

THE MECHANICS OF BINARY INTERACTIONS

Our system comprises an infinite number of mechanically identical, spherical particles known as monomers. These particles have masses m_1 and radii R_1 . When two monomers collide, they lose a certain amount of impact energy and rebound with a coefficient of restitution ε . If the impact energy is below a specific threshold value $E_{\text{imp}} \leq E_{\text{agg}}$, the monomers stick together due to surface forces like van der Waals forces, forming a larger aggregate particle with mass m_2 and radius R_2 . This process is known as *aggregation* and allows the creation of larger particles from individual monomers. A particle of mass m_k is an aggregate of k monomers, hence $m_k = k \cdot m_1$. We assume that the aggregates remain spherically shaped, and their radii scale as $R_k \sim m_k^{1/3} \sim k^{1/3}$.

Conversely, there is another mechanism called *fragmentation* that decreases the sizes of aggregates. If the impact energy is higher than a certain threshold value $E_{\text{imp}} \geq E_{\text{frag}}$, the colliding aggregates break into smaller pieces. The size distribution of the fragmented pieces are difficult to model analytically, and in this work we assume a simplistic model of fragmentation, called *shattering*. When two aggregates of masses m_i and m_j collide with a sufficient energy, both of them shatter into singular monomers, $m_i \rightarrow i \cdot m_1$ and $m_j \rightarrow j \cdot m_1$.

Generalized collisions

Let us consider a collision of particles of masses m_i , m_j and velocities \mathbf{v}_i , \mathbf{v}_j , and radii R_i , R_j . The collision geometry is characterized by the unit vector $\hat{\mathbf{n}}$, which is directed from the center of particle j to the center of particle i at the moment of contact of two particles

$$\hat{\mathbf{n}} = \frac{\mathbf{r}_i - \mathbf{r}_j}{R_i + R_j}, \quad (1)$$

where \mathbf{r}_i and \mathbf{r}_j are position vectors of the particles. The next parameter which describes the collision, is the *restitution coefficient* $0 \leq \varepsilon \leq 1$. This parameter controls the amount of energy dissipated after the collision. The total energy of this binary system, can be split into two parts, the translational energy and the internal energy

$$E = E_{\text{translation}} + E_{\text{internal}} = \frac{MV^2}{2} + \frac{\mu g^2}{2}, \quad (2)$$

where

$$\begin{aligned} \mathbf{V} &= \mu_i \mathbf{v}_i + \mu_j \mathbf{v}_j, \quad \mathbf{g} = \mathbf{v}_i - \mathbf{v}_j, \\ M &= m_i + m_j, \quad \mu = \frac{m_i m_j}{m_i + m_j}, \\ \mu_i &= \frac{m_i}{m_i + m_j}, \quad \mu_j = \frac{m_j}{m_i + m_j}. \end{aligned} \quad (3)$$

The translational energy does not change after the collision, but the internal part dissipates. Using $\hat{\mathbf{n}}$, we can split the relative velocity into normal and tangential parts

$$\mathbf{g}_n = (\mathbf{g} \cdot \hat{\mathbf{n}}) \hat{\mathbf{n}}, \quad \mathbf{g}_t = \mathbf{g} - \mathbf{g}_n, \quad (4)$$

and write the total energy as

$$E = \frac{MV^2}{2} + \frac{\mu g_t^2}{2} + \frac{\mu g_n^2}{2}. \quad (5)$$

Now, we can write the post-collision total energy E' as

$$E' = \frac{MV^2}{2} + \frac{\mu g_t^2}{2} + \varepsilon^2 \frac{\mu g_n^2}{2}, \quad (6)$$

where only the normal part of the internal energy dissipates.

In the most general case, we assume that the outcome of the collision is a collection of particles with various masses and velocities. Introducing the function $P_k(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j)$, which is the number of particles of mass m_k and velocity \mathbf{v}_k created after the collision of particles with velocities \mathbf{v}_i and \mathbf{v}_j and sizes i, j , or in other words, introducing the

velocity distribution function of the particles of mass m_k . Using this distribution function, we can write the total mass, momentum and energy of particles in the outcome of the generalized collision

$$\begin{aligned} M &= \sum_{k=1}^{i+j} \int d\mathbf{v} m_k P_k(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j), \\ M\mathbf{V} &= \sum_{k=1}^{i+j} \int d\mathbf{v} m_k \mathbf{v} P_k(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j), \\ \frac{MV^2}{2} + \frac{\mu g_t^2}{2} + \varepsilon^2 \frac{\mu g_n^2}{2} &= \sum_{k=1}^{i+j} \int d\mathbf{v} \frac{m_k v^2}{2} P_k(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j). \end{aligned} \quad (7)$$

Restitution

For a restitutive rebound of particles, the outcome velocities are analytic and given by

$$\begin{aligned} \mathbf{v}'_i &= \mathbf{v}_i - \mu_j(1 + \varepsilon)\mathbf{g}_n, \\ \mathbf{v}'_j &= \mathbf{v}_j + \mu_i(1 + \varepsilon)\mathbf{g}_n, \end{aligned} \quad (8)$$

Let us write the distribution function $P_k(\mathbf{v})$ for the restitutive collision. First of all, the masses of impacting particles do not change, hence the distribution function should contain δ -functions to control this. Together with the analytic expression for the outcome velocities, we can write

$$P_k^{\text{res}}(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j) = \delta_{k,i} \delta[\mathbf{v}_k - \mathbf{v}_i + \mu_j(1 + \varepsilon)\mathbf{g}_n] + \delta_{k,j} \delta[\mathbf{v}_k - \mathbf{v}_j - \mu_i(1 + \varepsilon)\mathbf{g}_n]. \quad (9)$$

The $\delta_{k,x}$ is a Kronecker-delta operator.

Aggregation

If the impact energy is smaller than a certain threshold $E_{\text{imp}} \leq E_{\text{agg}}$, the outcome of the collision is merging of two particles. From the momentum conservation we can write the outcome of the aggregative collision, which is a single particle with a mass and velocity

$$m' = m_i + m_j \quad \mathbf{v}' = \mathbf{V} = \frac{m_i \mathbf{v}_i + m_j \mathbf{v}_j}{m_i + m_j}. \quad (10)$$

The total energy loss is

$$\Delta E = \frac{MV^2}{2} - \frac{m_i v_i^2}{2} - \frac{m_j v_j^2}{2} = -\frac{\mu g^2}{2} = -E_{\text{internal}}, \quad (11)$$

so, all the internal energy is lost during the aggregative collision. The threshold energy value E_{agg} is in general a function of the sizes of particles.

Let us write the debris velocity distribution function for the aggregation process. Since the outcome is a single particle of mass $m_i + m_j$, with velocity \mathbf{V} , we have

$$P_k^{\text{agg}}(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j) = \delta_{k,i+j} \delta[\mathbf{v}_k - \mu_i \mathbf{v}_i - \mu_j \mathbf{v}_j]. \quad (12)$$

Fragmentation

If the impact energy exceeds the certain threshold value $E_{\text{imp}} \geq E_{\text{frag}}$, the two impactors break into into smaller particles in the collision. We cannot obtain the velocities of the monomers from only conservation laws, hence we have to assume that certain constraints are valid. Namely, we assume two constraints:

1. Both particles shatter into their constituent monomers;

2. Complete isotropy of the momenta of the monomers in CoM frame;

These two constraints allow us to write the outcome velocities of the fragmented pieces. Let us write the energy needed to release a single monomer from a particle as γ . Hence, the total energy needed for a complete decomposition of an aggregate of mass m_k can be estimated as

$$E_k = \gamma \cdot k. \quad (13)$$

The fragmentation process of two particles of masses m_i and m_j , with velocities \mathbf{v}_i and \mathbf{v}_j can be then described as a decay of a single particle of mass $m_k = m_i + m_j$ with velocity $\mathbf{v}_k = \mathbf{V} = \mu_i \mathbf{v}_i + \mu_j \mathbf{v}_j$. The decay energy can be estimated as

$$E_{\text{decay}} = E_{\text{imp}} - \gamma \cdot k, \quad (14)$$

which is the amount of energy which is equally distributed among all the shattered monomers. From this, we can see that the impact energy should be larger than $\gamma \cdot k$, which can be treated as the threshold energy. Since the impact energy is the normal part of the internal energy, we can write

$$E_{\text{decay}} = \frac{\mu g_n^2}{2} - \gamma \cdot k = \varepsilon^2 \frac{\mu g_n^2}{2}, \quad (15)$$

and the restitution coefficient for the fragmentation is

$$\varepsilon = \sqrt{1 - \frac{2\gamma k}{\mu g_n^2}}. \quad (16)$$

Since the decay energy has to be positive, we can write the threshold value for the normal relative velocity as

$$g_n \geq \sqrt{\frac{2\gamma k}{\mu}} = \sqrt{\frac{2\gamma}{m_1}} \cdot \frac{i+j}{\sqrt{ij}}. \quad (17)$$

In the CoM frame, each released monomer has an energy

$$E'_c = \frac{m_1 v_c'^2}{2} = \frac{E_{\text{decay}}}{k} = \varepsilon^2 \frac{\mu g_n^2}{2k}, \quad (18)$$

where v'_c is the speed of a monomer in CoM frame

$$v'_c = \frac{\sqrt{ij}}{i+j} \cdot \varepsilon g_n. \quad (19)$$

Let us estimate the number of monomers dN in a small solid angle $d\Omega$. From the second constraint, we deduce that this number has to be proportional to the angle itself, hence

$$dN = \frac{k}{4\pi} d\Omega, \quad k = i + j. \quad (20)$$

In the Lab frame, the speeds of monomers are not equal, but rather uniformly distribution in the range

$$v'_{\min} = V - v'_c, \quad v'_{\max} = V + v'_c. \quad (21)$$

Since the fragmented debris consist of only monomers, the distribution function $P_k(\mathbf{v}_k|\mathbf{v}_i, \mathbf{v}_j)$ has to contain the term $\delta_{k,1}$. In the CoM frame, we can write

$$P_k^{\text{frag, CoM}}(\mathbf{v}_k|\mathbf{v}_i, \mathbf{v}_j) = \delta_{k,1} \delta(v_k - v'_c) \frac{i+j}{4\pi}. \quad (22)$$

In this case, the integral of any velocity function $\varphi(\mathbf{v}_k)$ in the form of

$$\int d\mathbf{v}_k \varphi(\mathbf{v}_k) P_k^{\text{frag, CoM}}(\mathbf{v}_k|\mathbf{v}_i, \mathbf{v}_j) = \delta_{k,1} \frac{i+j}{4\pi} \int d\mathbf{v}_k \varphi(\mathbf{v}_k) \delta(v_k - v'_c), \quad (23)$$

can be written as

$$\delta_{k,1} \frac{i+j}{4\pi} \int d\hat{e} \int_0^\infty dv \varphi(v, \hat{e}) \delta(v - v'_c) = \delta_{k,1} \frac{i+j}{4\pi} \int d\hat{e} \varphi(v'_c, \hat{e}). \quad (24)$$

If $\varphi(\mathbf{v}) \equiv \varphi(v, \hat{e}) = \hat{e}\varphi(v)$, such as $\mathbf{v} = v\hat{e}$, then

$$\int d\hat{e} \hat{e} \varphi(v) = \mathbf{0}. \quad (25)$$

If $\varphi(\mathbf{v}) \equiv \varphi(v, \hat{e}) = \varphi(v)$, then

$$\int d\hat{e} \varphi(v) = 4\pi \varphi(v). \quad (26)$$

To write the debris velocity distribution function in the Lab frame, we have to add the center of mass velocity to all the velocities of the monomers. This can be written as

$$P_k^{\text{frag}}(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j) = \delta_{k,1} \frac{i+j}{4\pi} \int d\hat{e} \delta(\mathbf{v}_k - \mathbf{V} - v'_c \hat{e}). \quad (27)$$

Now, integrating over a function $\varphi(\mathbf{v}_k)$ becomes

$$\delta_{k,1} \frac{i+j}{4\pi} \int d\hat{e} \int d\mathbf{v}_k \varphi(\mathbf{v}_k) \delta(\mathbf{v}_k - \mathbf{V} - v'_c \hat{e}) = \delta_{k,1} \frac{i+j}{4\pi} \int d\hat{e} \varphi(\mathbf{V} - v'_c \hat{e}). \quad (28)$$

If $\varphi(\mathbf{V} - v'_c \hat{e}) = \varphi(\mathbf{V}) - \hat{e}\varphi(v'_c)$, then we have

$$\delta_{k,1} \frac{i+j}{4\pi} \int d\hat{e} \int d\mathbf{v} \varphi(\mathbf{v}) \delta(\mathbf{v} - \mathbf{V} - v'_c \hat{e}) = \delta_{k,1} (i+j) \varphi(\mathbf{V}). \quad (29)$$

DISTRIBUTION FUNCTION

The statistical description of the system is fully described by a set of distribution functions $f_k(\mathbf{r}, \mathbf{v}, t)$. It is normalized, such that $f_k(\mathbf{r}, \mathbf{v}, t) d\mathbf{r} d\mathbf{v}$ gives the number of particles of size k in the phase space volume $d\Gamma = d\mathbf{r} d\mathbf{v}$, around the point (\mathbf{r}, \mathbf{v}) . Hence, integrating over the whole phase space gives us the total number of particles of size k

$$N_k = \int d\mathbf{r} d\mathbf{v} f_k(\mathbf{r}, \mathbf{v}, t). \quad (30)$$

The spacial distribution of particles is not very important for us, hence in the following we assume that the system is spatially homogeneous, and we use only the velocity distribution function $f_k(\mathbf{v}, t)$

$$N_k = \int d\mathbf{r} \int d\mathbf{v} f_k(\mathbf{v}, t), \quad (31)$$

hence

$$n_k \equiv \frac{N_k}{V} = \int d\mathbf{v} f_k(\mathbf{v}, t), \quad (32)$$

is the number density of the subsystem of particles with size k . The other field functions, such as the mean flow velocity \mathbf{u}_k or granular temperature T_k can be defined as velocity moments of the distribution function

$$\begin{aligned} n_k \mathbf{u}_k &= \int d\mathbf{v} \mathbf{v} f_k(\mathbf{v}, t), \\ \frac{3}{2} n_k T_k &= \int d\mathbf{v} \frac{m_k c_k^2}{2} f_k(\mathbf{v}, t), \\ \mathbf{c}_k &= \mathbf{v} - \mathbf{u}_k. \end{aligned} \quad (33)$$

KINETIC EQUATIONS

The time evolution of the distribution functions obey the Boltzmann equations

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} - \frac{1}{m_k} \frac{\partial U(\mathbf{r})}{\partial \mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{v}} \right) f_k(\mathbf{r}, \mathbf{v}, t) = \sum_j \mathcal{I}(f_k, f_j), \quad (34)$$

where $U(\mathbf{r})$ is the potential of the external gravitational field. The LHS of the Boltzmann equation describes the change over time in the function f_k due to the local flow of the particles, subject to external driving. The function $\mathcal{I}(f_k, f_j)$ on the RHS is the *collision integral*, which describes the change over time in the function f_k due to collisions of particles k with particles of size j . Since we have three types of collisional outcomes, the collision integral \mathcal{I} has to take into account all these types of outcomes. Without the loss of generality, we can write the collision integral as a sum of three functions

$$\mathcal{I}(f_k, f_j) = \mathcal{I}^{\text{agg}}(f_k, f_j) + \mathcal{I}^{\text{res}}(f_k, f_j) + \mathcal{I}^{\text{frag}}(f_k, f_j), \quad (35)$$

each corresponding to the specific type of collision.

General structure of collision integrals

Let us consider a collision integral $\mathcal{J}(f_k, f_j)$ for a generalized collision. If we consider a small volume in the phase space $d\Gamma$ around a point (\mathbf{r}, \mathbf{v}) , the term $f_k(\mathbf{r}, \mathbf{v}, t) d\Gamma$ gives us the number of particles of size k in that volume at time t . The collision integral shows how many particles leave and enter this phase space volume per unit time, due to collisions only. So, the collision integral contains two terms, the gain term, which shows the number of particles that enter the phase space volume per unit time, and the loss terms, which shows the number of particles that leave this phase space volume per unit time

$$\mathcal{J}(f_k, f_j) = \mathcal{G}(f_k, f_j) - \mathcal{L}(f_k, f_j). \quad (36)$$

These terms are proportional to the number of collisions happening in unit volume per unit time. Estimation of the number of collisions between the particles of sizes i and j gives us

$$dN_{ij}^{\text{cols}} = \sigma_{ij}^2 d\mathbf{v}_i d\mathbf{v}_j \int d\hat{\mathbf{n}} \Theta(-\mathbf{g} \cdot \hat{\mathbf{n}}) |\mathbf{g} \cdot \hat{\mathbf{n}}| f_i(\mathbf{v}_i, t) f_j(\mathbf{v}_j, t). \quad (37)$$

Now, integrating over all possible pairs of velocities and mass combinations, we can write the gain and loss terms as

$$\begin{aligned} \mathcal{G}(f_k, f_j) &= \sum_i \sigma_{ij} \int d\mathbf{v}_i d\mathbf{v}_j \int d\Omega P_k(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j) f_i(\mathbf{v}_i, t) f_j(\mathbf{v}_j, t), \\ \mathcal{L}(f_k, f_j) &= \sum_i \sigma_{ij} \int d\mathbf{v}_i d\mathbf{v}_j \int d\Omega \delta_{k,i} \delta(\mathbf{v}_i - \mathbf{v}_k) f_i(\mathbf{v}_i, t) f_j(\mathbf{v}_j, t). \end{aligned} \quad (38)$$

The delta functions in the loss term make sure that one of the collision partners is always the considered particle of size k and velocity \mathbf{v}_k . Now, the collision integral for a general type of collision is written as

$$\mathcal{I}(f_k, f_j) = \sum_j \sigma_{ij} \int d\mathbf{v}_i d\mathbf{v}_j \int d\Omega [P_k(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j) - \delta_{k,i} \delta(\mathbf{v}_i - \mathbf{v}_k)] f_i f_j, \quad (39)$$

where

$$d\Omega = d\hat{\mathbf{n}} \Theta(-\mathbf{g} \cdot \hat{\mathbf{n}}) |\mathbf{g} \cdot \hat{\mathbf{n}}|, \quad \mathbf{g} = \mathbf{v}_i - \mathbf{v}_j. \quad (40)$$

For specific types of collisions, e.g. aggregation, fragmentation, restitution, we have to make sure that the integration domains are specified as well. Usually, this domains are the function of the relative velocity $\mathcal{D}(\mathbf{g})$. Hence, the specific collision integrals are written as

$$\mathcal{I}^{\text{type}}(f_k, f_j) = \sum_j \sigma_{ij} \int d\mathbf{v}_i d\mathbf{v}_j \mathcal{D}^{\text{type}}(\mathbf{g}) \int d\Omega [P_k^{\text{type}}(\mathbf{v}_k | \mathbf{v}_i, \mathbf{v}_j) - \delta_{k,i} \delta(\mathbf{v}_i - \mathbf{v}_k)] f_i f_j, \quad (41)$$

where *type* can be aggregation, fragmentation or restitution.