INSTABILITIES IN GRANULAR FLUIDS AT MODERATE DENSITIES

STATISTICAL PHYSICS in eXTREMADURA

European Union

European Regional Development Fund

Vicente Garzó

Departamento de Física, Universidad de Extremadura, Badajoz, Spain

Peter Mitrano and Christine Hrenya

Department of Chemical and Biological Engineering, University of Colorado, Boulder, USA

SigmaPhi2014, July 7-11, Rhodes, Greece

OUTLINE

1. *Smooth* inelastic hard spheres: Enskog kinetic equation for ***moderately dense*** systems

2. Granular hydrodynamic equations

3. Chapman-Enskog-like method

4. *Instabilities* in granular dense fluids

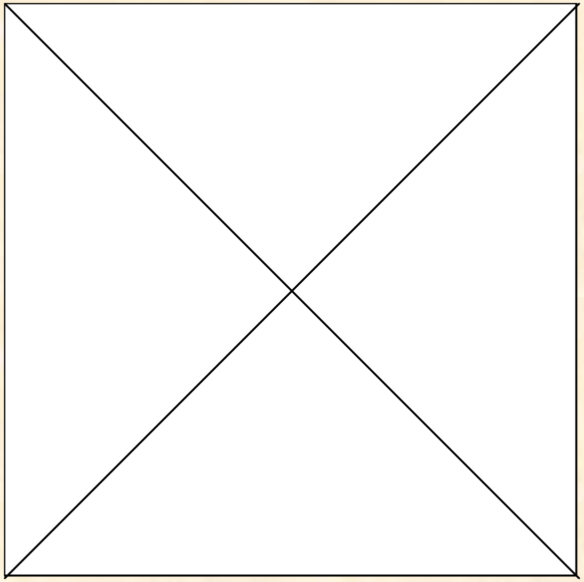
5. Conclusions

SigmaPhi2014, July 7-11, Rhodes,Greece

INTRODUCTION

Granular systems are systems constituted by macroscopic grains: Sand, rice, sugar, snow, pills,…….Ubiquitous in our daily lives

In some cases, they can behave as a solid. In others (external excitation), granular medium is more similar to a gas.



Smooth hard spheres with *inelastic* collisions

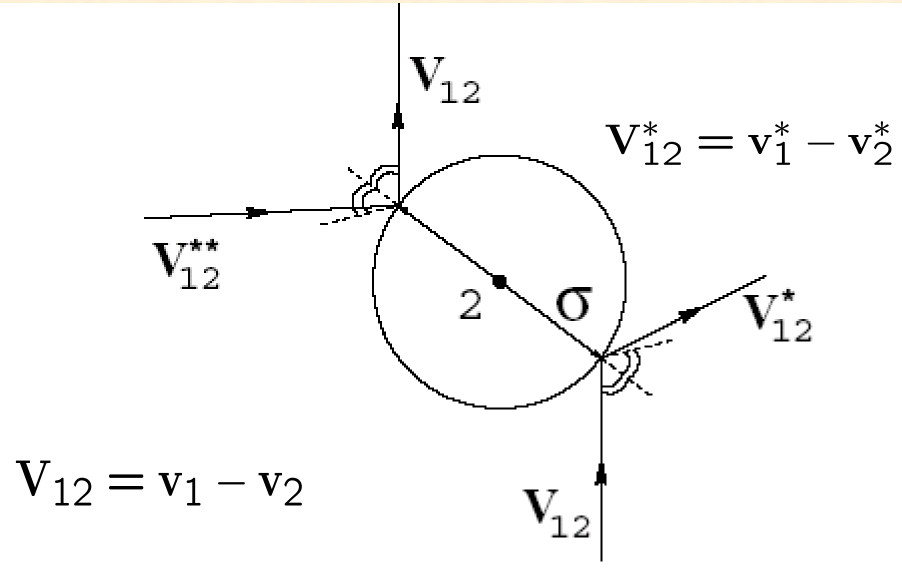


FIG. 1: Sketch of inelastic collisions (after T.P.C. van Noije & M.H. Ernst).

$$\mathbf{V}^*_{12} \cdot \hat{\boldsymbol{\sigma}} = -\alpha \mathbf{V}_{12} \cdot \hat{\boldsymbol{\sigma}}$$

Coefficient of normal restitution

$$0 < \alpha \leq 1$$

Direct collision

$$\mathbf{v}^*_1 = \mathbf{v}_1 - \frac{1}{2}(1+\alpha)\,(\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\hat{\boldsymbol{\sigma}}$$

$$\mathbf{v}^*_2 = \mathbf{v}_2 + \frac{1}{2}(1+\alpha)\,(\hat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\hat{\boldsymbol{\sigma}}$$

Momentum conservation

$$\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}_1^* + \mathbf{v}_2^*$$

Collisional energy change

$$\Delta E = \frac{1}{2} m \left(v_1^{*2} + v_2^{*2} - v_1^2 - v_2^2 \right) = -\frac{m}{4}(1-\alpha^2)(\mathbf{V}_{12}\cdot\widehat{\boldsymbol{\sigma}})^2$$

Very **simple** model that *captures* many properties of granular flows, especially those associated with dissipation

Real granular systems characterized by some degrees of *polidispersity* in density and size: *Multicomponent* granular systems

Mechanical parameters: $\{m_i, \sigma_i, \alpha_{ij}\}, \quad i = 1, \cdots, s$

Direct collision:

$$\mathbf{v}_1^* = \mathbf{v}_1 - \frac{m_j}{m_i + m_j}\left(1 + \alpha_{ij}\right)(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2^* = \mathbf{v}_2 + \frac{m_i}{m_i + m_j}\left(1 + \alpha_{ij}\right)(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

$$(\Delta E)_{ij} = \frac{1}{2}\left(m_i v_1^{*2} + m_j v_2^{*2} - m_i v_1^2 - m_j v_2^2\right) = -\frac{1}{2}\frac{m_i m_j}{m_i + m_j}(1 - \alpha_{ij}^2)(\mathbf{V}_{12}\cdot\widehat{\boldsymbol{\sigma}})^2$$

REVISED ENSKOG KINETIC THEORY

S-multicomponent mixture of smooth hard spheres or disks of masses m_i, diameters σ_i, and coefficients of restitution α_{ij}

At a kinetic level: $f_i(\mathbf{r}_1,\mathbf{v}_1;t)$

$$\left(\partial_t + \mathbf{v}_1 \cdot \nabla_{\mathbf{r}_1} + m_i^{-1}\mathbf{F}_i(\mathbf{r}_1) \cdot \nabla_{\mathbf{v}_1}\right) f_i(\mathbf{r}_1, \mathbf{v}_1; t) = C_i(\mathbf{r}_1, \mathbf{v}_1; t)$$

$$C_i(\mathbf{r}_1, \mathbf{v}_1; t) = \sum_{j=1}^{s} \sigma_{ij}^{d-1} \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}} \Theta(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \times \left(\alpha_{ij}^{-2} f_{ij}(\mathbf{r}_1, \mathbf{v}_1'', \mathbf{r}_1 - \boldsymbol{\sigma}_{ij}, \mathbf{v}_2''; t) - f_{ij}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + \boldsymbol{\sigma}_{ij}, \mathbf{v}_2; t)\right)$$

Two-particle distribution function

$$\mathbf{V}_{12} \equiv \mathbf{g}_{12}$$

Collision rules:

$$\mathbf{v}_1'' = \mathbf{v}_1 - \mu_{ji}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2'' = \mathbf{v}_2 + \mu_{ij}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

where $\mu_{ij}=m_i/(m_i+m_j)$

Kinetic theory approach: ***velocity*** correlations are neglected (molecular chaos hypothesis !!)

$$f_{ij}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_2,\mathbf{v}_2;t) \rightarrow \chi_{ij}\left(\mathbf{r}_1,\mathbf{r}_2 \mid \{n_i\}\right) f_i(\mathbf{r}_1,\mathbf{v}_1;t) f_j(\mathbf{r}_2,\mathbf{v}_2;t)$$

↓ (χ_{ij})

Spatial correlations (volume exclusion effects)

Bad news for the RET: Several MD simulations have shown that velocity correlations become *important* as density increases (McNamara&Luding, PRE (1998); Soto&Mareschal PRE (2001); Pagonabarraga et al. PRE (2002);…..)

Good news for the RET: Good agreement at the level of *macroscopic* properties for moderate densities and finite dissipation (**Simulations**: Brey et al., PF (2000) ; Lutsko, PRE (2001); Dahl et al., PRE (2002); Lois et al. PRE (2007); Bannerman et al., PRE (2009);…..
Experiments: Yang et al., PRL (2002); PRE (2004); Rericha et al., PRL (2002);…..)

RET is *still* a valuable theory for granular fluids for *densities* beyond the Boltzmann limit and *dissipation* beyond the quasielastic limit.

MACROSCOPIC BALANCE EQUATIONS

Hydrodynamic fields

$$n_i(\mathbf{r},t)=\int d\mathbf{v}\, f_i(\mathbf{r},\mathbf{v},t)$$

$$\mathbf{U}(\mathbf{r},t)=\frac{1}{\rho(\mathbf{r},t)}\sum_i \int d\mathbf{v}\, m_i \mathbf{v}\, f_i(\mathbf{r},\mathbf{v},t)$$

$$T(\mathbf{r},t)=\frac{1}{n(\mathbf{r},t)}\sum_i \int d\mathbf{v}\,\frac{m_i}{d}(\mathbf{v}-\mathbf{U})^2 f_i(\mathbf{r},\mathbf{v},t)$$

Macroscopic equations are ***exact*** since they are obtained from the first hierarchy equation (without the Enskog approximation)

VG, J. W. Dufty, C. M. Hrenya, PRE **76**, 031303; 031304 (2007)

Balance equation for the partial densities

$$D_t n_i + n_i \nabla \cdot \mathbf{U} + m_i^{-1} \nabla \cdot \mathbf{j}_i = 0$$

Balance equation for the flow velocity

$$\rho D_t U_\beta + \nabla_\gamma P_{\gamma\beta} = \sum_{i=1}^{s} n_i(\mathbf{r},t) F_{i\beta}(\mathbf{r})$$

Balance equation for the granular temperature

$$\frac{d}{2} n (D_t + \zeta) T + P_{\gamma\beta} \nabla_\gamma U_\beta + \nabla \cdot \mathbf{q} - \frac{d}{2} T \sum_{i=1}^{s} \frac{\nabla \cdot \mathbf{j}_i}{m_i} = \sum_{i=1}^{s} \frac{\mathbf{F}_i \cdot \mathbf{j}_i}{m_i}$$

Cooling rate

$$D_t \equiv \partial_t + \mathbf{v} \cdot \nabla$$

Mass flux

$$\mathbf{j}_i(\mathbf{r}_1,t)=m_i\int d\mathbf{v}_1\mathbf{V}_1 f_i(\mathbf{r}_1,\mathbf{v}_1;t)$$

V=v-U

Pressure tensor

$$P_{\gamma\beta}(\mathbf{r}_1,t)=P^k_{\gamma\beta}(\mathbf{r}_1,t)+P^c_{\gamma\beta}(\mathbf{r}_1,t)$$

Kinetic contribution **Collisional contribution**

$$P^k_{\gamma\beta}(\mathbf{r}_1,t)=\sum_{i=1}^{s}\int d\mathbf{v}_1 m_i V_{1\beta}V_{1\gamma}f_i(\mathbf{r}_1,\mathbf{v}_1;t)$$

$$P^c_{\gamma\beta}(\mathbf{r}_1,t) = \frac{1}{2}\sum_{i,j=1}^{s} m_j\mu_{ij}\left(1+\alpha_{ij}\right)\sigma_{ij}^d\int d\mathbf{v}_1\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^2 \times\widehat{\sigma}_\beta\widehat{\sigma}_\gamma\int_0^1 dx\, f_{ij}(\mathbf{r}_1-x\boldsymbol{\sigma}_{ij},\mathbf{v}_1,\mathbf{r}_1+(1-x)\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t).$$

Heat flux

$$\mathbf{q}(\mathbf{r}_1,t)=\mathbf{q}^k(\mathbf{r}_1,t)+\mathbf{q}^c(\mathbf{r}_1,t)$$

$$\mathbf{q}^k(\mathbf{r}_1,t)=\sum_{i=1}^{s}\int d\mathbf{v}_1\frac{1}{2}m_iV_1^2\mathbf{V}_1f_i(\mathbf{r}_1,\mathbf{v}_1;t)$$

$$\begin{aligned}\mathbf{q}^c(\mathbf{r}_1,t) \; = \; & \sum_{i,j=1}^{s}\frac{1}{8}\left(1+\alpha_{ij}\right)m_j\mu_{ij}\sigma_{ij}^d\int d\mathbf{v}_1\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\\ & \times(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^2\left[\left(1-\alpha_{ij}\right)\left(\mu_{ji}-\mu_{ij}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})+4\widehat{\boldsymbol{\sigma}}\cdot\mathbf{G}_{ij}\right)\\ & \times\widehat{\boldsymbol{\sigma}}\int_0^1 dx\,f_{ij}(\mathbf{r}_1-x\boldsymbol{\sigma}_{ij},\mathbf{v}_1,\mathbf{r}_1+(1-x)\,\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t),\end{aligned}$$

$\mathbf{G}_{ij}=\mu_{ij}\mathbf{V}_1+\mu_{ji}\mathbf{V}_2$ is the center-of-mass velocity

Cooling rate

$$\zeta = \frac{1}{2dnT}\sum_{i,j=1}^{s}\left(1-\alpha_{ij}^{2}\right)m_i\mu_{ji}\sigma_{ij}^{d-1}\int d\mathbf{v}_1\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}$$
$$\times\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^3 f_{ij}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_1+\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t)$$

Balance equations become a closed set of hydrodynamic equations for (n_i,**U,**T) once the *fluxes* and the *cooling rate* are expressed as ***functionals*** of (n_i,**U,**T) (“constitutive relations”)

CHAPMAN-ENSKOG NORMAL SOLUTION

Assumption: For long times (much longer than the mean free time) and far away from boundaries (bulk region) the system reaches a *hydrodynamic* regime.

Normal solution $f_i(\mathbf{r}, \mathbf{v}; t) = f_i(\mathbf{v} | \{n_i(\mathbf{r}, t)\}, \mathbf{U}(\mathbf{r}, t), T(\mathbf{r}, t)\})$

In some situations, gradients are controlled by boundary or initial conditions. Small spatial gradients:

$$f_i = f_i^{(0)} + f_i^{(1)} + \cdots$$

$f_i^{(0)}$ → "local" HCS

Constitutive equations (binary mixture)

$$\mathbf{j}_1 = -\frac{m_1^2 n}{\rho} D_{11} \nabla \ln n_1 - \frac{m_1 m_2 n_2}{\rho} D_{12} \nabla \ln n_2 - \rho D_T \nabla \ln T$$

$$P_{\gamma\beta} = p\delta_{\gamma\beta} - \eta \left(\nabla_\gamma U_\beta + \nabla_\beta U_\gamma - \frac{2}{d} \nabla \cdot \mathbf{U} \right) - \kappa \nabla \cdot \mathbf{U}$$

$$\mathbf{q} = -T^2 D_{q,1} \nabla \ln n_1 - T^2 D_{q,2} \nabla \ln n_2 - \lambda \nabla T$$

Eight transport coefficients: $\left\{ D_{11}, D_{12}, D_T, \eta, \kappa, D_{q,1}, D_{q,2}, \lambda \right\}$

Parameter space: $\{m_1/m_2, \sigma_1/\sigma_2, x_1, \phi, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$

SigmaPhi2014, July 7-11, Rhodes,Greece

INSTABILITIES IN FREELY COOLING *DENSE* GRANULAR BINARY MIXTURES

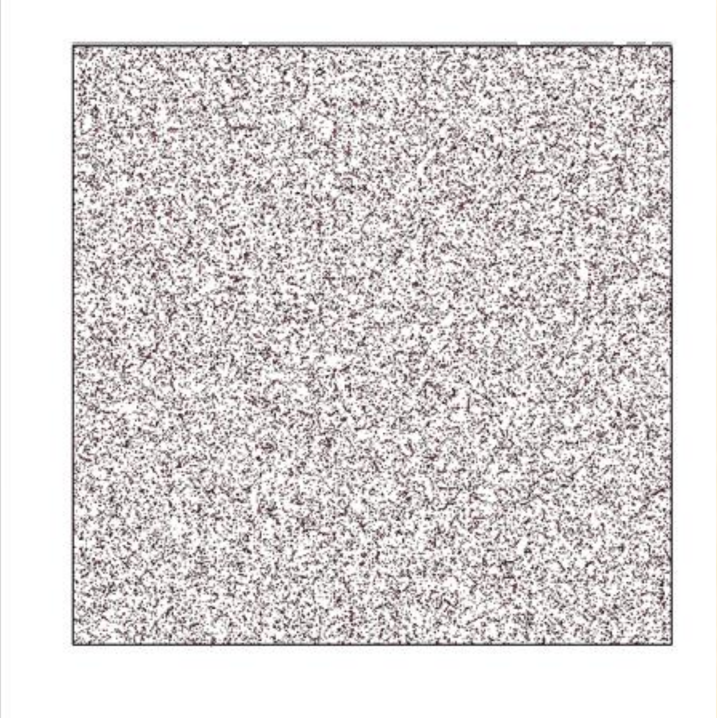
In contrast to ordinary fluids, *instabilities* (such as dynamic particle clusters) occur in the homogeneous cooling state (HCS) of granular gases

Pionnering work of Goldhirsch&Zanetti (PRL **70**, 1619 (1993))

Typical configuration of particles exhibing clustering

$$\alpha = 0.6, \phi = 0.05$$

(Peter Mitrano, CU)



General trends: (i) instabilities are more likely in larger domains; and (ii) velocity vortices manifest more readily than particle clusters

This is also a very ***clean*** problem to assess Navier-Stokes hydrodynamics derived from Kinetic Theory

For given values of the mechanical parameters of the system, there exists a **critical** system lenght demarcates (stable) homogeneous flow from one with *velocity-vortex* instabilities or one exhibiting the *clustering* instability

LINEAR STABILITY ANALYSIS

HCS is *unstable* with respect to long enough wave-length perturbations. Stability analysis of the nonlinear hydrodynamic equations with respect to HCS for small initial excitations

HCS solution

$$\nabla(n_{1H}/n_H) = \nabla n_H = \nabla T_H = 0,$$

$$\mathbf{U}_H = \mathbf{0}, \quad \partial_t \ln T_H = -\zeta_H$$

This basic solution is unstable to linear perturbations

We linearize the Navier-Stokes equations with respect to the HCS solution. Deviations of the hydrodynamic fields from their values in HCS are *small*

$$x_1 = \frac{n_1}{n}, n = n_1 + n_2$$

$$x_1(\mathbf{r}, t) = x_{1H} + \delta x_1(\mathbf{r}, t), n(\mathbf{r}, t) = n_H + \delta n(\mathbf{r}, t),$$

$$\mathbf{U}(\mathbf{r}, t) = \delta \mathbf{U}(\mathbf{r}, t), T(\mathbf{r}, t) = T_H + \delta T(\mathbf{r}, t)$$

Only linear terms in perturbations are retained

Linearization about HCS yields a set of partial differential eqs. with coefficients that are independent of space **BUT** depend on time. Time dependence can be eliminated by

$$\tau = \int_0^t dt' \nu_H(t'), \ell = \frac{\nu_H(t)}{v_H(t)}\mathbf{r}$$

$$\nu_H \propto n_H \sigma_{12}^{d-1} v_H, v_H = \sqrt{2T_H/(m_1+m_2)}$$

Set of coupled linear differential equations with *constant* coefficients

Set of Fourier transformed dimensionless variables:

$$\rho_{1,\mathbf{k}}(\tau) = \frac{\delta x_{1\mathbf{k}}(\tau)}{x_{1H}}, \quad \rho_{\mathbf{k}}(\tau) = \frac{\delta n_{\mathbf{k}}(\tau)}{n_H}$$

$$\mathbf{w}_{\mathbf{k}}(\tau) = \frac{\delta \mathbf{U}_{\mathbf{k}}(\tau)}{v_H(\tau)}, \quad \theta_{\mathbf{k}}(\tau) = \frac{\delta T_{\mathbf{k}}(\tau)}{T_H(\tau)}$$

$$\delta y_{\mathbf{k}\beta}(\tau) = \int d\boldsymbol{\ell} e^{-i\mathbf{k}\cdot\boldsymbol{\ell}} \delta y_\beta(\boldsymbol{\ell}, \tau)$$

$$\delta y_{\mathbf{k}\beta} \equiv \left\{ \rho_{1,\mathbf{k}}, \rho_{\mathbf{k}}, \mathbf{w}_{\mathbf{k}}, \theta_{\mathbf{k}} \right\}$$

Transversal component of the velocity field is *decoupled* from the other modes. This identifies "d-1" shear (transversal) modes

$$\left(\frac{\partial}{\partial\tau} - \zeta_H^* + \frac{1}{2}\eta_H^* k^2\right)\mathbf{w}_{\mathbf{k}\perp} = 0$$

$$\mathbf{w}_{\mathbf{k}\perp}(\tau) = \mathbf{w}_{\mathbf{k}\perp}(0)e^{s_\perp \tau}, s_\perp(k) = \zeta_H^* - \frac{1}{2}\eta_H^* k^2$$

There exists a critical wave number: $k_\perp^c = \sqrt{\frac{2\zeta_H^*}{\eta_H^*}}$

$k < k_\perp^c$ → Shear modes grow exponentially!!

The remaining 4 longitudinal modes are *coupled* and are the eigenvalues of a 4X4 matrix

There exists two critical wave numbers:

$$k_{\perp}^{c} = \sqrt{\frac{2\zeta_H^*}{\eta_H^*}}, \qquad k_{\parallel}^{c}$$

Solution of a quartic equation

For wave numbers smaller than these critical values, the system becomes unstable

Periodic boundary conditions, the smallest k is $2\pi/L$

If the system length L>Lc, then the system becomes unstable

$$\frac{2\pi}{L_c^*} = \max\left\{k_\perp^c, k_\parallel^c\right\}$$

In most of the studied cases, the linear stability analysis predicts that the instability is driven by velocity vortices

$$k_\perp^c > k_\parallel^c$$

Stringent *assessment* of kinetic theory calculations!!!

MONOCOMPONENT GRANULAR FLUIDS

VG, PRE **72**, 021106 (2005)

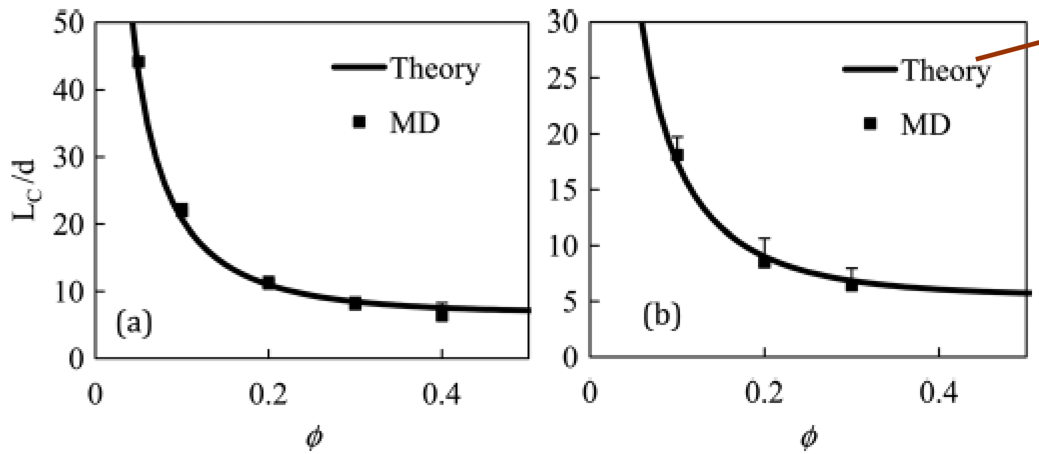


FIG. 8. Comparison of the critical length scale (L_C/d) for (a) $e=0.8$ and (b) $e=0.7$. The "error bars" correspond to the transition length scale range obtained from MD simulations (see Sec. IV A and Figure 5). Theoretical predictions are obtained from the linear stability analysis of Garzó (Ref. 23).

Mitrano, Dhal, Cromer, Pacella , Hrenya, Phys. Fluids **23**, 093303 (2011)

Standard Sonine approximation

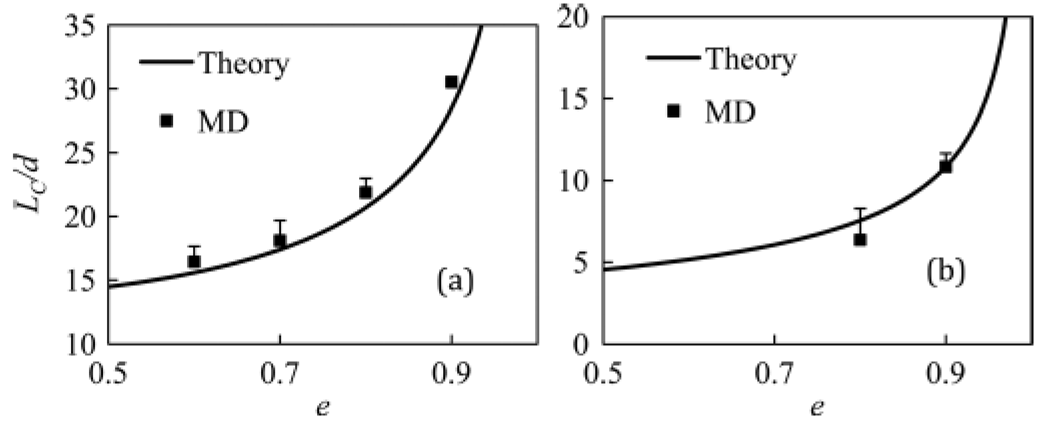


FIG. 9. Comparison of the critical length scale for (a) $\phi = 0.1$ and (b) $\phi = 0.4$. The "error bars" correspond to the transition length scale range obtained from MD simulations (see Sec. IV A and Figure 5). Theoretical predictions are obtained from a linear stability analysis of Garzó (Ref. 23).

HIGHLY DISSIPATIVE GRANULAR FLUIDS

Modified Sonine approximation (VG, Santos, Montanero, Physica A **376** 94 (2007))

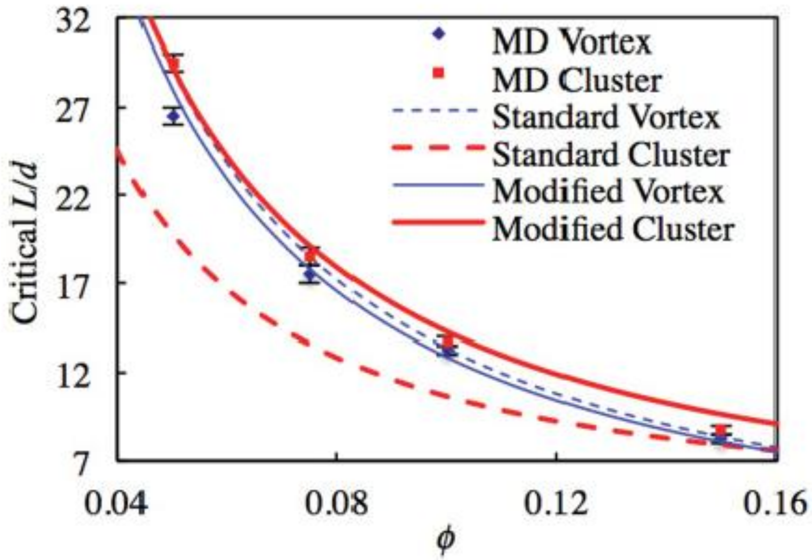


FIG. 4. (Color online) Critical length scale for vortex and cluster instabilities (i.e., L_{Vortex}/d and L_{Cluster}/d, respectively) plotted as a function of solids fraction for $e = 0.25$. The solid and dashed lines correspond to the modified and standard theories, respectively.

Mitrano, VG, Hilger, Ewasko, Hrenya, PRE **85**, 041303 (2012)

BINARY GRANULAR DENSE MIXTURES

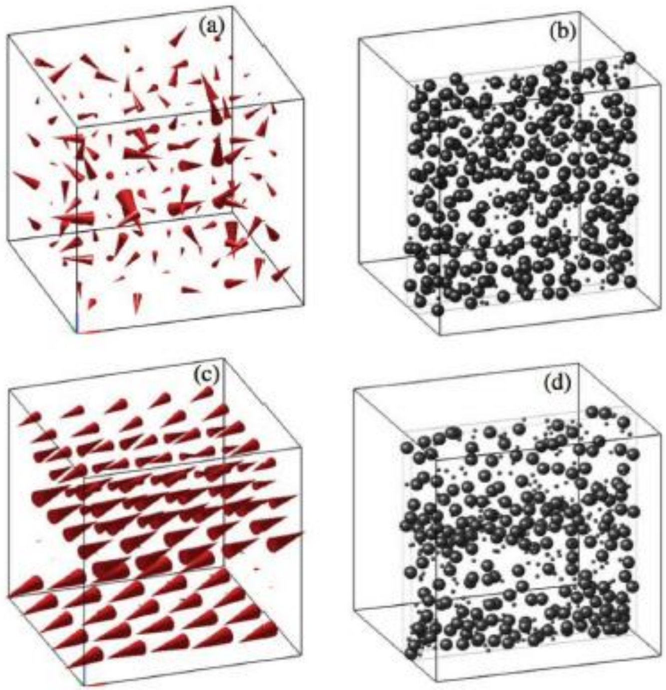


FIG. 1. (Color online) Visualizations from a MD simulation of an equimolar mixture ($x_1 = 0.5$) with $m_1/m_2 = 2$, $\sigma_1/\sigma_2 = 3$, $\phi = 0.2$, and $\alpha = 0.7$ of (a) stable, coarse-grained velocity field at five collisions per particle (or "cpp"), (b) stable particle positions at five cpp, (c) unstable, coarse-grained velocity field at 400 cpp, and (d) cluster systems at 400 cpp. A cell size of $L/5$ is used for local velocity averaging.

P. Mitrano, VG, C. Hrenya
PRE **89**, 0200201 (R) (2014)

BINARY GRANULAR DENSE MIXTURES

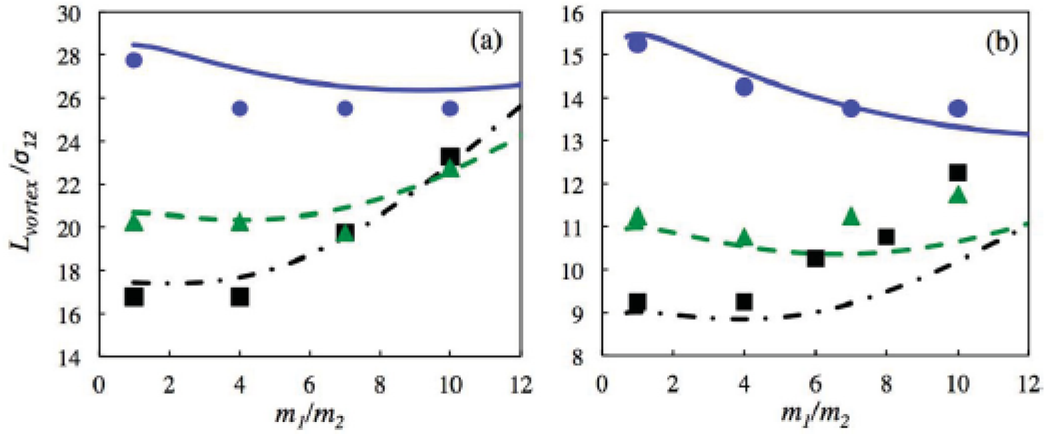


FIG. 2. (Color online) Critical length scale for velocity vortices as a function of the mass ratio m_1/m_2 with $x_1 = 0.1$, $\sigma_1/\sigma_2 = 1$ for (a) $\phi = 0.1$ and (b) $\phi = 0.2$. The data points correspond to MD simulations, while the lines are the theoretical predictions given by Eq. (3). (Blue) circles/solid line, (red) triangles/dashed line, and (black) squares/dot-dashed line correspond to $\alpha = 0.9$, $\alpha = 0.8$, and $\alpha = 0.7$, respectively. Error ranges are the size of the data points and are omitted.

BINARY GRANULAR DENSE MIXTURES

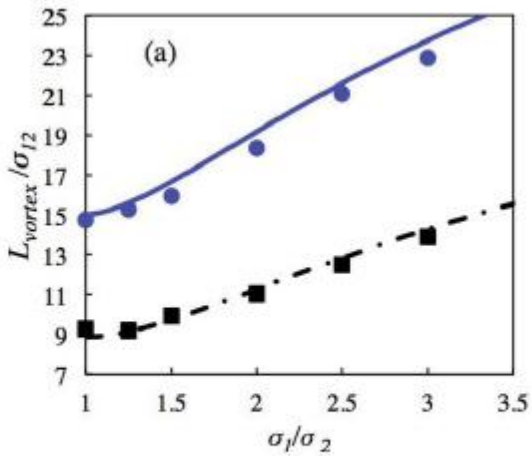


FIG. 3. (Color online) Critical length scale for velocity vortices as a function of (a) the ratio of diameters σ_1/σ_2 with $m_1/m_2 = 2$, $x_1 = 0.5$, and $\phi = 0.2$ and (b) the mole fraction x_1 with $m_1/m_2 = 6$, $\sigma_1/\sigma_2 = 1$, and $\phi = 0.2$. The meaning of symbols and lines is the same as that of Fig. 2.

CONCLUSIONS

✓Hydrodynamic description (derived from kinetic theory) appears to be a powerful tool for analysis and predictions of rapid flow gas dynamics of granular mixtures at ***moderate*** densities.

✓Instability of HCS: Good agreement with MD even for finite dissipation and moderate densities. Stringent test of kinetic theory results

Quantitative agreement could be improved at disparate masses by considering the second Sonine approximation to the ***shear viscosity***

Thanks for your attention