Using a New Scattering Order Formulation of the Discrete Dipole Approximation to Calculate Scattering by Irregularly Shaped Aerosols

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the discrete dipole approximation (DDA):

[e.g., Purcell and Pennypacker, 1973; Draine, 1988; Draine and Goodman, 1993; Draine and Flatau, 1994; Draine, 2000; Mc Donald, 2007; Yurkin and Hoekstra, 2007; Mc Donald et al., 2009; Yurkin and Hoekstra, 2011]

1. break up a target into a three-dimensional grid of polarizable points (dipoles)
2. near field dipole fields dictate the radiative interactions among the dipoles
3. far field dipole fields dictate the total radiance of radiation scattered by the target

conventional implementations of the DDA:

1. solve a matrix equation for the dipole moment per unit volume at each point

$$\bar{\alpha}_i^{-1}\mathbf{P}_i - \sum_{j\neq i}\mathbf{G}_{ij}\mathbf{P}_i = \mathbf{E}_i^{\text{inc}}$$

2. calculate the scattered radiance as a function of angle

the scattering order formulation of the DDA (SOF-DDA):

[e.g., Kirkwood, 1936; Chiapetta, 1980; Singham and Bohren, 1987, 1988, 1989]

1. A scattering target is divided into polarizable points. Points are only defined where material exists.
2. The dipole moment per unit volume at each defined point is calculated according to the electromagnetic field incident on the target from the outside only. This is called the 1st order dipole moment.
3. The 1st order scattered field in the far field is calculated.
4. Each dipole radiates onto every other dipole according to its 1st order dipole moment, adding to the 1st order scattered near field at each defined point.
5. The 2nd order dipole moment per unit volume at each defined point is calculated, which is in reaction to the vector sum of the electromagnetic field incident on the target from the outside and the 1st order scattered near field.
6. The 2nd order scattered field in the far field is calculated.
7. Each dipole radiates onto every other dipole according to its 2nd order dipole moment, adding to the 2nd order scattered near field at each defined point.
8. The 3rd order dipole moment per unit volume at each point is calculated, which is in reaction to the vector sum of the electromagnetic field incident on the target from the outside and the 2nd order scattered near field.
9. The 3rd order scattered field in the far field is calculated, etc.
10. The iterations are continued until convergence is achieved within the desired precision.

advantages of the SOF-DDA:

1. iterations are "physical" rather than numerical
2. dipoles may be placed with arbitrary spacing
3. no system of coupled equations, no matrix to invert
4. no grid points need to exist where there is no material
5. readily parallelizable with no theoretical maximum number of CPUs

the SOF-DDA on a small sphere:

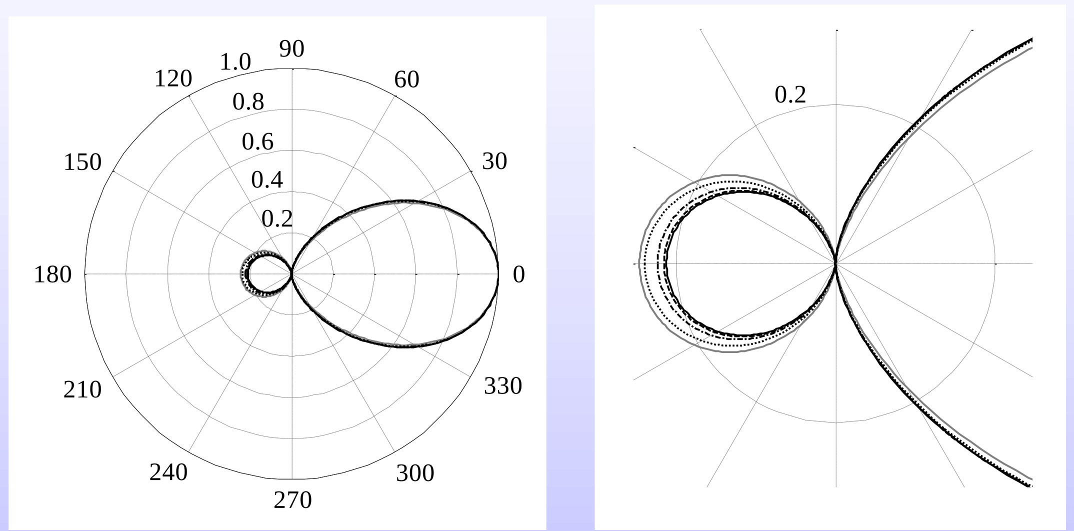

Figure 1. Left plot: polar plot of the scattering phase function at wavelength 0.500 microns, normalized by the radiance at scattering angle zero, for successive orders of scattering by a homogeneous water sphere of radius 0.1 microns, obtained using a SOF-DDA model with dipole spacing 0.01 microns. The electric field of the incident radiation is polarized parallel to the scattering plane. **Right plot:** a zoom-in on the backscatter lobe of the left plot. Solid grey line: 1st order, dotted line: 2nd order, dot-dashed line: 3rd order, dashed line: 4th order, solid black line: 5th and final order.

Note that the iterations converge after only 5 orders of scattering, demonstrating the efficiency of the SOF-DDA approach for this simple target.

Note also the interesting progression of the ratio of backward to forward scattering that one can observe using the SOF-DDA rather than a conventional numerical iteration procedure.

disadvantages of the SOF-DDA:

1. a single "physical" iteration may be slower than a single numerical iteration
2. does not always converge for larger compact scatterers

our new SOF-DDA "marching scheme":

1. The plane wave hits one side of the particle first, exciting a wall of dipoles nearest to the point of incidence. This wall of dipoles gets its 1st order dipole moments first.
2. The wave advances and the second wall gets its 1st order dipole moments while the first wall advances to its 2nd order dipole moments.
3. Continue advancing the wave one wall at a time.
4. Once the wave has passed through the entire particle, all dipoles have been "activated", but they are not all at the same scattering order as defined in the usual sense. They are all at the same "marching step".

How thick should the wall of dipoles be?

1. Use the model of an under-damped forced harmonic oscillator.
2. The e-folding time for transients to die down = $2/\Gamma$, where Γ is the FWHM of the absorption peak within which the frequency of the incident radiation is found.
3. Using a gross estimate for dielectric materials found in the atmosphere, Γ = ~100 nm, and the e-folding time = ~5.8e-15 seconds.
4. Multiplying by the speed of light in vacuum, the incident plane wave has traveled ~1.75-microns distance before the dipoles that it first reached come into steady state oscillation with it.

⇒ **The wall of dipoles should be no more than one-dipole thick.**

the SOF-DDA marching scheme on a larger sphere:

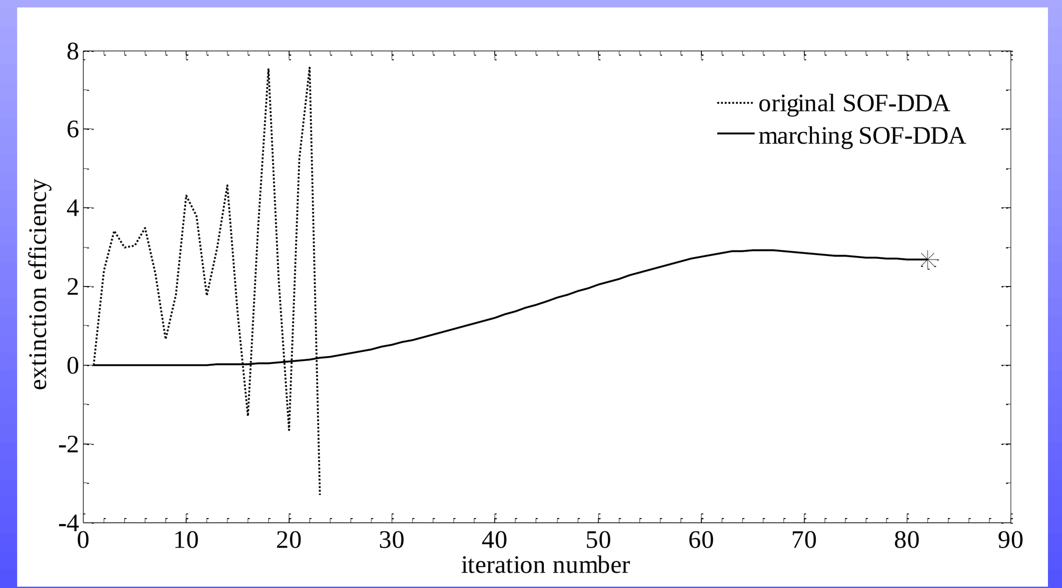

Figure 2. Successive values of extinction efficiency (Q_{ext}) at wavelength 0.500 microns for a homogeneous water sphere of radius 0.3 microns with dipole spacing 0.01 microns, obtained using the original SOF-DDA model (dotted line) and the marching SOF-DDA model (solid line). The electric field of the incident radiation is polarized parallel to the scattering plane. Asterisk: theoretical value computed using the Mie scattering subroutine of Bohren and Huffman [1983, Appendix A].

sample calculations for highly irregular shapes:

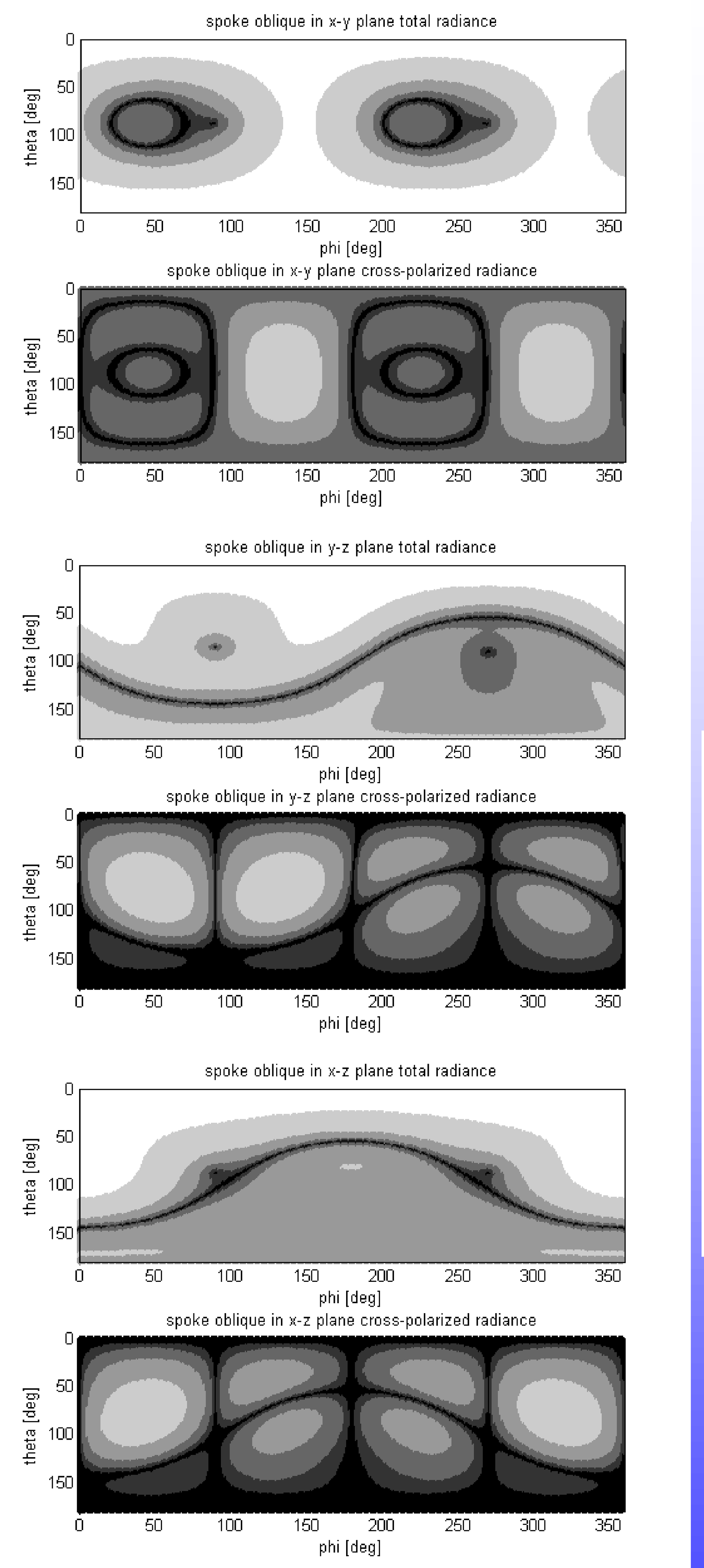

Figure 3. Contour plots of total scattered radiance and cross-polarized scattered radiance with logarithmic contour scaling, mapped over a total sphere of solid angle, for oblique finite cylinders of length 0.40 microns and refractive index 1.43+i0.005, in water of refractive index 1.335, at wavelength 0.500 microns.

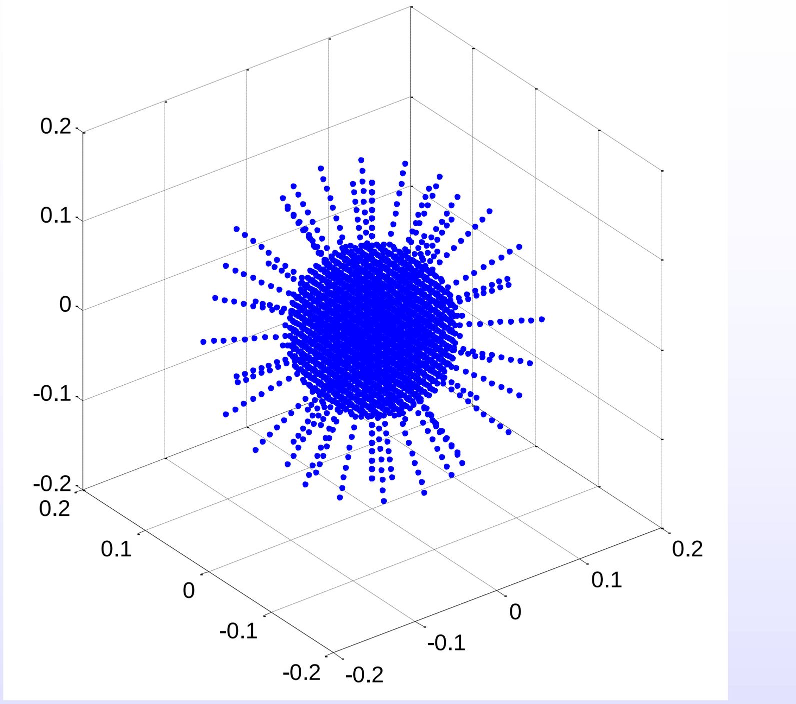

Figure 4a. Computer prototype of a small radiolaria (a plankton shaped like a sphere with spokes). Axes are in units of microns.

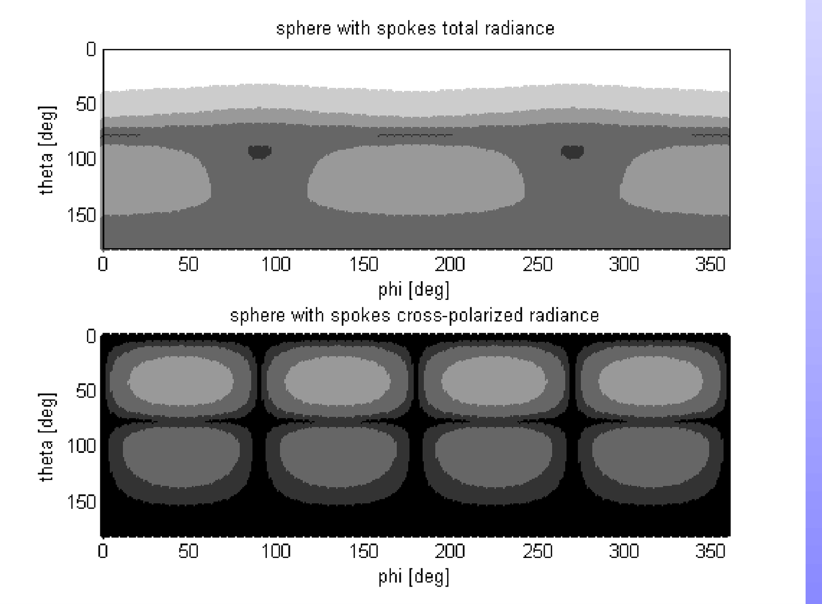

Figure 4b. Contour plot of total scattered radiance and cross-polarized scattered radiance with logarithmic contour scaling, mapped over a total sphere of solid angle, for a small radiolaria of refractive index 1.43+i0.005, in water of refractive index 1.335, at wavelength 0.500 microns.

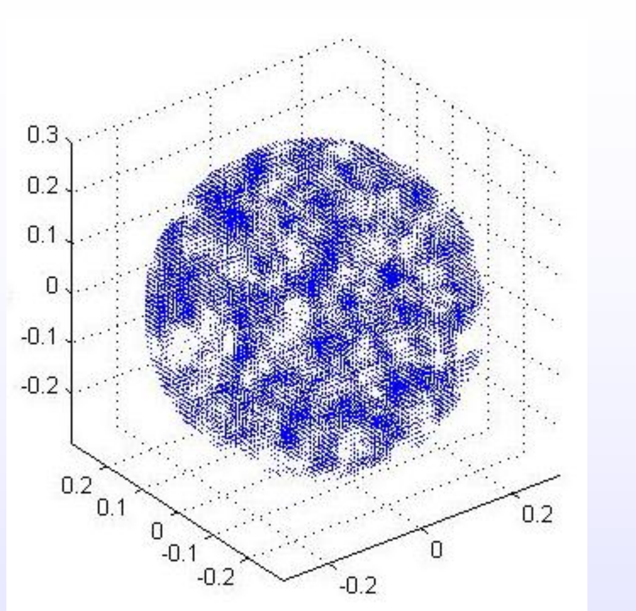

Figure 5. Computer prototype of a highly porous aerosol (HPA) composed of natural organic material (NOM), created by carving out voids of 0.03-microns radius using a random number generator. Axes are in units of microns. The refractive index of the filaments of NOM at wavelength 0.355 microns was taken to be 1.60 + i0.14 [Adler et al., 2014a,b].

Extinction calculations were performed on HPA for the first time using dipole spacing 1 nm, which is equivalent to 17,972,210 dipoles!

order of scattered field	dipole spacing	Q_{ext}
1	10 nm	0.2156746
1	5 nm	0.2156721
1	1 nm	0.2156556
2	10 nm	0.5915229
2	5 nm	0.5971381
2	1 nm	0.5995764

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