Outstanding Challenges in Computational Methods for Integral Equations

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1 Overview of the Field

Approximately 30 years ago, a class of algorithms known as fast multipole methods (FMMs) were developed by L. Greengard and V. Rokhlin at Yale University. These algorithms allow for the evaluation of N-body calculations, in which the interaction kernel obeys an inverse power law, in time proportional to $\mathcal{O}(N)$ instead of the naive $\mathcal{O}(N^2)$ needed for the direct calculation. While first popularized in the regime of purely N-body calculations (e.g. astrophysics and molecular chemistry), descendants of the original FMM recently revolutionized the field of computational electromagnetics via their ability to accelerate the solution of classical integral equations arising in problems such as capacitance extraction and radar scattering. Analogous FMM-type algorithms have been developed for other PDEs arising in classical mathematical physics, namely fluid dynamics, elasticity and elastodynamics, heat diffusion, and various aspects of magnetohydrodynamics.

Simultaneous with the continued development of the FMM and its algorithmic descendants, the last several decades have seen incredible developments in both the mathematical theory of integral equations and the associated computational tools needed for their efficient and accurate solution. In many important real-world applications, integral equation formulations of the partial differential equations (PDEs) of classical mathematical physics (e.g. electromagnetic scattering, large-scale fluid flow, etc.) are preferable for analytical as well as numerical reasons. They naturally handle unbounded domains, complex geometries, and the resulting numerical schemes almost always respect the physical conditioning of the underlying problem. However, there still exist a large collection of problems for which integral equations are not computationally feasible; current shortcomings include, among others, the lack of efficient algorithms for handling complex three dimensional geometries, robust algorithms for high frequency wave phenomena, and the limited existence of well-conditioned integral formulations for fields outside of classical mathematical physics.

It was our goal in this workshop to discuss many of the outstanding challenges in this field, and to build a roadmap for future mathematical and computational research.

2 Recent Developments and Open Problems

In this section we enumerate some recent developments in the field of computational integral equations and mention related open problems, many of which were discussed at length during the workshop:

- **Novel integral equation formulations**. Classic potential theory naturally gives rise to boundary integral equations associated with the Dirichlet and Neumann boundary value problems for the Laplace equation. Using analogous ideas and Green's functions for other constant coefficient PDEs (e.g. Helmholtz, Stokes, Maxwell), more involved integral equations can be derived for other physical phenomena. Only recently have integral equations been derived for the time-harmonic harmonic Maxwell equations which are immune from spurious resonances and valid in arbitrary topologies at all frequencies. Likewise, the development of integral equation formulations that are robust, even at so-called Wood's anomalies, for quasi-periodic scattering problems are also quite recent. There is still much work to be done in the area of designing well-conditioned integral equations for classic problems, such as variable media sound/electromagnetic wave propagation, anisotropic wave propagation, and non-linear PDEs such as compressible fluid flow.

- **Discretization, quadrature, and computational geometry**. While most commercial computer aided engineering and meshing software merely generate low-order surface meshes (i.e. flat triangles), in many instances (particularly in engineering design) more accuracy can be obtained with less computational effort if higher-order methods are used. Higher-order convergence requires all aspects of the discretization to be done to high-order: function approximation, quadrature for singular Green's functions, and surface meshing/parameterization. Only recently have robust, high-order quadratures been developed for weakly-singular integral operators, but the coupling with fast algorithms is rather detailed and, as-of-now, unfinished work. Furthermore, progress on the generation of high-order surface discretizations and function discretization along surfaces in three dimensions with edges and corners is in its infancy. Lastly, any design problem requires an optimization step; coupling high-order discretizations with optimization procedures which allow for automatic mesh refinement and geometric perturbations is a nascent field and many of the participants are focusing efforts on these tasks.

- **Analysis-based fast algorithms**. Very efficient algorithms based on low-rank operator compression (e.g. FMMs and fast direct solvers) have been developed for the Laplace equation and the low-frequency Helmholtz equation (and related PDEs) in two dimensions. These algorithms allow for solution of the corresponding boundary value problems in linear time/complexity. In three dimensions, while FMMs have been developed for both Laplace and low/high-frequency Helmholtz potentials, the computational algorithms are slightly less efficient and carry a larger constant implicit in the $\mathcal{O}(\cdot)$ notation. Furthermore, because of geometric considerations, the related fast direct solvers in three dimensions (which explicitly construct the inverse of the operator) are less efficient and often do not exhibit optimal asymptotic scaling. Lastly, there exist a class of algorithms known as butterfly algorithms which offer a purely linear algebraic alternative to the wideband FMM for large-scale electromagnetic calculations. Butterfly algorithms have shown early promise as a tool with which to develop a fast direct solver for high-frequency wave problems, and several of the participants for the workshop are actively working on this line of research.

- **Workhorse numerical algorithms**. At the core of almost all high-performance numerical codes – whether they be PDE solvers, machine learning algorithms, or signal processing tools – are dense linear algebra routines such as QR, SVD, or LU factorizations, Gaussian elimination, or eigenvalue computations. The analysis-based fast algorithms used in integral equation methods are no different, and recently there have been many developments in using randomized linear algebra techniques to accelerate (and stabilize) the underlying operator compression inherent in such algorithms (i.e. data-sparse matrix compression). Efficient randomized algorithms have been developed for solving least squares problems and for constructing special-purpose matrix factorizations; early indications show that related ideas may yield efficient dense linear-algebraic solvers for full-rank systems. Several participants are at the forefront of developing randomized linear algebra schemes and coupling them with the fast algorithms used in solving integral equations.

- **Applications**. While many of the algorithms and solvers usually associated with the theme of this workshop apply mainly to linear constant-coefficient PDEs, often they have applications to nonlinear PDEs (e.g. compressible fluid flow) and statistics/machine learning (e.g. Gaussian process modeling). Statistical applications of these algorithms was not a topic that was highlighted much during the pre-

		May 23, 2022	May 24, 2022	May 25, 2022	May 26, 2022	May 27, 2022
		Monday	**Tuesday**	**Wednesday**	**Thursday**	**Friday**
Panel discussions	09:00 – 10:20	*Geometry, quadrature*	*Fast direct solvers*	*Applications*	*Oscillatory problems*	*Community software*
Moderator		O'Neil	Martinsson	Chaillat	O'Neil	Gillman
Panelist 1		Anna-Karin Tornberg	Adrianna Gillman	George Biros	Euan Spence	Andreas Kloeckner
Panelist 2		Shidong Jiang	Steffan Borm	Shravan Veerapaneni	James Bremer	Timo Betcke
Panelist 3		Denis Zorin	Jianlin Xia	Antoine Cerfon	Alex Barnett	Manas Rachh
	Coffee					
Talk 1	11:00 – 11:30	Bowie Wu	Dan Fortunato	Charlie Epstein	Fruzsina Agocs	
Talk 2	11:30 – 12:00	Kirill Serkh	Yabin Zhang	Felipe Vico	Yang Liu	
Talk 3	12:00 – 12:30	Isuru Fernando	Abi Gopal	Timo Betcke	Jason Kaye	
	Break					
Lunch	13:30 – 15:00					
Working groups	15:00 – 16:00	In-person discussions	In-person discussions	FREE AFTERNOON	In-person discussions	CHECKOUT
Dinner	19:00 – 21:00					

Figure 1: The workshop schedule.

sentations, but will definitely be a topic of discussion in the subsequent virtual panel discussions that we plan to have as a result of this workshop.

3 Workshop format

Our workshop was run in a hybrid format, with a daily schedule structured as follows:

- *9:00 – 10:30: Panel discussion (hybrid).* Each day started with a panel discussion on a currently active research topic (see Section 4 for details). The discussion started with three brief (about 5 min each) discussion starters that were delivered by senior researchers who later served as panelists. These presentations were designed to highlight promising research problems and open questions. Each panel session was moderated by one of the organizers. After the brief introductions, the panels consisted of moderated discussions that involved the panelists, as well as both in person and zoom participants.
- *10:30 – 11:00: Coffee break.*
- *11:00 – 12:30: Research talks (hybrid).* Each day included three research talks given by junior participants, with a mix between in person and online presentations. The talks were well attended, and involved lively discussions between the virtual and in-person participants.
- *12:30 – 13:30: Discussions / individual collaborations (in person).* The workshop involved extensive discussions and collaborative research. There were also some impromptu informal presentations.
- *13:30 – 15:00: Lunch.*
- *15:00 – 17:00: Discussions / individual collaborations (in person).*

We decided to limit the hybrid component of the workshop to the morning sessions since many of our remote participants were based in Europe. We had also received feedback that while people were very keen to participate, there was a preference that the zoom sessions be somewhat contained in length.

In our opinion, the format worked out very well. The panel discussions in the mornings were particularly successful, with a large share of the participants engaged. We were impressed with the technical set-up in the room; this enabled good interactions between the in-person and the virtual participants.

Despite the fact that the hybrid format worked out quite well, the productivity of the workshop was still limited by the fact that only 15 participants were able to congregate on site. We appreciate the hard work done by BIRS and the local staff to enable to workshop to run despite the challenging circumstances. Nevertheless, we very much hope that the workshops will be brought back up to full capacity in the near future.

4 Presentation Highlights

As mentioned above each day saw a morning moderator discussion, and the first four days each saw an additional hybrid session involving three 30 minute research talks. The panelists in the first session generally consisted of mid- to late-career experts in their respective fields. The research talks in the second session were given by graduate students, post-docs, and early- to late-career faculty members. In this section, we summarize some highlights from the panelist discussions and research-focused talks.

4.1 Day One: Geometry and Quadrature

4.1.1 Panel discussion

Anna-Karin Tornberg and Sidong Jian both gave some general overview discussion of quadrature methods for integral equations along boundaries in two and three dimensions, and some brief comments regarding the outstanding problems for volume quadrature problems needed in, for example, solving inhomogeneous boundary value problems such as Poisson problems.

Then, Denis Zorin talked about some of the geometric considerations in solving boundary integral equations, namely, the interaction between the resulting numerical quadrature rule and various surface representations (i.e. CAD vs. locally triangulated, etc.). His comments spurned a very lively back and forth on how to best integrate Computer Aided Drawing (CAD) capabilities, meshing algorithms, and fast integral equation solvers. Questions regarding refinement under uncertainty were raised, and various trade-offs between low-order (but oversampled) and high-order (but not oversampled) discretizations were discussed. It was an open-ended panel discussion: there were many unanswered questions regarding how to best proceed (with regard to interfacing complex geometry, meshing, and solvers) mainly due to the fact that the overwhelming majoring of the community has been focused on building solvers which are theoretically compatible with complex geometries, but not epecially optimized to robustly handle complex geometry.

4.1.2 Invited talks

Titles and brief abstracts of research talks are given below:

- **A unified trapezoidal quadrature method for singular & hypersingular integral operators**
  Bowei Wu, UT Austin, TX
  A unified treatment of boundary integral operators in 2D and 3D using a simple trapezoidal quadrature method is presented. The method is based on generalized Euler-Maclaurin formulas and can be applied to weakly singular as well as hypersingular operators. The construction of such a quadrature rule for a given kernel can be done systematically in simple steps, which we will demonstrate in this talk and show numerical examples [11].

- **Applications of potential theory in computer graphics**
  Kirill Serkh, U. Toronto, ON, Canada
  Vector graphics image processing schemes will be presented that are based on solving integral equations along interfaces between objects [3].

- **Synthesis of translation operators and execution plans for the fast multipole method**
  Isuru Fernando, U. Illinois at Urbana-Champaign
  In the application of the Fast Multipole Method to the computation of potentials for elliptic PDEs and systems thereof, opportunities exist for lowering cost through knowledge of the kernel and the PDE operator. We present two methods that, given various small amounts of user-supplied problem knowledge (e.g. symbolic expression of the kernel, symbolic PDE), automatically exploit these opportunities. The first is devoted to the automatic synthesis of translation operators (e.g. multipole-to-local, point-to-multipole, etc.) for arbitrary kernels. We describe the asymptotic cost of variants of our algorithm available given certain pieces of information, as well as the methods by which they are attained. We present theoretical cost bounds as well as numerical evidence that our algorithms attain them. The second builds on the first and is devoted to the automatic synthesis of execution plans for expressions of potential operators involving multiple inputs and outputs, multiple different kernels, composition, as well as source and target derivatives. Given a symbolic description of such an operator, our system outputs a sequence of operations that realizes cost savings through an algebraic procedure based on syzygies. Finally, we describe the application of the combination of these approaches in a system for

the high-order accurate evaluation of layer potentials from unstructured geometries in two and three dimensions [8].

4.2 Day Two: Fast Direct Solvers

4.2.1 Panel discussion

This panel focused on methods for solving the linear systems that arise upon the discretization of the integral equations associated with linear elliptic PDEs. These equations involve coefficient matrices which are dense, but at this time there are well-established algorithms (e.g. the Fast Multipole Method) that can rapidly evaluate the matrix-vector multiplication. In cases where iterative methods such as GMRES converge fast, having a fast algorithm for the matrix-vector multiplication resolves the problem. The focus of this panel was on problems where iterative methods struggle, as happens, e.g., when modeling many acoustic and electromagnetic scattering problems. The techniques discussed aim to directly build an approximation to the inverse of the coefficient matrix, which sidesteps the issue of slow convergence of iterative solvers. Despite the density of the matrix, it turns out that this inversion problem can, in important environments, be carried out in linear or close to linear time. The three panelists briefly surveyed the state of the art, and pointed the attendees to opportune areas of future research. A lively discussion that involved both the panelists and the audience members followed. Questions discussed included how to choose between a plethora of methods that have been proposed; what applications may most benefit from direct solvers; how to attain high performance on modern communication bound hardware; how randomized algorithms may fit; and how machine learning may play a part going forwards.

4.2.2 Invited talks

Titles and brief abstracts of research talks are given below:

- **A fast direct solver for surface PDEs based on the hierarchical Poincaré–Steklov method**
  Daniel Fortunato, CCM, Flatiron Institute, New York, NY
  We introduce a fast direct solver for variable-coefficient elliptic partial differential equations on surfaces based on the hierarchical Poincaré–Steklov method [5]. The method takes as input a high-order quadrilateral mesh of a surface and discretizes surface differential operators on each element using a high-order spectral collocation scheme. Elemental solution operators and Dirichlet-to-Neumann maps tangent to the surface are precomputed and merged in a pairwise fashion to yield a hierarchy of solution operators that may be applied in $\mathcal{O}(N \log N)$ operations for a mesh with N elements. The resulting fast direct solver may be used to accelerate implicit time-stepping schemes, as the precomputed operators can be reused for fast elliptic solves on surfaces. We apply the method to a range of problems on both smooth surfaces and surfaces with sharp corners and edges, including the static Laplace–Beltrami problem, the Hodge decomposition of a tangential vector field, and some time-dependent reaction–diffusion systems.

- **Fast Algorithms for 2D Multilayer Quasi-Periodic Scattering**
  Yabin Zhang, U. Michigan, Ann Arbor, MI
  The talk presents a fast direct solution technique for solving two-dimensional wave scattering problems from quasi-periodic multilayered structures. The computational cost of creating the direct solver scales O(N) where N is the total number of discretization points on all interfaces. The bulk of the precomputation can be re-used for any choice of the incident wave. As a result, the direct solver can solve over 200 scattering problems involving an eleven-layer geometry with complex interfaces 100 times faster than building a new fast direct solver from scratch for each new set of boundary data. An added benefit of the presented solver is that building an updated solver for a new geometry involving a replaced interface or a change in material property in one layer is inexpensive compared to building a new fast direct solver from scratch. Numerical results illustrate the improved performance of the new solver over some previous approaches [12].

- **A fast algorithm for computing quadratures for bandlimited functions**
  Abinand Gopal, Yale University, New Haven, CT

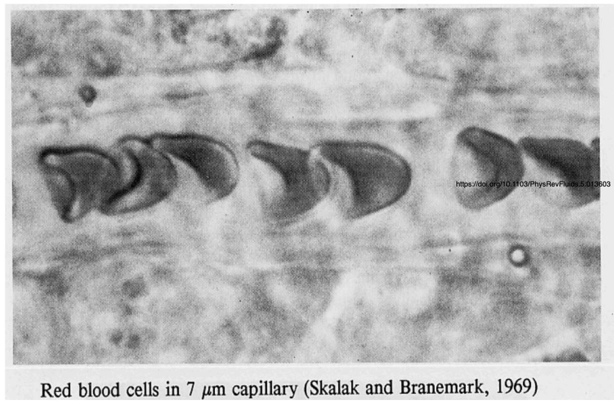

Figure 2: Intended application for BIE: simulation of red blood cells - from G. Biros introduction.

Bandlimited functions arise in a wide variety of applications in scientific computing and signal processing. In this talk, we present a fast algorithm for computing quadratures for bandlimited functions, based on recent advances in the numerical treatment of prolate spheroidal wave functions. The resulting quadrature rules are capable of integrating functions with a given bandlimited to high accuracy and can be computed rapidly, with only $\mathcal{O}(n)$ operations required to compute an n-point rule with fixed bandlimit [6].

4.3 Day Three: Applications

4.3.1 Panel discussion

Boundary integral equations are a very efficient tool for a lot of applications ranging from acoustics, electromagnetism, elastic wave propagations, blood flow, etc. We have used the panel discussion to review some major open questions to be solved by the community. The discussion has been led by George Biros, Shravan Veerapaneni and Antoine Cerfon that have complementary point of views on the existing issues.

Georg Biros began by describing some of the challenges that arising when solving massive fluid-structure interacting systems using integral equation methods accelerated via FMMs, in particular with applictions to simulating blood flow. Some of the challenges that present themselves in this situation are: Nonlinear interface mechanics, Lubrication effects (near contact), Surface biharmonic operators, Shear resistance / memory effects, Surface inextensibility, Weakly/nearly singular integrals, Stiff time-stepping, Chaotic dynamics, and Long range hydrodynamic interactions. Some of these challenges are mathematical, and some are computational in spirit.

Next, Shravan Veerapaneni gave an overview of some additional challenges that present themselves in large-scale fluid dyamics codes based on integral equation formulations. These challenges included: Modelling particulate Stokes flow, Control and optimization problems, Nonlinear fluid models (viscoelastic, nonlinear Stokes, ..), and developing methods for Time-dependent PDEs (Unsteady Stokes, Navier-Stokes, ...).

Finally, while fluid flow has historically been a target for integral equation formulations, Antoine Cerfon discussed some challenges and outstanding problems in Integral Equation Methods for Magnetic Fusion. In particular, these challenges include: Need of a FMM for an integral kernel that is not translation invariant, Efficient rules for singular on-surface quadratures, Accurate and efficient rules for singular off-surface quadratures (near surface), Surface and volume solvers for three-dimensional domains with corners, Formulation/numerical schemes for high-order accurate Fréchet derivative used in optimization.

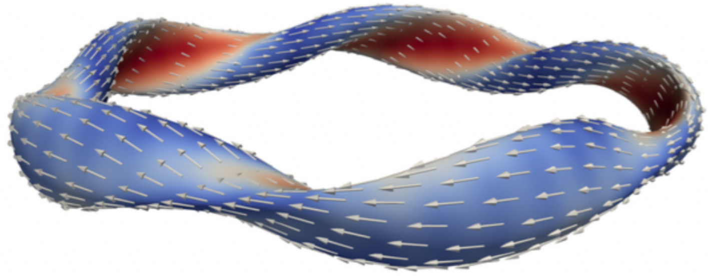

Figure 3: Challenges in magneric fusion for BIEs - from A. Cerfon introduction.

The panel discussion continued with a lively back-and-forth discussion of what fields seem to be amenable to solving problems using integral equation formulations; magneto-fluid dynamics seems quite rich for finding open problems.

4.3.2 Invited talks

Titles and brief abstracts of research talks are given below:

- **Type I Superconductors, Integral Equations and $\lambda_L \to 0$ Limiting Behavior**
  Charles Epstein, CCM, Flatiron Institute, New York, NY
  We analyze the classical magneto-static approach to the theory of type I superconductors, and a Debye source representation that can be used numerically to solve the resultant equations. We also prove that one of the fields found within the superconductor via the London equations is the physical current in that the outgoing part of the magnetic field is given via its Biot-Savart integral. Finally, we compute the static currents for moderate values of London penetration depth for a sphere, a stellarator-like geometry, and a two-holed torus [4].

- **Transpose method for quasi-Newton optimization problems in acoustics and electromagnetism**
  Felipe Vico, U. Valencia, Spain
  In this paper we present the transpose method for quasi-Newton optimization problems in acoustics and electromagnetism. In particular we use a fast algorithm for optimizing the location of p.e.c. spheres in free space such that a certain goal function is optimized. The goal function can be used to maximize the total field in a certain point in space (focal point) or any other function that depends on the scattered field produced by the spheres. The method can be used to create new materials (metamaterials) or goal-oriented materials with uncommon electromagnetic/acoustic properties [10].

- **Electrostatic simulations with Bempp and Exafmm - A black-box coupling approach**
  Timo Betcke, University College London, UK
  Biomolecular electrostatics is key in protein function and the chemical processes affecting it. Implicit-solvent models expressed by the Poisson-Boltzmann (PB) equation can provide insights with less computational power than full atomistic models, making large-system studies – at the scale of viruses, for example – accessible to more researchers. In this talk we present a Galerkin BEM approach to compute solvation for large protein models based on the black-box coupling of the Bempp software with the Exafmm kernel-independent FMM library (see Fig. 4). We discuss the implementation of the coupling and scalability for large problems. We conclude the talk with remarks on ongoing work to develop FEM/BEM coupled solvers for solvation problems with inhomogeneities, and an outlook to software development for extreme scale solvation models [2].

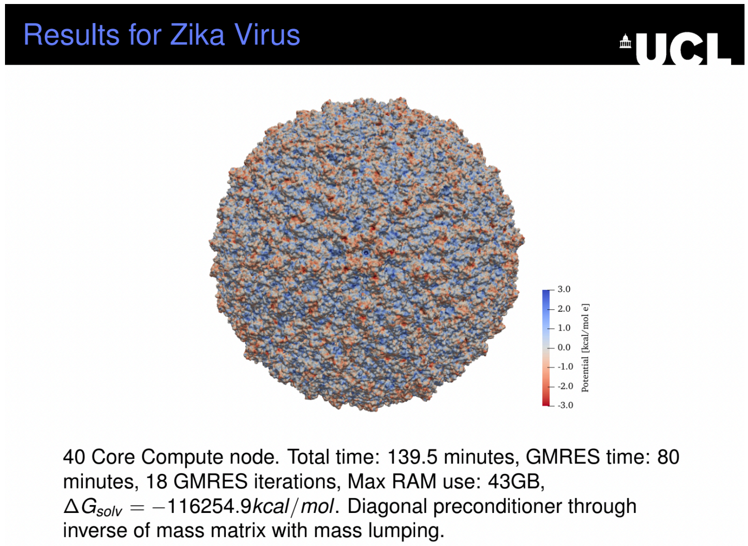

Figure 4: Illustration of the capacities of fast BEMs for model the Zika virus - from T. Bectke talk.

4.4 Day Four: Oscillatory Problems

A longtime outstanding problem in computational physics has been to build an efficient, i.e. asymptotically optimal, solver for high frequency (time-harmonic) wave propagation problems. The salient feature of these problems is that the characteristic wavelength of the solution/data is much smaller than the domain over which it propagates. A breakthrough algorithm was developed nearly 30 years ago in the High-Frequency Fast Multipole Method which allowed for the nearly linear time application of such operators; however, solving such a system using this algorithm requires coupling to an iterative solver. In these high-frequency regimes, iterative solvers generally fail to converge in suitable time. Therefore, a lot of effort recently has been devoted to building butterfly factorizations of such operators and inverting them directly. Such a factorization can be seen in Figure 5, and differs signifcantly from the usual ones based on low-rank considerations.

4.4.1 Panel discussion

The panel discussion began with an overview of various challengs in high frequency problems by Alex Barnett. This overview included various regimes of wave propagation (variable media, hard boundaries), discretization considerations, asympototic limits (e.g. geometric diffraction), alternative solution methods (solving for phase/amplitude separately), and on the standard failures of iterative solvers.

James Bremer talked in detail about an approach to high frequency problems based on an explicit separation of the amplitude and phase of the solution, efficient numerical methods for doing this in one dimension, and the general breakdown of the idea (or rather, the technical difficulties encountered) in higher dimensions. The consensus seemed to be that some approach along these lines has to be the way forward, otherwise the number of unknowns needed to discretize problems at something proportional to the Nyquist rate would be untenable.

Lastly, Euan Spence discussed challenges specifically related to the Galerkin and Nystrom discretization of high-frequency integral equations. In some regimes, and for some specific geometries, it is not known that such high-order accurate discretizations result in convergent schemes (or rather, one can construct situations in which the discretization is not convergent). It is likely that these are highly degenerate cases, constructed to exploit various aspects of the convergence theory, but that in practice they would occur very rarely. However, the resulting discussion was quite lively, as several people had strong opinions on the most efficient way to discretize such operators and deal with the result linear systems.

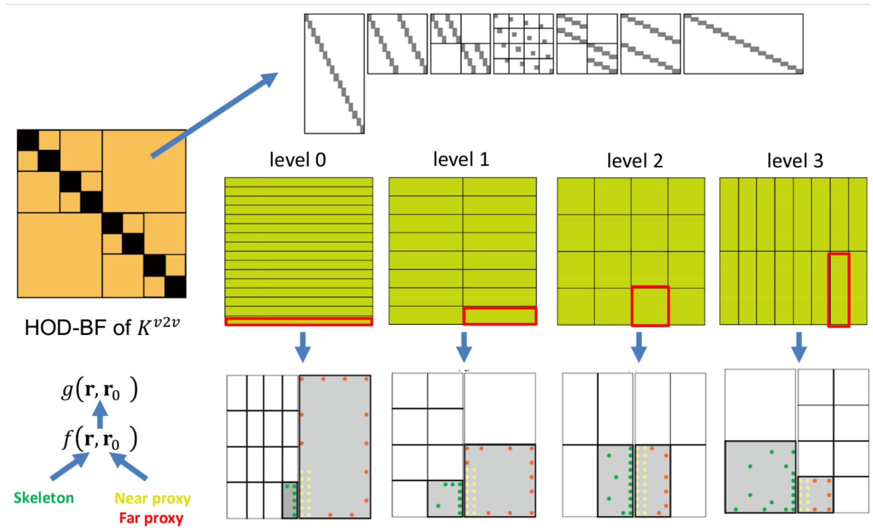

Figure 5: Depiction of the types of operator/matrix factorizations needed in order to build efficient algorithms for applying integral transforms with highly oscillatory kernels. Image from talk given by Y. Liu.

4.4.2 Invited talks

Titles and brief abstracts of research talks are given below:

- **A fast and accurate solver for highly oscillatory ODEs**
  Fruzsina Agocs, CCM, Flatiron Institute, New York, NY
  Oscillatory systems are ubiquitous in physics: they arise in celestial and quantum mechanics, electrical circuits, molecular dynamics, and beyond. Yet even in the simplest case, when the frequency of oscillations changes slowly but is large, the vast majority of numerical methods struggle to solve such equations. Methods based on approximating the solution with polynomials are forced to take O(k) timesteps, where k is the characteristic frequency of oscillations. This scaling can generate unacceptable computational costs when the ODE in question needs to be solved billions of times, e.g. as the forward modelling step of Bayesian parameter estimation. In this talk I will introduce an efficient method for solving 2nd order, linear ODEs with highly oscillatory solutions. The solver employs two methods: in regions where the solution varies slowly, it uses a spectral method based on Chebyshev nodes and with an adaptive stepsize, but in the highly oscillatory phase it automatically switches over to an asymptotic method. The asymptotic method constructs a nonoscillatory phase function solution of the Riccati equation associated with the ODE. In the talk I will present how the method fits in the landscape of oscillatory solvers, the theoretical underpinnings of the asymptotic solver, a summary of the switching and stepsize-update algorithms, some examples, and a brief error analysis [1].

- **Butterfly Compressed Babich Integrator for Solving Helmholtz Equations in Inhomogeneous Media**
  Yang Liu, Lawrence Berkeley National Laboratory, Berkeley, CA
  Time-harmonic wave phenomena in inhomogenous media are governed by Helmholtz and Maxwell equations with variable coefficients, and are typically simulated with finite-difference (FD)/finite-element-based differential equation solvers or volume integral equation based solvers (VIE). Fast, accurate and stable algorithms for solving these problems in the high-frequency regime are computationally very challenging. Although a few recent works have leveraged the so-called butterfly compression techniques to construct fast FD and VIE-based direct solvers, they suffer from a few other computational issues. The FD-based solver is plagued with numerical dispersion, PML truncation error and zero-pivoting during sparse matrix inversion, hence cannot handle large systems with high-order accuracy. The VIE solver, on the other hand, requires inverting a large dense linear system and turns

out to be still expensive even with butterfly acceleration. In this work, we consider another approach called Hadamard-Babich integrator, which represents a high-frequency ansatz of the Green's function for inhomogenous media. We first construct low-rank products of the phase and amplitude ingredients of the Babich integrator and use the results to construct butterfly compression of the discretized integral operator for the entire computation domain. The resulting Babich integrator-based solver is very accurate for smoothly varying media and computationally very efficient compared to FD or VIE solvers. When further combined with surface integral equation (SIE) formulations, the proposed solver also applies to large 2D and 3D domains with surface inclusions or multiple regions. This is a joint work with Jianliang Qian, Jian Song from MSU and Robert Burridge from UNM [9].

- **Algorithmic challenges in quantum many-body Green's function methods**
  Jason Kaye, CCQ, Flatiron Institute, New York, NY
  Many-body Green's function methods are of central importance in modern approaches to computational quantum physics which have attempted to reach higher accuracies than those provided by effective one-body approximations like density functional theory. These Green's functions satisfy nonlinear integral equations, called Dyson equations, and present an interesting set of algorithmic challenges which may be possible to address, in part, using ideas developed in the computational integral equations community. This talk will discuss a few of these challenges, compare and contrast them with those arising in more standard computational integral equations problems, and introduce new fast algorithms for Dyson equations [7].

4.5 Day Five: Community Software

The last day of the workshop consisted solely of a panel discussion on community software in the morning. The three panelist were Manas Rachh, Timo Betcke and Andreas Kloeckner. These are the three most prominent software developers in our community. Manas is leading the efforts to build and distribute FMM and quadrature packages through the Flatiron Institute. Timo is the main developer of BEM++. This is a software package based on boundary element formulations which contains linear algebra and quadrature tools that can be used independently. Andreas Kloeckner develops a software for a variety of partial differential equation solution techniques including kernel independent quadrature and FMM libraries. Additionally he develops a collection of `Python` interfaces to things like OpenCL, Cuda and mesh generation.

These experts presented their reasons for developing software and a common goal of having the software being able to interact with each other is a simple, accessible and clean manner. Each panelist had a wishlist of things they want for their software. Some of these were pointed problems that they want to tackle such as 10 times faster solution techniques for three dimensional problems where the solution is oscillatory. Others were general statements about how they think software should be managed. For example, it was suggested that there should be two versions of a package. The first version is for non-specialist users such as graduate students and practitioners. This will allow the impacts of the developments in the integral equation community to have a more immediate impact to the related areas and allow junior members of the community (such as graduate students and postdocs) to push new directions in the field by being able to use existing methods without having to develop code from scratch which is a time consuming nontrivial process. The second version will have more transparency in the lower levels of the code allowing for domain specific developers to modify and/or build from existing software packages. Again, this will allow researchers in the field of integral equations to more easily and rapidly build from existing work. By having access to the lower level components of the algorithms, these users will be able to make fundamental contributions to the field and be able to seamlessly use the other components of the software package.

5 Scientific Progress Made

A key goal of the workshop was that in addition to covering recent research and scientific progress, participants would spend significant time discussing problems that they want to solve but can't, or problems that they think are important in the field.

5.1 Organizing the community

One of the main outcomes of the workshop was to truly help organize a community of researchers and students working in computational integral equation methods across the world. There was a general attempt to provide a roadmap of important problems going forward, what types of software need to be developed in terms of both training, research, and standard use by those in other fields (i.e. engineering, physics, etc.). This roadmap will surely help to drive work in the field for at least the next several years, and generate many new interesting directions for students and early-career faculty.

Community pages[1] with references for papers and available software were assembled as a result of this meeting. Having access to these materials will allow new people entering the field, as practitioners or as graduate students, to easily know what techniques exist and make use of them without the huge overhead of having to build software from scratch.

5.2 In-person afternoon sessions

There was some variety in the afternoon sessions. Two afternoons were spent with in-person participants giving chalk talks at the boards around the garden about their current work and answering questions about their recently published papers. One afternoon the group went on a long walk together in the area around the hotel. This allowed for informal discussions about the academic job market, including standard time-lines for applications, what to include in application documents, how to chose letter writers, and what makes a good job talk. We also chatted about the experience of returning to in-person teaching and the challenges associated with that. On the Wednesday afternoon, we explored downtown Oaxaca. Everyday we continued to discuss the panel discussion topic, as there was never enough time to finish the discussions during the allotted time in the morning.

6 Outcome of the Meeting

As a direct result of the meeting, it was decided that some informal virtual meeting of the computational integral equations community should, and will, continue going forward on a monthly or bi-monthly basis. After the scientific isolation caused by the Covid-19 Pandemic, the excitement surround the exchange of ideas during this meeting far exceeded expectations. It served as the perfect crystallization seed to generate a long-term commitment by the members of this community to stay in touch, support graduate students and post-docs, and work to develop a fruitful roadmap forward for the field.

References

[1] F. J. Agocs, W. J. Handley, A. N. Lasenby, and M. P. Hobson, Efficient method for solving highly oscillatory ordinary differential equations with applications to physical systems, Phys. Rev. Research **2** (2020), 013030.

[2] T. Betcke and M. W. Scroggs, Designing a high-performance boundary element library with OpenCL and Numba, Computing in Science & Engineering **23** (2021), 18–28.

[3] K. Bower, K. Serkh, S. Alexakis, and A. R. Stinchcombe, Fast Computation of Electrostatic Potentials for Piecewise Constant Conductivities, https://arXiv.org/abs/2205.15354 (2022).

[4] C. L. Epstein and M. Rachh, Debye source representations for type-I superconductors, I: The static type I case, J. Comput. Phys. **452** (2022), 110892.

[5] A. Gillman, P. G. Martinsson, A Direct Solver with Complexity for Variable Coefficient Elliptic PDEs Discretized via a High-Order Composite Spectral Collocation Method, SIAM J. Sci. Comput. **36** (2014), A2023–A2046.

[1] `https://github.com/inteq-software/inteq-software-catalog`

[6] A. Gopal and P. G. Martinsson, An accelerated, high-order accurate direct solver for the Lippmann–Schwinger equation for acoustic scattering in the plane, Adv. Comput. Math. **48** (2022).

[7] J. Kaye and H. U. R. Strand, A fast time domain solver for the equilibrium Dyson equation, https://arxiv.org/abs/2110.06120, (2022).

[8] A. Kloeckner, I. Fernando, M. Wala, A. Fikl, G. Hao, and M. Knepley, sumpy: n-body kernels and translation operators, https://github.com/inducer/sumpy, (2022).

[9] S. B. Sayed, Y. Liu, L. J. Gomez, and A. C. Yucel, A butterfly-accelerated volume integral equation solver for broad permittivity and large-scale electromagnetic analysis, IEEE Trans. Ant. Propag. **70** (2021), 3549–3559.

[10] F. Vico-Bondia, M. Cabedo-Fabrés, M. Ferrando-Bataller, and E. Antonino-Daviu, Optimization of 2D Heterogeneous Lenses via BFGS and Volume Integral Equation Method, 2021 IEEE International Symposium on Antennas and Propagation and USNC-URSI Radio Science Meeting (2021), 1657–1658.

[11] B. Wu and P.G. Martinsson, Zeta correction: a new approach to constructing corrected trapezoidal quadrature rules for singular integral operators, Adv. Comput. Math. **42** (2021), 1–21.

[12] Y. Zhang and A. Gillman, A fast direct solver for two dimensional quasi-periodic multilayered media scattering problems, BIT Num. Math. **61** (2021), 141–171.