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Dust grain coagulation modelling: From discrete to continuous

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ABSTRACT

In molecular clouds, stars are formed from a mixture of gas, plasma and dust particles. The dynamics of this formation is still actively investigated and a study of dust coagulation can help to shed light on this process. Starting from a pre-existing discrete coagulation model, this work aims to mathematically explore its properties and its suitability for numerical validation. The crucial step is in our reinterpretation from its original discrete to a well-defined continuous form, which results in the well-known Smoluchowski coagulation equation. This opens up the possibility of exploiting previous results in order to prove the existence and uniqueness of a mass conserving solution for the evolution of dust grain size distribution. Ultimately, to allow for a more flexible numerical implementation, the problem is rewritten as a non-linear hyperbolic integro-differential equation and solved using a finite volume discretisation. It is demonstrated that there is an exact numerical agreement with the initial discrete model, with improved accuracy. This is of interest for further work on dynamically coupled gas with dust simulations.

1. Introduction

The matter which fills the space between the stars consists of rarefied gas, small dust particles – the so called interstellar medium (ISM) – magnetic fields and background radiation. While dust accounts only for a small part of the total mass of the ISM (∼1% (Spitzer, 1954)), its presence is of the utmost importance as its absorption and scattering (mainly at ultraviolet and optical wavelengths) and its (re-)emission (mainly in (far) infrared wavelengths) of incoming radiation provides the possibility to gain detailed knowledge of the ISM. Furthermore, as demonstrated in coupled gas–dust simulations of well-observed shear flow regions in the Orion nebula, performed in Hendrix et al. (2015), dust can influence the dynamics of the ISM, leading to the formation of observable structures in molecular cloud environments, in which stars and planets are ultimately formed. From recent observational data it is known that in molecular clouds, dust grains can reach micrometre scales (Pagani et al., 2010; Steinacker et al., 2010), becoming much larger than their typical size in the diffuse ISM ∼250 nm (Kim et al., 1994). By using adequate models of grain coagulation and accretion to simulate growth of dust grains in molecular clouds, one can try to understand the environment in which grains grow to a substantial size, and on which time scales such growth is to be expected. In combination with observations, this allows an estimation of the life expectancy of a molecular cloud, and can even provide insight into the typical time scales of star formation processes (Hirashita and Li, 2013).

The role of dust coagulation is also important in protoplanetary disks, and in that context, it has been investigated intensely in the last decade. We limit ourselves to discuss a selection of findings that are likely also relevant for dense molecular cloud cores. Dust evolution in terms of its particle size distribution and its tendency to settle towards the midplane of a (quiescent or turbulent) protoplanetary disk was studied by Nomura and Nakagawa (2006), for the case of the solar nebula. The authors solve a coagulation equation (their Eq. (12)) that includes a vertical mass transport term of interest for dust settling in protoplanetary disks, and use it to obtain dust size distributions as a function of time and disk height at the orbits of Earth, Jupiter or Neptune. The main finding was that a gravitationally unstable layer of dust, with particles up to centimetre sizes, can form at distances 1–30 AU in a quiescent disk. Ormel et al. (2007) also investigated the solar nebula case, and used a Monte Carlo approach to, in essence, avoid the direct numerical integration of the collision/coagulation model expressed by an (extended) Smoluchowski equation (their Eq. (20)). Using Monte Carlo traces growth of individual particles directly, and can recover the evolution of the particle size distribution function, when binning over particle masses. In the

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protoplanetary disk context, it was found that the collisional evolutions are influenced by the coupling between dust and gas motions, depending intricately on the internal structure of the grains (in particular, on their porosity). In the present paper, we will discuss equivalent ways to handle the direct integration of the Smoluchowski equation, inspired by the work by Hirashita (2012).

Mathematical models for grain–grain interactions have been improved in the last decade, and Hirashita's work in Hirashita and Yan (2009), Hirashita (2012) and Hirashita and Li (2013) presents discrete models for coagulation, accretion and fragmentation of dust, whilst keeping the dust decoupled from the gas dynamics. Focusing only on coagulation, the purpose of this paper is to validate the discrete model in Hirashita (2012), study its properties, and propose a different numerical implementation adapted to improve the coupling with gas dynamics. The crux of the study is the relationship identified with the well known Smoluchowski equation, introduced first in 1916 Smoluchowski (1916) and widely studied since. This result is obtained by deriving the continuous form of the discrete coagulation model in Hirashita (2012), which yields the Smoluchowski equation with a specific kernel.

The role of the Smoluchowski equation in coagulation and porosity evolution of dust species in protoplanetary disks is exploited fully in Okuzumi et al. (2009), where the distribution function of aggregates, whose evolution is governed by a Smoluchowski equation (their Eq. (1)), was allowed to depend on both mass and volume of the dust aggregates. A so-called volume-averaging procedure rephrases attention to evolution equations for the moments of the distribution function. In doing so, one needs a suitable truncation to circumvent the problem that this procedure introduces ever higher order moment dependences. In our work, we will use a simple dust coagulation model and demonstrate clearly the various equivalent means to formulate it discretely or continuously, and show the advantages of using a conservative formulation. This is needed in preparation for fully dynamic gas–dust evolutions, which simultaneously handle evolving dust size distributions. Once more, protoplanetary studies by Birnstiel et al. (2010) already made progress in handling the coupled gas plus dust evolution consistently, where a time-dependent viscous disk is incorporated as far as its radial dependences are concerned. In Birnstiel et al. (2010), the governing Smoluchowski equation was vertically integrated, using Gaussian kernels to handle some of the involved integrals analytically. A flux-conserving donor-cell scheme was then used to numerically integrate the set of two advection–diffusion equations for the surface densities of gas and dust species, together with the vertically integrated Smoluchowski equation.

The computational cost of correctly simulating dust in full 3D dynamical models (i.e. not relying on vertically integrated prescriptions) is considerable, as dust grains are highly diverse and have complex compositions and morphologies. Most importantly, they cover a size distribution range which spans more than ten orders of magnitude in locations such as protoplanetary disks (Testi et al., 2014). Only few numerical simulations have taken the effect of dust into account, and those that do have made simplifying assumptions: e.g. the works of Saito (2002), Miniati (2010) and Laibe and Price (2012) used a two-fluid approach in which only one discrete dust size is considered, while the work by Hendrix and Keppens (2014), Hendrix et al. (2015) and Hendrix and Keppens (2015) adopted a fixed size distribution for all times, where individual grain size bins do not communicate through coagulation or shattering processes, but where each size bin is coupled dynamically to the gas as a pressureless fluid subject to (size-dependent) drag-forces. This approach was pioneered in protoplanetary disk studies in Paardekooper and Mellema (2006). In an early study of protoplanetary disks, a 2.5D (axially symmetric) model by Suttner and Yorke (2001) did explore the coupling of gas with dust using up to 30 dust size bins, and showed the importance of dust coagulation in the first 1000 years of the protostellar accretion disk.

The outline of this paper is as follows. Since we focus on a specific model as studied in discrete form by Hirashita and Li (2013), Hirashita (2012) and Hirashita and Yan (2009), we opt to summarise Hirashita's work as presented in Section 2. The corresponding continuous model is derived in Section 3. The properties of the model are then studied in Section 4, where the existence of a unique mass conserving solution is proven, relying heavily on existing literature on the Smoluchowski equation. In Sections 5 and 6, a continuously conservative alternative form is outlined, together with its finite volume approximation, following the work in Filbet and Laurençot (2004). Ultimately, the initial and the modified numerical models are compared in Section 7.

2. The discrete model

This section focuses on the discrete coagulation model by Hirashita (2012), which describes how dust grain size distribution n evolves in time, in dense cores of molecular clouds. Discarding the spatial dynamics; which would require a coupling with the gas dynamics; it is possible to write the distribution as a function $n(a, t)$ only of particle size a and time t. In the discrete model used in Hirashita (2012), n is hidden in the discrete variable ρ_i which represents the mass density of all grains with mass in the range $[m_{i-1/2}, m_{i+1/2}]$:

$$\rho_i(t) = \int_{m_{i-1/2}}^{m_{i+1/2}} \hat{n}(m,t) m \, dm \sim \hat{n}(m_i,t) m_i [m_{i+1/2} - m_{i-1/2}], \quad (1)$$

where $\hat{n}(m, t)$ is the number density as a function of the grain mass m instead of the grain size, which is related to $n(a, t)$ through $dN_{gr}/V = n(a,t)\, da = \hat{n}(m,t)\, dm$, where $N_{gr}(t)$ is the total number of dust grains at time t in a volume V. The index i ranges from 1 to N, with N the total number of dust bins in the discrete model such that $\cup_i (m_{i-1/2}, m_{i+1/2})$ covers the total interval of grain masses considered.

The discrete model for dust coagulation taken from Hirashita (2012) reads:

$$\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} = -Q^- + Q^+, \quad (2)$$

at the left hand side, an explicit Euler scheme is used for the time evolution of the discrete variable ρ_i and the superscript index n (here, n is not the grain size distribution anymore) accounts for the time discretisation. At the right hand side, Q^- represents the loss term of the ith bin, due to the coagulation between grains in the ith bin and all grain sizes. Q^+ instead is the gain term of the ith bin, given by all the interactions between smaller grains that give rise to grains of ith mass. These terms are all evaluated at time level n (explicit) and characterised as follows

$$Q^- = m_i \rho_i \sum_{l=1}^{N} \alpha_{li} \rho_l, \quad (3)$$

$$Q^+ = \sum_{j=1}^{N} \sum_{l=1}^{N} \alpha_{lj} \rho_l \rho_j m_{coag}^{lj}(i). \quad (4)$$

In the expressions, α_{lk} is a weight matrix:

$$\alpha_{lk} = \frac{\sigma_{lk} v_{lk}}{m_k m_l}. \quad (5)$$

Here, $\sigma_{lk} = \pi(a_l + a_k)^2$ is the cross section, note that the sizes a_l, a_k can be seen as function of grain mass m, since the grains are