A02_Project Description – Application to the ETH Zurich Postdoctoral Fellowship programme

2.1 Summary

The project is concerned with the numerical simulation of acoustic and electromagnetic scattering of time-harmonic waves, which is a core task in computational science and engineering and enabling technology for optimization and imaging. A popular class of numerical methods relies on integral equations, which recast time-harmonic scattering problems into functional equations satisfied by surface densities defined on the scattering obstacle. Various techniques are known to approximate the solution of those equations numerically. However, the system matrix of the discrete problem may be ill-conditioned, which regularly happens for high-resolution discretizations and very low or high frequencies.
We aim at designing and analyzing rigourously a range new numerical schemes that yields well-conditions linear systems, are able to deal with complex geometry of the scatterers, and are robust in the low- and high-frequency limits. We focus on thin scatterers modeled as open curves or surfaces, so-called screens. Moreover, the new methods will be systematically implemented and tested numerically to illustrate the theoretical findings.
First, we will derive combined-field integral equations for multi-screens, which are among the most general and complex types of scatterers faced in applications. Combined-field methods have been very successful for massive scatterers but are not yet available for screens. Yet, the modern quotient-space treatment of multi-screens seems perfectly suited for the application of this idea.
Second, we will develop "conformal preconditioners" for integral equations on polygons. At the the heart of the idea is a simple identity relating the conformal mapping of a given polygon into a circle to the Dirichlet-Neumann operator. This leads to the formulation of new preconditioners and hints at a new kind of theoretical tools to analyze integral equations on polygons.
Promising partial theoretical and numerical results for acoustics in two dimensions are already available. The ideas naturally generalize to three dimension and, with suitable adaptations to electromagnetic scattering. Once elaborated for these problems, the full potential of our new methods will emerge and, we believe, they will have an impact in computational engineering.

2.2 Project details

2.2.1 Topic, state of research and open problems

Forward scattering problems in frequency domain

Assume that an incident time-harmonic wave with frequency k impinges on an obstacle, or a material heterogeneity, an airplane in the sky, a crack in a material, a tumor in the body, etc.. The presence of the obstacle generates a scattered field propagating away from it. The shape and intensity of this scattered field depends on the location, geometry and material properties of the scatterer. Scattering problems arise in different areas and different types of waves, like sound waves (acoustics), electromagnetic waves, and elastic waves, of which the first two will be in the focus of the project.

In many contexts it is fundamental to predict the scattered field from the *a priori* knowledge of the scattering object and incident wave. This can only be done by numerical computations, and one wants high accuracy at moderate computational cost. This is important for engineering (acoustics, electromagnetism) and is also an essential step in most algorithms for inverse problems.

This project aims to address on the following aspects of numerical simulation of scattering problems:

- We look for extensions and improvements of existing numerical methods in the specific case where the scatterer is a "screen", that is, an object modeled by an infinitely thin layer, its geometry described as an open curve (2D) or surface (3D). So-called multi-screens will also be considered, which are generalizations of screens, in particular featuring junctions.

- The key parameter is the wave frequency k. High-frequency problems are challenging because they require finer discretization. Moreover, methods that are efficient at medium frequencies are often haunted by instability in the high or low frequency ranges. In this project, we aim at designing methods with provably robust behavior with respect to frequency.

Integral equations and boundary element methods (BEM)

Among the standard mathematical tools most suitable for this task are integral equation formulations and the Galerkin boundary element method (BEM), see [31, 34]. The discretization of integral equations by BEM leads to dense linear systems, which, nowadays, routinely have more than 10^6 unknowns. The use of matrix-compression techniques like Fast Multipole Methods [23] and H-matrices [24] becomes mandatory. Unfortunately, this rules out the use of direct elimination solvers. The only remaining solver option are iterative methods such as GMRES [33].

For Galerkin BEM for first-kind boundary integral equations, a comprehensive convergence theory is available, but the arising linear systems are notoriously ill-conditioned for high-resolution discretizations, causing the iterative solvers to progress very slowly. Preconditioning becomes indispensable and much research has been devoted to it for about thirty years. The most successful approach has been operator preconditioning [7], also known as Calderón preconditioning, pioneered in [36] and further developed in [3, 11] for electromagnetics, and in [28] for screens.

An alternative are second-kind boundary integral equations. They enjoy better stability with respect to discretization parameters, and for this reason, in many instances, researchers have tried to avoid the use of first-kind integral equations despite their simplicity. However, second-kind boundary integral equations do not seems to exist for screens and, thus, they are not relevant for this project. Discuss this point.

Recent advances and open problems

Let us survey some recent advances in the field of integral equations, and related open problems.

Scattering by screens. We call an obstacle complex when its is not smooth domains or at least a Lipschitz domain, a class of scatterers well understood by now [31]. Issues also arise when singularities like edges or conical points are present. Particular attention has been devoted to BEM for screens and cracks, which provide important examples of non-Lipschitz domains, see [10, 22, 26–29, 32].

In the case of “simple” screens that can be viewed as parts of a boundary of a Lipschitz domain, the formulation of well-posed integral equations in a proper mathematical framework is well-understood [35, 38], and recent advances concern the design of more efficient numerical methods, including high-order approximation schemes and provably “optimal preconditioners”. Additionally, some more challenging geometries are considered, including multi-screens [18, 19] and fractal screens [16]. In those cases, the achievement was to obtain well-posed integral equations and study their theoretical properties. For those complex geometries, many natural questions remain open, e.g. convergence of the numerical methods, singularity analysis and efficient preconditioning.

Robustness in frequency. Although by now optimal preconditioners are available for scattering at Lipschitz domains and screens, [25, 36], it is difficult to precisely determine the dependence on frequency of the performance of preconditioners. S. Chandler-Wilde, D. Hewett, and E. Spence in the UK have been making progress in theoretical asymptotic analysis of the condition number of the classical integral equations without preconditioners [17] and the use of asymptotic-numerical methods [15].

Besides the popular Calderón preconditioners [13, 14] for closed surfaces (recently extended to screens [9]), "analytic preconditioners", based on pseudo-differential calculus which exhibit good frequency robustness [1, 4] have been proposed for closed surfaces, which entertain a close link with regularized combined-field integral equations [12]. Although the frequency robustness properties are clear in practice and thoroughly documented in [7], up to now there is no mathematical theory adapted to the study of this asymptotic robustness. Moreover, those analytic preconditioning methods fail for screens. In the expert community there is a belief that pseudo-differential analysis, which is often involved in constructing those robust preconditioners, should also pave the way for a quantitative estimate of frequency dependence, but such an desirable analysis has not been accomplished yet. Some recent activity centering around semi-classical analysis seems promising [21].

2.2.2 Own (preparetory) work

During my PhD thesis, I have contributed to the research on compression and acceleration methods for the linear systems coming from boundary element methods [5]. I then worked on new *high-frequency preconditioners* for acoustics integral equations on screens in two dimensions, following the paradigm of operator preconditioning. The first publication on this topic [2] presents the analytical framework and some numerical tests. The new preconditioners are inspired by those of [4]. For example, for the single-layer integral equation, the following preconditioning operator is introduced:

$$P_k = \sqrt{-(\omega\partial_\tau)^2 - k^2\omega^2}\,. \tag{2.1}$$

Compare this to the preconditioners of [4] which take the form

$$Q_k = \sqrt{-\Delta_S - k^2 I_d}$$

where Δ_S is the Laplace-Beltrami operator on the closed surface S. In (2.1), ω is a weight function defined on the screen Γ and proportional to $\sqrt{\mathrm{d}(x, \partial\Gamma)}$, while ∂_τ is the tangential derivative. Upon using Padé approximations for the square root, the preconditioner obtained is "quasi-local" in the sense that it involves only sparse matrices, as opposed to Calderón preconditioners which are dense and require an additional compression step. The numerical tests demonstrate the robustness of the method with respect to k and the relevance of the singular weight function ω.

Further, [6] is a more in-depth theoretical paper in which I develop a new type of *pseudo-differential calculus* on open curves, providing support for the definition of P_k. Indeed, it is proven that the term $k^2\omega^2$ is the optimal correction in terms of some pseudo-differential properties of the preconditioner. As in the case of closed surfaces, there remains to confirm the relevance of this pseudo-differential property in terms of numerical performance.

2.2.3 Goals and methods

Frequency-robust preconditioners on 3D screens

Although the numerical method published in [2] is only adapted to two-dimensional contexts, generalizations to three dimensions seem possible and has been attempted in the last chapter of my thesis, with promising empiric results. For instance, on an open surface Γ with the tangential gradient ∇, the preconditioner (2.1) becomes

$$P_k = \sqrt{-(\omega\,\nabla\,\omega)\cdot\nabla - k^2\omega^2}\,.$$

Once this theory is completed for acoustic problems, a natural extension to electromagnetic scattering will be possible, as a natural combination of my work and that of my host professor [27]. Indeed, in [27], from the knowledge of *closed-form inverses* of the single layer and hypersingular operators, a compact perturbation of the inverse of the Electric Field Integral Equation (EFIE) operator is constructed, which leads to uniform bounds for the condition number in the medium and low frequency domain. Replacing the exact inverses by the square-root operators (which are compact-equivalent to the exact inverses), it is expected to obtain similar results, while benefiting from the quasi-local form and the high-frequency robustness.

After dealing with electromagnetic problems, one can attempt to generalize this method to other operators (Hodge-Helmholtz, Dirac) and related scattering problems, which are actively investigated in my host group. Another natural research direction is the extension of the pseudo-differential calculus of [6] to open surfaces in 3D.

Conformal preconditioners

It is widely known that in generalized combined-field formulations, the exterior Dirichlet to Neumann (DtN) map is the optimal coupling operator. For a simply connected domain Ω in dimension 2, and for the Laplace problem ($k = 0$) it is possible to show that the exterior DtN Λ_0 is given by

$$\Lambda_0 = \sqrt{-(\omega\partial_\tau)^2}\ ,$$

where ∂_τ is the tangential derivative on the boundary of the polygon and

$$\omega(x) = |(\nabla f) \circ f^{-1}(x)|$$

where f is the conformal mapping that transforms the exterior of Ω to the exterior of the unit disk. This generalizes naturally the ideas of my thesis to more general domains in dimension 2. When Ω is the interior of a polygon, it is possible to compute efficiently the conformal mapping using the Schwarz-Christoffel formula [20]. By analogy with the results of my thesis, one is led to believe that, for the Helmholtz problem ($k \neq 0$), the operator

$$\sqrt{-(\omega\partial_\tau)^2 - k^2\omega^2}$$

may be a good approximation of the exterior DtN map Λ_k. In addition, using the conformal change of variables, the global pseudo-differential calculus on the circle [37] could provide a new, useful pseudo-differential class on the polygon, thus furnishing a natural tool to investigate this question. Preliminary theoretical and numerical investigation are very promising.

This work would also point to ways to attach 3D singularities such as wedges, which are very common in practical applications.

Quotient space framework for integral equations on multi-screens

Another promising idea is the possibility of formulating "combined-field" integral equations for multi-screens. Combined field formulations are well-known for smooth scatterers and have been introduced more than 50 years ago [8] as a way to guarantee the well-posedness of the equation at any frequency. For screens, combined field integral equations have been elusive, because they degenerate when the obstacle no longer has interior. However, we have recently discovered that the formalism of quotient-spaces for multi-screens restores a "virtual" interior to the obstacle, and a combined-field equation can be formulated mathematically without difficulty. Preliminary numerical simulations have shown the power of this idea and it will be an immediate objective of this project to implement this idea and analyze it rigorously. This also unlocks the possibility to implement regularized combined field equations on such geometries, hopefully leading to frequency-robust formulations. Motivation: Screen first-kind BIE are well-posed for all frequencies! + : possibility to make formulate regularized combined field equations, hopefully leading to well-conditioned, robust formulations.

Lastly, after my thesis, I have done a 6-month post-doctorate with Xavier Claeys. At LJLL, UPMC Paris, a former postdoc of my host professor R. Hiptmair, on the topic of preconditioning integral equations on multi-screens using an additive Schwarz approach, see e.g. [30].

Implementation and numerical testing

All the methods that will be developed in this project will be implemented and tested numerically. For BEM simulations in dimension 2, I have developed my own code during my thesis that I can reuse during my stay at ETH. For 3D simulations, I will either use the software Gipsylab, a matlab BEM software which is close in implementation to my code, or use another free software developed by the community like X. Claeys' Bemtools[1], already used in the host group or BEM++[2] by T. Betcke, UCL.

2.2.4 Timetable and research plan

A crude timetable of the research project can be proposed as follows:

- High-frequency preconditioners for 3D screens for scalar waves by December 2020.
- Robust preconditioners for 3D screens for electromagnetic waves by March 2021, collaboration with Dr. Urzua-Torres.
- Conformal preconditioners by July 2021, collaboration with Pr. Alouges.
- Combined-field multi-screens formulations by end of 2021, collaboration with Dr. Claeys.
- Additive Schwarz preconditioners before end of 2021, collaboration with Dr. Claeys.

I changed the format of the two biblio entries you added.

[1] `https://github.com/xclaeys/BemTool`

[2] `http://bempp.com/`

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[3] F. Andriulli, K. Cools, H. Bagci, F. Olyslager, A. Buffa, S. Christiansen, and E. Michielssen. A multiplicative Calderon preconditioner for the electric field integral equation. *IEEE Trans. Antennas and Propagation* 56:2398–2412, 2008.

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2.3 Available resources of the ETH host professor for the realization of the project

The proposed project is of a theoretical and computational nature without an experimental component and does not require any special equipment of facilities, beyond standard resources like office space and IT infrastructure. Researchers a the Seminar of Applied Mathematics have access to D-MATH compute servers and ETH's Euler and Leonhard Linux clusters, which can be used for large-scale computations to be carried out as part of the project.

2.4 Significance of the project for the ETH host professor

Prof. R. Hiptmair's research has had a focus on boundary integral equations, boundary element methods, and preconditioning techniques for many years. In particular he has worked on operator preconditioning, screen problems, and novel BIE approaches to electromagnetic scattering. The natural continuation of this work are investigations into operator preconditioning for complex screens and the development of preconditioning strategies that are robust for high and low (in the case of electromagnetics) frequencies. Thus Prof. Hiptmair's research interests are perfectly aligned with the goals of the fellowship application.

2.5 Planned use of requested budget for research costs

Beside kCHF 4 to be spent for travel, I am planning to use the remaining kCHF 8 of the standard budget of kCHF 12 to pay the salary of 1-2 student research assistants, who are to help me with coding jobs. I hope to be able to hire students after they have done term or thesis projects with me. Thus they can make a substantial contribution to software development in the project.

2.6 Proposed teaching duties of ETH Fellowship candidate

Upon arriving at ETH Zurich I would like to teach an MSc-level course on "Integral Equation Methods for Scattering" beside a Seminar on "Operator Preconditioning". I hope to attract several undergraduate students interested in doing MSc and BSc thesis or term projects under my supervision, thus building a small informal group. I expect a $\sim$30% workload due to teaching proper ($\sim$15%) and supervision ($\sim$15%), though the latter will be closely connected to my research.

2.7 Other requests for funding, especially applications submitted to other fellowship programs

I have not submitted any other applications.

2.8 List of relevant publications by the ETH Fellow candidate and the ETH host professor

[1] F. Alouges and M. Averseng. New preconditioners for Laplace and Helmholtz integral equations on open curves: Analytical framework and Numerical results. Accepted for publication in *Numerische Mathematik*, 2020.

[2] M. Averseng. Fast discrete convolution in $\mathbb{R}^2$ with radial kernels using non-uniform fast Fourier transform with nonequispaced frequencies. *Numerical Algorithms* 83(1):33–56, 2020.

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2.9 Relevant publications of other authors

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