THE OUTLINE OF THE DIRECT SIMULATION MONTE CARLO METHOD

In a DSMC method, the phase space is filled with quasi-particles, each representing a probability to find a particle at a certain location $\boldsymbol{r} \pm \mathrm{d}\boldsymbol{r}$ with a velocity $\boldsymbol{v} \pm \mathrm{d}\boldsymbol{v}$, at a given moment in time $t \pm \mathrm{d}t$. Hence, each simulated particle represents F_N number of real particles, where F_N can be a very large number. The simulated region in the coordinate space can be split into smaller cells. This is not important for homogeneous systems, however necessary when simulating inhomogeneous systems and flows. Denoting by V_c volume of cells and n number density of the real system, the number of real particles in the cell is given by $N = nV_c$, where index c means per cell. Now, we can write the number of simulated quasi-particles in a cell as $N_s = nV_c/F_N$. After a time step Δt in a simulation, each of the quasi-particles moves in the coordinate space according to $\boldsymbol{r}_i \to \boldsymbol{r}_i + \boldsymbol{v}_i \cdot \Delta t$ and the changes in the velocity space will be estimated from the collisional laws of the system $\boldsymbol{v}_i \to \boldsymbol{v}_i'$.

The main idea of the DSMC method is to correctly estimate the number of collisions for a given Δt. The probability of two simulated particles colliding could be estimated as a ratio of the volume swept out by their collision cylinder to the volume of the cell:

$$P = \frac{F_N \sigma g \Delta t}{V_c} \ , \tag{1}$$

where σ is the cross-section and g is the relative speed of two particles. For N particles in a cell, there are $N(N-1)/2$ possible collision pairs, and we can check each of the pairs for a possible collision. For each pair, we can generate a random number $rnd(0,1)$, uniformly distributed between zero and one, and accept the pair if this number is smaller than P. However, this is extremely ineffective, since the probability P are very small, and the number of collision pairs is very large. To increase effectiveness, we can reduce the number of collision pairs, while proportionally increasing the probability of acceptance (colliding). The maximal effectiveness $P_{\max}$ is obtained when the probability of acceptance is one, hence we can write

$$P_{\max} = \frac{F_N (\sigma g)_{\max} \Delta t}{V_c} \ . \tag{2}$$

The number of tested pairs is then estimated to be

$$N_p = \frac{F_N}{2V_c} \cdot N^2 (\sigma g)_{\max} \cdot \Delta t \ , \tag{3}$$

whit the probability of acceptance

$$P = \frac{\sigma g}{(\sigma g)_{\max}} \ . \tag{4}$$

In the case of a polydisperse system, the collision partners can have different masses, hence different mobilities and varying cross-section parameters. The number of tested pairs and acceptance probabilities can be then adjusted as

$$P_{kj} = \frac{\sigma_{kj} g_{kj}}{\{(\sigma g)_{\max}\}_{kj}} \,, \tag{5}$$

and

$$N_{p,kj} = \frac{F_N}{2V_c} \cdot N_k N_j \{(\sigma g)_{\max}\}_{kj} \cdot \Delta t \,. \tag{6}$$

Since $\{(\sigma g)_{\max}\}_{kj}$ is arbitrary, we can choose a single maximal value for the whole system, and write it as $(\sigma g)_{\max}$, which would be independent on k and j. Now, we can write

$$P_{kj} = \frac{\sigma_{kj} g_{kj}}{(\sigma g)_{\max}} \,, \tag{7}$$

and

$$N_p = \frac{F_N}{2V_c} \cdot (\sigma g)_{\max} \Delta t \cdot \sum_{k,j} N_k N_j \,. \tag{8}$$

THE DSMC ALGORITHM

The numerical simulation can be split into several steps:

1. Initialization of the system and constants, such as F_N, V_c, Δt and particle parameters;
2. Randomly distribute particles across the system, and initialize their velocities;
3. Choose the value of $(\sigma g)_{\max}$;
4. Propagate the positions of particles according to $\boldsymbol{r}_i \to \boldsymbol{r}_i + \boldsymbol{v}_i \Delta t$;
5. Calculate the value N_p according to (8);
6. Randomly choose two particles k and j in a cell;
7. Generate a random number $r \in (0, 1)$;
8. Generate a random direction vector $\boldsymbol{e}$;
9. If the value $\sigma_{kj} |\boldsymbol{e} \cdot (\boldsymbol{v}_k - \boldsymbol{v}_j)| > r \cdot (\sigma g)_{\max}$, accept the pair;
10. If the pair is accepted, perform a collision operation, and change velocities accordingly;

11. Go back to step 6 and repeat N_p times;

12. Set simulation time to $t \to t + \Delta t$;

13. Go back to step 4 and repeat until the end of the simulation;

AGGREGATION AND FRAGMENTATION PROCESSES

If we allow particles to stick together after a collision, or fragment into smaller particles, we need to adjust our simulation accordingly. The model dictates, that an aggregation happens if the impact energy of particles is less than a certain value $E_{\rm imp} < E_{\rm agg}$, or $g_{kj} < g_{\rm agg}$. Mechanically, the aggregation process is quite straightforward. Let us discuss the fragmentation process. First, we assume that it happens if the impact energy of particles is larger than a certain value $E^n_{\rm imp} > E_{\rm frag}$, or $g^n_{kj} < g_{\rm frag}$, where superscript n denotes the normal component of the impact velocity. In general, it is not possible to analytically obtain the velocities of each fragment after a shattering collision, however, we can make certain simplifications. First, we assume that during a fragmentation process, both impactors completely disassemble into monomers. Hence, if masses of colliding particles are $m_k = k \cdot m_0$ and $m_j = j \cdot m_0$, then after fragmentation we have $k + j$ monomers with masses m_0. Second, since in the center of mass frame of the colliding particles, there is no preferred direction of velocities, and since all monomers are identical, we can assume that they gain equal amounts of kinetic energy. These assumptions lead to the following conclusions. If the impact energy is

$$E_{\rm imp} = \frac{\mu_{kj} g^2_{kj}}{2} \ , \tag{9}$$

where $\mu_{kj} = m_k m_j/(m_k + m_j)$, and if $0 \leq \varepsilon_f \leq 1$ is a parameter which controls the amount of the energy which is dissipated during the fragmentation process, the energy we need to equally distribute among monomers can be calculated as

$$E_0 = \varepsilon^2_f \cdot \frac{\mu_{kj} g^2_{kj}}{2} = (k + j)\frac{m_0 u^2}{2} \ , \tag{10}$$

where u is the speed of each monomer in the center of mass frame of reference. Now, we can write

$$u = \frac{\sqrt{kj} \cdot \varepsilon_f g_{kj}}{k + j} \ . \tag{11}$$

If $\hat{\boldsymbol{u}}_i$ are direction vectors of each shattered monomer, their velocity vectors are given by

$$\boldsymbol{u}_i = \frac{\sqrt{kj} \cdot \varepsilon_f g_{kj}}{k+j} \hat{\boldsymbol{u}}_i \ , \quad i = 1, 2, \ldots, k+j \ . \tag{12}$$

Since the total momentum conserves, we can write $\sum_{i=1}^{k+j} \boldsymbol{u}_i = \boldsymbol{0}$. Now, we can write the velocity of each monomer in the laboratory frame of reference as

$$\boldsymbol{v}_i = \frac{k\boldsymbol{v}_k + j\boldsymbol{v}_j}{k+j} + \frac{\sqrt{kj} \cdot \varepsilon_f g_{kj}}{k+j} \hat{\boldsymbol{u}}_i \ . \tag{13}$$

THE DSMC ALGORITHM WITH AGGREGATION AND FRAGMENTATION

Now we can extend our simulation algorithm to include both aggregation and fragmentation processes:

1. Initialization of the system and constants, such as F_N, V_c, Δt and particle parameters;
2. Randomly distribute particles across the system, and initialize their velocities and size distributions, for instance monomers only initial distribution;
3. Choose the value of $(\sigma g)_{\max}$;
4. Propagate the positions of particles according to $\boldsymbol{r}_i \to \boldsymbol{r}_i + \boldsymbol{v}_i \Delta t$;
5. Calculate the value N_p according to (8);
6. Randomly choose two particles k and j in a cell;
7. Generate a random number $r \in (0, 1)$;
8. Generate a random direction vector $\boldsymbol{e}$;
9. If the value $\sigma_{kj} |\boldsymbol{e} \cdot (\boldsymbol{v}_k - \boldsymbol{v}_j)| > r \cdot (\sigma g)_{\max}$, accept the pair;
10. If the pair is accepted, perform a collision operation:
    (a) Calculate the impact energy $E_{\text{imp}} = \mu_{kj} g_{kj}^2 / 2$ of particles;
    (b) If $E_{\text{imp}} < E_{\text{agg}}$, then remove both particles, and add a new particle of mass m_{k+j} and velocity $\boldsymbol{V} = (m_k \boldsymbol{v}_k + m_j \boldsymbol{v}_j)/(m_k + m_j)$ at a random position;

(c) If the impact energy is larger than E_{agg} but $E^n_{\mathrm{imp}} < E_{\mathrm{frag}}$, then do not remove or add new particles, change the velocities of particles according to collision laws;

(d) If the impact energy $E^n_{\mathrm{imp}} > E_{\mathrm{frag}}$, then remove both particles. Add $k + j$ monomers at random positions. Generate $k + j - 1$ unit vectors $\hat{\boldsymbol{u}}_i$, and apply velocities from (13) to $k + j - 1$ newly created monomers. Set the velocity of the last monomer to be

$$\boldsymbol{v}_{k+j} = \frac{k\boldsymbol{v}_k + j\boldsymbol{v}_j}{k+j} - \frac{\sqrt{kj} \cdot \varepsilon_f g_{kj}}{k+j} \sum_{i=1}^{k+j-1} \hat{\boldsymbol{u}}_i \ . \tag{14}$$

11. Go back to step 6 and repeat N_p times;

12. Set simulation time to $t \to t + \Delta t$;

13. Go back to step 4 and repeat until the end of the simulation;

KINETIC PARAMETERS

The one-particle distribution function $f(\boldsymbol{r}, \boldsymbol{v}, t)$ is normalized to give us the number of particles in the system:

$$\int f(\boldsymbol{r}, \boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{v} = N \ .$$

If we consider a spatially homogeneous system, we can assume that the distribution function does not depend on the position in space, and that it describes only the velocity distribution, hence

$$\int \mathrm{d}\boldsymbol{r} \int f(\boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{v} = N \ , \quad \Rightarrow \quad \int f(\boldsymbol{v}, t) = \frac{N}{V} = n \ .$$

Given a velocity function $A(\boldsymbol{v}, t)$, its ensemble average $\langle A(t) \rangle$ can be obtained from

$$n \langle A(t) \rangle = \int A(\boldsymbol{v}, t) f(\boldsymbol{v}, t)\, \mathrm{d}\boldsymbol{v} \ . \tag{15}$$

Ensemble averages of parameters , that depend on two particles $B(\boldsymbol{v}_1, \boldsymbol{v}_2, t)$, can be obtained by the use of two-particle distribution function $f_2(\boldsymbol{v}_1, \boldsymbol{v}_2, t)$:

$$\begin{aligned} n^2 \langle B(t) \rangle &= \int B(\boldsymbol{v}_1, \boldsymbol{v}_2, t) f_2(\boldsymbol{v}_1, \boldsymbol{v}_2, t)\, \mathrm{d}\boldsymbol{v}_1\, \mathrm{d}\boldsymbol{v}_2 \ , \\ n^2 &= \int f_2(\boldsymbol{v}_1, \boldsymbol{v}_2, t)\, \mathrm{d}\boldsymbol{v}_1\, \mathrm{d}\boldsymbol{v}_2 \ . \end{aligned} \tag{16}$$

From the molecular chaos assumptions, we can write the two-particle distribution function in terms of two one-particle distribution functions as

$$f_2(\boldsymbol{v}_1, \boldsymbol{v}_2, t) = g_2(\sigma) f(\boldsymbol{v}_1, t) f(\boldsymbol{v}_2, t) \ , \tag{17}$$

where $g_2(\sigma)$ is the pair correlation function at contact. Now, the two-particle ensemble averages can be written as

$$n^2 \left\langle B(t) \right\rangle = g_2(\sigma) \int B(\boldsymbol{v}_1, \boldsymbol{v}_2, t) f(\boldsymbol{v}_1, t) f(\boldsymbol{v}_2, t) \, \mathrm{d}\boldsymbol{v}_1 \, \mathrm{d}\boldsymbol{v}_2 \ . \tag{18}$$

Estimation of the number of collisions

By the definition of the one-particle distribution function, the number of particles with velocity $\boldsymbol{v}$ at a position $\boldsymbol{r}$ at a time t is given by $\mathrm{d}N = f(\boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{r} \, \mathrm{d}\boldsymbol{v}$. Here $\mathrm{d}\boldsymbol{r} = \mathrm{d}V$ is an infinitesimal volume around the position $\boldsymbol{r}$. Let us take a particle at position $\boldsymbol{r}_1$ with a velocity $\boldsymbol{v}_1$, and consider its collision with another particle with velocity $\boldsymbol{v}_2$ within the given time interval Δt. Constructing a collision cylinder with a base area $\mathrm{d}S = \sigma \, \mathrm{d}\boldsymbol{e}$, and height $h = |\boldsymbol{g}_{12}| \Delta t$, where $\boldsymbol{g}_{12} = \boldsymbol{v}_2 - \boldsymbol{v}_1$ is the relative velocity, we can write its volume as

$$\mathrm{d}V_{cc} = h \, \mathrm{d}S = \sigma |\boldsymbol{g}_{12}| \Delta t \ . \tag{19}$$

Now, the number of particles with velocities $\boldsymbol{v}_1$ within this volume element is equal to $f(\boldsymbol{v}_1, t) \, \mathrm{d}\boldsymbol{v}_1 \, \mathrm{d}V_{cc}$. The number of particles with velocities $\boldsymbol{v}_2$ in the entire system is $f(\boldsymbol{v}_2, t) \, \mathrm{d}\boldsymbol{v}_2 \, V$, which is the number of collision cylinders in the system. Hence, the number of collisions ν between particles with velocities $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ that occur during Δt is equal to:

$$\nu(\boldsymbol{v}_1, \boldsymbol{v}_2) = \frac{1}{2} f(\boldsymbol{v}_2, t) \, \mathrm{d}\boldsymbol{v}_2 \, V \cdot f(\boldsymbol{v}_1, t) \, \mathrm{d}\boldsymbol{v}_1 \, \sigma |\boldsymbol{g}_{12}| \Delta t \ , \tag{20}$$

where the factor $1/2$ is added to account for double counting. Now, the total number of collisions ΔN_c within time interval Δt is obtained by integrating over the above expression

$$\Delta N_c = \frac{1}{2} V \sigma \Delta t \int \mathrm{d}\boldsymbol{v}_1 \, \mathrm{d}\boldsymbol{v}_2 \, |\boldsymbol{g}_{12}| f(\boldsymbol{v}_1, t) f(\boldsymbol{v}_2, t) \ . \tag{21}$$

The integral is nothing else but an ensemble average of the impact speed $|\boldsymbol{g}_{12}|$. Now we have

$$\Delta N_c = \frac{1}{2} V \sigma n^2 \left\langle |\boldsymbol{g}_{12}| \right\rangle \Delta t = \frac{1}{2} N \sigma n \left\langle |\boldsymbol{g}_{12}| \right\rangle \Delta t \ . \tag{22}$$

Maxwellian distribution function

We test our DSMC code against an analytic model, using the Maxwellian one-particle distribution function

$$f(\boldsymbol{v},t) = n\Big(\frac{m}{2\pi T}\Big)^{3/2} \exp\left(-\frac{mv^2}{2T}\right) , \tag{23}$$

where the dependence on time is given through the macroscopic parameters $n(t)$ and $T(t)$. Let us introduce a thermal speed $u_T(t)$ as

$$T(t) = \frac{1}{2} m u_T(t)^2 , \tag{24}$$

and the dimensionless velocity vector as $\boldsymbol{c}(t) = \boldsymbol{v}/u_T(t)$. Now, the distribution function is rewritten as

$$f(\boldsymbol{v},t) = \frac{n}{u_T(t)^3} \cdot \phi(\boldsymbol{c}) , \tag{25}$$

where

$$\phi(\boldsymbol{c}) = \pi^{-3/2} e^{-c^2} = \pi^{-3/2} e^{-\boldsymbol{c}\cdot\boldsymbol{c}} , \tag{26}$$

is the dimensionless distribution function. The two-particle distribution function can now be written as

$$f_{12}(\boldsymbol{v}_1, \boldsymbol{v}_2, t) = g_2 n^2 u_T^{-6} \cdot \phi_{12}(\boldsymbol{c}_1, \boldsymbol{c}_2) , \tag{27}$$

where

$$\phi_{12}(\boldsymbol{c}_1, \boldsymbol{c}_2) = \pi^{-3} \exp\left(-c_1^2 - c_2^2\right) . \tag{28}$$

Average relative speed for Maxwellian distribution of velocities

The average relative speed $\langle |\boldsymbol{g}_{12}| \rangle$ is obtained by solving the next integral

$$\langle |\boldsymbol{g}_{12}| \rangle = \frac{1}{n^2} \int \mathrm{d}\boldsymbol{v}_1 \, \mathrm{d}\boldsymbol{v}_2 \; |\boldsymbol{g}_{12}| f(\boldsymbol{v}_1, t) f(\boldsymbol{v}_2, t) . \tag{29}$$

Since $\boldsymbol{g}_{12} = u_T \boldsymbol{c}_{12}$ and $\mathrm{d}\boldsymbol{v} = u_T^3 \, \mathrm{d}\boldsymbol{c}$, we can rewrite the integral in a dimensionless form as

$$\langle |\boldsymbol{g}_{12}| \rangle = u_T \int \mathrm{d}\boldsymbol{c}_1 \, \mathrm{d}\boldsymbol{c}_2 \; c_{12} \phi_{12}(\boldsymbol{c}_1, \boldsymbol{c}_2) . \tag{30}$$

Changing into the center of mass system, we have

$$\begin{aligned} \boldsymbol{c}_1 &= \boldsymbol{C} - \frac{1}{2}\boldsymbol{c}_{12} , \\ \boldsymbol{c}_2 &= \boldsymbol{C} + \frac{1}{2}\boldsymbol{c}_{12} , \end{aligned} \tag{31}$$

where $\boldsymbol{C}$ is the dimensionless center of mass velocity. Since $\mathrm{d}\boldsymbol{c}_1\,\mathrm{d}\boldsymbol{c}_2 = \mathrm{d}\boldsymbol{C}\,\mathrm{d}\boldsymbol{c}_{12}$, and using

$$\boldsymbol{c}_1^2 + \boldsymbol{c}_2^2 = 2C^2 + \frac{1}{2}c_{12}^2 \,, \tag{32}$$

we have

$$\langle|\boldsymbol{g}_{12}|\rangle = 16u_T\pi^{-1}\int_0^\infty \mathrm{d}C\; C^2 e^{-2C^2}\int_0^\infty \mathrm{d}c_{12}\; c_{12}^3 e^{-\frac{1}{2}c_{12}^2} \,, \tag{33}$$

and solving these standard integrals, we obtain the average impact speed

$$\langle|\boldsymbol{g}_{12}|\rangle = \sqrt{\frac{8}{\pi}}\cdot u_T = 4\sqrt{\frac{T}{\pi m}} \,. \tag{34}$$

Now, the number of collisions in time Δt is

$$\Delta N_c = \frac{1}{2}N\sigma n\,\langle|\boldsymbol{g}_{12}|\rangle\,\Delta t = 2N\sigma n\sqrt{\frac{T}{\pi m}}\Delta t \,, \tag{35}$$

or since $\sigma = 4\pi R^2$, we write

$$\Delta N_c = 8NR^2 n\sqrt{\frac{\pi T}{m}}\Delta t \,. \tag{36}$$

Temperature decay and Haff's cooling

The dynamics of the granular temperature obey the next equation

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -\zeta T \,. \tag{37}$$

Here ζ is the cooling coefficient

$$\zeta = \frac{2}{3}n\sigma g_2 u_T\cdot\mu_2 \,, \tag{38}$$

where

$$\mu_2 = -\frac{1}{2}\int \mathrm{d}\boldsymbol{c}_2\,\mathrm{d}\boldsymbol{c}_1\int \mathrm{d}\boldsymbol{e}\;\Theta(-\boldsymbol{c}_{12}\cdot\boldsymbol{e})|\boldsymbol{c}_{12}\cdot\boldsymbol{e}|\phi_{12}(\boldsymbol{c}_1,\boldsymbol{c}_2)\Delta\left[c_1^2+c_2^2\right] \,, \tag{39}$$

where $\Delta\psi(\boldsymbol{c}) = \psi(\boldsymbol{c}') - \psi(\boldsymbol{c})$ is the change of parameter ψ due to a collision. From the mechanics of restitutive collisions, we know that the post-collisional velocities are

$$\begin{aligned}\boldsymbol{c}_1' &= \boldsymbol{c}_1 - \frac{1+\varepsilon}{2}(\boldsymbol{c}_{12}\cdot\boldsymbol{e})\boldsymbol{e} \,,\\ \boldsymbol{c}_2' &= \boldsymbol{c}_2 + \frac{1+\varepsilon}{2}(\boldsymbol{c}_{12}\cdot\boldsymbol{e})\boldsymbol{e} \,,\end{aligned} \tag{40}$$

which in term gives us

$$\Delta\left[c_1^2+c_2^2\right] = c_1'^2 + c_2'^2 - c_1^2 - c_2^2 = -\frac{1-\varepsilon^2}{2}(\boldsymbol{c}_{12}\cdot\boldsymbol{e})^2 \,. \tag{41}$$

Now, the factor μ_2 reads

$$\mu_2 = \frac{1-\varepsilon^2}{4} \int \mathrm{d}\boldsymbol{c}_2 \, \mathrm{d}\boldsymbol{c}_1 \int \mathrm{d}\boldsymbol{e} \; \Theta(-\boldsymbol{c}_{12}\cdot\boldsymbol{e})|\boldsymbol{c}_{12}\cdot\boldsymbol{e}|^3 \phi_{12}(\boldsymbol{c}_1,\boldsymbol{c}_2) \; . \tag{42}$$

Solving these integrals with the Maxwellian distribution functions, we get

$$\mu_2 = \sqrt{2\pi}\big(1-\varepsilon^2\big) \; . \tag{43}$$

Now, the cooling coefficient is

$$\zeta = \frac{4}{3}\big(1-\varepsilon^2\big) n\sigma g_2 \sqrt{\frac{\pi T}{m}} \; . \tag{44}$$

Using this value of ζ and solving the ordinary differential equation for the temperature dynamics, we obtain the time evolution function for the granular temperature

$$T(t) = \frac{T_0}{\left(1-t/t_c\right)^2} \; , \tag{45}$$

where

$$t_c^{-1} = \frac{8}{3}\big(1-\varepsilon^2\big) n R^2 \sqrt{\frac{\pi T_0}{m}} \; . \tag{46}$$

Here we assumed $g_2 = 1$.

DSMC SIMULATIONS

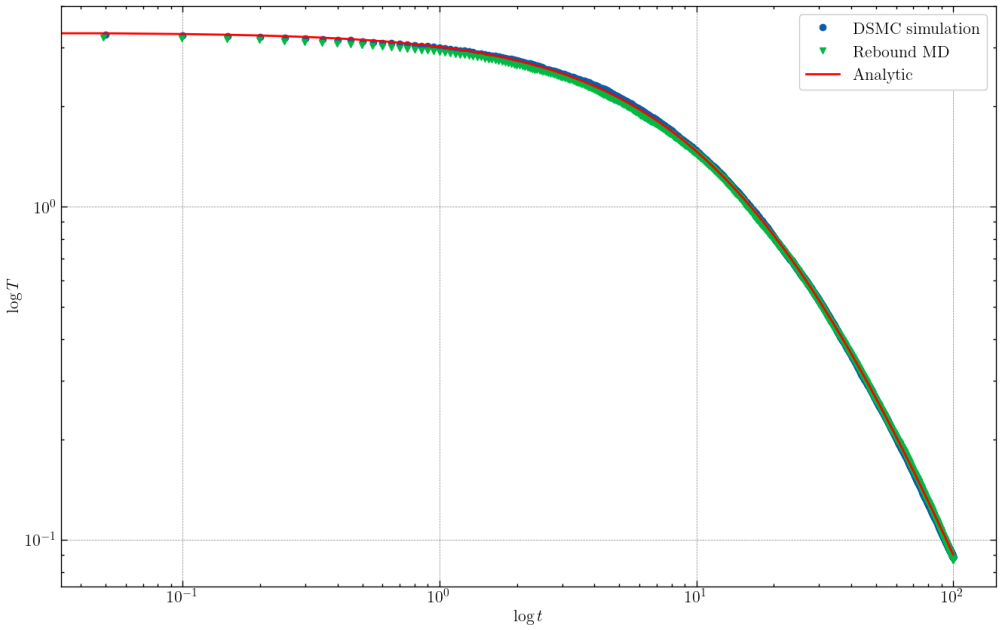

FIG. 1. Simulation of a monodisperse system, with $N = 2000$ particles. Time evolution of the granular temperature

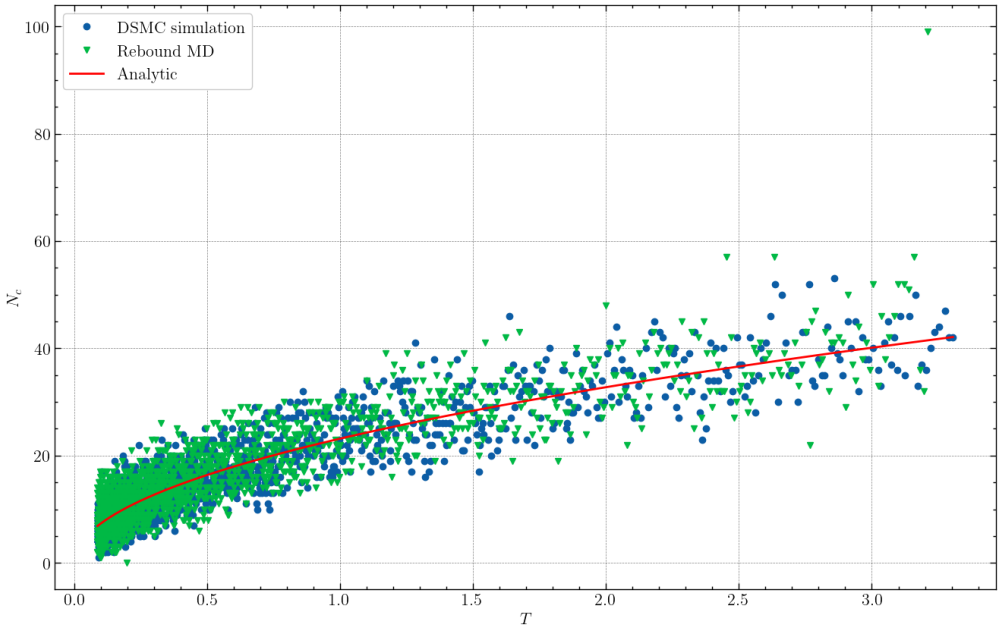

FIG. 2. Simulation of a monodisperse system, with $N = 2000$ particles. Dependence of the number of collision on the temperature of the system.

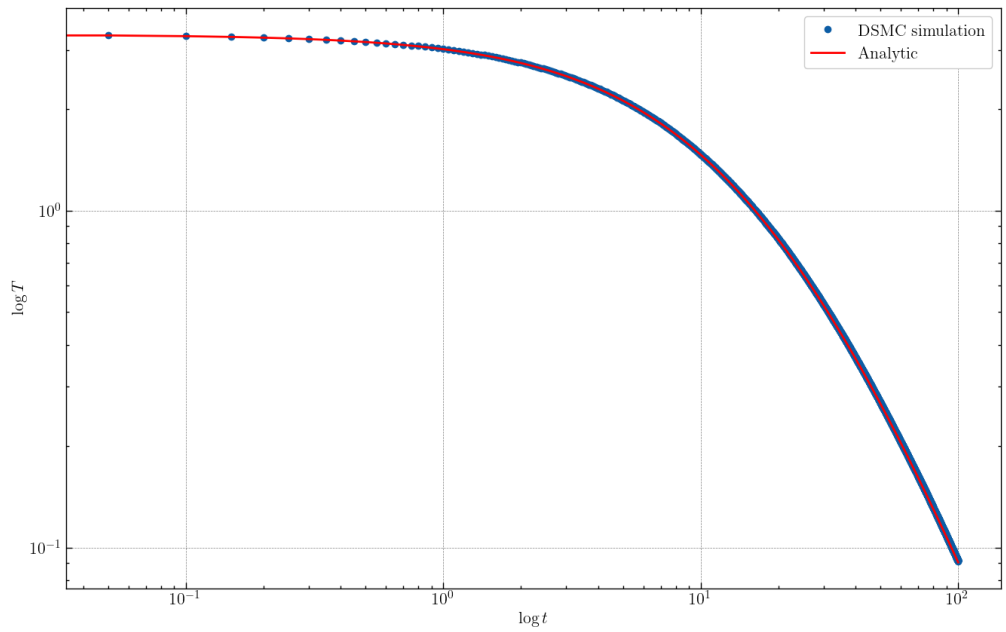

FIG. 3. Simulation of a monodisperse system, with $N = 1\,000\,00$ particles. Time evolution of the granular temperature

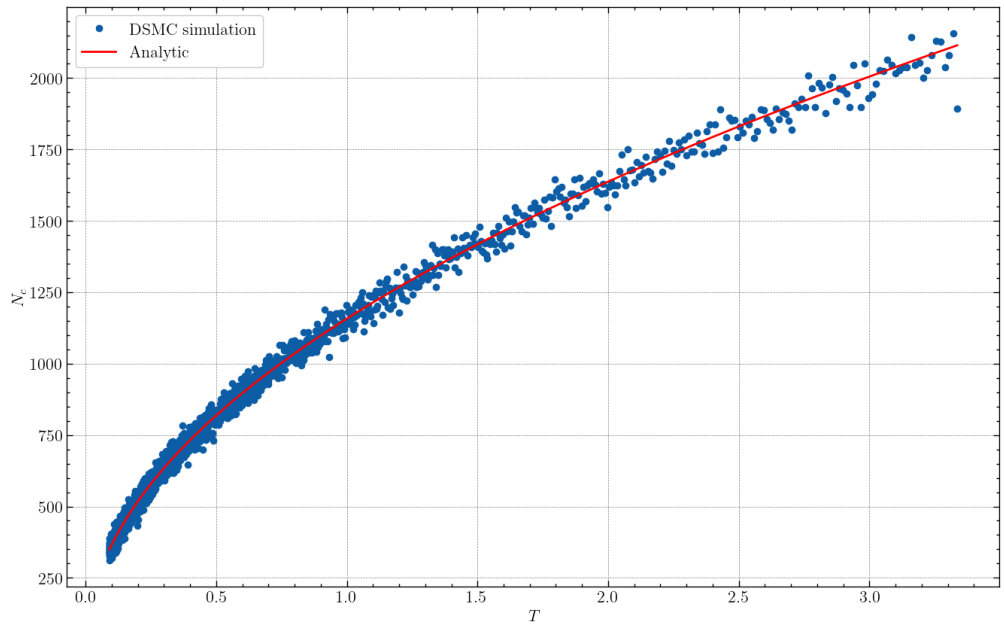

FIG. 4. Simulation of a monodisperse system, with $N = 1\,000\,00$ particles. Dependence of the number of collision on the temperature of the system.

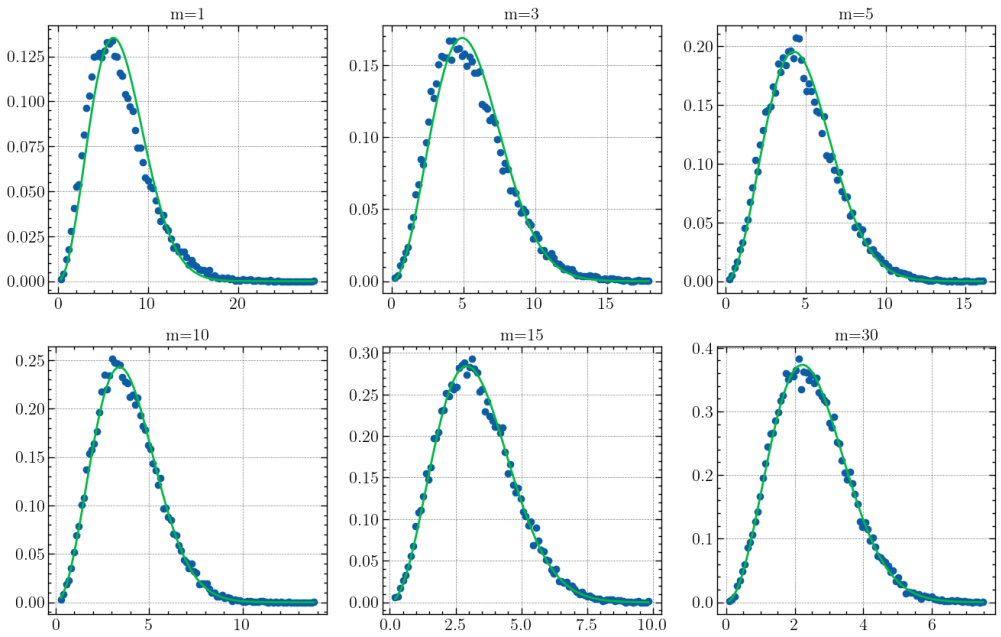

FIG. 5. Velocity distributions after $N_c \approx 1.5 \cdot 10^5$ collisions. Solid lines are theoretical Maxwellian curves.

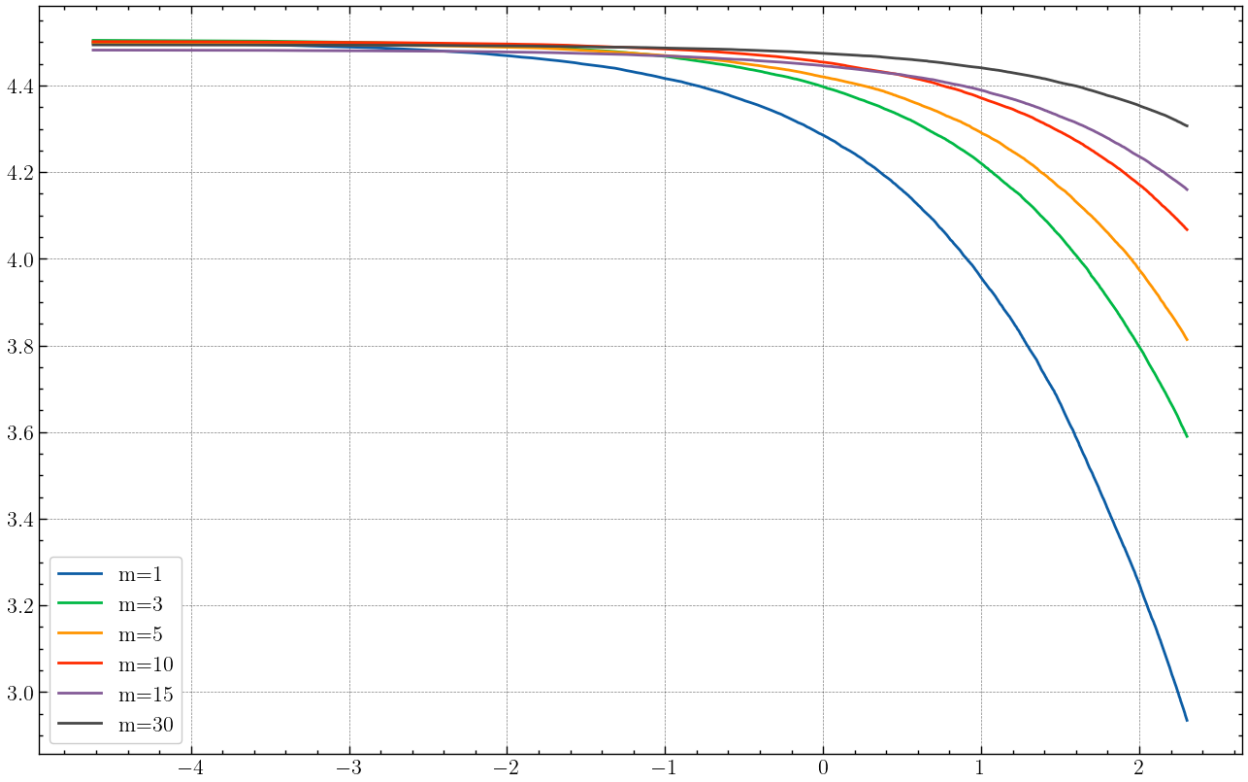

FIG. 6. Temperature evolution of polydisperse system, starting with identical temperatures. We can see that the smaller particles lose more energy over time and cool faster.