RESEARCH SUMMARY

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My recent research interests focus mainly on the following aspects of applied and computational mathematics: (i) inverse problems and imaging, including inverse boundary value problems, multi-physics inverse problems, and imaging in random media; (ii) random graphs, including graph limits, modeling of complex networks, and community detection; (iii) scientific computing, including fast algorithms for PDEs and numerical optimization; and (iv) kinetic modeling and simulation, including wave and paticle transport in complex media, and semiconductor equations.

1 Inverse Boundary Value Problems

Inverse boundary value problems aim at reconstructing coefficients in partial differential equations (PDEs) from the knowledge of over-determined boundary data. These inverse problems find applications in various modern imaging techniques. A prototype of such inverse boundary value problems is diffuse optical tomography (DOT). This is a non-invasive medical imaging modality that uses near infra-red (NIR) light sources to probe physical properties of biological tissues. In a DOT experiment, we send NIR photons into the tissue to be probed, say $\Omega \subseteq \mathbb{R}^d$. We then measure the photon currents that exit the tissue through its surface $\partial\Omega$. From the measurements, we attempt to recover the absorption and scattering properties of the tissue which could provide useful diagnostic information.

The distribution of NIR photon density $u(\mathbf{x})$ in tissue-like media is often modeled by the following linear diffusion equation:

$$\begin{aligned} -\nabla\cdot\gamma\nabla u + \sigma(\mathbf{x})u &= 0, && \text{in } \Omega \\ \mathbf{n}\cdot\gamma\nabla u + \kappa u &= g(\mathbf{x}), && \text{on } \partial\Omega \end{aligned} \tag{1}$$

where γ and σ are respectively the diffusion coefficient (which is related to the scattering property of the medium) and the absorption coefficient of the underlying medium, $\mathbf{n}(\mathbf{x})$ is unit outer normal direction at $\mathbf{x} \in \partial\Omega$, and g models the light source used to illuminate the medium.

Mathematically, diffuse optical tomography can be formulated as an inverse boundary value problem for the diffusion equation (1) that aims at reconstructing the diffusion coefficient γ and the absorption coefficient σ from boundary data given by the operator:

$$\Lambda_{(\gamma,\sigma)} : g(\mathbf{x}) \mapsto J(\mathbf{x}) = \mathbf{n}(\mathbf{x})\cdot\gamma\nabla u(\mathbf{x})_{|\partial\Omega}. \tag{2}$$

This inverse boundary value problem is a slightly more complicated version of the famous *Calderón's problem* in electric impedance tomography (EIT). The problem is mathematically challenging to analyze. Moreover, the problem is "severely ill-conditioned" in general. What this means is that even though the inverse problem may admit a unique solution in certain cases (for instance when $(\sigma, \kappa) = (0, 0)$), when no regularization is applied, noise contained in the measurements will be amplified more than what would result from an arbitrary number of differentiations during the numerical inversion procedure.

In a series of joint works with my collaborators [2, 15, 19, 35, 36, 37], we studied the DOT problem in the radiative transport regime. We developed an inverse transport algorithm based on frequency-domain data. Mathematical and numerical analysis in [18, 34, 38, 40] show that frequency-domain data stabilize the inversion significantly in certain situations, enabling us to reduce the "cross-talk" between the absorption and scattering properties during image reconstructions.

We also studied similar inverse boundary value problems in other imaging applications [5, 6].

2 Hybrid Multi-Physics Inverse Problems

Hybrid inverse problems refer to inverse problems of coupled systems of two or more PDEs of different types. These inverse problems are the mathematical foundations for emerging multi-modality coupled-physics imaging techniques where we combine two imaging modalities based on different physics to obtain the advantages of both. Photoacoustic tomography (PAT) is one of such modalities that combine the high-contrast DOT with the high-resolution ultrasound imaging.

As in the DOT case, we send a pulse of NIR light into a biological tissue. The tissue absorbs part of the incoming light and heats up due to the absorbed energy. The heating then results in the expansion of the tissue and the expansion generates compressive (acoustic) waves. We then measure the time-dependent *acoustic signal*, not the photon currents as in DOT, that arrives on the surface of the tissue.

The same diffusion equation (1) can be taken as the model for light propagation in PAT. The photon energy that is absorbed at location $\mathbf{x} \in \Omega$ per unit volume is the product of the absorption coefficient and the photon density. The heating due to this absorbed energy generates an initial pressure field, denoted by H, that is of the form:

$$H(\mathbf{x}) = \Xi(\mathbf{x})\sigma(\mathbf{x})u(\mathbf{x}) \tag{3}$$

where the positive function $\Xi(\mathbf{x})$ is the nondimensional Grüneisen coefficient that measures the photoacoustic efficiency of the tissue. The initial pressure field H then propagates according to the acoustic wave equation, with the wave speed $c(\mathbf{x})$,

$$\begin{aligned} \frac{1}{c^2(\mathbf{x})}\frac{\partial^2 p}{\partial t^2} - \Delta p = 0, \qquad & \text{in } \mathbb{R}_+ \times \mathbb{R}^d \\ p(0, \mathbf{x}) = H(\mathbf{x}), \quad \frac{\partial p}{\partial t}(0, \mathbf{x}) = 0 \quad & \text{in } \mathbb{R}^d. \end{aligned} \tag{4}$$

The objective is to reconstruct the coefficients γ, σ and Ξ from acoustic measurements, that is:

$$\Lambda_{(\gamma,\sigma,\Xi)} : g(\mathbf{x}) \mapsto p(t,\mathbf{x})_{|(0,T]\times\partial\Omega}. \tag{5}$$

We studied in [9, 10, 39] the quantitative step of the inverse problem. We showed that if one of the coefficients in (γ,σ,Ξ) is known, then the other two can be reconstructed uniquely with Lipschitz type of stability with internal data H collected from two illuminations g_1 and g_2. Moreover, we can construct an explicit reconstruction procedure, which only requires solutions of a transport equation with known vector field (given by the data) and a diffusion equation with known coefficients, to solve the nonlinear inverse problem. We showed that one can reconstruct all three coefficients (γ,σ,Ξ) simultaneously, again in a unique and stable way, with multi-spectral data, that is data collected from illuminations of different wavelengths [11]. These results are recently generalized in [29] to the radiative transport model in both the non-scattering regime with two illuminations, for applications in sectional PAT. In fact, we can simultaneously reconstruct the optical coefficients and the ultrasound speed under some additional constraints [16, 17, 45].

If we replace the NIR illumination source with microwave source in PAT, we obtain a hybrid imaging modalities that is often called thermoacoustic tomography (TAT). The propagation of microwave in tissue is described by the Maxwell's equation:

$$\begin{array}{ll} -\nabla\times\nabla\times\mathbf{E} + k^2\mathbf{E} + ik\mu(\mathbf{x})\mathbf{E} = 0, & \Omega \\ \mathbf{n}(\mathbf{x})\times\mathbf{E} = \mathbf{g}(\mathbf{x}), & \partial\Omega. \end{array} \tag{6}$$

The initial pressure field generated in this case is of the form

$$H(x) = \Xi(\mathbf{x})\mu(\mathbf{x})|\mathbf{E}|^2(\mathbf{x}). \tag{7}$$

The pressure field propagates following the same acoustic wave equation (4).

In [12] we proved the uniqueness of reconstructing the conductivity μ (assuming $\Xi = 1$) in quantitative TAT (QTAT) and showed that the inverse problem is stable in Lipschitz sense. We proposed a fixed point algorithm for the reconstruction of μ.

We propose recently to combine the classical fluorescence tomography with ultrasound tomography to obtain another hybrid imaging modality: fluorescence photoacoustic tomography (fPAT) [44, 42]. We also developed, along the same lines, two-photon PAT [13, 41], a PAT modality intends to image the two-photon absorption coefficient of tissue-like heterogeneous media.

3 Imaging in Random Media

Imaging in complex random media is a topic that is closely related, but also significantly different from, the inverse coefficient problems in DOT and PAT. The objective of imaging is to find scattering targets or emitting sources in (potentially unknown) complex media.

A prototype of the imaging problem can be described as follows. Let Ω be a target that is buried in a complex medium $V(\mathbf{x})$. We send electromagnetic waves into the medium and collect scattered waves at different locations. Let $u^i(\mathbf{x})$ and u^s be the incident wave field and u^s be the scattered wave field, then the total field $u = u^i + u^s$ solves the Maxwell equation which reduces to the Helmholtz equation in many practically relevant situations:

$$\Delta u + k^2(1 + V(\mathbf{x}))u = 0 \quad \text{in} \quad \mathbb{R}^d \backslash \Omega. \tag{8}$$

The scattered wave field has satisfy the radiation condition:

$$\lim_{r \equiv |\mathbf{x}| \to \infty} r^{\frac{d-1}{2}} \left(\frac{\partial u^s}{\partial r} - iku^s\right) = 0. \tag{9}$$

Depending on the properties of the target, appropriate boundary conditions have to be described on $\partial\Omega$.

In [7, 3], we consider the imaging problem in the regime where there are significant amount of multiple scattering between waves and the underlying medium so that the phase information carried in the waves is already lost by the time these waves arrive at the detectors. In this case most of the currently available techniques that make use of coherent wave information suffers in efficiency. We propose an imaging method that use *incoherent* data to reconstruct a few characteristics of the targets. Our method is based on the fact that the propagation of wave energy in such heterogeneous media follows a transport equation whose coefficients only depend on the statistics, not on individual realizations, of the media. The imaging problem is thus replaced by a parameterized inverse transport problem. Numerical inversions are based on the following least-square minimization procedure. Let $\mathcal{F}$ be a family of parameters we want to reconstruct. We define the minimization problem as:

$$\mathcal{F}_b = \arg \min_{\mathcal{F} \in \Pi} \mathcal{O}(\mathcal{F}) \tag{10}$$

where $\Pi = [\mathcal{F}_{min}, \mathcal{F}_{max}]$ is a family of box-constraints. The objective function is given by:

$$\mathcal{O}(\mathcal{F}) = \frac{1}{2} \sum_{i=1}^{I} \sum_{j=1}^{J} |E_t^{i,j} - E_w^{i,j}|^2, \tag{11}$$

where $E_t^{i,j}$ is the prediction of received wave energy calculated with the energy transport equation for source i on detector j, and $E_w^{i,j}$ is the corresponding experimental measurement. Reconstruction based on synthetic and real experimental measurement show that the proposed method works well in many situations.

In the above imaging method, the statistical properties (such as its transport mean free path) of the underlying medium are assumed fully known. Even though these are sufficient for the imaging method to work, the random fluctuations of the medium can still have an impact on the imaging result. In [8], we analyze this impact in a slightly different setting and proposed a computational strategy to minimize the impact. In simplified situations, such as the case of imaging point sources in unknown media [46], we were able to characterized precisely the impact of the uncertainty in the medium on the imaging results.

4 Kinetic Modeling and Simulations

Kinetic equations and systems often appear as mathematical models for collection behavior of large particle systems. For instance, it is often believed that the radiative transport equation is an accurate model for describing light propagation in biological tissues. Therefore, the equation is often used in inverse problems in DOT and PAT that we described in the previous sections.

We performed systematic numerical studies on the propagation of photon density waves in heterogeneous media in [1, 36] for applications in frequency-domain DOT. We proposed efficient computational algorithms for solving the related kinetic models for such wave propagation problems.

In [4, 6], we studied the problem of propagation of photons in highly scattering media with non-scattering regions. We showed that classical macroscopic description of the propagation fails in this case with extended void regions. Instead we derived a generalized macroscopic diffusion model in which we model the extended void regions as an interface on which a tangential diffusion process is supported. The model we derived is computationally as cheap as the classical diffusion model but is significantly more accurate.

In [3, 7] we studied the problem of propagation of high-frequency acoustic/electromagnetic waves in discrete random media. We considered the regime where there are significant amount of multiple scattering between waves and the underlying medium. In this case, the phase of the wave field contains mainly information of the multiple scattering due to the random media, and thus is not a robust quantity to be useful in applications. In stead, wave energy density is a more robust quantity. We showed that the wave energy density actually solves a kinetic equation whose coefficient are determined by low-order statistics of the random media.

In [14], we studied the transport of electrons and holes in semiconductor devices for applications in device optimization and design. We studied the problem of doping profiling where the aim is to recover doping profiles of devices from current-voltage characteristics of the devices. We proposed several numerical strategies to solve the Boltzmann-Poisson transport equation and the related design/inversion problem. We later generalized the ideas in [20, 21] to study the transport of charged particles in semiconductor-electrolyte solar cells, aiming at improving the efficiency of the cell through computational optimization of the charge transport process.

5 Fast Algorithms in Scientific Computing

One of the recent exciting developments we were able to make was on an integral equation based fast algorithm for linear kinetic equations of radiative transport type. A prototype of such equations can be written as:

$$\begin{aligned} \mathbf{v}\cdot\nabla u+\sigma(\mathbf{x})u &= \sigma_s(\mathbf{x})\int_{\mathbb{S}^{d-1}} K(\mathbf{v},\mathbf{v}')u(\mathbf{x},\mathbf{v}')\mathrm{d}\mathbf{v}', \quad \text{in } \ \Omega\times\mathbb{S}^{d-1} \\ u &= f(\mathbf{x},\mathbf{v}), \qquad\qquad\qquad\qquad\qquad \text{on } \ \Gamma_- \end{aligned} \tag{12}$$

where $\mathbb{S}^{d-1}$ is the unit sphere in $\mathbb{R}^d$, $d\mathbf{v}$ is the normalized surface measure on $\mathbb{S}^{d-1}$, and $K(\mathbf{v},\mathbf{v}')$ is the scattering phase function that describes the way that particles traveling in direction $\mathbf{v}$ getting scattered into direction $\mathbf{v}'$. The boundary sets $\Gamma_\pm$ are defined as $\Gamma_\pm = \{(\mathbf{x},\mathbf{v}) \in \partial\Omega\times\mathbb{S}^{d-1} \text{ s.t. } \pm\mathbf{v}\cdot\mathbf{n}(\mathbf{x})>0\}$ with $\mathbf{n}(\mathbf{x})$ the unit outer normal vector at $\mathbf{x}\in\partial\Omega$.

Due to the fact that such equations are posed in phase space (and thus is high-dimensional), it is computationally extremely challenging to solve the equations. In [43], we propose a fast multipole based algorithm for solving (12) when $K = 1$. Our method is based on a novel integral formulation of the equation. The integral formulation allows us to solve for macroscopic quantities directly without having to resolve the structure of the solution in the velocity variable. Numerical tests show that this new algorithm can easily be two order faster than exists algorithms in the field. Moreover, the new algorithm can be easily implemented into optimization or inversion calculations for kinetic models that we have recently developed [15]. We are currently trying to generalize our method for similar equations with anisotropic but symmetric scattering kernel K. In this case, we can use even parity formalism to derive integral representation of the solution to the kinetic equation which can then be efficiently solved using the idea in [43].

Another fast numerical algorithm we were able to develop recently is method for solve the linearized Poisson-Boltzmann equations that arise in mathematical models for the electrostatics of molecules in solvent [49]. This method use an implicit surface representations with an implicit boundary integral formulation to derived a linear system defined on Cartesian nodes in a narrowband surrounding the closed surface that separate the molecule and the solvent. The needed implicit surfaces is constructed from the given atomic description of the molecules, by a sequence of level set algorithms. We then use the fast multipole method to accelerate the solution of the linear system.

6 Random Graphs and Complex Networks

Modeling of large complex networks has a lot of practical applications. The subject has attracted tremendous amount of attention in recent years. One important inverse problem in the study of complex networks is to infer the structure of a network from some measured data on quantities, such as sub-network densities, related to the network.

We study recently this inverse problem assuming that we have data on certain sub-network (for instance, edge, two star, and triangle) statistics. To be a little more precise, consider a simple (i.e. vertices are distinguishable, edges are undirected, and there is no loops or multiple edges) and dense random network on n vertices. We could have at most $\binom{n}{2}$ edges, and $\binom{n}{3}$ triangles. Let $e := \frac{\text{\# of edges}}{\binom{n}{2}}$ and $t := \frac{\text{\# of triangles}}{\binom{n}{3}}$ be the edge and triangle densities in a network of n vertices. If we are given the edge density, say $e = \varepsilon$, and the triangle (or any other sub-network) density, say $t = \tau$, can we know the structure of the network?

In a series of joint work with my collaborators [22, 23, 24, 30, 32, 31], we partially answered the question. Roughly speaking, for truely large networks, if the edge-triangle (or edge-two-star) density datum is away from the datum predicted by the Erdős-Rényi network model, the datum uniquely determines the global structure of the network. More precisely, we proved in [23], in the case of edge-two-star density datum, that the graphs with the given density datum are all "multipodal": asymptotically in the number of vertices there is a partition of the vertices into $M < \infty$ subsets $V_1, V_2, \ldots, V_M$, and a set of well-defined probabilities g_{ij} of an edge between any $v_i \in V_i$ and $v_j \in V_j$. In fact, this remarkable feature of multipodality appears also in large random networks constrained by other subgraph densities. We showed in [22] that for an arbitrary fixed subgraph H, for all but finitely many values of the edge density, if the density of H is constrained to be slightly higher than that for the corresponding Erdős-Rényi graph, the typical large graph is bipodal with parameters varying analytically with the densities. Asymptotically, the parameters depend only on the degree sequence of H. In other words, the bipodal structure is kind of "universal" in large random networks with given edge-H density.

Our extensive numerical simulations and asymptotic analysis in [30, 32] shows that in fact, the number of podes in each of the multipodal structures that we mentioned above remains very small for a wide range of edge-H density values. This suggests that large network of this type can be described accurately with a small number of parameters, a feature that we are using right now for community detection in large dense complex networks.

7 Multiscale Analysis and Fluid Dynamics

In the earlier days of my career, I have done some research on multiscale analysis of nonlinear dynamical systems and fluid dynamics. Results of these analysis can be found in [25, 26, 27, 28, 47, 48, 50]. I remain interested in this fascinating subject.

Let $s(t)$ be a given sequence indexed by t coming out of a stochastic dynamical system. We define the so-called structure function $d_l(t) = s(t+l) - s(t)$ at scale l. We are interested in how the probability distributions and statistical behavior of $d_l(t)$ scale as a function of l. Intuitively, if $s(t)$ is a Brownian motion, then $d_l(t)$ follows the Gaussian distribution with variance scale linearly with l. For general $s(t)$, the behavior of $d_l(t)$ characterize the deviation of $s(t)$ from Brownian motion. In most cases, this deviation happens at the tails of the distribution function, which means that events of large amplitude but small probability actually play central roles in the statistical properties [26] of the system. We observe very similar structures in velocity fields of turbulent fluids in Taylor-Couette flow and wake flows [47, 50], nucleotides density profiles of DNA sequence [48] as well as solutions of other nonlinear dynamical systems [33]. These multiscale analysis in fact provided additional information for some phase space reconstruction problems in nonlinear dynamics [27]. They also enabled us to establish a relationship between wavelet transform and invariant measure of iterated function systems (IFS) [28] and to find homoclinic solutions (basically solitons) to many functional equations [25, 27].

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