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# Extrapolation of Simulated Scattering Matrix for Large Size Parameter Values

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## Introduction

Even though aerosol particles comprise only a small fraction of the total atmospheric mass, they are radiatively very important. Ultimately, their interaction with radiation is governed through their single-scattering properties, which are needed, e.g.,

1. to quantify the aerosol radiative effects;
2. for the aerosol remote sensing measurements; and
3. for aerosol corrections in other remote sensing measurements.

Among atmospheric aerosols, computation of the single-scattering properties of mineral dust is particularly challenging due to their irregular shapes and inhomogeneous compositions. Consequently, drastic simplifications are often made, such as assuming the particles to be homogeneous spheres.

For wavelength-scale particles, the single-scattering properties can also be computed using brute-force numerical methods, such as the discrete dipole approximation (DDA) [1]. With such methods, most simplifications to the model particle properties can be avoided. For example, [2] used model particles with real shapes and spatial distribution of component minerals derived by stereogrammetry and energy-dispersive spectroscopy. Unfortunately, the DDA and other similar methods become prohibitively slow when the particle size considerably exceeds the wavelength of radiation. Computations beyond size parameter $x = \pi D/\lambda = 20$, where $D$ is the diameter of the particle, are highly demanding even for supercomputers. Yet, larger size parameters are needed to cover the radiatively important dust particle sizes at the shortwave spectral range.

To extend DDA computations to larger size parameters, we propose a method based on extrapolation. This is feasible, because the scattering matrix elements for irregular particles generally become featureless and start converging towards the large-particle limit already at size parameters around 10. Through extrapolation, the use of simplified model particles will be avoided and consistency achieved, which may prove to be preferable. Here, we only consider extrapolation for the component $S_{11}$ of the scattering matrix, related to the scattered intensity.

## The extrapolation method

The optimal choice for extrapolation is a semi-phenomenological model that takes into account the underlying physics when constructing the extension. The scattered field consists of several distinct types of components: a relatively smooth radial field, forward and backward scattered peaks, and transitional oscillations. These should be modelled separately.

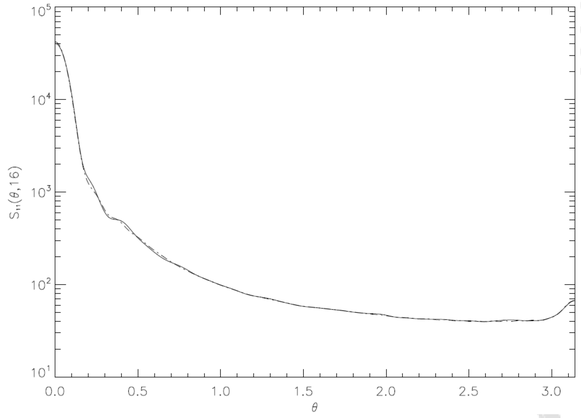
The behavior of the radial field as a function of size parameter follows an asymptotic power law that can be modeled reasonably well through simple scattering approximations. Specifically, it is feasible to express the radial field in the form $f_0(\theta)f(\theta,x)$, where $f_0(\theta)$ is the $\theta$ profile of the simulated field at the extrapolation boundary. Here we approximate $f_0(\theta)$ with a sparse spline curve.

The behavior of the forward and backward scattering peaks can be separated into $f(x\cos\theta)g(x\sin\theta)$, where $f(x\cos\theta)$ can be modeled with the same approach as $f(\theta,x)$ of the radial field. The shape function $g(x\sin\theta)$ is more complicated and sample type dependent. In order to accommodate for the variety of shapes of peaks in the simulated cases, we are approximating the shape by a series of generalized sinc functions

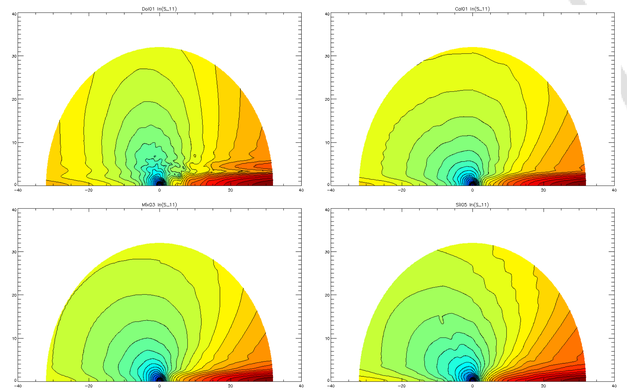
$$g(x\sin\theta) = \sum_n c_n \; sinc_n^2(qx\sin\theta),$$

where $q$ is a scale parameter.

When modeling the main $S_{11}$ moment, the transitional oscillations can be ignored for the cases considered here. For each sample type, we use non-linear least squares fitting to match the parameterized semi-phenomenological model with the simulated moment values for the size parameter range of 10 to 16. Assuming that this range is sufficiently close to the asymptotic limit, the expected errors in the extrapolation can be estimated by a comparison between the simulated values and the model in the matching range. As can be seen from Table 1, the mean relative error decreases as a function of size parameter, corresponding to the diminishing contribution from transitional oscillations.




The congruence of simulated (solid) and modeled (dash-dotted) profiles for $S_{11}$ of a test particle (Mix) from [2] at the extrapolation boundary.



Simulated $S_{11}$ for four test particles from [2] (Dol, Cal, Mix, Sil) computed for size parameters $x$ between 0.5 and 16 and subsequently extrapolated up to $x$= 32. The x-axis shows the size parameter.

| Type | 10 | 12 | 14 | 16 |
|---|---|---|---|---|
| Dol | 0.084 | 0.075 | 0.074 | 0.033 |
| Cal | 0.032 | 0.029 | 0.021 | 0.020 |
| Mix | 0.040 | 0.026 | 0.023 | 0.015 |
| Sil | 0.093 | 0.064 | 0.056 | 0.048 |

Mean relative error between simulated profile and extrapolation model of $S_{11}$ at the matching region for different sample types as a function of size parameter.

**References:**

[1] M. Yurkin and A. Hoekstra. *J. Quant. Spectrosc. Radiat. Transfer*, **112**:2234–2247, 2011.
[2] H. Lindqvist, et al. *Atmos. Chem. Phys.*, **14**:143–157, 2014.