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Interim Summary Report

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Title: **How good is dust emission as a tracer of star-forming regions in molecular clouds?**

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1. Introduction

Molecular clouds are dense regions of the Interstellar Medium (ISM) at temperatures < 20 K [1] that are home to some of the earliest phases of star formation. Much like the ISM, they are composed of gas and cosmic dust. Dust is a relatively small fraction of the total ISM mass, estimated as being only 1% according to Shetty et. al. [2]. Whilst the dust mass accounts for such a small mass component, it still presents an important role in star formation. Dust properties such as the spectral index β and temperature T have an effect on dust emission and therefore the ability to detect radiation from within a molecular cloud due to, for example, a prestellar core and therefore understand the processes governing its formation and evolution.

1.1 Cosmic dust

Molecular clouds are also known as stellar nurseries for their active star forming roles, and the dust density is key to this - it is significantly greater inside a molecular cloud than in the ISM. Ward-Thompson and Whitworth [3] estimate that the number density at the centre of a typical molecular cloud is approximately 10^{12} particles m^{-3} , whilst the mean ISM density is only of the order 10^6 particles m^{-3} : a factor of 10^6 particles m^{-3} less.

1.2 Dust emission

Furthermore, cosmic dust is opaque to visible light meaning that a molecular cloud will not radiate in the visible wavelengths. Given the temperature of dust in both the ISM and a typical molecular cloud, cosmic dust radiates mostly in the far infrared and sub-millimetre regimes.

Cosmic dust emission is best described by a modified blackbody function as described in Kelly et. al. [4]:

$$S_\nu = \Omega B_\nu(T) \kappa_0 \left(\frac{\nu}{\nu_0} \right)^\beta N \quad (1.1)$$

for optically thin dust i.e. emission only. Here, S_ν is the flux density, Ω is the solid angle of the observing beam, B_ν is the Planck function at dust temperature T , N is the dust column density and κ_0 is a reference opacity. The remaining fractional term is described as κ , the opacity of the dust. The dust opacity is highly frequency dependent in ν (the frequency of emission) whilst ν_0 is a reference frequency. Finally, β is the spectral index of the dust, or the dust emissivity index according to Ward-Thompson and Whitworth [3]. The optical depth of the dust can be retrieved from Equation 1.1 as $\tau = \kappa_0 N$.

1.3 Theoretical Spectral Energy Distribution fitting

Experimentally, both T and β remain unknown terms. However, observational data such as that from the Herschel PACS and SPIRE detectors can be used to construct Spectral Energy Distributions (SED). An SED is simply a plot of flux as a function of wavelength (or frequency). By fitting a theoretical SED to the observed SED from Herschel data, the values of both β and T can be recovered. However, as Kelly et. al. [4] describes, β and T are degenerate such that an underestimate of β leads to an overestimate of T and likewise overestimates of β lead to underestimates of T . This is especially true of wavelengths $\geq 200\mu\text{m}$ according to Shetty et. al. [5]. Interestingly, Shetty et. al. [5] also concluded that a potential inverse T - β dependence, as was also described in Kelly et. al. [4], could be the result of noise in observations, something which greatly affects the accuracy of β and T estimates; line of sight temperature variations also effect this.

1.4 RADMC-3D

RADMC-3D is a 3-dimensional Monte-Carlo radiative transfer and ray tracing code developed by Cornelis Dullemond and written in Fortran 90 for radiative transfer and emission astrophysics in dusty environments [7]. A Python ‘wrapper’, `radmc3dPy`, allows RADMC-3D to be called from a Python script. RADMC-3D can run simulations in both Cartesian and Spherical coordinates; simulations in Cartesian coordinates were used in this study.

RADMC-3D is able to compute both images as well as Spectral Energy Distributions (SED) and spectra for a number of different continua. This project focussed only on dust continuum. The images can be computed using 2 different methods: the thermal Monte-Carlo simulation, or an image ray trace. All computations require input files for RADMC-3D to read and use in its simulations. RADMC-3D’s Python port, `radmc3dPy`, is able to write these input files, however for this project a custom script was written such that file creation was independent of `radmc3dPy`.

The thermal Monte-Carlo simulation is able to compute dust temperatures – using the technique described in Bjorkman and Wood [8] – from user-defined dust densities, providing a source of flux (and therefore photons) exists. This source of flux can either be through a star in the image space or an Interstellar Radiation Field. The code then ‘fires’ photons out from the flux source into the image space. Conversely the image ray trace reads in both user-defined dust temperatures and dust densities, thus bypassing the computation of the dust temperatures as would have been the case in the thermal Monte-Carlo simulation.

1.5 Input files

Prior to these computations however, RADMC-3D by default writes input files to the working directory. These files have `.inp` extension whilst RADMC-3D output files have `.out` extensions. An intermediate file type with `.dat` extension is also used where the file is the result of a computational process, such as the dust temperature.

RADMC-3D performs its calculations on grids; the spatial and frequency grids are used to set up the model space. `amr_grid.inp` contains the coordinates, in cm, of all pixels, or cells, in in all dimensions applicable to the model (in this case, 3-dimensions). Likewise, `wavelength_micron.inp` contains wavelengths from $0.1\mu\text{m}$ to $1000\mu\text{m}$. Files containing radiation sources are not required for ray trace calculations however dust opacity and density information, along with dust temperature information, is. All dust files contain the same number of points as `amr_grid.inp`, only each point in these files is the dust property at that cell. Lastly, the `radmc3d.inp` file contains all parameters for the code to read, such as the boundaries of the image grid. Critically, all units must be CGS (centimetres – grams – seconds) consistent.

1.6 Image ray trace and visualisation

Because `radmc3dPy` is not strictly a Python version of RADMC-3D, any Python script using it must use an operating system interface such as ‘`os`’ to call and run the ray trace. During the ray trace, all `.inp` files are read and used by RADMC-3D to compute intensity along predefined, pre-calculated rays. This information is then written to `image.out`, where `radmc3dPy` plots a 2D version (x vs y) of the 3D results, given some parameters such as distance to the source, it’s size, and the wavelength at which to plot.

Multi wavelength images can be plotted using `radmc3dPy`. This can be achieved through generating a `camera_wavelength_micron.inp` file that contains a number of points in the wavelength range over which

the image is to be plotted. 3D data visualisation is possible through a VTK output that is viewable through Paraview [10].

2. Methodology

2.1 Model setup

Initially the examples provided with RADMC-3D were inspected and compiled in order to understand their operation. These examples were basic, consisting of both 1D and 2D sphere projections with user defined stars at their centres that ran thermal Monte-Carlo simulations to build dust temperatures. To begin building 3D models, specific input files needed to be created. As stated in Section 1.5, a custom Python script was written to handle this file creation. Traditionally, radmc3dPy would handle file creation at the model setup phase, however given that RADMC-3D is designed to be run from the command line, it was determined that reducing the number of dependencies would allow greater compatibility with different machines. This is critical if the code is to be run on a machine that may not have radmc3dPy installed, such as a supercomputer for larger computations. All code was version controlled using GitHub and stored in a private repository¹.

2.2 Spatial and frequency setup

To begin, a 3D sphere that represented a molecular cloud of uniform number density 10^5 cm^{-3} and uniform temperature 10 K surrounded by a warmer and less dense ISM of number density 10^2 cm^{-3} and temperature 15 K was created. This was performed by computing the cloud radius from its number density and user specified mass (in this case $1 M_{\odot}$). By providing the code with the number of cells in each dimension, as well as a distance boundary to place the cloud in, `amr_grid.inp` could be written. Furthermore, the writing of `wavelength_micron.inp` took a user defined number of wavelengths evenly spaced across the range specified in Section 1.6.

2.3 Dust property file setup

Each cell in the spatial grid (`amr_grid.inp`) was assigned a density and temperature by simply determining whether each point was within the cloud radius using the equation of a sphere. The resulting temperature data was then written to `dust_temperature.dat`, whilst the density data was written to `dust_density.inp`.

To compute the dust opacity, the opacity law defined in Equation 1.1 was used. The wavelength points in `wavelength_micron.inp` were looped through and the opacity determined for $\nu_0 = \lambda_0$ where λ_0 was the mean filter wavelength for the PACS and SPIRE filters. The value of β was taken from Ward-Thompson and Whitworth [3] as $\beta=1.7$.

2.3 Filter transmission

To accurately simulate data from Herschel, the optical transmission of its filters must be factored in to calculations. Data comprising the transmission curves for each filter were downloaded from the SVO Filter Profile Service [6]. This data was not linearly spaced in λ so function interpolation was performed using SciPy [11] – this allowed the transmission to be determined at the wavelength points written to `camera_wavelength_micron.inp`. These transmission coefficients will then be multiplied by each point in `image.out` that was computed at the corresponding wavelength and summed. The new image data, `image_trans.out`, will then be fed back in to radmc3dPy and plotted to give the synthetic Herschel data.

3. Results

At this stage, models have been set up to compute a $1 M_{\odot}$ molecular cloud with number density 10^5 particles cm^{-3} and temperature 10 K ray traced over the SPIRE passbands [10]. This cloud was placed at 150 parsecs away from the observer. An example image, dust emission intensity as a function of position for the PSW band, is shown in Figure 2.

¹ This private repository can be found at <https://github.com/tomasjames/ZiggyStarDust> but is only accessible to contributors

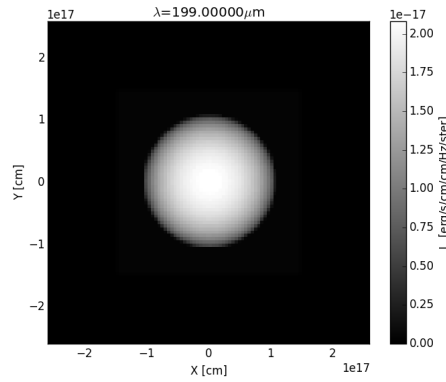


Figure 2: A $1 M_{\odot}$, 10 K molecular cloud with $10^5 \text{ particles cm}^{-3}$ at a distance 150 pc in the PSW passband.

4. Future work

Once the transmission compensated images can be computed – they were not complete in time to present in this report - an SED using RADMC-3D will be created. A standard χ^2 test will then be used to fit a theoretical SED to recover the values of temperature, T and column density, N . Dendrogram software will also then be used to extract prestellar cores in both synthetic and real data. This will allow comparison of the prestellar core populations in each dataset, as well as their masses to better understand how prestellar cores form. The accuracy of the recovered temperature could also be tested by performing a thermal Monte-Carlo simulation for a given Interstellar Radiation Field. This would allow the results given in Shetty et. al. [5] and Kelly et. al. [4] to be explored further.

5. References

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