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mcdust: A 2D Monte Carlo code for dust coagulation in protoplanetary disks

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Software

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Summary

The Solar System and other planetary systems are formed in a disk of gas and dust around the young, forming central star, called a protoplanetary disk. The micron-sized particles collide and grow through several processes to form the planetary architectures as we see them today. The overall gas dynamics, the interaction between the gas and dust, and the collisions between the dust particles leave an imprint on the formation pathways of the planets and, therefore, on life. Recent observations with telescopes such as ALMA (Andrews et al., 2018) show a diversity of dust structures in protoplanetary disks, and it is imperative that we have models that are able to describe the observations and, more generally, to help move forward towards the goal of an end-to-end planet formation theory. We present `mcdust`, a parallel Monte Carlo code aimed at modelling the evolution of dust in protoplanetary disks to better understand the dust size distributions and dust collisional evolution.

Statement of need

Modelling dust coagulation and evolution is an essential part of understanding protoplanetary disks and planet formation. The evolution of micrometer-sized dust grains to millimeter-sized aggregates sets the tone for planetesimal formation. Dust evolution is inextricably linked with the formation of substructures in disks (Pinilla et al., 2012) and is of prime importance when understanding disk chemistry (Houge et al., 2025; Woitke et al., 2016). Therefore, it is important to understand the processes involved in dust growth and dynamics and how they influence different aspects of disk dynamics and planet growth in detail.

Dust coagulation is generally modelled with the Smoluchowski equation (Smoluchowski, 1916), an integro-differential equation. The drawback of the method is that when we add a property to track (e.g, charge, composition, porosity), it adds a dimension to solving the Smoluchowski equation and necessitates a parameterized approach when considering dust properties to reduce the complexity in these methods (Blum, 2006; Okuzumi et al., 2009; Stammler et al., 2017).

One can also model dust coagulation by performing Monte Carlo simulations. Monte Carlo methods are well-suited for stochastic processes, making them suitable for dust coagulation (Gillespie, 1975). For such a method, the representative particle approach (Ormel et al., 2007; Zsom & Dullemond, 2008) is very suitable, allowing us to track the particles and hence their histories. We can add properties to the particles that can be tracked without much computational complexity. This advantage is very useful when we want to combine dust evolution and chemistry, allowing us to examine the thermal histories of particles and their compositions when chemical models are included (Flores-Rivera et al., 2025).

Although there have been several publications that have made use of the Monte Carlo method to model dust coagulation in protoplanetary disks (Houge & Krijt, 2023; Krijt et al., 2018), there is no available open-source code that models dust coagulation using Monte Carlo methods, and such a code would be very helpful.

State of the field

Several codes exist to model dust growth in protoplanetary disks, and we focus on discussing the open-source codes in the field. There are semi-analytical methods like `twopoppy` (Birnstiel et al., 2012) and `TriPoD` (Pfeil et al., 2024) that model the overall dust size distributions without modelling full dust coagulation. Some examples of open-source codes that model full dust coagulation are `dustpy` (Stammler & Birnstiel, 2022), a 1D code to simulate gas and dust evolution, and `cuDisc` (Robinson et al., 2024), a 2D (radial-vertical) code modelling dust coagulation and disk evolution. Both of these codes solving the Smoluchowski equation are Eulerian in nature, i.e., they follow volume rather than mass. `PHANTOM` (Price et al., 2018) is a smoothed-particle hydrodynamics code that models dust growth using a monodisperse growth approximation and does not solve the Smoluchowski equation for dust growth (Vericel et al., 2021). We refer the reader to Eriksson et al. (2026) for a comparison of the different dust evolution codes, including `mcdust`.

`mcdust` models dust coagulation and transport in the vertical and radial directions. The currently included collisional outcomes are dust growth by sticking, fragmentation of dust particles, and erosion, where a small particle chips a portion of the large particle. We employ a representative particle approach detailed in Zsom & Dullemond (2008) to track a limited number of particles instead of tracking every particle, saving computational time. We have a static power-law gas disk in the default version where the gas surface density is $\Sigma_g = \Sigma_{\mathrm{AU}}(r/\mathrm{AU})^{-1}$ with Σ_{AU} being the gas surface density at 1 AU. The temperature is assumed to be vertically isothermal, given by $T = T_{\mathrm{AU}}(r/\mathrm{AU})^{-0.5}$ with T_{AU} being the temperature at 1 AU. The static power-law gas disk is a good assumption for simulations less than Myr timescales. This can be modified as per the user's needs. Dust coagulation depends on the local gas properties, and therefore, we bin particles into grids in order to perform collisions. We make use of an adaptive grid approach where we make sure that each cell has an equal number of representative particles. This guarantees that there are always sufficient particles to resolve the physics of collisions. Figure 1 shows a sketch of our adaptive grid model and the different physical processes simulated by `mcdust`.

`mcdust` in its first iteration was introduced in Drążkowska et al. (2013). In its current version, the code has been optimized and modified to make it faster and adaptable to suit the needs of the user. But the physics of the code has largely remained the same, and we refer the reader to Drążkowska et al. (2013) for the details.

The particle-based approach makes `mcdust` useful for performing dust coagulation simulations with different properties (e.g., porosity) and compositions for dust with little computational overhead. Including dust growth/dynamics in hydrodynamic simulations of protoplanetary disks can be very expensive and computationally complex (Drążkowska et al., 2019). This is where `mcdust` can also be used to post-process data from hydrodynamic simulations to understand the dynamics and evolution of dust in different conditions. The current version of `mcdust` can take 2D (r-z) steady-state gas velocities as input and perform dust growth simulations for different gas velocity structures seen in hydrodynamic simulations.

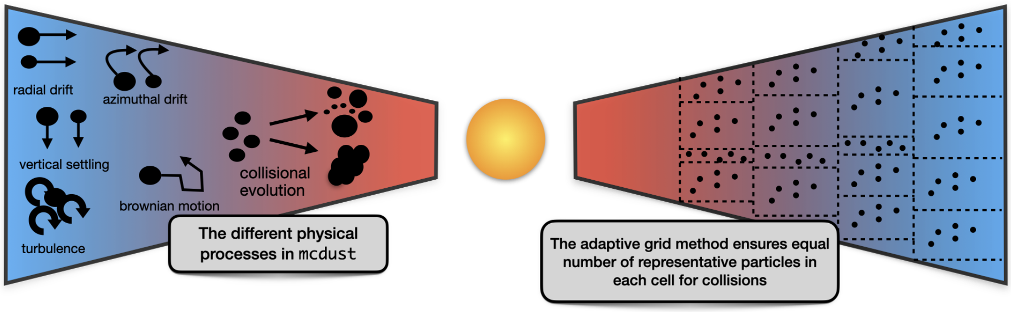

Figure 1: (Left) An overview of the different physical processes in `mcdust` and (right) a representative sketch of the adaptive grid method used in `mcdust` to group particles and perform collisions.

Software design

The representative particle approach can be computationally intensive and, therefore, time-consuming when running a simulation with enough resolution (Drążkowska et al., 2014). `mcdust` has been designed with the intention to overcome this aspect and is written in Fortran and parallelised with OpenMP, which enables the user to utilize high-performance computing systems on the node level. The modules of `mcdust` are written in such a way that the user can modify the specific module as per their requirements. For example, the major processes in the simulations can be turned off/on with the preprocessor directives before running the simulation. Large parts of the code, like the protoplanetary disk setup (`discstruct.F90`) and the initialisation of the dust particles across the disk (`initproblem.F90`), are written in a way that they can be adapted by the user for their specific needs. The data I/O is done with the HDF5 data format to ensure faster writing and reading of data for further analysis. We also provide a Python script that aids the user with the data visualisation, which can be modified to the user's needs.

Research impact statement

`mcdust` has already been used in its previous iterations to model the evolution of dust in protoplanetary disks. Drążkowska et al. (2013) used it to model the pile-up of dust in the inner edge of the dead zones in protoplanetary disks. We refer the reader to Drążkowska et al. (2014) and Drążkowska & Szulágyi (2018) for other instances where `mcdust` has been used to model dust growth in protoplanetary disks. Vaikundaraman et al. (2025) investigated the depletion of refractory carbon in the inner Solar System, and Gurrutxaga, Drążkowska, et al. (2026) modelled the formation of carbonaceous chondrites in a pressure bump using `mcdust`, demonstrating its capabilities of adding properties to particles and tracking them. Gurrutxaga, Vaikundaraman, et al. (2026) showed a more robust way to track particle properties using a modified version of `mcdust`, which will soon be implemented in `mcdust`. Vaikundaraman et al. (2026) used `mcdust` to post-process magnetohydrodynamic simulations to understand dust evolution in complex gas flows.

Benchmark

We compare a run of our code with a run from the open-source 1D dust coagulation code `dustpy` (Stammler & Birnstiel, 2022). The parameters used for the simulations are listed in Table 1. The gas evolution in both codes was switched off, and the codes were run with a static gas background to exclude any differences in gas treatment that might influence the outcome of dust evolution.

Table 1: Parameters used for the benchmark simulations to compare `mcdust` and `dustpy`.

Parameter	Value
gas surface density at 1 AU	$1000\ \mathrm{g/cm^2}$
temperature at 1 AU	280 K
turbulence strength (α)	10^{-3}
fragmentation velocity (v_{frag})	10 m/s
erosion mass ratio	10
gas surface density power law p	1
temperature power law q	0.5

We ran a simulation for 10,000 years. Figure 2 shows the dust surface density σ_d as a function of particle mass and distance from the star at the end of the simulation for both `mcdust` and `dustpy`.

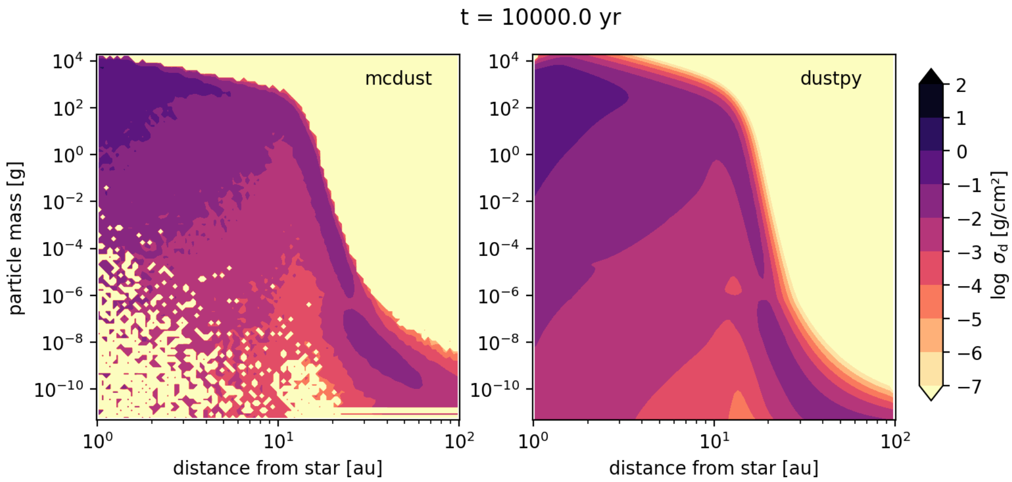

Figure 2: A comparison of the dust surface density σ_d as a function of particle mass and distance from the star between `mcdust` (left) and `dustpy` (right).

It is evident from Figure 2 that both codes have similar overall outcomes, but there are certain differences. The most striking one is that `mcdust` does not provide coverage of the regions of parameter space that do not include a sufficiently high fraction of the dust mass. This holds for all Monte Carlo-based codes. But with higher resolution simulations, this issue can be overcome. The other important factor is that `mcdust` does not face the issue of artificially sped-up growth (Drążkowska et al., 2014) that `dustpy` and other Smoluchowski equation-based codes tend to encounter (Stammler & Birnstiel, 2022). And the 2D r-z structure of `mcdust` also helps us to investigate processes like sedimentation-driven coagulation (Drążkowska et al., 2013) that are not usually seen in 1D simulations like `dustpy`. This can be seen in the image at around 50 AU, where `mcdust` has larger surface densities and higher masses when compared to `dustpy`. For a more detailed discussion of the differences between the Monte Carlo method and the Smoluchowski equation approach, we point the reader to Drążkowska et al. (2014). Benchmarking the simulations against analytical coagulation kernels is an important way to validate the coagulation models, and we refer the reader to Drążkowska et al. (2013) and the `mcdust` documentation for the different coagulation kernel tests.

AI usage disclosure

No AI tools, including generative AI tools, have been used in the development of the software, creation of the documentation, or writing of the paper.

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