# VICI Report (Project No. 10828)

*To:*        VICI and Industrial Partners of project VICI No. 10828

*From:*      Nicolás Rivas, PhD Student

*Subject:*   Bridging the gap between particulate systems and continuum theory

# Background

In the context of the VICI project 10828, *Bridging the gap between particulate systems and continuum theory*, the following is a progress report on the granular-hydrodynamics modeling of a vibrated quasi-two-dimensional granular system. Granular materials are ubiquitous in everyday life; we find them in cosmetic powders, cereals, vitamin pills, sand, rocky terrains, to name a few. They also constitute over 75% of all raw material feedstock to industry. This makes granular materials research relevant not only for the understanding of natural phenomena, but also for industry processes, where the prediction of their behavior under different circumstances may be fundamental.

Particle simulations can now correctly predict grains behavior in a wide range of circumstances, but are mainly limited to spherical geometries, or/and to a limited number of particles. On the other hand, several continuum equations that describe granular flows have been proposed, but fail to accurately predict the behavior for a wide range of densities and geometries. Our research focuses on establishing a connection between both approaches.

One common procedure in continuum theories for granular materials is taking the Navier-Stoke equations for regular fluids, interpret the fluid density $\rho$ as the granular number density $n$, and then modify the *transport coefficients*, expanding their validity for a wider range of densities and inelasticities[1, 2]. In this project we try to apply that approach to a complex, driven granular system, consisting in a vertically shaken shallow box filled with grains (see Fig. 1 for a sketch of the system setup). This system presents many different inhomogeneous stable states that depend on the parameters of energy injection, geometry, and grain properties and number[3, 4, 5]. Studying the transition and stability of these states, from both a microscopic and macroscopic approach, may lead to a better understanding of the out-of-equilibrium statistical physics behind complex granular systems. Two main aspects motivate this research: the development and comparison of a set of simulation tools, both microscopic (molecular dynamics), and macroscopic (granular-hydrodynamics equations solver), in order to see the limits and advantages of each approach in different scenarios; and the study of the vertically vibrated shallow granular system from a physical point of view, in order to further understand the complex behaviors present in driven granular systems.

# Progress Report

## Hydrodynamic Modeling

No substantial accomplishment has been made on the reproduction of the granular system using the granular hydrodynamic model. Initially, the simplest approach was tried, using a constant temperature boundary condition corresponding to the oscillating bottom wall, and a zero density upper boundary condition as the top free surface. The parameters of the simulations where set with the goal of observing the Leidenfrost state: a density inversion state, where a low density region near the vibrating bottom sustains a high density region. We where not able to obtain the known Leidenfrost density profile. Other classical boundary conditions where tried but none was adequate. We now strongly believe that more realistic boundary conditions are necessary.

The main drawback for the hydrodynamic modeling of the system has been the familiarization with *hpGEM*, a framework for the implementation of discontinuous Galerkin finite element methods. Lacking an adequate documentation and people with experience in the software, a considerable amount of time has been invested in understanding the algorithm, in order to implement the desired boundary conditions and hydrodynamic equations. A new collaboration and roadmap for the development of *hpGEM* has been recently proposed that should accelerate the implementation of the needed code.

## Event-Driven Simulations

Future granular hydrodynamic results will be compared with previous realized experiments[4], and simulations. For simulations we consider the inelastic hard sphere model (IHS) for particles, and thus are able to use an event-driven algorithm. The main advantage of this simulation approach is its speed, when compared to the more commonly used soft-particle simulations.

The parameters are set to correspond to the experimental setup described in [4]. This is: width $L_x = 101$ and depth $L_y = 5$, with $\sigma = 1$, the lengthscale and diameter of the particles. In the previous experimental and MD simulation study, three different amplitudes of oscillation where considered: $a = 2.0, 3.0, 4.0$. The frequency $\omega$ and the number of particles $N$ are determined by the parameters $F \equiv Nd^2/L_xL_y$, the number of particle layers; and
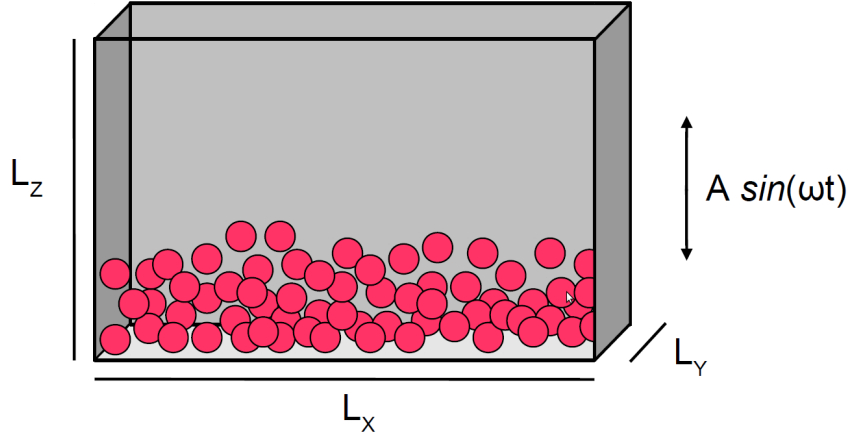
Figure 1: System setup: vibrated quasi-two-dimensional shallow box. The whole system oscillates sinusoidally with a given amplitude $A$ and frequency $\omega$.

$\Gamma \equiv a\omega^2/g$, the dimensionless acceleration, which we consider in the $F \in (2, 14)$ and $\Gamma \in (2, 50)$ ranges. This implies $N \in (1010, 7070)$, and $\omega \in (0.5, 3.5)$.

When comparing with the soft-particle linear spring-dashpot model, used in previous works, the only free parameters for the IHS model are the dynamic and static friction coefficients, and the tangential restitution coefficient $r_t$ of the particles, in particle-particle and particle-wall collisions. In our case we set both friction coefficients at $\mu = 0.15$, and $r_t = r_n$, the normal restitution coefficient, is taken to be $r_n = 0.95$.

Figure 2 shows a comparison between the previously obtained phase spaces, and the one obtained by our ED simulations. It can be seen that ED simulations are able to reproduce all previously observed phenomena, and that the regions mostly coincide, although there are some disagreements. Order parameters where constructed for most states in order to quantitatively distinguish between them. This was done for all transitions except for the Leidenfrost-Convection transition, where we are still working on an accurate order parameter. In that case the different states where identified by observing the configurations of the system. Care was taken to let the system evolve for a considerable amount of time, $20000T$ at least, to disregard any transient state.

Undulations seems to be the region where there are more differences between both kind of simulations; less energy is needed in the ED simulations for the Leidenfrost state to appear. Dark yellow simulations correspond to a state not mentioned in the previous experiments and simulations, of alternating bursts of energies, similar to undulations, but particles do not present a sinusoidal shape. Gray states correspond to intermediate states between convection and Leidenfrost or bouncing bed; a movement of the particles around two or one given point can be seen, but there are no clear convective roles, or these appear and disappear constantly.

We now focus on the Leidenfrost and Convective states, as this transition has been lately studied analytically by fellow researchers, and a comparison and extension of the results using ED simulations may be helpful in further research.

**Width dependency**

In simulations the width of the system is easily modifiable. The Leidenfrost state keeps all its fundamental characteristics as the width of the system $L_x$ is decreased. Figure 3a shows that the density profiles coincide almost perfectly for $L_x \in (10, 100)$. This is expected, as the state is horizontally symmetric, and it shows that walls do not play a fundamental role in the existence of the Leidenfrost state.

On contrary, in the convection state the width plays a fundamental role. The *natural* width of the convective rolls can be determined by changing the length of the system, $L_x$, and observing their stability. Figure 3b shows a density spatio-temporal diagram for $L_x = 60$. One can see that the end state is not stable, as the rolls move from one side of the system to the other. This is not the case for $L_x = 100$ (Figure 3c), where the low density regions remain roughly in the same position. Before reaching $L_x = 100$ the two rolls configuration is unstable, and it coexists with the one roll state. This transition between the stable and unstable one roll configuration can be used to define a characteristic length.
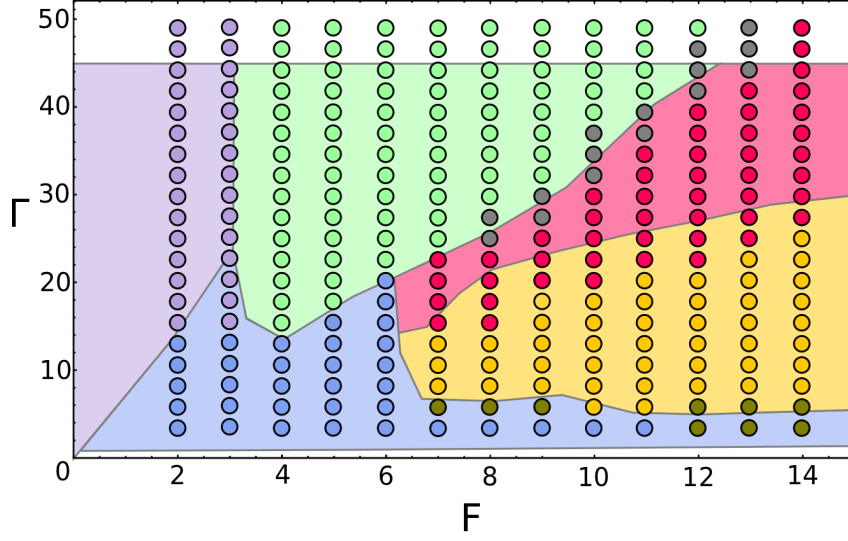
Figure 2: Phase diagram of the shallow granular bed with $a = 4$. Background is taken from [4], where experiments and simulations where used; dots correspond to ED simulations. Gaseous phase (purple), Bouncing Bed (blue), Undulations (yellow), Leidenfrost (red) and Convection (green).
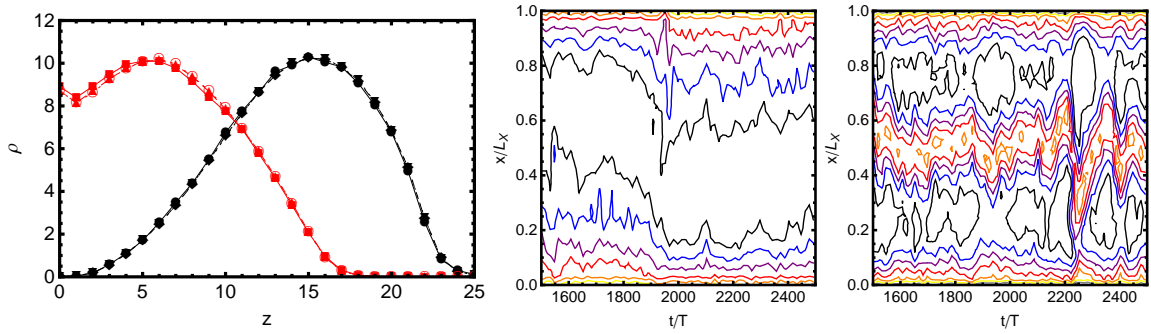


Figure 3: (Left) Vertical number density ($\rho$) profile, at $\phi = 0$ (black) and $\phi = \pi$ (red), for $L_x = 10$ (solid), $L_x = 50$ (dashed) and $L_x = 100$ (points). (Right) Density spatio-temporal diagram for $L_x = 60$, in the convective state. Black is low density.
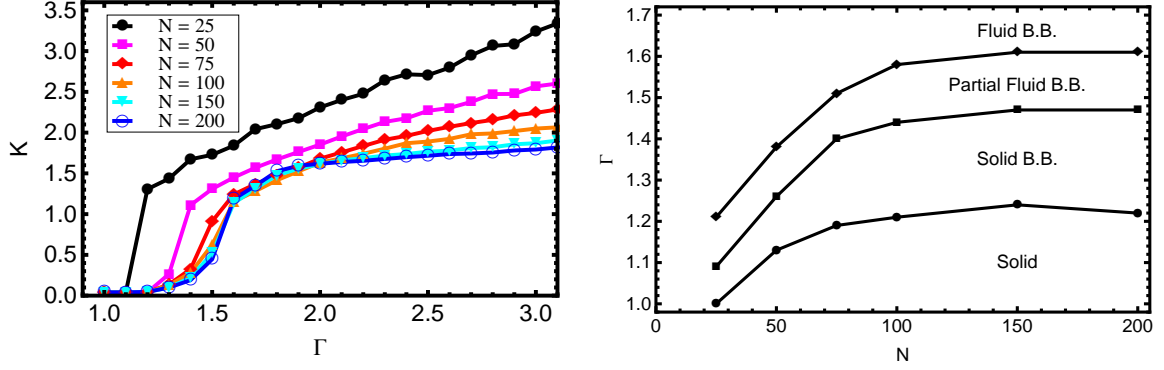
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Figure 4: (Left) Kinetic energy of the particles as a function of the amplitude of oscillation $A$, for several different total number of particles $N$. (Right) Phase diagram of the column system for low energy region, with $\omega = 1.0$.

In general, we see that the basic physics of the Leidenfrost-Convection transition is recovered in a system with $L_x = 50$, and can even be present for lower widths until $L_x = 20$, although in that case the walls have a bigger influence on the convective state. This can be very helpful for the hydrodynamic approach, as it shows that it is possible to have a much smaller system with the same physics, leading to a dramatic increase in simulation speed, as the hydrodynamic equation solver is very computationally expensive. The typical length-scale of the convective role also leads to a better characterization of the state, useful for further theoretical approaches.

**Column**

The width of the system can be reduced until the geometry corresponds to a tall square container. We study this geometry with the idea of understanding the basic behaviors of the vertically vibrated system.

When energy injection is low, all particles remain essentially still, only moving up and down with no relative velocity with respect to the base. We call this the *solid* state. For $\Gamma > 1.1$ the solid detaches from the base, essentially corresponding to a *bouncing bed* state. Particles in this case move only around their stable, almost crystalline positions. The system then goes through different types of bouncing beds, as particles progressively fluidize, from top to bottom. In Figure 4a the kinetic energy of the grains, $K$, is plotted against $\Gamma$, for several $N$ and fixed frequency $\omega = 1.0$. The transition is seen as a well defined, one order of magnitude change in $K$, when $\Gamma$ only changes, at most, 30%. After the transition the energy continues to increase at a much slower rate.

Looking closely at the transition region, one can observe that there are two different regimes with different slopes. First the energy increases with a similar rate as when already in the final state, and then a more abrupt region is observed.

All these regions can be identified with qualitatively different behaviors. When $K \ll 1$, the energy injection is not enough to lift any particle from its resting position. The energy of the system begins to increase when particles are given enough energy to leave the floor. First, only top particles move and only around stable positions, slightly increasing the energy by colliding with their neighbors. The change in slope occurs when the free flight of the top particles is large enough that they can go over their neighbors. This considerably increases the temperature of the top layer, as particle now don't have a stable position and are constantly moving in the horizontal direction.

In order to sketch a phase space, we interpolate $K$ for each of the different regions by a linear function, and define the critical points as those at which the lines intersect. Figure 4 shows the obtained map in the $(N, \Gamma)$ space; a convergence to critical points independent of $N$ is observed. It is necessary to remark, though, that as $N$ increases, the transition between the two middle regions tends to blur, but until $N = 200$ it is still possible to observe it. This convergence is expected; remember that the pressure in a granular pile is constant after a certain height.

In the low amplitude ($A \sim 0.1\sigma$), high frequency limit ($\Gamma > 1$), the previously observed transition of the kinetic energy vanishes. $K$ increases in a similar shape as in the middle frequency and amplitude region, but with no clear discontinuities. This fact agrees with our previous explanation of particles having enough energy to bounce over each other. For $N > 150$, $K(\Gamma)$ converges to a given form for all $N$ explored.

For higher amplitudes, $A \sim 4\sigma$ (the value used for the longer system), a qualitative change of behavior is seen. The system remains in essentially a bouncing bed state, but the center of mass of the grains starts oscillating with
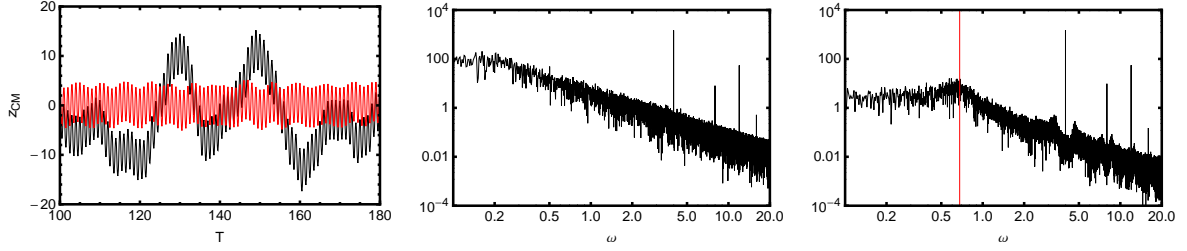
Figure 5: (Left) Vertical center of mass, $z_{cm}$, in time, for $F = 3.125$ (black) and $F = 25$ (red). (Right) Spectrum of the $z_{cm}$ time signal, for $F = 3.125$ (middle), and $F = 25$ (right).

a given frequency, much lower than the base one $\omega$. We pay attention to the vertical center of mass of the system:

$$z_{cm} = \frac{1}{N} \sum_i z_i$$

The temporal evolution of $z_{cm}$ clearly shows the oscillation of the whole system in phase with the oscillation of the base. This frequency coexists with bigger, longer fluctuations, that decrease their intensity as $F$ is increased. In Figure 5 two time series are shown, for $F = 3.125$ ($N = 50$) and $F = 25$ ($N = 400$). The difference between them is evident, although it must be noticed that both of them present long fluctuations, but for $F = 3.125$ this fluctuations are considerably larger. The existence of this second frequency of oscillation can be confirmed by observing the spectrum of this signal. This is shown in Figure 5b and 5c. Both show very defined peaks at and at the harmonics of the oscillation frequency ($\omega = 4$), although for the $F = 25$ case the frequencies are slightly larger and present other peaks around them. If data is taken stroboscopically with the base frequency, then this peaks disappear. The low frequencies oscillations can be seen as a not-so-defined but relevant peak at $\omega = 0.68$ in system with more particles, that is, when fluctuations are smaller they are more coherent in time.

### Segregation

Finally we considered binary mixtures in the vibrated shallow box geometry, where particles can differ in either mass or size. We label them $A$ or $B$ particles, where $A$ particles have unitary mass and diameter, that is, $m_A = 1$ and $\sigma_A = 1$. At least three new parameters are added when considering two particle species, that is $m_B$, $\sigma_B$ and the number of $B$ particles $N_B$, with $N = N_A + N_B$. This is considering that both $A$ and $B$ particles have the same elastic and friction coefficients between them, and with the walls.

As control parameters we consider the ratio of masses $m_r = m_B/m_A$, the ratio of diameters $\sigma_r = \sigma_B/\sigma_A$, and the concentration of $B$ particles, that is $n_B = N_B/N$. Of course, the control parameters in the mono-disperse system are still highly relevant: $\omega$, $A$ and $N$. This highly dimensional phase space is impossible to study extensively; in this report we just present preliminary observations for mass binary mixtures.

Useful to quantify and observe the segregated states are the number density profiles in the $x$ or $z$ direction, for each particle species, $\rho_{A,B}(x)$ and $\rho_{A,B}(z)$. The profiles are obtained by coarse-graining the system in the corresponding direction and counting the number of particles in each column or row.

In the Leidenfrost state, vertical segregation can be seen, where heavy particles gather in the middle of the system (see Figure 6a). For high enough $m_r$ and after a much longer timescale than vertical segregation, segregation increases even further as light particles gather in the sides, as shown in Figure 6b and 6c.

# Future Work

In general, until now, much progress has been made in reproducing known results using the event-driven approach, allowing for much faster simulations. This makes it feasible to explore the phase space; the first step was reducing the length of the system, with the goal of diminishing future hydrodynamic simulations time. The step of reaching a square geometry (column of grains) seemed obvious, and seems to provide further insight into how the non-homogeneous stable states come to be. A general refinement and deeper exploration of the results here presented is needed, in order to provide a more general picture of vertically vibrated granular systems.
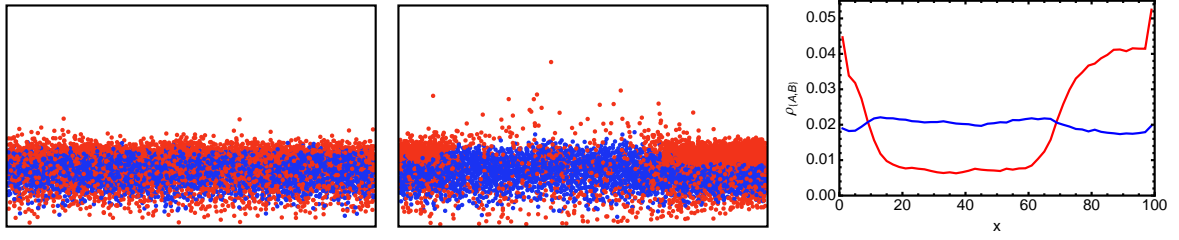
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Figure 6: (Left) Configuration of a mass binary system with $m_r = 2.0$ (left) and $m_r = 5$ (center), in the Leidenfrost state. (Right) Horizontal number density profiles for both $A$ (red) and $B$ (blue) particles, with $m_r = 5$ and $\omega = 2.3$.

On the other hand, hydrodynamic simulations have not produced any relevant output. Nevertheless, progress is being made in understanding the software needed for the solution of the granular-hydrodynamic equations, with the desired boundary conditions.

As main future objectives we consider:

- Take part in the development of the differential equation solver software hpGEM.

  - Implement the necessary boundary conditions for the Leidenfrost effect. This involves the familiarization with the moving grid methods, that are already implemented in hpGEM but without proper documentation or available previous work. A free surface would also be the ideal top boundary condition to observe the Leidenfrot-Convection transition.

  - Compare future simulation results with the ones obtained by ED, MD, and previous experimental works.

- Further collaboration with experimental studies of the granular Leidenfrost effect, using ED simulations.

  - Careful study of the Leidenfrost-Convection transition. This involves the creation of adequate order parameters in order to observe possible hysteresis and metastability (with frequency as control parameter).

  - Study the high-frequency, low-amplitude limit, and compare with previous results and analytical expressions. This regimes are hard to reach in experimental studies, but are expected to have a better agreement with hydrodynamics, as it corresponds better to a bottom with constant temperature boundary condition.

- Explore further the system phase space, using the speed advantage of ED simulations.

  - Study further the low frequency oscillations in the column geometry, and see its influence on the regular, long system.

  - Explore the binary mixtures case, and try to explain the segregation with previously known mechanisms.

- See the possibility of comparing the results in the new systems (column, binary mixtures) with experiments.

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