EXTENDED GRANULAR TEMPERATURE

Lou Kondic* and Robert P. Behringer**
* *Department of Mathematical Sciences & Center for Applied Mathematics & Statistics*
New Jersey Institute of Technology, Newark, NJ 07102, USA
** *Department of Physics & Center for Nonlinear and Complex Systems*
Duke University, Durham NC, 27708, USA

Summary We consider the role of elastic energy in the context of granular materials undergoing shear flow. Depending on the ratio of pressure to Young's modulus of the material from which grains are made and the typical velocity of shearing, there is a transition from a regime in which the fluctuations of kinetic energy are dominant to the regime where the fluctuations of elastic energy are dominant. This regime has likely been reached in recent experiments. We then consider a generalization of the granular temperature that includes both types of energy fluctuations and that changes smoothly from one regime to the other. We conclude by discussing related energy distributions and the degree to which the zeroth law of thermodynamics is satisfied by this new generalized temperature.

OVERVIEW

We explore the role of elasticity in the energy and energy fluctuations of sheared dense granular systems. For dilated gas-like granular states, energy fluctuations are frequently described in terms of a temperature, defined as the fluctuating part of the kinetic energy, $T_k \equiv m < v^2 > /2$. Here, v is the local random component of the velocity. This definition is predicated on assumptions such as molecular chaos, absence of correlations, and short-lived collisions, that do not always apply. For dense systems, a very different concept, Edwards entropy, has been proposed [1].

Both of these pictures assume that minimal energy is stored in compressional modes of the particles. This assumption is valid when the pressure is small compared to the Young's modulus. However, it can easily be shown that in particular for slow shearing, there are many physical situations when this need not be the case. In such a setting, neither T_k nor T_E is likely to provide a good measure of the random nature of the system.

The main goal of this work is to analyze via discrete element simulations (DES) the storage of energy and energy fluctuations for dense granular material subject to shearing. In this context, we propose an extension of granular "temperature" that contains information on fluctuations of the elastic energy, and then compare this extension to a temperature drawn from statistical mechanics. (A somewhat similar approach of applying equilibrium statistical theory to out-of-equilibrium systems has been recently used by other authors [4, 5].)

The generalization of "temperature" that we consider is based on the classical idea that for a lattice of elastic particles, the average fluctuating energy/particle is $3k_BT$. Using this as a heuristic guide, we define a generalized temperature that is roughly $T_g = m < v^2 > /2 + k < x^2 > /2$, where v corresponds to the fluctuating part of the velocity, and x to the fluctuating part of the compression of a particle. Note that this definition provides a simple bridge between the extremes of a gas-like state and a highly compressed slowly evolving state.

In the simulation, particles are confined between two inpenetrable straight parallel boundaries. The top boundary, which is 50 mean particle diameters (d_m) long, moves at a steady speed, and induces shearing in the system. The boundary conditions in the shearing direction are periodic. These simulations closely follow the soft-disk/sphere model (see [7, 8] and references therein), and are performed with approximately 2000 polydisperse particles, with a radius variability of 10%. The results that follow use t, the time it takes the shearing wall to travel once across the domain, as a time scale, and l/t ($l = 50d_m$) as a velocity scale. The quantities below are calculated using space-time averaging, see [8]. In particular, the elastic energy is obtained by averaging *per collision*, not per particle. The difference between the two is significant for dense granular systems considered here, since particles typically experience multiple collisions.

DISCUSSION OF THE RESULTS

By analyzing the elastic energy and kinetic temperature, as the volume fraction ν is slowly increased, we observe in our simulations that there is a transition region (about $\nu_c = 80\%$) where the energy stored in the internal degrees of freedom (elastic energy) becomes more relevant than the kinetic energy. In order to have a quantity that might play the same role as T_k in a dense granular system we propose a generalized granular 'temperature' by

$$T_g = T_k + T_e, \tag{1}$$

as a sum of T_k, and the 'elastic' part T_e. T_e is defined as the mean fluctuation of *elastic* energy, in a manner similar to T_k, which is the mean fluctuation of *kinetic* energy. This definition follows the classical statistical mechanics result where the mean fluctuations in the combined elastic and kinetic energy of an oscillator are proportional to the temperature. However, unlike this classical case, there is no reason to expect equipartition between elastic and kinetic modes. Rather, the ratio $T_e/(T_e + T_k)$ varies from 0 in the dilute limit, to 1 in the dense limit.

Figure 1 shows T_k, T_e, and average elastic energy, E_e vs. time, for four different ν's. For higher ν's, clearly $T_e \gg T_k$. Interestingly, there are rather large fluctuations of the results with ν just above $\nu_c \approx 80\%$, corresponding to the regime

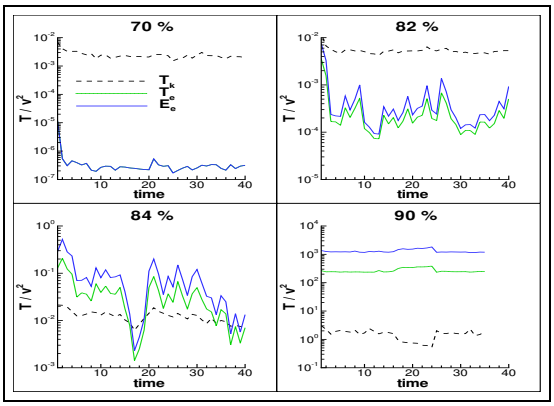

Figure 1. Elastic energy, kinetic and elastic temperatures for various ν's, scaled by v^2.

where elastic energy becomes predominant. Also, experiments have indicated a phase transition for comparable densities which may be related [2]. Generally, one might expect both glassy and/or jamming phenomena to dominate this regime.

We further interpret T_g by comparing it to an alternative definition from statistical mechanics. We consider the standard relation [6] $dU/dT = \delta U^2/T^2$ where U is the total energy in the (usually conservative) system, T is the temperature, and $\delta U^2 = \langle U^2 \rangle - \langle U \rangle^2$. We then ask whether it makes sense to define $T = T_g = T_k + T_e$. To check this idea, we now think of the relation above as a defining equation for $T_m = \sqrt{\delta U^2}/(dU/dT_g)$. The agreement between T_m and T_g will provide some indication of the utility of the definition for T_g. Note that we should not expect perfect or possibly even any agreement, since we are considering a strongly dissipative system far from equilibrium.

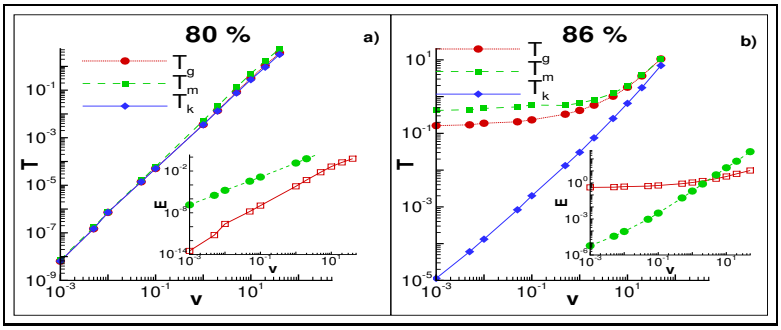

Figure 2. Generalized, kinetic, and 'model' temperature (see the text) for two volume fractions. The insets show kinetic energy (filled circles) and average elastic energy (squares).

Figure 2 contains a summary of the various types of temperatures considered in this study for two ν's. As already noted, for $\nu = 80\%$, most of the energy is still kinetic, while for $\nu = 86\%$, elastic energy is essential. For $\nu = 80\%$, T_k is dominant, and also it satisfies the model above since $T_k \approx T_m$. However, for $\nu = 86\%$ and for slow shearing, T_k is smaller by 4 orders of magnitude than T_g and T_m. Thus, T_k cannot be used to even approximately describe a dense slowly sheared granular system. This difference decreases for higher shearing rates, but only at very high shearing is there good agreement. We note that the presented results apply to any confined, sheared, granular system.

The agreement between T_g and T_m is not perfect; however prefect agreement is not to be expected. These studies demonstrate the clear need to incorporate elastic energy and elastic fluctuations, and that T_g has utility as a generalized granular temperature. Clearly, there remain many open questions regarding the extent to which the various temperatures serve similar functions to their molecular counterpart.

We acknowledge support by NASA NAG3-2367, NAG3-2372, NAG3-2372-05 and NNC04GA98G. RPB acknowledges support by NSF grants DMR-0137119, DMS-0204677 and DMS-0244492.

References

[1] S. F. Edwards. In A. Mehta, editor, *Granular Matter: An Interdisciplinary Approach*, 121, Springer,New York 1994.
[2] D. Howell, C. Veje, and R. P. Behringer. *Phys. Rev. Lett.*, 82:5241, 1999.
[3] W. Losert, J.-C. Geminard, S. Nasuno, and J. P. Gollub. *Phys. Rev. E*, 61:4060, 2000.
[4] I. K. Ono etal. *Phys. Rev. Lett.*, 89:095703, 2002.
[5] H. A. Makse and J. Kurchan. *Nature*, 415:614, 2002.
[6] D. A. McQuarrie. *Statistical Mechanics*. University Science Books, Sausalito, 2000.
[7] L. Kondic. *Phys. Rev. E*, 60:751, 1999.
[8] L. Kondic and R.P. Behringer. *cond-mat/0307555*, 2003.