Computational Cost Optimization via Stochastic Kernel Sampling for the Numerical Integration of the Smoluchovski Coagulation Equation

Vincent C. Mader

June 27, 2023

Contents

List of Figures

List of Tables

1 Preface

1.1 Acknowledgements

1.2 Abstract

What is the topic of this thesis?

- We want to `test whether` the numerical `integration` of the Smoluchovski `coagulation equation` can be `sped up` via `stochastic sampling` of the kernel.

- Depending on how accurate one wants to model the involved processes, the integration of the coagulation equation can become quite costly (from a computational standpoint).

- This is due to the "high dimensionality" of the problem.

    - 3 dimensions of space (in principle)

    - 3 dimensions of mass (explain why -> fragmentation)

    - X dimensions of porosity

    - + maybe other attributes of the dust particles

- Therefore, the idea is that a big gain in computational performance could be gained by only including the "relevant" parts of the kernel into the integration. ("relevant" according to what criterion?)

- Finding out whether this works (and by `how much` the computational cost can be reduced) is the big goal of this thesis.

2   Introduction

3   Definition of a Simplified Dust Coagulation Model

3.1   Prerequisites and Assumptions

Consider a distribution of dust particles with different masses m. For simplicity, all of them are assumed to share the same material density ρ_s, as well as all other properties except their particle mass and radius.

In this highly simplified model, the particles are furthermore assumed to be spherically shaped, such that the relationship between mass m and radius a can be expressed as

$$m = \frac{4\pi}{3}\rho_s a^3$$

3.2   The Dust Particle Mass Distribution Function

Let $n(m)$ label the *particle mass distribution function*, i.e. the number of particles per unit volume that possess a given mass value m. This distribution function shall be defined in such a way that the total number N of particles per unit volume is given by

$$N = \int_0^\infty n(m) \; \mathrm{d}m$$

The mass density ρ_s, i.e. the total mass per unit volume, can then be written as

$$\rho_s = \int_0^\infty m \cdot n(m) \; \mathrm{d}m$$

3.3   Dust Particle Collisions

The movement of particles inside a protoplanetary disk can be assumed to be partly systematic (due to velocity contributions of e.g. Keplerian motion) and partly random (due to effects of e.g. Brownian or turbulent motion). This leads to occasional collision events.

The probability of more than two particles being involved in the same collision is so small that the rate of simultaneous interactions between three (or more) bodies can be neglected entirely. Thus, in this model, all collisions are assumed to be two-body collisions.

When two particles collide, there can be a number of different collision outcomes that have to be taken into consideration. A simple approach of classifying these outcomes is to group them into the following three scenarios:

1. *Bouncing*: Here, nothing really happens from the point of view of the particle mass distribution function. The particles collide, but do not exchange any mass. The collision itself of course *can* have an effect on the particle kinematics via the exchange of momentum, but the distribution of masses stays unchanged. For that reason, this outcome does not have to be taken into account when modeling the evolution of the particle mass distribution.

2. *Merging*: The second case is more interesting for us: Here, the two colliding particles merge and form a single new particle. Thus, the two initial particles with mass values m_1 and m_2 disappear, while a new particle with mass $m_1 + m_2$ is created. The removal/addition of these masses from/to the mass distribution has to be handled in some fitting way, and we will take a look at how to do this in the next section.

3. *Fragmentation*: In the third case, the two colliding particles do also "disappear" during the interaction. In contrast to the case of merging though, here it is possible that a whole series of particles is brought into existence. When two particles collide and fragment, various smaller particles with different mass values can be created, under the condition that the sum of particle masses is equal to the total mass $m_1 + m_2$ before the interaction.

To summarize: In this model, the input to a collision event is assumed to *always* be two particles, while the output can be any (natural) number, from a single particle in the case of merging, to very many particles in the case of fragmentation.

3.4   The Smoluchovski Coagulation Equation

Let us now turn our attention towards the question of how to formulate a model for the particle mass distribution's evolution in time. One such model is given by the following integro-differental population balance equation:

$$\frac{\mathrm{d}n}{\mathrm{d}t}(m,t) = \int_0^\infty \int_0^\infty K(m, m', m'') \cdot n(m', t) \cdot n(m'', t)\ \mathrm{d}m'\ \mathrm{d}m''$$

This equation is typically referred to as the *Smoluchovski equation*, due to its treatment by Marian Smoluchovski in 1916 [cite]. It describes how the number n of particles (per unit volume) with mass m is affected by collision events at time t involving two particles with masses m' and m''.

The quantity $K(m,\ m', m'')$ is called the (coagulation) *kernel*. It encodes all the information about the collision events, their rates, and their outcomes.

3.5   The Coagulation Kernel

4 Discretization of the Dust Coagulation Model

4.1 ~~Introduction/General Idea~~

Due to the discrete nature of number representation on digital computers, it is necessary for numerical treatment to move away from a continuous representation. Instead, a discrete analogon has to be constructed for the mass grid, the evolution equations, as well as the coagulation kernel.

4.2 Discretization of the Mass Axis

4.2.1 ~~Introduction/General Idea~~

We will start with the discretization of the mass axis: Here, the goal is to partition the continuous range of particle masses m present in the disk into a set of $\mathcal{N}_m \in \mathbb{N}$ intervals, which from now on will be referred to as mass grid "bins". Each of these bins can be uniquely characterized by an index $i \in [0, \mathcal{N}_m - 1]$, and its corresponding mass value m_i^c, which are situated at the center of the bin (ergo the superfix "c").

To derive an expression for these mass values, let us first define the upper and lower boundaries of the discrete mass grid. We shall label them $m_{\max}$ and $m_{\min}$, respectively. Now, consider a collection of $\mathcal{N}_m + 1$ appropriately spaced grid points m_i^b, which will serve as the bin boundaries.

Figure 1: Illustration of the discretized mass axis.
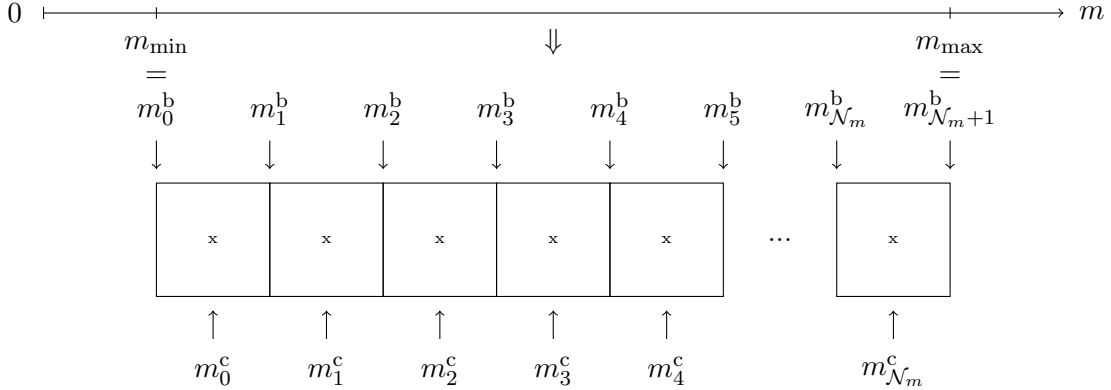
4.2.2 Discretization of the Mass Axis using a Linear Scale

The spacing of these grid points of course depends heavily on the utilized scaling, which for simplicity shall be assumed to be linear at the moment. Later on, we will make use of a logarithmic scaling to assure a better representation of all masses along the wide range of mass values present in the disk.

Analogously to the bin centers, the boundary points can be labeled by an index $i \in [0, \mathcal{N}_m]$. The corresponding mass value m_i^b can then be expressed as

$$m_i^b = m_{\min} + (m_{\max} - m_{\min}) \cdot \frac{i}{\mathcal{N}_m}$$

To calculate the the mass values for the grid points at the center of a bin, all we need to do now is take the arithmetic mean of its two neighboring boundary values, i.e.:

$$m_i^c = \frac{m_i^b + m_{i+1}^b}{2}$$

Thus, after having defined only the three numbers $\mathcal{N}_m$, $m_{\min}$, and $m_{\max}$, it is possible to interpolate the values of all mass grid points sitting on the boundaries and/or centers of the bins.

The inverse transformation from mass to index can be determined easily by rearranging the above relation. This leads to the following expression

$$i(m) = \mathcal{N}_m \cdot \frac{m - m_{\min}}{m_{\max} - m_{\min}}$$

Sidenote: In the linearily scaled mass grid, the bin "width" is constant, and independent of the bin index. This will change once the switch to a logarithmic grid is made! For now though, it is given by

$$\Delta m = m_{i+1}^{\mathrm{b}} - m_i^{\mathrm{b}}$$
$$= \frac{m_{\max} - m_{\min}}{\mathcal{N}_m}$$
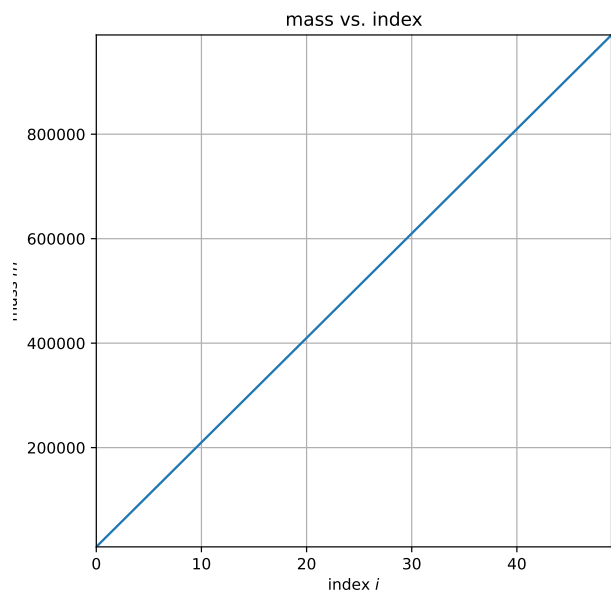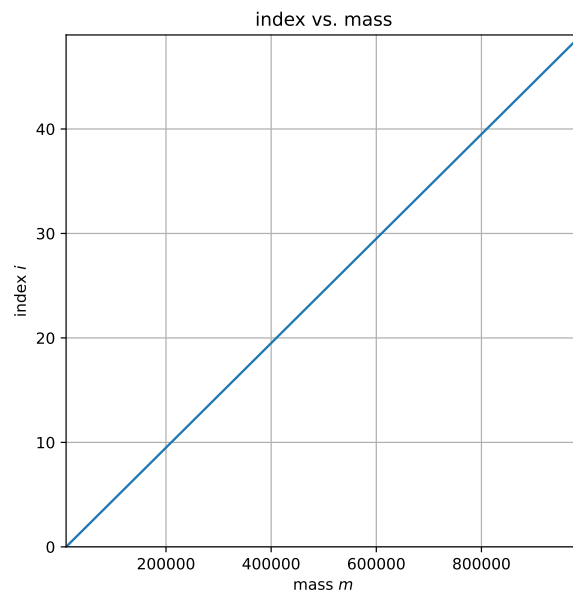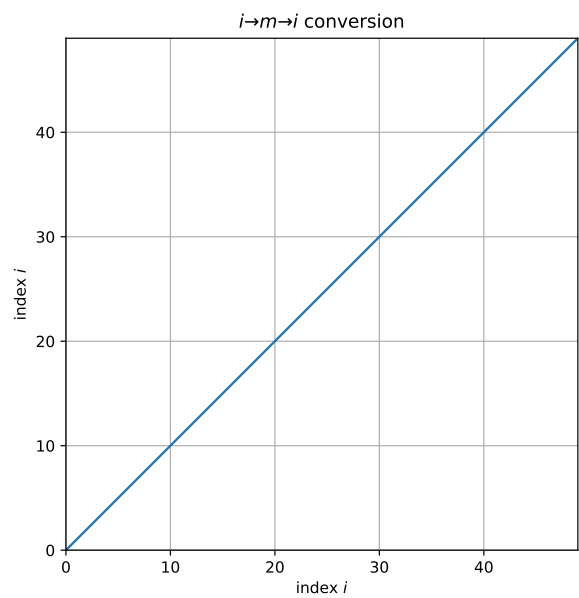
(a) CAPTION ...
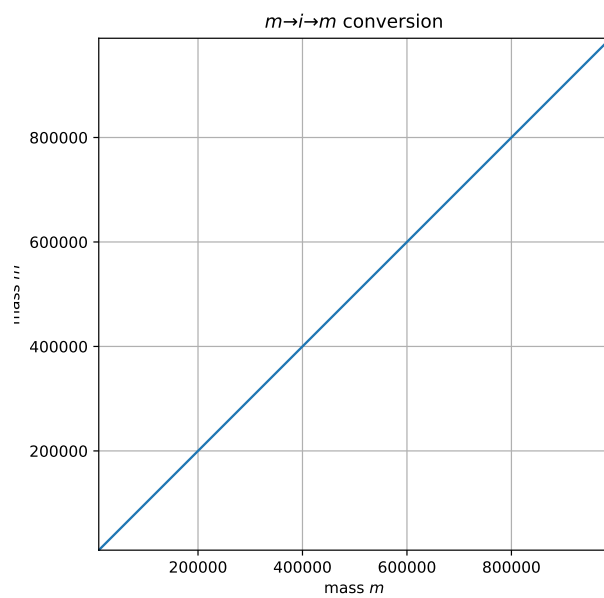
(b) CAPTION ...

(c) CAPTION ...

(d) CAPTION ...

Figure 2: CAPTION ...

4.2.3 Discretization of the Mass Axis using a Logarithmic Scale

As before, let $\mathcal{N}_m$ be used to label the number of bins, and let the upper and lower grid boundaries be given by $m_{\min}$ and $m_{\max}$, respectively.

Once again, we first define an expression for the grid points sitting directly on the bin boundaries. Making use of an index $i \in [0, N_m]$, they can be uniquely identified and calculated via

$$m_i^{\mathrm{b}} = m_{\min} \cdot \left(\frac{m_{\max}}{m_{\min}} \right)^{i/\mathcal{N}_m}$$

To arrive at the mass values at the bin centers, we again take the mean. Here, it's not the arithmetic mean though, but the geometric mean, i.e.

$$m_i^{\mathrm{c}} = \sqrt{m_i \cdot m_{i+1}}$$

In contrast to the linear grid, the bin "width", i.e. the additive offset from one bin to the next, is not the same for all bins in the logarithmic grid. Instead, what stays the same for is the *relative* mass increase from one bin to the next.

As above in the linear case, the inverse transformation can be arrived at by rearranging for i. This leads to the following expression:

$$i(m) = \mathcal{N}_m \cdot \frac{\log(m) - \log(m_{\min})}{\log(m_{\max}) - \log(m_{\min})}$$
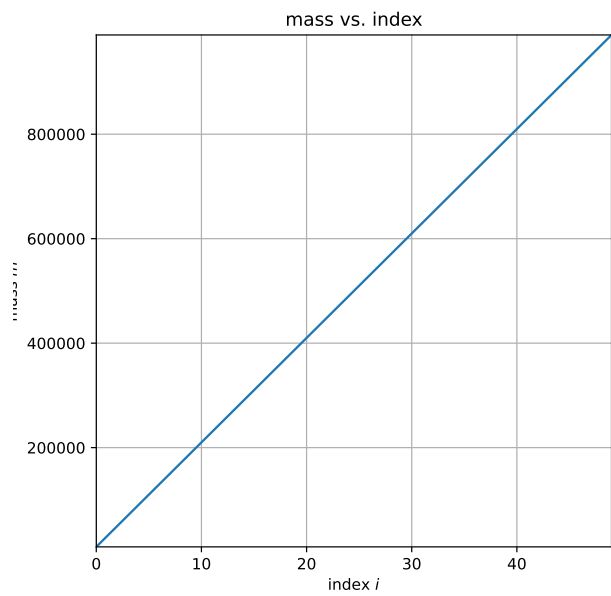
(a) CAPTION ...
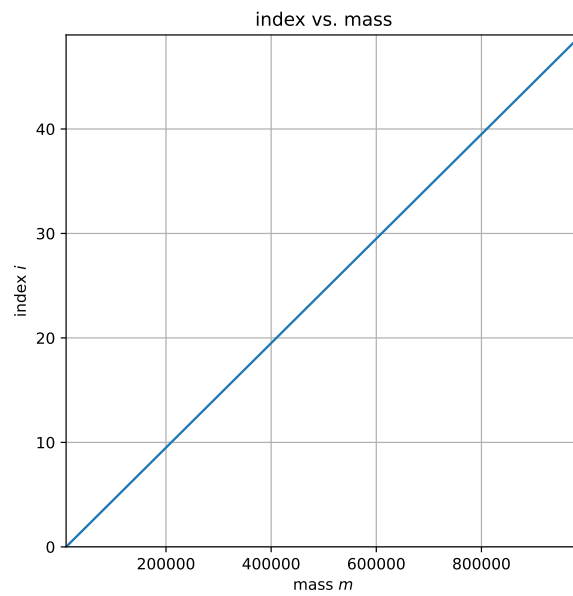
(b) CAPTION ...
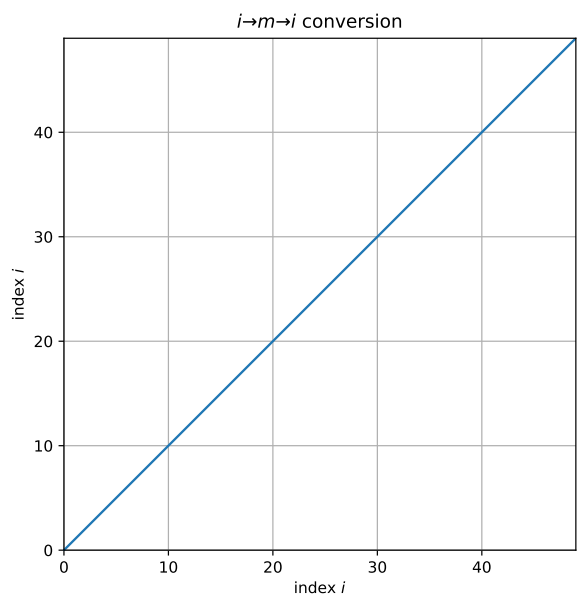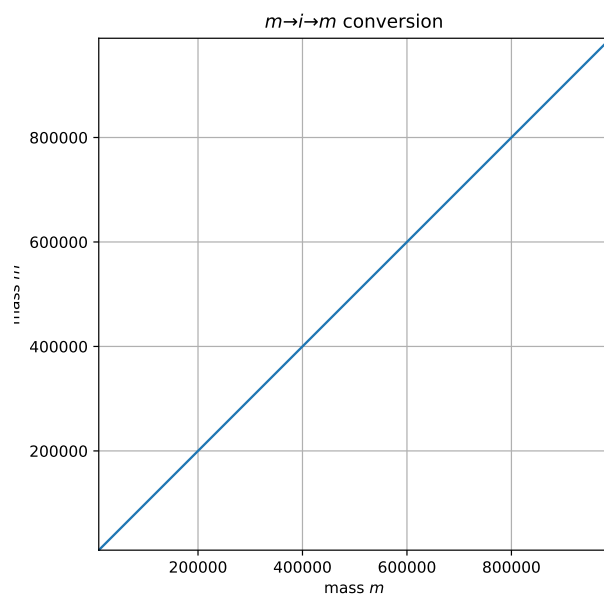
(c) CAPTION ...

(d) CAPTION ...

Figure 3: CAPTION ...

14

4.3   Discretization of the Particle Mass Distribution Function

Just as we discretized the range of masses, so we also have to discretize the particle mass distribution function. For this, we define:

$$n_i := n(m_i)$$

The number of particles per unit unit volume in bin i is then calculated by integration over the particle mass distribution function from the lower to the upper bin boundary:

$$N_i = \int_{m_{i-1/2}}^{m_{1+1/2}} n(m) \ \mathrm{d}m$$

The mass density ρ_i in the bin i is given by

$$\rho_i = \int_{m_{i-1/2}}^{m_{1+1/2}} m \cdot n(m) \ \mathrm{d}m$$

To arrive at the total mass density independent of particle mass, one has to sum over all bins:

$$\rho = \sum_{i=0}^{\mathcal{N}_m-1} \rho_i$$

4.4   Discretization of the Smoluchovski Coagulation Equation

With $i, j \in \mathbb{N}$ "being indices":

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_{i=1}^{\mathcal{N}_m} \sum_{j=1}^{\mathcal{N}_m} K_{kij} \cdot n_i \cdot n_j$$

Equivalent formulation: [which one to use? I like the lower one <3]

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_{i=0}^{\mathcal{N}_m-1} \sum_{j=0}^{\mathcal{N}_m-1} K_{kij} \cdot n_i \cdot n_j$$

5   Initialization of the Particle Mass Distribution Function

Now, let us turn our attention to the initialization of the particle mass distribution function.

Options:

1. Dirac-delta distribution
2. MRN distribution

What would be best?

- MRN is more physical than Dirac-delta. (see later chapter)
- It does not *really* make that much of a difference though.
- The information about the initialization is quickly lost anyways.
- Both 1. & 2. qualitatively lead to the same results (even if not quantitatively).

Observation:

- Using the MRN distribution leads to a significant slowdown of the integration. (minutes, instead of seconds)
- This might be because I chose $m_{\max}$ to be the largest mass grid bin.
    - Do not do this!
    - This is unphysical!
    - Instead use $\approx 0.5\mu$m
- Test whether this problem persists!

6 Integration of the Smoluchovski Equation

6.1 How to discretize the time axis in a linear fashion?

Let the temporal domain be divided into $\mathcal{N}_t$ discrete "bins". Then, let ξ be the index used to uniquely identify each time step, i.e.

$$\xi \in \mathbb{N} \cap [0, \mathcal{N}_m - 1]$$

When discretizing the time axis in a linear way, this leads to

$$t_\xi = t_0 + \xi \cdot \Delta t$$

Here, t_0 labels the time value at the start of the simulation (can be set to $t_0 = 0$ without loss of generality), and Δt labels the size of each time step.

The step size needs to be chosen sufficiently small as to assure stability of the integration scheme.

[...CFL criterion...] [...implicit integration...]

6.2 What is the difference between additive/multiplicative incrementation of time

- TODO: Move?

6.2.1 Additive time-steps

- straightforward approach
- incrementation of time via

$$t_{n+1} = t_n + \Delta t$$

6.2.2 Multiplicative time-steps

- more appropriate here [explain why]

$$t_{n+1} = t_n \cdot q_t$$

6.3 How to integrate the Smoluchovski equation using an explicit Euler scheme?

As above, we use the notation $n_{i,\xi}$ to label the dust particle mass distribution function evaluated for the mass m_i at a point in time t_ξ.

The goal now is to compute the distribution function's value after one additional step in time, i.e. at the time

$$t_{\xi+1} = t_\xi + \Delta t$$

This can be done by making use of an explicit Euler integration scheme [when?]. For a sufficiently small time step Δt, we can thus arrive at an approximate expression for the distribution function's updated value via the transformation

$$
\begin{aligned}
n_{k,\xi} \to n_{k,\xi} + \Delta t \cdot \frac{\mathrm{d}n_{k,\xi}}{\mathrm{d}t} \\
= n_{k,\xi} + \Delta t \cdot \sum_{i=0}^{\mathcal{N}_m-1} \sum_{j=0}^{\mathcal{N}_m-1} K_{kij} \cdot n_i \cdot n_j
\end{aligned}
$$

If the step size is chosen too large, the method will break down due to the insufficient stability properties of the explicit Euler integration scheme.

Instead, [... implicit Euler/Radau...] [see above]

6.4 How to discretize the time axis in a logarithmic fashion?

As the temporal domain spans over multiple orders of magnitude for the processes involved in planet formation, it makes sense to discretize the time axis in a logarithmic fashion. [write this differently?]

[...]

6.5 How to integrate the Smoluchovski equation using implicit schemes?

7 Construction of the Kernel for Simple Hit-and-Stick Coagulation

7.1 Introduction, Overview, & Goals for this Section

- Here, we only take a look at the simple case of...

    - ...simple *linear* mass axis discretization.

    - ...simple *Dirac-delta* initialization.

    - ...simple *explicit Euler* integration.

7.1.1 Construction of a Kernel for Hit-and-Stick Coagulation

Assuming simple hit-and-stick coagulation, the kernel can be written as

$$K(m, m_1, m_2) = \frac{1}{2} \big[\delta(m - m_1 - m_2) - \delta(m - m_1) - \delta(m - m_2) \big] \cdot R(m_1, m_2)$$

Here, the coefficient $R(m_1, m_2)$ labels the collision-and-merging rate.

7.2 Definition of the Kernel for simple Stick-and-Hit Coagulation

Let us first turn our attention to the simple case of stick-and-hit coagulation: Here, two particles with masses m_1 and m_2 collide, and subsequently merge into a single particle with combined mass $m_{\text{tot}} = m_1 + m_2$.

Let $C(m_1, m_2)$ be the rate at which collisions occur between such a pair of particles. Then, let

$$R(m_1, m_2$$

label the rate of collision events that lead to a merging of the two particles into a single new one.

Of course, in actuality not every collision leads to a merge event. For simplicity, we will for now will assume that it does. As such, we can write

$$R(m_1, m_2) = C(m_1, m_2)$$

Later on, we will more carefully examine how the collision+sticking rate can be calculated.

[... also talk about definition of collision rate...] [... also talk about "reaction rates"...] [... difference between "collision", "collision+merge", "reaction" rates (fragmentation?)...]

[... collision+sticking rate, sticking probability, "Dust evolution w/ binning methods" eq.1.6-1.11...]

[... move the above elsewhere? -> "collisions" section?] [...]

A kernel describing the stick-and-hit coagulation process can be written as

$$K(m, m_1, m_2) = \frac{1}{2}\left[\delta_D(m - m_1 - m_2) - \delta_D(m - m_1) - \delta_D(m - m_2)\right] \cdot R(m_1, m_2)$$

Here, δ_D labels the Dirac delta function.

[...]

7.3 Numerical Integration with the Explicit Euler Scheme

8 Implementation of a Logarithmic Mass Axis Representation

8.1 Introduction, Overview, & Goals for this Section

8.2 Reasons for Making Use of a Logarithmic Representation

8.3 Challenges Associated with a Logarithmic Representation

8.4 Definition of the Logarithmic Mass Axis

8.5 Implementation of the Kovetz-Olund algorithm

8.5.1 Reasons for the Necessity of the Kovetz-Olund Algorithm

Even in a highly simplified scenario, where only hit-and-stick coagulation is included, the definition of the kernel K_{kij} is not at all trivial. To assure both the consistency and accuracy of the algorithm, one has to take care of two separate problems, namely:

1. The conservation of mass *has* to be assured, otherwise the numerical solution can not be assumed to remain stable for long. In the case of stick-and-hit coagulation, this means that for every pair of colliding particles, a single new particle has to be created. At the same time, the two initial particles have to be removed from the distribution. During this process, the total mass should remain unaffected down to machine precision.

2. When using a logarithmically spaced grid for the discretized mass axis, it can not be assumed that after a collision of two dust particles with masses m_i and m_j the resulting particle will carry a mass $m_k = m_i + m_j$ whose value can be mapped trivially onto the grid. In general, the corresponding index will not be an integer, and instead lie between somewhere between the two neighboring grid points with indices k and $k+1$. Therefore, the result of the merging of m_i and m_j has to be divided in some sensible way between these two neighboring bins.

8.5.2 Implementation of the Kovetz-Olund Algorithm

An elegant way for solving the two problems listed above is given in the paper by [Kovetz & Olund, 1969], where they used the following procedure:

1. The stick-and-hit coagulation kernel is split into two parts. The first is the *gain* of particles in bin k due to the collision of particles from the bins i and j. The second is the *loss* of particles from bin k due to collisions of particles in bin k with particles from any other bin j.

   Using this separation into gain & loss, the dust particle mass distribution's temporal derivative can be expressed in the following form:

   $$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_{i,j} K_{kij}^{\mathrm{gain}} n_i n_j - \sum_j K_{kj}^{\mathrm{loss}} n_k n_j$$

   In other words, the total kernel [from above, cite eq.] can be written as

   $$K_{kij} = K_{kij}^{\mathrm{gain}} - K_{ij}^{\mathrm{loss}} \delta_{ki}$$

   Splitting the kernel like this into a gain & a loss term is a quite general approach, and can be used in more complex scenarios as well (including e.g. particle fragmentation processes).

2. For the scenario of pure hit-and-stick coagulation, a unique discretization of the kernel can be defined such that both the number of particles and the conservation of total mass are handled correctly. To

do this, consider a pair of colliding particles with indices i and j. Then, let the index $\bar{k}$ be chosen in such a way that the condition

$$m_{\bar{k}} \leq m_i + m_j < m_{\bar{k}+1}$$

is satisfied.

3. As stated before, in hit-and-stick coagulation, a single new particle emerges for each pair of colliding particles. Using the definitions from above, this condition can be expressed as follows:

$$K_{\bar{k},ij}^{\text{gain}} + K_{\bar{k}+1,ij}^{\text{gain}} \stackrel{!}{=} K_{ij}^{\text{loss}}$$

4. The second condition is that of mass conservation, which can be written as:

$$m_{\bar{k}} K_{\bar{k},ij}^{\text{gain}} + m_{\bar{k}+1} K_{\bar{k}+1,ij}^{\text{gain}} \stackrel{!}{=} (m_i + m_j) K_{ij}^{\text{loss}}$$

5. Now, for the mapping of the resulting particle's mass onto two neighboring bins, let us define a parameter ε such that

$$K_{\bar{k},ij}^{\text{gain}} = K_{ij}^{\text{loss}} \cdot (1 - \varepsilon), \text{ and}$$
$$K_{\bar{k}+1,ij}^{\text{gain}} = K_{ij}^{\text{loss}} \cdot \varepsilon$$

This assures that [equation from pt 3] is satisfied. If we now plug this definition into [equation from pt 4] and solve for ε, we arrive at

$$\varepsilon := \frac{m_i + m_j - m_{\bar{k}}}{m_{\bar{k}+1} - m_{\bar{k}}}$$

This is the algorithm of [Kovetz & Olund (1969)], and it was also used in subsequent papers like [Brauer et al. (2008)] and [Birnstiel et al. (2010)].

8.6 Implementation of Near-Zero-Cancellation Handling for Coagulation

8.6.1 What is Near-Zero-Cancellation and where can it occur in general?

When using floating-point numbers following the representation defined by the IEEE-754 standard, it can occur that

$$a + b = a \quad \text{for} \quad b \neq 0$$

Typically, this happens when

$$|b| < \varepsilon_m \cdot |a|$$

Here, ε_m labels the *machine precision.*

[Add: How big is ε_m for an f32, how big for an f64?]

8.6.2 Where can Near-Zero-Cancellation occur in our model?

Let i and j once again be the indices used to label two colliding particles. Additionally, assume now that particle i is *much smaller* than particle j.

The detailed balance approach from above requires the removal of both the big and the small particle from the mass distribution, followed by the re-insertion of a new particle carrying the initial pair's combined mass. This new particle would then have a mass which is nearly identical to that of the bigger one of the original two particles, it would be only a tiny bit heavier.

In the approach defined above this would mean that $\bar{k} = j$, i.e. the resulting particle will reside in the same bin as the larger original one. Also, it would follow that $\varepsilon \ll 1$.

Let us now take a look at the particle mass distribution in the bin $\bar{k}$ and, more specifically, by how much it changes from one timestep to the next. For this particular pair of i and $\bar{k} = j$, we can write:

$$\frac{\mathrm{d}n_{\bar{k}}}{\mathrm{d}t} = K_{\bar{k},i\bar{k}}^{\text{gain}} n_i n_{\bar{k}} - K_{\bar{k}i}^{\text{loss}} n_i n_{\bar{k}}$$

Plugging in [equation from above] leads to

$$\frac{\mathrm{d}n_{\bar{k}}}{\mathrm{d}t} = (1 - \varepsilon) K_{\bar{k}i}^{\text{loss}} n_i n_{\bar{k}} - K_{\bar{k}i}^{\text{loss}} n_i n_{\bar{k}}$$

Here, the two terms alsmost cancel each other out. What remains is a contribution which is proportional to ε.

If ε is small enough, the double-precision accuracy of the floating point representation will lead to breakdown of the method. [rewrite this sentence, copied almost exactly from Kees]

8.6.3 Handling Near-Zero-Cancellation for Stick-and-Hit Coagulation

It is relatively easy to identify the particle pairs (i, j) for which the scenario detailed above will occur. Let i (without loss of generality) be the index of the larger one of the two colliding masses. Cancellation may then occur when the resulting k is equal to j.

In that case, we carry out the subtraction in [previous equation] analytically, and write:

$$\frac{\mathrm{d}n_{\bar{k}}}{\mathrm{d}t} = -\varepsilon K_{\bar{k}i}^{\text{loss}} n_i n_{\bar{k}}$$

[Elaborate on this, see "Dust Evolution with Binning Methods"]

9 Inclusion of Fragmentation Processes into the Kernel

9.1 "First/Simple/Naive Attempt"

9.1.1 How to implement naive fragmentation?

- "Pulverization"

9.2 The MRN Distribution

- introduced by Mathis-Rumpl-Nordsieck, 1977

9.2.1 How to implement MRN distribution (for initialization)?

Particle mass distribution function is defined by the condition:

$$\rho = \int_{m_{\text{min}}}^{m_{\text{max}}} n(m) \cdot m \, \mathrm{d}m$$

Ansatz: power law with $q = -11/6$ (see 'sizedistributions.pdf')

$$n(m) \sim m^q$$

Choose constant A such that

$$n(m) = A \cdot m^q$$

Plug into the integral from above

$$\rho = \int A \cdot m^q \cdot m \, \mathrm{d}m$$

$$= \int A \cdot m^{q+1} \, \mathrm{d}m$$

$$= \frac{A}{q+2} \, m^{q+2} \Big|_{m_{\text{min}}}^{m_{\text{max}}}$$

$$= \frac{A}{q+2} \, (m_{\text{max}}^{q+2} - m_{\text{min}}^{q+2})$$

Rearanging for A leads to

$$A = \frac{(q+2) \cdot \rho}{m_{\text{max}}^{q+2} - m_{\text{min}}^{q+2}}$$

Now we only need to choose values for m_{min} and m_{max}.

- For the minimum mass, no lower limit exists. For it, the value corresponding to the smallest bin can be chosen [citation needed].

- For the maximum mass, an upper limit has to be chosen. It can be left as a free parameter to be set in 'config.toml', or set to something approximating 0.5 μm. [see 2004 Dullemond & Dominik] ^ max. in interstellar medium (use for m_{min}?)

9.2.2 How to implement MRN distribution for fragmentation?

Let m_i and m_j be the masses of two particles that are involved in a collision leading to fragmentation.

How do we model this?

- Distribute the mass $m_{\text{tot}} = m_i + m_j$ onto bins with $m < m_{\text{tot}}$.

- For this, use the MRN distribution $n(m) = Am^q$.

- For this, find the value of A.

- For this, use the formula from [Summarize: How to implement MRN distri].

- For this, find a value for $m_{\max}$.

How do we choose a value for $m_{\max}$?

- Can it be larger than $\max(m_i, \; m_j)$?

    - "Some merging, some fragmenting"

    - "$1 + 1 \to 1.5 + 0.1 + 0.1 + 0.1 + 0.1 + 0.1$"

- If...

    - ...yes: It can at most be equal to $m_i + m_j$

    - ...no: It can at most be equal to $\max(m_i, m_j)$

- In either case, it can't really be *equal* to either of the two values.

    - That would be stick-and-hit in case "yes", and bouncing in case "no".

    - It can at most be equal to the mass corresponding to the next-lower bin.

Answer:

- We don't really know.

- It doesn't *really* matter that much anyhow.

- One could specify the method in 'config.toml', or just use one of the methods.

9.2.3   Test integration speed with MRN distribution enabled. Is there a slowdown?

9.3   "Implementation of Near-Zero-Cancellation Handling for Fragmentation" (?)

10 Definition of the Dust Particle Reaction Rates

10.1 Definition of the Dust Particle Reaction Rates

10.2   Definition of the Dust Particle Collision Rates

The collision rate for a pair of masses m_1 and m_2 can be written as

$$C(m_1, m_2, \Delta v) = \sigma(m_1, m_2) \cdot \langle |\vec{v}_1 - \vec{v}_2\rangle$$

  - ˆ TODO: Is there not a "number density" term missing here? Otherwise, the unit would be 'm^3 / s'.

Here, $\sigma(m_1, m_2)$ labels the cross section for a collision event. The relative velocity between such two particles is given by the difference $\vec{v}_1 - \vec{v}_2$, its absolute value is $|\vec{v}_1 - \vec{v}_2|$, and $\langle |\vec{v}_1 - \vec{v}_2| \rangle$ is the expectation value of that quantity.

[Simplification was done here] [Elaborate: Give more precise formula]

In our notation:

$$C_{ij} = \sigma_{ij} \cdot \langle \Delta v_{ij} \rangle$$

10.3 Definition of the Collision Cross Section

The cross section for a collision of two particles i and j with radii a_i and a_j can be written as

$$\sigma_{ij} = \pi \cdot (a_i + a_j)^2$$

Here, the radii can be computed from the corresponding masses m_i and m_j from equation [Summarize: Assumptions needed for the (naive/simple) particle mass distribution.].

[Add plot here]

10.4 Definition of the Relative Particle Velocity

11   Calculation of the Relative Dust Particle Velocities

11.1   Definition of the Relative Velocity due to Radial Drift

$$\Delta u_{\mathrm{RD}} = \left| u_r(m_1) - u_r(m_2) \right|$$

dust radial velocity:

$$u_r = \frac{u_g}{1 + \mathrm{St}^2} - \frac{2u_n}{\mathrm{St} + \mathrm{St}^{-1}}$$

gas radial velocity:

$$u_g = -\frac{3}{\Sigma_g \sqrt{r}} \cdot \partial_r \left(\Sigma_g \nu_g \sqrt{r} \right)$$

particle maximum drift velocity:

$$u_n = -\frac{E_d}{2\rho_g \, \Omega_K} \cdot \frac{\partial P_g}{\partial r}$$

../../msc-thesis.py/figures/22/dv_RD.pdf

11.2 Definition of the Relative Velocity due to Differential Settling

$$\Delta u_{\mathrm{DS}} = \left| u_i - u_j \right|$$

$$u_i = ts \cdot \Omega_K^2 \cdot z$$

$$\mathrm{St} = \Omega_K \cdot t_s$$

../../msc-thesis.py/figures/22/dv_DS.pdf

11.3 Definition of the Relative Velocity due to Brownian Motion

$$\Delta u_{ij}^{\mathrm{BR}} = \sqrt{\frac{8k_B T}{\pi} \cdot \frac{m_i + m_j}{m_i \cdot m_j}}$$

$$= \sqrt{\frac{8}{\pi \beta \mu_{ij}}}$$

../../msc-thesis.py/figures/22/dv_BR.pdf

11.4 Definition of the Relative Velocity due to Turbulence

../../msc-thesis.py/figures/22/dv_TU.pdf

11.5 Definition of the Azimuthal Relative Velocity

$$\Delta u_{ij} = \left| u_n \cdot \left(\frac{1}{1 + \text{St}_i^2} - \frac{1}{1 + \text{St}_j^2} \right) \right|$$

../../msc-thesis.py/figures/22/dv_AZ.pdf

11.6   Total Relative Velocity

$$\Delta u_{ij} = \Delta u_{\mathrm{BR}} + \Delta u_{\mathrm{RD}} + \Delta u_{\mathrm{AZ}} + \Delta u_{\mathrm{TU}} + \Delta u_{\mathrm{DS}}$$

$$\Delta u_{ij} = \sqrt{\Delta u_{\mathrm{BR}}^2 + \Delta u_{\mathrm{RD}}^2 + \Delta u_{\mathrm{AZ}}^2 + \Delta u_{\mathrm{TU}}^2 + \Delta u_{\mathrm{DS}}^2}$$

../../msc-thesis.py/figures/22/dv_tot.pdf

12 Implemention of Stochastic Kernel Sampling

13   Summary of Results

14 Thesis Discussion & Outlook

15 Appendix

15.1 Glossary

a [4] b [3] c [2] d [1]

16 ~~References~~

References

[1] Birnstiel, T., Dullemond, C. P., and Brauer, F. Gas- and dust evolution in protoplanetary disks. *A&A*, 513:A79, 2010.

[2] Brauer, F., Dullemond, C. P., and Henning, Th. Coagulation, fragmentation and radial motion of solid particles in protoplanetary disks. *A&A*, 480(3):859–877, 2008.

[3] Dullemond, C. P. and Dominik, C. The effect of dust settling on the appearance of protoplanetary disks. *A&A*, 421(3):1075–1086, 2004.

[4] J. S. Mathis, W. Rumpl, and K. H. Nordsieck. The size distribution of interstellar grains. , 217:425–433, October 1977.