N-BODY CALCULATIONS OF CLUSTER GROWTH IN
PROTO-PLANETARY DISKS

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We investigated numerically the dust growth driven by Brownian motion in a proto-
planetary disc around a solar-type young stellar object. This process is considered
as the first stage in the transformation of the initially micron-sized solid particles
to a planetary system. In contrast to earlier studies the growth was investigated at
the small particle number densities typical for the conditions in a proto-planetary
disc. Under such circumstances, the mean particle distance exceeds the typical
aggregate diameter by orders of magnitude, and a collision will be a very rare
event. We derived a criterion which allows an efficient detection of candidates for
imminent collisions. The N-particle-method we used is based upon an adaptive
time step scheme respecting the individual dynamical states of the aggregates. Its
basic concept is to perform on average constant “length steps”, instead of using
constant time steps. The numerical cost of the algorithm scales with the particle
number better than $N \log N$. In order to minimise the influence of the decreasing
number of particles within the simulation box, a new rescaling method is used
throughout the aggregation process. Our numerical results indicate that at very
low number densities, the growth process is influenced by spatial number density
fluctuations.

1 Introduction

Since the advent of high performance computers, scientists have been able to
numerically investigate complex astronomical phenomena that have interested
astronomers and physicists for centuries. The first problems in numerical astrophysics
were hydrodynamical and radiative transfer problems. Then, starting
in the early 1980s, several workers began modeling the gravitational clustering
of stars and galaxies efficiently using tree codes. Since the beginning of
the 90’s Particle codes are although used to investigate smaller-scale astrophysical
problems, such as the formation of the precursors of the planets (planetesimals).

Nowadays it is a generally accepted view among the astrophysicists, that the
genesis of a planetary system coincides with the formation of sun-like young stellar
objects surrounded by a gaseous disc. The building bricks of the planetesimals
are micron-sized solid particles (the so-called cosmic dust) embedded in the gas
of the disc. The formation of a planetary system is a surprisingly fast process.
From both, the astronomical observations of proto-planetary discs and geophysical
studies, one can derive a formation time scale of a few million years. Up to the
mid-90s the majority of the astrophysicists were convinced that the transition
of the micron-sized dust grains to the kilometre-sized planetesimals were due to
gravitational instabilities. So it was quite a surprise for the community, when
Weidenschilling and Cuzzi et al. demonstrated that the inherent gas turbulence prevents dense dust layers from collapsing into a planetesimal. Another possible process for forming a planetesimal in a proto-planetary disc is the dust growth due to collisional sticking - the so-called coagulation. For particles to collide and stick, there must be a relative velocity component between the grains. In the onset of grain growth Brownian motion dominates other motions. However, it cannot be the source of an effective grain growth leading to planetesimals, because the growth time scales are much longer than the few million years. Consequently, there has to be a much more effective mechanism for driving the dust coagulation. Such a source of relative velocities could be the turbulent gas motion if the typical time \( \tau_f \) a dust aggregate needs to couple with the gas stream, is larger than the typical life time of the smallest turbulent eddy. If one considers realistic values for a proto-planetary disc around a solar-like protostar, then one finds that the \( \tau_f \) of the initial particles must increase by five orders of magnitude in order to have grain growth driven by turbulence. Consequently, during the Brownian stage of dust growth the typical friction time of the dust aggregates has to grow rapidly. However, Monte-Carlo type simulations of the cluster growth indicate that the growth tends to form fractal aggregates characterised by an almost constant coupling time \( \tau_f \). In these simulations, particles are added to the growing dust grain according to some given rule. The disadvantage of such Monte-Carlo methods is that they require significant simplification of the astrophysical conditions. In addition, the Monte Carlo approach cannot address the inherently dynamic nature of the coagulation process.

To overcome the disadvantages of Monte-Carlo astrophysical simulations, we developed a self-consistent N-particle code. In order to obtain a detailed understanding of the coagulation in proto-planetary discs, we considered the influence of the aggregate structure in the coagulation process. The “classical” tool for a numerical study of this phenomenon is the molecular dynamic (MD). However, since the dust grains are performing a non-deterministic, diffusive motion, it is not straightforward to apply the MD concept for modeling this process. Another difficulty with the MD approach is that we wish to study the coagulation at very low particle number densities. Or more precisely, the mean particle distance \( \langle x \rangle = \{3/4\pi n\}^{1/3} \) (\( n \)-particle number density) exceeds the typical aggregate size by at least four orders of magnitude. Under such circumstances, a mutual collision of two particles is a rare event. In order to model the coagulation exactly, it is essential that no collisions are missed. To meet this requirement one needs a good estimate for the particle position after a certain period of time. In the following we demonstrate that, for sufficient small time steps, we can use the MD methods even for diffusing particles.

2 Computational technique
2.1 Simulation of diffusive trajectories

Since the motion of growing dust grains is only affected by the gas-grain interaction (diffusion), and in some cases by the gravitational field, the particle dynamics between successive collisions can be treated independently. The “equation of motion” for diffusive particles is given by the Langevin equation

\[
d_t x = v, \\
d_t v = -\tau_f^{-1}v + m^{-1}F_{fl}. \tag{1}
\]

Here, \(x\) and \(v\) are the Cartesian components of the position and velocity of the particle. Furthermore, the friction time \(\tau_f\) is the mean interval the particle needs to dissipate its relative kinetic energy with respect to the suspending gas. The influence of the gas-grain interaction is approximated by the stochastic force \(F_{fl}\) having the properties \(\langle F_{fl} \rangle = 0\) and \(\langle F_{fl}^2 \rangle = 2mkT/\tau_f\) (\(m\) - particle mass, \(T\) - kinetic gas temperature, \(k\) - Boltzmann constant).

The diffusive path of the particle can be obtained by successive integration of (1). After a time interval \(\tau = \delta t/\tau_f\), the new particle position and velocity are given by

\[
x = x_0 + \tau_f(v + v_0) \tanh(\tau/2) + \left\{2\tau_f^2(v^2)[\tau - 2\tanh(\tau/2)]\right\}^{1/2} \xi_1 \tag{2}
\]
\[
v = v_0e^{-\tau} + \left\{\langle v^2 \rangle[1 - e^{-2\tau}]\right\}^{1/2} \xi_2, \tag{3}
\]

where \(\xi_1\) and \(\xi_2\) are normalised Gaussian random numbers, i.e. \(\langle \xi_i \rangle = 0\), \(\langle \xi_1\xi_2 \rangle = 0\), and \(\langle \xi_i^2 \rangle = 1\) (\(i = 1, 2\)). As mentioned before, the MD concept requires knowledge of the particle position after a period of time. For a particle following a diffusive trajectory, it is impossible to obtain such an expression for an arbitrary interval \(\delta t\), since only the probability of the particle being at position \(x\) after \(\delta t\) can be derived. However, on time scales \(\delta t \ll \tau_f\), the particle dynamics is still strongly correlated with its initial state. Performing a first order series expansion of Eq. (2) and (3) yields

\[
x = x_0 + v_0\delta t + \mathcal{O}(\tau^3/2), \tag{4}
\]
\[
v = v_0[1 - \tau] + \sqrt{2\langle v^2 \rangle\tau}\xi + \mathcal{O}(\tau^3/2). \tag{5}
\]

Although Eq. (4) describes the motion of a free particle following a ballistic trajectory, the particle is moving stochastically for \(\tau \ll 1\). Due to the “stochastic force” \(\xi\) in Eq. (5), the motion is not reversible in time. For this reason, stochastic path segments described by Eq. (4) and (5) are called pseudo ballistic.

To obtain a test criterion for particle collisions, we make use of the fact that on time scales \(\tau \ll 1\) the deviation of the actual trajectory from the ballistic path is small. From the higher terms of Eq. (5), one finds, that on average the dispersion of the particle position is

\[
\langle (x - x_0 - v_0\delta t)^2 \rangle = \langle \Delta x^2 \rangle = 2\tau^2\tau_f\tau^3 + \mathcal{O}(\tau^4). \tag{6}
\]

The dispersion in the direction of the ballistic trajectory \(\xi\) is negligible, while perpendicular to the trajectory, \(\langle \Delta x^2 \rangle\) contributes significantly. Heuristically, this
result can be interpreted that the particle is moving towards its ballistic path (4) within a cone having the time-dependent opening radius $\langle \Delta x'^2 \rangle^{1/2}$. Consequently, the prerequisite for an aggregate collision within $\tau \ll 1$ is the intersection of their probability cones. If a particle pair fulfills this criterion, the trajectories of the two aggregates will be simulated with a high temporal resolution according to Eq. (4) and (5). The time step interval is obtained by the requirement that the faster particle move one diameter of the larger aggregate during that time. If the particles become closer to each other than the distance of the sum of their radii, then they will be combined into a new cluster.

2.2 Numerical realisation: Calendar algorithm

As mentioned before the coagulation of particles following a diffusive trajectory can be represented by MD methods if the applied time step $\delta t$ is much smaller than the friction time $\tau_f$. In the course of a time step $\delta t \ll \tau_f$, only particles closer than a critical separation are likely to collide. Only for these pairs the test of the collision criterion is required. Therefore, at each time step the nearest neighbour of the considered particle has to be determined. Experience shows that, due to the large velocity dispersion of the growing ensemble, algorithms with global time step schemes are inefficient for simulating the coagulation. Therefore we utilised a time step scheme respecting the dynamical state of the particles. The algorithm is similar to MD methods simulating hard sphere fluids. The basic idea is to perform average constant length steps, instead of constant time steps. To implement this idea, the simulation volume is divided into cubical cells of the same size. Next, the individual time step $\delta t_i$ for a particle is defined by the interval $\delta t_i = t'_i - t_i$ that the particle needs to move from its current cell to a neighbouring one, where $t_i$ and $t'_i$ are the instant of the last update of its coordinates (its “local time”) and the instant of crossing the cell boundary, respectively. Obviously, within the interval $(t_i \ldots t'_i)$, a particle can only collide with particles also belonging
to its cell. It is essential that for the ensemble particle $i$ leaving its cell first (ie $t'_i = \min(t'_1 \ldots t'_N)$), all possible collision partners have moved into its cell before $t_i$. This leads to the following procedure: First, for each cell, build a list of the embedded particles. Next, for the particle with the smallest cell crossing time $t'_i$, the collision criterion is checked with respect to the other particles in its cell. If no collision is found, the particle position and velocity are updated according to Eq. (4) and (5). Finally, the cell list is updated and the procedure is repeated for the next particle with the momentarily smallest $t'_i$ (see Fig. 2). It should be noted that in contrast to “classical” MD, touching the cell boundary at $t'_i$ does not necessarily mean that the particle will instantaneously leave its embedding cell. Due to the stochastic nature of its motion, the particle can be “reflected” on the boundary. For a more detailed consideration of such effects we refer to the description of our method\(^1\).

The prerequisite for an efficient numerical implementation of the described procedure is a fast search algorithm for the smallest cell crossing time $t'_i$ (the so-called “event”). Therefore, the cell-crossing events are arranged in a tree-like structure (the so-called “calendar”) as demonstrated in Fig. 3.

\subsection*{2.3 Rescaling of the particle number}

Every N-particle method suffers from finite size effects due to the restricted number of simulated particles $N$. In order to minimise such effects, one chooses $N$ as large as possible. However, for aggregation studies it is not sufficient just to start with a large $N$, since the particle number density decreases due to the collisional sticking. In previous aggregation studies, the growth was simulated in a box of constant

![Figure 2. A 2-dimensional example of three time steps according to the presented event-driven algorithm. The arrows show the predicted trajectories within the cells, while the italic numbers are the predicted instants $t'_i$ of crossing the cell boundaries. For each time step the trajectory of the bold-printed particle is simulated. Before the first time step all particles have the local time $t_i = 0$ (Fig. a). Due to $\delta t_{11} = \min(t'_1 \ldots t'_{12}) = 0.3$, the first time step has to be conducted for particle 11. After this, the new local time for particle 11 is $t_{11} = 0.30$ (Fig. b), while after the second time step ($\delta t_{12} = \min(t'_1 \ldots t'_{12}) = 0.35$) the local time for particle 12 is $t_{12} = 0.35$ (Fig. c). Note that for particle 12 periodic boundary conditions were used.](image)
volume. In that case, the total number \( N \) of simulated particles in the course of the simulation decreased, leading to strong finite size effects. In extreme cases, the box contained eventually only a single huge particle (e.g., Ziff), which is an unphysical result. Such effects can be avoided if the number of simulated aggregates is kept constant on average. For maintaining an almost constant \( \langle N \rangle \) we rescale the size

\[
\Delta N = N(t) - \langle N \rangle
\]

by rescaling the box size. Fig. (a) shows the box before the rescaling. The hatched parts mark the areas copied to the new volume as demonstrated in Fig. (b). On the average the rescaled box contains again \( \langle N \rangle \) particles (Fig. (c)).

\[
L \rightarrow L' = L \sqrt{1 + \Delta N(t)/\langle N \rangle}
\]

if the particle loss \( \Delta N \) exceeds a given threshold. The new volume is refilled with copies of clusters of the original box (Fig. (b)). Note, that the global observables of the simulation (mass density, cluster size spectrum) are not changed by this rescaling method.
3 Results

In this section we give a brief overview of the results we obtained from simulations using scalar machines. We investigated the coagulation driven by Brownian motion for the typical conditions in a proto-planetary disc at 10 AU. All simulations were started with \( N \) randomly distributed spheres of 1 micron diameter. The simplification of an initially mono-disperse size distribution is justified by the fact that the growth driven by Brownian motion tends to form aggregates of similar size. In order to study the influence of the initial dust number density \( n_0 \) simulations with \( n_0 \) between \( 10^7 \ldots 10^9 \text{m}^{-3} \) were performed. Most of the simulations were carried out with 10,000 particles. For each parameter set at least six runs with different seeds of the random generator were executed.

3.1 Structure of the growing aggregates

As outlined in Sec. 1 the prerequisite for an effective grain growth driven by turbulence is a rapid increase of the aggregate friction time \( \tau_f \). Both, theoretical studies and experiments show, that for particles, which are small compared to the mean free path of the gas, \( \tau_f \) is proportional to their mass–surface ratio. This has the consequence, that the \( \tau_f \)-evolution is determined by the structure of the growing aggregates. The increase of the particle mass \( m \) with respect to a typical radius \( R \) is a characteristic scaling property of any growth regime and can be expressed by a fractal dimension \( D_m \)

\[
m(\lambda R) = \lambda^{D_m} m(R).
\]

All published models for the dust coagulation assume that there is a unique value of the fractal dimension \( D_m \) describing all aggregates of the dust ensemble. However, real growth processes produce a wide variety of different particle structures. In (Fig. 5a) the distribution of the fractal dimension of a simulated dust ensemble for fixed times is shown. We found that the mean fractal dimension \( \langle D_m \rangle \) is about 1.8. This value is in good agreement with the results of Monte-Carlo simulations of the ballistic Cluster-Cluster-Aggregation (BCCA). In order to analyse the \( \tau_f \) evolution also the scaling of the projected aggregate area \( \sigma \) with the typical radius has to be known. Our studies show (Fig. 5b) that the often used assumption of \( \sigma \sim R^2 \) implies the wrong picture of the \( \tau_f \) evolution. We found that \( \sigma \) scales approximately as \( R^{1.6} \), corresponding to a friction approximately proportional to the eighth root of the typical aggregate mass (Fig. 5c). Although we obtained in contrast to simpler models a size-dependent friction time our result still shows that growth solely driven by Brownian motion cannot form aggregates with friction times comparable to the lifetime of the smallest turbulent eddies within a million years. However, due to the broad distribution of the fractal dimension there are some aggregates growing as compact particles. These particles are of great importance because they could be possible seed grains for a runaway growth due to differential sedimentation.

\* We considered a disc of 80 AU with a mass accretion of \( \dot{M} = 10^{-6}M_\odot\text{yr}^{-1} \) and an “alpha” viscosity of \( \alpha = 10^{-2} \). Using the one-dimensional hydrodynamical disc model of Ruden&Pollack we determined the gas temperature \( T_g \) and pressure \( p_g \) at 10 AU as about 100 K and \( 2 \cdot 10^{-4} \text{Pa} \), respectively.
3.2 Evolution of the mass spectrum

In the previous section we discussed the friction time growth with the aggregate size. Equally important for the understanding of the formation of larger aggregates in proto-planetary discs is the dynamics of the growth. The evolution of the cluster ensemble is characterised by the number density $n_s$ of clusters of the mass $s$. For the simulated spectra of the Brownian coagulation we observed a self-similar evolution. For such growth processes the mass spectrum can be described by the scaling ansatz

$$n_s(t) \sim t^{-w} s^{-\tau} f(s/t^z),$$

where $w$, $\tau$, and $z$ are scaling exponents and $f(x)$ is the scaling function of the growth process. In the asymptotic limit, the scaling exponents are related by $w = (2 - \tau)z$. Furthermore, the mean cluster mass $S(t) \sim \sum s n_s s^2$ evolves asymptotically as $S(t) \sim t^z$ while the cluster number density $n(t) = \sum s n_s$ scales as $n(t) \sim t^{-w}$ for $\tau < 1$ and $n(t) \sim t^{-w}$ otherwise. From the averaged spectra...
we calculated the mean cluster size and the cluster number density for different initial number densities \(n_0\) (Fig. 6). The calculated scaling exponents are related to each other as predicted by this concept. Consequently, the scaling ansatz (7) is appropriate to describe the dust growth driven by Brownian motion at low number densities. The scaling exponents \(z\) derived from the asymptotic growth of the mean cluster mass for different \(n_0\) are smaller than 2. Consequently, the fastest increase of the mean friction time due to Brownian growth is \(\langle \tau_f \rangle \sim t^{1/4}\). This result supports the point made in the previous section that the short time scales of dust growth required by astronomical and geophysical constraints can not be due to coagulation driven by Brownian motion.

In numerical studies of the cosmic dust growth the aggregation process is very often described by a rate equation approach. As the spatial dependence of the number densities is neglected, this approach is a mean field description of the growth. In this framework the scaling exponents \(z\), \(w\), and \(\tau\) are ruled by the scaling behaviour of the rate coefficients and do not depend on the initial number density \(n_0\). However, as indicated in Fig. 6, our simulation results show a significant dependence upon \(n_0\), which might be due to spatial fluctuations of the number densities. Our results suggest that using the Smoluchowski theory should be done with caution for describing the dust growth in proto-planetary discs.

4 Conclusions

In the early stages of dust growth the coagulation of dust particles driven by Brownian motion plays an important role. In order to explain the short time
scales of dust growth as constrained by astronomical and geophysical studies not only the mass of the dust particles but also their friction time has to increase quickly. We developed an N-particle model that allowed us to study coagulation driven by Brownian motion. In contrast to earlier studies, the dust growth was investigated at astrophysically relevant small number densities. Under such conditions the mean particle distance exceeds the typical aggregate diameter by orders of magnitude, and a collision will be a rare event. We derived a criterion which allows an efficient detection of candidates for imminent collisions. The N-particle-method is based upon an adaptive time step scheme respecting the individual dynamical states of the aggregates. Its basic concept is to perform on average constant “length steps”, instead of using constant time steps. In order to minimise the influence of the decreasing number of particles within the simulation box, a new rescaling method is used throughout the aggregation process.

We found that the structural properties of a dust cloud is characterised more completely by the distribution of the fractal dimensions of its constituent clusters. The mean of this distribution of $D_m \sim 1.8$ is in good agreement with the results of Monte-Carlo simulations of the ballistic Cluster-Cluster Aggregation (BCCA). The friction time of the aggregates growing due to Brownian coagulation scales with the mass as $\langle \tau_f \rangle \sim m^{1/10}$.

In addition, the dynamical evolution of the dust ensemble has been investigated. We found that the mass spectrum of the ensemble evolves self-similar. For that reason, the mass spectrum of the dust growth due to Brownian motion at low number densities can be described by a scaling ansatz. We derived from the simulated spectra that the mean friction time of the dust ensembles increases with time as $\langle \tau_f \rangle \sim t^{1/4}$. This indicates that the fast dust growth in proto-planetary is not due to the Brownian coagulation.

Acknowledgments

The authors are indebted to R. Mucha, J. Blum, H. Klahr, and A. Graps for helpful and stimulating discussions. This work was made possible by the support of the DFG to SK (DFG grant He1935 within the special programme “Physics of Star-formation”) and SP (DFG-Habilitation grant). The numerical simulations were partially carried out at the super-computing centre Jülich, Germany and we wish to thank for generous allocation of computing time.

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