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On spurious solutions in finite element approximations of resonances in open systems

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ABSTRACT

In this paper, we discuss problems arising when computing resonances with a finite element method. In the pre-asymptotic regime, we detect for the one dimensional case, spurious solutions in finite element computations of resonances when the computational domain is truncated with a perfectly matched layer (PML) as well as with a Dirichlet-to-Neumann map (DtN). The new test is based on the Lippmann–Schwinger equation and we use computations of the pseudospectrum to show that this is a suitable choice. Numerical simulations indicate that the presented test can distinguish between spurious eigenvalues and true eigenvalues also in difficult cases.

1. Introduction

Open resonators are common in many applications including acoustic properties of musical instruments, laser cavities, and multilayer X-ray resonators [1–3]. A widely applicable technique to terminate the computational domain in resonance as well as in scattering problems is a perfectly matched layer (PML). It is possible to prove that the Galerkin method converges (in gap), which implies that in the asymptotic regime there are no Galerkin eigenvalues that are unrelated to the spectrum of the original operator. However, under realistic conditions it is very costly to use sufficiently fine meshes and most computations are therefore done in the pre-asymptotic regime. The PML problem is highly non-normal and there are frequently numerous eigenvalues that are unrelated to the spectrum of the original operator. These eigenvalues are called spurious eigenvalues and they are a major challenge in engineering applications. The origin of these spurious eigenvalues is spectral instability [4–6]. For example, even if the inequality $\|Au - k^2u\| < \epsilon\|u\|$ holds for a very small ϵ, k^2 may still not be close to the spectrum of A.

A common approach that aims to detect spurious solutions is to compute numerical approximations with several sets of PML parameters. Then a perturbation argument is used to distinguish true resonances from spurious solutions [7–9]. This requires several computations of the eigenvalues for different parameters. The basic assumption in this approach is that spurious eigenvalues react more strongly to perturbations than approximations to resonances. However, eigenvalues may also react strongly due to an insufficient approximation and it is unclear how much an eigenvalue should move to be marked as a spurious eigenvalue.

In this paper, we propose a new test based on a volume integral formulation of the problem called the Lippmann–Schwinger equation and argue that this is a suitable choice. This test is applied to numerical solutions obtained with a finite element method where the computational domain is truncated with a PML as well as with a DtN map. Numerical simulations

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indicate that the presented test can distinguish between spurious eigenpairs and true eigenpairs also in complicated cases when the spurious solutions mix with true approximations of resonances. The new test determines if a computed eigenvalue numerically is in an ϵ-pseudospectrum of the integral operator and the corresponding vector is an ϵ-pseudomode. The Lippmann–Schwinger equation is frequently used in acoustic and electromagnetic scattering theory [10] and it has previously been used directly to determine resonances [7,11,12]. The resonant modes grow exponentially at infinity but the integration in the Lippmann–Schwinger equation is only over the resonator where the solutions are well behaved. This is a computationally significant advantage in particular for large structures that contain many air holes. However, the direct approach with an integral equation is demanding since it results in a nonlinear eigenvalue problem (NEP), matrices are full, and each evaluation (e.g. solver iteration) requires a matrix assembly.

An advantage with the DtN map in one dimension is that the resulting eigenvalue problem only has a quadratic nonlinearity and the formulation contains no free parameters. The PML has the advantage that the resulting eigenvalue problem is linear. However, the method contains several parameters, which influence the computational result.

For the DtN formulation, we use a block operator representation and apply standard techniques to prove an estimate for the gap between the discrete and continuous eigenspaces. Moreover, based on the results [13,14] we state the corresponding estimate for the gap in the PML setting. Convergence in gap proves for the DtN formulation that no spurious solutions exist when the finite element space is large enough but the rate of convergence depends critically on resolvent norms that may be very large. The same conclusions hold in the PML formulation with the additional requirement that the PML layer is thick enough [14]. The eigenvalue problem with a truncated PML will have more eigenvalues inside a given region in the complex plane compared with a DtN formulation of the same problem. We introduce a DtN for the truncated PML and determine a region in the complex plane where it is possible to obtain convergence for given PML parameters. Then, we derive a new estimate of the difference between a resonance and an eigenvalue of the finite PML problem. Finally, the integral equation based test is then used to detect spurious solutions in the DtN and PML formulations. The numerical examples indicate that the test can detect spurious eigenvalues in solutions computed with relatively coarse discretizations (computed with h-FEM) as well as for fine discretizations obtained using p-FEM.

The results in this paper are stated for the one-dimensional case, which for the considered test problems, it is possible to reach the asymptotic regime and compute resonances without spurious solutions on a standard computer. This is an advantage, since in this case it is possible to evaluate numerically the performance of the new filtering technique. The filtering process can be extended to higher dimensions and it will then provide a new practical tool for many challenging applications in physics and engineering.

A procedure to efficiently compute resonances with the PML or DtN formulation is then: (i) Use a coarse discretization and e.g. ARPACK with several shifts to compute a selection of Galerkin eigenvalues. (ii) Use the new filtering process to sort out approximations of interest and reduce the number of shifts. (iii) Use hp-adaptivity, e.g. a technique similar to [15] for PML and [16] for DtN, to reduce the errors in the target eigenvalues. (iv) Check that the new eigenpairs significantly reduce the residual in the Lippmann–Schwinger equation.

2. Convergence of Galerkin spectral approximations for the DtN and PML formulations

In this section we introduce the DtN and PML formulations used to truncate the exterior domains and prove convergence of the Galerkin method. Our approach to analyze the DtN formulation follow [17,18] and we state convergence results proved by Bramble and Osborn, et al. [19]. The results stated for the infinite PML formulation are contained in [14]. For the finite PML problem we introduce a DtN map, which is used to derive a new error estimate and reference solutions.

2.1. Computing resonances with the DtN map

Resonance problems are closely related to the underlying scattering problem and we begin therefore with the Helmholtz scattering problem on $\mathbb{R}$ [20]. Consider the scattering of a given incoming wave u_i by an obstacle n with support in $\operatorname{supp}(n^2 - n_0^2) \subset (-d, d)$. Then the outgoing radiation condition on the scattered wave u_s is

$$u_s'(-x_0) = -ik\, n_0\, u_s(-x_0), \quad u_s'(x_0) = ik\, n_0\, u_s(x_0), \quad x_0 \geq d \tag{2.1}$$

and a function that satisfies (2.1) is called *outgoing* [20]. The scattering problem is then: Find for given k^2 with $\Im k^2 \geq 0$ the total wave $H^2(\mathbb{R}) \ni u = u_i + u_s$ with u_s outgoing, that satisfies

$$-u'' - k^2 n^2 u = 0. \tag{2.2}$$

The condition (2.1) on u_s ensures uniqueness of the solution [21, p. 348], [20].

For $x \notin \Omega_d$ and given non-zero $k \in \mathbb{C}$, Eq. (2.2) has the linearly independent solutions $e^{\pm ikn_0x} \in H^2_{\text{loc}}(\mathbb{R})$. For $x \geq d$, we have that $u_s(x) = e^{ikn_0x}$ is the outgoing solution and $u_s(x) = e^{-ikn_0x}$ is called the *incoming* solution. Similarly, for $x \leq -d$ the function $u_s(x) = e^{-ikn_0x}$ is outgoing and $u_s(x) = e^{ikn_0x}$ is the incoming solution.

The standard definition of resonances as the poles of the analytical continuation of the resolvent operator is discussed in Section 4. However, these resonances can also be determined by solving a nonlinear eigenvalue problem, where the nonlinearity comes from the Dirichlet-to-Neumann (DtN) map [3,22]. In one space dimension, the problem formulation