Eigenvalues/singular values and fast PDE algorithms: acceleration, conditioning, and stability

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1 Overview of the Field

Partial Differential Equation (PDE) theory constitutes a cogent set of theoretical and computational methods that enable qualitative and quantitative understanding in vast areas of science and engineering, including the fields of physics, chemistry, biology, economics and ecology, amongst many others. With increasing computational power, the ambitions to produce physically faithful numerical solutions have been raised to exceedingly high levels; in recent years it has become clear, however, that the advances in computer technology alone will not enable accurate solution of complex scientific PDE problems. It is the sound techniques of numerical analysis, grounded in solid theoretical foundations that will unleash the computational power of modern computer systems in the area of computational science.

While many high-quality tools are currently available for the numerical solution of Partial Differential Equations, a large number of important problems have remained intractable, or nearly so, due to the shear scale of the computer power their solutions require. Interestingly, most of the difficulties that hinder applicability and/or performance of numerical methods concern the structure of spectra (eigenvalues and singular values) of various discrete operators associated with numerical solvers.

Thus, unfavorable spectral distributions give rise to

- Lack of stability or restricted stability of explicit time-domain solvers, including Finite-Difference solvers, Finite-Element solvers, Discontinuous Galerkin solvers, Finite Volume solvers, methods based on Radial Basis Functions, Spectral solvers, etc.
- Slow convergence of iterative linear-algebra methods for implicit time-stepping.
- Large iteration counts in iterative algorithms for elliptic problems, such as those based on domain decomposition, overlapping meshes, etc.
- Accuracy limitations owing to ill-conditioning in high-frequency solvers based on use of Oscillatory Basis Functions.
- Oversampling requirements to meet accuracy tolerances in acceleration methods for frequency-domain and time-domain integral-equation solvers.
- Slow convergence of iterative linear-algebra solvers for integral-equation methods.

- Conditioning difficulties arising from presence of geometric singularities and associated accuracy limitations for both volumetric and integral-equation PDE solvers.

While it is clear that these difficulties have common sources, which relate to spectral distributions of various operators, such connections have not been systematically explored. We believe such studies, which lie at the heart of the contributions presented in this workshop, are greatly beneficial to a wide range of areas in computational PDE. For example, the existence of geometric singularities gives rise to spectral distributions that affect the convergence of iterative steady state solvers as well as the time steps of the time-domain solvers, and thus, an understanding of one impacts on the other. Recent advances in QR decomposition techniques to resolve conditioning issues that have been successfully implemented for Radial Basis Function solvers, further, could yield significant improvement for other methodologies including time-domain, frequency-domain and steady state methods based on Oscillatory Basis Functions, Discontinuous Galerkin and, indeed, most of the approaches listed above. Similarly, recent progress on elimination of time-step constraints on the basis of Alternating-Direction approaches might be applicable to remedy or eliminate stability restrictions arising in the area of Discontinuous Galerkin or other methods.

2 Recent Developments and Open Problems

A number of important new ideas have recently emerged in the field of Numerical Solution of Partial Differential Equations, many of which relate to eigenvalues/singular-values of the associated discrete systems. These include topics concerning the following areas.

Stability - Regardless of the accuracy of a particular method for time-dependent problems, if it is not in some measure stable it will not be useful: failing stability, the numerical approximation of a bounded solution becomes infinite (and thus totally inaccurate) in finite time. The stability of the system is indeed governed by certain eigenvalues and singular values. Recent ideas, including temporal sub-cycling in high-order Discontinuous Galerkin methods and boundary projections in Fourier based methods, can nearly (even completely, in some cases) overcome stability constraints without sacrificing computational efficiency.

High-Order/Spectral Accuracy - Relying on methods that ensure agreement of solutions to their Taylor/Fourier expansions to some (adequately high) order n, higher-order/spectral methods generally use fewer unknowns to reach a prescribed solution accuracy. At the same time the eigenvalues of the resulting systems are often correlated to the order of the method and the problems associated with poorly behaved eigenvalues are exacerbated as the order is increased. Further, the eigenvalues are often very sensitive to the specific geometry and/or mesh of the problem. The advent of certain embedded-boundary methods, high-order integral methods, and overlapping meshes has greatly broadened the applicability of high-order and spectral methods.

Fast Iterative Methods - Relying on ideas related to the Fast Fourier Transform, use of approximate inverses (preconditioners) to accelerate convergence of iterative methods and low-rank matrix approximations, the advent of fast integral-equation solvers and multi-grid methods, as well as wavelet-based and fast direct solvers has inaugurated a new research direction in the field of numerical solution of PDEs. The overall computational cost of these methods is often tied directly to behavior of eigenvalues. Poorly behaved eigenvalues often lead to the requirement of larger numbers of linear-algebra iterations which can then only be reduced by finely tuned preconditioners. Emerging hybrid methods, which employ, say, a combination of a fast algorithm and a classical method (e.g., a hybrid of integral equation solvers and high-order finite-element approximations), are promising and currently a subject of much activity.

3 Presentation Highlights

Highlights of the presentations are included below, organized according to the thematic areas of the workshop. This organization is to some extent arbitrary, since the topics are inherently interconnected—as the presentations themselves made it abundantly clear, and as necessitated by the nature of the workshop.

Presentation highlights in the area of *Stability and Efficiency* The presentation by **B. Henshaw** on high-order accurate algorithms for overlapping grids, touched on several of the themes of the workshop. The focus was the use of overlapping grid meshes that can be applied to both static and dynamic geometries to avoid several complications. The overlapping grids allow greater structure to the meshes and dramatically reducing mesh anomalies. Generation of the mesh becomes less cumbersome for complicated geometries, and the eigenvalues of the resulting system of equations are generally more predictable and better behaved. Thus the stability of the solvers can be significantly better than alternate methods if the geometry is nominally complex. These overlapping mesh methods are adaptable and can be utilized by essentially any mesh dependent PDE solver. The presentation by **S. Jin**, in turn, concerned Semiclassical Computation of High Frequency Waves in Heterogeneous Media. In this presentation semiclassical Eulerian methods were presented, which can be used to evaluation of the evolution of high frequency waves through heterogeneous media without explicit numerical resolution of the small wavelengths. The method is based on the classical Liouville equation in phase space, with discontinous Hamiltonians; the presentation provided relevant interface conditions consistent with the correct transmissions and reflections.

The adaptability of overlapping meshes was once again considered in the presentation by **N. Albin** entitled *Fourier Continuation Methods Long-Range Propagation and Transport*. Fourier Continuation methods, essentially a method to overcome the Gibbs' phenomenon for non-periodic functions, was applied to the solution of PDEs in complex geometries. A key component of the geometric flexibility of this effort was the overlapping mesh approach. On the other hand, the idea of using generalized Fourier methods in of itself is a promising idea which addresses accuracy, stability, and the computational speed of algorithms. A different perspective on Fourier Continuation methods was presented by **M. Lyon**, who presented new methods for evaluation of FC continuation functions, giving rise to algorithms that are both fast and are capable of spectral accuracy throughout the computational domain. Fourier methods for non-periodic problems were also presented by **R. Platte** and **A. Gelb** in their presentation entitled *A hybrid Fourier-polynomial method for partial differential equations*. Similarly, **R. Braverman** presented a discussion of methods based on local Fourier bases obtained from use of windowing functions. All of these presentations showed that Fourier methods could be employed in a manner which allows the solver to avoid time step inherent in Chebyshev methods (due to the tight boundary discretizations in those methods) were to be used. In a related context, the presentation by **T. Driscoll** considered various powerful functions provided by Chebyshev-based methods that can be accessed from the Matlab application *Chebfun*, and the presentation by **S. Lau** demonstrated a multidomain spectral-tau method for the solution of the three dimensional helically reduced wave equation. Finally, the use of adaptive meshes applied to the pricing of financial derivatives was discussed in a the presentation by **C. Christara** entitled *Adaptive and high-order PDE pricing of financial derivatives*. A space-time adaptive and high-order method was developed for valuing options using a PDE approach. Both finite difference and finite element methods were considered for the spatial discretization of the PDE, while classical finite differences were used for the time discretization. To control the space error, an adaptive gridpoint distribution based on an error equidistribution principle was used.

A major concern for stability is the way in which the boundary conditions are enforced, especially for high-order methods. Many presenters, including those listed above addressed the manner in which the boundary conditions can be enforced within their specific methodologies throughout the presentation. Additionally, **T. Hagstrom** (Southern Methodist University) focused on the specifics of applying boundary conditions in the context high-order differentiation schemes and the resulting difficulties along with varies partial resolutions that have been developed. Significant progress has been made to stabilize high-order differentiation schemes by controlling the behavior at the boundary and this presentation overview of strategies in this area will be important for all workshop participants working on high-order methods to consider. A discussion of stability in the context of integral equation methods was presented by **X. Antoine** for the iterative solution of the Helmholtz equation in by means of finite element methods. In particular, the presentation introduced certain *Shifted Laplace Preconditioners*, which can stabilize the conditioning of the associated weak formulation, with controlled dependence on the wave number.

Presentation highlights in the area of *High-Order/Spectral Accuracy* Several issues related to the stability of high-order numerical methods have been discuss in the workshop. Amongst these, **Victor Dominguez** presented a convergence analysis of a Nyström method for 3D BIEs in acoustic scattering problems, in which he outlined a much needed rigorous analysis of a high-order Nyström method for the combined Boundary Integral Equation (BIE) that arises in 3D sound-soft acoustic scattering by a smooth obstacle S.

The workshop hosted several presentations on the design and analysis of efficient numerical methods for solution of PDEs in periodic media via periodic and quasi-periodic Green's functions. These are timehonored challenging problems, whose solution has escaped the scientific computing community in several important cases. Most notably, the issues of Wood anomalies (that is frequencies for which classical quasi-periodic Green's functions put forth in the literature do not exist) in 3D is not entirely resolved. In this connection, **M. Siegel** presented a small-scale decomposition for 3D boundary integral computations with surface tension, in which he showcased an efficient, non-stiff boundary integral method for 3D interfacial flow with surface tension, with an application to porous media flow. For these problems, the velocity of the interface is typically given in terms of the Birkhoff-Rott integral, and a new method to compute this efficiently by Ewald summation was presented. The stiffness was removed by developing a small-scale decomposition. In order to develop this small scale decomposition, the problem was formulated using a generalized isothermal parametrization of the free surface.

Several important contributions related to rapidly convergent quasi-periodic Green's functions throughout the frequency spectrum were highlighted in the presentation by **S. Shipman** presented an efficient solver for acoustic and electromagnetic scattering problems in three-dimensional periodic media. The speaker presented an accurate and efficient numerical method, based on integral Nyström discretizations, for the solution of three dimensional wave propagation problems in piece-wise homogeneous media that have two-dimensional (in-plane) periodicity (e.g. photonic crystal slabs). The approach uses (**1**) A fast, high-order algorithm for evaluation of singular integral operators on surfaces in three-dimensional space, and (**2**) A new, representation of the three-dimensional quasi-periodic Green's functions, which, based on use of infinitely-smooth windowing functions and equivalent-source representations, converges super-algebraically fast throughout the frequency spectrum—even for high-contrast problems and at and around the resonant frequencies known as Wood anomalies. A related periodic problem was discussed by **J. Tausch**: in this case, an eigenvalue problem on periodic waveguides was considered, where periodicity was enforced through appropriate uses of *Dirichlet-to-Neumann maps*. **M. Melenk**, in turn, considered the convergence properties of numerical methods for boundary value problems for the Helmholtz equation at large wave numbers k. At the heart of the analysis lies a decomposition of solutions into two components: the first component is an analytic, but highly oscillatory function and the second one has finite regularity but features wavenumber-independent bounds. An important contribution results: for a conforming high order finite element method quasi-optimality is guaranteed provided (a) the approximation order p is selected as $p = O(\log k)$ and (b) the mesh size h is such that kh/p is small. **J. Ovall** considered issues concerning error estimation and adaptivity for finite element approximation of eigenvalues, with a focus on the use of efficient hp finite elements that robust with respect to singularities and near-singularities in the eigenfunctions, degeneracies and near-degeneracies in the spectrum, and discontinuities or other undesirable behavior in the differential operator.

A focus also developed in the workshop on the general area of efficient numerical methods for fluid-dynamics. **J-C. Nave** discussed a variety of numerical methodologies for fluid-dynamics and other PDE problems and interface problems, including methodologies based on level set methods and finite-difference schemes. In particular, Nave presented an approach that augments the level set function values by gradient information, and evolves both quantities in a fully coupled fashion. This procedure allows the algorithm to maintain the coherence between function values and derivatives, while exploiting the extra information carried by the derivatives. The method is of comparable quality to WENO schemes, but with optimally local stencils. In addition, structures smaller than the grid size can be located and tracked, and the extra derivative information can be employed to obtain simple and accurate approximations to the curvature. **G. Wright**, in turn, presented an efficient methodology based on Radial Basis Functions in conjunction with Partitions of Unity for solution of atmospheric transport (advective) fluid motions.

Several contributors discussed eigenvalues of important classical operators. **N. Nigam** discussed recent progress on eigenvalue problems related to the Laplace operator. In particular, discussion dealt with sharp bounds on the eigenvalue of the Laplace-Beltrami operator of closed Riemannian surfaces of genus higher than one, and eigenvalue problems for the Laplacian, with mixed Dirichlet-Neumann data. **P. Monk** (University of Delaware) discussed the "Interior Transmission Problem" (ITP), which gives rise to a non-standard eigenvalue problem. Properties of the ITP were discussed in several applications and numerical schemes for computing the related eigenvalues were explored. Remarkably, transmission eigenvalues can be observed from far field data, and the resulting eigenvalues can be used to estimate properties of the scatterer. **M. Costabel and M. Dauge** presentation, in turn, concerned the Cosserat eigenvalue problem, that is, the Dirichlet problem for the Lame equations of linear elasticity, where the bulk modulus is considered as the eigenvalue parameter. This problem is notoriously difficult from the computational point of view; this presentation included recent progress on theoretical and on numerical aspects of this problem.

Another very important area of research that was featured in the workshop is efficient solutions of PDEs with a large number of possibly random parameters. The presentation given by **M. Ganesh** concerned a model reduction algorithm for parametrized multiple particle electromagnetic configurations. In this approach, a parameterized multiple scattering wave propagation model in three dimensions is considered as a function of the parameters in the model—describing the location, orientation, size, shape, and number of scattering particles as well as properties of the input source field such as the frequency, polarization, and incident direction. For such dynamic parameterized multiple scattering models, the standard discretization procedures are prohibitively expensive due to the computational cost associated with solving the full model for each online parameter choice. In the work presented, an iterative offline/online reduced basis approach for a boundary element method was proposed in order to simulate a parameterized system of surface integral equations reformulation of the multiple particle wave propagation model. In a related connection, **Y. Chen** presented certified fast algorithms for electromagnetic problems based on the use of reduced basis methods. In particular, like Ganesh's method, this approach was concerned with offline/online solution strategies for electromagnetic scattering problems to effect dramatic reductions in the computational costs for parameterized PDEs. The discussion concerned a posteriori error estimation to control the accuracy of the reduced basis methods as well as generalization of the applicability of the approach through use of domain decomposition.

Presentation highlights in the area of *Fast Iterative Methods* The area of numerical solutions for wave propagation problems in the high-frequency regime has been extremely active in the past decade. Our workshop hosted several speakers that have made key contributions in this area. **S. Chandler-Wilde, S. Langdon and E. Spence** considered numerical-asymptotic boundary integral methods for problems of high-frequency acoustic scattering, and discussed the authors' recent progress on the design and analysis of hybrid numerical-asymptotic boundary integral methods for boundary value problems for the Helmholtz equation that model time harmonic acoustic wave scattering in domains exterior to impenetrable obstacles. Their presentation included new results on the analysis of highly oscillatory boundary integral operators and on the high-frequency asymptotics of scattering problems as well as the fundamental question of whether the Helmholtz equation is sign-indefinite.

One important issue that several speakers in our workshop addressed is the design of numerical solutions of PDEs that are based on formulations of the PDEs whose spectral properties lead to rapidly convergent algorithms. For instance, boundary integral equations are a viable approach for the solution of linear PDEs as they offer an important dimensional reduction, yet the classical integral equations of many PDEs may not possess good spectral properties. Several of our participants have been made significant progress in the design and implementation of hybrid integral formulations that exhibit nearly optimal spectral properties. The presentation by **D. Levadoux** presented certain inherently well-conditioned formulations for time-harmonic scattering/transmission problems of electromagnetism. These equations form a family of source integral equations for the solution of time-harmonic Maxwell scattering and/or transmission problems. Regardless of the composition of the obstacle—metallic, full dielectric or coated with an impedance layer—the general methodology presented by the speaker is able to guide the construction of well-conditioned integral equations.

The very important issue of spectral properties of boundary integral operators for scattering problems has been recently investigated in relation to convergence properties of linear algebra solvers. In connection with spectral properties of various possible formulations of PDEs, nonnormality is a well studied subject in the context of partial differential operators. Yet, only little is known for boundary integral operators.The presentation by **T. Betcke**, on nonnormality of boundary integral operators in acoustic scattering, addressed issues related to the lack of normality of boundary integral operators and the impact of this property on the convergence of associated iterative solvers. In particular, recent results presented by the speaker for the analysis of spectral decompositions and nonnormality of boundary integral operators on general domains were discussed. One particular application is the analysis of stability constants for boundary element discretizations.

Boundary integral techniques have been extensively used for simulation of wave propagation phenomena, including scattering by penetrable and non-penetrable obstacles. The collection of potentials and integral operators associated to a particular operator (the acoustic wave propagation at fixed frequency, for instance, leads to Helmholtz's operator) can be used to build a Calderón Calculus—which amounts to a set of rules to handle potentials and operators, leading to well posed integral operators of the first and second kind, resonance-free combined field formulations, preconditioners, etc. In the presentation by **F. J. Sayas**, a recently completed fully discretized Calderón Calculus for the two dimensional Helmholtz equation was discussed. This full discretization can be understood as a highly non-conforming Petrov-Galerkin discretization of the continuous calculus, based on two staggered grids, Dirac delta distributions substituting acoustic charge densities and piecewise constant functions substituting dipole densities. It was pointed out in the presentation that the frequency-domain approximations and the convolution quadrature black-box introduced by C. Lubich can be combined, yielding a simple approach for simulation of scattering of transient waves in the plane.

Other workshop highlights The workshop fostered a wide variety of research connections and the development of collaborations in ways traditional conferences do not—ample time afforded opportunities for meaningful exchanges leading, in particular, to consolidation of ideas, methods, and even research efforts amongst the participants. The organizers believe that these informal discussions played a significant role towards making the workshop a great success.