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FREQUENCY-EXPLICIT CONVERGENCE ANALYSIS FOR FINITE ELEMENT DISCRETIZATIONS OF WAVE PROPAGATION PROBLEMS IN HETEROGENEOUS MEDIA

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We consider the Helmholtz equation in a heterogeneous domain $\Omega \subset \mathbb{R}^d$ with $d \in \{2,3\}$. The domain is characterized by its bulk modulus and density $\kappa, \rho : \Omega \to \mathbb{R}^+$, and the boundary $\partial\Omega$ is split into two subdomains Γ_{A} and Γ_{D}. Then, given $f : \Omega \to \mathbb{C}$, we seek a function $u : \Omega \to \mathbb{C}$ such that

$$\left\{ \begin{array}{rcll} -\dfrac{\omega^2}{\kappa} u - \boldsymbol{\nabla} \cdot \left(\dfrac{1}{\rho} \boldsymbol{\nabla} u \right) & = & f & \text{in } \Omega \\ u & = & 0 & \text{on } \Gamma_{\mathrm{D}} \\ \dfrac{1}{\rho} \boldsymbol{\nabla} u \cdot \boldsymbol{n} - \dfrac{1}{\sqrt{\kappa\rho}} u & = & 0 & \text{on } \Gamma_{\mathrm{A}}, \end{array} \right. \tag{1}$$

where $\omega > 0$ is the (given) angular frequency.

We assume that the heterogeneous coefficients κ and ρ are piecewise smooth. Specifically, we assume that there exists a partition $\mathscr{P} = \{\Omega_\ell\}$ of Ω such that each Ω_ℓ has a smooth boundary of class $\mathscr{C}^{m+1,1}$ and that $\kappa, \rho \in \mathscr{C}^{m,1}(\overline{\Omega_\ell})$ for all $\Omega_\ell \in \mathscr{P}$ where $m \geq 0$ is a given integer.[1]

We consider finite element discretizations to problem (1) of degree $p \leq m+1$ that are built on shape-regular meshes $\mathscr{T}_h$ compatible with the partition $\mathscr{P}$. We perform a stability and convergence analysis under the assumption that the problem is solvable for all frequencies. Then, for every $\omega > 0$, there exists a real number $\beta_{\mathrm{s}}(\omega)$ such that

$$\|u\|_{0,\Omega} \leq \frac{\beta_{\mathrm{s}}(\omega)}{\omega^2} \|f\|_{0,\Omega}. \tag{2}$$

The behaviour of $\beta_{\mathrm{s}}(\omega)$ is known for several configurations of interest, and in particular, it depends linearly on ω for non-trapping domains.

Our key result is the following: under the assumption that $\omega h + \beta_{\mathrm{s}}(\omega)(\omega h)^p \leq C$, the finite element solution is quasi-optimal, and we have

$$k\|u - u_h\|_{0,\Omega} + |u - u_h|_{1,\Omega} \leq C \left(h + \frac{\beta_{\mathrm{s}}(\omega)}{\omega} (\omega h)^p \right) \|f\|_{0,\Omega}.$$

Recalling that $N_\lambda = (\omega h)^{-1}$ is a measure of the number of elements per wavelength, our analysis shows that the finite element scheme provides a quasi-optimal solution under the assumption that

$$N_\lambda \geq C \max\left(1, \beta_{\mathrm{s}}(\omega)^{1/p}\right). \tag{3}$$

Following estimate (3), our key conclusion is that high order finite element methods are stable on coarser meshes than low order ones, especially in the high-frequency regime.

This crucial observation is corroborated by numerical experiments, which show that the main estimates we derive are sharp, and that higher order methods generally need much less degrees of freedom to achieve a desired accuracy in the high frequency regime.

ADAPTIVE MULTILEVEL SOLVERS FOR THE DISCONTINUOUS PETROV-GALERKIN METHOD WITH AN EMPHASIS ON HIGH-FREQUENCY WAVE PROPAGATION PROBLEMS

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The work focuses on the development of fast and efficient solution schemes for the simulation of challenging problems in wave propagation phenomena. In particular, emphasis is given in high frequency acoustic and electromagnetic problems which are characterized by localized solutions in problems like ultrasonic testing, laser scanning and modeling of optical laser amplifiers. In wave simulations, the computational cost of any numerical method, is directly related to the frequency. In the high-frequency regime very fine meshes have to be used in order to satisfy the Nyquist criterion and overcome the pollution effect. This often leads to prohibitively expensive problems. Numerical methods based on standard Galerkin discretizations, lack of pre-asymptotic discrete stability and therefore adaptive mesh refinement strategies are usually inefficient. Additionally, the indefinite nature of the wave operator makes state of the art preconditioning techniques, such as multigrid, unreliable.

A promising alternative approach is followed within the framework of the discontinuous Petrov-Galerkin (DPG) method. The DPG method offers numerous advantages for our problems of interest: mesh and frequency independent discrete stability even in the pre-asymptotic region, and a built-in local error indicator that can be used to drive adaptive refinements. Combining these two properties together, reliable adaptive refinement strategies are possible which can be initiated from very coarse meshes. The DPG method can be viewed as a minimum residual method, and therefore it always delivers symmetric (Hermitian) positive definite stiffness matrix. This is a desirable advantage when it comes to the design of iterative solution algorithms. Conjugate Gradient based solvers can be employed which can be accelerated by domain decomposition (one- or multi- level) preconditioners for symmetric positive definite systems.

Driven by the aforementioned properties of the DPG method, an adaptive multigrid preconditioning technology is developed that is applicable for a wide range of boundary value problems. Unlike standard multigrid techniques, our preconditioner involves trace spaces defined on the mesh skeleton, and it is suitable for adaptive hp-meshes. Integration of the iterative solver within the DPG adaptive procedure turns out to be crucial in the simulation of high frequency wave problems. A collection of numerical experiments for the solution of linear acoustics and Maxwell equations demonstrate the efficiency of this technology, where under certain circumstances uniform convergence with respect to the mesh size, the polynomial order and the frequency can be achieved. The construction is complemented with theoretical estimates for the condition number in the one-level setting.

PARALLEL CONTROLLABILITY METHODS FOR THE HELMHOLTZ EQUATION

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The Helmholtz equation is notoriously difficult to solve with standard iterative methods, increasingly so, in fact, at higher frequencies. Controllability methods instead transform the problem back to the time-domain, where they seek the time-harmonic solution of the corresponding time-dependent wave equation. Two different approaches are considered here based either on the first (mixed) or second-order formulation of the wave equation. Both are extended to general boundary-value problems governed by the Helmholtz equation and lead to robust and inherently parallel algorithms. Numerical results illustrate the accuracy, convergence and strong scalability of controllability methods for the solution of high frequency Helmholtz equations with up to a billion unknowns on massively parallel architectures.

INTERPOLATION PROPERTIES OF GENERALIZED PLANE WAVES FOR THE CONVECTED HELMHOLTZ EQUATION

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Trefftz methods are commonly used for wave propagation problems in frequency domain, and rely on basis functions that solve exactly the driving equation, such as classical plane waves. In order to take advantage of Trefftz methods for problems with variable coefficients, in which case there is usually no known exact solution of the PDE to discretize the Trefftz formulation, Generalized Plane Waves (GPWs) have been developed as approximated solutions to the given PDE.

We will discuss the design and interpolation properties of GPWs for the 3D convected Helmholtz equation, emphasizing the similarities with the 2D Helmholtz equation as well as the challenges arising from inhomogeneity and anisotropy of the 3D medium.

ELECTROMAGNETIC TRANSMISSION PROBLEMS: WAVENUMBER-EXPLICIT BOUNDS

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We consider the time-harmonic Maxwell's equations with rough, possibly discontinuous, permittivity ϵ and magnetic permeability μ. Under a natural assumption on ϵ and μ, which excludes ray trapping, we prove bounds on the solution in terms of the data, with these bounds explicit in all parameters. The L^2 norms of the electric and the magnetic fields are bounded by the L^2 norm of the source term, independently of the wavenumber. The range of problems covered includes, e.g., the scattering by a penetrable star-shaped Lipschitz obstacle.

Such explicit bounds are key to developing frequency-explicit error analysis for numerical methods such as FEM and BEM. The "shape-robustness" allows to quantify how variations in the shape of the obstacle affect the solution and makes the bounds particularly suitable for uncertainty quantification (UQ) applications. Our bounds are obtained using identities first introduced by Morawetz (essentially integration by parts).

RIGOROUS COUPLE WAVE ANALYSIS OF ONE DIMENSIONAL DIFFRACTION GRATINGS

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Rigorous Coupled Wave Analysis (RCWA) is a technique for approximating the electromagnetic field in a diffraction grating. It is widely used to obtain rapid solutions for heterogeneous gratings where the relative permittivity varies periodically in one direction. This semi-analytical approach expands all the electromagnetic field phasors as well as the relative permittivity as Fourier series in the spatial variable along the direction of periodicity, and also replaces the relative permittivity with a stairstep approximation along the direction normal to the direction of periodicity. Thus, there is error due to Fourier truncation and also due to the approximation of grating permittivity.

We study the convergence properties of RCWA for s- and p-polarized monochromatic incident light on a one dimensional grating. We prove that the RCWA is a Galerkin scheme, which allows us to employ techniques borrowed from the Finite Element Method to analyze the error.

Fo s-polarization an essential tool is a Rellich identity that shows that certain continuous problems have unique solutions that depend continuously on the data with a continuity constant having explicit dependence on the relative permittivity. We prove that for s-polarization the RCWA converges with an increasing number of retained Fourier modes and with a finer approximation of the grating interfaces. Numerical results show that our convergence results for increasing the number of retained Fourier modes are seen in practice, while our estimates of convergence in slice thickness are pessimistic.

For p-polarization the analysis via a Rellich identity is much more delicate. However, for a grating consisting of absorbing media, we prove convergence both with an increasing number of retained Fourier modes and with a finer approximation of the grating interfaces. Our analytical results suggest a slow rate of convergence depending on the singularities occurring in the solution due to material interfaces.

NEARBY PRECONDITIONING FOR MULTIPLE REALISATIONS OF THE HELMHOLTZ EQUATION, WITH APPLICATION TO UNCERTAINTY QUANTIFICATION

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Let $\mathbf{A}^{(j)}$, $j = 1, 2$, be the Galerkin matrices corresponding to the h-FEM discretisation of the Helmholtz equations

$$\nabla \cdot (A^{(j)} \nabla u^{(j)}) + k^2 n^{(j)} u^{(j)} = -f, \quad j = 1, 2$$

in the exterior of some bounded set with Dirichlet boundary conditions. In this work we answer the following question: when is $\mathbf{A}^{(1)}$ a good left- or right-preconditioner for $\mathbf{A}^{(2)}$? More precisely, we ask: How small must $\|A^{(1)} - A^{(2)}\|_{L^\infty}$ and $\|n^{(1)} - n^{(2)}\|_{L^\infty}$ be (in terms of k-dependence) for GMRES applied to either $(\mathbf{A}^{(1)})^{-1}\mathbf{A}^{(2)}$ or $\mathbf{A}^{(2)}(\mathbf{A}^{(1)})^{-1}$ to converge in a k-independent number of iterations for arbitrarily large k?

We prove that, if

$$k\|A^{(1)} - A^{(2)}\|_{L^\infty} \text{ and } k\|n^{(1)} - n^{(2)}\|_{L^\infty} \text{ are both sufficiently small} \tag{1}$$

then $\mathbf{A}^{(1)}$ is a good preconditioner for $\mathbf{A}^{(2)}$ when using *weighted* GMRES, and numerical experiments show the conditions (1) are sharp. Moreover, numerical experiments show that the conditions (1) are sharp for standard GMRES, but to prove $\mathbf{A}^{(1)}$ is a good preconditioner for $\mathbf{A}^{(2)}$ for standard GMRES we require a slightly stronger condition on $A^{(1)}$ and $A^{(2)}$ than that in (1).

Our motivation for tackling this question comes from calculations in uncertainty quantification (UQ) for the Helmholtz equation with *random* coefficients A and n. Such a calculation requires the solution of many deterministic Helmholtz problems, each with different A and n. The answer to the question above dictates to what extent a previously-calculated preconditioner of one of the Galerkin matrices can be used as a preconditioner for other Galerkin matrices. The extent to which one can reuse preconditioners reduces the cost of the UQ calculation.

SOME CONTRIBUTIONS OF THE NUMERICAL SIMULATION FOR WAVES PROPAGATION IN COMPLEX MEDIA

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In this talk, I will present two numerical methods we have widely used to obtain nice physical results regarding wave propagation in complex heterogeneous media: the moment or volume integral method [3] and the coupled dipoles method [4]. For both I will present the advantages and limitations in term of accuracy and requested computing resources. Two physical systems will be considered as illustrations: near-field optics of semi-continuous metallic films [2] and light propagation in disordered clouds of correlated dipolar nanoparticles [5, 1]. With these examples, I will show the important contribution of the numerical simulation in the understanding and control of wave propagation in strongly scattering media.

References

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A STUDY OF LIGHT-MATTER INTERACTION AT THE NANOSCALE: THEORETICAL AND NUMERICAL CONSIDERATIONS

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Nanophotonics is the area of physics that tries to exploit the interaction of light with nanoscaled structures. By using metallic nanostructures, one is able in particular to obtain impressive exaltation of light and subwavelength confinement. This opens up new possibilities for controlling and enhancing optical wave-matter interactions and leads to a lot of interesting applications such as (to cite but a few) efficient design of nanolasers, nanoantennas, solar cells or biosensing.

In this domain, numerical modelling is fundamental in order to envisage any expensive experimental scenario. The deep understanding of the phenomenon itself is also essential for physicists. A precise study of the possible models are thus essential. The modelling relies on the accurate description of the propagation of an optical wave in a dispersive metallic medium. At the scales and frequencies considered, several effects have to be taken into account. In particular, a correct characterization of the response of the electrons in the metal to the applied electromagnetic field is crucial and can lead to new models. In this work, we propose to focus on a model that incorporates some quantum effects. It consists of a linear coupling between the time domain Maxwell's equations and a linearized hydrodynamic model with a quantum pressure term. Both theoretical and numerical interesting challenges emerge from this PDE model.

We are especially interested in providing a complete study in this context: from theoretical issues of well-posedness and stability, to the development of adapted and efficient numerical algorithms (here we choose to use a discontinuous Galerkin numerical framework) and the study of their academic properties, to finally, efficient numerical simulations on realistic test cases. We will go through several results that we recently obtained for this particular model.

SCATTERING PROBLEMS WITH OSCILLATING, NON-PERIODIC AND DISCONTINUOUS WAVE SPEED

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We study the Helmholtz equation in heterogeneous media in $\mathbb{R}^d$, $d = 1, 2, 3$ modelled in the frequency domain. For a class of oscillatory discontinuous coefficients with spherical symmetry, we present a new theoretical approach to bound the norm of the solution operator by a term which is exponential in the frequency and independent of the number of discontinuities. We present examples of coefficients showing that our estimates are sharp. In particular our examples in 3D differ from the wave localisation effects appearing at a single discontinuity in the geometry or the material ("whispering gallery" modes). Instead, the growth of the stability constant is caused by a highly varying wave speed.

COMPUTATIONAL HIGH-FREQUENCY WAVE PROPAGATION IN HETEROGENEOUS HIGH-CONTRAST MEDIA

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(Wave) scattering and propagation in heterogeneous high-contrast media experiences a rising interest because such materials can develop unusual optical or acoustic properties, such as a negative refractive index or wave guiding, which are important in practical applications. From the numerical side, the solution of such problems exhibits several challenges: (i) spatially rough PDE coefficients and (ii) the high-frequency regime of wave propagation. Through the high contrast in the coefficients even moderate wave numbers can suddenly imply a high-frequency regime in certain parts of the computational domain, thereby even amplifying the aforementioned numerical challenges.

In this talk, we discuss a computational multiscale method in the spirit of the Localized Orthogonal Decomposition to deal with the combination of rough high-contrast coefficients and high-frequency regime. The method does not require additional structures in the coefficients, such as periodicity or scale separation. In the spirit of a generalized finite element method, special multiscale and problem-adapted basis functions are constructed based on the solution of local fine-scale problems. For the global computation, however, only coarse meshes are used, which do not need to resolve the oscillations and discontinuities of the coefficients. Rigorous numerical analysis allows to estimate the discretization error a priori and is confirmed by numerical examples. Furthermore, the numerical experiments also illustrate some astonishing effects of wave scattering in heterogeneous high-contrast media, such as band gaps, flat lenses, or wave guides.