Kinetic Theory and Hydrodynamics for Rapid Granular Flow - A Perspective

James W. Dufty

Department of Physics, University of Florida, Gainesville, FL 32611, USA

(August 1, 2001)

Abstract

These are preliminary notes prepared for presentation at the workshop "Challenges in Granular Matter" at the Abdus Salam Institute for Theoretical Physics, Trieste, August 2001. Revisions and figures will be added at a later date.

Many features of real granular fluids under rapid flow are replicated by a system of smooth hard spheres with inelastic collisions. For such a system, it is tempting to apply standard methods of kinetic theory and hydrodynamics to calculate properties of interest. The domain of validity for such methods is *a priori* uncertain due to the inelasticity, but recent systemmatic studies continue to support the utility of kinetic theory and hydrodynamics as both qualitative and quantitative descriptions for many physical states. The current status of kinetic theory and hydrodynamics is reviewed and interpreted, with the optimistic conclusion that much existing phenomenology can be placed on firm grounds for further understanding of complex states observed in rapid granular flow.

I. INTRODUCTION

Granular media in rapid, dilute flow exhibit a surprising similarity to ordinary fluids and the utility of a hydrodynamic description for such conditions has been recognized for many years [1]. This phenomenology has come under scrutiny in recent years with questions about the domain of its validity and the associated constitutive equations appearing in the hydrodynamic equations [2,3]. Answers to such questions can be found in a more fundamental microscopic description where the tools of nonequilibrium statistical mechanics are available for critical analysis. An intermediate mesoscopic description between statistical mechanics and hydrodynamics is that of kinetic theory, whose applicability to granular matter also poses questions. Attention here is restricted to an idealized microscopic model system that captures only the primary feature of grains: inelastic collisions. The system is composed of smooth, hard spheres whose energy loss on binary collisions is characterized by a restitution coefficient $0 < \alpha \leq 1$. This single parameter distinguishes the ideal granular fluid ($\alpha < 1$) from the ideal normal fluid ($\alpha = 1$). For normal fluids, extensive studies during the past thirty years confirm the validity of a wide range of many-body methods to analyze states near and far from equilibrium. These studies include applicability of kinetic theory (Boltzmann, Enskog, and corrections due to correlated collisions), and on longer space and time scales, a hydrodynamic description. The foundations for kinetic theory and hydrodynamics, including practical calculation of properties such as the equation of state and transport coefficients, is most complete for the elastic hard sphere system.

How much of this body of knowledge can be translated to rapid flow granular media using the same system with the only change being $\alpha < 1$? At the most fundamental level of Newton's equations there is little evident change for the fluidized state; the microstate of the system at time t is completely characterized by the positions and velocities of all spheres. The sequence of free streaming and instantaneous velocity changes on binary collisions determines the evolution uniquely for given initial conditions at $t' < t$. Only the binary collision rule changes, such that the relative velocity $\mathbf{g}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ for particles i and j after the collision is given by

$$\widetilde{\mathbf{g}}_{ij} = \mathbf{g}_{ij} - (1+\alpha)\widehat{\boldsymbol{\sigma}}(\mathbf{g}_{ij} \cdot \widehat{\boldsymbol{\sigma}}). \tag{1.1}$$

where $\widehat{\sigma}$ is a unit vector along the line from particle j to i. This is the usual rule for reflection of relative velocities except that the magnitude of the normal component $|\widetilde{\mathbf{g}}_{ij} \cdot \widehat{\boldsymbol{\sigma}}|$ after the collision has been decreased by a factor α to $\alpha\,|\mathbf{g}_{ij} \cdot \widehat{\boldsymbol{\sigma}}|$. Thus, the standard event driven molecular dynamics (MD) simulation method developed for normal fluids can be applied directly to granular fluids with this small change in the collision rule[1]. Given the microstates and dynamics prescribed in this way, the tools of nonequilibrium statistical mechanics can be applied as well. In particular, the formulation of a kinetic theory and its application to derive the equations of fluid dynamics for granular systems can be addressed. The objective here is to summarize the current status of such investigations and to address some of the early and continuing concerns about the validity of kinetic theory and hydrodynamics for granular media. Relevant literature prior to 1990 has been reviewed by Campbell [4]. More recent reviews addressing the statistical mechanical foundations have been given by Ernst [5] and by van Noije and Ernst [6]. The reader is advised to consult the extensive references in these articles. Here, a personal perspective on the current status of kinetic theory and hydrodynamics for granular gases is provided as a supplemental orientation to this rapidly growing field. The references given are selective and apologies are offered at the outset to the many other important contributions not recognized explicitly.

Contributions to this field come from increasingly diverse areas: chemical engineering, fluid dynamics, statistical mechanics, condensed matter physics, computational physics.

[1]The phenomenon of "inelastic collapse" can stop the MD simulation due to condensation of small arrays of particles with rapid collisions at high density and strong dissipation [2]. This is an artifact of the instantaneous hard sphere collision that appears to have no macroscopic consequences, and which can be avoided in several different ways. It will not be considered further in the discussion here.

Each has its priority for problems to be solved, in some cases focused more on urgent practical concerns while in others addressing more abstract "points of principle". The material selected for discussion here reflects the author's personal view that a fundamental (microscopic) basis for rapid flow granular media can be found within the general framework of nonequilibrium statistical mechanics, and that its explication will impact practical applications under realistic conditions. This perspective approaches granular media via idealized models for which controlled molecular dynamics simulation, many-body theory, and real experiments reasonably can be performed to answer specific questions with clear consequences.

II. KINETIC THEORY AT LOW DENSITY

It is taken for granted in all of the following that a microscopic formulation of non-equilibrium statistical mechanics for inelastic, smooth hard spheres is justified [6–8]. Concerns at this level are the same as those for open systems (inherently non-equilibrium states) with elastic collisions - e.g. the required "mixing" property for the dynamics in phase space to justify the relevance of average values and fluctuations about them. Once it is recognized that granular states are always "non-equilibrium" the distinction between systems with elastic and inelastic collisions diminishes considerably, as emphasized below. A first order question is whether the reduction of non-equilibrium statistical mechanics to a more practical kinetic theory description can be justified. This is a difficult problem even for the case of elastic collisions which, as noted above, has been addressed extensively and successfully for the hard sphere system over the past thirty years. It is not the purpose here to summarize the status of that research but rather to explore any *additional* questions and concerns for its application to granular gases arising from the inelasticity of the collisions. The general conclusion below is that while there are significant differences in many derived properties of interest, there are few new qualitative limitations on the equations describing these properties based on analytic and simulation studies to date. Some of the confusion and disagreement in the literature is due to differing perceptions of the necessary conditions for a kinetic theory (e.g., Boltzmann or Enskog kinetic equations), and the necessary conditions for a hydrodynamic description (e.g., Navier-Stokes or non-linear rheological equations). In principle and in practice, the validity of kinetic theory and the validity of hydrodynamics are independent questions. However, for gases (no compact structures) it is expected that existence of a kinetic theory should provide the basis for investigating hydrodynamics as well.

To set the stage for the discussion here, a brief formal "derivation" of the kinetic description for both the distribution function and fluctuations at low density is given as an illustrative example. A small parameter expansion of the reduced distribution function leads to a formal solution to the BBGKY hierarchy [9,10]. The analysis is similar to an expansion proposed by Grad for the hard sphere gas with elastic collisions [11]. In this approach, there is no reference to concepts such as "approach to equilibrium", Maxwellian distribution, or "molecular chaos", and the distinction between inelastic or elastic collisions plays no explicit role. Thus, superficially at least, it appears the basis for the low density kinetic theory is the same in both cases. Closely related results follow from a cluster expansion of the reduced distribution functions, again with no formal reference to whether the collisions are elastic or inelastic [5,6,12].

The s-particle reduced distribution functions, $f^{(s)}(x_1,\cdots,x_s,t)$, obey the BBGKY hierarchy where $x_i=(\mathbf{q}_i,\mathbf{v}_i)$. A dimensionless form of this hierarchy is obtained by scaling the space and time with the mean free path $\ell\equiv 1/(n\sigma^2)$ and the mean free time $t_0\equiv \ell/v_0$. Here, n is the density, σ is the hard sphere diameter, and v_0 is some characteristic velocity. Similarly, the reduced distribution functions are scaled with $(n/v_0^3)^s$. The resulting dimensionless BBGKY hierarchy has the form

$$\begin{aligned}&\left(\partial_t+\sum_{i=1}^{s} v_i\cdot\nabla_i-\lambda^2\sum_{i<j}^{s}\overline{T}(i,j)\right)f^{(s)}(x_1,\cdots,x_s,t)\\&=\sum_{i=1}^{s}\int dx_{s+1}\,\overline{T}(i,s+1)f^{(s+1)}(x_1,\cdots,x_{s+1},t).\end{aligned}\tag{2.1}$$

The binary scattering operator $\overline{T}(i,j)$ for a pair of particles $\{i,j\}$ is defined by

$$\overline{T}(i,j)=\int d\hat{\sigma}\ \Theta(\mathbf{g}_{ij}\cdot\widehat{\sigma})(\mathbf{g}_{ij}\cdot\widehat{\sigma})[\alpha^{-2}\delta(\mathbf{q}_{ij}-\lambda\widehat{\sigma})b_{ij}^{-1}-\delta(\mathbf{q}_{ij}+\lambda\widehat{\sigma})], \tag{2.2}$$

where $\hat{\sigma}$ is a unit vector along $\mathbf{q}_{ij}=\mathbf{q}_i-\mathbf{q}_j$ and $d\hat{\sigma}$ denotes a two dimensional solid angle integration over the sphere for particles at contact. Also, $\mathbf{g}_{ij}\equiv\mathbf{v}_i-\mathbf{v}_j$ is the relative velocity, and b_{ij}^{-1} is the scattering operator defined for any function $X(\mathbf{v}_i,\mathbf{v}_j)$ by

$$b_{ij}^{-1}X(\mathbf{v}_i,\mathbf{v}_j)\equiv X(\mathbf{v}_i',\mathbf{v}_j'). \tag{2.3}$$

The "restituting" velocities (i.e., the inverse of those in (1.1)) are

$$\mathbf{v}_i'\equiv\mathbf{v}_i-\frac{1+\alpha}{2\alpha}(\mathbf{g}_{ij}\cdot\hat{\sigma})\hat{\sigma},\qquad \mathbf{v}_j'\equiv\mathbf{v}_j+\frac{1+\alpha}{2\alpha}(\mathbf{g}_{ij}\cdot\hat{\sigma})\hat{\sigma}. \tag{2.4}$$

The α dependence of $\overline{T}(i,j)$ contains all aspects of the inelasticity, and plays no explicit role in the following expansion.

In this dimensionless form the BBGKY hierarchy depends on the single dimensionless parameter $\lambda\equiv\sigma/\ell=n\sigma^3$, the ratio of the "force range" to the mean free path. This parameter is small at low density, suggesting an expansion for a solution to the entire hierarchy as a power series in λ. The dependence on λ occurs explicitly as shown on the left side of (2.1) and implicitly through the finite separation of the colliding particles in $\overline{T}(i,j)$. The structural features of the expansion in λ are simplest if it is performed at fixed $\overline{T}(i,j)$. The s-particle reduced distribution functions are taken to have the representation

$$f^{(s)}(x_1,\cdots,x_s,t)=f_0^{(s)}(x_1,\cdots,x_s,t)+\lambda^2f_1^{(s)}(x_1,\cdots,x_s,t)+... \tag{2.5}$$

It is then readily shown that the hierarchy is solved exactly to order λ^2 in the form

$$f_0^{(s)}(x_1,\cdots,x_s,t)=\prod_{i=1}^{s}f_0^{(1)}(x_i,t), \tag{2.6}$$

$$f_1^{(s)}(x_1,\cdots,x_s,t)=\sum_{j=1}^{s}\prod_{i\neq j}^{s}f_0^{(1)}(x_i,t)f_1^{(1)}(x_j,t)+\sum_{i<j}^{s}\prod_{k\neq i,j}^{s}f_0^{(1)}(x_k,t)G(x_i,x_j,t), \tag{2.7}$$

where the expression for $f_1^{(s)}$ holds for $s\geq 2$. Thus, the reduced distribution functions for any number of particles is determined as a sum of products of the single particle functions

$f_0^{(1)}(x_1,t)$ and $f_1^{(1)}(x_1,t)$, and the pair function $G(x_1,x_2,t)$. These are determined from the set of three kinetic equations

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\nabla_1\right) f_0^{(1)}(x_1,t)=J(x_1,t\mid f_0^{(1)}). \tag{2.8}$$

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\nabla_1-I_1+\mathbf{v}_2\cdot\nabla_2-I_2\right) G(x_1,x_2,t)=\overline{T}(1,2)f_0^{(1)}(x_1,t)f_0^{(1)}(x_2,t) \tag{2.9}$$

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\nabla_1-I_1\right) f_1^{(1)}(x_1,t)=\int dy_2\,\overline{T}(1,2)G(x_1,x_2,t), \tag{2.10}$$

Here $J(x_1,t\mid f_0^{(1)})$ is the Boltzmann-Bogoliubov collision operator and I_1, defined over functions of x_1, is its linearized form

$$J(x_1,t\mid f_0^{(1)})=\int dx_2\,\overline{T}(1,2)f_0^{(1)}(x_1,t)f_0^{(1)}(x_2,t) \tag{2.11}$$

$$I_1h(x_1)\equiv\int dx_2\,\overline{T}(1,2)\left(f_0^{(1)}(x_1,t)h(x_2)+h(x_1)f_0^{(1)}(x_2,t)\right). \tag{2.12}$$

These low density results (2.8)-(2.10) are remarkably rich. The leading order distribution function $f_0^{(1)}$ is the solution to the Boltzmann equation. The two particle correlations are generated from the uncorrelated product of Boltzmann solutions through inelastic binary collisions $\overline{T}(1,2)f_0^{(1)}(x_1,t)f_0^{(1)}(x_2,t)$ on the right side of (2.9). Finally, corrections to the Boltzmann solution due to correlations are given by a coupling of the distribution function to the correlations in (2.10) (the so-called "ring" recollision effects). In the following sections, it is noted that the solutions and implications of these kinetic equations can be quite different for elastic and inelastic collisions. But these differences come from the equations themselves and should not be interpreted as signatures of their failure to apply. For example, at $\alpha=1$ a possible solution for an isolated system is $f_0^{(1)}(x_1,t)\to f_M(v_1)$, $G(x_1,x_2,t)=0=f_1^{(1)}(x_1,t)$, where f_M is the Maxwell-Boltzmann distribution. Equation (2.10) supports f_M because energy is conserved, and $G(x_1,x_2,t)=0$ because $T(1,2)f_M(\mathbf{v}_1)f_M(\mathbf{v}_2)=0$ for the same reason. Since energy conservation no longer holds with $\alpha<1$ it is not surprising that the isolated system does not approach equilibrium, the Maxwellian is not a stationary solution, and that finite correlations exist. Indeed, the extent to which such predicted differences agree with observations from molecular dynamics provide *support* for the kinetic theory, not *limitations* on it as is sometimes implied.

Clearly, the above derivation has not restricted this kinetic description to isolated systems. In fact, the most interesting cases of practical interest are response to boundary conditions and/or external fields. The similarities between normal and granular fluids is closest for such "nonequilibrium" conditions. Too often, properties of granular gases are contrasted only to those of the equilibrium state for normal gases. It is important to note that practical access to the solutions to the above kinetic equations is possible for a wide range of conditions by direct simulation Monte Carlo (DSMC) [13]. Analytic results for complex states have been obtained using accurate kinetic models for the above equations [14], as discussed in Section 7. The benchmark for validity of these kinetic equations is molecular dynamics (MD) simulation of the idealized granular fluid microdynamics. Frequently, these simulations are performed at higher densities than can be supported by the low density approximation. However, there is a corresponding Enskog approximation that extends the above low density kinetic theory to moderate densities as well [7,15]. It is appropriate to emphasize also that the terminology "kinetic theory" is not limited to Boltzmann and Enskog equations. Indeed, at high densities and long times it is known that there are important (even dominant) corrections due to correlated many-body collisions of the type described by (2.10) at low density. Thus, observed deviations from Boltzmann-Enskog for $\alpha < 1$ do not necessarily imply a failure of a kinetic theory description in general.

III. HOMOGENEOUS COOLING STATE

An isolated homogenous fluid with elastic collisions rapidly approaches the stationary equilibrium Gibbs state after a few collisions. The single particle distribution function is Maxwellian and there are no correlations on length scales large compared to the hard sphere diameter. In contrast, for inelastic collisions no stationary state is possible for the isolated system. Instead, it is straightforward to show that the temperature (defined in the usual way from the average kinetic energy) is monotonically decreasing due to the inelastic collisions. Still, on the same time scale as the approach to equilibrium for elastic collisions, the granular fluid approaches a special "homogeneous cooling state" (HCS) for which all time dependence of the distributions occurs only through this cooling temperature. This implies a scaling form for the single particle distribution

$$f_0^{(1)}(\mathbf{v},t) = v_0^{-3}(t) n \phi\left(v/v_0(t)\right), \quad v_0^2(t) = 2T(t)/m. \tag{3.1}$$

The pair correlations have a similar scaling form. The existence of a scaling solution and corresponding time dependence of $T(t)$, its approach from general homogeneous states, the form of $\phi\left(v\right)$, and the space dependence of correlations in this state provide specific tests for the kinetic theory. The scaling property implies an exact time dependence $T(t) = T(0)(1+ct)^{-2}$ (Haff's law) which has been confirmed by MD [16] and by DSMC solution to the Boltzmann and Enskog equations [17]. In both the MD and DSMC the approach to a scaling solution is observed to occur rapidly after a few collisions, similar to the approach to equilibrium for normal fluids. The velocity dependence of $\phi\left(v\right)$ has been calculated approximately from the the Boltzmann and Enskog equations by an expansion about the Gaussian ($\alpha = 1$ form) in polynomials [18,19]. Deviations from the Gaussian have been measured by MD and DSMC and compared with a low order truncation of the expansion. The agreement is excellent for all $0.3 < \alpha \leq 1$. Finally, the form of this scaling distribution has been analyzed from the Boltzmann equation for large velocities and predicted to have an exponential rather than Gaussian form [19]. This also has been confirmed in detail by DSMC [20] and the effect has been observed by MD simulation as well [16].

Recently, the scaling solutions to the Boltzmann equations for a mixture have been studied [21]. A new effect is the occurrence of different temperatures for each species, although each with the same cooling rate given by Haff's law. This difference is a reflection of the failure of energy equipartition in the HCS, an exact property of the Gibbs state. The polynomial solutions for the mixture distribution functions can be constructed in the same way as for the one component fluid. The rapid approach to this HCS, the dependence of the different temperatures on species parameters (size, concentration, mass), and the velocity dependence of the scaling solutions have been confirmed in detail by DSMC [22], for $\alpha \geq 0.5$. To date there have been no MD simulations for comparison.

Correlations in the HCS are described by Eq.(2.9) for $G(x_i, x_j, t) = f^{(2)}(x_1, x_2, t) - f^{(1)}(x_1, t) f^{(1)}(x_2, t)$. The origin of these correlations is the source term in this equation $\overline{T}(1,2)\phi\left(v_1/v_0(t)\right)\phi\left(v_2/v_0(t)\right) \neq 0$. This vanishes for elastic collisions because in that case ϕ becomes the Maxwellian, and $\overline{T}(12)$ regains the detailed balance property. For $\alpha < 1$ this finite source gives non-zero *short ranged* spatial correlations $\sim \delta(q_{ij} - \sigma)$. The generators for the two particle dynamics on the left side of (2.9) include in their spectrum the inelastic fluid hydrodynamic modes (discussed below). These modes give rise to *long ranged* spatial correlations in $G(x_i, x_j, t)$, including algebraic decay at large distances for velocity moments corresponding to density, energy, and momentum correlations. A detailed study of the predictions for these correlations based on (2.9) has been given by Brey et al. [10]. These calculations require analysis of the spectrum for $\mathbf{v}_1 \cdot \nabla_1 - I_1$ at long wavelengths, and confirm the existence of hydrodynamic modes as spontaneous fluctuations in the granular gas. These modes agree with those obtained for the decay of imposed spatial gradients described in the Section 6, and this spectral analysis can be viewed as an independent confirmation of hydrodynamics (in effect, this is Onsager's regression hypothesis extended to granular fluids). The dispersion relations for these modes as a function of α and wavevector is more complex than for normal fluids and the spatial dependence cannot be obtained from simple scaling without specification of a domain for α. The calculated space dependence of the correlation functions is in excellent agreement with DSMC simulation of the kinetic equation (2.9).

Correlations on such macroscopic scales in normal fluids also can be described by the usual hydrodynamic equations extended to include thermal fluctuations characterized by white, Gaussian noise. Averaging products of solutions to these stochastic equations over the noise provides the correlation functions. van Noije et al. [23] have extended this approach to granular fluids as well. The agreement with the kinetic theory and DSMC results above is good, except for large inelasticity where the use of elastic fluid transport coefficients in [23] is not justified. Furthermore, these results are in good agreement with MD simulations. In summary, the consistency of kinetic theory and hydrodynamics to predict a new effect for granular gases - long range correlations in an isolated homogeneous system - appears to be established.

Spatial correlations on short length scales have been described in detail by Lutsko [24,25]. The analysis is based on an exact boundary condition for hard spheres at contact, $\mathbf{q}_{12} = \sigma$ [26]

$$\begin{aligned}\Theta\left(\mathbf{q}_{12}\cdot\mathbf{g}_{12}\right) f^{(2)}(x_1, x_2, t) &= \Theta\left(\mathbf{q}_{12}\cdot\mathbf{g}_{12}\right)\alpha^{-2}b^{-1}f^{(2)}(x_1, x_2, t)\\ &= \alpha^{-2}b^{-1}\Theta\left(-\mathbf{q}_{12}\cdot\mathbf{g}_{12}\right) f^{(2)}(x_1, x_2, t)\end{aligned} \tag{3.2}$$

The left side describes the distribution of particles on the post-collision hemisphere. The right side is the distribution of particles on the pre-collision hemisphere as a function of their restituting velocities, and the equality represents their relationship by a two particle collision. Lutsko observes that the class of generalized mean spherical approximations (GMSA) for the equilibrium radial distribution $g\left(\mathbf{q}_1 - \mathbf{q}_2, \alpha = 1\right)$ function requires primarily the value of this function at contact and the equation of state. Consequently the GMSA can be extended to the HCS for $g\left(\mathbf{q}_1 - \mathbf{q}_2, \alpha \leq 1\right)$ with appropriate changes in these quantities. The value at contact is obtained by using the approximation

$$\Theta\left(-\mathbf{q}_{12}\cdot\mathbf{g}_{12}\right) f^{(2)}(x_1, x_2, t) \rightarrow \Theta\left(-\mathbf{q}_{12}\cdot\mathbf{g}_{12}\right) g\left(\mathbf{q}_1 - \mathbf{q}_2, 1\right) f^{(1)}(x_1, t) f^{(2)}(x_2, t) \tag{3.3}$$

on the pre-collision hemisphere, i.e. neglect of velocity correlations on this hemisphere. The boundary condition (3.2) then gives the remaining half of the distribution on the post-collision hemisphere *with velocity correlations* determined from the binary collision. The equation of state is determined from the Enskog kinetic equation which can be obtained in this context as follows [26]. The exact first equation of the BBGKY hierarchy (Eq.(2.1) with $s = 1$), is written in the equivalent form

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1\right) f_0^{(1)}(x_1, t) = \sigma^2 \int d\overrightarrow{x}_2 \int d\widehat{\sigma}\, \delta\left(\mathbf{q}_{12} - \sigma\widehat{\sigma}\right)\left(\widehat{\sigma}\cdot\mathbf{g}_{12}\right)\left[\alpha^{-2}\widehat{b}_{ij}^{-1} + 1\right]$$

$$\times\Theta\left(-\widehat{\sigma}\cdot\mathbf{g}_{12}\right)f_2(x_1,x_2,t). \tag{3.4}$$

This shows that any approximation for $f_2(x_1,x_2,t)$ need only be imposed for the pair of particles at contact and on the pre-collision hemisphere. In particular, the use of (3.3) in (3.4) leads to the Enskog kinetic equation. This route to the Enskog (and hence Boltzmann equation at low density) provides a precise meaning to the phenomenological terminology "molecular chaos assumption ": neglect of two particle velocity correlations for a pair of particles at contact on the pre-collision hemisphere. The pressure in the HCS follows from the Enskog equation by evaluating the trace of the average momentum flux. In this way, the radial distribution function at contact and pressure are found to be $g\left(q_{12}=\sigma,\alpha\right)=\frac{1+\alpha}{2}g\left(q_{12}=\sigma,\alpha=1\right)$ and $p\left(\alpha\right)=nk_BT\left[1+\frac{\pi n\sigma^3}{6}g\left(q_{12}=\sigma,\alpha\right)\right]$, respectively. Using $g\left(q_{12}=\sigma,\alpha\right)$ and $p\left(\alpha=1\right)$ in the GMSA Lutsko obtains a model for $g\left(q_{12},\alpha\right)$ as a function of q_{12}, α, and the density. The agreement with MD simulation is very good even at extreme conditions of high density, $n\sigma^3=0.5$ and strong dissipation $\alpha=0.5$, for the domain tested $\sigma\leq q_{12}\leq 3\sigma$. This is an indirect confirmation of the molecular chaos assumption (3.3), supporting as well the basis for the Enskog kinetic equation. In detail, however, there are deviations for $\alpha<0.7$ that have a system size dependence being larger for the larger system (in particular, the molecular chaos value at contact appears to fail). The explanation for this is a long wavelength hydrodynamic shear mode becoming unstable at about $\alpha=0.7$, as discussed in the next section. When this is compensated for in the simulation the system size dependence no longer occurs, but significant deviations from the "molecular chaos" approximation remain at high density for $\alpha<0.6$. A similar limitation on the "molecular chaos" assumption was observed in a two dimensional MD simulation [27] where the distribution of impact parameters on the pre-collision hemisphere was found to become non-uniform (particularly for large impact parameters) at values of the restitution coefficient for which significant shear fluctuation is observed.

The validity of (3.3) has been tested by MD simulation more directly [29], although for the limited domain $0.98\leq\alpha\leq 1$, $0.05\leq n\sigma^3\leq 0.2$. These authors study a generalization of the pair correlation function obtained by integrating $f^{(2)}$ over the center of mass velocity and the magnitude of the relative velocity. This defines a pair correlation function $g\left(q_{12}=\sigma,\theta,\alpha\right)$ depending on the angle between the relative velocity and the relative coordinate. The MD results for $g\left(q_{12}=\sigma,\theta,\alpha\right)$ as a function θ for $n\sigma^3 = 0.1$ and $\alpha = 0.98$ show good agreement with the molecular chaos approximation except near $\theta = \pi/2$ (large impact parameters). To resolve small differences the pressure is measured directly from the virial and an order parameter for pre-collision velocity correlations is measured. The pressure shows a systematic deviation from the Enskog pressure of less than one percent for the density range considered. The order parameter for velocity correlations has a significant system size dependence and an extrapolation of MD results to large systems is required. Signatures of finite pre-collision velocity correlations are found in this way, indicating deviations from (3.3). In spite of the good agreement found for $g\left(q_{12}=\sigma,\theta,\alpha\right)$, the authors emphasize limitations of the Enskog kinetic theory based on the pressure and order parameter measurements. To put this in context, it should be recognized that the same small corrections to the Enskog equation can occur at these densities also with elastic collisions, *except* for the equilibrium state. Indeed, they can be calculated from Eq. (2.9) for $\alpha = 1$. Once it is recognized that the HCS is a nonequilibrium state the role of the Enskog kinetic theory as a good approximation at low and moderate densities is seen to be supported for both elastic and inelastic collisions. However, it appears from the discussion of the last paragraph that the range of densities for which this is true decreases with increased dissipation.

The strongest objections to the above description for properties of the HCS and the validity of the Boltzmann equation for granular gases have been offered in reference [30]. However, both the DSMC simulation and theoretical analysis presented there have subsequently been criticized as invalid [31,32].

Related studies of homogeneous *steady* states (HSS) also have been studied as tests of kinetic theory [33–36]. Such steady states are produced by insertion of a random external force to accelerate the particles and hence compensate for collisional cooling. This has the advantage of avoiding the intrinsic time dependence of the HCS, but at the price of introducing unknown new effects induced by the external force. It should be noted that the time dependent HCS can be mapped formally onto a stationary state for time independent study as well, by a suitable change of variables for the velocities and time [25]. There are considerably more MD results for the HSS, with similar conclusions regarding the deviations of the velocity distribution from Maxwellian, excess population at large velocities, and velocity correlations that are generally consistent with kinetic theory as described above for the HCS. Fluctuating Navier-Stokes order hydrodynamics, including noise from the external random force predicts well both spatial correlations and fluctuation-renormalization of mean values [40,33].

This section has focused on the velocity distribution and correlations for the simplest state of a granular gas, isolated and uniform. Significant differences are observed from the corresponding equilibrium state for the same gas with elastic collisions. In some of the literature quoted the existence of such differences from the equilibrium state interpreted as a failure of conditions for kinetic theory for granular gases. As the discussion above shows, it is quite the other way around - these differences are quite well predicted from the kinetic theory. Deviations from Enskog kinetic theory at higher densities are expected due to correlated collisions, just as for fluids with elastic collisions [37]. There is some indication that the effects of correlated collisions are enhanced at strong dissipation, and hence appear at lower densities, due to unstable fluctuations in the transverse flow field as discussed in the next section. It would be interesting to translate this qualitative statement into a more quantitative one by careful comparison of such effects for normal fluids in a nonequilibrium state with those of the HCS, since they are certainly present in both cases.

IV. INSTABILITIES AND CLUSTERING

It was first observed in MD simulations that the HCS is unstable to sufficiently long wavelength perturbations [38]. For systems large enough to support such spontaneous fluctuations the HCS becomes inhomogeneous at long times. In MD simulations the inhomogeneities may grow by the formation of clusters, ultimately aggregating to a single large cluster [39]; if cluster growth is suppressed a vortex field may grow to the system size where periodic boundary conditions can induce a transition to a state of macroscopic shear. The mechanism responsible for the growth of inhomogeneities can be understood at the level of Navier-Stokes hydrodynamics where linear stability analysis shows two shear modes and a "heat" mode to be unstable. Qualitatively [38], spontaneous vortex fluctuations of sufficient size grow due to this instability and provide excess local temperature and pressure; a particle flux is then established from high to low shear domains increasing the density and cooling rate; this further enhances the pressure difference to continue the particle flow. A more quantitative description poses a challenging test for both kinetic theory and hydrodynamics.

Perhaps the simplest signature of inhomogeneities is a deviation of the global temperature from the form given by Haff's law. In the presence of local flow fields the average kinetic energy for the system decays more slowly than that implied by the homogenous scaling form (3.1). If the local flow fields are assumed to be dominated by vortex flow, the decay law can be calculated from hydrodynamics [40]. The agreement of the slower decay predicted in this way with MD simulation is excellent, confirming both the instability and the relevance of hydrodynamics for its description. Another signature of vortex growth is provided by the time dependence of the transverse velocity field spatial correlations. As discussed above they can be calculated from the kinetic equation (2.9) as was done in references [10,41], or from fluctuating hydrodynamics as in references [23,40]. The amplitude of the correlations in the transverse velocity field is seen to increase by an order of magnitude on the time scale for growth of the hydrodynamic shear mode. The agreement between MD, DSMC, kinetic theory, and hydrodynamics is very good.

A more complete investigation of the mechanism for cluster formation has been carried out by Brey and collaborators [42], based on DSMC solution to the Boltzmann equation and an approximate solution to the nonlinear Navier-Stokes hydrodynamic equations derived from it (Section 6). The linear stability analysis for the hydrodynamic equations provides a prediction for the critical wavelength for the instability as a function of α. This was measured by DSMC for the energy at fixed α to determine the smallest system size for which secular growth occurs. The agreement between hydrodynamics and simulation for this critical wavelength is excellent for all $0.7 \leq \alpha \leq 0.9$, i.e. including strong dissipation. Next, the evolution of an initial flow field with sinusoidal space dependence of wavelength λ was considered. As expected from the linear stability analysis, the transverse component grows in time preserving the same imposed wavelength. In contrast the initially uniform density and energy becomes sinusoidal at *half* the original wavelength, suggesting a bilinear coupling of these fields with the transverse flow field. Indeed, this is consistent with the mechanism proposed by Goldhirsch, Tan, and Zanetti [38] described above, where the hydrodynamic viscous heating provides such a bilinear coupling in the temperature equation. A detailed comparison between a nonlinear hydrodynamic solution and DSMC for the growth of this second harmonic in the density and temperature shows excellent agreement [42]. This confirms that the mechanism for initial cluster growth is initiated by the unstable shear mode and its nonlinear coupling to the density.

There are also MD confirmations of a hydrodynamic description for the instabilities. Deltour and Barrat [28] study the onset of shear and cluster instabilities for a two dimensional system, showing good agreement with predictions of linear hydrodynamics. A nonlinear hydrodynamic analysis has been compared with MD simulation at much weaker dissipation, $\alpha \geq 0.95$ [43]. The density and temperature are assumed to be slaved by the linearly unstable transverse velocity field and quadratic nonlinearities are retained. For fixed system size there is a critical value of α below which the nonlinear equations support a stable inhomogeneous macroscopic shearing state. The critical value of α and the values of the Fourier components for the flow field, density, and temperature are found to be in very good agreement with the MD simulation results.

In summary, for sufficiently large systems the HCS develops spatial inhomogeneities at times long compared to that required for growth of a local shear fluctuation. The existence, onset, and early evolution of the instability is well-described by Navier-Stokes order hydrodynamics. The kinetic equation also can be used to explore the late stage evolution as well via DSMC. It appears [42] that the density field approaches an inhomogeneous steady form, independent of initial conditions, for fixed α. This suggests that the isolated system supports a more complex, but stable, state whose form is yet to be clarified. MD simulations do not yet confirm this, perhaps due to the smaller system sizes and time scales considered.

V. HYDRODYNAMICS

Consider now a spatially inhomogeneous state, created either by initial preparation or by boundary conditions. In the bulk, there are local balance equations for the density $n(\mathbf{r},t)$, temperature $T(\mathbf{r},t)$ (or energy density), and flow velocity $\mathbf{U}(\mathbf{r},t)$

$$D_t n + n\nabla\cdot\mathbf{U} = 0, \tag{5.1}$$

$$D_t T + \frac{2}{3nk_B}\left(P_{ij}\partial_j U_i + \nabla\cdot\mathbf{q}\right) = -T\zeta, \tag{5.2}$$

$$D_t U_i + (mn)^{-1}\partial_j P_{ij} = 0, \tag{5.3}$$

where $D_t = \partial_t + \mathbf{U}\cdot\nabla$ is the material derivative, $P_{ij}(\mathbf{r},t)$ is the pressure tensor and $\mathbf{q}(\mathbf{r},t)$ is the heat flux. The form of these balance equations is the same as for fluids with elastic collisions except for the source term on the on the right side of (5.2) due to the dissipative collisions, where $\zeta \propto (1-\alpha^2)$ is identified as the cooling rate. Haff's law follow's directly from (5.2) for spatially homogeneous states and the scaling law $\zeta \propto \sqrt{T}$. The fluxes P_{ij}, $\mathbf{q}$ and the cooling rate ζ are given as explicit low degree moments of the distribution functions $f^{(1)}(x_1,t)$ and $f^{(2)}(x_1,x_2,t)$.

These balance equations are an exact consequence of the Liouville dynamics for the system. Their utility is limited without further specification of P_{ij}, $\mathbf{q}$, and ζ which, in general, have a complex space and time dependence. However, for a fluid with elastic collisions this dependence "simplifies" on sufficiently large space and time scales where it is given entirely through a functional dependence on the fields n, T, and $\mathbf{U}$. The resulting functional dependencies of P_{ij} and $\mathbf{q}$ on these fields are called constitutive equations and their discovery can be a difficult many-body problem. The above balance equations, together with the constitutive equations, become a closed set of equations for n, T, and $\mathbf{U}$ are called *hydrodynamic equations.* This is the most general and abstract notion of hydrodynamics, which encompasses both the Navier-Stokes form for small spatial gradients and more general forms for nonlinear rheological transport. The primary feature of a hydrodynamic description is the reduction of the description from many microscopic degrees of freedom to a set of equations for only five local fields.

How does this reduction come about? For the case of elastic collisions the chosen fields are local densities of globally conserved number, energy, and momentum. Consequently, the dynamics of these variables can be made as slow as desired by considering long wavelength phenomena. In this way a time scale can be chosen such that all other excitations have decayed to zero, leaving a time dependence for all properties only through these conserved densities. In practice, the hydrodynamic fields dominate for times large compared to the mean free time, and for wavelengths large compared to the mean free time. This explains the wide domain of applicability for a hydrodynamic description of physical phenomena.

The extension of these ideas to granular flow raises several questions: 1) since energy is not conserved, why should the equation for T be included in the set of slow hydrodynamic fields?, 2) is the new time scale associated with the cooling rate ζ microscopic or macroscopic?, 3) without any equilibrium Gibbs state, what is the reference state toward which these fields are relaxing? These issues are quite different from the those regarding the validity of a kinetic theory, so to address them consider values of the density and restitution coefficient for which the Enskog kinetic equation is reliable. This is given by the exact first BBGKY hierarchy equation (3.4) with the molecular chaos assumption [7]

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\boldsymbol{\nabla}_1\right)f(\mathbf{r}_1,\mathbf{v}_1,t,)=J_E[\mathbf{r}_1,\mathbf{v}_1|f(t)], \tag{5.4}$$

where J_E is the Enskog collision operator,

$$J_E[\mathbf{r}_1,\mathbf{v}_1|f(t)] \equiv \sigma^2 \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}) \left\{\alpha^{-2} f^{(2)}(\mathbf{r}_1,\mathbf{r}_1-\boldsymbol{\sigma},\mathbf{v}_1',\mathbf{v}_2',t) \right.$$
$$\left. -f^{(2)}(\mathbf{r}_1,\mathbf{r}_1+\boldsymbol{\sigma},\mathbf{v}_1,\mathbf{v}_2,t)\right\}, \tag{5.5}$$

$$f^{(2)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{v}_1,\mathbf{v}_2,t) \equiv g(\mathbf{r}_1,\mathbf{r}_2|n(t)) f(\mathbf{r}_1,\mathbf{v}_1,t,) f(\mathbf{r}_2,\mathbf{v}_2,t). \tag{5.6}$$

(Here and in the following the superscript on $f^{(1)}$ will be suppressed to simplify the notation). The balance equations in the form (5.1) - (5.3) above follow directly from this equation without further approximation. Similarly, P_{ij}, $\mathbf{q}$, and ζ are found to be bilinear functionals of f [7]

$$P_{ij} = \int d\mathbf{v}\, mV_iV_j\, f(\mathbf{r},\mathbf{v},t) + \frac{1+\alpha}{4} m\sigma^3 \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\Omega\ \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})((\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})^2 \widehat{\sigma}_i\widehat{\sigma}_j$$
$$\times \int_0^1 d\lambda f^{(2)}(\mathbf{r}-(1-\lambda)\boldsymbol{\sigma},\mathbf{r}+\lambda\boldsymbol{\sigma},\mathbf{v}_1,\mathbf{v}_2,t), \tag{5.7}$$

$$\mathbf{q} = \int d\mathbf{v}\, \frac{1}{2} mV^2 \mathbf{V} f(\mathbf{r},\mathbf{v},t) + \frac{1+\alpha}{4} m\sigma^3 \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\Omega\ \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})((\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})^2 (\mathbf{G}\cdot\widehat{\boldsymbol{\sigma}})\widehat{\boldsymbol{\sigma}}$$
$$\times \int_0^1 d\lambda f^{(2)}(\mathbf{r}-(1-\lambda)\boldsymbol{\sigma},\mathbf{r}+\lambda\boldsymbol{\sigma},\mathbf{v}_1,\mathbf{v}_2,t), \tag{5.8}$$

$$\zeta = \left(1-\alpha^2\right) \frac{\beta m\sigma^2}{12nT} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\Omega\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})^3\, f^{(2)}(\mathbf{r},\mathbf{r}+\boldsymbol{\sigma},\mathbf{v}_1,\mathbf{v}_2,t), \tag{5.9}$$

where $\mathbf{V} = \mathbf{v} - \mathbf{U}(\mathbf{r},t)$ is the peculiar velocity and $\mathbf{G} = \frac{1}{2}(\mathbf{V}_1 + \mathbf{V}_2)$. Equations (5.1) - (5.9) provide an unambiguous basis to study the existence and criteria for a hydrodynamic description. Although these equations are complicated, DSMC provides direct numerical access to solutions to the kinetic equation to determine the fields and fluxes without any assumptions regarding hydrodynamics for critical tests and benchmarks.

Hydrodynamics results from the balance equations supplemented with constitutive equations for P_{ij}, $\mathbf{q}$, and ζ. Since the former are exact, the critical issue is the existence and form of the constitutive equations. It is clear from (5.7) - (5.9) that they will be obtained if the Enskog equation admits a "normal" solution, whose space and time dependence occurs entirely through its functional dependence on the fields

$$f(\mathbf{r},\mathbf{v},t) = F\left(\mathbf{v}\,|n,T,\mathbf{U}\right) \tag{5.10}$$

The fluxes and cooling rate then inherit this space and time dependence and become constitutive equations. The space and time dependence of the fields follows from solution to the resulting hydrodynamic equations to complete the self-consistent description of F. A hydrodynamic description for granular gases can be justified if it can be shown that such a "normal" solution exists, and that it represents a wide class of more general solutions on a large space and time scale. This is a difficult task even for the case of elastic collisions, and detailed results exist only for a few special nonequilibrium states using model kinetic equations (see Section 7 below). For the Boltzmann and Enskog equations partial answers exist for gases with elastic collisions and states with small spatial gradients. In that case, the Chapman-Enskog method [44] generates the normal solution explicitly by a systematic expansion in the small gradients . To lowest order the resulting constitutive equation for the pressure tensor is Newton's viscosity law, while that for the heat flux is Fourier's law. The pressure and associated transport coefficients in these expressions (shear and bulk viscosities, thermal conductivity) also are given by the method in terms of the Enskog collision operator. The balance equations become the familiar Navier-Stokes hydrodynamic equations. The dominance of the hydrodynamic description at large space and time scales is justified by a study of the spectrum of the linearized Enskog equation. It can be shown that there are five smallest eigenvalues (hydrodynamic modes) that scale with the wavelength such that they are isolated from all other eigenvalues [45] for wavelengths long compared to the mean free path. Thus a general excitation of the system will be dominated by the hydrodynamic modes after a short transient time during which all other excitations decay. It is verified that the spectral hydrodynamic modes are the same as those obtained from the linearized Navier-Stokes equations obtained by the Chapman-Enskog method, at long wavelengths.

While questions of convergence of the Chapman-Enskog solution and the nature of the constitutive equations and boundary conditions beyond Navier-Stokes order remain open, in general, the conceptual basis for hydrodynamics in fluids with elastic collisions seems clear and convincing. In the next section, the extent to which a similar analysis applies for granular gases is discussed.

VI. LOCAL HCS AND NAVIER-STOKES EQUATIONS

The mean free path $\ell = 1/n\sigma^2$ is a characteristic microscopic length both for fluids with elastic and inelastic collisions. Consider a state for which the spatial variations of n, T, and $\mathbf{U}$ are small on the scale of the mean free path (e.g., $\ell\nabla \ln n << 1$). Then it is expected that the functional dependence of the normal solution on the hydrodynamic fields can be made local in space through a Taylor series expansion about the point $\mathbf{r}$ and time t for which the distribution function is being evaluated. Similarly, since the solution is normal, all time derivatives occur only through the fields which obey the balance equations (5.1)–(5.3). For fluids with elastic collisions, these time derivatives are proportional to gradients of the fluxes which in turn are proportional to the small gradients of the fields. As discussed above, this is the basis for the dominance of hydrodynamics at long times and long wavelengths. The first difference for granular fluids appears at this point in the analysis since the time derivative of the temperature is not simply proportional to the gradients but also has a contribution from the cooling rate $-\zeta$. Since this is proportional to $(1-\alpha^2)$ it can be made small for sufficiently weak dissipation, although this is *not a condition* for the Chapman-Enskog expansion described below. It is only necessary that ζ remains smaller than the decay rates for the non-hydrodynamic excitations at large dissipation, a condition for the dominance of a closed set of equations including the temperature at late times.

Let ϵ denote a formal small "uniformity" parameter measuring the small spatial gradients in the fields (e.g. a term of order ϵ is of first order in a hydrodynamic gradient, ϵ^2 is either a product of two first degree hydrodynamic gradients or one second degree hydrodynamic gradient). As anticipated above, there is no restriction that the cooling rate ζ be of order ϵ; only the spatial gradients are being ordered by the uniformity parameter. The distribution function, collision operator, and time derivative are given by the representations

$$F = F^{(0)} + \epsilon F^{(1)} + \cdots, \qquad J_E = J^{(0)} + \epsilon J^{(1)} + \cdots, \qquad \partial_t = \partial_t^{(0)} + \epsilon \partial_t^{(1)} + \cdots \tag{6.1}$$

The coefficients in the time derivative expansion are identified from the balance equations with a similar expansion for P_{ij}, $\mathbf{q}$, and ζ generated through their definitions (5.7) - (5.9) as functionals of F. The leading term $F^{(0)}$ is further constrained to have the same moments with respect to $1, v^2$, and $\mathbf{v}$ as the full distribution F. To zeroth order in ϵ the macroscopic balance equations become $\partial_t^{(0)} n = 0, \quad \partial_t^{(0)} \mathbf{u} = 0, \quad T^{-1} \partial_t^{(0)} T = -\zeta^{(0)}$, and the time derivative in the Enskog kinetic equation to this order can be evaluated as

$$\partial_t^{(0)} F^{(0)} = -\zeta^{(0)} T \partial_T F^{(0)} = \frac{1}{2} \zeta^{(0)} \boldsymbol{\nabla}_V \cdot \left(\mathbf{V} f^{(0)} \right) \tag{6.2}$$

The first equality follows from the normal form of $F^{(0)}$, and the second equality follows from dimensional analysis which requires the form

$$F^{(0)} = n(\mathbf{r}, t) v_0^{-3/2} \phi(V/v_0), \qquad v_0^2 = 2T(\mathbf{r}, t)/m \tag{6.3}$$

The dependence on the magnitude of $\mathbf{V} = \mathbf{v} - \mathbf{U}(\mathbf{r}, t)$ is due to the requirement that to zeroth order in ϵ the distribution function must be isotropic with respect to the peculiar velocity.

The Enskog kinetic equation to zeroth order in ϵ determines the velocity dependence of $F^{(0)}$

$$\frac{1}{2} \zeta^{(0)} \boldsymbol{\nabla}_V \cdot \left(\mathbf{V} F^{(0)} \right) = J^{(0)} [F^{(0)}, F^{(0)}]. \tag{6.4}$$

Comparison of (6.3) with (3.1) shows a close similarity with the HCS. In fact, Eq. (6.4) is the same as that for the HCS so the scaling function $\phi(x)$ is exactly the same[2]. Here, however, $F^{(0)}$ is normal so the density, temperature, and flow velocity of the HCS must be replaced by their corresponding exact values for the *inhomogeneous* state considered, as indicated explicitly in (6.3). This is referred to as the *local* HCS distribution (a misnomer,

[2] In Section 3 the Boltzmann equation is considered, while here the Enskog equation is used. However, for the HCS and to zeroth order in ϵ the Enskog and Boltzmann collision operators differ only by a constant which can be absorbed in $\zeta^{(0)}$.

since it is no longer homogeneous). The fluxes can be calculated to this order using only the symmetry of this distribution with the results $\mathbf{q}^{(0)} = 0$, $P_{ij} = p\delta_{ij}$. The pressure p is the same as that for the HCS, $p = nk_BT\left[1 + \frac{1+\alpha}{2}\frac{\pi n\sigma^3}{6}g\left(q_{12} = \sigma\right)\right]$, except now evaluated at the true nonuniform temperature and density. The evaluation of the cooling rate $\zeta^{(0)}$ requires the detailed form for the local HCS, which can be obtained approximately by the polynomial expansion method described in Section 3. At low density, i.e. the Boltzmann limit, the resulting hydrodynamic equations are the counterpart of the Euler equations for a fluid with elastic collisions: first order partial differential equations in space and time. The only qualitative difference is the source term $-T\zeta^{(0)}$ in the temperature equation. At finite density, the Enskog equation gives an additional contribution to the cooling rate proportional to $\nabla \cdot \mathbf{U}$ at the next order in the Chapman-Enskog method, which must be retained as well at Euler order (hydrodynamic equations to first order in the spatial gradients). The dense fluid Euler equations were first obtained from a consistent application of the Chapman-Enskog method by Goldstein and Shapiro [18].

At this point the most significant differences in the application of the Chapman-Enskog method to granular gases have been exposed and it is an appropriate point to address some misconceptions. Early derivations of hydrodynamics from kinetic theory used the local Maxwellian for the reference state $F^{(0)}$, as is done in the case of elastic collisions [46–48]. Since the Maxwellian is only a good approximation for granular fluids at weak dissipation the applicability of the resulting hydrodynamics also has this limitation to weak dissipation. Similarly, it has been argued that hydrodynamics is a process of relaxation towards equilibrium and therefore can apply only if the granular gas is close to the local Maxwellian, implying the same limitation. However, the local Maxwellian is not a representation of the equilibrium state but rather of the macroscopic non-equilibrium state through its dependence on the hydrodynamic fields. Only its velocity dependence is equilibrium-like. Furthermore, the analysis here shows that even this velocity dependence is not free to be chosen, neither for computational convenience nor to match conceptual bias from experience for fluids with elastic collisions. Rather it is determined by the expansion itself. For elastic collisions the left side of (6.4) vanishes and the solution is indeed the *local* Maxwellian as a consequence of detailed balance. The physical interpretation is that a wide class of solutions for spatially inhomogeneous states evolve in two stages. During a short transient period of the order of the mean free time (the kinetic stage), the velocity distribution approaches closely the local Maxwellian and becomes normal as in (6.3). Subsequently, on a longer time scale the space and time dependence of the distribution occurs only through the fields that are governed by hydrodynamic equations. A similar interpretation holds for the granular gas. During the kinetic stage the velocity distribution rapidly approaches a normal solution close to the local HCS, now determined from (6.4) with the non-zero contribution from the cooling rate. The velocity distribution is no longer Maxwellian and the balance equations do not conserve energy, but the conceptual basis for this two stage relaxation and the mathematical implementation of the Chapman-Enskog method for the normal solution is not compromised by these changes.

It also has been argued that the instabilities of the HCS limit the time scale for validity of hydrodynamics. This is a valid question for calculating the linear response of the actual HCS to small spatial perturbations. In that case a solution to the kinetic equation is sought by expanding about an unstable state. While the derived linear hydrodynamic modes may apply through the early stages of instability, eventually the growing perturbation will invalidate the description. The Chapman-Enskog method generates a quite different solution, which agrees with linear response only when the local HCS is linearized about the HCS. The method generates the velocity dependence of a spatially *inhomogeneous* distribution from the Enskog equation through its parameterization by the hydrodynamic fields. Its space and time dependence is governed through these fields by the full nonlinear hydrodynamic equations. Consequently, it is capable of describing late stage stabilization of linear instabilities as long as spatial gradients remain relatively small. Examples have been given in the previous section for linear instabilities associated with vortex fluctuations that appear to evolve nonlinearly to stationary inhomogeneous states. Similar situations occur for fluids with elastic collisions, where the hydrodynamic equations describe well a wide range of bifurcation phenomena. In such cases both Euler level nonlinearities and the nonequilibrium state dependence of the transport coefficients (temperature and density) can be important, and both are incorporated in the Chapman-Enskog method.

Mathematically, the changes in this method for granular gases arise from the fact that the time derivative of the temperature does not vanish to lowest order in ϵ, as it does for a gas with elastic collisions. In fact, the reference state $F^{(0)}$ incorporates the time dependence of the temperature even for strong dissipation. It has been remarked that the validity of the Chapman-Enskog expansion is questionable for such a time dependent reference state [3]. However, since $F^{(0)}$ is normal, it necessarily has the time dependence of all hydrodynamic fields even in the case of elastic collisions. The primary difference for granular gases is the introduction of a new time scale $1/\zeta^{(0)}$ in the reference state. However, there is nothing *a priori* inconsistent with a description of slow spatial decay towards a time dependent reference state. Instead, the key question is whether the new time scale is smaller than that of other excitations active during the kinetic stage and negligible on the longer time scale. If so, the inclusion of the temperature as one of the hydrodynamic fields is justified for these long times. Further comment on this is given in Section 8.

Implementation of the Chapman-Enskog method to the first order in ϵ is now straightforward and has been carried out in detail and without approximation recently for the Boltzmann equation [49] and for the Enskog equation [50]; the case of a two component mixture is considered in [51]. The constitutive equations for the one component fluid found to this order are

$$P_{ij} \rightarrow p\delta_{ij} - \eta \left(\partial_j U_i + \partial_i U_j - \frac{2}{3}\delta_{ij} \nabla \cdot \mathbf{U} \right) - \gamma \delta_{ij} \nabla \cdot \mathbf{U}, \tag{6.5}$$

$$\mathbf{q} \rightarrow -\kappa \nabla T - \mu \nabla n, \tag{6.6}$$

$$\zeta^{(1)} = \frac{p - p^k}{p^k} \psi \nabla \cdot \mathbf{U}. \tag{6.7}$$

The form of the pressure tensor is the same as that for fluids with elastic collisions, where $\eta\left(n, T, \alpha\right)$ is the shear viscosity and $\gamma\left(n, T, \alpha\right)$ is the bulk viscosity, depending on the restitution coefficient as well as the local density and temperature. The heat flux is similar to Fourier's law, where $\kappa(n,T,\alpha)$ is the thermal conductivity. However, there is a new transport coefficient $\mu(n,T,\alpha)$ coupling the heat flux to a density gradient, and a coefficient $\psi(n,T,\alpha)$ coupling the cooling rate to the divergence of the velocity field. These latter two coefficients vanish at $\alpha = 1$. The transport coefficients are given in terms of solutions to inhomogeneous integral equations involving the linearized Enskog operator. Solubility conditions for the existence of solutions have been proven and approximate solutions in terms of polynomial expansions have been obtained for practical purposes, just as for the case of elastic collisions [50]. Consequently the transport coefficients are known as explicit functions of the density, temperature, and restitution coefficient. The Chapman-Enskog method places no explicit restriction on these parameters, so their domain of applicability with respect to density and dissipation is the same as that for the underlying Enskog kinetic equation. In particular, there is no restriction to weak dissipation introduced by the method.

The hydrodynamic equations associated with (6.5) - (6.7) are the Navier-Stokes equations or Newtonian hydrodynamics (constitutive equations that are linear in the gradients). Under some circumstances large gradients occur and more complex constitutive equations are required (e.g., shear flow discussed below). The need for more complex constitutive equations does not signal a breakdown of hydrodynamics [65], only a failure of the Navier-Stokes approximation [66]. Although the Chapman-Enskog method can be carried out to second order in ϵ (Burnett order), it is likely that failure of the Navier-Stokes approximation signals the need for other methods to construct the normal solution that are not based on a small gradient expansion. There are reasons to expect that such non Newtonian transport may be more prevalent for granular flows [3].

The validity of Navier-Stokes hydrodynamics and the dependence of the transport coefficients on the restitution coefficient has been verified in a number of simulations, both DSMC and MD, giving good agreement with the predictions from the Chapman-Enskog method. The tests at low density based on the Boltzmann equation have been review recently by Brey and Cubero [52]. The details described there will not be repeated; only a summary of the properties studied and the results obtained is given. The Navier-Stokes equations described above, with the low density transport coefficients as explicit functions of α are considered in reference [53]. Using DSMC the evolution of an initial sinusoidal transverse component of the velocity field is measured. After a few collisions it is found to decay according to shear diffusion, characterized by the shear viscosity. In this way the shear viscosity is measured as a function of α for $\alpha > 0.6$, showing very good agreement with the results from the Chapman-Enskog method. Similarly, the longitudinal modes were excited by an initial sinusoidal perturbation of the density. The evolution of the density and temperature fields, changing an order of magnitude over 30 collision times, is in excellent agreement with the theory using transport coefficients evaluated at the chosen $\alpha = 0.7$ (no adjustable parameters). Finally a similar perturbation to excite the diffusive mode of a labelled particle allowed measurement of the self-diffusion coefficient in two dimensions; a second measurement of the mean square displacement was made for comparison as well [54]. Both results are in excellent agreement with the Chapman-Enskog prediction for $\alpha > 0.6$ and with MD results performed for $\alpha > 0.7$. More recently, the self-diffusion coefficient has been compared with MD simulation at finite densities [55]. The agreement is very good for $\alpha > 0.6$ and $n\sigma^3 \leq 0.25$. Significant deviations are observed at higher densities and smaller α. The mean square displacement remains linear in time so that hydrodynamic diffusion still occurs, although its description by the Enskog equation is no longer accurate. Presumably, this is due to the enhanced shear fluctuations at larger densities and smaller α discussed in Section 4. The dependence of the shear viscosity on density and α has been compared to results from a DSMC measurement of viscous heating [56]. The agreement with the Chapman-Enskog prediction is excellent for $\alpha > 0.6$ and $n\sigma^3 \leq 0.5$ (in this case the shear fluctuations are implicitly suppressed by the method). These results show clearly the direct verification of hydrodynamics and the quantitative predictions for transport coefficients from kinetic theory for states with small spatial gradients but including strong dissipation.

VII. KINETIC MODELS AND EXACT RESULTS

In the last Section a precise question was posed: does the Enskog kinetic equation for a granular gas imply a corresponding hydrodynamic description on appropriate space and time scales. For Newtonian flows and relatively simple nonequilibrium states, the answer appears to be "yes". It is possible and of great interest to explore non Newtonian flows as well (e.g. steady shear flow), where the Navier-Stokes equations no longer apply. While this is possible using DSMC, the Chapman-Enskog method is no longer appropriate to construct the normal distribution and associated constitutive equations. This problem has been addressed for the Boltzmann equation with elastic collisions by considering model kinetic equations with structurally simpler collision operators that allow more penetrating analysis. In this way a small set of exact normal solutions has been obtained for spatially inhomogeneous states far from equilibrium, providing results in semi-quantitative agreement with DSMC studies of the underlying Boltzmann equation [57]. Recently, the method of kinetic models has been proposed for granular gases based on the Boltzmann and Enskog kinetic equations [58]. In the former case the Boltzmann equation is rewritten as

$$\left(\partial_t + \mathbf{v}\cdot\nabla\right) f - \frac{\zeta}{2}\frac{\partial}{\partial\mathbf{v}}\cdot\left(\mathbf{V}f\right) = J^{'}(f), \tag{7.1}$$

$$J^{'}(f) \equiv J(f) - \frac{\zeta}{2}\frac{\partial}{\partial\mathbf{v}}\cdot\left(\mathbf{V}f\right). \tag{7.2}$$

where $J(f)$ is the Boltzmann collision operator defined in (2.11). The velocity derivative term on the left side compensates for the time dependence of the temperature in the HCS. Consequently, the "new" collision operator $J^{'}(f)$on the right side has properties similar to that for elastic collisions: an invariant state and 5 vanishing low velocity moments

$$J^{'}(F^{(0)}) = 0, \qquad \int d\mathbf{v}\psi_\alpha\left(\mathbf{v}\right) J^{'}(f) = 0, \qquad \psi_\alpha \longleftrightarrow (1, m\mathbf{v}, \frac{1}{2}mV^2). \tag{7.3}$$

Now the usual BGK kinetic model for elastic collisions can be used to represent $J^{'}(f)$ rather than $J(f)$, preserving the properties (7.3)

$$J^{'}(f) \rightarrow -\omega\left(f-F^{(0)}\right). \tag{7.4}$$

where $F^{(0)}$ is the local HCS distribution. The collision frequency ω has a space and time dependence that occurs only through the density and temperature, and is a free parameter of the model. With this choice the model kinetic equation becomes

$$\left(\partial_t+\mathbf{v}\cdot\nabla\right)f=-\omega\left(f-F^{(0)}\right)+\frac{1}{2}\zeta\frac{\partial}{\partial\mathbf{v}}\cdot\left(\mathbf{V}f\right). \tag{7.5}$$

A review of some applications of kinetic models for granular gases is given in reference [14]. Such methods are potentially more important for granular gases since the states of interest are typically driven by external boundary conditions, posing intractable difficulties for analytic studies of the Enskog equation.

Exact solutions in kinetic theory for spatially inhomogeneous states are exceedingly rare. When, furthermore, such a solution is normal and corresponds to a hydrodynamic state far from equilibrium an important benchmark is obtained for both conceptual and computational issues. In the case of granular gases at low density there are two interesting examples: uniform shear flow [59] and planar nonlinear Couette flow [60]. Both allow controlled discussion of nonlinear rheological properties (e.g., shear thinning, normal stresses) that are important for a wide class of real granular flows. For uniform shear flow the model results predict the components of the pressure tensor as a function of shear rate and α, as well as the velocity distribution function itself which is manifestly normal. For nonlinear Couette flow the hydrodynamic fields, heat and momentum fluxes, and velocity distribution function are determined for conditions such that viscous heating dominates collisional cooling, including large gradients. Explicit expressions for the generalized transport coefficients (e.g., viscosity and thermal conductivity) are obtained as nonlinear functions of the shear rate and α. Comparison of such non Newtonian transport properties with DSMC results for the Boltzmann equation in each case shows surprisingly good agreement, confirming that the simplifications of the model do not compromise the physical implications of the Boltzmann equation. For the present discussion, these examples demonstrate the existence of a normal solution and hydrodynamics under conditions for which the Chapman-Enskog expansion is no longer justified.

VIII. SEPARATION OF SCALES

It remains to discuss the conditions for dominance of a hydrodynamic description. Simply put, the time scale for hydrodynamic processes must be long compared to that required for all other ("kinetic") excitations to decay and become negligible. The characteristic longest time scale for the kinetic excitations is of the order of the mean free time τ_m. The analysis is simplest for states near the homogeneous state (equilibrium or HCS). Then the amplitudes of the hydrodynamic fields do not deviate much from their uniform values, but their spatial variation can be complex. For fluids with elastic collisions the hydrodynamic frequencies, $\omega_H(k)$, are functions of the wavevector k (inverse wavelength) such that $\omega_H(k) \to 0$ as $k \to 0$. Consequently, a sufficient condition for the separation of time scales is a restriction to sufficiently small $k < \ell^{-1} =$ (mean free path)$^{-1}$, or in terms of the frequency $\omega_H(k) < \omega_0 = v_0\ell^{-1} = \tau_m^{-1}$ collision frequency. Note that this does not require that the mean free path should be large compared to the particle size. For example, in dense fluids the mean free path can be smaller than the hard sphere diameter and an accurate (but not Navier-Stokes) hydrodynamics applies from macroscopic length scales down to those of the order of the particle size. The analysis for inelastic collisions is similar, except that there is the additional condition that the cooling rate must be smaller than the collision rate, $\zeta < \omega_0$, in order to include the temperature as one of the hydrodynamic variables.

For states near the HCS, the separation of time scales (or frequencies) for a granular gas can be studied from the spectrum of the associated linear kinetic equation. There are two cases for which precise and unambiguous results have been obtained: the Enskog-Lorentz equation for a heavy impurity particle diffusing through a fluid in its HCS, and a kinetic model for the Boltzmann equation. In the first case a mass ratio expansion of the Enskog-Lorentz equation leads to a Fokker-Planck equation [58,62]. While there are many qualitative differences from the corresponding equation for elastic collisions, there is an exact mapping of the case $\alpha < 0$ to that with $\alpha = 1$ for all values of the impurity-gas restitution coefficient. The spectrum of the Fokker-Planck equation can be obtained exactly in this way. It shows a diffusive mode smaller than infinitely many other discrete kinetic modes, bounded away from them at a smallest distance of the order of the impurity-gas collision frequency. Furthermore this distance remains the same independent of the wavelength considered. Thus the justification and conceptual basis for hydrodynamic diffusion in this granular "Brownian motion" is the same as for elastic collisions; it dominates after a few collisions. The predictions of this Fokker-Planck description have been confirmed in detail by DSMC for the Boltzmann-Lorentz equation and by MD [63].

Similar conclusions follow for the linearized kinetic model for the Boltzmann equation (7.5). As an example, consider an initial state that excites transverse shear excitations (a perturbation of the transverse flow field) [58]. The complete spectrum can be determined in this case as well, although it is more complex including branch cuts as well as discrete points. There is an isolated shear diffusion mode with dimensionless frequency

$$\begin{aligned}\omega_H^*(k,\alpha) &= \frac{\zeta^*}{2} - \left(1+\frac{\zeta^*}{2}\right)\omega_H^*\left(\frac{k^*}{1+\frac{\zeta^*}{2}}, \alpha = 1\right) \\ &\rightarrow \frac{\zeta^*}{2} - \frac{k^{*2}}{2+\zeta^*}\end{aligned} \tag{8.1}$$

where $\zeta^* = \zeta/\omega_0$ is the dimensionless cooling rate. The second line indicates the small wavevector limit of $\omega_H^*(k^*, \alpha = 1)$. This is the unstable shear mode discussed in Section 4. In this case it is extended to larger wavevectors, beyond the Navier-Stokes form in the second line, but there is a restriction on the wavevector to be less than the inverse mean free path (more precisely $k^* = k\ell \leq \left(1+\frac{\zeta^*}{2}\right)\sqrt{\pi}$), just as for elastic collisions. The remainder of the spectrum is at larger frequencies with a smallest separation of the order of the collision frequency. Hence shear diffusion dominates after a few collisions. The longitudinal excitations can be studied exactly in the same way for this kinetic model, with the same conclusion that the hydrodynamic spectrum remains bounded away from the kinetic modes and sufficiently small wavevectors.

In both cases the analysis holds without any restriction to weak dissipation, and the cooling rate always remains separated from the kinetic modes. This provides an illustration of a contracted description including the temperature as one of the variables, even though it is not associated with a conserved quantity. Within the set of hydrodynamic excitations there can be a second separation of time scales when $k^{*2} << \zeta^*$, i.e. long wavelengths and strong dissipation. This is possible since some of the hydrodynamic modes vanish as $k^{*2} \to 0$ while others are coupled to the temperature whose dominant time scale ζ^{*-1} is fixed by α. Calculations based on the Boltzmann and Enskog equations lead to the necessary condition for the temperature to be a hydrodynamic field, $\zeta^* < \omega_0$. Then hydrodynamics includes the two qualitatively different regimes, $\zeta^* << k^{*2} < \omega_0$ and $k^{*2} << \zeta^* < \omega_0$. Occurrence of this separation within the hydrodynamic domain should not be confused with the last inequality, which assures the hydrodynamic description. The inclusion of a non-conserved degree of freedom, temperature, is not unique to granular gases. Some complex molecular gases have internal molecular modes with frequencies comparable to the sound velocity, and these modes can be considered as "hydrodynamic" on the dominant long time scale.

The above analysis refers to states near the HCS, confirming the *sufficient* conditions of hydrodynamic fields whose space and time variation is smooth on the scale of the mean free time and mean free path. When the hydrodynamics is non Newtonian, the field variations are large and these sufficient conditions are necessarily violated. Nevertheless, it is possible that the characteristic hydrodynamic frequencies can still be small compared to the mean free path and the separation of time scales can still be valid. This is the case for polymer fluids, where rheological properties imply shear rates large compared to the collision frequency. It is difficult to provide a general characterization of non Newtonian hydrodynamics since the constitutive equations are not known and may not be universal. However, uniform shear flow is a rare case for which exact results can be obtained [64] to illustrate the existence of hydrodynamics for large spatial gradients. An exact, closed set of equations for the components of the pressure tensor can be obtained from the Boltzmann equation for the special case of Maxwell molecules. The solution shows an exponentially fast approach to the hydrodynamic state (uniform shear flow with viscous heating, as obtained from the hydrodynamic equations) for times large compared to $\tau\left(a^*\right)$

$$\tau\left(a^*\right)=\tau_m\left[2\left(1+9a^{*2}+3a^*\sqrt{2+9a^{*2}}\right)^{1/3}+2\left(1+9a^{*2}-3a^*\sqrt{2+9a^{*2}}\right)^{1/3}-3\right]^{-1} \quad (8.2)$$

where $a^*=a\tau_m$ is the shear rate times the mean free time, measuring the hydrodynamic gradient. It is seen that $\tau\left(a^*\right)\leq\tau_m$, for *all* values of a^*, so the hydrodynamic description applies as expected for $t\gg\tau_m$ even if $a^*>>1$. A corresponding approximate analysis for hard spheres based on a kinetic model can be extended to inelastic collisions [59], leading to similar conclusions. The steady shear flow of a granular gas necessarily entails large a^* (see comments below) and this has been interpreted as a breakdown of hydrodynamics for granular systems [65]. However, as the above example illustrates, this conclusion confuses the failure of conditions for Navier-Stokes hydrodynamics with those for hydrodynamics more generally [66].

It is appropriate at this point to remark on the conjecture by Goldhirsch in his recent review [3]: "The main thesis of this paper is that granular gases should be considered to be mesoscopic in the sense that both the microscopic spatial and temporal scales are typically not well separated from the relevant corresponding macroscopic scales and this property of granular gases is at the root cause of many and perhaps most of the peculiar properties of granular gases." The terminology "not well separated" requires analysis in each case. It is not sufficient to make estimates based on dimensional analysis of macroscopic fields in terms of characteristic mesoscopic (kinetic) scales. As the example of the last paragraph shows, such analysis can lead be misleading (i.e. $a^*>>1$ does not imply the time scales are not well separated). The test for the validity of a hydrodynamic description for granular gases must be more precise: how do the true hydrodynamic frequencies compare to the true kinetic frequencies? For granular gases both the physical states and the forms for these frequencies can be more complex than those for normal fluids. The failure of familiar properties for the latter to hold for the former does not necessarily imply a failure of hydrodynamics, and there appears to be no precise example of hydrodynamic frequencies exceeding the collision frequency. Still, Goldhirsh is correct to warn that granular systems frequently support states outside the Navier-Stokes domain and therefore properties based on the latter cannot be trusted.

It is argued in [3] that mean free paths in granular systems can be macroscopic, leading to a failure to separate microscopic and macroscopic space scales. The primary example is a mean free path defined in the laboratory frame rather than the local rest frame for the fluid element. Such a definition allows arbitrarily large mean free paths for sufficiently large convection of the fluid, and can be anomalously large for both normal and granular fluids. Reasons for rejecting this definition are given in [66]. In general, when properly formulated it appears that the mean free path in a granular medium is qualitatively similar to that in a normal fluid. Of course, in strongly heterogeneous states of dense clusters and large voids the average mean free path is no longer a useful concept.

The title of this review article "Granular gases: probing the boundaries of hydrodynamics" recognizes an important motivation for studying rapid granular flow. The hydrodynamics is indeed different for many reasons and commonly occuring states often sample a different domain of the relevant parameter space than is accessible for normal fluids. The single feature of an energy sink allows a wide range of phenomena that are not possible otherwise. For example, the steady states of uniform shear flow or Couette flow described in Section 7 are possible only because of the balance between viscous heating and collisional cooling. In the steady state, therefore, the temperature, shear rate a, and restitution coefficient α are no longer independent variables. In dimensionless terms the relationship gives $a^* \propto (1-\alpha^2)$ and it is possible to show that the fluid is always non Newtonian for any $\alpha < 1$ [56]. A similar conclusion applies for a granular gas confined between walls with fixed temperature. The resulting steady state has a nonuniform temperature profile resulting from competition between the energy source at the wall and collisional cooling in the interior. The profile is fixed by the restitution coefficient and wall temperatures. Again, it can be shown that a correct description of the profile cannot be obtained from the Navier-Stokes equations due to inherent non Newtonian effects induced by the steady state. This is probably a characteristic of most steady states obtained by driving the system. Such non Newtonian behavior of simple atomic systems is impossible to observe experimentally (except in computer simulations) but seems to be the norm for granular gases. This makes the search for complex constitutive equations an interesting and challenging research area to be pursued. Rather than abandoning hydrodynamics for granular gases, it appears profitable to embrace such a description for new horizons and new opportunities.

IX. BOUNDARY VALUE PROBLEMS

Most problems of practical interest involve finite geometries and associated boundary conditions. Such problems can be addressed directly at the level of the Navier-Stokes hydrodynamics but, as with normal fluids, become less straightforward for non Newtonian flows. In any case, boundary value problems do not appear to pose any inherent problem for kinetic theory or its implementation via DSMC. As noted by Grad in his discussion of the Boltzmann equation [11] a normal solution of the form 5.10 can be expected to apply only outside certain domains of initial and boundary "slip" (a third slip across a shock layer is also discussed). The initial slip layer is the transient period of a few collisions required for the kinetic excitations to decay relative to those of hydrodynamics, as described above. Similarly, there is a domain of the order of a few mean free paths near the boundaries for which the solution to the kinetic equation is more complex than that which can be represented by the normal form. Away from these slip domains a description in terms of the five hydrodynamic fields can be expected. The boundary conditions for these fields necessarily require an independent means for extrapolation across the slip domains (modified initial and boundary conditions, relative to the actual given conditions).

For large systems and Navier-Stokes order gradients, the slip conditions are often negligible and the interesting physical phenomena resulting from boundary sources are not dependent on the mesoscopic details of the boundary layer. Recently, Brey et al. [67] have applied the Navier-Stokes hydrodynamic equations derived from the Boltzmann equation as described in Section 6 to describe a vibrated granular gas in an external gravitational field. It is worth repeating that the transport coefficients and cooling rate are specified functions of the restitution coefficient so there are no adjustable parameters. The system was driven at $z = 0$ and unbounded for $z > 0$. In appropriate dimensionless variables, non-trivial temperature and density profiles are obtained independent of the details of the boundary conditions (frequency and amplitude of vibration) although a transition to a collisionless Knudsen gas eventually occurs at asymptotically large z. These predictions from Navier-Stokes hydrodynamics are in very good agreement with corresponding results from both MD and DSMC for the Boltzmann equation. Similar good agreement between Navier-Stokes hydrodynamics, MD, DSMC, and experiment has been observed for gravitational flow of grains past a fixed wedge [68]. In this case the flow is supersonic leading to formation of a shock profile at the tip of the wedge and an expansion fan below the wedge, all well-described by the hydrodynamic boundary value problem.

It is interesting to note that the Navier-Stokes equations are capable of describing some of the more exotic behavior exhibited by granular gases, even though structurally they are quite similar to the equations for normal fluids. Symmetry breaking is one such phenomenon. Consider the above shaken system now partitioned vertically into two domains initially with the same density profiles. If a hole in the partition is introduced at a certain height, an asymmetry of the density in the two partitions develops depending on the amplitude of the vibration and degree of dissipation. The description in terms of a simple effusion process is in reasonable agreement with results from experiment and MD [69]. A more detailed Navier-Stokes analysis of a different symmetry breaking mechanism also is in good agreement with MD [70]. In this case a closed container of N particles is vibrated at $z = 0$ (no gravity) and an exact solution to the Navier-Stokes equations with constant pressure is constructed. Next, the system is partitioned normal to z starting at a height $z = h$. At sufficiently low density the hydrodynamic fields are symmetric with respect to the two sides of the partition, but above a critical density an asymmetry in the density occurs (a bifurcation in the hydrodynamic solution). The asymmetry (high and low density sides) continues to increase with larger density. The hydrodynamic analysis again is in excellent quantitative agreement with MD and DSMC results.

If some dimensions of the system are small, the details of the boundary conditions can become more important. For granular systems the boundaries may be rough, e.g. consisting of frozen layers of other grains, and the geometry of this roughness (local curvature) also can play a role. Coulomb friction is another mechanism for momentum transfer at the boundary. The problem of constructing realistic boundary conditions for granular gas hydrodynamics has been reviewed and illustrated recently by Jenkins [71]. As in the case of normal fluids, the objective is not to describe in detail the boundary layer near the surface, but rather to construct representative conditions for the hydrodynamic equations on the other side of the slip. Practical boundary conditions have been found in many cases for the accurate application of hydrodynamics for experimental analysis. This is an active and evolving field.

X. DISCUSSION

Two questions have been addressed here: 1) can kinetic theory provide a valid mesoscopic description of rapid flow (fluidized) granular media?, and 2) can a hydrodynamic description be formulated and justified for a macroscopic description? The evidence presented here has emphasized idealized conditions and states for which controlled numerical simulations and theoretical approximations can be compared. At this level, it appears that many of the questions, concerns, and objections raised regarding the kinetic theory have been removed and the domain of validity has been clarified in the past few years. Certainly, kinetic theory (Enskog or more sophisticated) appears to be a powerful tool for analysis and predictions of rapid flow gas dynamics. Combined with the numerical solution via DSMC, almost any boundary or initial value problem for moderate densities can be explored in detail. The most practical version of kinetic theory, the Enskog equation, appears to have a somewhat more restricted domain in the parameter space of density and restitution coefficient than for fluids with elastic collisions, but remains a remarkably rich and accurate basis for analysis of moderately dense granular gases. Any observable differences from Enskog provide a new opportunity to study correlated collision phenomena whose effects for normal fluids are typically small except for the dense fluid.

The hydrodynamic description for the same class of idealized conditions and states, also appears justified even though the phenomena can be considerably more complex than for normal fluids. Nevertheless, this complexity (e.g., instabilities, clustering, rheology) appears to be captured quantitatively by a properly formulated hydrodynamics. The required separation of time scales, including the temperature field, appears justified even at strong dissipation based on the few cases for which this question can be addressed quantitatively. For weakly inhomogeneous states the Chapman-Enskog method, properly implemented, gives both the Navier-Stokes hydrodynamics for a granular gas and the detailed forms for the transport coefficients as functions of density and α. Quantitative confirmation of these results, as indicated above in many studies, should remove most reservations about the basis of hydrodynamics for such states. Non Newtonian hydrodynamics for states in which the gradients of hydrodynamic fields are not small is less well-understood, just as for normal gases. However, in the latter case such states are rare or unphysical for simple atomic systems. In contrast, they appear frequently for granular gases in steady states where the gradients are strongly correlated to the coefficient of restitution. Kinetic models and DSMC for shear and Couette flow provide instructive examples of non Newtonian hydrodynamics, and support for the expectation that hydrodynamics with appropriate constitutive equations is applicable to such complex rheological states as well.

The optimistic view about hydrodynamics for granular media presented here appears at odds with the conclusion by Kadanoff in [2]: "Can a granular material be described by hydrodynamic equations, most specifically those equations which apply to an ordinary fluid? It seems to me the answer is "No!"". This conclusion is based on a number of observed phenomena: weakly shaken compact material showing composite effects and patterns, compaction (volume reduction) of dense material by tapping, clustering as described in Section IV, inelastic collapse (see footnote in Section 2), and one dimensional examples. It is important to note first that Kadanoff has in mind Navier-Stokes-like hydrodynamics (universal, local, partial differential equations). Indeed, in many of these cases it is difficult to imagine a hydrodynamic description of the type requested. These are not the fully fluidized states considered here, and it is clear that the presence of compact structures or large voids entail heterogenous materials for which Navier-Stokes hydrodynamics was never intended. The case for hydrodynamics improves considerably when that term is extended to include more general constitutive equations and when the states considered are fully fluidized in two or three dimensions. Polymer and colloidal fluids, liquid crystals, and emulsions all admit a hydrodynamic descriptions although more complex than Navier-Stokes, which are neither universal nor necessarily local. A single granular material can manifest properties similar to many different states of complex fluids, and it is possible that many different forms of constitutive equations will be required for an adequate hydrodynamic description of each. A single normal material also can have multiple types of macroscopic continuum descriptions for different states (fluid, metastable, elastic). One conclusion here is that granular media exhibit a wide range of interesting phenomena for which a Navier-Stokes hydrodynamics is an accurate and practical tool. More generally, however, there is agreement with Kadanoff that granular fluids are in a class of complex materials "with behaviors which are, at this moment, not fully understood." Kinetic theory and hydrodynamics (in the broader sense) can be expected to provide much of this understanding.

XI. ACKNOWLEDGEMENTS

It is a pleasure to acknowledge the essential assistance of Javier Brey, Vicente Garzó, James Lutsko, and Andrés Santos in their roles as collaborators, mentors, and critics for much of the material discussed here. This research was supported in part by National Science Foundation grant PHY 9722133.

REFERENCES

[1] P. K. Haff, "Grain flow as a fluid mechanical phenomenon", J. Fluid Mech. **134**, 187 (1983).

[2] L. P. Kadanoff, "Built upon sand: theoretical ideas inspired by the flow of granular materials", Sand Review V2.2, 1 (1997); Rev. Mod. Phys. **71**, 435 (1999).

[3] I. Goldhirsh, "Granular gases - probing the boundaries of hydrodynamics", in *Granular Gases*, eds. T. Poschel and S. Luging (Springer, NY, 2001).

[4] C. S. Campbell, "Rapid granular flows", Ann. Rev. Fluid Mech. **22**, 57 (1990).

[5] M. H. Ernst, "Kinetic theory of granular fluids: hard and soft inelastic spheres", in *Dynamics: Models and Kinetic Methods for Non-equilibrium Many Body Systems*, J. Karkheck editor (Kluwer Academic, Boston, 2000).

[6] T. P. C. van Noije and M. H. Ernst, "Kinetic theory of granular gases", in *Granular Gases*, eds. T. Poschel and S. Luging (Springer, NY, 2001).

[7] J. Brey, J. W. Dufty, and A. Santos, "Dissipative Dynamics for Hard Spheres", J. Stat. Phys. **87**, 1051 (1997).

[8] J. W. Dufty, "Statistical mechanics, kinetic theory, and hydrodynamics for rapid granular flow", J. Phys.: Condens. Matter 12, A **47** (2000).

[9] J. W. Dufty, M. Lee, and J. Javier Brey, "Kinetic model for pair correlations", appendix A in Phys. Rev. E **51**, 297 (1995); see also M. C. Marchetti, Ph. D. thesis, University of Florida, Appendix D, (1982).

[10] J. Javier Brey, F. Moreno, and M. J. Ruiz-Montero, "Spatial correlations in dilute granular flows: a kinetic model study", Phys. Fluids **10**, 2965 (1998).

[11] H. Grad, "Principles of the kinetic theory of gases", in *Encyclopedia of Physics*, ed. S. Flugge (Springer, NY, 1958); application of Grad's limit for granular gases also has

been considered by J. Piasecki (private communication).

[12] T. P. C. van Noije, M. H. Ernst, and R. Brito, "??", Physica A **251**, 266 (1998).

[13] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon, Oxford, 1994).

[14] J. Javier Brey, "Model kinetic equations for rapid granular flow", in *Dynamics: Models and Kinetic Methods for Non-equilibrium Many Body Systems*, J. Karkheck editor (Kluwer Academic, Boston, 2000).

[15] J. Dufty and M. Marchetti, "Non-equilibrium Fluctuations in Simple Fluids", in *25 Years of Non-equilibriuum Statistical Mechanics*, M. Rubi editor (Springer-Verlag, Berlin, 1994).

[16] M. Huthmann, J. Orza, R. Brito, "Dynamics of deviations from the Gaussian state..", Granular Matter **2**, 189 (2000).

[17] J. Javier Brey, M. J. Ruiz-Montero, and D. Cubero, "Homogeneous cooling state of a low-density granular flow", Phys. Rev. E **54**, 3664 (1997).

[18] A. Goldstein and M. Shapiro, "Mechanics of collisional motion of granular materials. part 1. general hydrodynamic equations", J. Fluid Mech. **282**, 75 (1995).

[19] T. P. C. van Noije and M. H. Ernst, "Velocity distributions in homogeneous granular fluids: the free and heated case", Granular Matter **1**, 57 (1998).

[20] J. Javier Brey, D. Cubero, and M. J. Ruiz-Montero, "High energy tail in the velocity distribution of a granular gas", Phys. Rev. E **59**, 1256 (1999).

[21] V. Garzo and J. Dufty, "Homogeneous Cooling State for a Granular Mixture", Phys. Rev. E **60**, 1 (1999).

[22] J. M. Montanero and V. Garzó, "Monte Carlo simulation of the homogeneous cooling state for a granular mixture", preprint 2001.

[23] T. P. C. van Noije, M. H. Ernst, R. Brito, and J. Orza, "Mesoscopic theory of granular fluids", Phys. Rev. Lett. **79**, 411 (1997); T. P. C. van Noije, R. Brito , and M. H. Ernst, "Spatial correlations in compressible granular flows", Phys. Rev. E **57**, R4891 (1998).

[24] J. F. Lutsko, "Velocity correlations and the structure of nonequilibrium hard core fluids", Phys. Rev. Lett. **86**, 3344 (2001).

[25] J. F. Lutsko, "Model for the atomic-scale structure of a dense, nonequilibrium fluid: the homogeneous cooling state of granular fluids", Phys. Rev. E **63**, 061211 (2001).

[26] J. F. Lutsko, "Molecular chaos, pair correlations, and shear-induced ordering of hard spheres", Phys. Rev. Lett. **77**, 2225 (1996).

[27] S. Luding, M. Muller and S. McNamara, "The validity of "molecular chaos" in granular flows", in: *World Congress on Particle Technology* (Brighton, 1998, CD: ISBN 0-85295-410-9).

[28] P. Deltour and J-L Barrat, "Quantitative study of a freely cooling granular medium", J. Phys. I **7**, 137 (1997).

[29] R. Soto and M. Mareschal, "Statistical mechanics of fluidized granular media: short range velocity correlations", Phys. Rev. E **63**, 041303 (2001).

[30] J. M. Salazar and L. Brenig, "Inelastic granular gas: Computer simulations and kinetic theory of the cooling state". Phys. Rev. E **59**, 2093 (1999).

[31] Y. Elskens, "Comment on "Inelastic granular gas .." ", cond-mat/9911276 v1 (1999).

[32] M. H. Ernst, "Comment II on "Inelastic granular gas.." ", cond-mat/9911436 v1 (1999).

[33] T. P. C. van Noije, M. H. Ernst, E. Trizac, and I. Pagonabarrga, "Randomly driven granular fluids: large scale structure", Phys. Rev. E **59**, 4326 (1999).

[34] C. Bizon, M. Shattuck, J. Swift, and H. Swinney, "Transport coefficients for granular media from molecular dynamics simulations", Phys. Rev. E **60**, 4340 (1999).

[35] C. Bizon, M. Shattuck, J. Swift, and H. Swinney, "Velocity correlations in driven two-dimensional granular media" in *Dynamics: Models and Kinetic Methods for Nonequilibrium Many-Body Systems*, J. Karkheck editor (Kluwer Academic, Boston, 2000).

[36] J. M. Montanero and A. Santos, "Computer simulation of uniformly heated granular fluids", Gran. Matt. **2**, 53 (2000).

[37] F. Vesely and G. Evans, "Pair dynamics in hard sphere fluids: recollision time correlation functions", J. Chem. Phys. **92**, 1275 (1990).

[38] I. Goldhirsh, M. -L. Tan, and G. Zanetti, "A molecular dynamical study of granular fluids I: the unforced granular gas in two dimensions", J. Sci. Comput. **8**, 1 (1993).

[39] S. Luding and H. J. Herrmann, "Cluster growth in freely cooling granular matter", Chaos **9**(3), 673 (1999).

[40] R. Brito and M. H. Ernst, "??", Europhys. Lett. **43**, 497 (1998); Int. J. Mod. Phys. C **9**, 1339 (1998).

[41] J. Javier Brey, F. Moreno, and M. J. Ruiz-Montero, "Instability and spatial correlations in a dilute granular gas", Phys. Fluids **10**, 2976 (1998).

[42] J. Javier Brey, M. J. Ruiz-Montero, and D. Cubero, "Origin of density clustering in a freely evolving granular gas", Phys. Rev. E **60**, 3150 (1999).

[43] R. Soto, M. Mareschal, and M. Malek Mansour, "Nonlinear analysis of the shearing instability in granular gases", Phys. Rev. E **62**, 3836 (2000).

[44] J. Ferziger and H. Kaper, *Mathematical Theory of Transport Processes in Gases* (North-Holland, Amsterdam, 1972).

[45] J. A. McLennan, *Introduction to Nonequilibrium Statistical Mechanics* (Prentice-Hall, New Jersey, 1989).

[46] J. T. Jenkins and S. B. Savage, "A theory for the rapid flow of identicle, smooth, nearly

elastic, spherical particles", J. Fluid Mech. **130**, 187 (1983).

[47] C. K. W. Lun, S. B. Savage, D. J. Jeffrey, and N. Chepurniy, "Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flow field", J. Fluid Mech. **140**, 223 (1984); C. K. K. Lun, "Kinetic theory for granular flow of dense, slightly inelastic, slightly rough, spheres", J. Fluid Mech. **233**, 539 (1991).

[48] J. T. Jenkins and M. W. Richman, "Grad's 13 moment system for a dense gas of inelastic spheres", Arch. Ration. Mech. Anal. **87**, 355 (1985); Phys. Fluids **28**, 3485 (1986).

[49] J. J. Brey, J. W. Dufty, C. S. Kim, A. Santos, "Hydrodynamics for Granular Flow at Low Density", Phys. Rev. E **58**, 4638 (1998).

[50] V. Garzo and J. Dufty, "Dense fluid transport for inelastic hard spheres", Phys. Rev. E **59**, 5895 (1999).

[51] V. Garzo and J. Dufty, "Hydrodynamics for a granular mixture at low density", cond-mat/0105395 v1.

[52] J. J. Brey and D. Cubero, "Hydrodynamic transport coefficients of granular gases" in *Granular Gases*, eds. T. Poschel and S. Luging (Springer, NY, 2001).

[53] J. Javier Brey, M. J. Ruiz-Montero, and D. Cubero, "On the validity of linear hydrodynamics for low density granular gases described by the Boltzmann equation", Europhys. Lett **48**, 359 (1999).

[54] J. Javier Brey, M. J. Ruiz-Montero, D. Cubero, and R. García-Rojo, "Self-diffusion in freely evolving granular gases", Phys. Fluids **12**, 876 (2000).

[55] J. F. Lutsko, J. Dufty, and J. J. Brey, unpublished.

[56] J. M. Montanero, A. Santos, V. Garzó, and J. Dufty, "Shear viscosity for a dense granular gas", unpublished.

[57] J. W. Dufty, “Kinetic theory of fluids far from equilibrium - exact results”, in *Lectures on Thermodynamics and Statistical Mechanics*, M. Lopez de Haro and C. Varea, ed. (World Scienfic, N.J., 1990).

[58] J. Brey, J. Dufty, and A. Santos, “Kinetic Models for Inelastic Hard Spheres”, J. Stat. Phys. J. Stat. Phys. **97**, 281, (1999).

[59] J. Javier Brey, M. J. Ruiz-Montero, and F. Moreno, ”Steady uniform shear flow in a low density granular gas”, Phys. Rev. E **55**, 2846 (1997).

[60] M. Tij, E. Tahiri, J. M. Montanero, V. Garzó, A. Santos, and J. Dufty, ”Nonlinear Couette flow in a low density granular gas”, J. Stat. Phys. **103**, 1035 (2001).

[61] J. M. Montanero, V. Garzó, A. Santos, and J. J. Brey, ”Kinetic theory of simple granular shear flows of smooth hard spheres”, J. Fluid Mech. **389**, 391 (1999).

[62] A. Santos and J. Dufty, ”Nonequilibrium phase transition for a heavy particle in a granular fluid”, cond-mat/0106205; “Critical Behavior of a Heavy Particle in a Granular Fluid”, Phys. Rev. Lett. **86**, 4823 – 4826 (2001).

[63] J. Brey, M. Ruiz-Monero, R. Garcia-Rojo, and J. Dufty, “Brownian Motion in a Granular Gas”, Phys. Rev. E **60**, 7174 (1999).

[64] A. Santos and J. J. Brey, Physica A **174**, 355 (1991).

[65] M. L. Tan, I. Goldhirsch, ”Rapid granular flows as mesoscopic systems”, Phys. Rev. Lett. **81**, 3022 (1998).

[66] J. Dufty and J. Brey, “Comment on “Rapid Granular Flows as Mesoscopic Systems”, Phys. Rev. Lett. **82**, 4566 (1999).

[67] J. Javier Brey, M. J. Ruiz-Montero, and F. Moreno, ”Hydrodynamics of an open vibrated granular system”, Phys. Rev. E **63**, 061305 (2001).

[68] E. Rericha, C. Bizon, M. Shattuck, and H. Swinney, ”Shocks in Supersonic Sand”,

cond-mat/0104474.

[69] J. Eggers, "??", Phys. Rev. Lett. **83**, 5322 (1999).

[70] J. Javier Brey, F. Moreno, R. García-Rojo, and M. J. Ruiz-Montero, "A hydrodynamic Maxwell demon in granular systems", Phys. Rev. Lett. (submitted).

[71] J. T. Jenkins, "Boundary conditions for collisional grain flows at bumpy, frictional walls", in *Granular Gases*, eds. T. Poschel and S. Luging (Springer, NY, 2001).