

Abstracts.

Dr. Thomas J. O'Brien
U.S. Department of Energy
National Energy Technology Laboratory (NETL)

On a turbulence theory of multiphase flow

Since the transient simulations of multiphase flow are very computationally intensive, there has been some effort to develop RANS-like turbulence theories for gas/particle flows, such as those in circulating fluidized beds. Several of these theories are being implemented in the MFIX code and their performance in being evaluated by comparison with (the available) experimental data. This talk will emphasize some recent results with the "Simonin" and discuss the proposed LANL model.

Dr. Jie Li (with Igor Aranson , Wai Kwok and Lev Tsimring)
Argonne National Laboratory

Controlling gas-solid contacting by modulated air flow in a shallow granular layer

Our understanding on spontaneous flow pattern in gas-fluidized beds will be presented based on discrete particle method. On this base, the possible ways in achieving the intimate gas-solid contacting are proposed which include the powder fabrication, effective gas suspension and the modulated air flow. This talk will then focus on the method by employing the modulated air flow.

We report experimental study of thin granular layer fluidized by periodically-modulated gas flow. Hopefully we find a sequence of well-defined transition between disordered states dominated by spontaneous bubbling-fluidization to ordered periodic sub-harmonic patterns as the frequency, the amplitude of modulation and the flow rate varied. Ordered states include periodic square and stripes and some more complicated structures. The wavelength of observed patterns is determined by the frequency of the modulation and mean flow rate. The transition to periodic patterns is associated with noticeable pressure difference drop across the granular layer. The patterned structures are also found to be closely related to the bed natural frequency. The potential

application in industries will also be highlighted. This will be demonstrated by an example of uniformly fluidizing for an ultra-fine powder in Geldart “C” group.

Dr. Sreekanth Pannala, ORNL

MFIX Simulations: Square CFB and ANL Flower Bed

MFIX (Multiphase Flow with Interphase eXchanges), a code for modeling reactive multiphase flow in fluidized beds has been recently declared open-source and is available for the multiphase modeling community for their research (<http://www.mfix.org>). This presentation will address some of the steps in the process of validating MFIX for different applications. Two applications have been chosen for this presentation. The first one is a circulating fluidized bed (CFB) of square cross-section very similar to the one used in the experiments of Zhou, Grace et al. (1994, 1995). A detailed grid-independent study has been performed on this case and some of the comparisons with the experiments will be presented. The next sample problem simulated is a very shallow bed with pulsing inflow (same as the experiments performed at Argonne National Laboratory by Igor Aronson and Jie Lie). The pattern formation in this experiment is very sensitive to the running conditions and thus very ideal to characterize the accuracy of computational models. The talk will touch upon the initial efforts in modeling the fascinating patterns formed in this simple experiment. The talk will conclude with summarizing what was learnt and elucidating future work.

Prof. Troy Shinbrot, Rutgers University ,
Banding and Scaling in Powders and Suspensions

In this talk I present recent results indicating:

- 1) that banding segregation encountered in tumbling drums depends crucially on scale, and inexplicably on the ratio between *particle* diameter to drum diameter.
- 2) that scale dependence can be understood in terms of an underlying Rayleigh-like instability in a core of fines in a tumbling drum
- 3) that much of what is known of segregation banding is duplicated in spontaneous pattern formation in suspensions.

These results suggest first that there may be a great deal that is to be learned by granular researchers from parallel research avenues long pursued by colleagues involved in colloid and suspension research, and second that the otherwise impractical problem of banding segregation can be used to reveal underlying -- and largely invisible -- principles of subsurface granular dynamics.

Prof. Heinrich Jaeger and Prof. Sid Nagel, University of Chicago,
Effects of Interstitial Fluid on Granular Size Segregation

Dr. Cynthia Olson, LANL

Grain ordering, stability, and dynamics for anisotropic grains and chains

Prof. Olivier Pouliquen (with Yoel Forterre),
IUSTI, Marseille

Dense granular flows on inclined planes

Granular flows are classically divided in two regimes depending on the kind of interactions experienced by the particles : a rapid regime where collisions are important, and a dense regime where multi particles interactions exist and friction is important. In this last regime the lack of constitutive equations has motivated many recent studies.

We will report experimental results we obtained in the inclined plane configuration. We will show that scaling laws observed in the experiments and in recent numerical simulations can serve as an empirical input in depth averaged hydrodynamics equations leading to quantitative predictions in several problems. The implication for constitutive equations for dense granular flows will be discussed.

Dr. Leo Silbert, U. of Chicago (and J. W. Landry and G. S. Grest)

Granular Flow down a Rough Incline Plan

A brief overview of the simulation studies of gravity-driven, dense granular flows is given. Particular attention will be paid to depth profiles of quantities typically measured in experiment, such as density and flow velocity. These profiles depend greatly on the height of the flowing material and how close the system is to jamming. A rescaling of the data shows good agreement with experimental results from inclined plane flows.

Dr. Deniz Ertas
Corporate Strategic Research
ExxonMobil Research & Engineering

Clusters and the rheology of dense granular flows

The bulk rheology of dense gravity-driven granular flows observed in experiment and large-scale simulations can be understood using a phenomenological scaling theory based on clusters that are continuously formed by granular gravitational collapse, whose sizes are limited by gradients in the strain rate [1]. If these clusters have characteristic contact lifetimes comparable to the inverse strain rate rather than the binary collision time, then they will predominantly transmit stresses through a contact network rather than through collisions. The size of these clusters determines the minimum depth of a flowing pile, connecting rheology and flow arrest through Pouliquen's empirical *flow rule* [2]. Furthermore, the ubiquity of "surface flows" observed in experiments with an erodible bed can be explained by the natural tendency of the system to evolve towards the flow arrest condition. After reviewing this scaling theory, I will describe ongoing investigations [3] of the existence of such

clusters in large-scale, 3-D granular dynamics simulations, which are known to faithfully reproduce experimentally observed flow properties.

[1] D. Ertas and T.C. Halsey, Europhys. Lett. **60**, 931 (2002).

[2] O. Pouliquen, Phys. Fluids **11**, 542 (1999).

[3] In collaboration with T.C. Halsey, G.S. Grest and J.W. Landry.

Prof. Tom Lubensky, Penn State
Hydrodynamic Theory of Shear Granular Flows

Prof. Michel Louge, Cornell University
A model for dense granular flows down bumpy inclines

We consider dense flows of spherical grains down an inclined plane on which spherical bumps have been affixed. We propose a theory that models stresses as the superposition of a rate-dependent contribution arising from collisional interactions and a rate-independent part related to enduring frictional contacts among the grains.

We show that dense flows consist of three regions. The first is a thin basal layer where grains progressively gain fluctuation energy with increasing distance from the bottom boundary. The second is a core region where the solid volume fraction is constant and the production and dissipation of fluctuation energy are nearly balanced. The last is a thin collisional surface layer where the volume fraction abruptly vanishes at the free surface. We also distinguish basal flows with the smallest possible height, in which the core and surface layers have disappeared.

We derive simple closures of the governing equations for the three regions with insight from the numerical simulations of Silbert, et al [PRE 64, 051302-1 (2001)] and the physical experiments of Pouliquen [Phys Fluids 11, 542 (1999)]. The theory captures the range of inclination angles at which steady, fully-developed flows are observed, the corresponding shape of the mean and fluctuation velocity profiles, the dependence of the flow rate on inclination, flow height, interparticle friction and normal restitution coefficient, and the dependence of the height of basal flows on inclination.

Dr. L.S. Tsimring, Institute of Nonlinear Science, UCSD (with D. Volfson, and I.S. Aranson)

Partially fluidized granular flows: continuum theory versus MD simulations

We carry out a comparison of 2D soft particle molecular dynamics simulations with the continuum theory of partially fluidized shear granular flows based on the order parameter description. We introduce the order parameter as a fraction of persistent contacts among total number of contacts between particles. The constitutive relation is deduced by representing the shear stress tensor as a sum of the "fluid part" depending on the strain rate tensor, and a "solid part". Using simulations of a model Couette flow between two rough planes, we construct the constitutive relation and fit the free energy which controls the dynamics of the order parameter.

Dr. Dmitri Volfson, Institute of Nonlinear Science, UCSD (with Lev Tsimring and Igor Aranson)

Granular flows in a deep Couette cell: continuum theory versus MD simulations.

We used soft-particle 2D MD simulations to study the structure of the shear flows in a deep granular layer under gravity. The flow is driven by the upper boundary pulled with either constant force or velocity. When the whole layer is drawn into the flow we recover the solution described by the kinetic theory of granular gases. In the case of partially fluidized layer we find that the velocity field and stresses are well described by the continuum theory based on the order parameter description. In particular, the partial stresses produced by the short-lived collisions in the closely packed regions comply surprisingly well with the kinetic theory.

J. S. Olafsen, University of Kansas

Energy injection and non-Gaussian velocity statistics in driven granular gases.

A variety of experiments have examined velocity fluctuations in driven granular gases, large collections of macroscopic particles that interact primarily through hard sphere collisions. While many experiments of differing geometries and forcing find non-Gaussian behavior in the tails of the velocity distributions that is nearly of the form $\exp(-v^{-3/2})$, this behavior has not been shown to be universal. One necessary question that has been largely overlooked in the details of the various experiments is how energy is injected into the system to compensate for dissipation so that the dynamics may be studied over long periods of time. A subset of the driven granular gas experiments will be discussed along with two new experiments designed to provide alternative methods for injecting energy into a driven granular gas system. The goal is to better understand the relationship between the external driving and the observed behavior of velocity fluctuations in driven granular gases.

Dr. Daniel Blair, Clark University

Experimental study on the collision statistics in a granular gas

We present an experimental investigation of a granular gas constrained on a two dimensional surface and excited by side wall forcing. Using high speed digital imaging we are able to locate all of the particles in our system and link their positions to form long time trajectories. Thus we are able to accurately identify collision events which allows us to measure the effective coefficient of restitution, path length and time between collisions. The distribution of the path length and collision time are found to strongly deviate from the exponential function derived from kinetic theory. We propose an empirical fitting form that captures the power-law behavior for short distances and times. We utilize this form for the distribution to calculate the average speed, v , from the mean free path and time. We compare v to the average speed $\langle v \rangle$ measured from the distribution of velocities and find agreement over a broad range of density. We use our experimental results

measure the granular temperature and pressure variation in our system and compare them with hydrodynamic models of rapid granular flow.

Prof. Paul. L. Krapivsky
Department of Physics, Boston University, Boston, MA

The Inelastic Maxwell Model

I shall talk about the dynamics of spatially homogeneous inelastic gases in the framework of random collision processes for which a Boltzmann equation with uniform collision rate is exact. I shall begin by analyzing the freely cooling gas and showing that the velocity distribution develops an algebraic high-energy tail, with an exponent dependent on the dimension and the degree of dissipation. Moments of the velocity distribution exhibit a multiscaling asymptotic behavior, and the autocorrelation function decays algebraically with time. I shall proceed by showing that in the forced case, the steady state velocity distribution decays exponentially. I then outline the behavior of mixtures and impurities. Finally, I will discuss a lattice gas version of the Maxwell model.

Prof. James Dufty
Department of Physics, University of Florida

The Current Status of Kinetic Theory for Granular Fluids

Recent developments in the application of kinetic theory to activated granular fluids are summarized. Most comments are restricted to the Boltzmann equation and its dense fluid generalization, the Enskog equation. The domain of validity for these equations, and their limitations, are indicated through calculations of transport properties for simple gases and two component mixtures for comparisons with molecular dynamics simulation. Their utility in the exploration of a hydrodynamic description for granular fluids also is discussed.

Dr. Xiaobo Nie, John Hopkins University (with Eli Ben-Naim and Shiyi Chen)
Velocity Statistics and Collective Motion of Granular Gases

We study dynamics of freely cooling granular gases in two-dimensions using large-scale molecular dynamics simulations. We find that for dilute systems the typical kinetic energy decays algebraically with time in the long time limit. Asymptotically, velocity statistics are characterized by a universal Gaussian distribution, in contrast with the exponential high-energy tails characterizing the early homogeneous regime. We show that in the late clustering regime particles move coherently as typical local velocity fluctuations are small compared with the typical velocity. Furthermore, locally averaged shear modes dominate over acoustic modes. The small thermal velocity fluctuations suggest that the system can be heuristically described by Burgers-like equations.

Prof. Rodney Fox, Iowa State University
Continuum Modeling of Multiphase Flows

Prof. Jerry Gollub (with JC Tsai)
Haverford College and University of Pennsylvania

Dynamics of 3D Sheared Granular Flow in a Fluid

We have measured both the internal grain motion and the total volume change of a thick three-dimensional boundary-driven shear flow in a fluid-filled annulus, over a wide range of shear-rates and timescales. The vertical velocity profile (perpendicular to the upper shearing surface) is measured over 5 orders of magnitude in velocity. It deviates strongly from an exponential, with a larger decay rate in the deeper regions of the flow.

For deep layers (about 25 particle diameters), and starting from an initially disordered state, an abrupt transition to an ordered state consisting of hexagonal layers occurs after an accumulated displacement at the shearing surface of about 10^5 particle diameters. In the process, the total volume shrinks by about 3%. For thinner layers, the ordering process occurs much more quickly. The flow structure is sensitive to the amount of granular material (for fixed load), revealing quantization effects when the filling is sufficient to produce an integral number of layers, even when that number is fairly large.

The ordered and disordered states have distinct rheology and flow structures. The grain velocity in the disordered state decays near the smooth sidewalls, while in the ordered state, the layers move rigidly and there is little decay. The disordered state also responds more slowly to a change in the boundary shear rate.

We find shear-induced size segregation of a binary mixture: Larger beads consistently rise over time at a certain angle with respect to the horizontal.

Finally, we find shear-induced diffusion of particles perpendicular to the shear. The mean-square displacement approaches a linear time-dependence, but the displacement statistics are clearly non-Gaussian.

We use these various results to comment on timescales that are important for slowly sheared granular flows.

Dr. James Landry
Sandia National Labs

Confined granular packings: structure, stress, and forces

The structure and stresses of static granular packs in cylindrical containers are studied using large-scale molecular dynamics simulations in three dimensions. We generate packings by both pouring and sedimentation

and examine how the final state depends on the method of construction. The vertical stress becomes depth-independent for deep piles and we compare these stress depth-profiles to the classical Janssen theory. The majority of the tangential forces for particle-wall contacts are found to be close to the Coulomb failure criterion, in agreement with the theory of Janssen, while particle-particle contacts in the bulk are far from the Coulomb criterion. In addition, we show that a linear hydrostatic-like region at the top of the packings unexplained by the Janssen theory arises because most of the particle-wall tangential forces in this region are far from the Coulomb yield criterion. The distributions of particle-particle and particle-wall contact forces $P(f)$ exhibit exponential-like decay at large forces in agreement with previous studies.

Prof. Michael Shearer
Department of Mathematics
NC State University

The effect of discreteness in continuum models of granular flow

Continuum models for granular flow typically exhibit dynamic ill-posedness. In this talk, we discretize in space a continuum model for rigid-plastic antiplane shear, with the result that the semi-discrete equations are well-posed (though unstable). Oscillations that develop initially are resolved through coarsening and long-time convergence to a shear band solution. When elasticity is included, the shear band solution loses stability, as the shear modulus enters the physically relevant range, giving way to a periodic solution with a complicated elastic-plastic structure. These results and numerical experiments are for solutions that depend on one space dimension. Recent simulations in two-dimensions show additional interesting structure that suggest the equilibrium equations (used extensively for engineering design) may have physically meaningful solutions, despite the property of ill-posedness.

Dr. Alan Hurd, LANL
Using scattering to study 3D stresses in a granular compact

Prof. Arshad Kudrolli
Department of Physics, Clark University

Clustering, Jamming and Segregation in Cohesive Granular Materials

The presence of cohesive forces between particles can have a considerable influence on the properties of granular materials. For example, the angle of repose of a wet granular pile is greater than that of a dry pile made of the same material due to liquid bridges which introduces capillary forces. Cohesion causes jamming in the flow of granular matter even in a regime where dry granular matter may flow. Wet granular matter is also observed to segregate less compared to dry granular materials. Although these qualitative facts are well known and often exploited in industrial process, a detailed knowledge of the properties even in comparison with dry granular matter has not yet been attained. In this context, we discuss a series of experiments where cohesion forces are important due to either presence of small amounts of liquid or because particles are magnetized. High resolution digital imaging is used to measure the angle of repose and the extent of segregation of bi-disperse mixtures poured into a quasi-two dimensional silo. We will discuss the effect of particle size, volume fraction, viscosity and surface tension of the liquid. It can be noted that small particles preferentially clump in a bi-disperse mixture and this is observed to lead to subtle effects on the nature of the particle spatial-distribution at certain volume fractions of the liquid. In an attempt to understand the cohesion effects in a model system, we

also study the clusters observed when magnetized steel beads are vibrated in a shallow container. We will discuss the formation of chains, rings and more compact clusters as the granular temperature is varied.

Work in collaboration with Azadeh Samadani and Daniel L. Blair

Thomas C. Halsey
ExxonMobil Research and Engineering
Route 22 East, Annandale
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A Ball in a Groove: Kinematics of Static Loading

We study the static equilibrium of an elastic sphere held in a rigid groove by gravity and frictional contacts, as determined by contact mechanics [1]. As a function of the opening angle of the groove and the tilt of the groove with respect to the vertical, we identify two regimes of static equilibrium for the ball. In the first of these, at large opening angle or low tilt, the ball rolls at both contacts as it is loaded. This is an analog of the "elastic" regime in the mechanics of granular media. At smaller opening angles or larger tilts, the ball rolls at one contact and slides at the other as it is loaded, analogously with the "plastic" regime in the mechanics of granular media. I will discuss implications of this calculation for the general problem of granular statics.

[1] T.C. Halsey and D. Ertaş, Phys. Rev. Lett. **83**, 5007 (1999).

Dr. Bob Ecke, LANL

Experiments in Granular Media: Chains, Particle-Fluid Interactions and Granular Flows

Dr. Maksim V. Sapozhnikov (with Yuriy V. Tolmachev, Igor S. Aranson, Wai-Kwong Kwok),
Argonne National Laboratory

Self-assembly of Electrostatically Driven Microparticles in a Poorly Conducting Liquid.

We performed experimental studies of electrostatically driven granular media (40 and 120 mm Bronze particles) immersed in a poorly conducting non-polar liquid (toluene). The conductivity of the liquid was adjusted by adding ethanol (up to 10%). Depending on the ethanol concentration and the value of applied DC electric field (up to 20 kV/cm) the microparticles self-assemble into a rich variety of novel phases. These phases include static precipitate (honeycombs and Wigner crystals); and novel dynamic condensate (toroidal vortices and pulsating rings). The discovered asymmetry of the phase diagram with the respect to polarity of the applied voltage is related to the excess of negative ions in the bulk of the liquid when current is present. The observed

dynamic phenomena are attributed to interaction between particles and electro-hydrodynamic flows produced by the action of electric field on ionic charges in the bulk of liquid.

Prof. Julio M. Ottino
Northwestern University

Mixing and Segregation in Granular Matter: Competition between Chaos and Order

Building up understanding in terms of elementary building blocks is the cornerstone of modern science: If one understands building blocks one can then infer consequences marching upwards in scales. There are, however, many systems where interaction among the elementary building blocks – no matter how well understood – does not even give a glimpse of the behavior of the global system itself. It is now recognized that there are many examples in science and engineering belonging to this class. Characteristic for these systems is the ability to display structure without any external organizing principle being applied. A class of examples is provided by dry and wet granular matter. In dry systems the surrounding media is air; in wet systems – or slurries – a liquid. How the grains interact with each other is reasonably well understood; as to how particles move, the governing law is Newton's second law. There are no surprises at this level. However, when the particles are many and the material is vibrated or tumbled, surprising behavior emerges. Systems self-organize in complex patterns that cannot be deduced from the behavior of the particles alone.

Mixtures of tumbled granular materials tend to separate radially, in 2D containers, and axially, in long cylinders, $2D+1$, due to small differences in particles' size, density, surface properties, or shape. The 2D case is reasonably understood. The axial case much less so. Although the mechanism for segregation is understood qualitatively in certain situations, quantitative analysis is still limited. The phenomena occur in both dry material and slurries. It is also becoming apparent that the phenomenon is richer than people had initially anticipated. Band merging, formation, and wave propagation all seem to occur. Careful experimental results are essential to give insight into the fundamental mechanisms. More challenging still are cases of full 3D segregation. Here experimental results give two seemingly contradictory insights. (1) axial segregation persist under conditions one could regard as unthinkable (very large perturbations with respect to axial rotation) and (2) the final segregation patterns in biaxial motions – though not the dynamics – can be predicted from an analysis of particle trajectories and an identification of regular and chaotic regions assuming no segregation exists.

Prof. R.P. Behringer, Duke University

Force Transmission in Granular Materials

Understanding the mechanisms by which forces are carried in granular materials at the microscale and the way that these mechanisms affect the larger scale response of granular systems is a considerable challenge. Older models, such as those used in soil mechanics, assume that granular materials are elastic up to yield. Hence, below yield, the regime of interest here, these models are captured by elliptic PDE's. However, these models

assume a priori that a continuum description is adequate. Recently, several new models have been proposed that draw on microscopic pictures. These models differ substantially from each other, and the range of long-wave-length descriptions includes parabolic, elliptic and hyperbolic PDE's. In recent experiments, we have characterized force propagation using photoelastic materials in 2D to carry out effective Green's function measurements. In these studies, we have probed the effects of order and disorder of packings, and of induced texture. Several important findings include: 1) in relatively ordered systems, the response tends to follow along principal lattice directions, 2) with sufficient disorder, the response is similar to that of an elastic medium, 3) Modest shear induces a highly anisotropic stress network, with power-law force correlations along the preferred direction, 4) The force response is preferentially along this strong direction. Our results are not consistent with diffusive (parabolic PDE) models, but both anisotropic elastic and hyperbolic models can still describe data for relatively ordered packings, within experimental resolution. Hence, it is crucial to develop new more precise photoelastic techniques and additional experimental tests.

Zeina S. Khan (with Wayne A. Tokaruk, Stephen W. Morris)
University of Toronto

Traveling Waves in Axial Segregation: Simultaneous Surface Concentration and Angle Measurements

Axial segregation is a striking phenomenon which is often observed when granular materials of different sizes are rotated in a horizontal cylindrical drum: the grains separate according to their size into bands along the axis of the drum. Surprisingly, a decaying transient traveling wave state has been found to occur prior to axial segregation in a mixture of salt and sand grains [1]. The existence of this state cannot be explained by earlier models of the process which were based on reverse diffusion. A new model [2] describes both wave behavior and axial segregation in terms of the coupled dynamics of two local variables: the concentration difference of large to small grains and the dynamic angle of repose, the angle formed by the flowing surface of grains. This model predicts that these fields oscillate out of phase during the initial transient traveling wave state and are in phase for the later axially segregated state. We used a scanning laser profilometer to simultaneously measure both these quantities during their whole spatio-temporal evolution. We find, contrary to the model, that they are simply correlated and maintain the same phase relationship at all times. From this, we infer that purely surface processes are insufficient to explain the traveling wave dynamics. We report progress on new bulk visualization techniques which are sensitive to the 3D structure of the segregation and the coupling between the surface concentration and the radially segregated core.

[1] K. Choo, T. Molteno, S. Morris, Phys. Rev. Lett., 79, 2975 (1997); K. Choo, M. Baker, T. Molteno, S. Morris, Phys. Rev. E, 58, 6115 (1998).

[2] I. Aranson, L. Tsimring, Phys. Rev. Lett., 82, 4643 (1999); I. Aranson, L. Tsimring, V. Vinokur, Phys. Rev. E, 60, 1975 (1999).