Research statement and plans — Alex H. Barnett, November 2013

My research group and I create new numerical algorithms that enable the solution of challenging linear partial differential equation (PDE) problems efficiently, robustly, and to high accuracy. Our recent focus is on wave scattering and eigenvalue (resonance) problems in complex geometries such as periodic light-guiding structures, or at very high frequencies. The PDE in question is usually some variant of the Helmholtz equation

$$(\Delta + \omega^2)u \ = \ 0 \qquad \text{in } \Omega \subset \mathbb{R}^d, \qquad d = 2 \text{ or } 3 \tag{1}$$

where Δ is the Laplacian, $\omega > 0$ the frequency, and Ω an interior or exterior domain with boundary $\partial\Omega$, on which various boundary conditions are enforced. Our tools—potential theory, integral equations, analytic and other basis set expansions, compression of low-rank operators, quadratures—have in common *high-order accuracy* (i.e. extremely rapid convergence of errors), and *rigorous mathematical foundations.* In several cases myself and collaborators are responsible for the latter, using PDE, microlocal, complex, and functional analysis.

The application areas are broadly in wave devices, nano-optics, and quantum physics, including radar, acoustics, imaging, gratings, photonic crystals, solar cells, resonators and filters, and questions in mathematical physics. Many digits of accuracy—beyond the 1-2 digits common in engineering codes using finite elements (FEM) or finite differences (FD)— are crucial for applications such as: systems close to resonance, field singularities, assessing sensitivity with respect to geometry, and device design and optimization. In most cases we achieve 10 or more digits of accuracy without sacrificing efficiency. In two distinct practical settings we achieve around a factor 10^3 faster computation than the existing state-of-the-art algorithms on the same CPU.

Our work blends new algorithms, analysis, documented software, and applications, often in a single publication. A significant fraction is interdisciplinary, collaborating with biologists, engineers, pure mathematicians, and musicologists.

1 Wave scattering: computational acoustics and electromagnetics

Here I overview our recent progress, and future directions, in solvers for Helmholtz-type boundary-value problems.

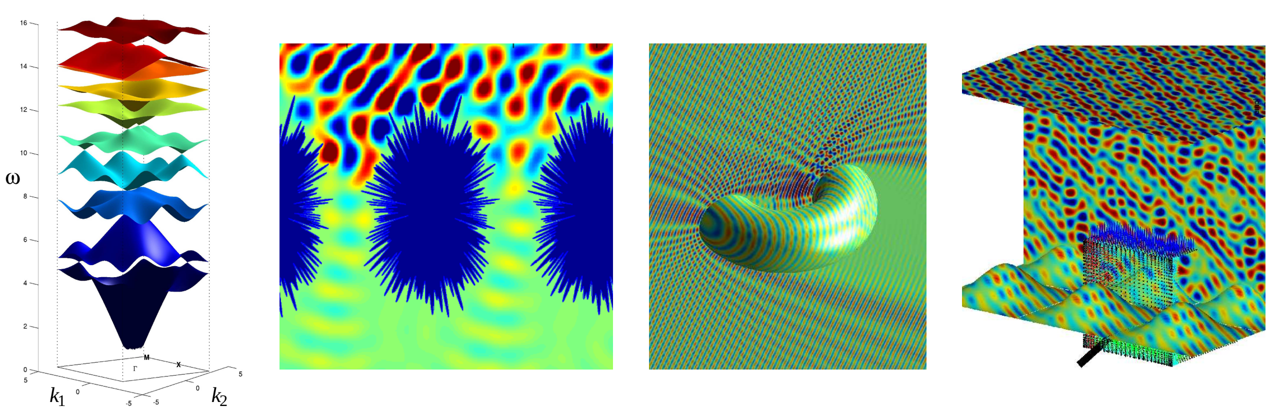

Figure 1: Left to right: (a) Band structure of 2D dielectric photonic crystal, error 10^{-9}, 30 mins CPU time (laptop). (b) Scattering from 2D diffraction grating of Dirichlet obstacles demanding $N = 10^5$ boundary unknowns (two periods shown), error 10^{-10}, 600 times faster than GMRES plus fast multipole method. (c) Sound-soft 3D acoustic scattering from torus 30λ in size using QBX, error 10^{-5}, 2 hrs. (d) 3D acoustic scattering from doubly-periodic bumpy surface, period 8λ, error 10^{-6}, 8 mins (also shown: unit cell collocation points).

1.1 Corner singularities, accurate field evaluations, inhomogeneous media

Boundary value problems and particular solutions. Wave scattering at a fixed frequency ω from the exterior Ω of an obstacle with boundary $\partial\Omega$ is described in 2D (or z-invariant 3D) by

$$(\Delta + \omega^2)u = 0 \quad \text{in } \Omega, \qquad u = -u^{\text{inc}} \quad \text{or} \quad u_n = -u_n^{\text{inc}} \quad \text{on } \partial\Omega, \qquad \frac{\partial u}{\partial r} - i\omega u = o(r^{-1/2}) \tag{2}$$

where u^{inc} is the incident wave, u the scattered wave, and the total (physical) field is $u^{\text{tot}} = u + u^{\text{inc}}$. Here $u_n := \partial u/\partial n$, and $r := |\mathbf{x}|$. Corners in $\partial\Omega$ induce singularities in u which make a high-accuracy solution challenging with finite elements (and especially with finite difference methods popular with engineers). In work with Timo Betcke (UCL) [15][1] we split Ω into subdomains, one for each corner, and exploit an analytic expansion of the local polar form $u^{\text{tot}}(r,\theta) = \sum_{m=1}^{\infty} c_m J_{m\alpha}(\omega r)\sin m\alpha\theta$ in each subdomain; this assumes corners are locally wedges of angle α. This is the *method of particular solutions* (MPS): we set up a linear system to impose continuity of values and derivatives at subdomain boundaries, using the *method of fundamental solutions* (MFS) [13] to impose the radiation condition, and use a dense least-squares solve. We handle complex geometries with Dirichlet and Neumann boundary conditions, with errors around 10^{-10} for domains with around 10 corners, and prove exponential convergence: doubling the number of unknowns N doubles the number of correct digits.

Remark 1 *The schemes I develop are efficient because only boundaries are discretized, rather than the entire domain as with conventional FEM or FD solvers. This reduction by one of the dimensionality of the problem means that N is much smaller (10^3, say, rather than 10^6). Radiation conditions are automatic, so no artificial absorbing boundaries (PMLs) are needed as for FEM/FD. At high ω, $N = O(\omega^{d-1})$ rather than $O(\omega^d)$, a huge advantage that allows scattering problems hundreds of wavelengths in size to be solved on a laptop in a minute.*

Integral equations. We overview another approach to scattering (2) sharing the advantages of high-order accuracy, and efficient boundary representation. Recall the fundamental solution (Green's function) for (1),

$$G_\omega(\mathbf{x},\mathbf{y}) = \frac{i}{4}H_0^{(1)}(\omega|\mathbf{x}-\mathbf{y}|), \quad \mathbf{x},\mathbf{y} \in \mathbb{R}^2 , \qquad \text{or} \qquad G_\omega(\mathbf{x},\mathbf{y}) = \frac{e^{i\omega|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}, \quad \mathbf{x},\mathbf{y} \in \mathbb{R}^3 . \tag{3}$$

The scattered wave is then represented by a layer potential on $\partial\Omega$, such as (choosing a simple case),

$$u(\mathbf{x}) = (\mathcal{D}_\omega \tau)(\mathbf{x}) := \int_{\partial\Omega} \frac{\partial G_\omega(\mathbf{x},\mathbf{y})}{\partial n_{\mathbf{y}}}\tau(\mathbf{y})ds_{\mathbf{y}}, \qquad \mathbf{x} \in \Omega. \tag{4}$$

Applying, for instance, the Dirichlet boundary condition and *jump relations* turns this into integral equation for the unknown ('density') function τ, of the Fredholm 2nd kind,

$$(\tfrac{1}{2}I + D_\omega)\tau = -u^{\text{inc}} , \tag{5}$$

where D_ω is the 'double-layer operator' (the restriction of $\mathcal{D}_\omega$ to $\partial\Omega$). The 2nd-kind form guarantees that it is *well-conditioned*; this cannot be said of FEM or FD solvers, nor of the MPS. 2nd-kind formulations also exist for Neumann, transmission and other problems. Upon discretization, the system matrix is again dense, but now an iterative solution (via GMRES) is often practical, and by using fast multipole acceleration (FMM) to apply the matrix-vector products, one achieves $O(N)$ solution time. N up to the billions have been solved in this way. However, for such ideas to be widely applied, many technical challenges remain. This motivates much of my recent and ongoing work.

Accurate quadrature and near-field evaluations. One persistent problem, caused by the *singularity* in the kernel (3), is that special singular quadratures [23] are needed to discretize (5) to high order, by, e.g., the Nyström method, and to evaluate the representation (4) *close to the boundary* $\partial\Omega$. Existing high-order methods (e.g. Bruno–Kunyansky or Bremer polar transformations) are especially CPU-intensive in 3D, needing interpolation onto a new polar grid for each target node. In 2011 I devised a simple new local-expansion scheme [24] for near-boundary evaluation, with proven exponential convergence for the 2D Laplace case, and analyzed the quadrature evaluation error of (4) for the first time. In this scheme, a single refinement step from N nodes

[1] references are to works as numbered in my CV.

to roughly $4N$ achieves machine precision accuracy in field evaluations arbitrarily close to $\partial\Omega$. In collaboration with Klöckner, Greengard, and O'Neil, we applied this to create a panel-based Nyström method *free of singular quadratures* [21], known as QBX. A big advantage is that the scheme generalizes simply to 3D: Fig. 1c shows my implementation of QBX in 3D acoustic scattering from a smooth torus with $N = 145000$: the quadrature costs about the same time as 50 GMRES iterations using the Helmholtz FMM [27]. Our future plans are:

- extending the QBX quadrature scheme to handle high aspect ratio panels in 3D
- combination of QBX with fast direct solvers in 3D (with Adrianna Gillman)
- handling edges and corners accurately using adaptive panel-clustering

Media with smoothly-varying properties. One area of ongoing research is the generalization of (1) to

$$(\Delta + \omega^2 n(\mathbf{x})^2)u = 0 \qquad \text{in } \mathbb{R}^d, \qquad d = 2 \text{ or } 3$$

where the refractive index $n(\mathbf{x})$ varies smoothly in space. Important applications exist in seismic and ultrasonic imaging, quantum potential scattering, and underwater acoustics. With postdoc Adrianna Gillman (Dartmouth) and Gunnar Martinsson (Boulder), we created a *direct solver* for 2D scattering problems for arbitrary smooth $n(\mathbf{x})$, when $n-1$ has compact support. We cover a square containing its support with small "leaf" boxes: for each box we use a spectral Chebyshev product grid to approximate its interior impedance-to-impedance (Robin-to-Robin) map. Recursive dense Schur complement operations up the quad-tree merge the box ItI maps, to give the ItI map—and then Dirichlet-to-Neumann (DtN) map—for the entire square. My contributions include proposing the ItI (the DtN is not robust due to resonances), a new leaf solve, and the proof that it is 2nd-kind. The algorithm is $O(N^{3/2})$ for N total unknowns, and $O(\sqrt{N})$ per new incident angle. It solves problems 100λ across to 9 digits in a few minutes; each new incident angle takes a fraction of a second [25]. The scheme will simply generalize to 3D.

With former graduate student Matt Mahoney and undergraduate Brad Nelson '13 we focused on a special case of a *graded-index* medium $n^2(x_1, x_2) = x_2 + c$, where $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$, and found an integral form for $G_\omega(\mathbf{x}, \mathbf{y})$ whose integrand involves only the exponential function. Using numerical steepest descent we evaluate this Green's function with effort independent of frequency, hence can scatter to 10-digit accuracy from 2D obstacles 100λ in size embedded in this graded medium.

1.2 Fast solvers for diffraction gratings and photonic crystal band structure

Many wave devices and technologies exploit periodic structures, including optical filters, nano-optics, plasmonics, and lithography. Related structures periodic on the wavelength scale include *photonic crystals* and *metamaterials*, which can produce wave guiding impossible in naturally-occurring materials, with applications to communications and ultra-fast optical computing. There are other applications to water waves and radar measurement of ocean waves. Since such materials are usually piecewise homogeneous, integral equation methods—generalizations of (3)–(5) with unknowns living on material interfaces—can be efficient and high-order accurate. However, modeling of the scattering of waves from such gratings is numerically challenging, due to (a) the existence of so-called *Wood's anomalies* (parameters where one or more Bragg diffracted waves lies parallel to the grating), (b) the common need for solution at a large number (e.g. 10^2) of incident wave angles in design and optimization problems, and (c) ill-conditioning of the BVP problem itself due to guided modes (resonances) and complex geometries, which slows the convergence of an iterative solution.

Integral equation methods are traditionally applied to periodic problems by replacing the free-space Green's function (3) by its phased sum over the periodic lattice. However, at Wood's anomalies (issue (a) above) this sum is infinite and the method fails. In work with Leslie Greengard, we devised a robust scheme immune to this failure in two contexts: the *band structure* (see Fig. 1a) of a 2D photonic crystal [16], and dielectric grating scattering [18] as in Fig. 1b. We combine the free-space Green's function with layer potentials *on unit-cell walls*, and in the grating case exploit the spectral (plane wave) representation

$$G_\omega(\mathbf{x}, \mathbf{0}) \;=\; \frac{i}{4\pi} \int_{-\infty}^{\infty} e^{ikx_2}\, \frac{e^{i\sqrt{\omega^2 - k^2}\,|x_1|}}{\sqrt{\omega^2 - k^2}}\, dk\,, \qquad \mathbf{x} = (x_1, x_2)\,. \tag{6}$$

We devised spectrally-accurate complex-plane quadratures for this integral, giving accuracies approaching machine precision in rapid solution times (sometimes a fraction of a second).

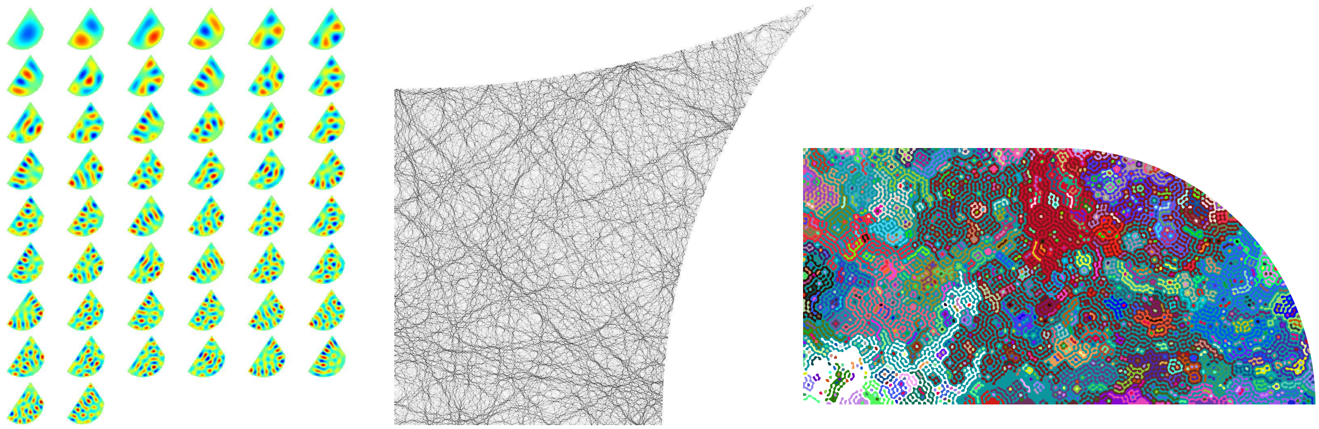

Figure 2: (a) Lowest 50 Dirichlet eigenmodes of domain with an arc and three corners computed to 10 digits accuracy in 16 s on a single core. (b) 10^5th Dirichlet eigenmode of a chaotic 2D domain (320 wavelengths across). (c) Chaotic stadium eigenmode showing 1277 nodal domains (each painted a different, random, color).

We recently tackled both issues (b) and (c) with Adrianna Gillman by creating [22] a *fast direct solver* for scattering from gratings of obstacles. We combine the fast hierarchical operator compression schemes of Gillman–Martinsson for the obstacle's self-interaction integral operator, with a factorization exploiting the low-rank nature of the periodic part of the interaction. By grouping multiple incident wave angles intelligently, for a complicated obstacle demanding $N = 10^5$ unknowns (see Fig. 1c) we reach a solution time of 6 seconds per angle, at a Wood's anomaly. This is a factor *600 times faster* than the previous state of the art ([18] combined with FMM and a GMRES iterative scheme). The generalization to multi-layer media and the full Maxwell equations poses no technical barriers; we expect this to have important applications in optics problems such as designing efficient thin-film solar cells.

I have created a simpler periodizing scheme based up on collocation on the walls of the unit cell via a dense least-squares system. I have tested this in 2D and 3D cases, the latter using QBX for the surface quadrature; this is a promising basis for accurate scattering solvers. See Fig. 1d. The multi-layer periodic dielectric grating case has been implemented in 2D, and with postdoc Min Yung Cho we plan to release software for this.

Graduate student Yuxiang Liu has implemented the MFS (see Sec. 1.1) for the full Maxwell equations in 3D time-harmonic scattering, and for 3D axi-symmetric bodies, and will combine this with the above periodizing scheme, for micro-magnetic sensor applications in collaboration with engineer Fridon Shubitidze.

2 Eigenvalue problems: high accuracy and high frequency

Eigenvalue problems for PDEs arise in modeling acoustic, electromagnetic and quantum cavity resonators, nanoscale devices, vibrating membranes, and data analysis. The paradigm example is to compute the Laplacian eigenfrequencies k_j, $j = 1, 2, \ldots$, and corresponding eigenmodes ϕ_j of the Dirichlet 'drum' $\Omega \subset \mathbb{R}^d$, i.e.

$$-\Delta\phi_j = k_j^2\phi_j \qquad \text{in } \Omega, \qquad\qquad \phi_j = 0 \qquad \text{on } \partial\Omega\ . \tag{7}$$

E.g. see Fig. 2a. Neumann and mixed boundary conditions also arise in applications. The high frequency (large mode number j) case is extremely challenging, and is of ongoing interest in *quantum chaos* (see section 2.1) and architectural acoustics.

In recent years we have advanced the state of the art for this problem such that high-frequency examples (where Ω is hundreds of wavelengths across) can be computed around 10^3 times faster than with any competing method; see Fig. 2b–c. The fast method [20] exploits a weighted Neumann-to-Dirichlet operator for the Helmholtz equation in Ω, in particular, the flow with respect to frequency parameter k of the *spectrum* of this operator. The latter is numerically computed in $O(N^3)$ time using Nyström discretization with N boundary points. However, each such spectrum provides approximations to *many* k_j and ϕ_j that lie in a frequency window: the cost per mode j is thus only $O(N^2)$. The method is for general dimension, but is limited to Ω star-shaped.

In a rare pure-meets-applied collaboration with Andrew Hassell (ANU), we have proven [20] the first known bounds on the errors in this algorithm, including that the k_j errors are 3rd-order in the frequency window width; this required heavy microlocal analysis machinery. We also devised an improved version that is observed to be 5th-order, including high-order methods for the modes. The motivation (originating with my thesis) is the desire to turn a mysterious method from quantum physics (the 'scaling method') into a mathematically rigorous algorithm that engineers can use. We have achieved the first part of this goal; the vital future work now demands general domains, and Neumann boundary conditions. A promising idea for the latter (already successful in a similar context) is to replace the boundary weight by a suitable pseudo-differential operator.

Other recent results include rigorous analysis showing that the errors of eigenvalues and modes computed by the MPS (see section 1.1) or other boundary methods can be orders of magnitude less than previously thought. Let an approximate eigenvalue k^2 and mode u satisfy $(\Delta + k^2)u = 0$ in Ω, with small relative boundary norm $t := \|u\|_{L^2(\partial\Omega)}/\|u\|_{L^2(\Omega)}$. We improved errors in k and u from $O(k^2 t)$ to $O(kt)$, giving 3 extra digits of accuracy in high-frequency applications [14] [19].

Ongoing and future plans: We have developed a new integral-equation algorithm for low-to-medium eigenvalues for general geometries and boundary conditions, with cost $O(N^3)$ per mode but with a prefactor 10 times smaller than prior schemes. Define the operator Fredholm determinant, whose roots lie are precisely the eigenfrequencies $\{k_j\}_{j=1}^{\infty}$,

$$f(\omega) := \det(I - 2D_\omega)$$

where D_ω is the Helmholtz double-layer operator on $\partial\Omega$ at frequency ω. Then $f(\omega)$ is an analytic function, and thus roots are efficiently found *to spectral accuracy* using the method of Boyd: evaluation of f (via the Nyström method) at N Chebyshev points, conversion via FFT to a Laurent series, thence to a polynomial whose roots are found via diagonalization of the companion matrix. Fig. 2a shows many modes of a domain with corners computed to 10 digit accuracy in a few seconds; it would be difficult to reach such efficiency and accuracy with finite elements (FEM). With graduate student Lin Zhao we have shown that an exterior near-resonance problem can occur for highly concave domains, and cured it with a robust "combined-field" representation $f(\omega) := \det(I - 2D_\omega + 2i\eta S_\omega)$. A paper is in progress with graduate student Lin Zhao.

Andrew Hassell and I are developing a fast solver for Neumann eigenvalues of star-shaped domains, and have plans to break the star-shaped restriction. Other plans include 3D eigenvalue solvers, using our QBX quadrature scheme and fast direct solvers.

2.1 Applications: quantum chaos and experimental mathematics

Quantum chaos is the mathematical (and sometimes physical) study of the above drum modes (7). It turns out that the statistical behavior of the distribution of modes ϕ_j as one tends to very high frequencies ($j \to \infty$) depends on the type of motion that a "billiard ball" (or geodesic, or ray of light reflecting off the walls) would undergo in that same domain. If the billiard ball motion is regular (as induced by e.g. a rectangular billiard table), one gets a distribution of eigenvalue spacings and modes that is very different from the case of *chaotic* billiard motion (e.g. a table with defocusing walls). This idea has deep connections to quantum physics, spectral geometry, number theory, and wave models of the early universe. I am known for contributions to this field in 'experimental mathematics', where specialized numerical methods are essential to make headway.

Let me give a little mathematical background. The large-eigenvalue asymptotics depends upon the integrability of the 'geodesic flow' (ray motion) on the manifold. For ergodic flow, we have a partial understanding in the form of rigorous results such as the Quantum Ergodicity Theorem, which states that *almost all* modes ϕ_j become asymptotically equidistributed (spatially, and also in phase space). The mode in Fig. 2b illustrates this equidistribution. The Quantum Unique Ergodicity (QUE) conjecture of Rudnick–Sarnak is that, for uniformly-hyperbolic flow, this holds for *every* mode. It is believed that we are far from a proof of this conjecture (apart from arithmetic cases, for which proof in part Lindenstrauss recently received the Fields medal).

The above motivated my large-scale numerical study [9] of a billiard with uniformly-hyperbolic flow; see Fig. 2b. I analyzed 30000 modes up to number $j \approx 7 \times 10^5$, and found strong evidence for QUE, as well as for conjectures in the physics literature on the power-law decay of the fluctuations in $|\phi_j|^2$. This work featured on the cover of *Notices of the American Mathematical Society*, and related images of mine have appeared in four recent review articles, including the one by Peter Sarnak (Princeton). Then, with Timo Betcke [11], we computed 16000 modes of the 'mushroom' billiard, whose flow is *mixed*: it has two invariant regions in phase space, one integrable and one ergodic. We verified (to an accuracy of 1%) Percival's conjecture on the localization of modes, and proposed and tested a model for so-called dynamical tunneling from the integrable into the ergodic region. In both of these works, via specialized algorithms, we reached eigenvalues, and amounts of data, 10–100 times higher than attained before.

My senior thesis student Kyle Konrad '12 recently studied, on an unprecedented scale, the statistics of *nodal domains* (regions of constant sign) in chaotic eigenfunctions; see Fig. 2c. By counting 10^9 domains from 10^5 eigenfunctions using 200 CPU-days of computation, we were surprised to discover that the (heretofore believed) conjecture of Bogomolny–Schmit on the mean number of nodal domains is too large by $5 \pm 1\%$. And yet, we found that the power-law exponent (187/91) for the distribution of domain areas agrees with deviation as small as 0.1%. A preprint is in progress. This suggests that the percolation idea upon which their conjecture is based could be modified to give the correct mean.

Our group's studies continue to impact the mathematical and quantum physics community. Future research plans include the study of intensity distribution in the random wave model for chaotic eigenmodes, and of resonances in partially-open chaotic cavities.

3 Other interdisciplinary research avenues

Incompressible Stokes flow for blood vesicles and micro-fluidics. I have generalized the near-field layer potential global quadrature schemes of Helsing to multiple new cases: exterior, single-layer, and first-derivatives. This builds upon, and improves upon, *barycentric interpolation* schemes for the Cauchy integral. With Shravan Veerapaneni and Bowei Wu (Michigan) we are building a complete toolkit for close-evaluation of 2D Stokes potentials for time-stepping vesicle flow in arbitrary wall geometries [26]. We plan to extend this to 2D and 3D periodic problems.

Ecology and home range modeling. The way animals use their habitat is controlled by factors such as food, water, terrain, predators, their 'home ranges', and social interactions; revealing these effects is key for conservation efforts. In a collaboration with Paul Moorcroft (Harvard), we developed a new animal movement Markov model [10], [12]. This unifies two standard approaches: resource selection analysis (a spatially implicit approach), and mechanistic home range analysis (an explicit probabilistic kinetic model). Our model's kernel may be factorized to derive an analytic steady state solution, yet has the flexibility to model variation in habitat via a general spatial *preference function* w. As a result, such models could be fit to data much more rapidly than before, and the time-evolution (probability density functions) of moving animals can be simulated quickly using fast Fourier transform methods. The analytic solution allowed us to predict that steady state animal density scales like w on small scales but like w^2 on large scales, with consequences for current practices of real-world telemetry data analysis and model-fitting.

Diffuse optical tomography. Near-infrared light is a promising tool for non-invasive medical imaging, yet requires the solution of a complex inverse problem to reconstruct the images. Following on earlier work on Bayesian statistical solution of the inverse problem [6], and the development of a rapid solver for the PDE forward problem (heat equation) in multi-layer geometries [7], I have continued to contribute in this area with work validating the diffusion approximation against the more accurate, but much more computationally intensive, radiative transport model, in 3D models of the human head [8]. One conclusion is that the diffusion approximation may often be used, allowing a much faster solution of the inverse problem for brain imaging.

Mathematics of music. In collaboration [17] with Larry Polanksy (Dartmouth) and Michael Winter (UCSB), we have analyzed a framework for the random generation of musical melodies with varying amounts of temporal correlation. This simplifies and generalizes methods of James Tenney, one of the first composers to apply computer code to the creation of music in the 1960s. Our cross-disciplinary approach combines stylistic analysis, numerical experimentation, and rigorous mathematical analysis.