# High-order methods for computational wave propagation and scattering

organized by
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Workshop Summary

This workshop was concerned with the development of numerical methods for wave propagation with a focus on high-order convergence for general scattering configurations (with applicability to complex and singular geometries and high frequency problems), including integral equations, finite-difference and finite-element algorithms, spectral and Fourier based approaches and hybrids of asymptotic and numerical methods.

A rich set of exchanges occurred during the five days of this workshop; the organizers feel much was accomplished in this period of time with regards to bridging gaps between experts in different fields of the general area under consideration. In what follows the minutes of the workshop are presented in some detail. The organizers are thankful for Prof. Catalin Turc's careful records in these regards, without which this report could not have reached the desired level of detail and quality.

## 1. Monday, September 10 2007

In the morning of this first day of the workshop lectures by Dr. Penny Davies (entitled "Numerical Solution of Time Domain Boundary Integral Equations"; delivered by herself) and by Drs. C. Geuzaine, R. Reitich and Catalin Turc, (entitled "Frequency Domain Integral Equations for Acoustic and Electromagnetic Scattering Problems"; delivered by C. Turc) were presented. In the afternoon discussions concerning the morning lectures as well as the general topic "Time-domain vs. frequency-domain solvers" and involving the complete group of attendees were conducted. A summary of salient points of these discussions are provided in what follows.

**Question 1** (raised by Ralf Hiptmair) : Is there a theory of preconditioning for Nyström methods? In particular, if the original operator and the preconditioner are individually discretized, can one prove that the composition of the discretized operators (i.e. the products of matrices) is uniformly well-conditioned? More precisely, if $A$ and $B$ are two integral operators of opposite order such that $AB \sim I$ (meaning their composition differs from identity by a compact operator), and $A_h$ and $B_h$ are approximations to the integral operators obtained via a Nyström method, we are interested whether there exist $c_1$ and $c_2$ such that $0 < c_1 \leq \kappa(A_h B_h) \leq c_2$ for all $h \leq h_0$. As a model problem, we can consider the case when the operators of opposite order are given by the single layer potential operator $S$ and the Neumann trace of the double layer potential operator $N$ corresponding to the Laplace equation. In this connection, it would be relevant to study in what sense the Calderon relations translate to the discrete level of the operators $S_h$ and $N_h$. Once this particular problem is understood, one could pursue the same questions in the case of layer potential operators for the Helmholtz and Maxwell equations.

In the classical sense, if the integral operator $A$ is defined as

$$(Au)(x) = \int K_A(x,y)u(y)dy,$$

a Nyström approximation of $A$ is given by

$$(A_h u)(x) = \sum_j K_A(x,y_j)u(y_j)w_j$$

where the $y_j$ form a grid of size $h$ and the $w_j$ are quadrature weights, so that $A_h$ converge spectrally to $A$ in a certain norm of interest, i.e. $||A_h - A|| \leq Ce^{-ch}$ for $h$ small enough. In a larger , a Nyström approximation is any super-algebraic or possibly spectral approximation of the operator $A$ that does not simply amount to discrete formulas of the previous type. For example, such approximations were proposed by Bruno et al. and Beale.

**Question 2** (raised by Tom Hagstrom): In the case of time-domain scattering from a sphere or more generally convex obstacle, the solution decays exponentially in any compact set as time goes to infinity (Morawetz et al.) when the object is illuminated with a finite-time pulse. Yet, numerical instability was observed when attempting to solve the time-domain scattering problem using retarded single layer potentials. The question is whether there is a relationship between the unique solvability of single layer potential integral equation formulations in time domain and the spurious resonances introduced by single layer potential integral equation formulations in the frequency domain. Moreover, is it possible to extend the resonances-free combined field integral equation approach from the frequency domain to the time domain in order to remedy the issue of instability?

**Question 3** (raised by Penny Davies): It is well established that in the frequency domain the solutions to scattering problems from objects that exhibit geometric singularities are themselves singular, and the nature of their singularity is fairly well understood and employed with various degree of success in the design of high-order numerical methods for such applications. For, instance, in the case of acoustic scattering from open surfaces, the scattered fields can be expressed as single layer potential in the sound-soft case and as double layer potentials in the sound-hard case, leading to the integral equations of the first kind $S_k\phi = -u^{inc}$ in the former case and $N_k\psi = -\partial u^{inc}/\partial n$ in the latter. In the neighborhood of the edge the fields are known to behave asymptotically as $\phi \sim 1/\sqrt{d}$ and $\psi \sim \sqrt{d}$ where $d$ is the distance to the edge measured along the normal to the edge. In order for such singular asymptotic behaviors of the densities be used to great effect in numerical schemes for time-domain integral equation formulations, more refined estimates of the previous kind are needed that should express the dependence of the asymptotic constants on the wavenumber and incident field (e.g. the direction of propagation of the plane wave). The question is whether you can control the constants in the previous asymptotic formulas for all plane-wave incident fields of varying frequencies?

## 2. Tuesday, September 11 2007

In the morning of this second day of the workshop lectures by Dr. Thomas Beale (entitled “Computing with Singular and Nearly Singular Integrals”; delivered by himself) and by Drs. S. Chandler-Wilde, M. Dauge and R. Potthast, (entitled “On Singularities in Direct and Inverse Scattering Problems”; delivered by R. Potthast) were presented. In the afternoon discussions concerning the morning lectures as well as the general topic "Geometric singularities and high-frequency scattering problems" and involving the complete group of attendees were conducted. A summary of salient points of these discussions are provided in what follows.

**Question 1** (raised by Penny Davies) : How much information about geometric singularities can be determined from the far-field data? This issue plays a central part in the engineering design of aircrafts, where the paradigm is to design geometric configurations whose RCS are the most challenging to compute accurately. In particular, in the framework of the geometric theory of diffraction, it has been suggested by Joe Keller that the edge and corner singularities are visible in the far-field pattern.

**Question 2** (raised by Ralf Hiptmair): How can one best handle geometric singularities in the context of Nyström methods? One of the main challenges of Nyström methods is to integrate to high-order the singularity of the kernels of the integral operators. This is exacerbated when geometric singularities in the domain of integration, as in addition to the more singular nature of the integral operators, the densities are themselves singular in the neighborhood of the geometric singularities of the domain. Recently, Bruno et al. devised a successful strategy to obtain high-order Nyström methods for domains with edges in three dimensions. The question was directed toward a detailed explanation of this strategy.

**Question 3** (raised by Simon Chandler-Wilde): How would you best design graded meshes for high-frequency methods for objects with and without geometric singularities? The recent success of high-frequency numerical methods for scattering problems relies in one hand on the choice of the ansatz in the solution and on localized integration techniques to certain regions of the obstacles that contribute the most to the scattered field on the other hand. These two aspects are handled in numerical methods with graded meshes that are designed to capture the relevant feature of the fields and of the underlying geometry in the special regions of interest. However, there is a need to understand the manner in which such graded meshes should be optimally designed, and the question was aimed precisely at this issue.

**Question 4** (raised by Tom Hagstrom): Can one handle the issue of geometric singularities by avoiding them altogether in some clever way? Since posing the problems on the actual boundary needs to address the issue of geometric singularities as the singular solutions need to be appropriately represented, the question is whether it would be possible to reformulate the problem on ficticious domains around the geometric singularities via transparent boundary conditions. The possible gains of this approach should stem form the fact that on the newly introduced domains, the solutions to the reformulation of the problem are no longer singular.

## 3. Wednesday, September 12 2007

In the morning of the third day of the workshop lectures by Drs. R. Hiptmair and P. Monk (entitled "Plane Wave Discontinuous Galerkin Methods", delivered by R. Hiptmair and by Dr. T. Hagstrom, (entitled "Towards Efficient Volume-Based Time-Domain Solvers for Scattering Problems", delivered by himself) were presented. In the afternoon discussions concerning the morning lectures as well as the general topic "Finite element vs. finite difference methods" and involving the complete group of attendees were conducted. A summary of salient points of these discussions are provided in what follows.

**Question 1** (raised by Thorsten Hohage, Rainer Kress and Oscar Bruno): Is the Lippman-Schwinger integral equation formulation a viable alternative for scattering problems from inhomogeneous media? The scattering problems from inhomogeneous media have been traditionally approached within a FEM methodology based on variational formulations of the governing differential equations. As an alternative, methods based on the Lippman-Schwinger have been developed, and these methods appear to be more versatile than generally believed, since they can handle discontinuities in the material properties while still being overall efficient. The purpose of the question is to explain the details behind numerical schemes based on Lippman-Schwinger equations developed by Hohage, Bruno and Hyde, details which will facilitate putting in perspective the possible merits of such strategies.

**Question 2** (raised by Ralf Hiptmair): Numerical dispersion in domain and surface methods. The problem stems from the fact that volumetric (domain) methods that rely on variational formulations of the differential operators for wave equations, while local, introduce numerical dispersion, and this pollution effect seems to be unavoidable. On the other hand, surface methods that rely on integral equation formulations, introduce highly non-local operators, but do not appear to suffer from numerical dispersion.

**Question 3** (raised by Peter Monk): Is there a way to overcome the ill-conditioning in the Ultra Weak Variational Formulation (UWVF) for wave equations? The ill-conditioning of the UWVF stems from the approximation properties of the plane-wave expansions. To overcome this issue, other basis expansions based on exact solutions to the Helmholtz equation could be pursued. In this regard, several other possibilities such as the Method of Fundamental Solutions and Wave-ray were mentioned.

**Question 4** (raised by Tom Hagstrom): Can embedded boundary methods be used for time-domain solvers for scattering problems? The main difficulties associated with this approach come from maintaining the high-order accuracy at the boundaries while avoiding the small cells instability. A recent approach based on a combination of ADI methods and continuation methods was developed by Bruno and Lyon, and their method does not seem to suffer from the aforementioned issues.

## 4. Thursday, September 13 2007

On Thursday morning of the lectures by Drs. F. Cakoni and D. Colton (entitled “Qualitative Methods in Inverse Scattering”, delivered by F. Cakoni) and by Drs. M. Ganesh and M. Pieper (entitled “Spectrally Accurate Algorithms for Direct and Inverse Electromagnetic Scattering in Three Dimensions”, delivered by M. Ganesh) were presented. In the afternoon discussions concerning the morning lectures as well as the general topic “Inverse Problems” and involving the complete group of attendees were conducted. A summary of salient points of these discussions are provided in what follows.

**Question 1** (raised by Fioralba Cakoni): Are there any ideas for how to extend the qualitative inverse methods in the time domain? This question pertains to a recurring theme throughout this workshop, that is, a significant body of work has been devoted to frequency domain methods both in direct and inverse scattering problems, yet relatively few efforts were directed to translate these methods to the time-domain counterpart.

**Question 2** (raised by Fioralba Cakoni, Roland Potthast, etc.): Can one couple qualitative and Newton methods in inverse problems? On one hand, Newton methods work well as long as certain a priori information and good initial guesses are available, and only few incident waves guarantee good reconstruction. On the other hand, qualitative methods need not require any a priori information, but multi-static data should be available. The question is thus whether a combination of the particular advantages of two main approaches is possible.

**Question 3** (raised by Hanyou Chu): Are the backscattered data only enough for the purposes of the inverse problems? The question stems from practical considerations, as most technical devices are geared toward measurements of the backscattered data (scattering amplitude) rather than the phase of the far-field. On the other hand, most numerical methods in inverse problems assume that information about the phase of the scattered far-field is available.

**Question 4** (raised by Simon Chandler-Wilde): Conditioning in integral equations for acoustic and electromagnetic scattering. The question of interest is the asymptotic dependence for large wave numbers of the condition numbers of the linear systems obtained through various possible discretizations. Various studies have been carried out for geometries for which these operators are diagonal, and explicit asymptotic expansions have been obtained. In the case of more complicated configurations such as cavities, new results suggest that the rate of growth of the condition number increases more dramatically with the wavenumber, and the question is how effective the regularization techniques are in this case.

## 5. Friday, September 14 2007

On Friday morning of the lectures by Dr. T. Hogage (entitled "Computing Complex Resonances", delivered by himself) and by Drs. H. Haddar and P. Monk (entitled "Asymptotic Models for EM scattering: Theoretical and Numerical Issues for General Impedance Boundary Conditions", delivered by H. Haddar) were presented. In the afternoon discussions concerning the morning lectures as well as the general topic " Resonances and Impedance Boundary Conditions" and involving the complete group of attendees were conducted. A summary of salient points of these discussions are provided in what follows.

**Question 1** (raised by Oscar Bruno): Is it possible to use an iterative solver for scattering problems near or at resonances? The issue is related to the fact that resonances correspond to zero eigenvalues, and, as a result, iterative solvers take more iterations while incurring losses in the accuracy. However, once a priori information is available about the location of such resonances, one can use deflation techniques to solve the linear system in a space that does not contain eigenvectors corresponding to small eigenvalues, and, thus, the number of iterations is controlled.

**Question 2** (raised by David Colton): Is there a connection between transmission eigenvalues and resonance states?

**Question 3** (raised by Tom Beale): Can one construct an incomplete system of eigenfunctions for the scattering matrix?

**Question 4** (raised by Ralf Hiptmair, Fioralba Cakoni, Monique Dauge): Could the far field data behave better than the near-field data in the case when geometric singularities such as corners are present? The question stems from the fact that geometric singularities complicate significantly the analysis and the design of high-order methods for scattering problems. The asymptotic nature of the singularities of solutions is fairly complicated even at the level of the leading order singularity, hence the judicious use of this knowledge in the design of efficient, high-order numerical methods is far from obvious, regardless of the framework of the approach. Thus, naturally, the question arises whether it would be possible to use the effect of the geometric singularities into the far-field solution, which is not as singular as the effect on the solution in the near-field.

Finally, at the conclusion of the workshop the following research directions were identified as holding significant promise.

(1) Qualitative methods in time-domain inverse scattering problems via the work on qualitative methods in frequency domain
(2) Towards full fidelity computations for scattering from complicated obstacles and reliable error analysis
(3) High-frequency scattering from polygonal and polyhedral objects
(4) Numerical advantages of combined field integral equations in the time-domain
(5) A priori and a posteriori adaptivity in plane-wave methods
(6) Clarify the wave number dependence of numerical methods for scattering applications