Introduction to the cda package

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Abstract

The cda package implements the coupled-dipole approximation for electromagnetic scattering by sparse collections of subwavelength particles, with a particular focus on plasmonic nanoparticles in the visible regime. The interaction matrix is formed in C++ code for speed; convenient wrapper functions are provided at the R level to calculate the extinction, scattering, and absorption of light by particles with linearly and circularly polarised light. Functions are also provided to calculate orientation-averaged circular dichroism, and display clusters of nanoparticles in three dimensions using RGL or povray.

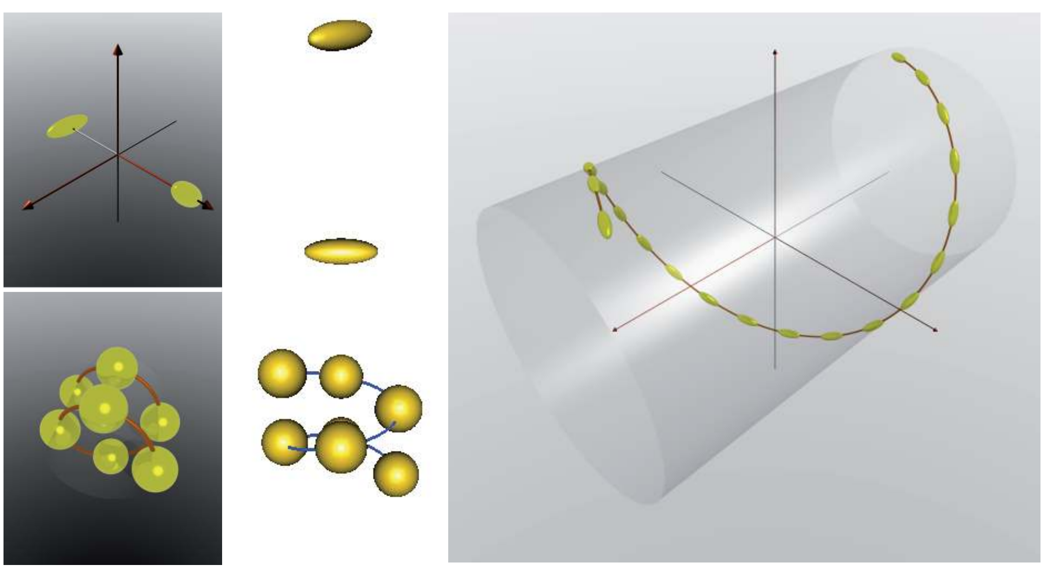

Figure 1: Rendering of particle clusters using RGL or povray. The figures may be reproduced with demo(clusters_3d).

1 Extinction of linearly polarised light

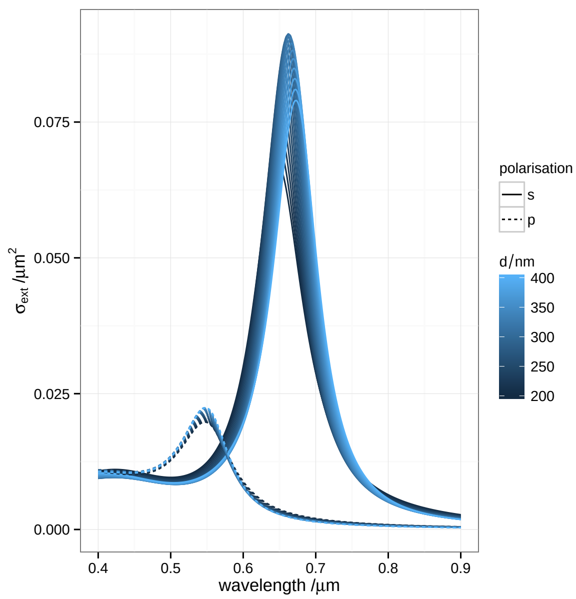

Figure 2: `demo(dimer_linear)` from the cda package. Extinction spectra of a dimer of gold nanorods excited by linearly polarised light, with varying separation. The two rods are parallel, with a distance varied from 200 nm to 400 nm. The particle shape is described by a prolate ellipsoid of semi-axes 50 nm and 30 nm, immersed in a homogeneous medium of refractive index 1.5 (glass).

Figure 2 presents the extinction spectrum of a dimer of gold nanorods excited by linearly polarised light. The code for `demo(dimer_linear)` calls the functions

- `makeRodChain(N=2, pitch = 0.5, a = 0.05, b = 0.03, c = b)` to create the dimer cluster of two prolate ellipsoids
- `linear_extinction_spectrum(cluster, material = gold, n = 1.33)` to solve the electromagnetic scattering of linearly polarised light.

Some values such as the particle size are set by default.

When the incident electric field is along the long axis of the particles, the coupling between the two longitudinal localised plasmon resonances (LSPR) yields a blue-shift of the resonance. Conversely, the transverse LSPR red-shift with decreasing interparticle separation.

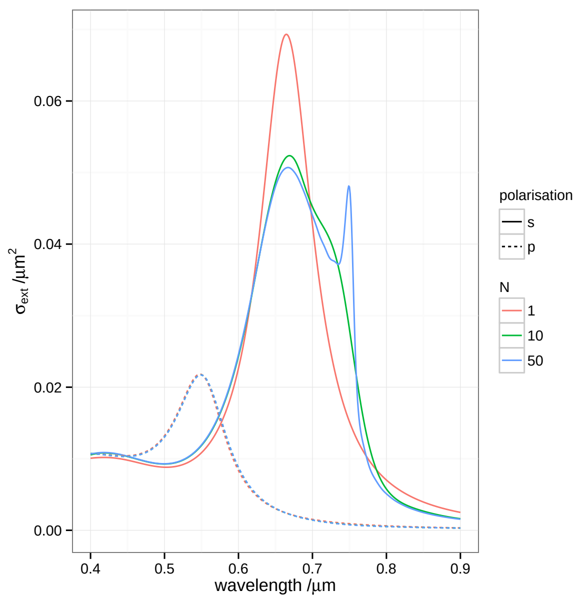

Figure 3: `demo(diffractive_chain)` from the cda package. A linear chain of $N = 1, 10, 50$ ellipsoidal gold particles with regular spacing 500 nm is modelled. The extinction cross-section is calculated for linearly polarised light along the short and long axis of the particles.

To simulate a diffractive chain, we simply call the same functions with a larger number of particles in the cluster. The code for figure 3 is in `demo(diffractive_chain)`. We note the appearance of a peak associated with light diffraction for chains with a sufficient number of particles, and polarisation orthogonal to the chain axis[3, 4, 2]. For infinite, two-dimensional arrays of identical particles illuminated at normal incidence, a lattice sum can be used to write the self-consistent effective polarizability of the particles $\alpha^* = \frac{1}{1/\alpha - S}$. The code in `demo(lattice_sum)` (figure 4) uses the following functions,

- `array_factor(wavelength, N, pitch)` to calculate a truncated sum of dipole sources.
- `interpolate.fun(G0$wavelength, G0$Gxx)` to interpolate the (complex) tabulated results of the rigorous calculation made available with `data(G0)`.

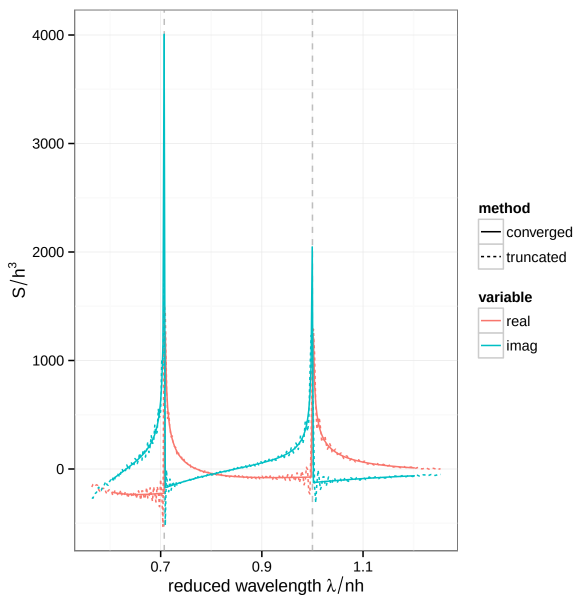

Figure 4: `demo(lattice_sum)` from the cda package. The truncated evaluation of the lattice sum S is compared with the rigorous, converged solution obtained by an Ewald-type summation.

2 Circular dichroism

Calculations of circular dichroism in chiral assemblies of plasmonic nanoparticles are demonstrated in two examples. First, the code in `demo(dimer_cd)` illustrates the optical activity of a dimer of gold nanorods arranged in a chiral configuration[1]. Specifically, it uses the pre-defined functions,

- `makeDimerCluster(d, phi = pi/4, psi = 0, right = TRUE, ...)` to define a chiral dimer cluster with inter-particle distance d, dihedral angle φ, and tilt ψ.

- `circular_dichroism_spectrum(clust, gold, n=1.33)` solves the electromagnetic scattering of circularly polarised light, performing angular averaging over incident light directions.

Finally, the code in `demo(helix_cd)` uses the function `makeSpheresCluster(N, radius, R0, pitch,delta, right=TRUE)` to generate a helical cluster of nanospheres[6, 5]. Circular dichroism spectra are obtained, with the separated contribution from absorption and scattering.

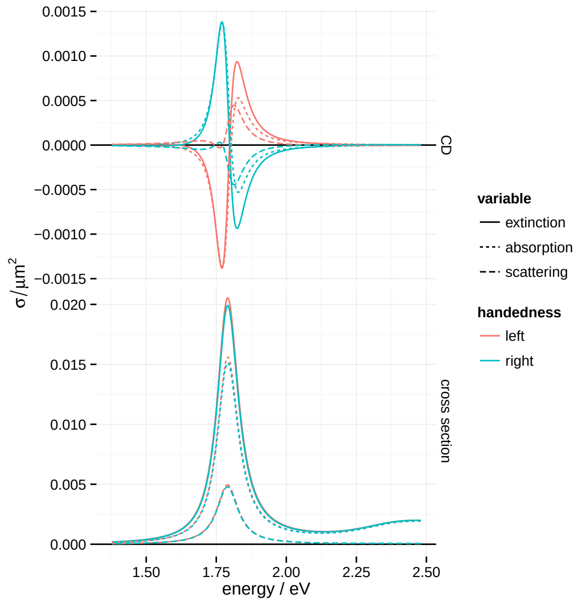

Figure 5: `demo(dimer_cd)` from the cda package. A chiral cluster of two nanorods is used with a separation $d = 200\,\text{nm}$ and dihedral angle $\varphi = \pm\pi/4$. Opposite handedness yields a mirror-image circular dichroism spectrum.

References

[1] Baptiste Auguié, José Lorenzo Alonso-Gómez, Andrés Guerrero-Martínez, and Luis M. Liz-Marzán. Fingers crossed: Optical activity of a chiral dimer of plasmonic nanorods. *The Journal of Physical Chemistry Letters*, 2(8):846–851, 2011.

[2] Baptiste Auguié and William Barnes. Collective resonances in gold nanoparticle arrays. 101(14):143902, Sep 2008.

[3] Baptiste Auguié and William L. Barnes. Diffractive coupling in gold nanoparticle arrays and the effect of disorder. *Opt. Lett.*, 34(4):401–403, Feb 2009.

[4] Baptiste Auguié, Xesús M. Bendaña, William L. Barnes, and F. Javier García de Abajo. Diffractive arrays of gold nanoparticles near an interface: Critical role of the substrate. *Phys. Rev. B*, 82(15):155447, Oct 2010.

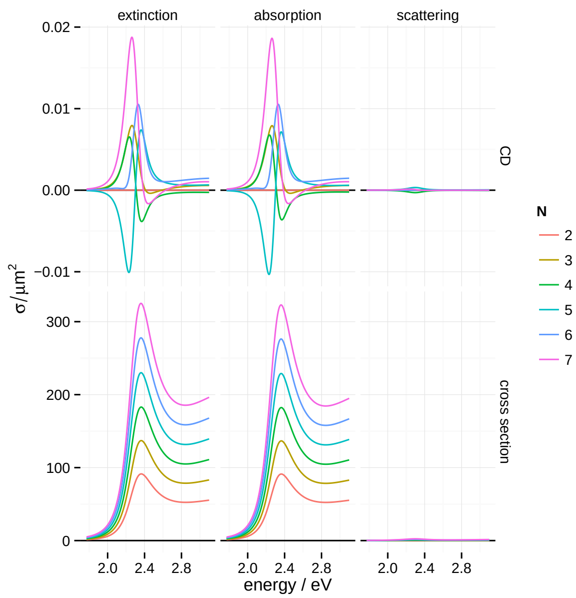

Figure 6: `demo(helix_cd)` from the cda package. The extinction, scattering and absorption spectra of a helical arrangement of gold nanospheres are simulated, with varying number of particles.

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[6] Andrés Guerrero-Martínez, Baptiste Auguié, José Lorenzo Alonso-Gómez, Zoran Džolić, Sergio Gómez-Graña, Mladen Žinić, M. Magdalena Cid, and Luis M. Liz-Marzán. Intense optical activity from three-dimensional chiral ordering of plasmonic nanoantennas. *Angewandte Chemie International Edition*, 50(24):5499–5503, 2011.