# SIMULATIONS OF VIBRATED GRANULAR MEDIA IN TWO AND THREE DIMENSIONAL SYSTEMS

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We use the direct simulation Monte Carlo (DSMC) method to simulate spheres in two- (2D) and three-dimensional (3D) vibrating boxes. The results obtained by DSMC are compared with results from event driven (ED) simulations and agreement is observed if the density is not too large. With an excluded volume correction for the DSMC method we may access even higher densities. After the agreement between ED and DSMC is established in 2D we extend our simulations to 3D.

## 1 Introduction

In this study we focus on granular media in vibrated containers in two and three dimensions. If dissipation is not too strong and enough energy is fed into the system, e.g. via vibration of the container, the surface of the material may fluidize [1,2] and the energy scales with the typical velocity of vibration rather than with the typical acceleration. [2,3,4] Simulations in 1D [1,2,5] were complemented by two dimensional simulations [2,6] and experiments.[3,7] In 1D and 2D the potential (or kinetic) energy $E$ scales with the typical velocity $V$, i.e. $E \propto V^\alpha$, with $\alpha = 2$ in 1D and $\alpha \approx 1.4$ in 2D. The latter result is obtained from experiments [7], consistent with simulations, with respect to the fact that they lead also to an exponent $\alpha < 2$. Theoretical approaches usually lead to the exponent $\alpha = 2$ in 1D and 2D, see Ref. [8] and references therein.

In the following we introduce the numerical methods used and establish coincidence in 2D and 3D. We will discuss different boundary conditions and their effect on the exponent $\alpha$ in 2D and 3D. We are interested in the influence of the boundary because it always exists in the experiments and often determines the behavior.

## 2 Simulation Aspects

The container is made of a horizontal bottom, two vertical walls, and it is open to the top. The position of the bottom is $z_0(t) = A\sin(2\pi f t)$ , as a function of time $t$, with the amplitude $A$ and the frequency $f$, so that the typical velocity is $V = 2\pi A f$. Before we start the simulations $N$ particles with diameter $d$ are filled into the container with random initial positions and velocities. We assure that the system reaches a steady state before performing averages.

### *2.1 ED simulation method*

In the event driven (ED) method the particles follow an undisturbed Newtonian motion, under the influence of gravity, until an event occurs. An event may be e.g. the collision of two particles and the duration of an event is implicitly zero. We introduce dissipation on contact via the restitution coefficient $\varepsilon$, with $\varepsilon = 1$ in the

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elastic, and $\varepsilon = 0$ in the completely inelastic case. A second restitution coefficient $\epsilon_w$ is used for the collisions with the walls. For details concerning the ED method see references.[6,9]

### *2.2 DSMC simulation method*

Direct simulation Monte Carlo (DSMC) is a method first proposed by Bird for the simulation of rarefied gas flows[10], and was also used for liquid-solid flow simulations (see Ref. [11] and references therein). One of the algorithms advantages is its suitability for parallelization. Here we introduce dissipation and an excluded volume correction and apply the method to dry granular media.

In DSMC the evolution of the system is integrated in time steps $\tau$. At each time step every particle is first moved without interaction with other particles. The particles are then sorted into spatial cells with length $L$ and volume $V_c = L^D$, where $D$ is the dimension. $L$ is set to one half of the mean free path but not less than two diameters of the beads. The time step $\tau$ is chosen small enough to assure that even the fastest particle needs several time steps to cross a cell. Between particles in the same cell we assume stochastic collisions to take place. The rules for this collisions are taken from kinetic theory. First we choose

$$M_c = \frac{N_c(N_c-1)\sigma v_{max}\tau}{2V_c} \tag{1}$$

collision pairs in each cell. $N_c$ is the number of particles in the cell, $v_{max}$ is an upper limit for the relative velocity between the particles, $\sigma$ the scattering cross section of spheres ($\sigma_{2D} = 4R$, $\sigma_{3D} = 4\pi R^2$). To get $v_{max}$ we sample the velocity distribution from time to time and set $v_{max}$ to twice the maximum particle velocity found. In order to get the correct number of collisions with regard to the actual relative velocities we apply an acceptance-rejection method: For a pair of particles $i$ and $j$ the collision is performed if

$$\frac{|\vec{v}_i - \vec{v}_j|}{v_{max}} < Z, \tag{2}$$

where $Z$ is independent uniformly distributed in the interval $[0,1]$. This method leads to a collision probability proportional to the relative velocity of the particles.

Since the collision takes place regardless of the position in the cell, we have to choose an impact parameter $b$ in order to calculate the post collision velocities. Molecular chaos is assumed here, $b$ is drawn from a uniform distribution in the interval $[-2R, 2R]$ in 2D or in a circle with radius $2R$ in 3D. We tested the validity of this assumption with ED and found no deviations in the parameter range discussed below. The rest of the collision scheme is identical with the event driven procedure, so that the normal component of the post collision velocity is $\vec{u}^{(n)} = -\epsilon\vec{v}^{(n)}$, whereas the tangential component remains unchanged.

To get better results at higher densities we extend the DSMC method in two respects and refer to the modified method as DSMC2. Firstly we add an offset of $2R$ to the particle distance along the direction of the momentum transfer[12]. Secondly we correct $M_c$ in equation (1) by replacing the volume $V_c$ of a cell with the effective

free volume $V_c - V_0$, where $V_0$ is the volume the particles in that cell would need in a random close packing (packing fraction 0.82 in 2D [13] and 0.64 in 3D [14] ).

## 3 Results

### *3.1 Comparison of DSMC and ED in 2D*

We chose the height of the center of mass to measure the energy in the system. To evaluate the validity of the DSMC method for this application we first compare ED, DSMC and DSMC2 in two dimensional simulations. In figure 1 we plot the height of the center of mass $H$ vs. velocity $V$ for elastic walls and inelastic particles as well as the particle number density as a function of height for $f$=100Hz and $V$=0.11m/s. At low excitations of the bottom plate ($V < 0.6$m/s) the DSMC method is not longer valid. However, the improved DSMC2 method still gives good agreement with ED down to $V = 0.06$m/s. In this case the density is about 84% of the density the system has at rest. The much better agreement of DSMC2 with ED can also be seen in the density distribution.

In figure 2 we plot the probability distribution for the horizontal ($U_x$) and vertical ($U_z$) velocities. Again we see agreement of DSCM2 and ED. The mean square velocity is larger for elastic walls compared to dissipative walls and the distribution of the vertical component is asymmetric with the maximum shifted towards negative velocity. The decay for positive velocities is slower, due to the dissipation in the system and a net energy flux from the bottom upwards.

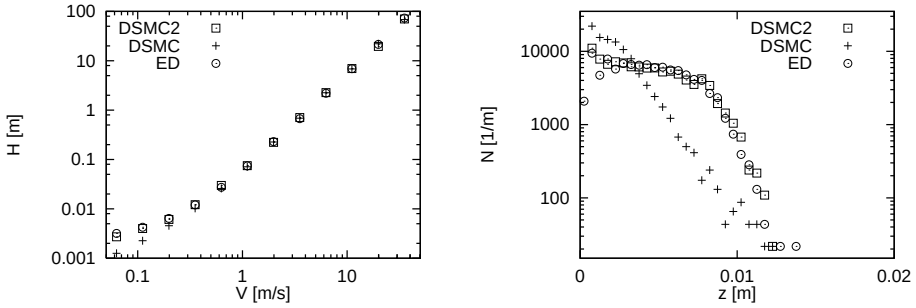


Figure 1: Comparison of the three different methods: DSMC2, DSMC and ED. Left: height of the center of mass vs. $V$. Right: density distribution for $V = 0.11$m/s.

### *3.2 Different boundary conditions in two dimensions*

The scaling behavior was investigated like in Refs. [6,9] The results of DSMC2 are in reasonable agreement with the previous results of ED (see figure 3). This is true for the overall scaling and for the deviation from the theoretical expected power law $H \sim V^2$ at small $V$ values. This proves that the reason for these phenomena is neither long range correlation nor a likewise multiple particle memory effect, since both are not explicitly included in DSMC2.

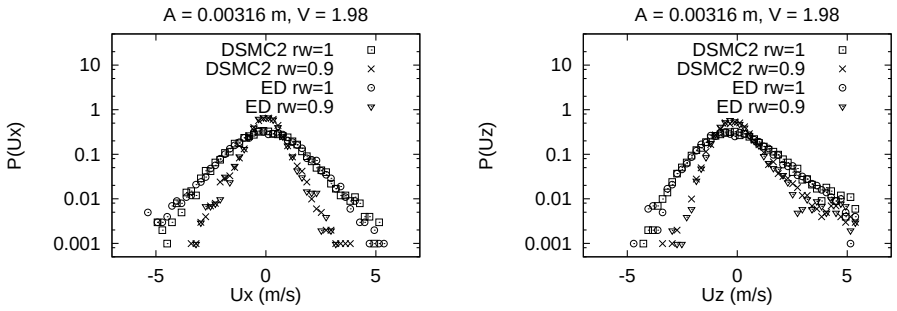


Figure 2: Semilog plot of the probability distribution $P(U)$ vs. horizontal velocity $U_x$ (left) and vertical velocity $U_z$ (right).

To understand the reason for the strange dependency of $H$ on $V$ with dissipative particles and walls we plot $H(V) - H(0)$ with the height of the center of mass at rest $H(0) = 2.492 \times 10^{-3}$m for all possible combinations of $\epsilon$ and $\epsilon_w$. The agreement between DSMC2 and ED for all boundary conditions shows that the particle particle and particle wall interaction is represented correctly. For elastic walls and dissipative particles we find $\alpha \approx 2$ above $V \approx 0.6$m/s. For inelastic walls we observe a smaller $\alpha \approx 1.5$ over two decades, whereas we see two different regimes in the case of elastic particles and inelastic walls. In the latter case we find $H \sim V$ for small $V$ and $H \sim V^2$ for large $V$. For $V > 5$m/s the density is low enough that many collisions with the walls occur before the next particle collision. Therefore the horizontal velocity of a particle decays between two particle collisions if the walls are inelastic. Thus the dissipation of energy per unit time through the walls decreases due to decreasing collision frequency. Particle particle collisions are necessary to trigger dissipation and the system behaves similar to a system with dissipative particle collisions.

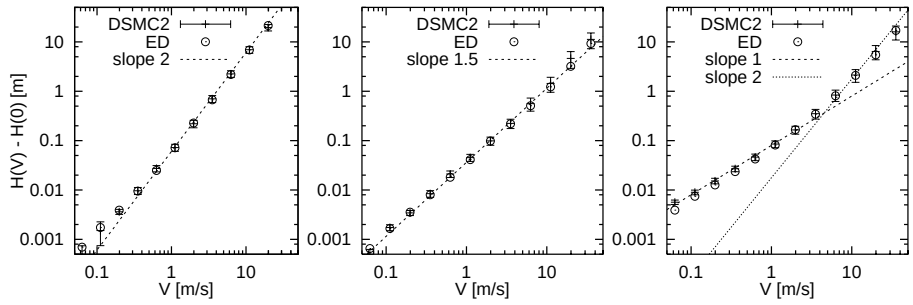


Figure 3: Reduced height $H(V) - H(0)$ with different dissipation combinations. Left: $\epsilon_w = 1, \epsilon = 0.9$ , middle: $\epsilon_w = 0.9, \epsilon = 0.9$, right: $\epsilon_w = 0.9, \epsilon = 1$. The error bars indicate the standard deviation.

### *3.3 Investigation in three dimensions*

After the agreement between ED and DSMC2 is established in 2D, we can now investigate the behavior in 3D. In order to obtain densities comparable to 2D we increase the number of beads by a factor 10, because the system is 10 diameters wide and deep. We estimate the height of the center of mass at rest to $H_{3D}(0) = 2.2 \times 10^{-3}$m using an ED simulation with dissipative beads and a fixed bottom plate.

We do not find new qualitative aspects of the system's behavior when we make the transition from 2D to 3D irrespective of the particular boundary condition chosen. Thus effectively, we recover the physics of a 2D system, because of the equivalence of the two horizontal dimensions.

## 4 Discussion and Conclusion

We apply the DSMC method to dry granular media simulations, accounting for dissipation and excluded volume. With the corrections described above we get reasonable quantitative agreement between the deterministic ED method and the partially stochastic DSMC2 algorithm. This proves that the assumptions made for DSMC are correct in the parameter range discussed here and that the behavior of the system does not depend on possible correlations between collisions. We compared various boundary conditions and report that the system shows qualitatively the same behavior of the height of the center of mass in 2D and 3D, what proves that the scaling observed is not a 2D artifact. Still open is the extension of DSMC to densities up to the stable packing density.

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