A Python library for computing light scattering by multilayered non-spherical particles

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We present a new library of routines for computing light scattering by axially symmetric particles with multiple layers. The library is written in Python and relies on the modern scientific framework SciPy. The tool is based on the generalized separation of variables method with a spherical basis. We discuss capabilities of the code and present results of extensive computations giving insight in the dependence of optical properties on the scatterer size and structure. We also share some experience of Python/SciPy usage.

INTRODUCTION

FORTRAN and C++ are traditionally used for computations in light scattering. They provide very fast codes, but using them is known to require development skills from researchers. A programming language that is more convenient to develop with and at the same time allowing as fast computations as with traditional languages is Python (*http://python.org*). This modern powerful scripting language is used in a wide variety of application domains. Its major advantages are cross-platform compatibility, open source, very clear and readable syntax, large amount of standard and third-party libraries for different tasks. Python code is very easy to develop, maintain and scale.

Python has recently become widely used in scientific applications mostly because of development of SciPy. SciPy (*http://scipy.org*) is a Python library for scientific computations, including modules for linear algebra, special functions, multiprecision arithmetic, symbolic mathematics and many others. Using Python allows researches to utilize standard functions for most of the tasks and focus on the algorithm implementation. SciPy also provides MATLAB-like environment for interactive computations and rich data visualization tools. As Python/SciPy nowadays are widely used in various fields of science there are a lot of packages for astronomy, biology, geosciences, chemistry, etc. Using SciPy makes integration with these packages quite easy.

The speed of SciPy-based code is comparable with that of MATLAB codes. However, Python provides facilities for integration with FORTRAN and C++ that allow one to have the speed of the low level languages, while keeping the code simplicity of Python.

GENERALIZED SEPARATION OF VARIABLES METHOD

To solve the light scattering problem we generalize the separation of variables method [1], that is most suitable for layered particles among the methods using field expansion [2].

We consider a particle with L layers embedded in a homogeneous medium. Each layer surface $\partial\Gamma^{(i)}$ is axisymmetric with the symmetry axis coinciding with z-axis. An incident

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plane wave propagates at the angle α to the z-axis. The electromagnetic fields in each of the domains $\Gamma^{(i)}$ satisfy the boundary conditions

$$\vec{E}^{(i)}(\vec{r}) \times \vec{n}^{(i)}(\vec{r}) = \vec{E}^{(i+1)}(\vec{r}) \times \vec{n}^{(i)}(\vec{r}), \quad \vec{r} \in \partial\Gamma^{(i)}, \quad i = 1, \ldots, L, \tag{1}$$

where $\vec{n}^{(i)}$ is an outward normal to the layer surface $\partial\Gamma^{(i)}$. The field in $\Gamma^{(1)}$ is a sum of the incident and scattered fields $\vec{E}^{(1)} = \vec{E}^{\mathrm{inc}} + \vec{E}^{\mathrm{sca}}$.

All fields are expanded in terms of spherical wave functions. The expansions are substituted in the boundary conditions (1). Multiplication of these conditions by the angular part of different index wave functions and integration over the corresponding surface $\partial\Gamma^{(i)}$ yield a system of linear algebraic equations relative to the expansion coefficients $\vec{x}^{(i)}$

$$P_i^{(i)} \vec{x}^{(i)} = P_{i+1}^{(i)} \vec{x}^{(i+1)}, \quad i = 1, \ldots, L,$$

where $P_j^{(i)}$ are some infinite matrices (see for details [3]), $\vec{x}^{(1)} = (\vec{x}^{\mathrm{inc}}, \vec{x}^{\mathrm{sca}})^{\mathrm{T}}$. The expansion coefficients of the incident field $\vec{x}^{\mathrm{inc}}$ are known. The unknown coefficients of the scattered field expansion can be found from a smaller system [1]

$$P_1^{(1)} \vec{x}^{(1)} = P_2^{(1)} \prod_{i=2}^{L} \left[(P_i^{(i)})^{-1} P_{i+1}^{(i)} \right] \vec{x}^{(L+1)}.$$

TOOL IMPLEMENTATION AND TESTING

The algorithm was implemented as a Python code. SciPy routines were used for linear algebra and for computing values of spherical functions. For massive computations Python's standard data storage and plotting methods were effectively used. The most resource-hungry part (computation of elements of matrices $P_j^{(i)}$) was implemented as a FORTRAN77 module and imported with *f2py*. The use of object oriented programming allowed efficient code reuse and more scalable design. With Python we achieved a significantly more clear and smaller code than with FORTRAN77 (1700 versus 2600 lines of code) and richer functionality, while preserving the same speed as with FORTRAN.

The new tool was compared with available codes based on the extended boundary condition [4], null-field [5], and DDA [6] methods. For example, see Fig. 1, where normalized intensity of multilayered prolate spheroids (F_{11}/g) computed with different techniques is plotted. Here g is the cross section of equivolume sphere. The computations have shown that our results perfectly match with those given by the other codes for particles with a relatively small number of layers and provide more accurate results for particles with a large number of layers.

Fig. 1 shows that our code is highly effective for multilayered particles, providing reliable results for small scatterers with several hundreds of layers and for large scatterers ($x_{\mathrm{V}} = 30$) with up to 4 layers. Relative difference between the scattering and extinction cross sections $\delta = |C_{\mathrm{sca}} - C_{\mathrm{ext}}|/(C_{\mathrm{sca}} + C_{\mathrm{ext}})$ was utilized as an accuracy measure.

NUMERICAL RESULTS

Using the code we have performed extensive computations to analyze the impact of particle size, shape and structure on different optical properties. A detailed graphical library of computational results is presented at the Database of Optical Properties (DOP) at *http://www.astro.spbu.ru/DOP/8-GLIB/op3*.

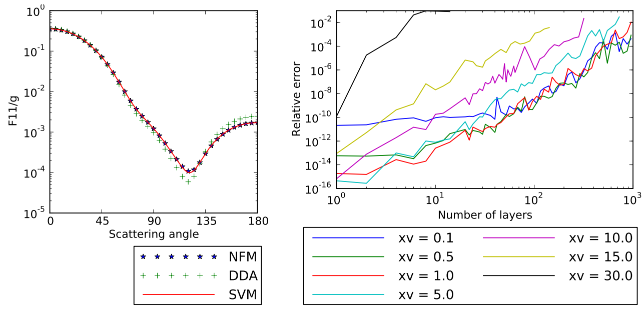

Figure 1. Results validation for multilayered particles. In left, comparison with NFM and DDA, and in right, relative error vs. the number of layers. The particle layers are equivolume prolate spheroids with aspect ratio $a/b = 1.4$, the materials are ice ($m = 1.3$) and vacuum ($m = 1$) repeating cyclically. The incident wave propagation angles are $\alpha = 0°$ (left) and $45°$ (right), effective size parameters $x_V = 3$ (left) and from 0.1 to 30 (right), number of layers $L = 8$ (left) and from 1 to 1000 (right).

Fig. 2 illustrates comparison of intensity and degree of linear polarization of porous scatterers approximated by 2- and 16-layered particles and homogeneous particles having the refractive index derived from the effective medium theory. These results extend the well-known work [7] where dependence of the scattering matrix elements on homogeneous particle size and orientation was discussed in detail. One can see that *the main effect of scatterer structure is appearance of strong polarization maxima and minima in a very wide range of the scattering angle values*. This and other revealed effects of scatterer structure are discussed in detail in [3].

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REFERENCES

[1] A.A. Vinokurov, V.G. Farafonov, and V.B. Il'in. Separation of variables method for multilayered nonspherical particles. J. Quant. Spectr. Rad. Transf. **110** (2009).

[2] V.B. Il'in, V.G. Farafonov, and A.A. Vinokurov. Theoretical and computational aspects of the SVM, EBCM, and PMM methods in light scattering by small particles. Abstr. ELS12 Conf. (2010).

[3] A.A. Vinokurov, V.B. Il'in, and V.G. Farafonov. On optical properties of nonspherical inhomogeneous particles. Opt. Spectr. (submitted) (2010).

[4] V.G. Farafonov, V.B. Il'in, and M.S. Prokopjeva. Light scattering by multilayered nonspherical particles: a set of methods. J. Quant. Spectr. Rad. Transf. **79–80** (2003).

[5] A. Doicu, Y.A. Eremin, and T. Wriedt. *Light scattering by systems of particles*. Springer (2006).

[6] B.T. Draine and P.J. Flatau. User guide to the Discrete Dipole Approximation code. Preprint arXiv.1002.1505v1 (2010)

[7] M.I. Mishchenko and L.D. Travis. Light scattering by polydispessions of randomly oriented spheroids with sizes comparable to wavelength of observation. Appl. Opt. **33** (1994).

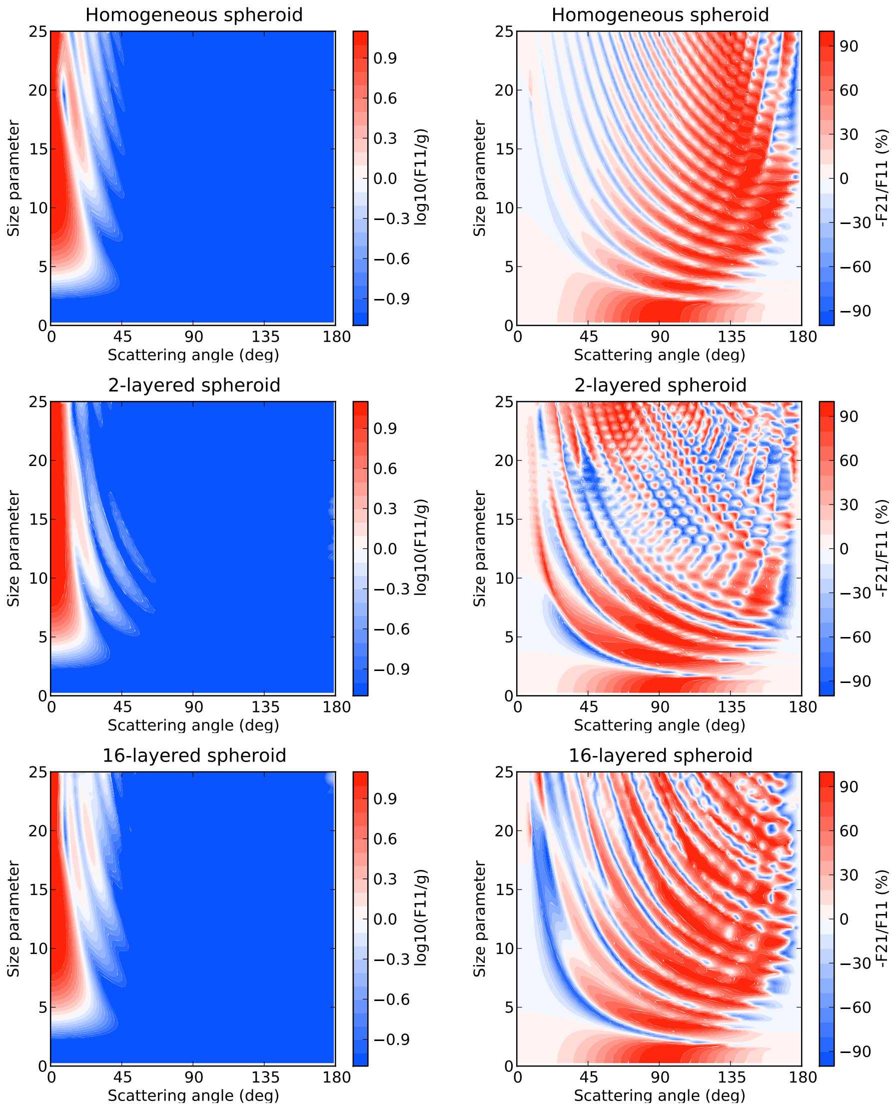

Figure 2. Normalized intensity and the degree of linear polarization vs the scattering angle and effective size parameter for homogeneous and layered prolate spheroids. The particle symmetry axis is parallel to the incident beam ($\alpha = 0°$). The particle layers are equivolume spheroids with aspect ratio $a/b = 1.4$, the materials are ice ($m = 1.3$) and vacuum ($m = 1$) repeating cyclically.