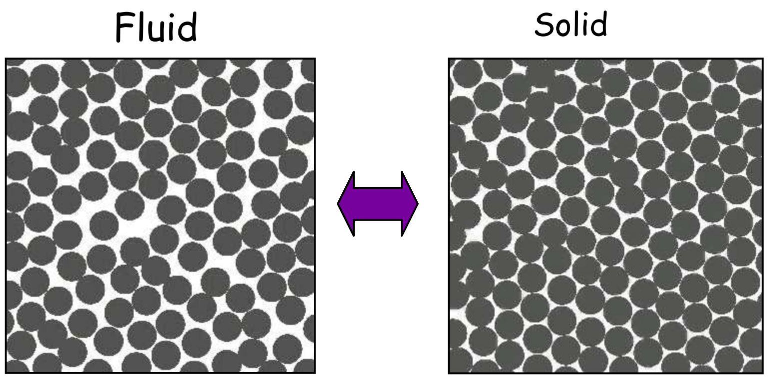
Caging Dynamics



Identical scenario to that for
MD in Q2D system of colloidal particles!

Nonequilibrium phase transition

Constant Volume (isochoric)



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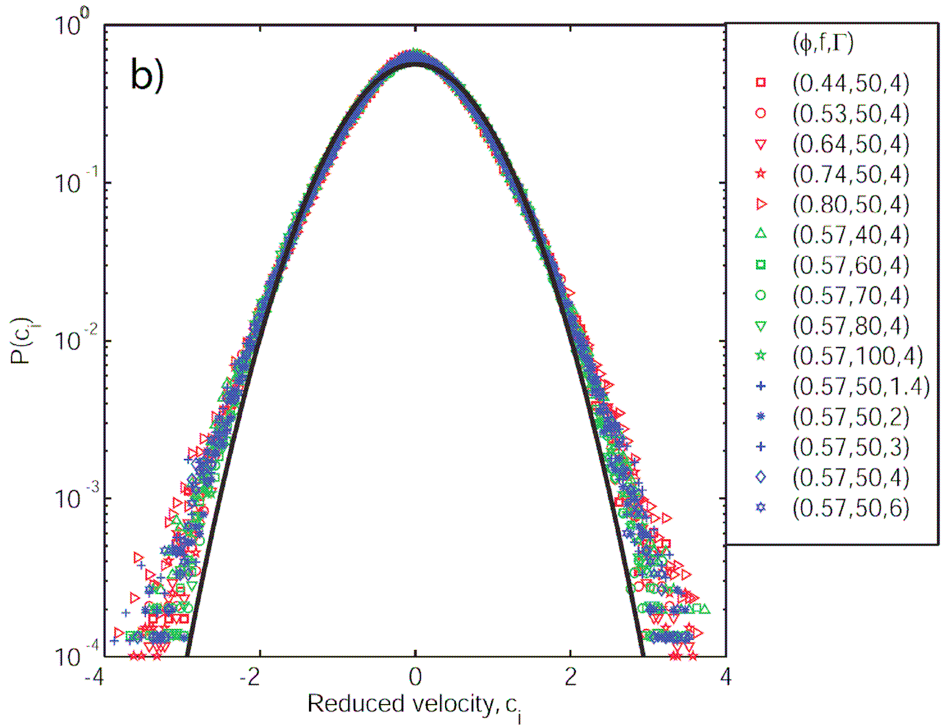
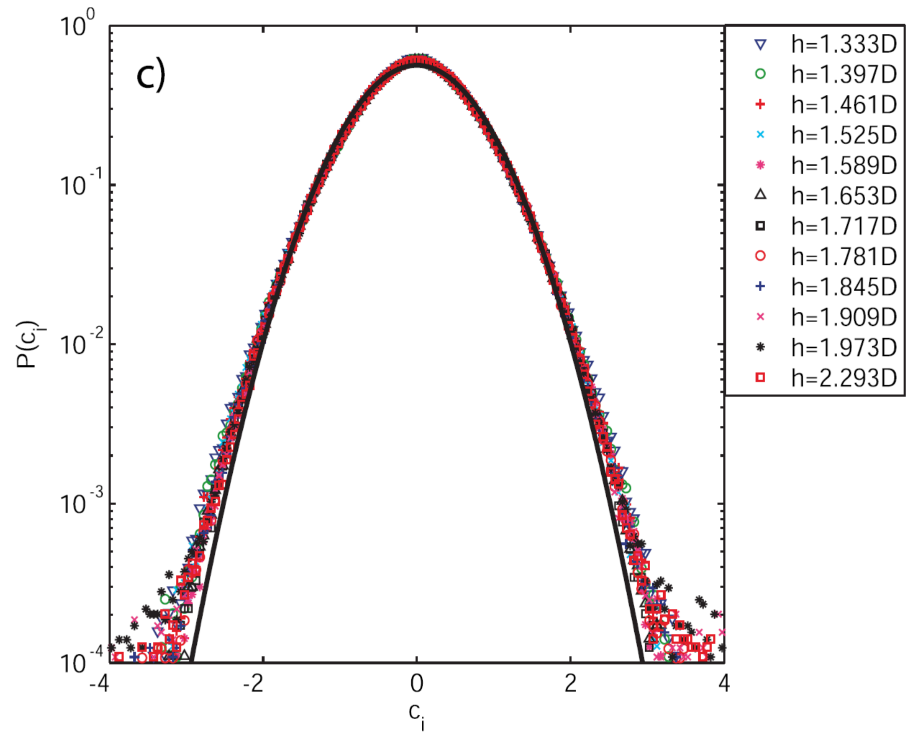
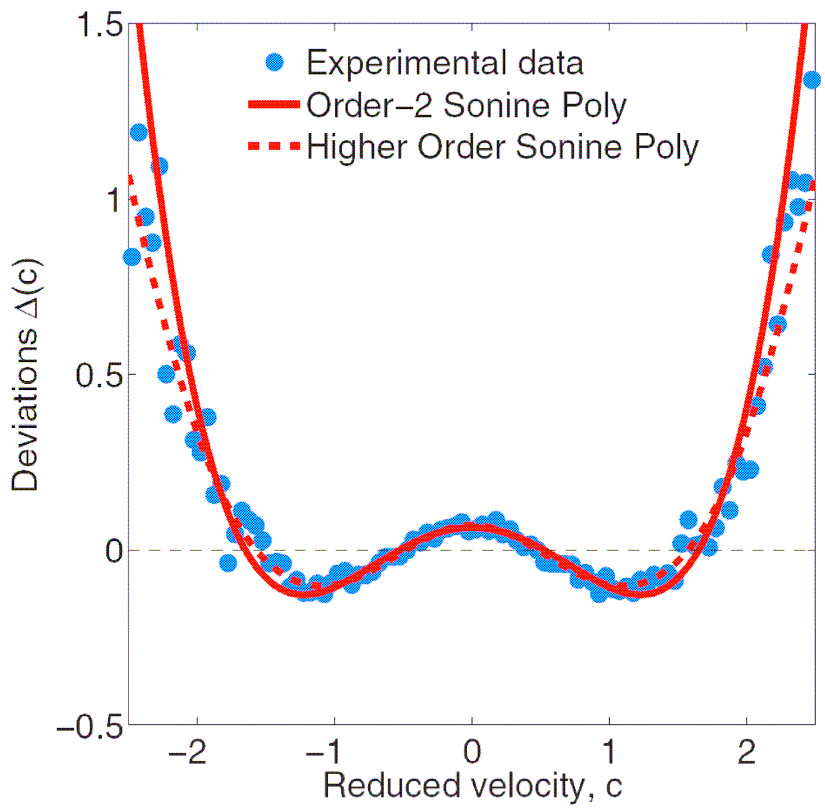
Forcing Independent Velocity Distribution





$$f(c) = f_{MB}(c)\left[1 + \left(\frac{K}{3} - 1\right)\left(\frac{c^4}{8T^2} - \frac{3c^2}{4T} + \frac{3}{8}\right)\right]$$

Forcing Independent Velocity Distribution



$$f(c) = f_{MB}(c)\left[1 + \left(\frac{K}{3} - 1\right)\left(\frac{c^4}{8T^2} - \frac{3c^2}{4T} + \frac{3}{8}\right)\right]$$

Isobaric Granular Fluid

First-order phase transition in a
non-equilibrium-steady-state

Phase transition & Thermodynamics

First order phase transition

- Discontinuity in one or more physical properties (like density, heat capacity etc.)
- Freezing, melting, sublimating

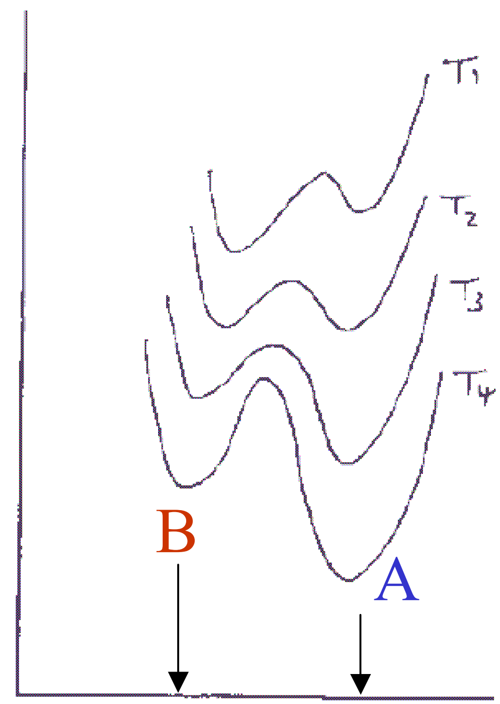
Illustrating a first-order phase transition

Probability of a particular state:

$$P(v,T) = A\,\mathrm{e}^{-F(v,T)}$$

Thermodynamic potential

F: Free energy

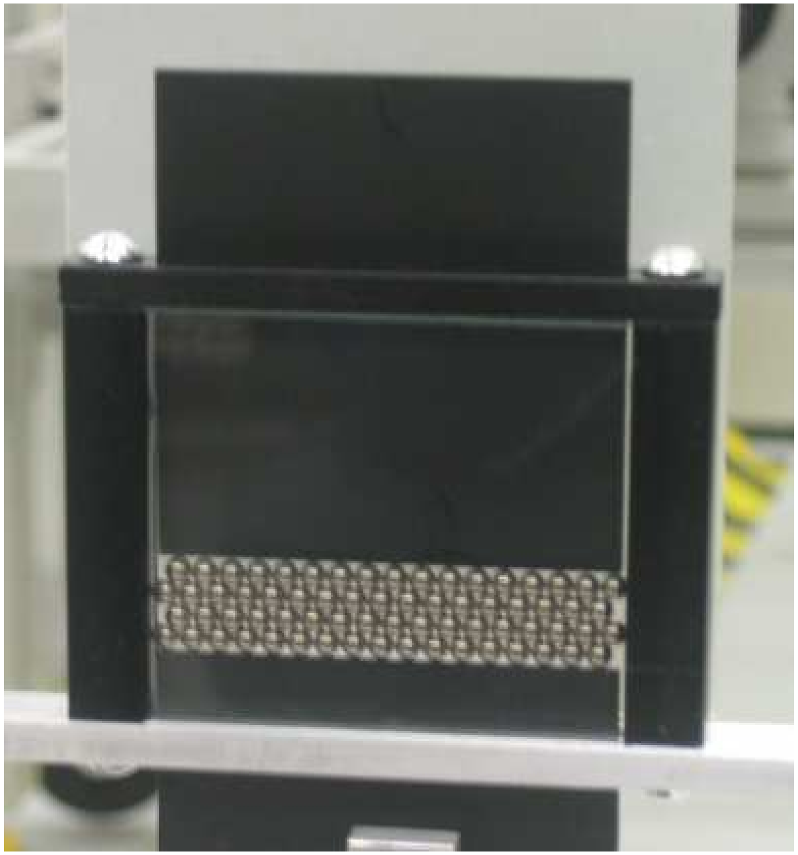


Volume/Density

Equilibrium thermodynamics!!

Experimental setup: Isobaric

- Stainless steel ball bearings
  - N=68, D=3.175mm
- Thin (2D) container dimensions
  - Width=17.5D x Height=20D x Depth≅1D
- Constant external pressure (isobaric)
  - Floating weight on top: $W/W_P \cong 1$
- Heated from below
  - Oscillating sinusoidally (f=50Hz)
  - $y(t)=A\sin(2\pi ft)$
- 840fps High speed digital camera
- High intensity LED light source

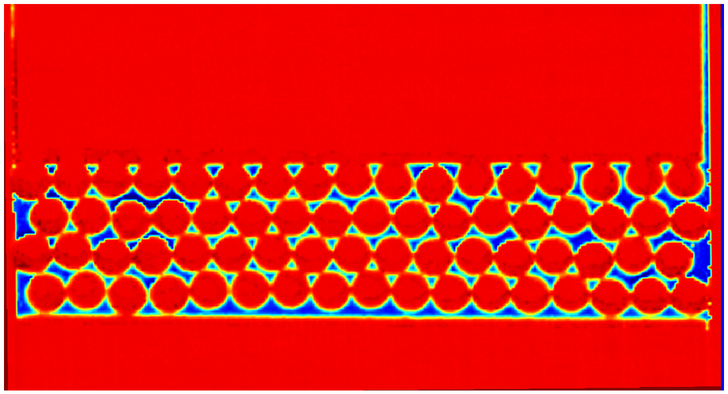


Fixed: P,N,Q   Q(A,f)=Heat Flux

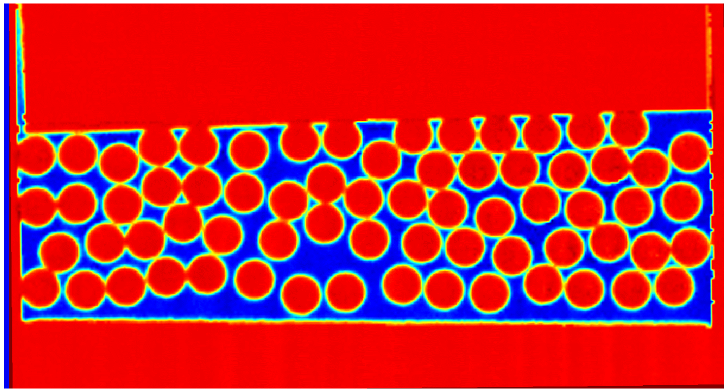
Free: T,V   Area Fraction ν or $\phi=NV_P/V$

Sublimation Transition

Crystalline State

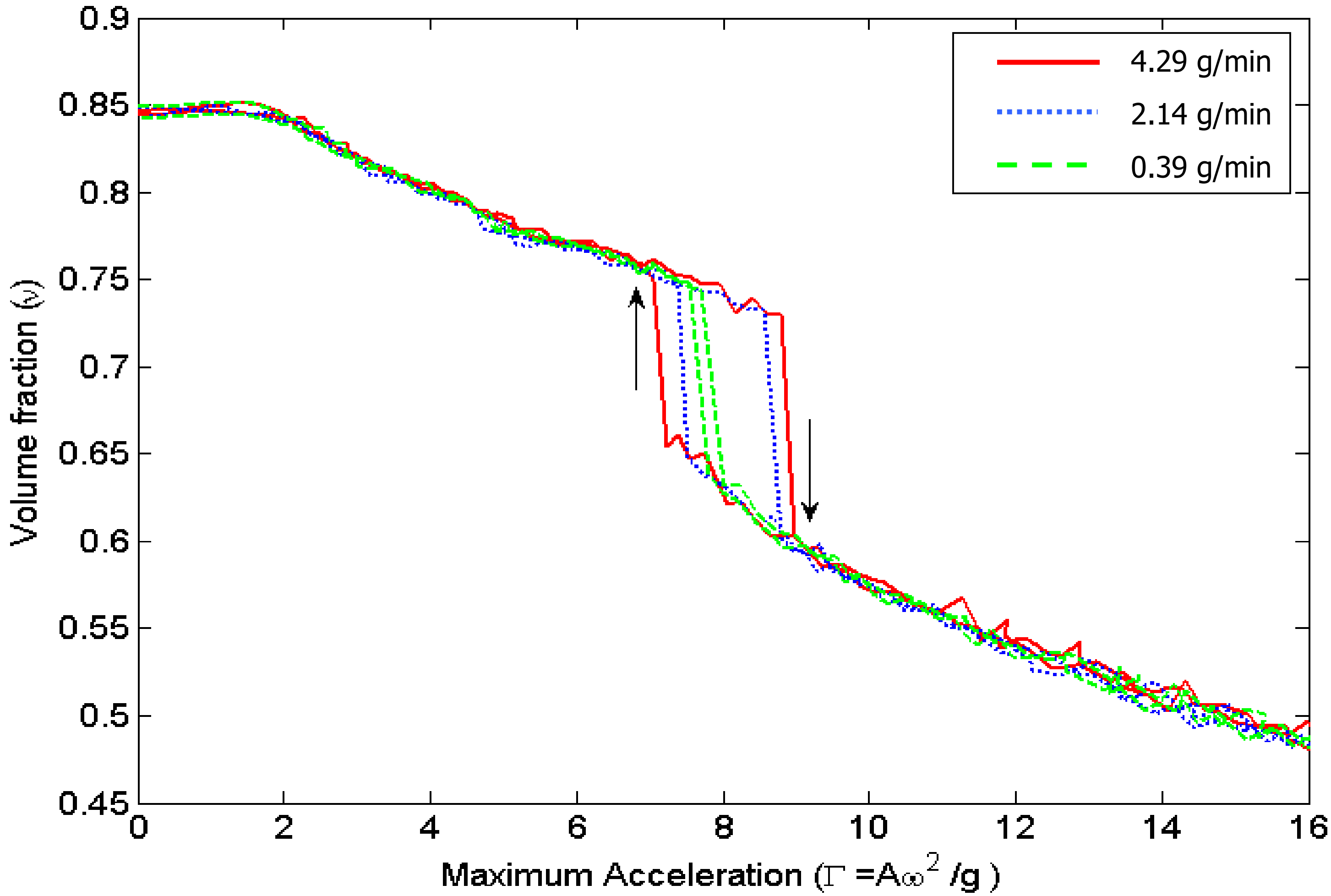


Gas State



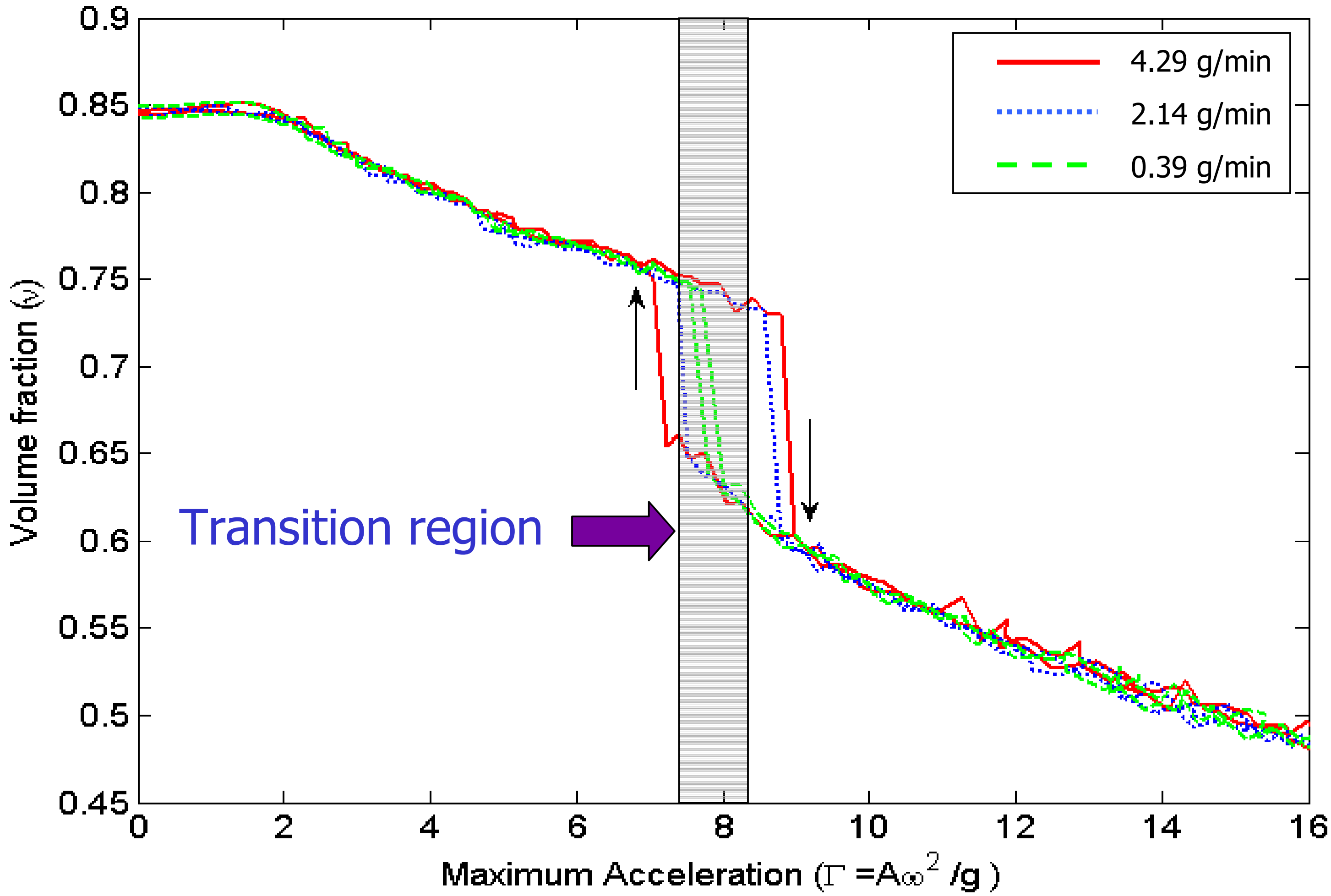
Sublimation Transition

With Rate Dependent Hysteresis

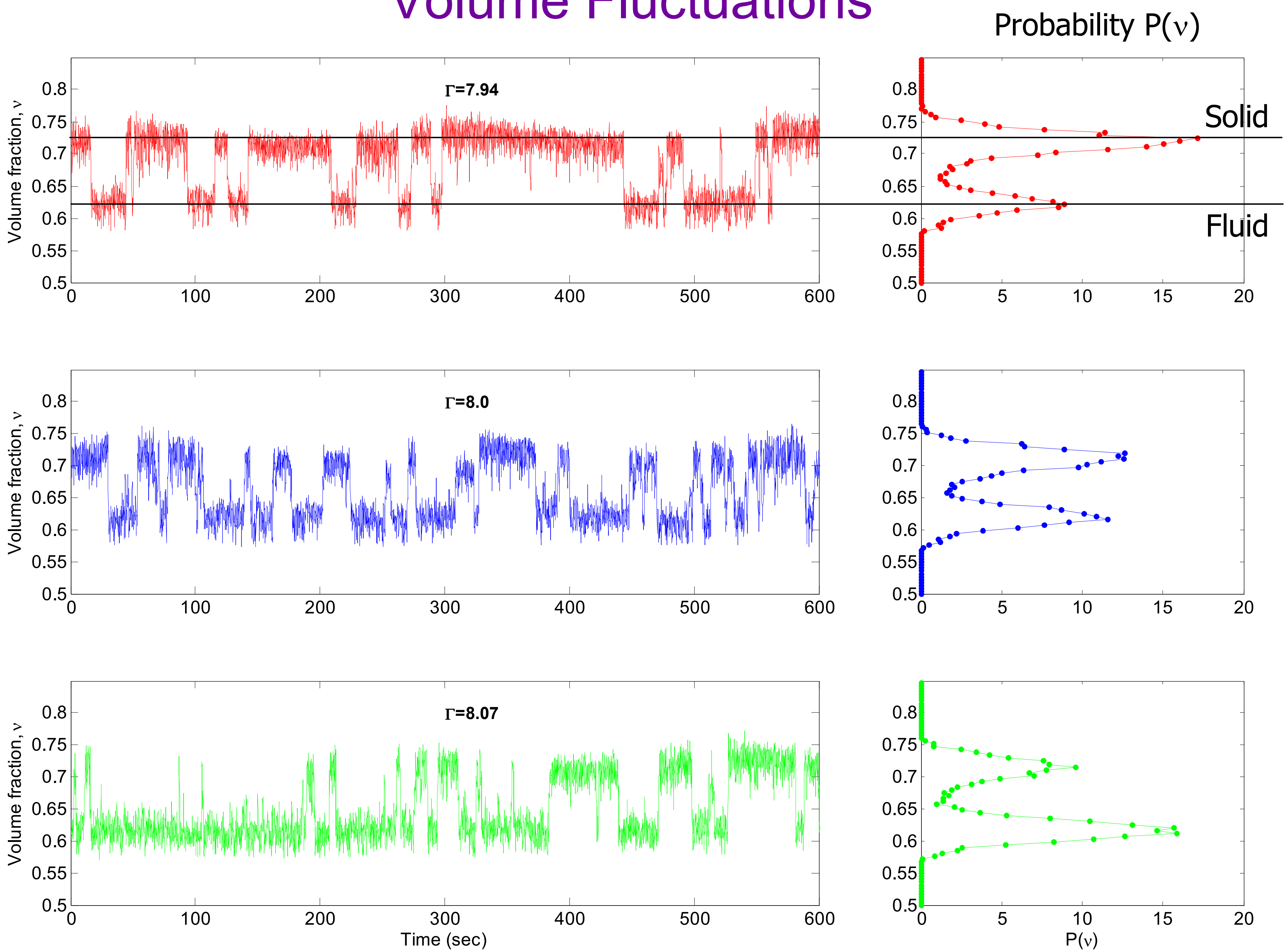


Sublimation Transition

With Rate Dependent Hysteresis



Volume Fluctuations



Functional Form of P(ν)

$$P(\nu) = A\mathrm{e}^{-F(\nu)}$$

$$F(\nu) = \frac{B}{4}\left(\nu^4 - \frac{4C}{3}\nu^3 + 2D\nu^2 - 4E\nu\right)$$

O(4) polynomial

Analogous to Ginzburg-Landau free energy functional.

$$C = \nu_f + \nu_o + \nu_s$$

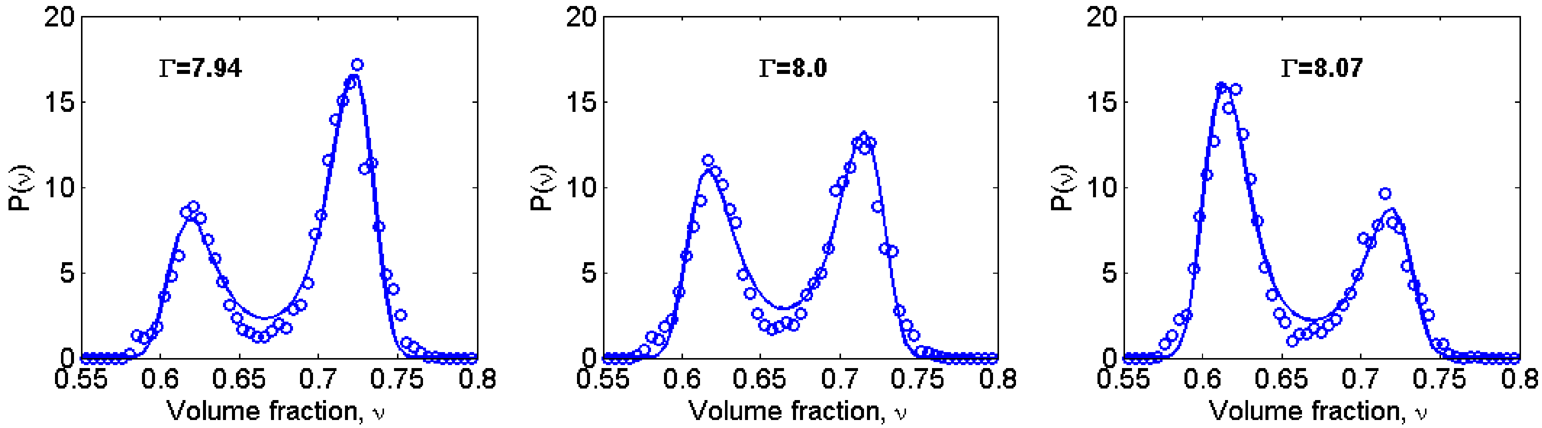
$$D = \nu_f\nu_s + \nu_s\nu_o + \nu_f\nu_o$$

$$E = \nu_f\nu_o\nu_s$$

ν_f =Fluidus point
ν_s =Solidus point
ν_o =Minima location

Results

Phenomenological Model



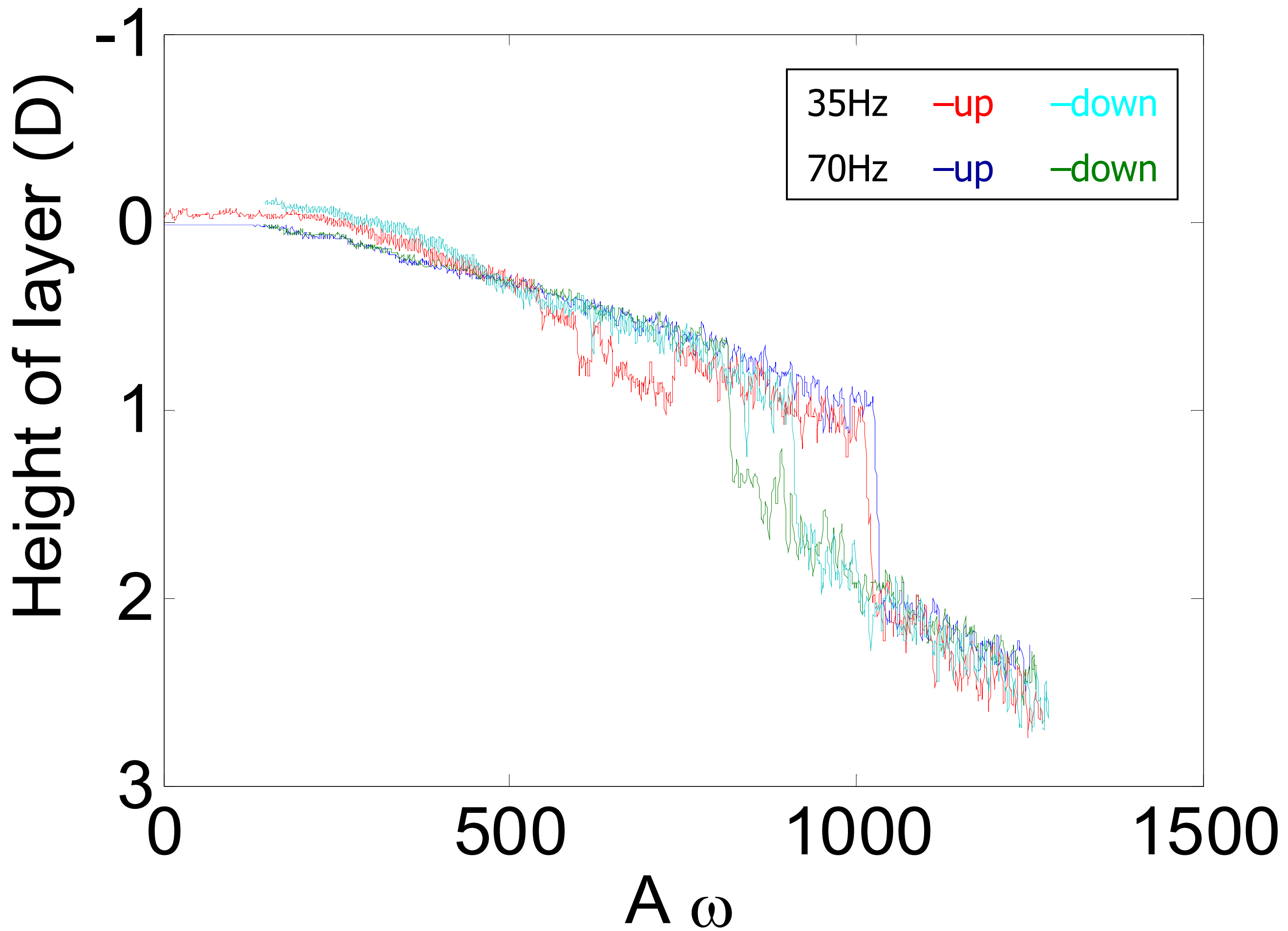
– System state corresponds to minimum F(ν) i.e., maximum P(ν).

– Analogous to free energy minimization in equilibrium systems.

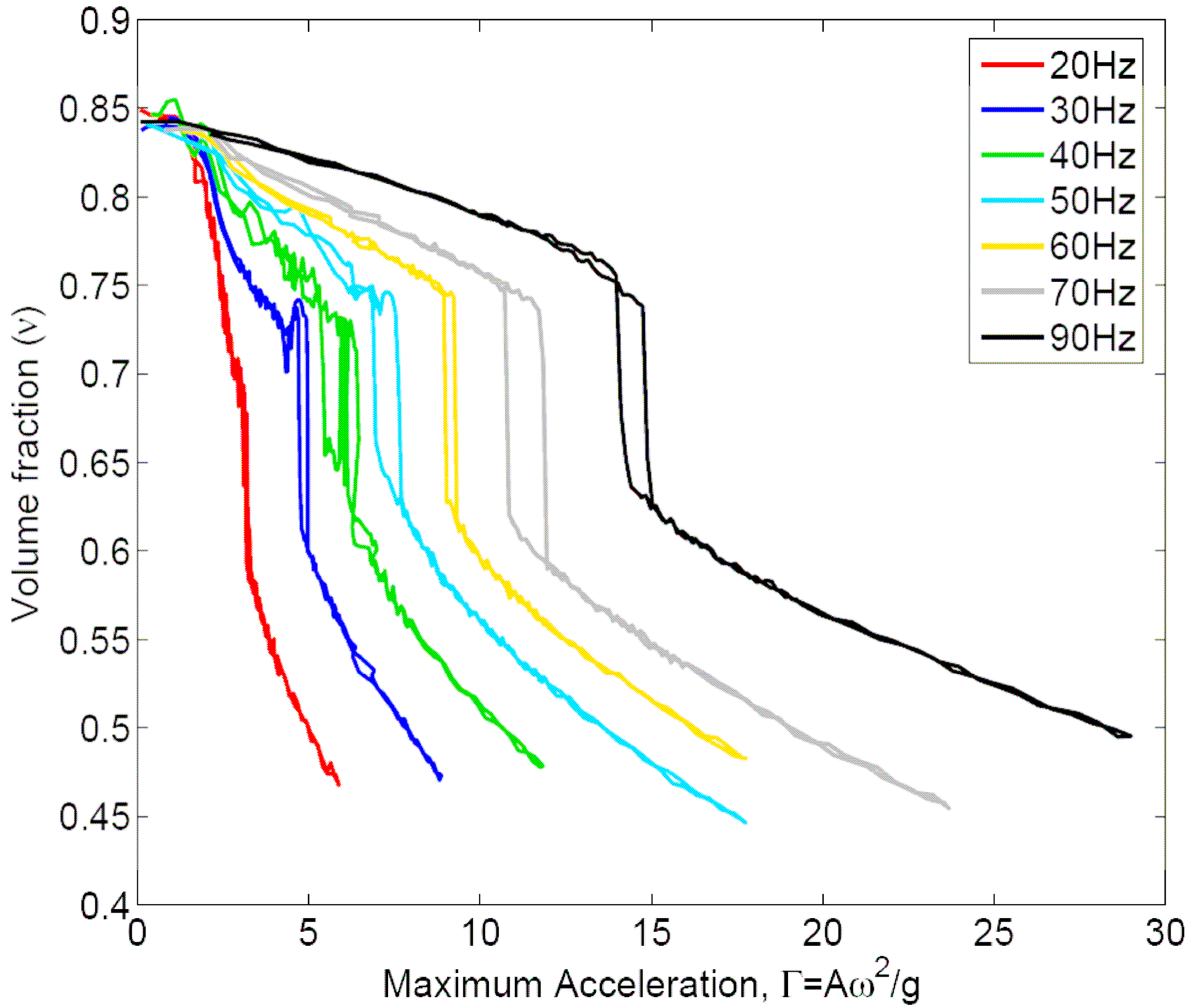
$$P(v) = A\mathrm{e}^{-F(v)}$$

Thermodynamic State Variable

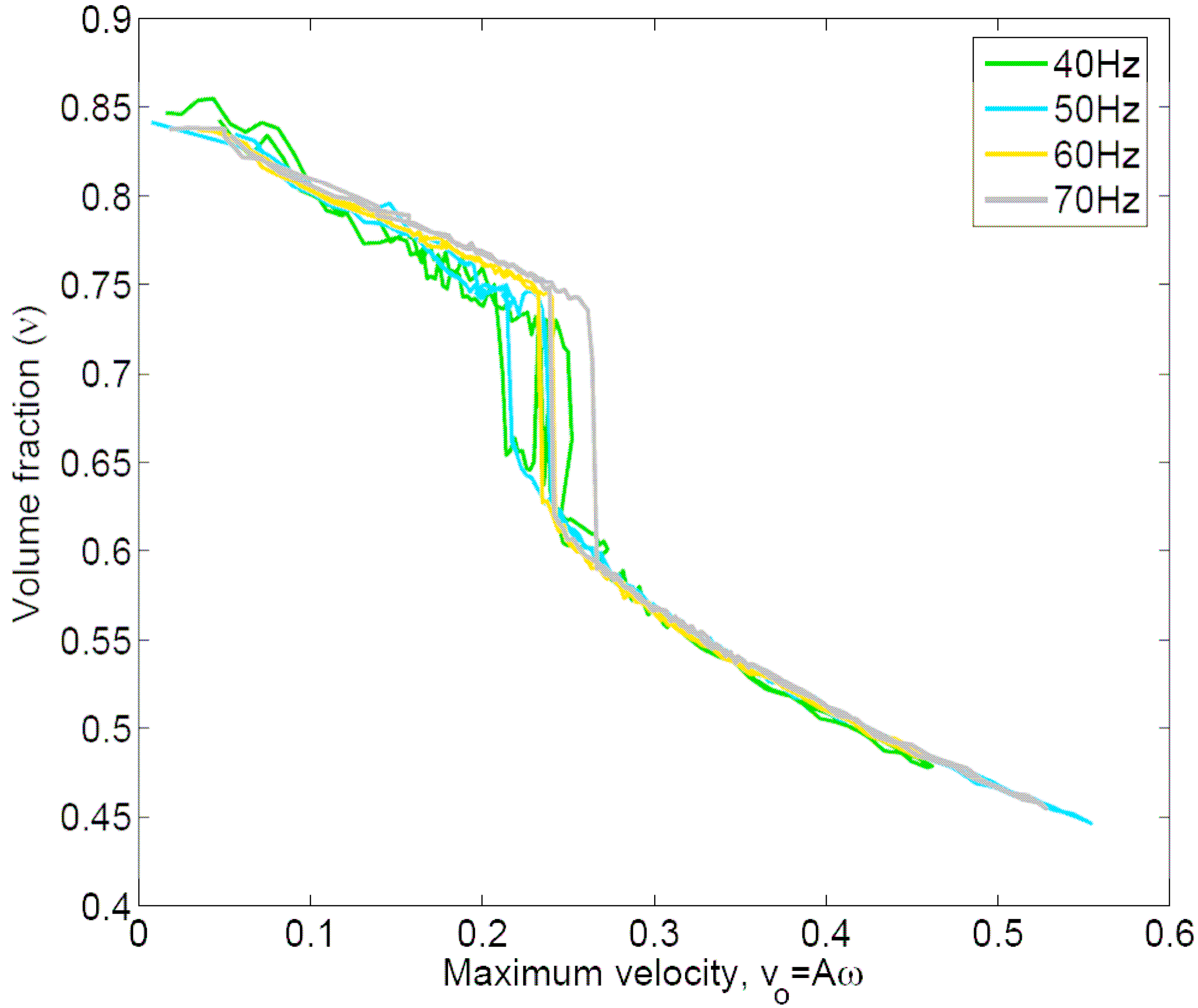
Energy Flux? => Aω



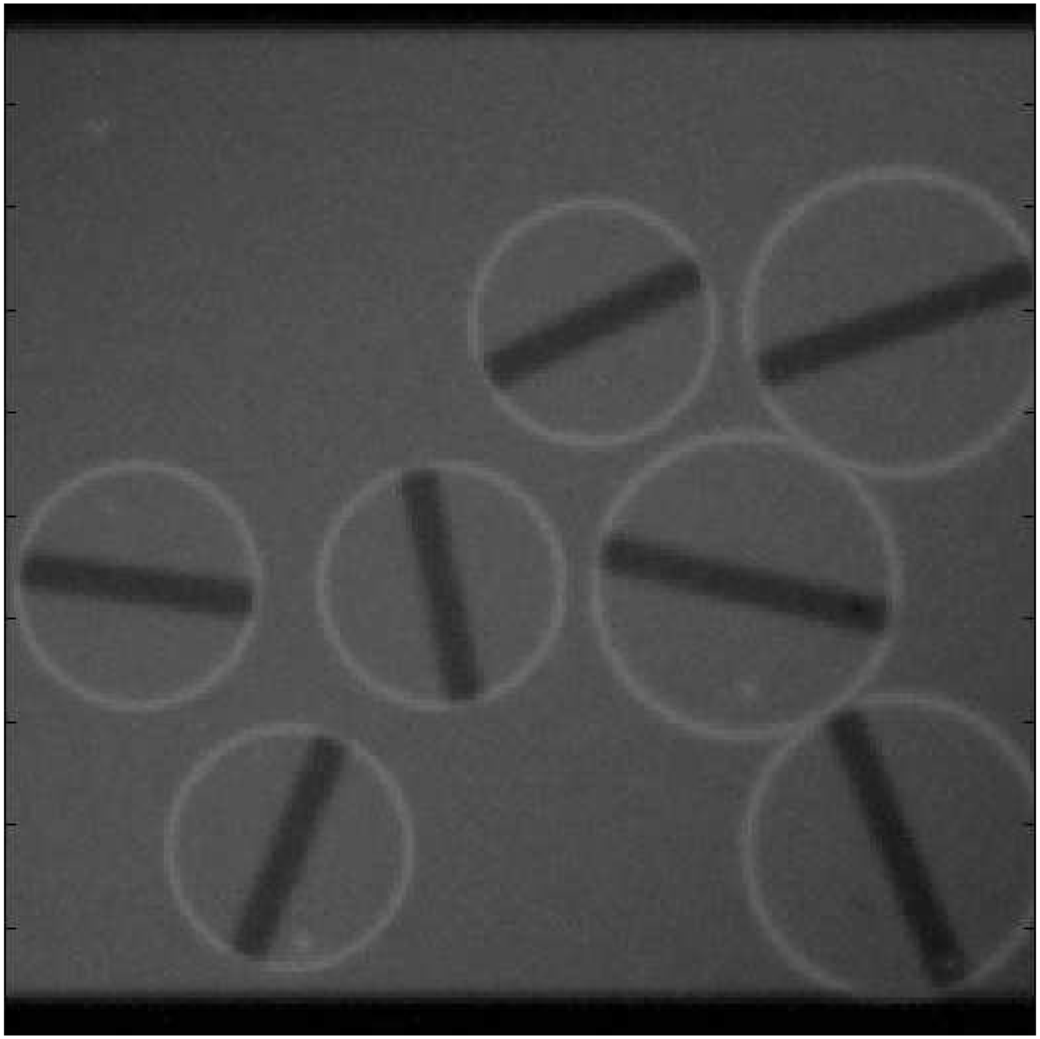
Effect of Frequency

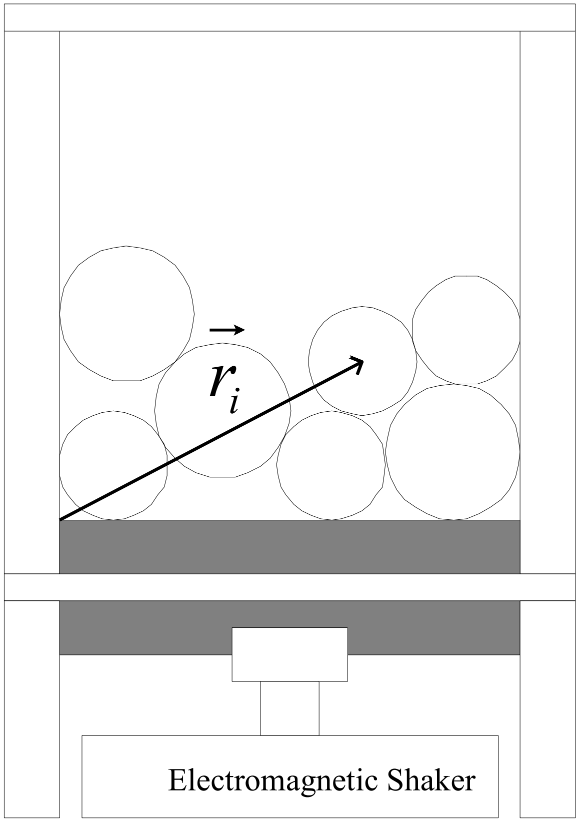


Collapse for High Frequencies



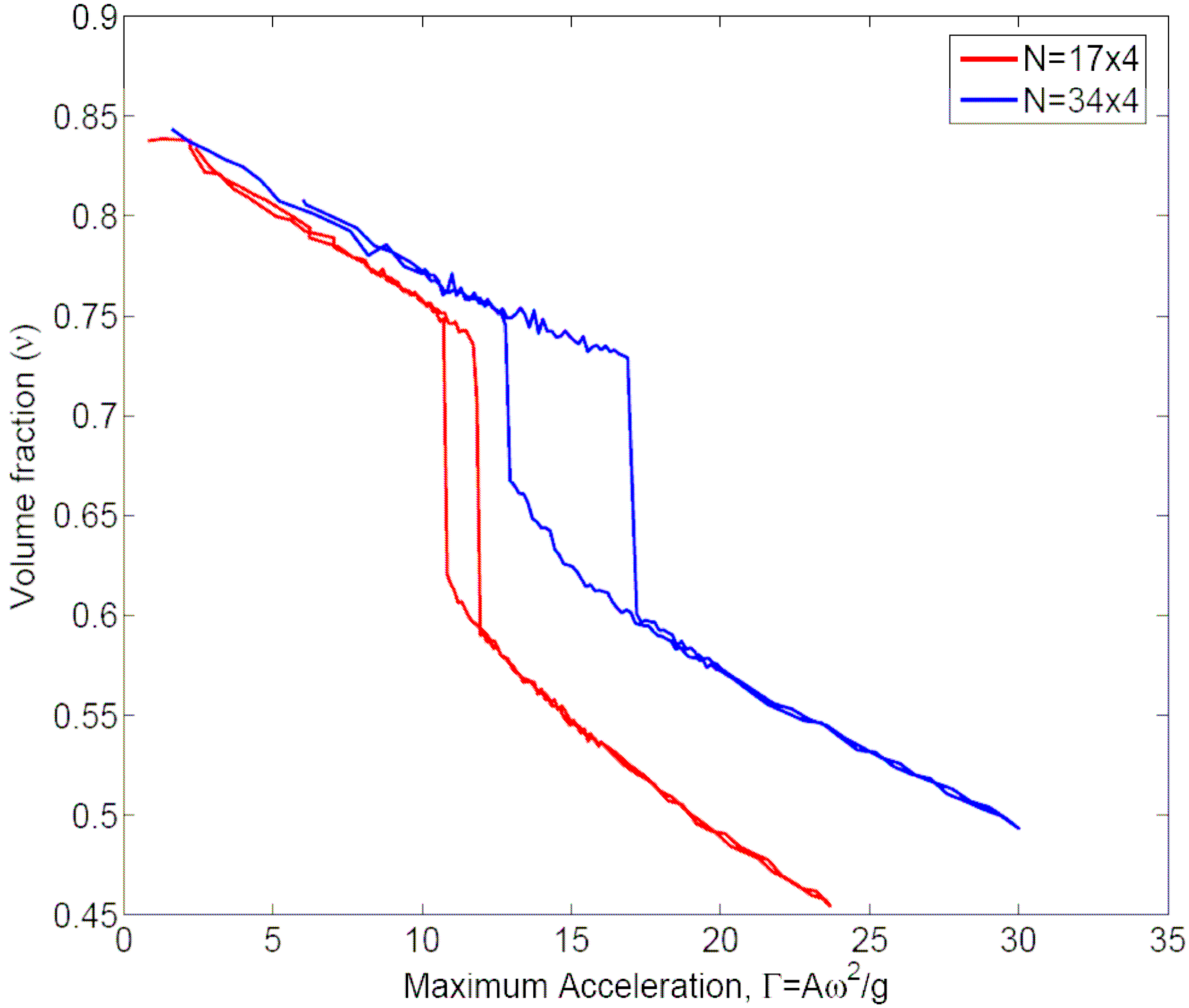
Friction Elimination



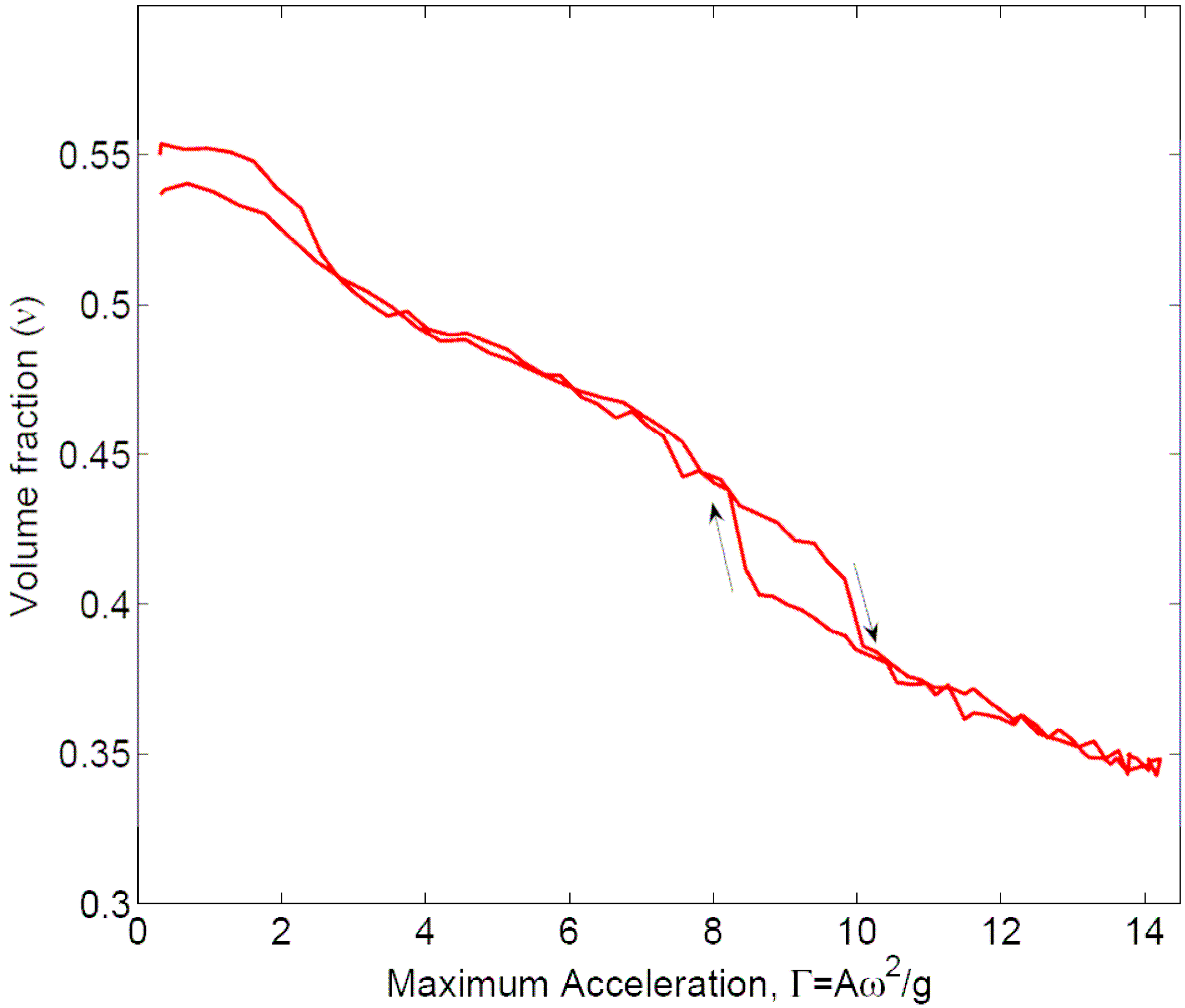


The End

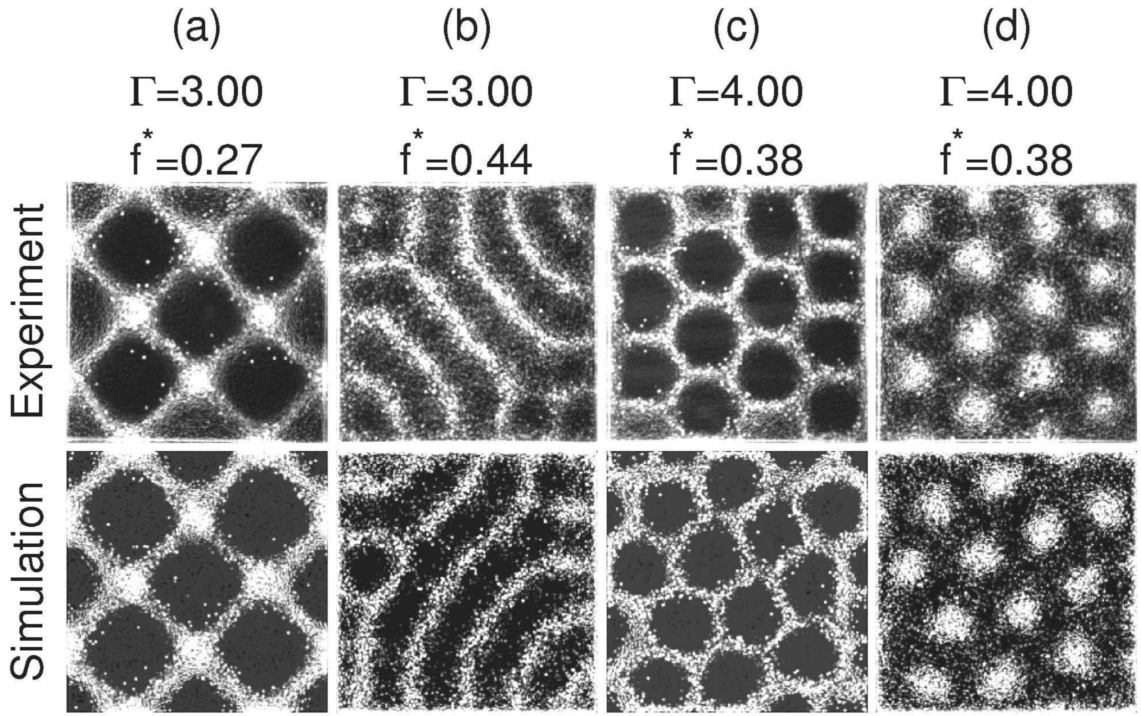
Effect of System Size



3D Phase Transistion



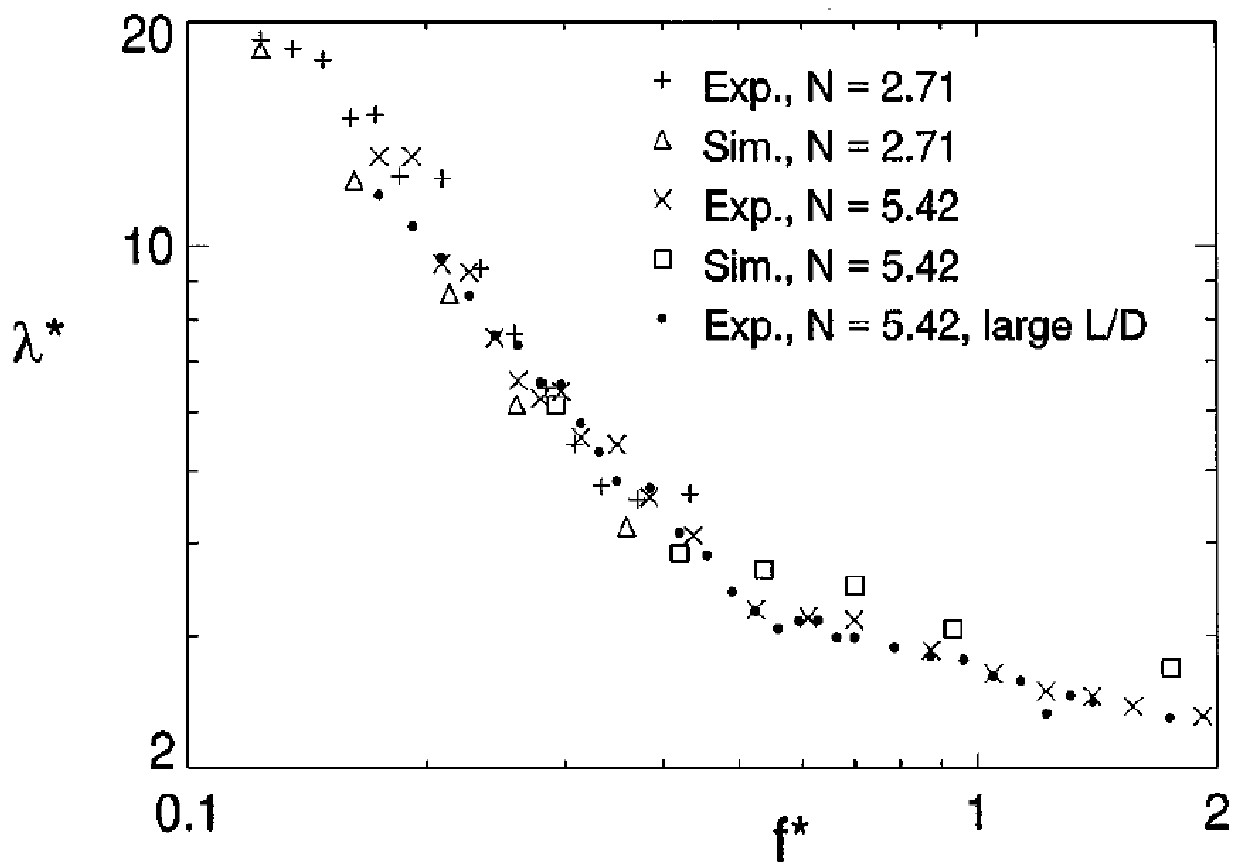
Simple Microscopic Law



- Hard Sphere
- Binary Collisions
  - Conserve Momentum
  - Dissipate Energy
- Rotations

Bizon, MDS, McCormick, Swift, Swinney
PRL 1998

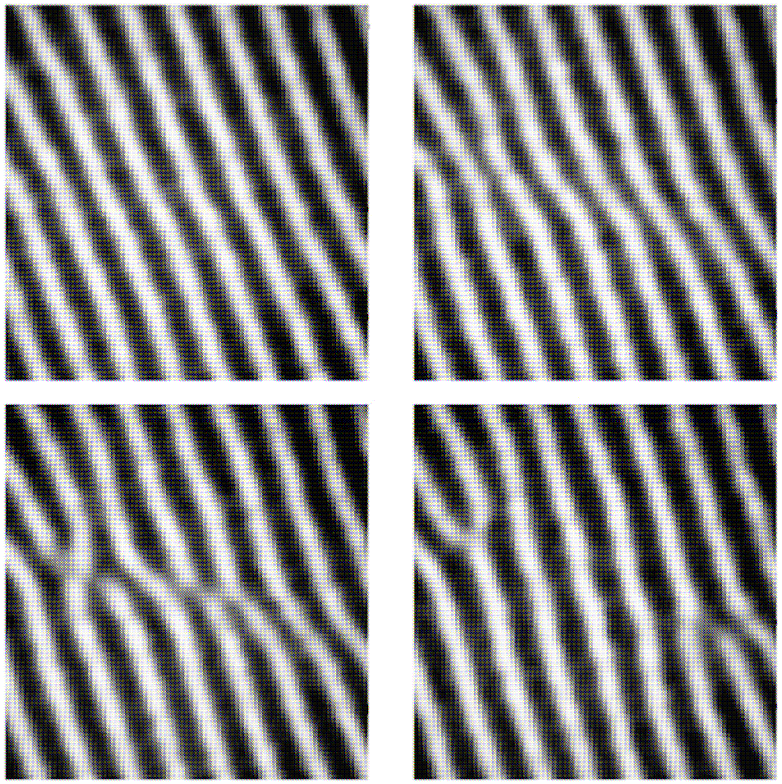
Pattern Wavelength vs. Frequency



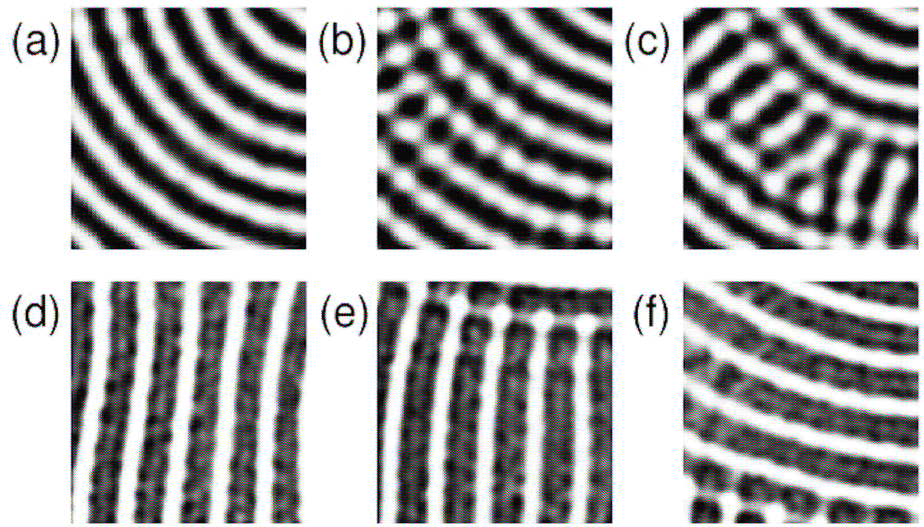
Bizon, MDS, McCormick, Swift, Swinney
PRL 1998

Instabilities of Stripe Patterns

Skew-Varicose

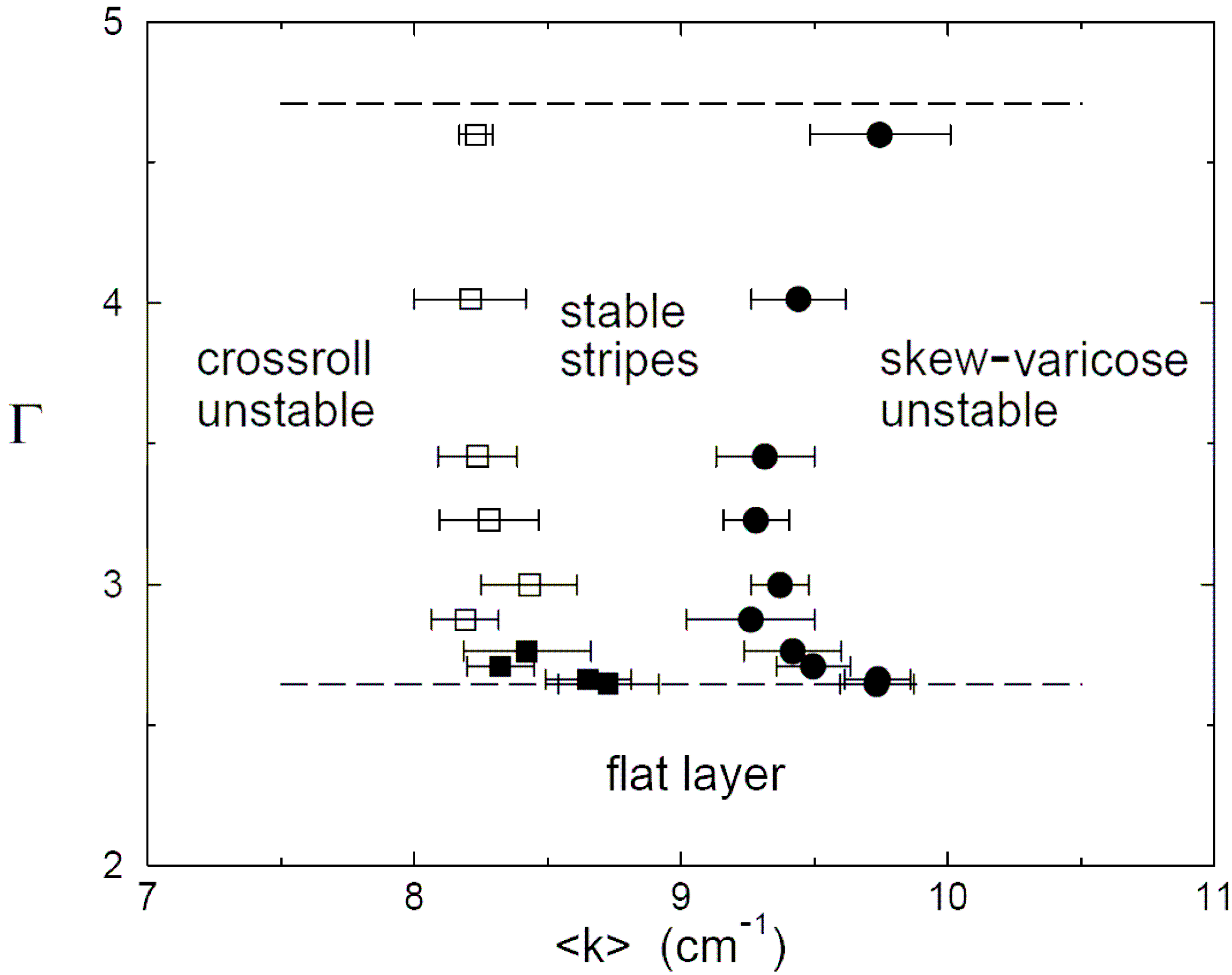


Cross Roll



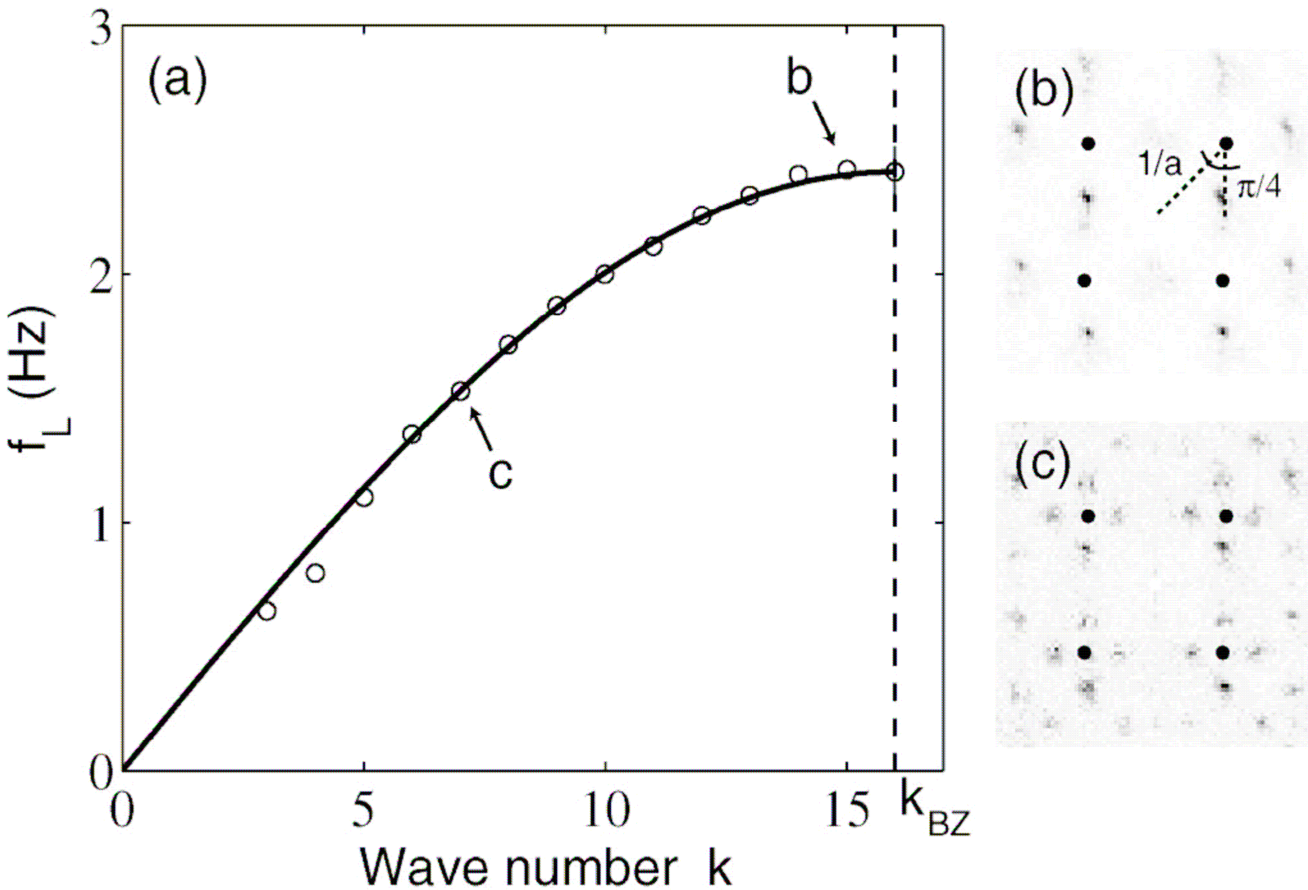
de Bruyn, Bizon, MDS, Goldman, Swift, Swinney PRL 1998

Stripe Stability Domain



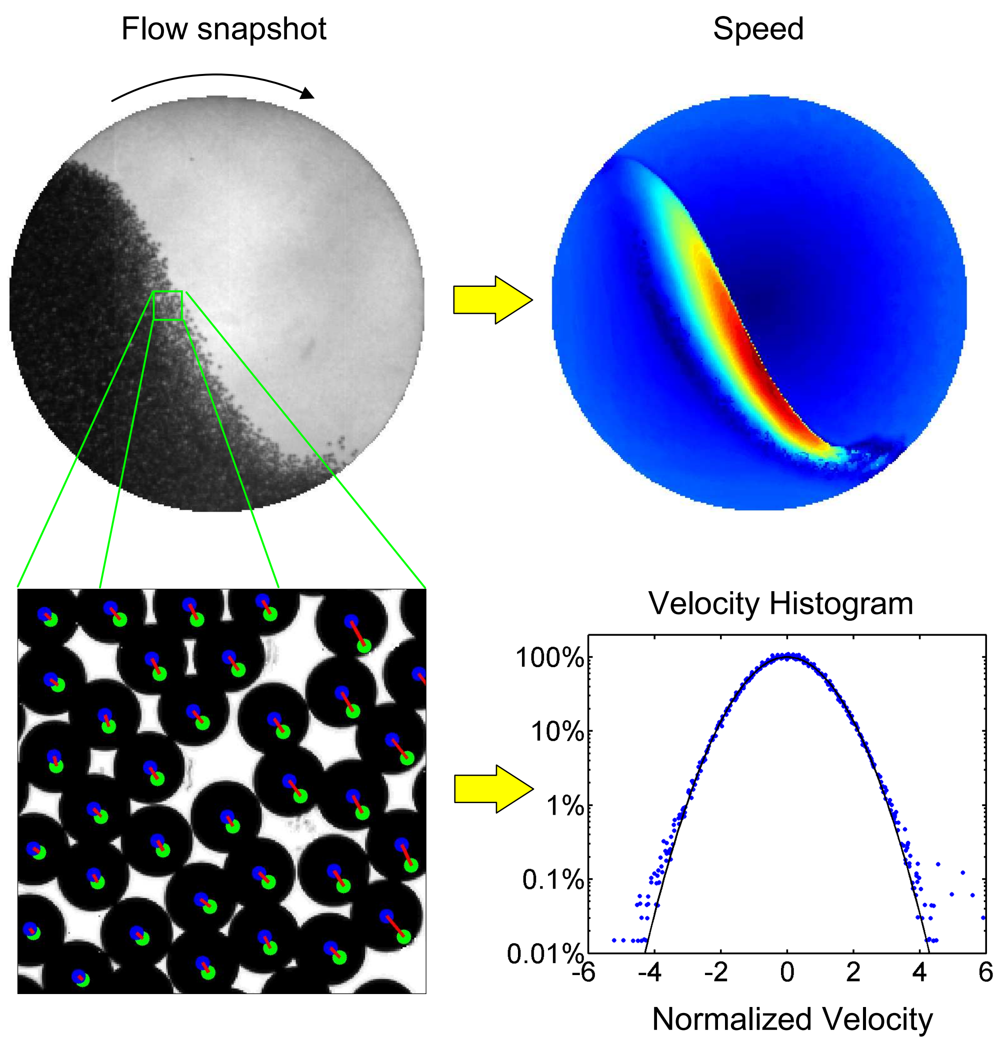
de Bruyn, Bizon, MDS, Goldman, Swift, Swinney PRL 1998

Dispersion Relation for Square Lattice

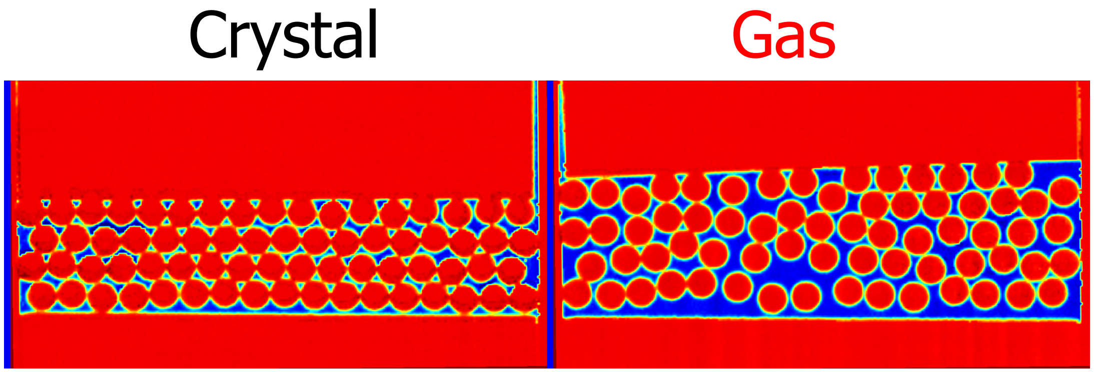


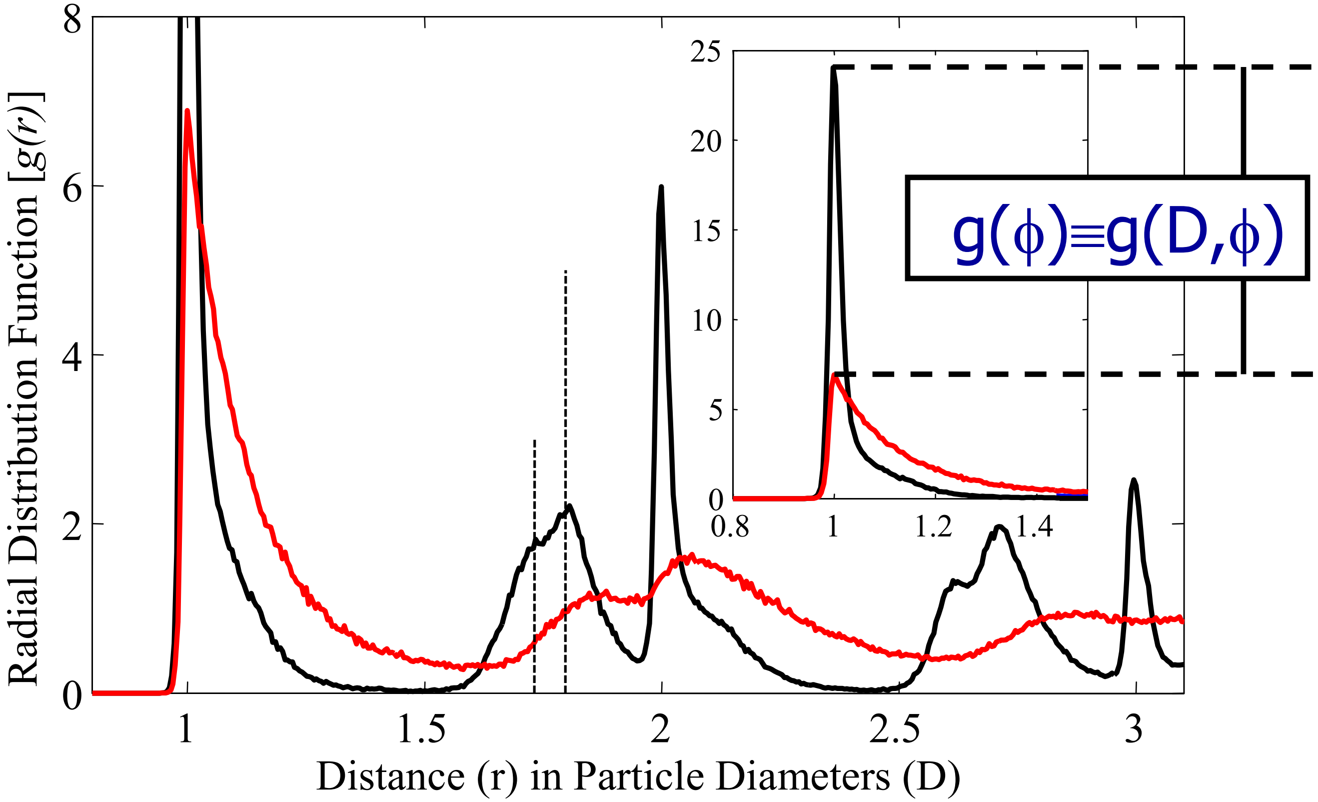
Goldman, MDS,Moon, Swift, Swinney PRL 2003

Dense Granular Flow



Radial Distribution Function





Granular Temperature

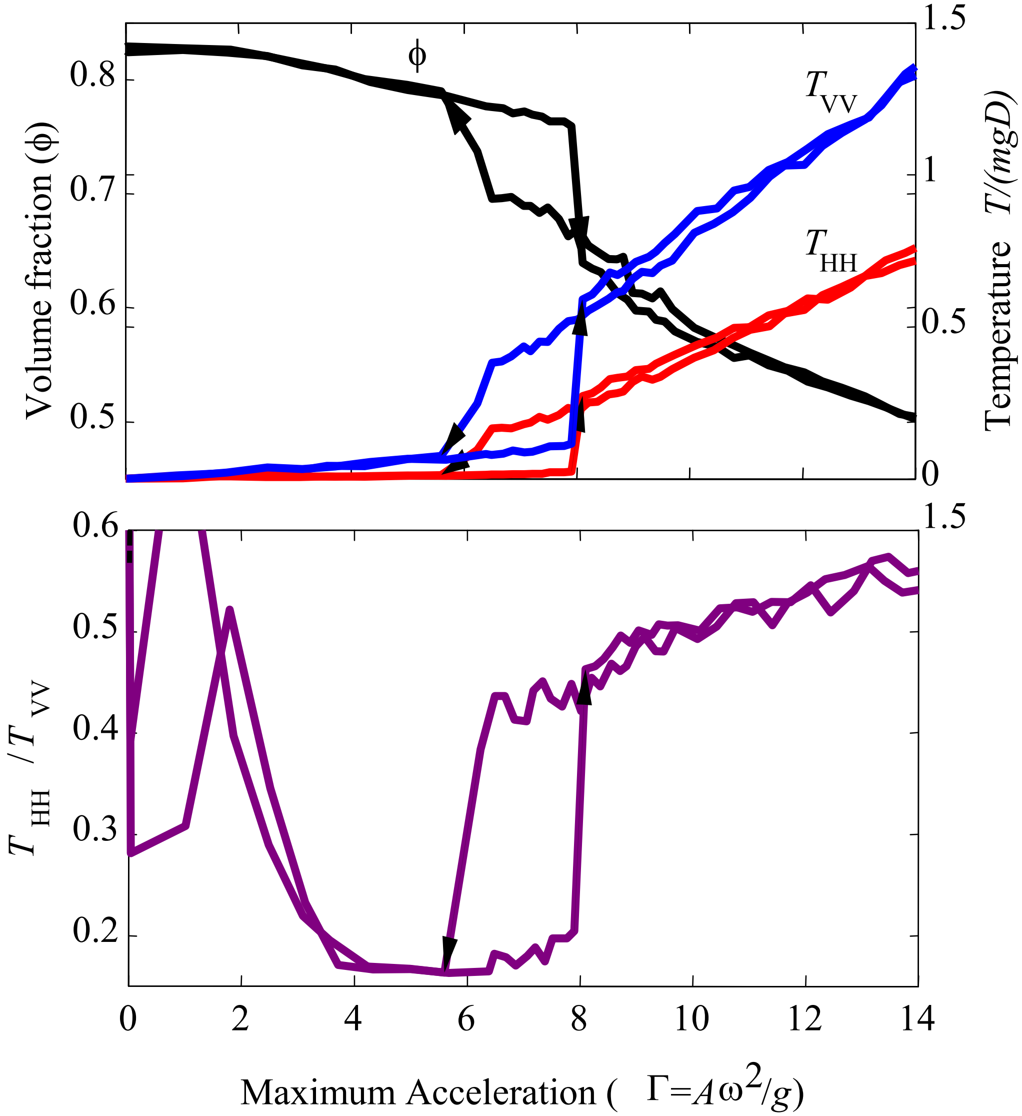
Ordinary Temperature
Equipartion of Energy

$$T = \frac{E}{N} = \left\langle \frac{1}{2} m \mathbf{v} \cdot \mathbf{v} \right\rangle = 2\left\langle \frac{1}{2} m v_x^2 \right\rangle = 2\left\langle \frac{1}{2} m v_y^2 \right\rangle$$

Granular Temperature
NO Equipartion of Energy

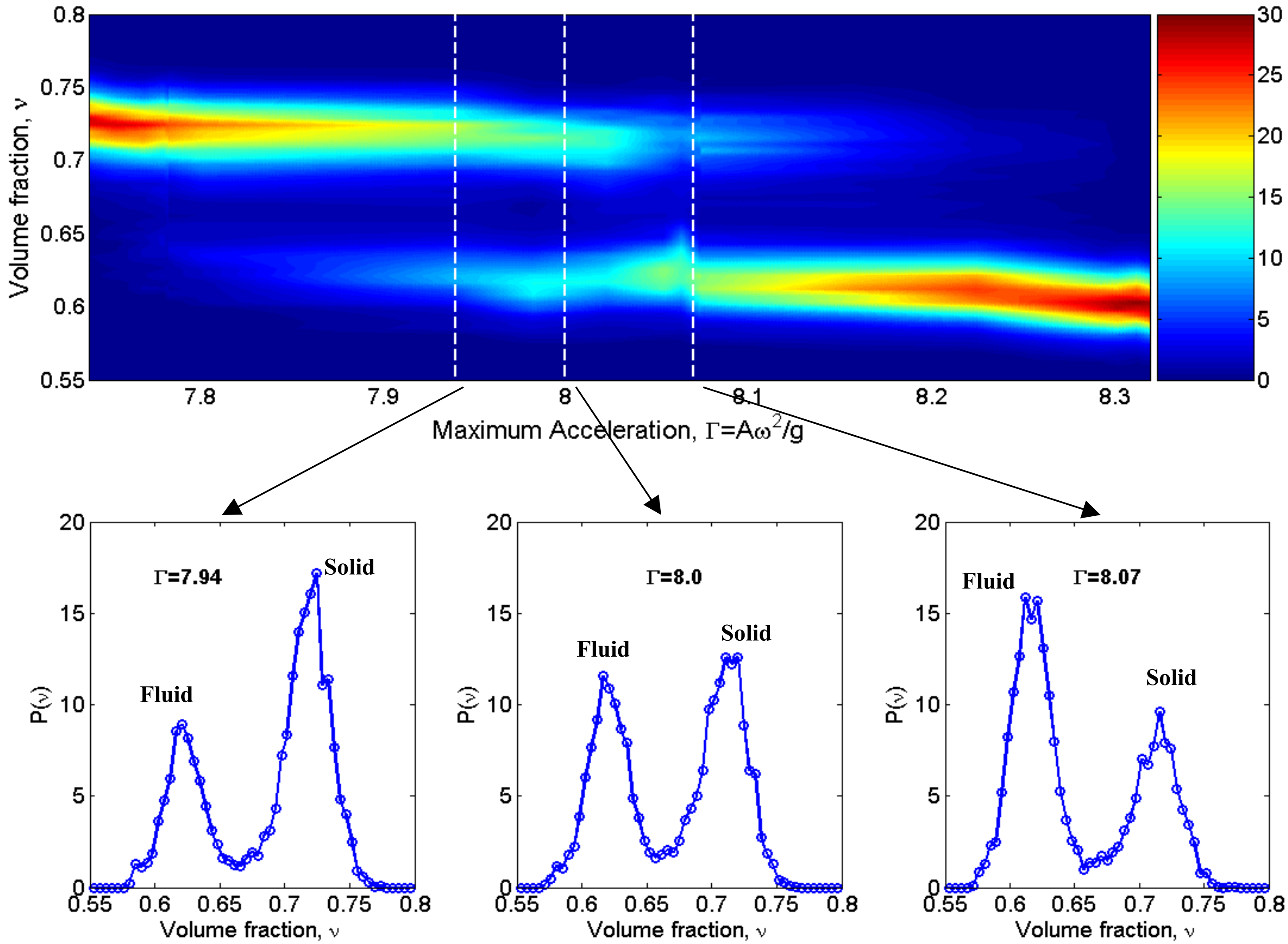
$$T_{HH} = \left\langle \frac{1}{2} m v_x^2 \right\rangle \neq T_{VV} = \left\langle \frac{1}{2} m v_y^2 \right\rangle \neq T_{VH} = T_{HV} = \left\langle \frac{1}{2} m v_x v_y \right\rangle$$

Temperature Dependence



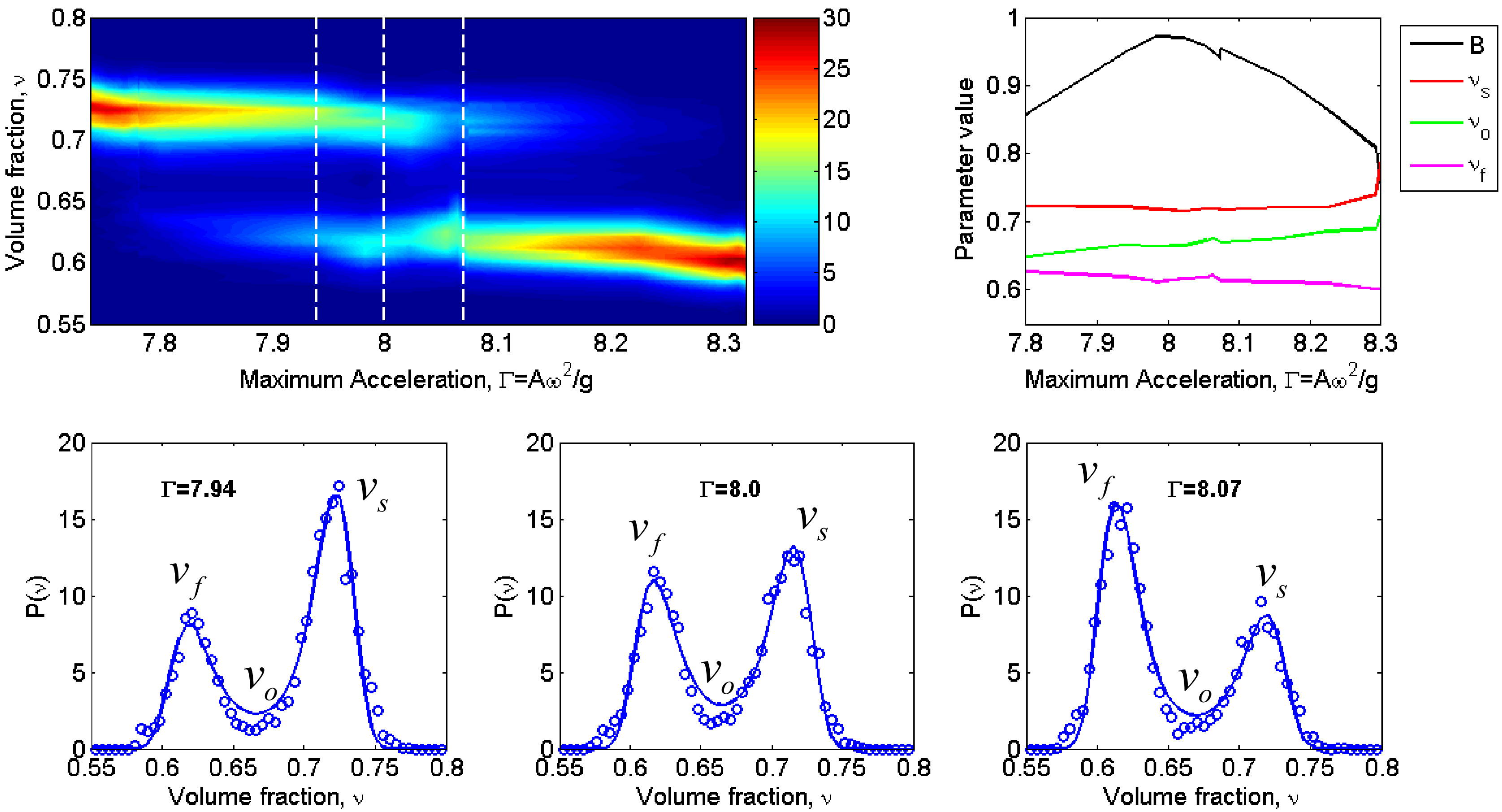
Results

PDF of volume fraction



Results

Phenomenological Model



Excellent agreement with experiments!

Solid-Fluid transitions

- Rapid flow: fluid like regime; theory and experimental analysis are cast in framework of kinetic theory.
- Slow flow: solid like regime; commonly described using tools of soil mechanics and plasticity theory and analogy to glasses.
- No well understood region of overlap.
- Few studies focus on solid to fluid transition.