

# <sup>1</sup> growopacity: A computationally efficient dust opacity model suitable for coagulation models

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## Summary

growopacity is a Python and C toolkit for calculating dust opacities in astrophysical environments. It provides a framework for generating, storing, and interpolating Rosseland and Planck mean opacities over customizable grids of grain size distributions, temperature, and powerlaw exponents. This package is designed as a wrapper around [OpTool](#), allowing users to specify a grain composition and obtain tabulated 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 growopacity, we outline a method to construct such a model and provide a python package that interfaces to [OpTool](#) to compute 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  $\kappa_{\text{abs}}(\nu)$  and  $\kappa_{\text{sca}}(\nu)$  (in  $\text{cm}^2/\text{g}$ ) as well as the asymmetry factor  $g(\nu)$  ([Henyey & Greenstein, 1941](#)) over a frequency grid  $\nu$ . This calculation is done using the Distribution of Hollow Spheres method (DHS, [Min et al., 2005](#)). The Rosseland and Planck mean opacities  $\kappa_R$  and  $\kappa_P$  can then be computed as

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

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  $q$  and  $a_{\max}$ . The above equation can then be used to compute and tabulate  $\kappa_R$  and  $\kappa_P$  over

<sup>35</sup>  $q$ ,  $a_{\max}$ , and  $T$ . The resulting 3D tables can be used in any context where  $q$  and  $a_{\max}$  are  
<sup>36</sup> dynamically evolved according to a dust coagulation model (Birnstiel et al., 2017; Pfeil et al.,  
<sup>37</sup> 2024; Robinson et al., 2024; Stammler & Birnstiel, 2022).

## <sup>38</sup> Interpolation algorithm

<sup>39</sup> Once the 3D tables of  $\kappa_R(q, a_{\max}, T)$  and  $\kappa_P(q, a_{\max}, T)$  have been computed, they can be  
<sup>40</sup> interpolated within the range of tabulated values. We interpolate for  $\log \kappa$  as a function of  $q$ ,  
<sup>41</sup>  $\log a_{\max}$ , and  $\log T$ , with regular sampling in this space (i.e., logarithmic spacing for  $a_{\max}$  and  
<sup>42</sup>  $T$ ). This works best when the mean opacities follow a powerlaw with respect to temperature  
<sup>43</sup>  $\kappa \propto T^b \Rightarrow \log \kappa \propto b \log T$ , which is a reasonable approximation and especially holds for small  
<sup>44</sup> grains (Bell & Lin, 1994; Semenov et al., 2003). It also ensures that the interpolated opacities  
<sup>45</sup> are always positive in case extrapolation is needed.

<sup>46</sup> We use a trilinear interpolation scheme, which is fast and simple to implement, and takes  
<sup>47</sup> advantage of the fact that the arrays  $q$ ,  $\log a_{\max}$ , and  $\log T$  are sorted and regularly spaced  
<sup>48</sup> to efficiently locate the indices of the grid points that surround the point of interest. For  
<sup>49</sup> each array  $x \in \{q, \log a_{\max}, \log T\}$  and for a target value  $x_t$ , we first find the index  $i$  such  
<sup>50</sup> 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  
<sup>51</sup> sampling space and  $\Delta x = x_{i+1} - x_i$  is the (constant) sampling spacing. As this information  
<sup>52</sup> is known *a priori*, this reduces the complexity of finding the required indices from  $\mathcal{O}(\log N)$  to  
<sup>53</sup>  $\mathcal{O}(1)$ , where  $N$  is the number of grid points in  $x$ , and is especially efficient for larger grids. Of  
<sup>54</sup> course, care must be taken to ensure that the indices are within the bounds of the grid.

## <sup>55</sup> Implementation

<sup>56</sup> The above method is implemented in the growpacity package. The package provides a simple  
<sup>57</sup> python interface to OpTool to compute accurate dust opacities for a given grain composition  
<sup>58</sup> (provided in OpTool format) and for a fixed  $a_{\min}$ , over a grid of  $a_{\max}$ ,  $q$ , and  $T$ . The resulting  
<sup>59</sup> 3D tables of  $\kappa_R$  and  $\kappa_P$  are saved in binary files that can be easily loaded with python. We  
<sup>60</sup> also provide an implementation of the interpolating function in C, that can be readily used in  
<sup>61</sup> radiation hydrodynamics codes. These files are especially lightweight: a typical calculation  
<sup>62</sup> involving  $q \in [-4.5, -2.5]$  with  $\Delta q = 0.25$ ,  $a_{\max} \in [0.1 \mu\text{m}, 1 \text{ m}]$  sampled twice per decade,  
<sup>63</sup> and  $T \in [1, 2000] \text{ K}$  with 100 points results in two arrays of  $9 \times 15 \times 100$  elements, or  
<sup>64</sup> about 220 kB of memory. This choice of spacing means that opacities are exactly evaluated  
<sup>65</sup> for  $q \in [-3.75, -3.5, -3]$ , corresponding to dust size distributions in equilibrium due to  
<sup>66</sup> small/large-scale turbulence, radial drift, or in a non-equilibrium growth regime (for more  
<sup>67</sup> information, see Pfeil et al., 2024).

<sup>68</sup> The code and documentation are available at  
<sup>69</sup> <https://github.com/alexziab/growpacity>.

## <sup>70</sup> Limitations and extensions

<sup>71</sup> We underscore that our intent is not to provide a new or more realistic dust opacity model,  
<sup>72</sup> but rather one suitable for use in coagulation models, where dust densities and distributions  
<sup>73</sup> can vary as a function of position and time—the applicability of the model depends on entirely  
<sup>74</sup> user-defined choices. The method can be easily extended to include gas opacities (e.g., Malygin  
<sup>75</sup> et al., 2014; Semenov et al., 2003) and prescriptions for the sublimation of dust species (e.g.,  
<sup>76</sup> Isella & Natta, 2005), for a more complete opacity model in regimes where gas opacities are  
<sup>77</sup> significant.

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