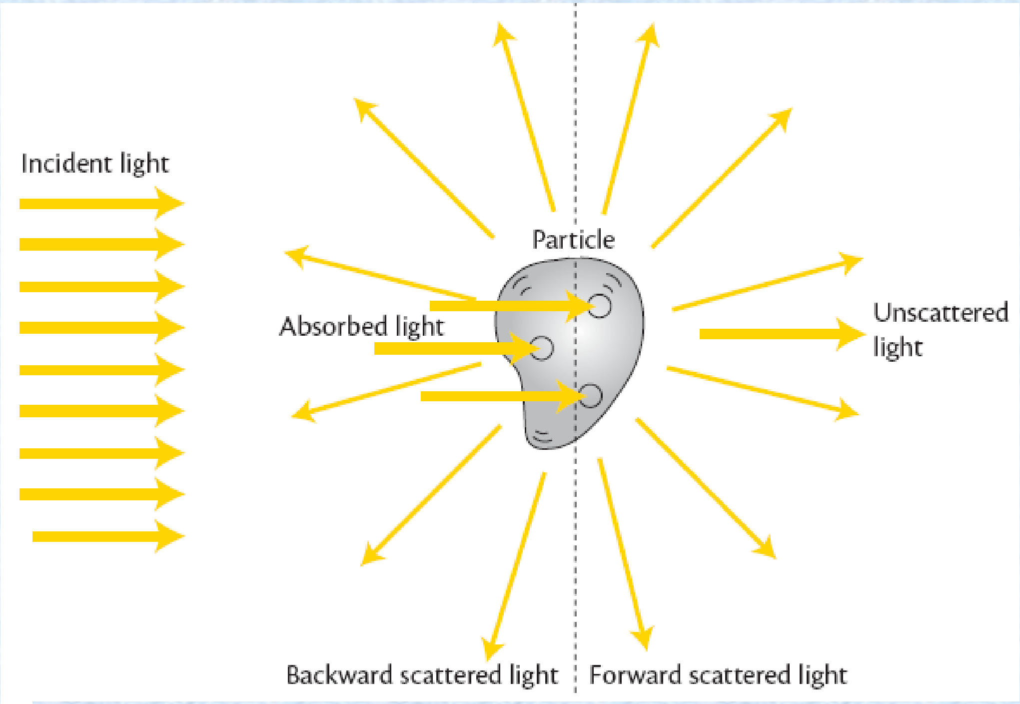
Lecture + Lab (this afternoon): Interaction of light with spherical particles.

Mie's (1905) solution + more.

Scattering of light by spherical particles (Mie scattering).

The problem (Bohren and Huffman, 1983):

Given a particle of a specified size, shape and optical properties that is illuminated by an arbitrarily polarized monochromatic wave, determine the electromagnetic field at all points in the particles and at all points of the homogeneous medium in which it is embedded.



We will assume that the incident wave is a non-polarized plane harmonic wave impinging on a spherical particles.

Why should you care about optical theory and Mie's solution?

These solutions provide a calibration to our sensors (LISST, b_b, flow-cytometers).

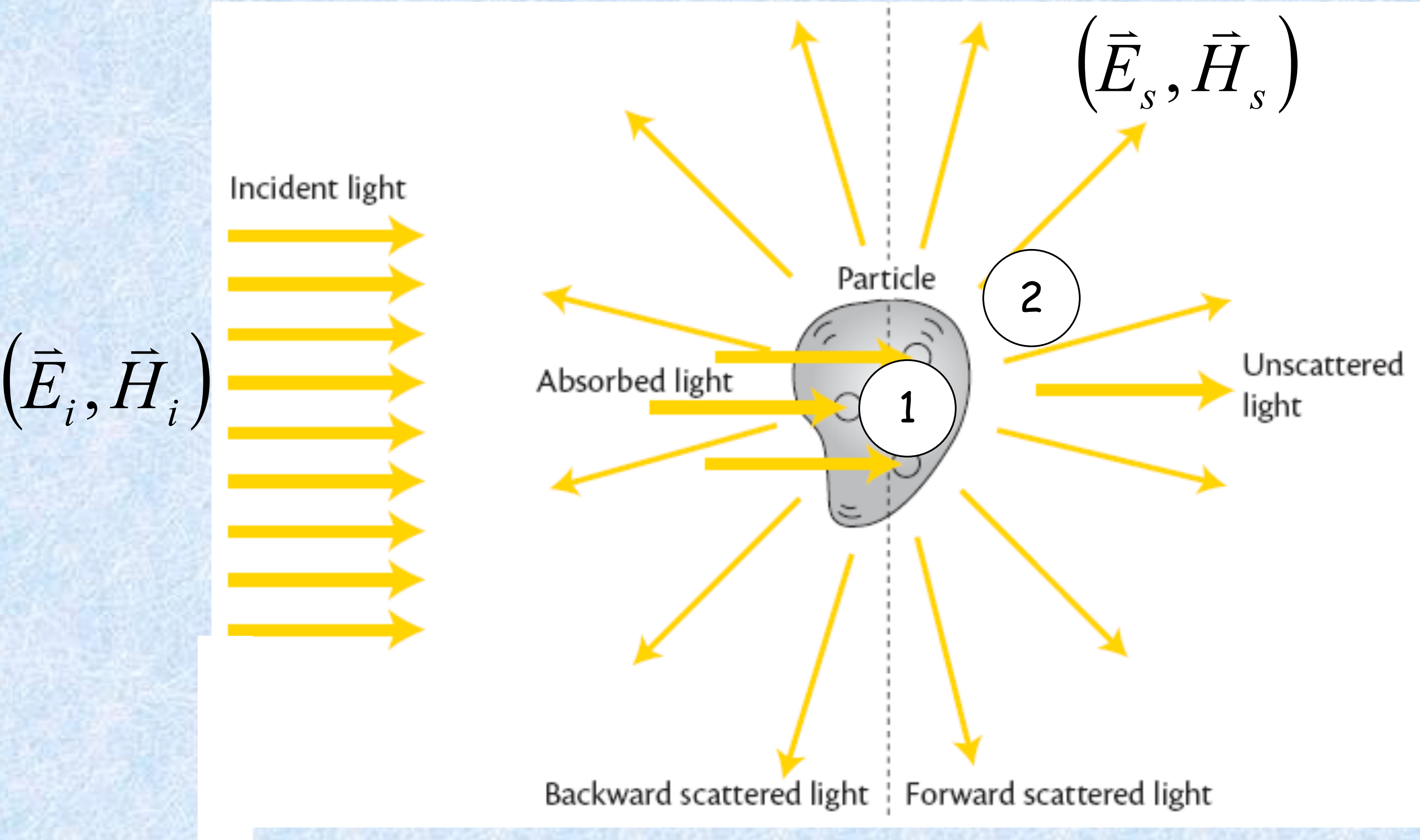
In addition, for a given concentration of particles of a given *size/wavelength* and *index of refraction* we expect a given signal (examples coming at the end…).

Tiho Kostadinov – used Mie theory to look at effects of changes of population PSD on Rrs.

Giorgio Dall'Olmo – used Mie theory to analyze diel cycles in optical properties.

Rebecca Green – used Mie theory to analyze flow-cytometer data, assigning size based on forward and backscattering of single cells.

Define four fields: $\left(\vec{E}_1, \vec{H}_1\right), \left(\vec{E}_2, \vec{H}_2\right), \left(\vec{E}_i, \vec{H}_i\right), \left(\vec{E}_s, \vec{H}_s\right)$



Outside the particle: $\vec{E}_2 = \vec{E}_i + \vec{E}_s, \vec{H}_2 = \vec{H}_i + \vec{H}_s$

Plane parallel harmonic wave:

$$\vec{E}_i = \vec{E}_0 \exp\left(i\left(\vec{k} \cdot x - \omega t\right)\right)$$
$$\vec{H}_i = \vec{H}_0 \exp\left(i\left(\vec{k} \cdot x - \omega t\right)\right)$$

Must satisfy Maxwell's equation where material properties are constant:

$$\nabla \cdot \vec{E} = 0$$

$$\nabla \cdot \vec{H} = 0$$

$$\nabla \times \vec{E} = i\omega\mu\vec{H}$$

$$\nabla \times \vec{H} = -i\omega\varepsilon\vec{E}$$

ε is the *permittivity* μ is the *premeability*.

define:

$$k^2 = \varepsilon\mu\omega^2$$

The vector equation reduce to:

$$\nabla^2\vec{E} + k^2\vec{E} = 0$$

$$\nabla^2\vec{H} + k^2\vec{H} = 0$$

Boundary conditions: the tangential components of the electric and magnetic fields must me continuous across the boundary of the particle (analogous to energy conservation):

$$\left[\vec{E}_2 - \vec{E}_1\right]\times\hat{n} = 0$$

$$\left[\vec{H}_2 - \vec{H}_1\right]\times\hat{n} = 0$$

The equations and BCs are linear → superposition of solutions is a solution.

An arbitrarily polarized light can be expressed as a supperposition of two orthogonal polarization states:

Amplitude scattering matrix

$$\begin{pmatrix} E_{l,s} \\ E_{r,s} \end{pmatrix} = \frac{\exp(ik(r-z))}{-ikr} \begin{pmatrix} S_2(\theta,\varphi) & S_3(\theta,\varphi) \\ S_4(\theta,\varphi) & S_1(\theta,\varphi) \end{pmatrix} \begin{pmatrix} E_{l,i} \\ E_{r,i} \end{pmatrix}$$

For spheres:

$$\begin{pmatrix} E_{l,s} \\ E_{r,s} \end{pmatrix} = \frac{\exp(ik(r-z))}{-ikr} \begin{pmatrix} S_2(\theta) & 0 \\ 0 & S_1(\theta) \end{pmatrix} \begin{pmatrix} E_{l,i} \\ E_{r,i} \end{pmatrix}$$

$$\Rightarrow \begin{aligned} E_{l,s} &= \frac{\exp(ik(r-z))}{-ikr} S_1(\theta) E_{l,i} \\ E_{r,s} &= \frac{\exp(ik(r-z))}{-ikr} S_2(\theta) E_{r,i} \end{aligned}$$

Taking the real part of the squares of the electric fields we get the radiant intensity [W Sr^{-1}]:

$$\Rightarrow \begin{aligned} I_{r,s} &= \frac{\left|S_1(\theta)\right|^2}{k^2 r^2} I_{r,i} \\ I_{l,s} &= \frac{\left|S_2(\theta)\right|^2}{k^2 r^2} I_{l,i} \end{aligned}$$

For unpolarized light:

$$I_s = \frac{\frac{1}{2}\left\{\left|S_1(\theta)\right|^2 + \left|S_2(\theta)\right|^2\right\}}{k^2 r^2} I_i$$

Solution is in the form of a series of orthogonal harmonics.
The larger the particle, the slower the convergence.

Polarization- Stokes notation and the scattering matrix:

$$I_s = \frac{k}{2\omega\mu}\left\langle \left|E_{l,s}\right|^2 + \left|E_{r,s}\right|^2 \right\rangle$$

No polarizers

$$Q_s = \frac{k}{2\omega\mu}\left\langle \left|E_{l,s}\right|^2 - \left|E_{r,s}\right|^2 \right\rangle$$

Horizontal - vertical polorizers

$$U_s = \frac{k}{2\omega\mu}\left\langle E_{l,s}E^*_{r,s} + E_{r,s}E^*_{l,s} \right\rangle$$

45° - (-45°) polorizers

Right handed – left handed circular polorizers

$$V_s = i\,\frac{k}{2\omega\mu}\left\langle E_{l,s}E^*_{r,s} - E_{r,s}E^*_{l,s} \right\rangle$$

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{k^2r^2}\begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{pmatrix}\begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix}$$

For a sphere, the Mueller matrix reduces to:

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{k^2 r^2} \begin{pmatrix} S_{11} & S_{12} & 0 & 0 \\ S_{12} & S_{11} & 0 & 0 \\ 0 & 0 & S_{33} & S_{34} \\ 0 & 0 & -S_{34} & S_{33} \end{pmatrix} \begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix}$$

Link to amplitude scattering matrix: $\begin{pmatrix} E_{l,s} \\ E_{r,s} \end{pmatrix} = \frac{\exp(ik(r-z))}{-ikr} \begin{pmatrix} S_2(\theta) & 0 \\ 0 & S_1(\theta) \end{pmatrix} \begin{pmatrix} E_{l,i} \\ E_{r,i} \end{pmatrix}$

$$S_{11} = \left\{ |S_1|^2 + |S_2|^2 \right\}, \qquad S_{12} = \left\{ |S_1|^2 - |S_2|^2 \right\}$$

$$S_{33} = \left\{ S_2^* S_1 + S_1^* S_2 \right\}, \qquad S_{34} = \left\{ S_2^* S_1 - S_1^* S_2 \right\}$$

$$S_{11}^2 = S_{12}^2 + S_{33}^2 + S_{34}^2, \qquad P \equiv -\frac{S_{12}}{S_{11}}$$

Solution method:

Expand incident and scattered fields in spherical harmonic functions for each polarization. Match solutions on boundary of particle and require them to be finite at large distances.

Input to Mie code:

Wavelength in medium (λ).

Size (diameter, D) in the same units as wavelength.

Index of refraction relative to medium ($n + in'$).

Solution depends on:

Size parameter: $\pi D/\lambda$

Index of refraction of particle relative to medium

Output to Mie code:

Efficiency factors:

Q_a, Q_c (also called Q_{ext}). Unitless.

$$Q_c = \frac{\text{Light attenuated on particle}}{\text{Light impinging on particle}}$$

Scattering matrix elements:

S_1 and S_2

From which we can calculate:

$Q_b = Q_c - Q_a$

$\beta \propto S_{11} = |S_1|^2 + |S_2|^2$

Other polarization scattering matrix elements:

$S_{12} \propto |S_1|^2 - |S_2|^2$

$P = -S_{12}/S_{11}$

$S_{33} = \mathrm{Real}(S_2 \times S_1^*)/S_{11}$

$S_{34} = \mathrm{Imag}(S_2 \times S_1^*)/S_{11}$

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{k^2 r^2} \begin{pmatrix} S_{11} & S_{12} & 0 & 0 \\ S_{12} & S_{11} & 0 & 0 \\ 0 & 0 & S_{33} & S_{34} \\ 0 & 0 & -S_{34} & S_{33} \end{pmatrix} \begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix}$$

How to go from Mie code output to IOPs:

$$C_{ext} = \text{Geometric cross section} \times \frac{\text{Light attenuated by particle}}{\text{Light impinging on particle}}$$

$C_{ext} = G \times Q_c$

What are the units?

Now, if we have 1 particle for m^3 of medium.

What will the the beam attenuation be?

$C = C_{ext}\ [m^2] \times 1/m^3$

Same algebra for other IOPs.

Populations of particles:

Monodispersion- example, obtaining the scattering coefficient:

$b = NQ_bG, \quad G = \pi D^2/4.$

Polydispersion: discrete bins:

$b = \Sigma N_i Q_{b,i} G_i$

When using continuous size distribtion:

$$N(D, \Delta D) = \int_{D-\Delta D/2}^{D+\Delta D/2} f(D)\,dD$$

$$b = \frac{\pi}{4} \int_{D_{\min}}^{D_{\max}} Q_b(D) D^2 f(D)\,dD$$

Similar manipulations are done to obtain the absorption and attenuation coefficients, as well as the population's volume scattering function.

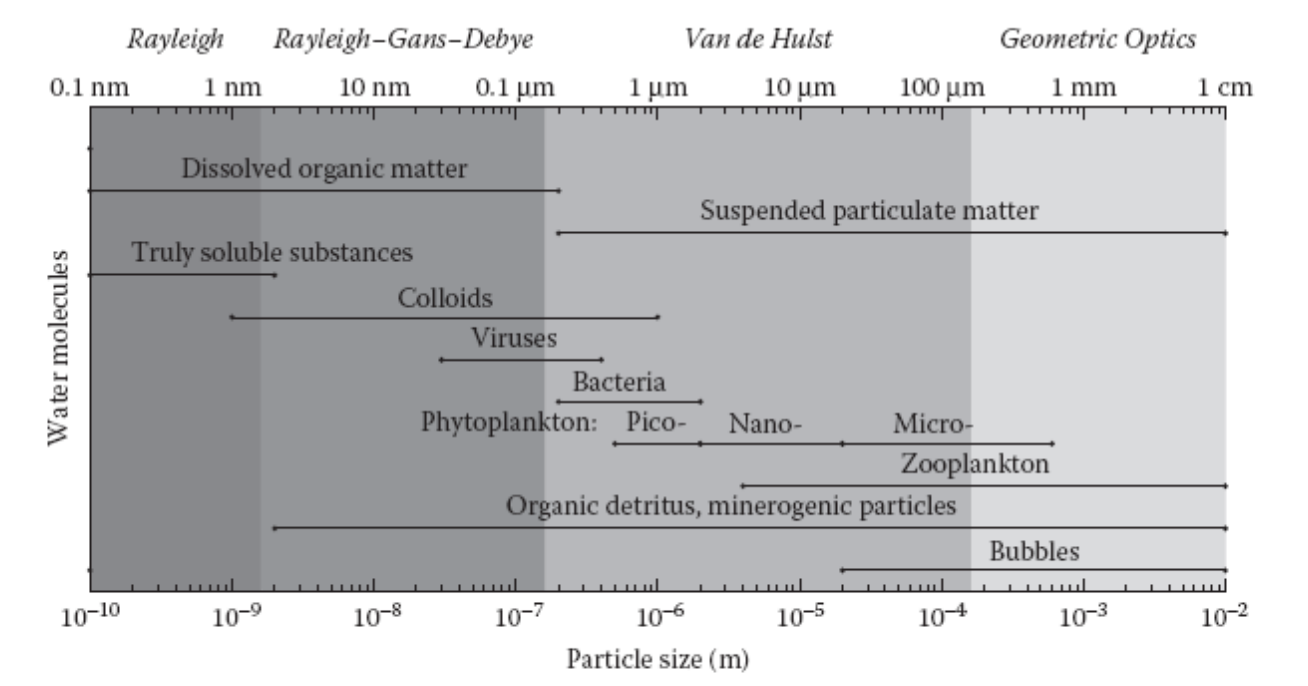
Optical regimes

Table 1 Size ranges roughly corresponding to the size regions defined for two different refractive indices given $\lambda = 676$ nm

Size region	$n = 1.05$	$n = 1.17$	Equivalent ρ
RAY	$D \ll 0.2\ \mu m$	$D \ll 0.2\ \mu m$	$\rho \ll 0.1$
RGD	$D < 5\ \mu m$	$D < 2\ \mu m$	$\rho < 3$
VDH	$5 < D < 200\ \mu m$	$2 < D < 65\ \mu m$	$3 < \rho < 100$
GO	$D \gg 200\ \mu m$	$D \gg 65\ \mu m$	$\rho \gg 100$

Useful before computers

Builds intuition to likely dependencies



Analytical solutions for light interaction with a sphere

Definitions: $x \equiv \pi D/\lambda$-size parameter

$m=n+in'$-index of refraction relative to medium

$\rho \equiv 2x(n-1)$-phase lag suffered by ray crossing the sphere along its diameter

$\rho' \equiv 4xn'$-optical thickness corresponding to absorption along the diameter

$\beta \equiv \tan^{-1}(n'/(n-1))$

D- Diameter

λ-wavelength in medium (=wavelength in vacuum/index of refraction of medium relative to vacuum)

Rayleigh regime: $x<<1$ and $|m|x<<1$

$Q_a=4x \operatorname{Im}\{(m^2-1)/(m^2+2)\}$ 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: $<\beta>=0.75(1+\cos^2\theta)$

Rayleigh-Gans regime: $|m-1|<<1$ and $\rho<<1$

$Q_a=8/3\, x \operatorname{Im}\{(m-1)\}$ 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 $x<<1$: $Q_b=32/27\, x^4 |m-1|^2$, $Q_{bb}= Q_b/2$

For $x>>1$: $Q_b=2\, x^2 |m-1|^2$, $Q_{bb}= 0.31|m-1|^2$

Anomalous diffraction (VDH): $x>>1$, $|m-1|<<1$ (ρ can be $>>1$)

$Q_c=2-4\exp(-\rho\tan\beta)[\cos(\beta)\sin(\rho-\beta)/\rho+(\cos\beta/\rho)^2\cos(\rho-2\beta)]+4(\cos\beta/\rho)^2\cos2\beta$

$Q_a=1+2\exp(-\rho')/\rho'+2(\exp(-\rho')-1)/\rho'^2$

$Q_b=Q_c-Q_a$

Geometric optic: $x>>>1$

$Q_c=2$

Absorbing particle: $Q_b=1$, $Q_a=1$

Exactly Non-absorbing particle: $Q_b=2$, $Q_a=0$

Angular scattering cross section: $\widehat{\beta}_{diff}(\theta)=\frac{Gx^2}{16\pi}\left[\frac{2J_1(x\sin\theta)}{x\sin\theta}\right]^2(1+\cos\theta)^2$, where G is the cross sectional area ($\pi D^2/4$).

From: Van de Hulst, 1957 (1981), Light scattering by small particles, Dover.

Why should you care about optical theory?

These solutions provide a calibration to our sensors (LISST, b_b, flow-cytometers).

In addition, for a given concentration of particles of a given *size/wavelength* and *index of refraction* we expect a given signal.

Examples:
1. what is the likely c(660) for a given concentration of phytoplankton ?

$r=20\mu m$
$[Conc.]=10^5/L= 10^8 m^{-3}$
$C_{ext}\sim 2\cdot Area= 2\cdot\pi\cdot(20)^2 10^{-12} m^2$
$\rightarrow c=C_{ext}\cdot[Conc]\sim 0.25 m^{-1}$

2. Hill shows that $c^*_{660}\sim 0.5 m^2/gr$. Is it sensible?

$C_{ext}\sim 2\cdot Area$.
$c^*_{6c0}=0.5=[conc.]*C_{ext,660}/ \{[conc.]*volume*density\}=0.75/\{r*density\}$.
For sediments, $density=2.5 gr/cm^3 =2.5\cdot 10^6 gr/m^3$
$\rightarrow$ average $r\sim 1.2\mu m$, a realistic size for clay.

Resources (among many others…):

Barber and Hill, 1990.

Bohren and Huffman, 1983.

Kerker, 1969.

Van de Hulst, 1981 (original edition, 1957).

Codes (among many others):
https://code.google.com/p/scatterlib/wiki/Spheres

We will use a translation of ‘bhmie’ to Matlab this afternoon