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growpacity: A computationally efficient dust opacity model suitable for coagulation models

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Summary

growpacity is a Python and C toolkit for calculating dust opacities in astrophysical environments. It provides a class (OpacityCalculator) for generating, storing, and interpolating mean opacities (Rosseland and Planck) over customizable grids of grain size distributions, temperature, and power-law exponents. This package is designed as a wrapper around OpTool, allowing users to specify grain composition and obtain temperature-, maximum grain size-, and dust size distribution-dependent mean opacities. The resulting tables are lightweight and optimized for use in radiation hydrodynamics and dust coagulation models, where grain size distributions evolve dynamically.

Statement of need

Radiation hydrodynamics simulations often require a dust opacity model under the assumption of a particular grain size or size distribution. It is however not straightforward to implement a dust opacity model that accounts for the dynamical evolution of this grain size distribution. With growpacity, we outline a method to construct such a model and provide a python package that implements it. The model is a wrapper around the OpTool package, with the user providing a grain composition and receiving temperature-, maximum grain size-, and dust size distribution-dependent mean opacities, tabulated in a lightweight format and complemented with efficient interpolation methods for usage in radiation hydrodynamics simulations.

Method

For a given grain composition and assuming a grain size distribution with number density $n(a) \propto a^q$ for grains with size a between minimum and maximum grain sizes $a_{\min}$ and $a_{\max}$, the OpTool package (Dominik et al., 2021) can compute the absorption and scattering opacities κabs(ν) and $\kappa_{\mathsf{sca}}(\nu)$ (in cm^2/g) as well as the asymmetry factor $g(\nu)$ (Henyey & Greenstein, 1941) over a frequency grid ν. This calculation is done using the Distribution of Hollow Spheres method (DHS) (Min et al., 2005). The Rosseland and Planck mean opacities κ_{R} and κ_{P} can then be computed as

$$\kappa_{\mathsf{P}}(T) = \frac{\int_0^\infty \kappa_{\mathsf{abs}} B_\nu(T) d\nu}{\int_0^\infty B_\nu(T) d\nu}, \quad \kappa_{\mathsf{R}}(T) = \frac{\int_0^\infty u_\nu(T) d\nu}{\int_0^\infty [\kappa_{\mathsf{abs}} + (1-g)\,\kappa_{\mathsf{sca}}]^{-1} u_\nu(T) d\nu}, \quad u_\nu(T) = \left.\frac{dB_\nu}{dT}\right|_T,$$

where $B_\nu(T)$ is the Planck function at temperature T. By fixing the grain composition and $a_{\min}$, OpTool can be used to calculate the absorption and scattering opacities over a grid of

a_{max} and q. The above equation can then be used to compute and tabulate κ_{R} and κ_{P} over a_{max}, q, and T. The resulting 3D tables can be used in any context where a_{max} and q are dynamically evolved according to a dust coagulation model (Birnstiel et al., 2017; Pfeil et al., 2024; Robinson et al., 2024; Stammler & Birnstiel, 2022).

Interpolation algorithm

Once the 3D tables of $\kappa_{\mathrm{R}}(q, a_{\mathrm{max}}, T)$ and $\kappa_{\mathrm{P}}(q, a_{\mathrm{max}}, T)$ have been computed, they can be interpolated within the range of tabulated values. We interpolate for $\log\kappa$ as a function of q, $\log a_{\mathrm{max}}$, and $\log T$, with regular sampling in this space (i.e., logarithmic spacing for a_{max} and T). This works best when the mean opacities follow a powerlaw with respect to temperature $\kappa \propto T^b \Rightarrow \log\kappa \propto b\log T$, which is a reasonable approximation and especially holds for small grains (Bell & Lin, 1994; Semenov et al., 2003). It also ensures that the interpolated opacities are always positive in case extrapolation is needed.

We use a trilinear interpolation scheme, which is fast and simple to implement, and takes advantage of the fact that the arrays q, $\log a_{\mathrm{max}}$, and $\log T$ are sorted and regularly spaced to efficiently locate the indices of the grid points that surround the point of interest. For each array $x \in \{q, \log a_{\mathrm{max}}, \log T\}$ and for a target value x_t, we first find the index i such that $x_i \leq x_t < x_{i+1}$ as $i = \lfloor (x_t - x_0)\,\Delta x^{-1} \rfloor$, where x_0 is the first (smallest) value in the sampling space and $\Delta x = x_{i+1} - x_i$ is the (constant) sampling spacing. As this information is known *a priori*, this reduces the complexity of finding the required indices from $\mathcal{O}(\log N)$ to $\mathcal{O}(1)$, where N is the number of grid points in x, and is especially efficient for larger grids. Of course, care must be taken to ensure that the indices are within the bounds of the grid.

Implementation

The above method is implemented in the `growpacity` package. The package provides a simple `python` interface to `OpTool` to compute accurate dust opacities for a given grain composition (provided in `OpTool` format) and for a fixed a_{min}, over a grid of a_{max}, q, and T. The resulting 3D tables of κ_{R} and κ_{P} are saved in binary files that can be easily loaded with `python`. We also provide an implementation of the interpolating function in `C`, that can be readily used in radiation hydrodynamics codes. These files are especially lightweight: a typical calculation involving $q \in [-4.5, -2.5]$ with $\Delta q = 0.25$, $a_{\mathrm{max}} \in [0.1\,\mu\mathrm{m}, 1\,\mathrm{m}]$ sampled twice per decade, and $T \in [1, 2000]$ K with 100 points results in two arrays of $9 \times 15 \times 100$ elements, or about 220 kB of memory. This choice of spacing means that opacities are exactly evaluated for $q \in [-3.75, -3.5, -3]$, corresponding to dust size distributions in equilibrium due to small/large-scale turbulence, radial drift, or in a non-equilibrium growth regime. For more information, see (Pfeil et al., 2024).

The code and documentation are available at **https://github.com/alexziab/growpacity**.

Limitations and extensions

We underscore that our intent is not to provide a new or more realistic dust opacity model, but rather one suitable for use in coagulation models, where dust densities and distributions can vary as a function of position and time—the applicability of the model depends on entirely user-defined choices. The method can be easily extended to include gas opacities (Malygin et al., 2014; Semenov et al., 2003) and prescriptions for the sublimation of dust species (Isella & Natta, 2005), for a more complete opacity model in regimes where gas opacities are significant.

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