Hands-on Mie lab.
Ocean Optics class, 2023.

Introduction:
Mie theory provides the solution for a plane-parallel EM energy interacting with a *homogeneous sphere*. It assumes that a single scattering event is taking place. It is in the form of a series solution. The code provided (translated from the textbook by Bohren and Huffman, 1983) was designed to sum up the series elements based on a given convergence criterion. We will also use simple approximations based on the anomalous diffraction approximation (developed by van de Hulst, 1957) which is applicable to many marine particles.

Code is available on: https://tinyurl.com/oo23miecode

The inputs to the Mie code:
1) Wavelength of light interacting with the particle in the medium (λ).
2) Index of refraction of the medium, assumed to be non-absorbing.
3) The diameter of the particle (with the same length units as the wavelength).
4) Complex index of refraction of the particle ($m=n+in'$), with both real (n) and imaginary (n') parts relative to the medium in which the particle is immersed. The imaginary part of the index of refraction relates to the absorption of the material it is made of *in solution*: $n'=a_{sol}\lambda/4\pi$.

The solution of the Mie code is often given in terms of 'cross section' and/or 'efficiency factor' for absorption and attenuation (scattering is obtained as a difference). For example, the attenuation cross-section, C_{ext},[1] has units of length^2 (L^2) and provides the amount of light that is attenuated by a single particle in one m^3. If we had N such particles in a m^3 of water the beam attenuation would be:

$$c=C_{ext}\, N \,/\, \text{volume} = \alpha_{ext}\, N\ .$$

where α_{ext} is the single-particle attenuation cross section per volume (or it could be thought of as the beam attenuation of a single particle).

[1] Note that attenuation is often referred to as extinction in the literature, hence the 'ext' subscript.

The efficiency factor (Q_{ext}) is the cross section divided by the particle's geometric cross-sectional area, e.g. for attenuation:

$$Q_{ext}=C_{ext}/\pi r^2,$$

Where r is the radius of the particle. The efficiency factors are dimensionless. Another output of the code is the phase function. The optical properties of an ensemble of particles are, by the Beer-Lambert law, the sum of the optical properties of each of the individual particle present.

Mie theory part I: optical properties of a single particle.

Review: analytical limits for Mie's solution *(homogeneous spheres)*.
See appendix.

Class examples:
1. What is the likely c(660) for a large HAB forming phytoplankton (D=20μm) with concentration of N=10^5 cells/L?

2. Hill et al., 2011, shows that $c^*_{660}\sim 0.5m^2/g$. Is it sensible?

3. Let's assume a phytoplankton with m=1.05+0.01i, D=2μm & λ=440nm. What analytical regime is applicable for such a cell?

What is its attenuation I, scattering (*b*) and absorption (*a*) per cell based on that approximation? Assuming $5*10^4$ phytoplankton per ml compute the absorption, scattering and attenuation coefficients of this ensemble of mono-dispersed particles (i.e., particles of all the same size)?

Using the Matlab routine **callbh.m** and the Mie solver (**bhmie.m**) get Q_a, Q_b, Q_c, Q_{bb}, $\beta(\theta)$ and $\tilde{\beta}(\theta)$. Calculate *a, b, c* and b_b per cell and for a population of $5*10^4$ phytoplankton per ml. Compare your results with the theoretical approximation you used above.

Extra credit: what if the phytoplankton in question were prolate spheroids with an axis ratio of b/a=5 (see Tab. 1 below). Based on a theorem by Cauchy, their average cross-sectional area over all orientations is ¼ x surface-area. If we assumed they had the same volume (biomass) as the above spherical cell, how would their absorption, scattering, and attenuation cross-sections be different? If Q_a was approximately the same, how would their absorption differ?

Shape	*Surface area*	*Volume*
Oblate spheroid ($b/a<1$)	$\frac{2\pi}{\sqrt{a^2-b^2}}\left[a^2\sqrt{a^2-b^2}+ab^2\ln\left(\frac{a+\sqrt{a^2-b^2}}{b}\right)\right]$	$\frac{4\neq}{3}a^2b$
Sphere ($a=b$)	$4\pi a^2$	$\frac{4\neq}{3}a^3$
Prolate spheroid ($b/a>1$)	$2\pi a^2+\frac{2\pi ab^2}{\sqrt{b^2-a^2}}\sin^{-1}\left(\frac{\sqrt{b^2-a^2}}{b}\right)$	$\frac{4\neq}{3}a^2b$

Table 1. Surface area and volume of spheroids (Beyer, 1987)

4. Let's assume we are dealing with non-absorbing rain drops (n=1.33) and a wavelength in air of 550nm (0.55µm). How does the mass-specific attenuation (*c*=Q_{ext}*cross-section/volume/density*) vary as function of size for drops varying in size D=0.01, 0.1, 1, 10, 100, 1000 micron. Use the Matlab routine **callbh.m** and the Mie solver (**bhmie.m**) to get $Q_{ext}=Q_c$.

Given a water fraction of 1g/m^3 calculate the transmission ($Tr=L/L_0=e^{-cR}$) through a cloud R=1km thick for water distributed uniformly with the above diameters. How do these result it explain visibility differences between fog and rain?

Part II: Optical properties of a population of particles

1. Assume a phytoplankton population with m=1.05+0.01i relative to water. Assume the particles' size distribution to be a power law distribution with a 'differential' size distribution function $f(D)=5*10^4D^{-4}$ particles per ml per µm for particles ranging from 0.2-100µm. Subdivide this range logarithmically into 35 size bins. Assume a wavelength of 440nm.

- Using the Mie code (**callbh_variedsizes_part2.m**) obtain *a, b, c,* b_b the volume scattering function (VSF; β(θ)) and the phase function ($\tilde{\beta}$ (θ)) for each size group.
- Add them up to get the IOPs of the population (use **Junge_population.m**).
- Compare the phase function for all sizes (plot them all on a semi-logarithmic plot).
- How do they compare to the shape of the total VSF?

- How does b_b/b change as function of size?
- Which contributes more to the attenuation in each size group, *a* or *b*? (plot them as function of D).
- How do the optical characteristics change if $f(D) \propto D^{-3}$?
- How does your answer change if the range is 1-100 μm (i.e. what does the range 0.2-1μm contribute most to)?
- Do the results change significantly when we used the finer spaced size bins (i.e. 100 versus 35 bins)?

Part III: Inverse calculation

1. Using a phytoplankton absorption curve (obtained with an ac-9) for T. Pseudonana we find $a(676)=0.14m^{-1}$. Assuming all cells had the same size (4μm) find n'(λ), for λ=676nm. Assume $N=5*10^5$cells/ml

   - Use $a(\lambda)=Q_a(\lambda)\pi D^2/4*N$ and the **AD.m** code. Notice: in the anomalous diffraction approximation, Q_a is *not* a function of n, and thus the assumed n value will not affect Q_a.
   - For the same cells it was found that $c(676)=0.8m^{-1}$. Using **AD.m** vary n between 1.02 and 1.2 and find which is most consistent with this observation. Notice: there may be more than one solution. Choose the one that seems most reasonable.

2. A given population of inorganic particles (n(660)=1.15, n'(660)=0.001) is distributed according to a power-law with ξ=3.5 between 2 and 30μm. If $c(660)=3m^{-1}$, what is the amplitude of the PSD (in # per ml per μm) at 2 μm? Use **AD_population.m**.

Note: a similar inverse approach can yield the population size exponent or size range for a population with given n and n' and with the full Mie code.

References

Bohren CF, Huffman DR. 2004. *Absorption and Scattering of Light by Small Particles*. Weinhem: Wiley-VCH.

Hill, P.S., E. Boss, J.P. Newgard, B.A. Law, and T.G. Milligan, 2011. Observations of the sensitivity of beam attenuation to particle size in a coastal bottom boundary layer. J. Geophys. Res., 116, C02023, doi:10.1029/2010JC006539.

van de Hulst HC. 1957. *Light Scattering by Small Particles*. New York: John Wiley and Sons.

Appendix: A brief survey of some analytical solutions for Mie theory (based mostly on *Light Scattering by Small Particles* by Van de Hulst):

Definitions: D- Diameter .
G is the cross-sectional area ($\pi D^2/4$).
λ-wavelength in medium (=wavelength in vacuum/index of refraction of medium relative to vacuum).
$x\equiv\pi D/\lambda$-size parameter (nondimensional).
$m=n+in'$-index of refraction relative to medium.
$\rho\equiv 2x(n-1)$-phase lag suffered by ray crossing the sphere along its diameter compared to a beam propagating in the medium.
$\rho'\equiv 4xn'$-optical thickness corresponding to absorption along the diameter.
$\beta\equiv\tan^{-1}(n'/(n-1))$

<u>Rayleigh regime</u>: $x\ll 1$ and $|m|x\ll 1$
$Q_a=4x\ \mathrm{Im}\{(m^2-1)/(m^2+2)\}$ note: proportional to λ^{-1}
$Q_b=8/3\ x^4\ |(m^2-1)/(m^2+2)|^2$ note: proportional to λ^{-4}
$Q_c= Q_a+ Q_b$
$Q_{bb}= Q_b/2$, Phase function: $<\beta>=0.75(1+\cos^2\theta)$

<u>Rayleigh-Gans regime</u>: $|m-1|\ll 1$ and $\rho\ll 1$
$Q_a=8/3\ x\ \mathrm{Im}\{(m-1)\}$ note: proportional to λ^{-1}
$Q_b=|m^2-1|\ [2.5+2*x^2-\sin(4x)/4x-7/16(1-\cos(4x))/x^2+(1/(2x^2)-2)\{\gamma+\log(4x)-Ci(4x)\}]$,
where $\gamma=0.577$ and $C_i(x)=-\int_x^\infty \frac{\cos(u)}{u}du$
$Q_c= Q_a+ Q_b$
For $x\ll 1$: $Q_b=32/27\ x^4\ |m-1|^2$, $Q_{bb}= Q_b/2$
For $x\gg 1$: $Q_b=2\ x^2\ |m-1|^2$, $Q_{bb}= 0.31|m-1|^2$

<u>Anomalous diffraction (VDH)</u>: $x\gg 1$, $|m-1|\ll 1$ (ρ can be $\gg 1$)
$Q_c=2-4\exp(-\rho\tan\beta)[\cos(\beta)\sin(\rho-\beta)/\rho+(\cos\beta/\rho)^2\cos(\rho-2\beta)]+4(\cos\beta/\rho)^2\cos 2\beta$
$Q_a=1+2\exp(-\rho')/\rho'+2(\exp(-\rho')-1)/\rho'^2$, $Q_b= Q_c-Q_a$

<u>Geometric optic</u>: $x\ggg 1$
$Q_c=2$, Absorbing particle: $Q_b=1$, $Q_a=1$
Exactly Non-absorbing particle: $Q_b=2$, $Q_a=0$

Angular scattering cross section: $\hat{\beta}_{diff}(\theta) = \frac{Gx^2}{16\pi}\left[\frac{2J_1(x\sin\theta)}{x\sin\theta}\right]^2 (1+\cos\theta)^2$.