MAFELAP 2019 abstracts for the mini-symposium PDE Eigenvalue Problems: Computational Modeling and Numerical Analysis

Organisers: Christian Engström, Stefano Giani, Nilima Nigam, Xuefeng Liu and Jeffrey Ovall

THE JONES EIGENVALUE PROBLEM IN FLUID-STRUCTURE INTERACTION

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The Jones eigenvalue problem first described by D.S. Jones in [2] concerns unusual modes in bounded elastic bodies: time-harmonic displacements whose tractions and normal components are both identically zero on the boundary. This problem is usually associated with a lack of unique solvability for certain models of fluid-structure interaction. The boundary conditions in this problem appear, at first glance, to rule out any non-trivial modes unless the domain possesses significant geometric symmetries. Indeed, Jones modes were shown to not be possible in most C^∞ domains in [1]. However, while the existence of Jones modes sensitively depends on the domain geometry, such modes do exist in a broad class of domains. This talk presents both theoretical and computational investigations of this eigenvalue problem in Lipschitz domains.

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COMPUTATION OF SCATTERING RESONANCES IN ABSORPTIVE AND DISPERSIVE MEDIA

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Scattering resonances that refer to a meta-stable behavior in time are for open resonators a natural replacement of eigenvalues for closed systems. The most common finite element methods to approximate scattering resonances uses a perfectly matched layer, infinite elements, or a Dirichlet-to-Neumann map. However, these methods encounter severe spectral instability, which in general results in a large number of spurious (unphysical) eigenvalues in addition to approximations of true scattering resonances. Those spurious solutions are a major problem in scattering resonance computations.

In this talk, we consider Helmholtz type of scattering resonance problems in several dimensions with piecewise constant coefficients as well as graded material properties. For electromagnetic problems we assume that the resonators consist of frequency dependent and lossy materials, such as metals at optical frequencies.

Volume integral based methods are in principle applicable and we encounter, in contrary to the differential operator based methods, no spurious solutions in scattering resonance computations. However, this approach is computationally very demanding, in particularly in higher dimensions. Therefore, we compute first approximations of scattering resonances of a differential operator and use a volume integral equation as residual for removing spurious solutions. This is a joint work with Juan Carlos Araujo-Cabarcas.

CONFORMING AND NONCONFORMING VIRTUAL ELEMENT METHODS FOR EIGENVALUE PROBLEMS

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We analyse the conforming and nonconforming Virtual Element Method (VEM) [1, 2, 3, 4] for the approximation of second order elliptic eigenvalue problems. As a model problem we consider the Laplace eigenvalue problem. We present two possible formulations of the discrete problem, derived respectively by a nonstabilized and stabilized approximation of the L^2-inner product, and we study the convergence properties of the corresponding discrete eigenvalue problem. The proposed schemes provide a correct approximation of the spectrum, in particular we prove optimal-order error estimates for the eigenfunctions and the usual double order of convergence of the eigenvalues. Moreover, we show a large set of numerical tests supporting the theoretical results, including a comparison between the conforming and the nonconforming schemes and present some possible applications of the theory.

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A DISCONTINUOUS GALERKIN METHOD FOR SOLVING ELLIPTIC EIGENVALUE PROBLEMS ON POLYGONAL MESHES WITH HP-ADAPTIVITY

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We present a discontinuous Galerkin method for solving elliptic eigenvalue problems on polygonal meshes [1] based on the discontinuous Galerkin composite finite element method (DGCFEM) [2]. In this talk, the key idea of generally shaped element domains in DGCFEM is used to construct polygonal elements and applied to eigenvalue problems. Polygonal and polyhedral meshes are advantageous to discretize domains of complicated shape reducing the overall number of elements needed.

A priori convergence analysis is presented for the method and tested on several numerical examples. Some of the numerical examples use non-convex elements that could be considered pathological in the finite element context.

Further, adaptive techniques are presented for DGCFEM and applied to complicated domains [3]. The mesh-adaptivity is based on a residual error estimator specific for DGCFEM. The robustness and accuracy of the adaptive techniques are supported by numerical examples. Interestingly, the convergence rate of the *hp*-adaptive technique is exponential also for polygonal meshes.

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FEAST ITERATION APPLIED TO PERTURBED PARTIAL DIFFERENTIAL OPERATORS

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Filtered subspace iteration with Rayleigh-Ritz eigenvalue extraction is a recently reviewed method in the form of the FEAST algorithm. In this talk we present a method motivated by the FEAST iteration and apply it directly on the operator level. The core of the algorithm is a numerical resolvent calculus based on contour quadratures coupled with a perturbation analysis of the resolvent evaluation motivated by the results in Numerical Linear Algebra. We prove convergence rate which depends on the properties of the filter (even in the presence of perturbations). Perturbations which we consider can originate both from the projection/truncation of infinite dimensional operators (necessary to evaluate resolvents) or from the uncertainty in the parameters of the underlying problem. This is a joint work with J. Gopalakrishnan and J. Ovall.

EIGENLOCKING ON THIN SHELLS OF REVOLUTION

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The finite element modelling of thin shells is known to be a very demanding task because of the many different ways parametric error amplification or locking phenomena can occur. Here we consider locking in connection with eigenvalue problems in shells, especially in inhibited pure bending shells or shells with clamped support. Our purpose is not to suggest ways for alleviating or circumventing eigenlocking, but to analyse, predict, and demonstrate its existence when the lowest eigenfrequency is computed. Here one has to account for the fact that unlike in second order problems, the lowest mode can have a higher multiplicity. Furthermore, it is possible that the lowest mode is part of such a narrow cluster that the only meaningful interpretation for convergence is to the cluster rather than to the mode itself. The concept of locking in parabolic shells was first identified in [1], but never fully demonstrated through numerical experiments. The results obtained for hyperbolic shells are new.

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WAVE BLOW-UP THROUGH MIXING OF NEUMANN AND DIRICHLET BOUNDARY CONDITIONS

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This talk aims at showing a new and efficient approach for maximizing the transmission between two points at a chosen frequency in terms of the boundary conditions. The proposed approach makes use of recent results on the monotonicity of the eigenvalues of the mixed boundary value problem and on the asymptotic expansion of the Green s function to small changes in the boundary conditions.

More precisely, starting with a Dirichlet boundary condition, we search for a location on the boundary, in which we can apply a short Neumann boundary condition to get an increase in the transmission intensity. As it turns out, there exists a critical length for the Neumann boundary, which will make the transmission-wave blow up. Our algorithm tries to find that domain-depending length, and as we will show, the algorithm succeeds whenever the critical length is small enough.

The switching of the boundary condition from Dirichlet to Neumann can be performed through the use of the recently modeled concept of metasurfaces comprised of coupled pairs of Helmholtz resonators.

A variety of numerical experiments are presented to show the applicability and the accuracy of the proposed new methodology.

EIGENPROBLEM WITH LOW-REGULARITY SOLUTION FOR NUCLEAR REACTOR CORE MODELING

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The behaviour of a nuclear reactor core depends on the nuclear chain reaction, which is described by the neutron transport equation. This equation is a balance statement that conserves neutrons. It governs the neutron flux density, which depends on 7 variables: 3 for the space, 2 for the motion direction, 1 for the energy (or the speed), and 1 for the time. In the steady-state case, one must solve an eigenvalue problem. The energy variable is discretized using the multigroup theory (G groups). Concerning the motion direction, an inexpensive approach to approximate the transport equation is to solve the simplified PN equations ($\frac{N+1}{2}$ coupled diffusion equations). It can be shown that the basic building block which allows to solve the general multigroup simplified PN equations, is the so-called neutron diffusion equation ($G = 1$, $N = 1$), which reads as the following eigenproblem, set in a bounded domain Ω of $\mathbf{R}^3$:
Find $\phi \in H^1(\Omega), \lambda \in \mathbf{R}^+$ such that:

$$\left\{ \begin{array}{rcll} -\mathrm{div}\, D\, \mathbf{grad}\, \phi + \Sigma_a\, \phi & = & \lambda\, \nu \Sigma_f \phi & \text{in } \Omega \\ \phi & = & 0 & \text{on } \partial\Omega. \end{array} \right. \tag{1}$$

Above, the data D, Σ_a, ν and Σ_f denote respectively the diffusion coefficient, the macroscopic absorption cross section, the fission yield and the fission cross section. Note that the data D can be a tensor and the fission cross section can vanish in some area. Concerning the resolution of the eigenproblem (1), we look for the criticality factor: $1/\min_\lambda \lambda$, together with the associated ϕ which corresponds to the averaged neutron flux density. Special attention is paid to the case where the eigenfunctions ϕ can be of low regularity. Such a situation commonly arises in the presence of three or more intersecting material components with different characteristics, as it appears in reactor cores studies. Indeed, the nuclear reactor cores have often a cubic or parallelepipedic geometry and the cross sections are averaged in each square or rectangular cell. They may be constant or piecewise polynomial. They may differ from one cell to another by a factor of order 10.

We analyze matching and non-matching domain decomposition methods for the numerical approximation of the eigenproblem (1). The domain decomposition method can be non-matching in the sense that the meshes of the subdomains, and more generally the finite elements spaces, may not fit at the interface between subdomains. We prove well-posedness of the discrete eigenproblems with the help of a uniform discrete inf-sup condition, and we provide optimal a priori convergence estimates. Numerical experiments illustrate the accuracy of the method.

RIGOROUS EIGENVALUE ESTIMATION AND ITS APPLICATION IN COMPUTER-ASSISTED SOLUTION PROOF FOR THE NAVIER–STOKES EQUATION

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The explicit eigenvalue bounds for differential operators play an important role in the field of computer-assisted proof. For example, to provide mathematically correct solution verification for no-linear partial differential equations, e.g., the Navier–Stokes equation, there appears many quantities reducing to the eigenvalue problem of differential operators. A brief list includes the Poincare constant, the constant in trace theorem, the interpolation error constants, etc.

In this talk, I will first review recently developed numerical methods with the aim of explicit bounds of eigenvalues, especially the ones based on the finite element methods. Particularly, the method proposed in [1] will be mainly introduced, due to its generality in solving various eigenvalue problems, including the ones of the Laplacian [1], the biharmonic [3, 2], the Stokes [4], the Steklov operators [5]. As a direct application of explicit eigenvalue bounds, the case of the solution verification for stationary Navier–Stokes equation in 2D and 3D domains will be introduced [6].

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DISCRETIZATION ERRORS IN FILTERED SUBSPACE ITERATION FOR SELF-ADJOINT OPERATORS

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In recent years, a variety of contour-integral based methods for approximating targeted clusters of eigenvalues, together with their corresponding invariant subspaces, have been proposed and analyzed for finite rank operators (matrices). One particularly popular approach in this vein is the so-called FEAST method, which is essentially a subspace iteration scheme employing a rational function of the operator that "filters" its spectrum in the sense that the eigenvalues of interest of the original operator become the dominant eigenvalues of the filtered operator, while their corresponding invariant subspaces remain the same. Analyses of such methods for matrices, regardless of whether or not they arise from discretizing an infinite rank (unbounded) operator, have focused on *iterative error*, i.e. how rapidly the approximate eigenvalues and invariant subspace converge to the corresponding true eigenvalues and invariant subspace *of the matrix* with respect to the number of iterations.

The focus of our study is on *discretization error*. In other words, if subspace iteration is applied using a discretized version of the filtered operator, how well do the computed eigenvalues and invariant subspace returned by this iteration approximate the corresponding true eigenvalues and invariant subspace *of the original (unbounded) operator* with respect to discretization parameters? We provide a general framework for analyzing filtered subspace iteration for (unbounded) selfadjoint operators that addresses discretization error in approximating both the invariant subspace and the collection of eigenvalues, highlighting a small set of practically-verifiable abstract assumptions that, if satisfied, guarantee convergence with respect to discretization parameters. Because our analysis is carried out on the level of Hilbert spaces, we naturally achieve convergence results in norms appropriate to such settings. We illustrate our key results on one or, if time permits, two types of discretizations of second-order elliptic operators, providing numerical experiments to gauge the sharpness of our results.

GUARANTEED A POSTERIORI BOUNDS FOR EIGENVALUES AND EIGENVECTORS: MULTIPLICITIES AND CLUSTERS

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In this talk we present a posteriori error estimates for conforming numerical approximations of eigenvalue clusters of second-order self-adjoint elliptic linear operators with compact resolvent. Given a cluster of eigenvalues, we estimate the error in the sum of the eigenvalues, as well as the error in the eigenvectors given through the density matrix, i.e., the orthogonal projector on the associated eigenspace. This allows us to deal with degenerate (multiple) eigenvalues within the framework. All the bounds are valid under the only assumption that the cluster is separated from the surrounding smaller and larger eigenvalues; we show how this assumption can be numerically checked. Our bounds are guaranteed and converge with the same speed as the exact quantities. They can be turned into fully computable bounds as soon as an estimate on the dual norm of the residual is available, which is presented in two particular cases: the Laplace eigenvalue problem discretized with conforming finite elements, and a Schrödinger operator with periodic boundary conditions of the form $-\Delta + V$ discretized with planewaves. For these two cases, numerical illustrations are provided on a set of test problems.

FINITE ELEMENT APPROXIMATIONS FOR SEVERAL NON-SELFADJOINT EIGENVALUE PROBLEMS

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In this talk, we shall discuss the finite element approximations for several non-selfadjoint eigenvalue problems including a Steklov eigenvalue problem, a transmission eigenvalue problem, and a scattering resonance problem in a narrow metallic slit. A new eigenvalue solver for the non-Hermitian matrices resulting from the discretization of the above problems will be introduced. Numerical examples are presented as well.

BOUNDARY ELEMENT METHODS FOR ELECTROMAGNETIC RESONANCE PROBLEMS IN OPEN SYSTEMS

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We consider Galerkin boundary element methods for the approximation of different kinds of electromagnetic resonance problems in open systems. Examples are the scattering-resonance problem for dielectric and plasmonic scatterers. An analysis of the used boundary integral formulations and their numerical approximations is presented in the framework of eigenvalue problems for holomorphic Fredholm operator-valued functions. We employ recent abstract results [3] to show that the Galerkin approximation with Raviart-Thomas elements provides a so-called regular approximation of the underlying operators of the eigenvalue problems. This enables us to apply classical results of the numerical analysis of eigenvalue problems for holomorphic Fredholm operator-valued functions [1, 2] which implies convergence of the approximations and quasi-optimal error estimates [4].

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RIGOROUS AND FULLY COMPUTABLE A POSTERIORI ERROR BOUNDS FOR EIGENFUNCTIONS

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Using Laplace eigenvalue problem

$$-\Delta u_i = \lambda_i u_i \quad \text{in } \Omega, \qquad u_i = 0 \quad \text{on } \partial\Omega,$$

as a model problem, a generalization of error bounds from [1] to the case of tight clusters and multiple eigenvalues is presented. Individual eigenfunctions do not depend continuously on problem data, in general, and they are sensitive to small perturbation of the problem in the case of tight clusters and multiple eigenvalues. Therefore, we propose to estimate entire spaces of eigenfunctions corresponding to clusters and multiple eigenvalues.

We derive a guaranteed and fully computable upper bound on a distance between the space of exact and the space of approximate eigenfunctions. The derived bound depends on the width of the cluster, spectral gap between the last cluster and the following eigenvalues, and on the possible non-orthogonality of approximate spaces corresponding to the preceding clusters. The derived bound can be easily computed from two-sided bounds on eigenvalues and the approximate eigenfunctions. No flux reconstructions are needed. It is naturally evaluated recursively, starting from the lowest cluster. Numerical experiments compare several versions of the bound both in the energy and $L^2(\Omega)$-norms. Optimal rates of convergence are observed. More details are presented in [5].

An alternative approach [4] is a generalization of concepts from [2, 3] to the case of clusters and multiple eigenvalues.

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INFINITE ELEMENTS FOR EXTERIOR HELMHOLTZ RESONANCE PROBLEMS BASED ON A FREQUENCY DEPENDENT COMPLEX SCALING

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Complex scaling is a popular method to treat scattering and resonance problems in open domains. Thereby the unbounded domain is decomposed into a bounded interior and an unbounded exterior part. Subsequently the technique of complex scaling is applied to the exterior domain to obtain exponentially decreasing solutions. Finally the complex scaled exterior is usually truncated and discretized using finite elements.

In our work we suggest a number of improvements to the method described above. To resonance problems usually frequency independent scalings are applied, to conserve the linearity of the resulting eigenvalue problem. Unfortunately, a frequency independent complex scaling works well only for a very narrow range of frequencies and the quality of the approximation depends heavily on the specific choice of the scaling function. To overcome this problem we use frequency dependent scaling functions, as it is common when treating scattering problems, for resonance problems as well. This approach leads to polynomial or rational eigenvalue problems instead of linear ones (cf. [2]).

For discretizing the exterior complex scaled problems we use a tensor product method, describing the exterior by a normal and an interface coordinate. Due to this ansatz we evade having to explicitly mesh the exterior domain. To avoid truncation and obtain super-algebraic approximation properties we make use of infinite elements in normal direction, which are based on Hardy space infinite Elements (cf. [1]).

We solve the resulting discrete eigenvalue problems by making use of an adapted version of the shift-and-invert Arnoldi algorithm. Applying this method requires no significant extra computational effort compared to solving linear eigenvalue problems.

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