Research projects about the multiple scattering of light

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I study direct and inverse problems involving *multiple scattering of light* (and related problems).

This research includes the following applied mathematics topics.

- PDEs and integral equations
- Asymptotics and perturbations
- Numerical analysis and scientific computing
- Waves in random media
- Inverse problems
- Multiscale modeling and simulation
Multiple scattering of light

Light scattering by a medium composed of a distribution of scattering centers.

Examples

- Biological tissues
- Rain, fog, and clouds
- Atmospheric turbulence

Waves in random media. Model a medium as one realization of an ensemble with an associated probability space.

Objective. Find canonical features in scattered light measurements that contain information about the medium or targets contained within.
Current related projects

- Boundary integral equations
- Me, Joe & William
- Intensity-only imaging
- Machine learning for SAR
- Time-dependent scattering
- Diffuse optical imaging of tissues
- Nano assembled hybrid materials
- Directed assembly of optically bound colloids
Current related projects

Boundary integral equations

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Intensity-only imaging

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Directed assembly of optically bound colloids
Plasmonic cloaking

All-angle scattering cancellation in free space with simple, homogeneous, and isotropic cloaks.

- Works by *cancelling scattering*
- Supports a wide band of frequencies
- Convenient to fabricate
- No external power required

**Research objective.** Develop a computational model of these plasmonic cloaks for investigating factors that lead to effective cloaking.

*Mühlig et al.* (2013)

Egel *et al.* (2017)
Modeling plasmonic cloaking

We model this plasmonic cloak as a dielectric sphere surrounded by a random distribution of point-like, gold scatterers.

- Foldy-Lax theory for scattering by point-like scatterers
- Method of fundamental solutions for scattering by the sphere

By combining these two scattering methods, we develop a computational model capable of studying optical properties of plasmonic cloaks.
Foldy-Lax theory

The scattered field for $N$ point-like scatterers located at $r_n$ for $n = 1, \cdots, N$ is

$$
\psi^s(r) = \sum_{n=1}^{N} \alpha_n \frac{e^{ik|r-r_n|}}{|r-r_n|} \psi^E(r_n),
$$

with $\alpha_n$ denoting the scattering strength and $\psi^E$ denoting the exciting field at $r_n$. 
Foldy-Lax theory

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with $\alpha_n$ denoting the scattering strength and $\psi^E$ denoting the exciting field at $r_n$.

The exciting field at $r_n$ is given by

$$\psi^E(r_n) = \psi^{inc}(r_n) + \sum_{n' \neq n}^{N} \alpha_{n'} \frac{e^{ik|r-r_{n'}|}}{|r-r_{n'}|} \psi^E(r_{n'}).$$

This is just a linear system of equations for $\psi^E(r_n)$ for $n = 1, \cdots, N$. 
Scattering strength

For a single point-like gold scatterer located at the origin, the scattered field is given by

$$\psi^s(r) = \alpha \frac{e^{ikR}}{R} \psi^{inc}(0).$$

It follows that the scattering cross-section is

$$\sigma_s = \int_{S^2} \lim_{R \to \infty} \left[ R^2 \frac{|\psi^s(r)|^2}{|\psi^{inc}(0)|^2} \right] d\omega = 4\pi |\alpha|^2$$

Using the optical theorem, we find that the total scattering cross-section is

$$\sigma_t = \sigma_s + \sigma_a = \frac{4\pi}{k} \text{Im}[\alpha].$$

Thus, knowing $\sigma_s$ and $\sigma_a$ for a gold nanoparticle allows us to determine $\alpha$. 
Method of fundamental solutions

- Introduced as a numerical method by Mathon and Johnston (1977).
- Approximate the interior and scattered fields by a superposition of finitely many spherical waves, each of which is an *exact* solution of the PDE.
- Strength of each spherical wave is determined through the boundary conditions.
Plasmonic cloaking model

The field inside the sphere with wavenumber $k_1$ is approximated by

$$\psi^{\text{int}}(r) \approx \sum_{m=1}^{M} \frac{e^{ik_1 |r-\rho_m^{\text{int}}|}}{|r - \rho_m^{\text{int}}|} c_m^{\text{int}}.$$ 

The field outside of the sphere with wavenumber $k_0$ is approximated by

$$\psi^{\text{ext}}(r) \approx \sum_{m=1}^{M} \frac{e^{ik_0 |r-\rho_m^{\text{ext}}|}}{|r - \rho_m^{\text{ext}}|} c^{\text{ext}}_m + \sum_{n=1}^{N} \frac{\alpha_n e^{ik_0 |r-r_n|}}{|r - r_n|} \psi^{E}_n.$$
Plasmonic cloaking model

We determine $c_m^{\text{int}}$, $c_m^{\text{ext}}$, and $\psi_n^E$ by requiring that

$$\psi^{\text{inc}} + \psi^{\text{ext}} = \psi^{\text{int}},$$

and

$$\partial_n \psi^{\text{inc}} + \partial_n \psi^{\text{ext}} = \partial_n \psi^{\text{int}}$$
on $|\rho_{m}^{\text{bdy}}| = a$ for $m = 1, \cdots, M$, and

$$\psi_n^E = \psi_n^{\text{inc}}(r_n) + \psi_n^{\text{ext}}(r_n) + \sum_{n' = 1}^{N} \alpha_{n'} e^{ik_0 |r-r_{n'}|} \psi_n^{E},$$

for $n = 1, \cdots, N$.

Doing so yields a $2MN \times 2MN$ linear system of equations.
Preliminary results

Preliminary results for a 500nm dielectric sphere with relative refractive index 1.5 and 5000 point scatterers (not gold) randomly distributed over the spherical shell 500nm < r < 520nm.
Future considerations

▶ Compute scattering strengths for gold nanoparticles and test the model for various parameter settings.
▶ Use experimentally realistic number densities and volume fraction of gold nanoparticles.
▶ Compare results with those obtained using effective medium theory.
▶ Compare with experimental measurements.
▶ Speed up computations by considering hierarchical matrix compression techniques.
▶ Consider ensembles of these plasmonic cloaking structures.
Diffuse optical imaging of tissues

We seek to image subsurface objects situated in strongly scattering tissues from measurements of backscattered light.

- Light becomes “diffuse” in strongly scattering tissues.
- Even though objects are situated just below the surface, measurements are dominated by light scattered deep in the tissue.
- Need to extract information contained in measurements of strongly scattered/fully incoherent light.
Spatially modulated light

- Introduced by Cuccia et al. (2005) as a means for imaging tissues.
- Projects Fourier patterns of light onto the tissue sample.
- Images in the spatial frequency domain.
- Intuitively, the higher spatial frequencies have a shorter penetration depth than lower spatial frequencies because tissues act as a low-pass filter.

Can we use spatially modulated light sources to image scattering and absorbing objects in tissues?
Light propagation in tissues

Light propagation and scattering in tissues is governed by radiative transfer theory.

- Developed in the early 20th century to describe light scattering by planetary atmospheres.
- It takes into account scattering and absorption by inhomogeneities.
- This theory assumes no phase coherence in its description of power transport (addition of power).
- The specific intensity $I(\Omega, r)$ quantifies the power flowing in direction $\Omega$ and at position $r$. 
Light rays

In a homogeneous medium, there is no absorption or scattering, and so the intensity of light is constant along straight lines or “rays.”

Mathematically, we write

\[ \Omega \cdot \nabla I = 0. \]
Absorption

When there is absorption, but no scattering, the intensity of light attenuates (exponentially decays) along rays.

Mathematically, we write

\[ \Omega \cdot \nabla I + \mu_a I = 0. \]
Scattering

When there is scattering, but no absorption the intensity of light is attenuated by light that scatters away from direction $\Omega$.

However, the intensity of light increases due to light scattering from some other direction $\Omega'$ into direction $\Omega$.

Mathematically, we write

$$\boldsymbol{\Omega} \cdot \nabla I + \mu_s - \mu_s \int_{S^2} f(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') I(\Omega', r) d\Omega' = 0.$$
The scattering phase function \( f \) gives the fraction of light scattered in direction \( \Omega \) due to light incident in direction \( \Omega' \).

The integral 
\[
\int_{S^2} f(\Omega \cdot \Omega') I(\Omega', r) d\Omega'
\]

is the light scattered in direction \( \Omega \) due to the continuous sum of light incident over all possible directions.
The radiative transfer equation

By combining our results for absorption and scattering, we come to an understanding of the radiative transport equation

$$\Omega \cdot \nabla I + \mu_a I + \mu_s I - \mu_s \int_{S^2} f(\Omega \cdot \Omega') I(\Omega', r) d\Omega' = Q.$$ 

Here, $Q$ denotes an emitting source.

This equation governs light propagation in tissues taking into account absorption, scattering, and emission of light.

It is a partial differential/integral equation with 5 independent variables.
Boundary conditions

To solve
\[ \Omega \cdot \nabla I + \mu_a I + \mu_s I - \mu_s \int_{S^2} f(\Omega \cdot \Omega') I(\Omega', r) d\Omega' = Q \]

in a domain \( D \) with boundary \( \partial D \), we must prescribe boundary conditions of the form

\[ I = I_b \quad \text{on } \Gamma_{in} = \{ (\Omega, r) \in S^2 \times \partial D, \Omega \cdot \nu < 0 \}. \]
The direct scattering problem

The direct scattering problem is related to the following boundary value problem for the radiative transfer equation

\[
\mathbf{\Omega} \cdot \nabla I + \mu_a(r) I + \mu_s(r) \left[ I - \int_{S^2} f(\mathbf{\Omega} \cdot \mathbf{\Omega}') I(\mathbf{\Omega}', r) d\mathbf{\Omega}' \right] = 0 \quad \text{in } z > 0,
\]

\[
I = \delta(\mathbf{\Omega} - \hat{z}) \left( I_0 + I_1 e^{i2\pi f_m x} \right) \quad \text{on } \Gamma_{in},
\]

\[
I \to 0 \quad z \to \infty.
\]

We would like to solve this problem with piecewise constant parameters: \( \mu_a \) and \( \mu_s \).

This is a computationally challenging problem to solve.
The inverse scattering problem

We take as measurements

\[ b_m(x, y) = \int_{\text{NA}} I(\Omega, x, y, 0) \Omega \cdot \hat{z} \, d\Omega \]

sampled over \( N \) \((x, y)\)-pairs corresponding to pixel locations on the detector.

By considering \( M \) spatial frequencies, \( f_m \) for \( m = 1, \cdots, M \), we form the \( M \times N \) data matrix \( B \),

\[
B = \begin{bmatrix}
  b_1(x_1, y_1) & \cdots & b_1(x_N, y_N) \\
  b_2(x_1, y_1) & \cdots & b_2(x_N, y_N) \\
  \vdots & \ddots & \vdots \\
  b_M(x_1, y_1) & \cdots & b_M(x_N, y_N)
\end{bmatrix}.
\]

Given the \( M \times N \) data matrix \( B \), we seek to recover the locations and shapes of scattering and/or absorbing objects in tissues.
Asymptotic analysis

In the limit of strong scattering and weak absorption, we can rescale the radiative transfer equation using the small, dimensionless parameter $\epsilon$ according to

$$
\epsilon \Omega \cdot \nabla I + \epsilon^2 \mu_a + \mu_s \left[ I - \int_{S^2} f(\Omega \cdot \Omega') I(\Omega', \mathbf{r}) d\Omega' \right] = 0.
$$

The asymptotic solution in the limit as $\epsilon \to 0^+$ is given as (Larsen & Keller, 1974)

$$
I = \Phi_{\text{bdy layer}} + \Psi_{\text{interior}}.
$$

Rohde and Kim (2017) showed that the measurements in this asymptotic limit are given by

$$
b_m(x, y) = \alpha_0 \left( I_0 + I_1 e^{i2\pi f_m x} \right) + \alpha_1 U_z(x, y, 0) + O(\epsilon^2).
$$
Diffusion approximation

The function $U$ satisfies the diffusion equation,

$$-\nabla \cdot (\kappa \nabla U) + \mu_a U = 0$$

with

$$\kappa = \frac{1}{3\mu_s(1 - g)},$$

where $g$ is the anisotropy factor.

- The diffusion approximation is well known and has been used extensively for imaging in strongly scattering media.
- Conventional wisdom is that this diffusion approximation is not valid near sources nor boundaries, but the boundary layer theory corrects these issues.
- Asymptotic theory of Rohde and Kim (2017) shows that diffusion is the correct forward model for this imaging problem.
Reduced imaging problem

Instead of the radiative transfer equation, we solve

$$-\nabla \cdot (\kappa \nabla U) + \mu_a U = 0 \quad \text{in } z > 0,$$

$$U = I_0 + I_1 e^{i2\pi f_m x} \quad \text{on } z = 0,$$

and take as measurements

$$b_m(x, y) = -\kappa \partial_z U(x, y, 0).$$

We model the portion of the measurements that contain information about the subsurface objects.

To solve the direct scattering problem with piecewise constant coefficients, we use the Method of Fundamental solutions again.
Modeling the measurements

By linearizing the direct scattering problem for a point-like obstacle at \( r_k \), we find that

\[
 b_m(x, y) \approx U^0_m(r_k) \alpha_k G_z(x, y, 0; r_k),
\]

with \( U^0_m \) denoting the homogeneous solution, \( \alpha_k \) denoting an absorbing strength, and \( G \) denoting the fundamental solution satisfying

\[
 -\Delta G + k_0^2 G = \delta(r - r_k), \quad k_0^2 = \mu_0 / \kappa_0.
\]

Here, \( \mu_0 \) and \( \kappa_0 \) are the known background values.

For a medium composed of \( K \) point-like absorbers, the model for the measurements is given by

\[
 B = \underbrace{A \Lambda X}_{U^0_m(r_k) \text{ diag indicator}}.
\]
Multiple signal classification

For an imaging region, we introduce a mesh with \( K \) nodes. Using the point-like absorber model, we approximate measurements by

\[
B = A (\Lambda X).
\]

- Measurements are linear combinations of the columns of the \( M \times K \) matrix \( A \).
- The columns of \( A \) that explain \( B \) correspond to the mesh nodes where there is an object.
- By computing \( B = U\Sigma V^H \) to determine \( P = I - \tilde{U}\tilde{U}^H \), we identify the columns of \( A \) that explain \( B \), and hence determine the mesh nodes where objects are located.

To construct an image, we plot \( \log_{10} [\eta_{\text{min}} / \eta_k] \) where

\[
\eta_k = \|Pa_k\|, \quad k = 1, \ldots, K.
\]
Numerical results
Numerical results
Numerical results
Future considerations

▶ Consider realistic parameter settings and any restrictions on the number of spatial frequencies possible.

▶ Develop algorithms that allow for this method to be used on experimental data.

▶ Develop a resolution analysis for this imaging problem in terms of the key inverse-length scale

$$k_0 = \sqrt{\mu_a/\kappa}.$$  

This imaging method is depth-limited and also size-limited.
Summary

Through these two problems, I have tried to show consistent themes that emerge in my research projects.

- Collaboration.
- Strong connection to experimental science.
- Seek to make progress by combining elements of asymptotics, numerics, modeling, etc.
- Emphasize care and systematic methods, but not necessarily rigor.