Computational Photonics
Tutorial 6:
Green's function and the discrete dipole approximation

19 July 2023

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Exercises for everyone:

- Task 1: Green's function in homogeneous space
- Task 2: Discrete dipole approximation

Extended exercises:

- Task 3*: Scattering cross section

Green's function in a homogeneous medium

Source at $\mathbf{r}_1$, find the field at $\mathbf{r}_2$. Let $\mathbf{R} = \mathbf{r}_2 - \mathbf{r_1}$. Then,

$$\mathbf{G}(\mathbf{R}) = \frac{k^2 e^{ikR}}{4\pi\epsilon_0\epsilon_\mathrm{r} R}\left[\left(\frac{3}{k^2R^2} - \frac{3i}{kR} - 1\right)\frac{\mathbf{RR}}{R^2} - \left(\frac{1}{k^2R^2} - \frac{i}{kR} - 1\right)\mathbf{I}\right]$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{RR}$ is the outer product of $\mathbf{R}$ with itself. In Cartesian coordinates,

$$\mathbf{RR} = \begin{bmatrix} x^2 & xy & xz \\ xy & y^2 & yz \\ xz & yz & z^2 \end{bmatrix}$$

where $x = x_2 - x_1$ and so forth.
Now, the field created by a collection of point electric dipoles $\mathbf{p}_1$, $\mathbf{p}_2$, ...

$$\mathbf{E}(\mathbf{r}) = \sum_n \mathbf{G}(\mathbf{r}_n - \mathbf{r})\mathbf{p}_n$$

Discrete dipole approximation for scattering

Consider polarizable electric dipoles, all with the same polarizability α,

$$\mathbf{p}_m = \alpha \mathbf{E}(\mathbf{r_m})$$

where $\mathbf{p}_n$ is located at $\mathbf{r}_n$. With many dipoles,

$$\mathbf{p}_m = \alpha \mathbf{E}_{\text{inc}}(\mathbf{r}_m) + \alpha \sum_{n \neq m} \mathbf{G}(\mathbf{r}_n - \mathbf{r}_m)\mathbf{p}_n$$

where self-interaction / self-field is accounted for in the polarizability.
Now we have the equation system $\mathbf{Ap} = \mathbf{b}$ where

$$\mathbf{A} = \begin{bmatrix} \mathbf{I} & -\alpha\mathbf{G}(\mathbf{r}_2 - \mathbf{r}_1) & -\alpha\mathbf{G}(\mathbf{r}_3 - \mathbf{r}_1) & \dots \\ -\alpha\mathbf{G}(\mathbf{r}_1 - \mathbf{r}_2) & \mathbf{I} & -\alpha\mathbf{G}(\mathbf{r}_3 - \mathbf{r}_2) & \dots \\ -\alpha\mathbf{G}(\mathbf{r}_1 - \mathbf{r}_3) & -\alpha\mathbf{G}(\mathbf{r}_2 - \mathbf{r}_3) & \mathbf{I} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

and

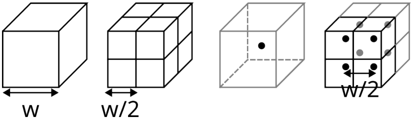
$$\mathbf{b} = \begin{bmatrix} \alpha\mathbf{E}_{\text{inc}}(\mathbf{r}_1) \\ \alpha\mathbf{E}_{\text{inc}}(\mathbf{r}_2) \\ \dots \end{bmatrix}$$

Discretization and material parameters

To represent a piece of homogeneous material with an array of polarizable dipoles, calculate the required polarizability by using the Clausius-Mossotti relation

$$\frac{n\alpha}{3\epsilon_0} = \frac{\epsilon - 1}{\epsilon + 2}$$

where n is the number density and ϵ the relative permittivity of the material in question. For a cubic lattice $n = 1/d^3$ where d is the distance between adjacent dipoles.
Along one dimension, a cube of width w can be divided into m unit cells with $m + 1$ boundaries at $-w/2 + [0, w/m, ...]$ and m centers at $-w/2 + w/(2m) + [0, w/m, ...]$. The dipoles should be located at the centers of the unit cells.



Implementation hints

- This time, all matrices are dense
- Outer products of vectors: `numpy.outer()`
- Block matrices: `numpy.block()`
- Useful for array manipulations: `np.stack()`, `numpy.ndarray.flatten()`

Task 1: Green's function

Implement the Green's function for a homogeneous medium

```
def green(r1, r2, k):
    # Arguments:
    #   r1: length 3 vector containing (x1,y1,z1)
    #   r2: (x2,y2,z2)
    #   k: wave number
    # Returns the 3-by-3 Green's tensor.
    return G
```

Sanity check: let $\mathbf{r}_1 = (0,0,0)$ and $\mathbf{r}_2 = (1,1,1)$, $k = 2\pi$ and $\epsilon_0\epsilon_\mathrm{r} = 1$.

```
In [25]: G
Out[25]:
array([[-0.13608234-1.20151788j, -0.09929022+0.60429807j, -0.09929022+0.60429807j],
       [-0.09929022+0.60429807j, -0.13608234-1.20151788j, -0.09929022+0.60429807j],
       [-0.09929022+0.60429807j, -0.09929022+0.60429807j, -0.13608234-1.20151788j]])
```

Task 2: Discrete dipole approximation

Implement the discrete dipole approximation.

```
def dda_dipole_moments(c, alpha, k, Ei):
    # Calculate the electric dipole moments for N dipoles under a prescribed
    # illumination.
    # Arguments:
    #   c: coordinates, N-by-3 matrix, each row holds the (x,y,z) coordinates of
    #      a dipole
    #   alpha: polarizability, scalar
    #   k: wave number
    #   Ei: incident field, vector of length 3N such that Ei[0::3] = Ex for each
    #       dipole, Ei[1::3] = Ey for each dipole etc.
    # Returns p, vector of length 3N with p[0::3] being the x-components, p[1::3]
    # the y-components et cetera.
    return p
def field_sc(X,Y,Z, c, p, k):
    # Knowing N dipole moments, calculate the scattered field at given coordinates.
    # Arguments:
    #   X,Y,Z: arrays containing the x,y,z coordinates of the points at which we
    #          want to calculate the scattered field
    #   c: coordinates of the dipoles, N-by-3 matrix
    #   p: dipole moments, as returned by 'dda_dipole_moments'
    #   k: wave number
    # Returns E, vector of length 3N where E[0::3] are the x-components of the
    # scattered field at each (x,y,z) point, E[1::3] are the y-components, etc.
    return E
```

Use the test case specified on the next slide.

Task 2 test case

Nearly zero backscattering from a silicon nanocube close to a Mie resonance

- Silicon ($\epsilon = 12.8$) nanocube of width 0.2 µm in vacuum
- Illuminated by a x-polarized plane wave propagating in the z-direction, frequency 310 THz
- Discretize the cube with 9-by-9-by-9 dipoles
- Calculate the intensity distribution on a circle in the xz-plane, radius 100 µm, and plot it in polar coordinates

Task 3*: Scattering cross section

Implement a function that takes the output of a DDA calculation and calculates the scattering cross section. Use the task 2 test case to test your function; the cross section should be on the order of $0.15\,\mu\text{m}^2$ (but as long as you're within 20 % of this it's good enough).
The scattering cross section can be calculated using the following equations:

$$\sigma_{\text{sc}} = \frac{P_{\text{sc}}}{I_{\text{inc}}}$$

$$P_{\text{sc}} = \frac{1}{2Z_0} \int_0^{2\pi} \int_0^{\pi} |\mathbf{E}_{\text{sc}}(r, \theta, \phi)|^2 r^2 \sin(\theta) d\theta d\phi$$

$$I_{\text{inc}} = \frac{1}{2Z_0} |\mathbf{E}_{\text{inc}}|^2$$

where the incident wave is a plane wave with the amplitude $\mathbf{E}_{\text{inc}}$.
Either discretize the integral "manually" or use `scipy` methods if you can.