NON-NEWTONIAN TRANSPORT PROPERTIES IN GRANULAR COUETTE FLOWS

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STATISTICAL PHYSICS in EXTREMADURA

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Granular and active fluids, 12-15 September, 2011, ZCAM, Zaragoza

SUMMARY

1. Introduction

2. Boltzmann description of steady Couette flows

3. Theoretical approaches: Grad's moment method and BGK-type kinetic model

4. Comparison with DSMC and MD

5. Impurity under steady Couette flow

6. Conclusions

INTRODUCTION

"*Smooth* hard spheres with *inelastic* collisions"

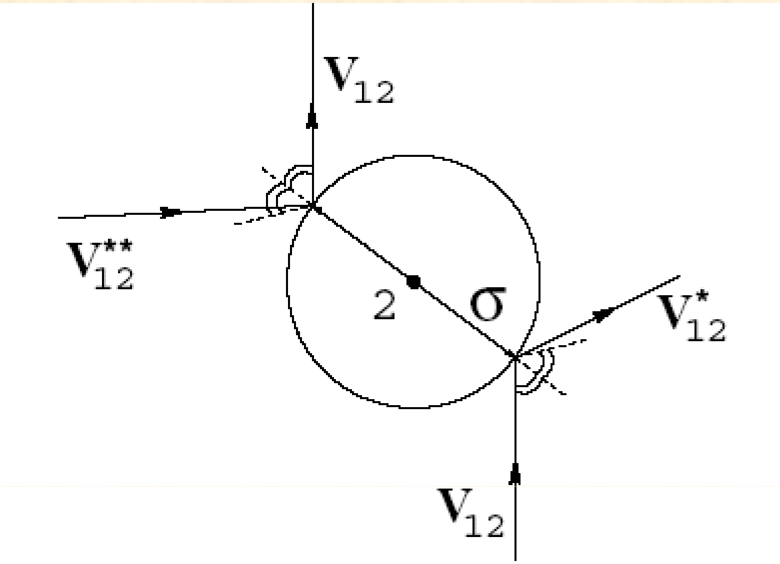


FIG. 1: Sketch of inelastic collisions (after T.P.C. van Noije & M.H. Ernst).

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

Coefficient of normal restitution

$$0 < \alpha \leq 1$$

Inelastic collisions → $$\Delta E = -\frac{m}{2}(1-\alpha^2)(\mathbf{V}_{12} \cdot \widehat{\boldsymbol{\sigma}})^2$$

KINETIC DESCRIPTION

One-particle velocity distribution function

$f(\mathbf{r}, \mathbf{v}, t) d\mathbf{r} d\mathbf{v}$ → Average number of particles at t located around **r** and moving with **v**

Boltzmann kinetic equation

- ***Dilute gas*** (binary colisions)
- ***"Molecular chaos"***

$$(\partial_t + \mathbf{v}\cdot\nabla) f(\mathbf{v}) = J[\mathbf{v}|f(t), f(t)]$$

$$J[\mathbf{v}_1|f,f] = \sigma^{d-1}\int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}) \times \left[\alpha^{-2} f(\mathbf{r},\mathbf{v}_1';t) f(\mathbf{r},\mathbf{v}_2';t) - f(\mathbf{r},\mathbf{v}_1;t) f(\mathbf{r},\mathbf{v}_2;t)\right]$$

$$\mathbf{g} = \mathbf{v}_1 - \mathbf{v}_2$$

Collision rules:

$$\mathbf{v}_1' = \mathbf{v}_1 - \frac{1}{2}\left(1+\alpha^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2' = \mathbf{v}_2 + \frac{1}{2}\left(1+\alpha^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

Differences with elastic BE: Presence of α^{-2} in gain term and collision rules

$$D_t n + n\nabla \cdot \mathbf{U} = 0$$

$$D_t \mathbf{U} + \rho^{-1} \nabla \cdot \mathsf{P} = 0$$

$$D_t T + \frac{2}{dn} (\nabla \cdot \mathbf{q} + \mathsf{P} : \nabla \mathbf{U}) = -\zeta T$$

$$P_{ij}(\mathbf{r}, t) = \int d\mathbf{v}\; m\mathbf{V}\mathbf{V} f(\mathbf{v})$$

$$\mathbf{q}(\mathbf{r}, t) = \int d\mathbf{v}\; \frac{m}{2} V^2 \mathbf{V} f(\mathbf{v})$$

"Normal" or hydrodynamic solution

•All the space and time dependence of vdf is given through its dependence on the hydrodynamic fields

$$f(\mathbf{r},\mathbf{v},t) = f[\mathbf{v}|n,\mathbf{U},T]$$

• For small spatial gradients, this functional dependence can be made ***local*** in space through an expansion in gradients of the hydrodynamic fields (Chapman-Enskog method)

First order: Navier-Stokes (NS) equations

$$P_{ij} = p\delta_{ij} - \eta\left(\nabla_i U_j + \nabla_j U_i - \frac{2}{d}\nabla\cdot\mathbf{U}\right)$$

$$\mathbf{q} = -\lambda\nabla T - \mu\nabla n$$

Brey, Dufty, Kim, Santos, PRE **58**, 4638 (1998)

$$\eta = \eta_0\eta^*_{\mathsf{NS}}(\alpha), \quad \lambda = \lambda_0\lambda^*_{\mathsf{NS}}(\alpha), \quad \mu = \frac{T\lambda_0}{n}\mu^*_{\mathsf{NS}}(\alpha)$$

$\eta_0, \lambda_0 \longrightarrow$ elastic Boltzmann coefficients

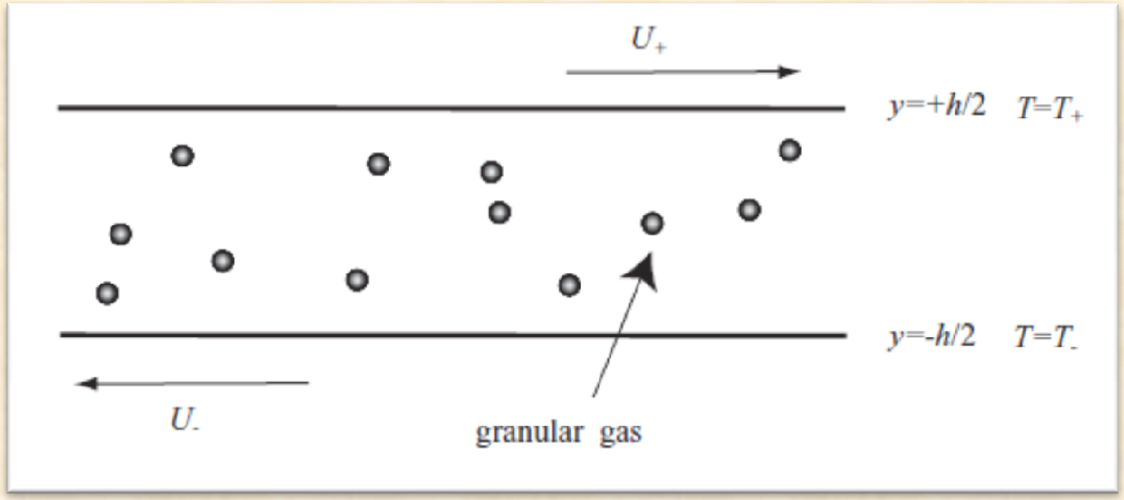
Ranges of interest of the physics of granular gases fall sometimes *beyond* NS description

Example: **Steady** states due to the coupling between inelasticity and spatial gradients. Large gradients as the gas becomes more inelastic

In these states (***large*** spatial gradients) , the *hydrodynamic* description is still possible but with more **complex** constitutive eqs. than that of NS

Extremely mathematical complex task!!

STEADY PLANAR COUETTE FLOW PROBLEM



Hydrodynamic fields: $U_x(y), n(y), T(y)$

Hydrodynamic balance equations

$$\partial_y P_{xy} = 0, \qquad \partial_y P_{yy} = 0$$

$$\partial_y q_y = -\frac{d}{2}\zeta n T - P_{xy}\partial_y U_x$$

Three independent hydrodynamic fields: $\{p(y), T(y), U_x(y)\}$

$$p = nT = \frac{1}{d} P_{ii}$$

Dimensionless local shear rate: $a = \nu^{-1}\partial_y U_x, \qquad \nu \propto n\sqrt{T}$

Assumptions (to be consistently confirmed):

$$p = \text{constant}, a = \text{constant}$$

$$P_{xy} = -\eta_0 \eta^*(\alpha, a) \partial_y U_x, \qquad q_y = -\lambda_0 \lambda^*(\alpha, a) \partial_y T$$

Scaling laws for the NS coefficients: $\eta_0, \lambda_0 \propto p/\nu \propto \sqrt{T}$

Generalized shear viscosity: $\eta^*(\alpha, a) \neq \eta^*_{\text{NS}}(\alpha)$

Generalized thermal conductivity: $\lambda^*(\alpha, a) \neq \lambda^*_{\text{NS}}(\alpha)$

Since $\zeta \propto n\sqrt{T} \propto T^{-1/2}$, then the steady temperature equation is

$$\left(\nu^{-1}\partial_y\right)^2 T = -2m\gamma(\alpha, a)$$

$$\gamma = \frac{d-1}{d(d+2)}\lambda^{*-1}\left(\eta^* a^2 - \frac{d}{2}\zeta^*\right)$$

Dimensionless quantity

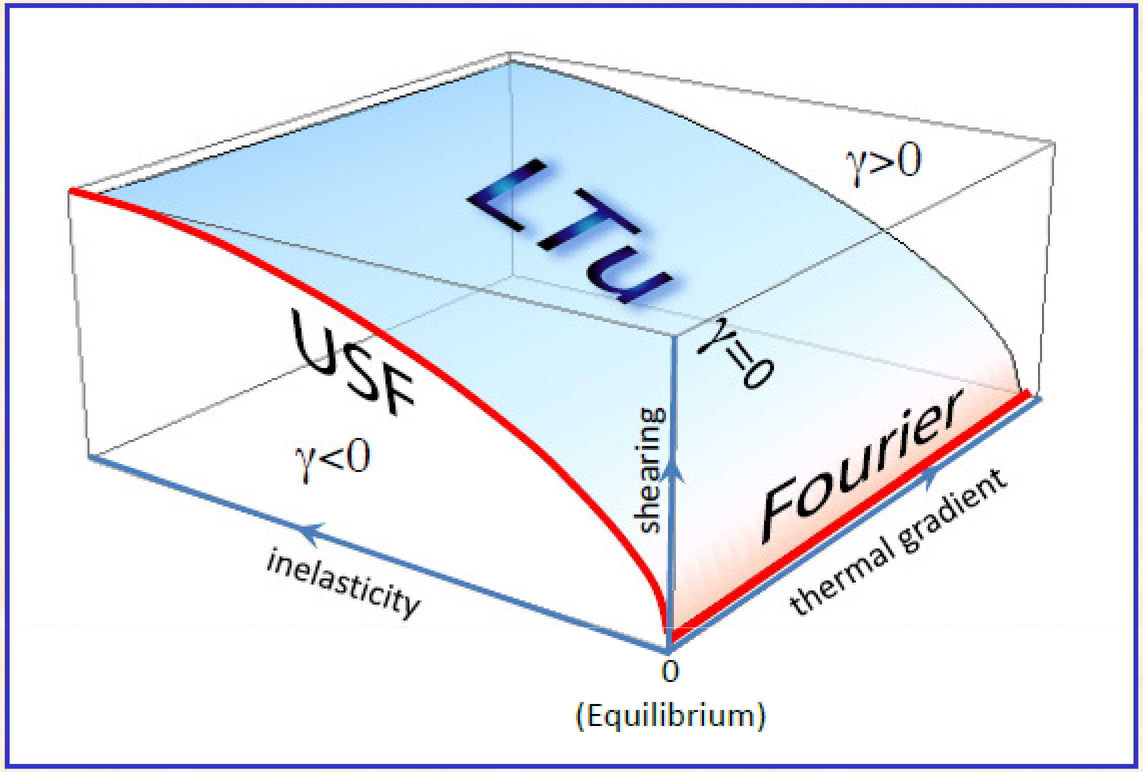
Reduced cooling rate: $\zeta/\nu \equiv \zeta^*(\alpha)$

Types of *flows*:

- If $\gamma < 0 \longrightarrow$ Collisional cooling predominates over viscous heating (granular)

- If $\gamma > 0 \longrightarrow$ Viscous heating predominates over collisional cooling (elastic, granular)

- If $\gamma = 0 \longrightarrow$ Viscous heating =collisional cooling (elastic, granular) $(\partial_y q_y = 0)$ (**LTu class**)



Each point represents a steady Couette flow state. The surface defines the LTu class (Fourier flow for ordinary gases and USF for granular gases as special cases)

Normal stress differences $$\theta_x = \frac{P_{xx}}{p}, \quad \theta_y = \frac{P_{yy}}{p}$$

$$\theta_x + \theta_y + (d-2)\theta_z = d, d \geq 3$$

Directional temperatures with respect to the granular temperature

Non-Newtonian coupling between shearing and thermal gradient

$$q_x = \lambda_0 \phi^*(\alpha, a) \partial_y T$$

Cross coefficient. Generalization of a Burnett transport coeficient

THEORETICAL APPROACHES

A. Grad's moment method

To check the consistency of the hydrodynamic profiles and the fluxes, one has to solve the BE

$$v_y \frac{\partial f}{\partial y} = J[f, f]$$

Truncated polynomial expansion for vdf
to solve the hierarchy of moment equations up to a given order

Retained moments $\longrightarrow$ $\left\{n, \mathbf{U}, T, P_{ij} - p\delta_{ij}, \mathbf{q}\right\}$

$$f \to f_M \left\{1 + \frac{m}{2pT}\left[(P_{ij} - p\delta_{ij})V_iV_j + \frac{4}{d+2}\frac{m}{nT^2}\left(\frac{mV^2}{2T} - \frac{d+2}{2}\right)\mathbf{V}\cdot\mathbf{q}\right]\right\}$$

Local equilibrium

$$\mathbf{V} = \mathbf{v} - \mathbf{U}$$

Grad's moment method **consistent** with the above Couette solution. Explicit expressions of *all* the rheological properties in terms of the (reduced) shear rate and dissipation. Results apply for **any** value of the thermal curvature parameter $\gamma(\alpha, a)$

B. BGK-type kinetic model

$$v_y \frac{\partial f}{\partial y} = -\beta(\alpha)\nu(f - f_M) + \frac{\zeta}{2}\frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{V} f$$

J. J. Brey, J. W. Dufty, A. Santos, JSP **97**, 281 (1999)

Exact hydrodynamic solution of the kinetic model is ***consistent*** with the above Couette flow description. Solution exists *only* for

$$\gamma(\alpha, a) \geq 0$$

Tij, Tahiri, Montanero, VG, Santos, Dufty JSP **103**, 1035 (2001)

SIMULATION METHODS

In order to assess the reliability of the theoretical results:
DSMC simulations of the BE and MD simulations
for a granular gas of hard spheres

Two objectives:

- to ***confirm*** the existence of Couette flows in the bulk domain under strong dissipation
- to ***assess*** the theoretical predictions for the generalized transport coefficients

I. $\gamma > 0$ Viscous heating dominates collisional cooling (BGK-type results)

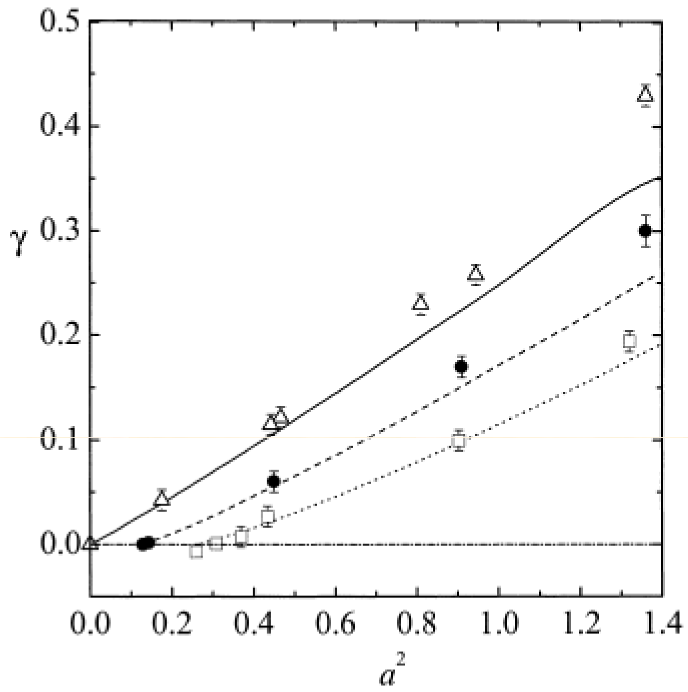
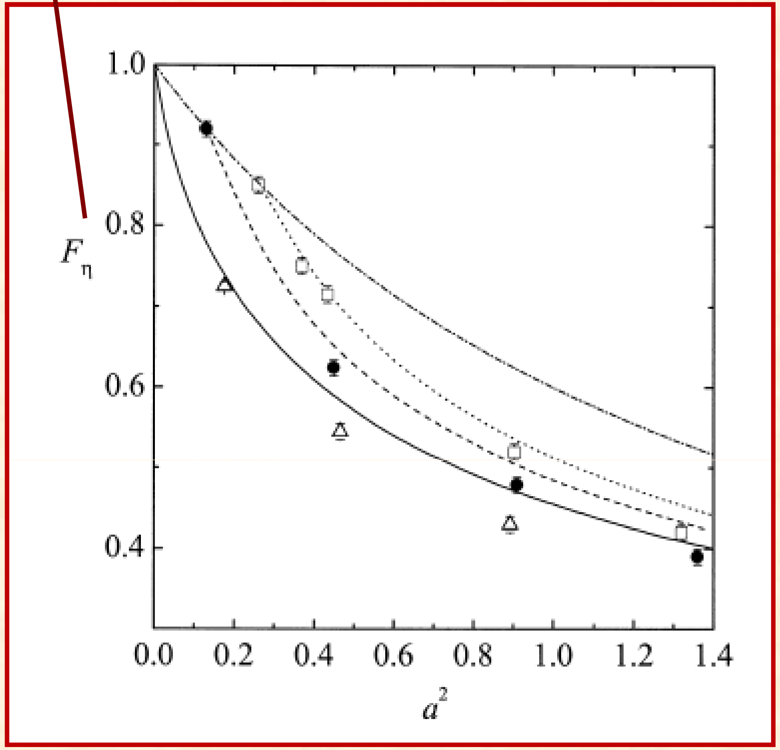
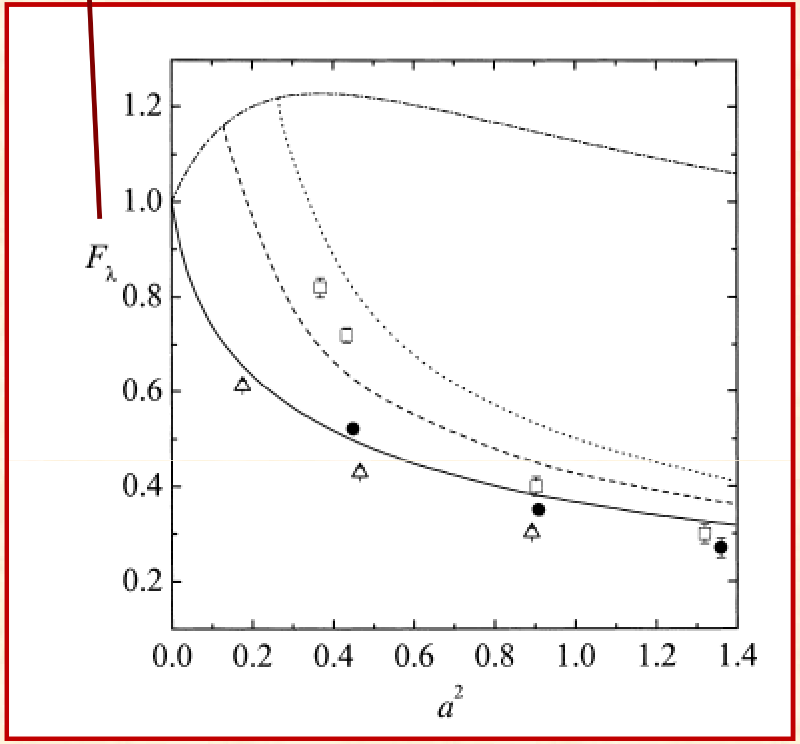


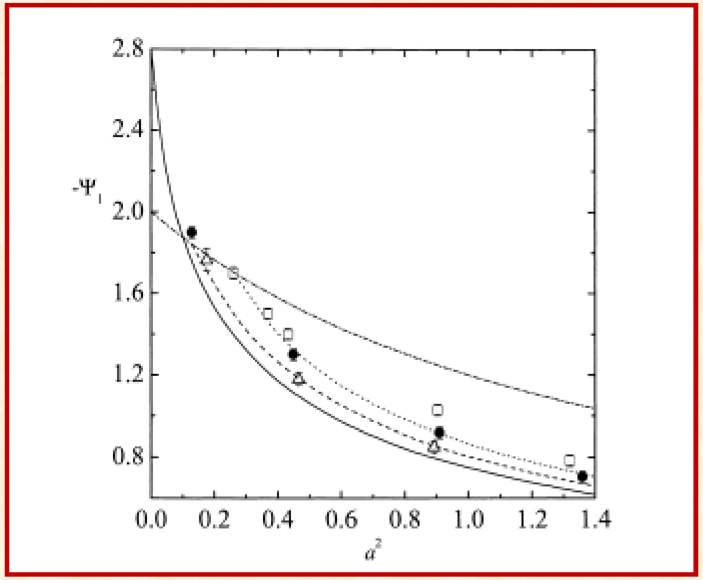
Fig. 3. Plot of the thermal curvature parameter γ as a function of a^2, as obtained from the kinetic model (lines) and from simulation (symbols), for $\alpha = 1$ (solid line and triangles), 0.9 (dashed line and circles), and 0.8 (dotted line and squares).

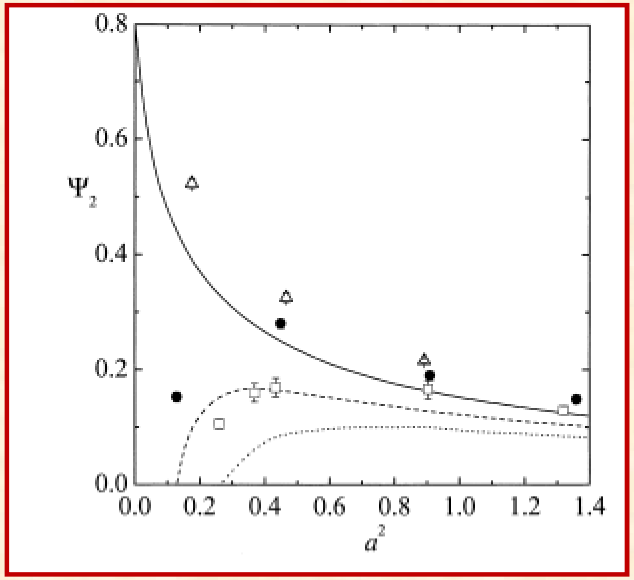
Tij, Tahiri, Montanero, VG, Santos, Dufty JSP **103**, 1035 (2001)

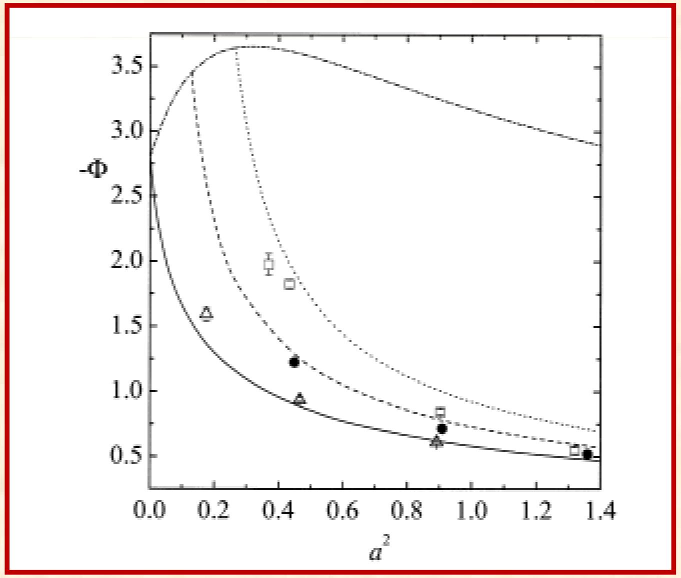
$\eta^*(\alpha, a)$ $\lambda^*(\alpha, a)$











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II. $\gamma < 0$ Collisional cooling dominates viscous heating (Grad's solution)

10 *F. Vega Reyes, V. Garzó and A. Santos*

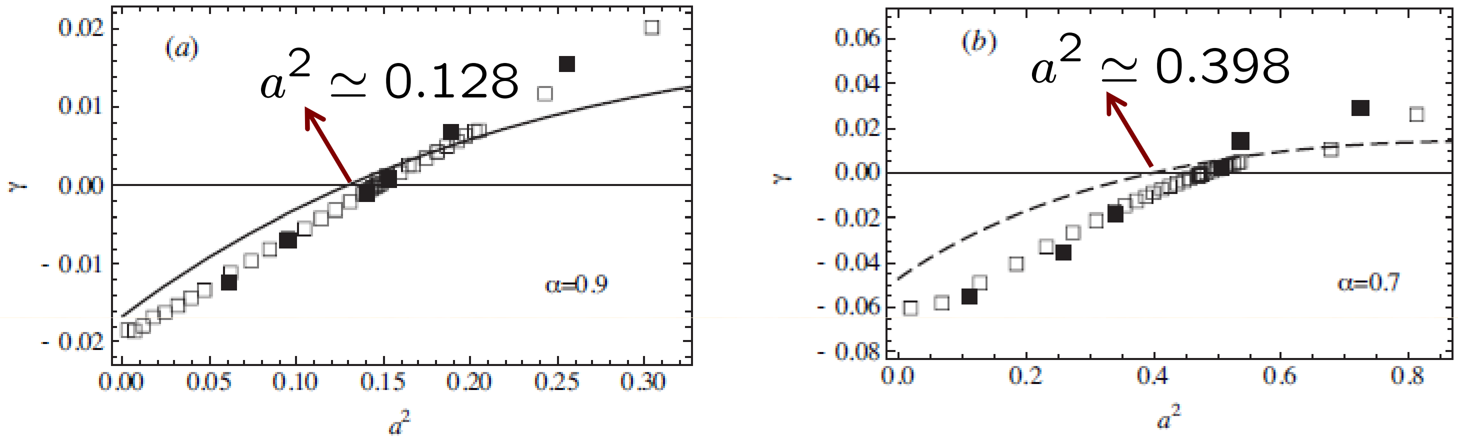


FIGURE 3. The thermal curvature γ as a function of shear rate squared a^2 for two values of the coefficient of restitution: $\alpha = 0.9$ in (a) and $\alpha = 0.7$ in (b). Lines represent results from Grad's method analytical solution while symbols stand for simulations: (□) for DSMC and (■) for MD.

12 F. Vega Reyes, V. Garzó and A. Santos

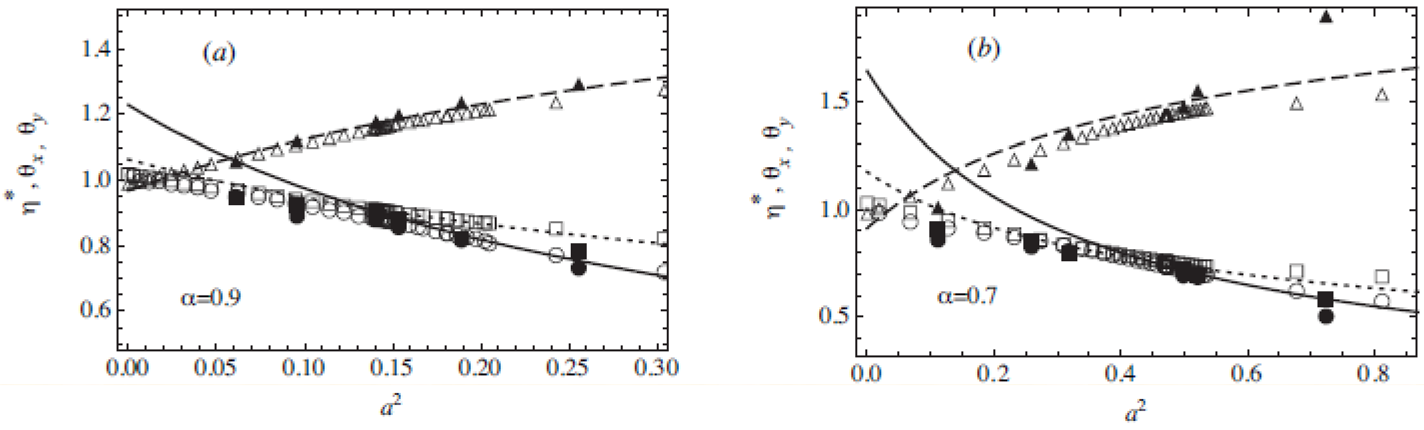


FIGURE 5. Viscosity η^* (solid line, circles) and normal stress components θ_x (dashed line, triangles) and θ_y (dotted line, squares). Lines stand for Grad's method solutions and open symbols for DSMC and solid symbols for MD simulations. (a) $\alpha = 0.9$, (b) $\alpha = 0.7$.

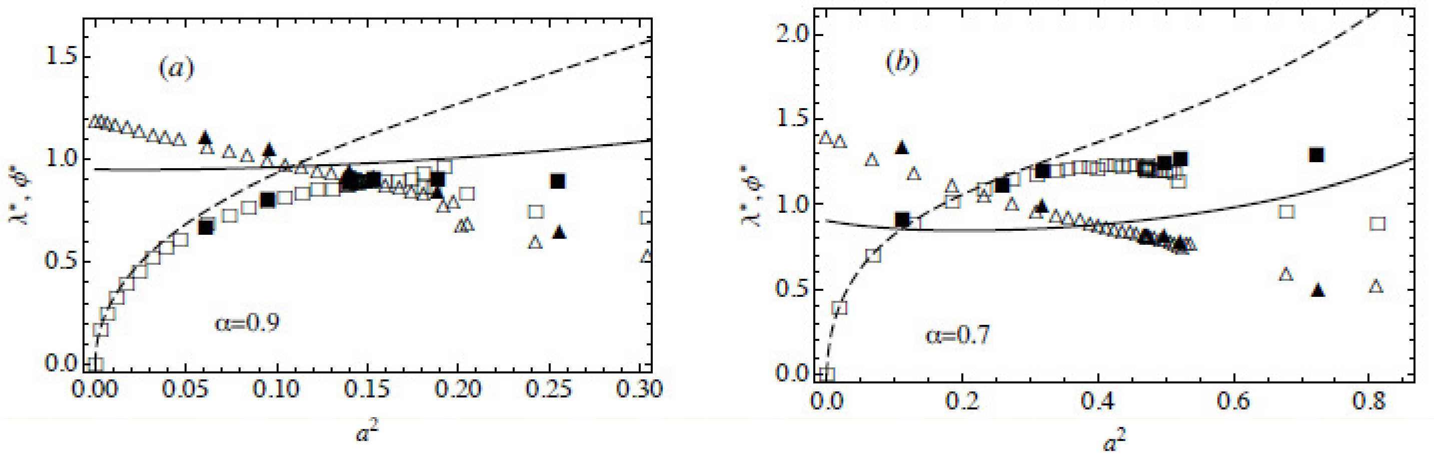


FIGURE 6. Heat flux transport coefficients: thermal conductivity λ^* (solid line, triangles) and cross coefficient ϕ^* (dashed line, squares). Again, lines stand for Grad's method solutions and open symbols for DSMC and solid symbols for MD simulations.

III. LTu flow class $\gamma = 0$

Viscous heating **exactly** balances collisional cooling

Theoretical and simulation results show a *manifold* of steady states such that

$$\nu^{-1}\partial_y U_x = a(\alpha) = \sqrt{d\zeta^*(\alpha)/2\eta^*(\alpha)} = \text{const.}$$

$$(\nu^{-1}\partial_y)T = A = \text{const.}$$

Independent of α, i.e, temperature profiles only depend on the boundary conditions for T

Implications:

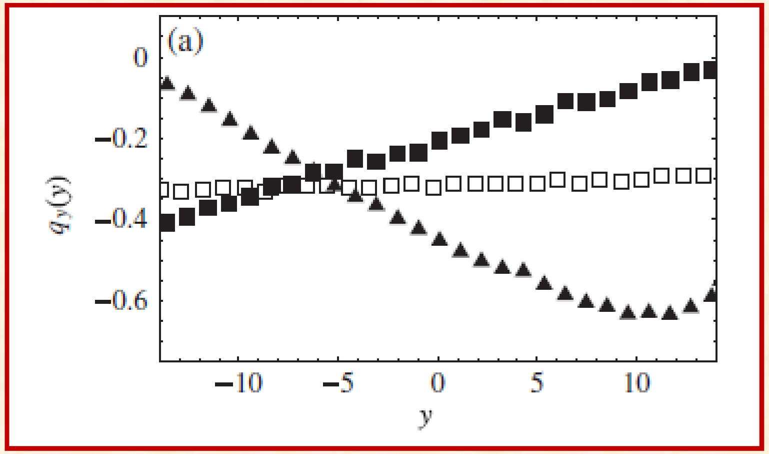
1. Profiles T(Ux) are linear ("LTu" class) $$\frac{\partial T}{\partial U_x} = \frac{A}{a(\alpha)} = \text{const.}$$

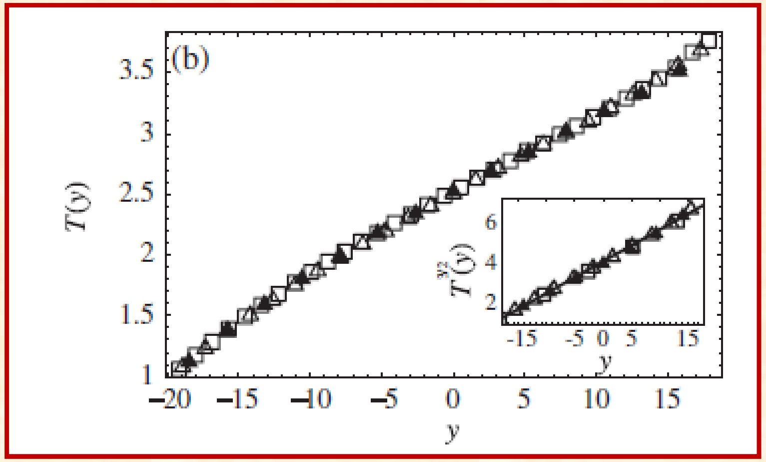
2. Heat flux components are uniform.

Special cases of LTu

- Elastic limit, *a*=0, conventional Fourier flow for ordinary gases $(A \neq 0)$
- USF is recovered for a granular gas in the limit $A \to 0$

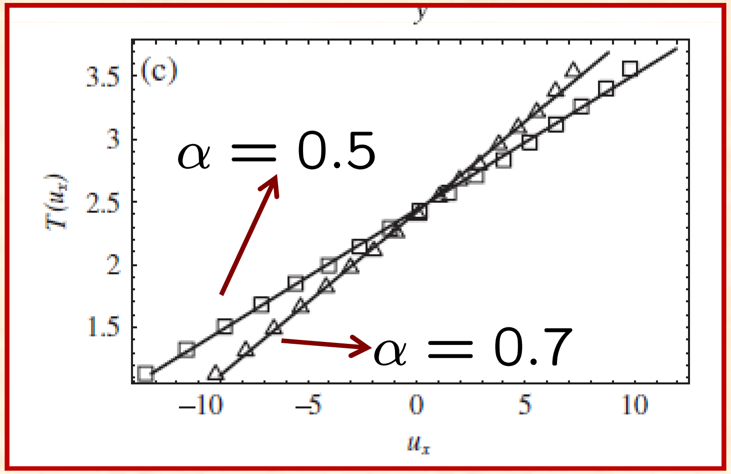
Hydrodynamic profiles from DSMC data





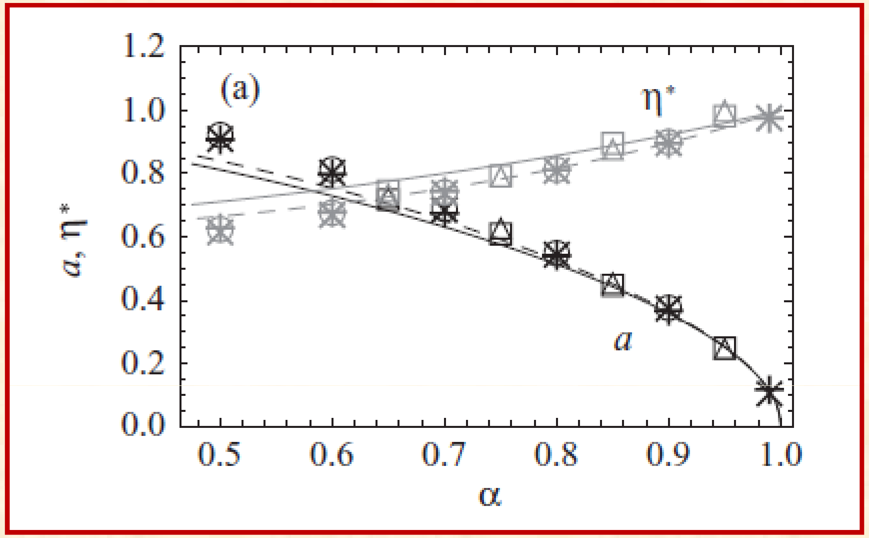
a) $\Delta T = T_+/T_- - 1 = 5, \alpha = 0.7$

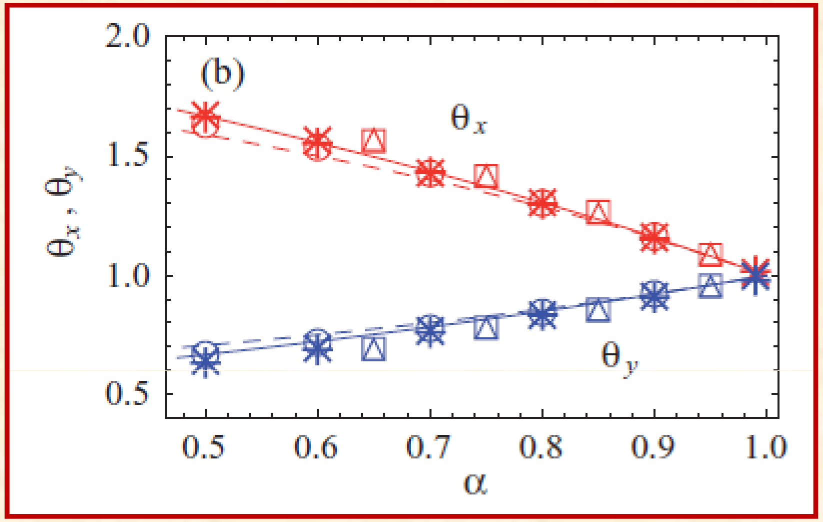
b) $\Delta T = 4, \alpha = 1, 0.7, 0.5$



F. Vega, A. Santos, VG, PRL **104**, 028001 (2010)

Rheological properties

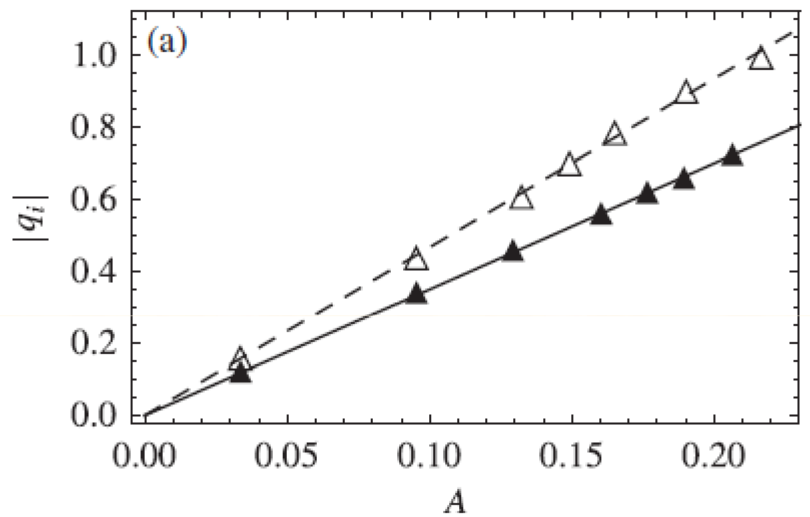


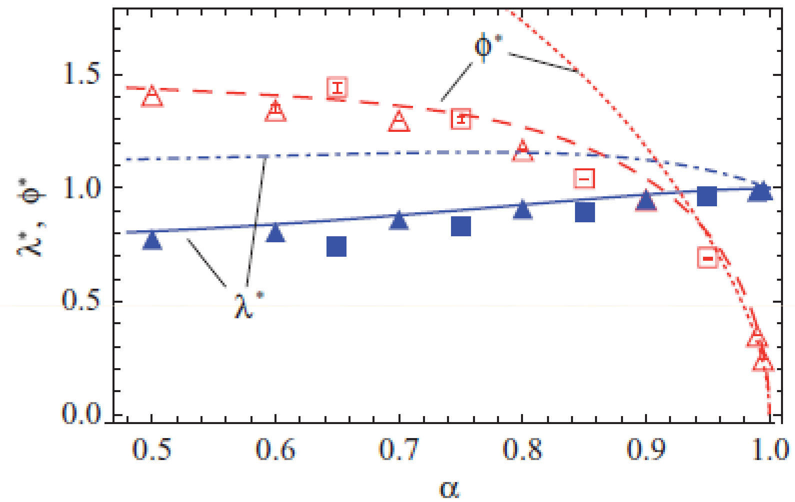


Triangles and squares: MD data, Rest of symbols: DSMC data, for different values of thermal gradient. Solid lines: Grad's theory. dashed lines: BGK model

F. Vega, VG, A. Santos, PRE **83**, 021302 (2011)

<u>Heat flux</u>





DSMC data
Open triangles: qx (α=0.7)
Filled triangles: - qy (α=0.9)

Squares: MD data, triangles: DSMC for different values of *A*. Solid and dashed lines (Grad's theory). Dot-dashed and dotted lines (BGK results)

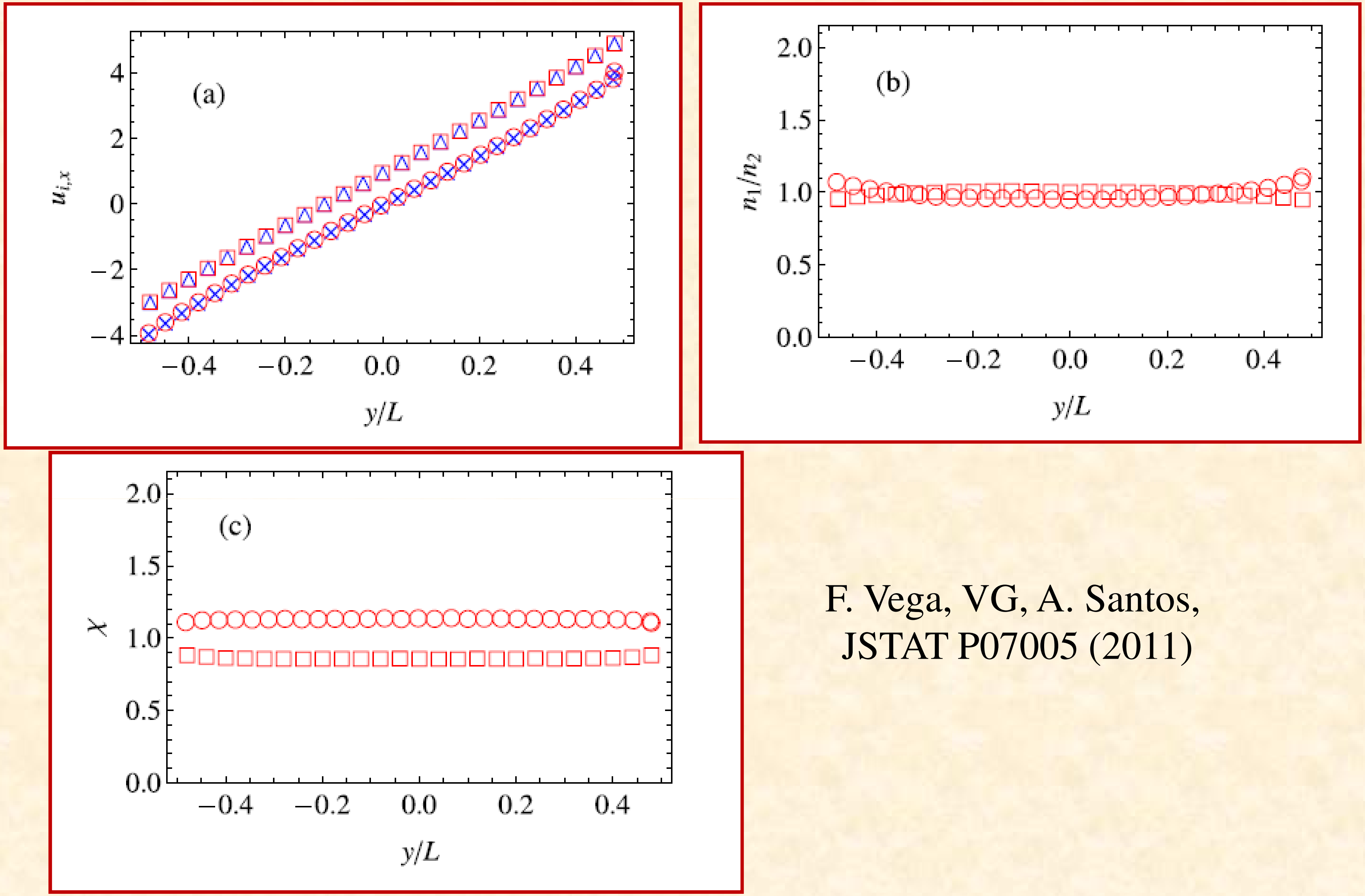
IMPURITY UNDER COUETTE FLOW

Dynamics of an impurity in a dilute granular gas under Couette flow

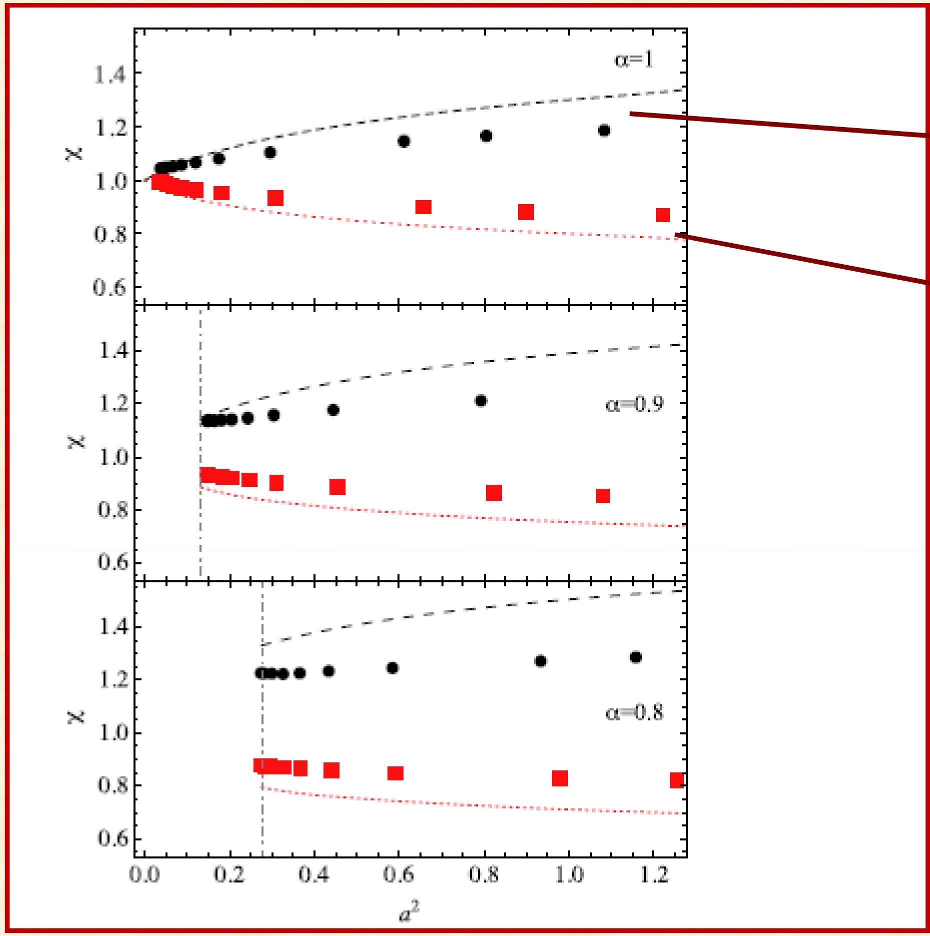
State of impurity is *enslaved* to that of the gas

$$\mathbf{U}_1 = \mathbf{U}_2, \quad x_1 = \frac{n_1}{n_2} = \text{const.}, \quad \chi = \frac{T_1}{T_2} = \text{const.}$$

Analytical results: kinetic model

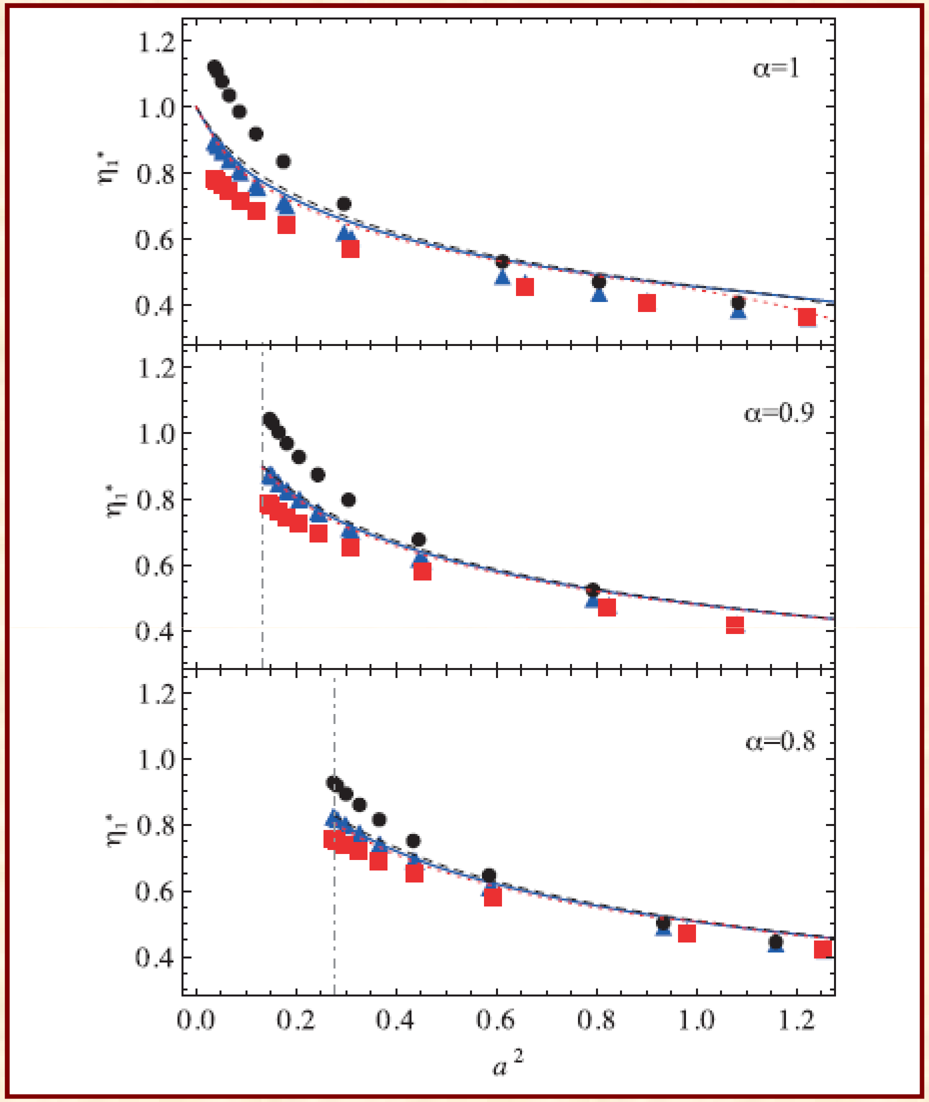


F. Vega, VG, A. Santos,
JSTAT P07005 (2011)



$m_1/m_2 = 2$

$m_1/m_2 = 1/2$



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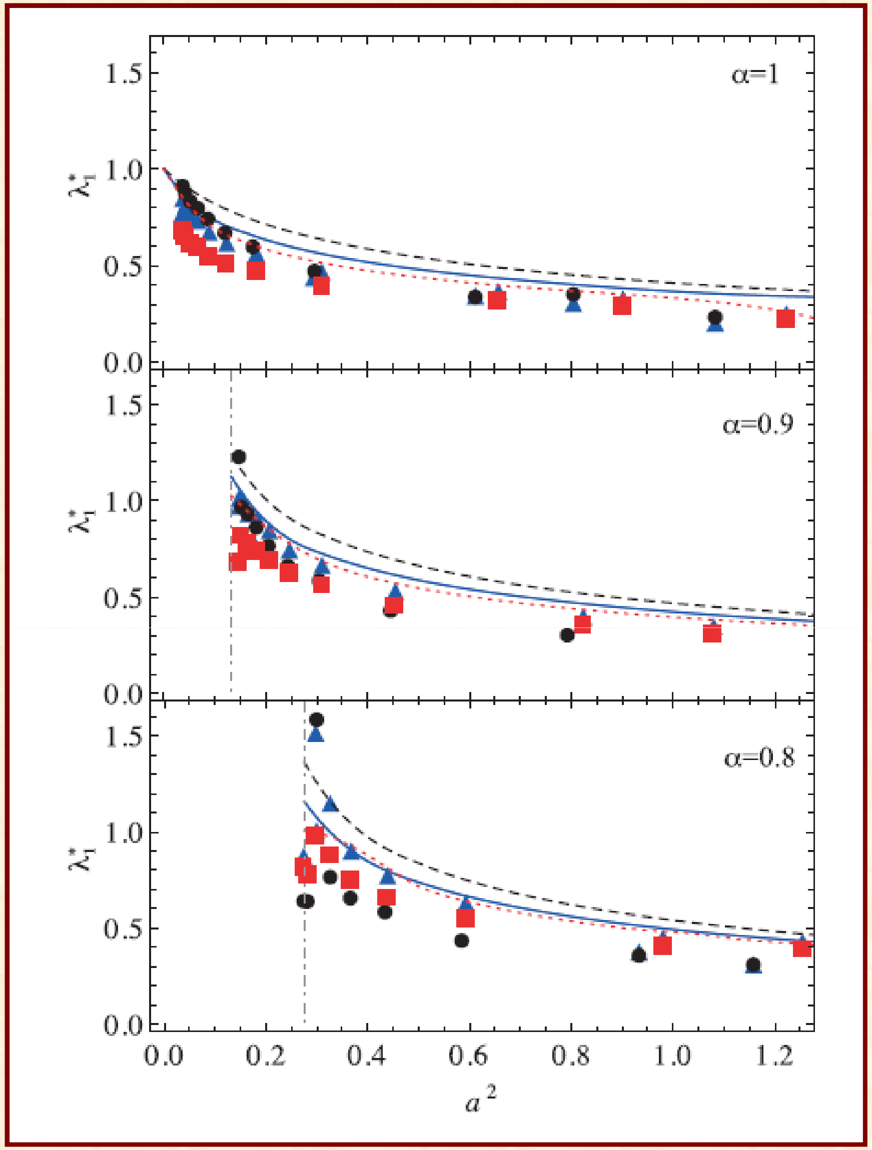
α=1
α=0.9
α=0.8
λ_1^*
a^2

CONCLUDING REMARKS

• Computer simulations have confirmed the existence of steady states in the bulk domain under *strongly* inelastic conditions

• Theoretical predictions from two approaches (Grad's method and BGK-type model) have been assessed for the generalized non-Newtonian transport coefficients

• Very good agreement between kinetic theory (Grad's method) and computer simulations, specially for the Ltu flows

• Existence of hydrodynamics beyond the NS domain for a dilute granular gas

THANKS FOR YOUR ATTENTION !!