Modeling for Process Control: High-Dimensional Systems

Final report

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September 12, 2008

Our research within this grant has been devoted to the modeling of complex temporal and extended spatio-temporal high-dimensional systems with the aim of applying these models for controlling the corresponding physical processes. The main direction of our research was modeling of complex dynamics of granular materials.

Among the highlights of our research in this area during the lifetime of the grant (2004-2006) are the advances in understanding the behavior of anisotropic granular matter under external driving, theoretical description of granular impact, modeling of the thermal collapse of hot granular gas under gravity, as well as development of theory for pattern formation by microtubules and molecular motors.

1 Partial fluidization theory and applications

In this part of work we applied our previously developed theory of partial fluidization to various problems of granular dynamics. In particular, we studied the stick-slip dynamics of a sold body moved over a granular bed, and found a good agreement between our theoretical modeling and direct molecular dynamics simulations as well as the earlier experiments. This work was published in Ref. [15].

In collaboration with French group of Dr. Anne Mangeney (Paris University) we applied the theory of partial fluidization to the problem of erosion of granular mass in order to compare and validate the Saint-Venant modeling approach and develop novel order-parameter based modeling tools. Using these new tools we studied avalanche dynamics in realistic geophysical conditions. In particular we addressed the problem of enhanced avalanche mobility in erodible bed conditions and explained it by entrainment of granular material underneath the avalanche. Our results on this subject were published in [9, 10].

2 Modeling of anisotropic granular dynamics

We discovered the novel mechanism of transport of granular medium related to the anisotropic shape of the grains. In our prior DOE-funded work we elucidated the mechanisms of collective motion of rods on a vibrating plate and developed phenomenological continuum model which demonstrated the transition to directed motion and onset of vortices. In our work within the grant period we focused on more specific properties of the inelastic frictional interaction between the anisotropic grains and the vibrating bottom. In particular, we studied the various regimes of motion of a bouncing dimer comprised of two spheres connected with a rigid rod. The first excited mode has a novel horizontal drift in which one end of the dimer stays on the plate during most of the cycle, while the other end bounces in phase with the plate. The speed and direction of the drift depend on the aspect ratio of the dimer. We employed both a novel soft-particle molecular dynamics algorithm and the event-driven simulations based on the detailed treatment of frictional interactions between the dimer and the plate in order to elucidate the nature of the transport mechanism in the drift mode. This work has been done in collaboration with experimental groups of Arshad Kudrolli (Clark University) and Igor Aranson (Argonne). This work has been published in [13, 6, 5, 8].

3 Granular crater dynamics

We performed extensive numerical simulations of granular craters and in general the impact of large objects falling into a granular bed. We systematically explored the various densities of the falling objects compared with the density of grains, sizes, impact velocities, frictional properties of the grains. These simulations allowed us to elucidate the mechanisms of energy loss during impact. Our findings indicate that most of energy is dissipated due to friction among the grains. Using our computational data, as well as the data from experiments performed by several groups (H. Swinney, D. Durian, J. DeBruyn) we developed a theoretical model which helps explain and predict various regimes of object penetration into a granular medium. This model generalizes classical Poncelet model of impact for the case of shallow cratering. This work has been published in Ref. [12].

4 Thermal collapse of a granular gas under gravity

Free cooling of a gas of inelastically colliding hard spheres represents a central paradigm of kinetic theory of granular gases. At zero gravity the temperature of a freely cooling *homogeneous* granular gas follows a power law in time. WE studied the role of gravity in the dynamics of colling of initially hot granular gas. We combined molecular dynamics simulations, a numerical solution of hydrodynamic equations and an analytic theory to show that a granular gas cooling under gravity undergoes thermal collapse: it cools down to zero temperature and condenses on the bottom of the container in a finite time. This work has been done in collaboration with Prof. B. Meerson (Jerusalem) [14].

5 Pattern formation of microtubules and motors: inelastic interaction of polar rods

We proposed and investigated a model describing spatio-temporal organization of an array of microtubules interacting via molecular motors. Starting from a stochastic model of inelastic polar rods with a generic anisotropic interaction kernel and we obtain a set of continuum equations for the local rods concentration and orientation. At large enough mean density of rods and concentration of motors, the model describes orientational instability. We demonstrate numerically and analytically that the orientational instability leads eventually to the formation of vortices and (for large enough density and/or kernel anisotropy) asters seen in recent experiments. We extended this model to include the effects of crosslinks. This work is done in collaboration with Igor Aranson and his group (Argonne) [2, 3, 7, 16].

6 Other accomplishments

Together with Igor Aranson we published a large review article [1] on pattern formation in granular systems in the Reviews of Modern Physics, the most influential review journal in physics community. We participated in writing the Encyclopedia for Nonlinear Science for which we have written an article “Avalanches” [11]. We also prepared a monograph “Granular patterns” [4] which is scheduled for publication by Oxford University Press in November 2008.

7 Impact

In the course of work within this grant we developed a number of theoretical models and algorithms which significantly advanced the fields of nonlinear dynamics, pattern formation, and granular physics. Our result have been published in 12 papers in leading international journals including Physical Review Letters, Physical Review, Review of Modern Physics, Geophysical Research Letters, New Journal of Physics. Our algorithms were implemented in MFIX (Multiphase Flow with Interphase eXchanges) code developed at the National Energy Technology Laboratory. We continued and established new productive collaborations with a number of institutions, including Argonne National Laboratory, University of Texas, Clark University, Paris University, etc.

One postdocs has been trained with the support of this grant (Dmitri Volfson).

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