RESEARCH STATEMENT

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A dominant theme in my work is the development of numerical methods for the solution of the partial differential equations (PDEs) of mathematical physics using integral equation-based methods. Some of the prominent problems in this area are: the selection of suitable integral representations, the development of fast solvers for inhomogeneous PDEs in complex geometries, the analysis of elliptic PDEs on regions with geometric singularities, and the analysis and evaluation of eigenfunctions of differential operators. It has become more and more clear since the advent of analysis based fast algorithms that the fastest and most efficient numerical solvers will be the ones that take advantage of the detailed analytical structure of the underlying equations. Thus, two central themes of my research are (a) advancing the development of black-box solvers in highly complicated environments and (b) revealing new analytic features of the solutions to the PDEs of mathematical physics.

Over the last three decades, integral equation methods have become powerful tools for the numerical solution of PDEs, owing primarily to the development of well-conditioned integral representations, efficient quadrature formulas for their discretization, and fast multipole based algorithms for the obtained dense linear algebraic systems. The resulting solvers have CPU time complexity that grows linearly (or almost linearly) with the number of unknowns. These "fast" algorithms have vastly increased the scale and complexity of problems which can be analyzed numerically, and have had a significant impact in a wide variety of applications: chip design, radar cross-section analysis, design of acoustic and audio equipment, the study of colloidal suspensions, etc. (see, for example, [1, 2, 3]). However, well-conditioned integral formulations for many equations are notably absent from the classical theory, and one of the directions of my research is the construction of such representations (see, for example, [4, 5, 6, 7, 8]).

Even with stable integral formulations, the development of fast and robust numerical solvers for complex geometries in two and three dimensions presents a number of challenges. While the existing fast methods scale almost linearly in the number of degrees of freedom, the associated constants tend to be large, especially in three dimensions. Automatically adaptive methods that resolve the complexity of the geometry and the input data (material properties, volume densities, and boundary conditions) have yet to be designed and implemented. The same is true when seeking to evaluate singular or nearly singular integrals robustly and to high order accuracy. One focus of my research is the development of a new approach, called "quadrture by expansion" (QBX), which exploits the smoothness of the induced field and carefully chosen expansion centers located off surface. QBX produces accuracy that turns out to be surprisingly insensitive to the geometry (see, for example, [9, 10, 11]).

At present, integral formulations for the solution of elliptic PDEs on regions with geometric singularities (corners, edges, etc.) rely on hierarchical refinement towards the singularity combined with numerical compression. This approach is viable, but tends to be very expensive in three dimensions. Surprisingly, the analysis of the densities which emerge as solutions to integral equations has received relatively little attention. Recently, K. Serkh and I observed that the densities corresponding to solutions of the biharmonic equation on regions with corners can be represented by rapidly convergent series of explicitly determined elementary functions; these expansions seem to have been overlooked in the classical literature [12]. A focus of my research is the development of such explicit analytical representations for various elliptic PDEs (Laplace, Helmholtz, Stokes,

Maxwell, etc.), and their application to the development of highly accurate and fast numerical solvers on domains with geometric singularities.

In addition to the solution of linear PDEs in complex geometry, my recent work deals with the localization behavior of ground-state (low frequency) eigenfunctions of elliptic differential equations. The problem naturally arises in several fields, including the study of vibrating membranes, spectral clustering, and quantum mechanics; the analysis of the detailed behavior of these eigenfunctions is an active area of research. In a joint paper with S. Steinerberger, we prove a universal bound for the distance of the maxima to the boundary for Schrödinger type equations (the Laplace and Helmholtz equations are a special case) [13]. Subsequently, we observe that, surprisingly, these methods also extend to the analysis of spectral clustering algorithms [14]. A focus of my research is to further extend our analysis to more general classes of elliptic PDEs (including non-linear ones), and develop numerical tools for the evaluation of eigenfunctions.

Finally, some of my research involves computational biology and applications to biomedicine. With J. Pulupa, J. Mincer, M. Tomasini, and S. Simon at Rockefeller University, we have designed efficient numerical algorithms for coarse grained dynamics of the nuclear pore complex [15]. I am also developing fast algorithms for the visualization of single-cell mRNA data in collaboration with Y. Kluger and G. Linderman at the Yale Medical school.

In the sections below, I elaborate on several of my recent and ongoing projects.

1. Boundary integral representations

Until recently, numerical solutions of PDEs were computed almost exclusively via direct discretizations of the differential operators (finite difference methods, finite element methods, etc.). Over the last three decades, the use of integral equations for the numerical solution of PDEs has rapidly increased—in part due to the development of fast multipole methods for handling the resulting dense linear systems. Carefully designed integral equation methods result in well-conditioned linear systems, where the condition number does not grow as the mesh is refined. The combination of well-conditioned integral equations, high-order discretizations, and fast algorithms often results in extremely fast and highly accurate numerical tools for the solution of PDEs. Surprisingly, for many physical applications, well-conditioned integral equations are not available from the classical theory.

In viscous flow, the mobility problem consists of determining the translation and rotation velocities of rigid bodies for which the forces and torques are prescribed. The existing integral formulations, while allowing for the accurate solution of the mobility problem, result in significant loss of accuracy for computing fluid stresses, since they necessitate the evaluation of hyper-singular integrals. In a series of papers with E. Corona, L. Greengard, and S. Veerapaneni, we derived well-conditioned integral representations for mobility problems in two and three dimensions which encounter none of these difficulties [4, 5]. The fluid stresses in our representations require the evaluation of singular integrals, as opposed to hyper-singular integrals. We use an essentially identical approach to the elastance problem in electrostatics, which consists of determining the potential on perfect conductors given the net charge on each conductor.

The biharmonic equation with Dirichlet boundary conditions arises naturally in the study of thin elastic plates. Direct discretization of the differential equation poses several numerical challenges, since the condition number of the discretized linear systems grows like $O(\frac{1}{h^4})$, where h is the grid spacing. Existing integral representations also encounter difficulties: they are not applicable to multiply connected regions, and the resulting integral equations are ill-conditioned on regions whose boundaries have high curvature. In a paper [7], with T. Askham, we address both of these difficulties by developing a novel integral representation based on the Sherman-Lauricella representation for Stokes flow. We prove the invertibility of the representation for multiply connected domains and develop numerical solvers capable of achieving machine precision accuracy even on regions with extremely high curvature (see fig. 1).

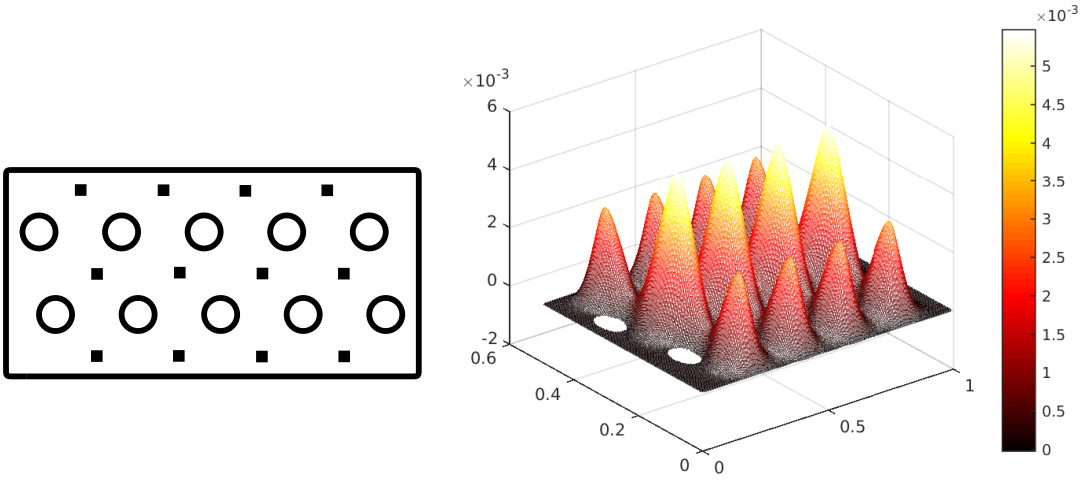

FIGURE 1. The solution of biharmonic equation with zero Dirichlet boundary conditions in a multiply connected region due to point forces at the squares.

Even with ideal integral representations, many PDEs are physically ill-conditioned in environments involving difficult geometries (for example, close-to-touching scatterers). In such cases, iterative schemes for solving the resulting integral equations tend to perform poorly. On the other hand, fast direct solvers (as opposed to iterative ones) have evolved rapidly over the last decade to solve various ill-conditioned boundary value problems, however, these solvers are often memory intensive, particularly in three dimensions. It turns out that, in this environment, efficient preconditioners can be obtained by computing inverses of smaller subproblems using fast direct solvers. The resulting preconditioned iterative schemes often have significantly lower memory requirements, and converge in a much smaller number of iterations. This work is currently in progress in collaboration with L. Greengard and A. Rahimian.

2. Fast and robust solvers for inhomogeneous elliptic PDEs in complex geometries

The solution of inhomogeneous elliptic PDEs via integral equation methods usually proceeds in two steps. First, the free space Green's function is convolved with the volume density and then boundary conditions are corrected using boundary integral methods. A persistent difficulty in the practical application of this procedure is its demand for accurate, robust, and efficient evaluation of boundary layer potentials everywhere in the volume, including targets very close to boundary. Current methods tend to be computationally expensive in three dimensions and, more importantly, there has been very little work on coupling these methods with fast algorithms in a manner that guarantees high-order accuracy, independently of the complexity of the geometry or the regularity of the discretization.

Targets close to the boundary present a different challenge than on-surface targets: the corresponding integrals are computable, e.g. by adaptive quadrature, but maintaining efficiency has proven nontrivial. Quadrature by expansion (QBX), is a recent approach which uses the one-sided smoothness of the layer potentials to create local expansions centered off the boundary; these expansions can be accurately evaluated both near and on the boundary. In theory, QBX can achieve high-order accuracy at targets anywhere in the volume. In joint work with A. Klöckner and M. O'Neil, we have made QBX into a viable numerical tool capable of accurately evaluating boundary layer potentials, scalably, anywhere in space, in a black-box fashion [10].

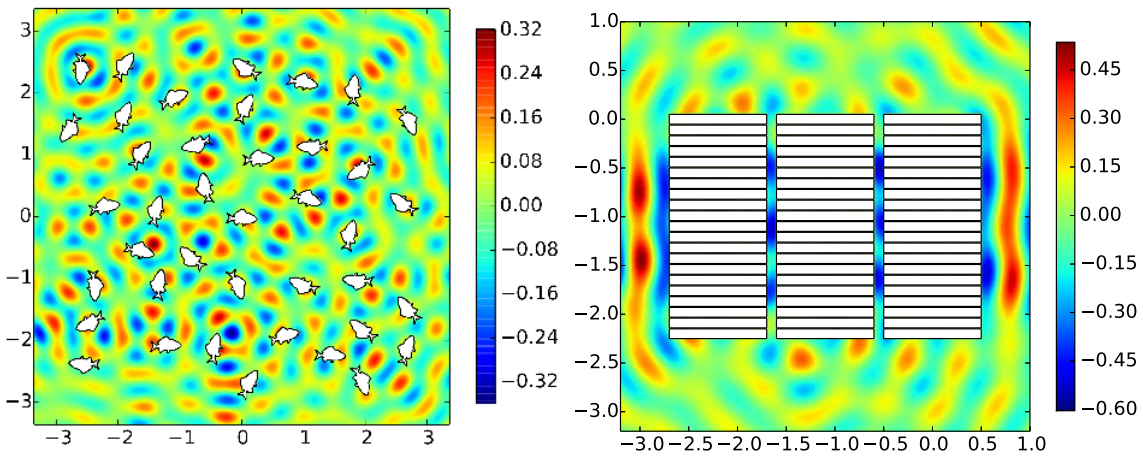

FIGURE 2. Solutions to the Helmholtz equation evaluated using QBX with error less than 10^{-12} everywhere in the volume. The spacing between the capacitor plates on the right is $\lambda/50$ where λ is the wavenumber.

In two dimensions, many existing solvers address the evaluation of volume and layer potentials in a fully adaptive manner, but few such tools exist for analogous problems in three dimensions. Along with T. Askham, Z. Gimbutas, L. Greengard, L. Imbert-Gerard, M. O'Neil, and F. Vico, we are developing adaptive, fast, high-order accurate numerical tools for Laplace, Helmholtz, Stokes, and Maxwell volume and layer potentials for complex geometries in three dimensions. Our work in this area is focused on addressing the following issues: accelerating the far-field computation for the Helmholtz volume and layer potentials; designing special purpose fast multipole methods for Maxwell potentials based on "generalized Debye" representations for the electric and magnetic fields; and reducing the memory requirements of the near-field quadrature computation which tends to be memory intensive, especially in three dimensions.

3. Elliptic PDEs on regions with geometric singularities

The numerical solution of elliptic PDEs on regions with geometric singularities (corners, edges, etc.) has been a notoriously refractory problem. Recently, integral equation methods have been successfully used in this environment, due to the fact that the condition numbers of the resulting discretized linear systems are essentially independent of the number of degrees of freedom. The development of these highly accurate and efficient numerical solvers has largely relied on adaptive refinement followed by numerical compression. While this approach is effective in two dimensions, the additional degrees of freedom required to compute the solution tend to be problematic in three dimensions. It turns out that if enough is known about the analytical behavior of the solution near the geometric singularities, then the required number of degrees of freedom can be made surprisingly small. However, the analytical apparatus for this is largely absent in the classical theory.

The biharmonic equation on regions with corners, for example, has been traditionally difficult to analyze. On two-dimensional regions with corners, the biharmonic Green's function has been conjectured to have infinitely many oscillations in the vicinity of the corner [16]. The complicated structure of the biharmonic Green's function emerges, in part, due to the fact that the governing equation does not satisfy a maximum principle. The solutions to the associated integral equations have a similarly complicated analytical structure, which has been largely unknown.

In a paper with K. Serkh, we demonstrate that on polygonal domains, the solution has a surprisingly straightforward and explicit analytical representation near corners [12]. In particular, the solutions are expressible as rapidly convergent series consisting of functions of the form t^{z_j}, where

z_j's are complex, and depend on the angle at the corner. While the general approach is similar to the analysis of the Laplace and Helmholtz case, the structure of the singularities for the biharmonic equation is significantly more intricate [17, 18]. We use the explicit series representation to construct (albeit using fairly modern techniques [19]) highly efficient special purpose discretizations and associated quadrature formulas. We solve the biharmonic equation on polygonal domains to nearly machine precision, using a small number of degrees of freedom in the vicinity of corners.

In three dimensions, the numerical solution of elliptic PDEs and corresponding integral equations on regions with geometric singularities is further complicated due to the singular behavior of the solution along the edges. The apparatus in two dimensions admits a generalization to surfaces with edge singularities where the surface subtends at a constant angle along the edge. The generalization to case of edges with more complicated geometric structure is work in progress, in cooperation with J. Hoskins, V. Rokhlin, and K. Serkh.

4. Eigenfunction analysis and evaluation

The localization behavior of eigenfunctions of elliptic PDEs is practically significant, but has been largely resistant to analysis. In joint work with S. Steinerberger, we prove that solutions to Schrödinger type equations cannot achieve their maximum and minimum values close to the boundary, unless the $\mathbb{L}^\infty$ norm of the Schrödinger operator is large [13]. Using the stochastic interpretation of Schrödinger's equation via the Feyman-Kac formula, we derive universal estimates for the likelihood of the first exit time for Brownian paths starting at the location of maxima. We also prove a related result demonstrating that the torsion function is very strongly correlated with the first eigenfunction of the domain. It has been observed previously that the location of maxima of the torsion function and the first eigenfunction tend to be extremely close on convex domains [20]. While this observation is not true for generic simply connected domains, we prove the existence of a universal constant c such that for every simply connected region, the torsion function v satisfies the inequality, $v(x_0) > c \max |v(x)|$, where x_0 is the location of the maximum of the first eigenfunction.

The discrete analogue of the analysis above is related to spectral embeddings for the classification of large datasets. In joint work with X. Cheng and S. Steinerberger, we show that spectral clustering algorithms preserve certain aspects of the geometry of the clustered data [14]. We observe that the eigenfunctions of the graph Laplacians on directed graphs are strongly correlated to the diffusion distance from the bottlenecks in the graph.

Oftentimes, computing eigenfunctions and corresponding eigenvalues to high accuracy in simple geometries can provide valuable insight into their analytical behavior under more general conditions. The calculation of eigenfunctions involves the solution of elliptic PDEs near resonances, which poses several challenges for their fast and accurate evaluation. In [13], we use randomized algorithms to regularize the eigenvalue problem and reduce it to related non-singular problems. We intend to extend this approach to enable the stable and fast evaluation of eigenfunctions and eigenvalues in a black-box manner.

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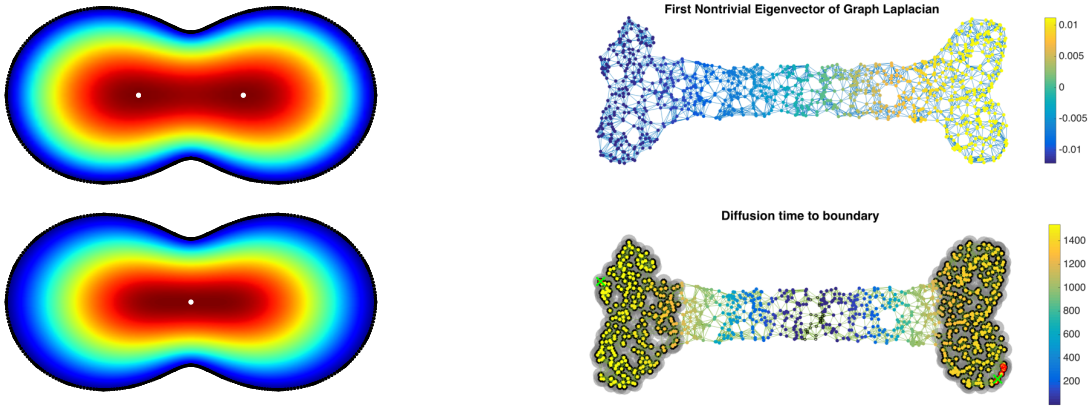

FIGURE 3. (left) The correlation between the torsion function (top) and the first harmonic eigenfunction (bottom). The white dots indicate the location of the maxima of the functions. (right) The correlation between the diffusion time to the boundary and the first eigenvector of the graph Laplacian.

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