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Iterative solution applied to the Helmholtz equation: Complex deflation on unstructured grids

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ABSTRACT

Extensions of deflation techniques developed for the Poisson and Navier equations (Aubry et al., 2008; Mut et al., 2010; Löhner et al., 2011; Aubry et al., 2011) [1–4] are presented for the Helmholtz equation. Numerous difficulties arise compared to the previous case. After discretization, the matrix is now indefinite without Sommerfeld boundary conditions, or complex with them. It is generally symmetric complex but not Hermitian, discarding optimal short recurrences from an iterative solver viewpoint (Saad, 2003) [5]. Furthermore, the kernel of the operator in an infinite space typically does not belong to the discrete space. The choice of the deflation space is discussed, as well as the relationship between dispersion error and solver convergence. Similarly to the symmetric definite positive (SPD) case, subdomain deflation accelerates convergence if the low frequency eigenmodes are well described. However, the analytic eigenvectors are well represented only if the dispersion error is low. CPU savings are therefore restricted to a low to mid frequency regime compared to the mesh size, which could be still relevant from an application viewpoint, given the ease of implementation.

1. Introduction

The Helmholtz equation is the archetype of the wave equation in the time domain. Applications of this equation are numerous and include acoustic scattering, geophysical seismic imaging, wireless communications. Due to this vast area of applications, a substantial effort has been invested in their numerical resolution. After discretization, these methods give rise to large, possibly sparse, matrices and their inversion may be time consuming. For large three dimensional problems, iterative methods in a broad sense (geometric or algebraic multigrid, iterative solvers, domain decomposition methods) represent the methods of choice due to memory (and possibly CPU) requirements. However their robustness is often criticized beyond the elliptic case. The main motivation of this work is given by the challenge of solving iteratively the coupled elastodynamic acoustic problem. The first building block for the elastic part consisted in extending the results of the scalar Poisson solver to the static elastic system. This was presented in [4]. The present work constitutes the first departure from the symmetric definite positive (SPD) case for scalar equation. In the literature, the Helmholtz equation has been mainly studied from two apparently different viewpoints, either from a discretization and accuracy viewpoint, or from an algebraic solver viewpoint. However, in both approaches plane waves, which are solutions of the Helmholtz equation in free space play a special part.

From an accuracy viewpoint, the oscillating nature of the Helmholtz equation gives rise to the famous pollution effect for high wave numbers [6–9]. Beside refining the mesh in the Finite Element h-refinement approach and increasing the polynomial order in the p-refinement paradigm, numerous methods have been designed to stabilize the Helmholtz equation. The Generalized Finite Element Method (GFEM) [10] modifies a bilinear stencil to have minimum pollution effect by minimizing the distance between the zeros of the discrete symbol and the one of the continuous symbol. The Partition of Unity Method (PUM) [11], uses analytical functions in the shape function definition. Extensions in three dimensions are presented in [12] in a Finite Element context and [13] in a Boundary Element context. The ultraweak method [14] relies on test functions that are solutions of the adjoint problem. The least square method [15] uses plane waves or Bessel functions in a discontinuous manner inside each element. The Galerkin Least Square (GLS) method [16] intends to stabilize the Helmholtz equation by adding consistently new weighted terms. The Residual Free Method (RFM) [17] relies on a bubble which verifies the analytical solution of the Helmholtz equation inside each element. A discontinuous Galerkin method [18] enriches the classical polynomial space with plane waves, and continuity is enforced weakly through Lagrange multipliers. The

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Discrete Singular Convolution (DSC) [19] method applies singular convolution with a special kernel for high wave numbers. The residual based method [20] belongs to the variational multiscale methods but includes the residual on inter-element boundaries. As underlined, most of these methods rely on a continuous or discontinuous introduction of plane waves to improve the classical finite element discretization.

From an algebraic solver viewpoint, numerous techniques have also been attempted, including preconditioning, geometric and algebraic multigrid, and domain decomposition methods. A review is given by Erlangga in [21]. For the first class of methods, Magolu Monga Made et al. [22,23] proposes to use an imaginary perturbation of the original matrix as preconditioner. A large class of preconditioners begins with the work in Bayliss et al. [24], where the normal equation is solved with a symmetric successive over relaxation (SSOR) preconditioner relying only on the discrete Laplacian part of the Helmholtz operator. The preconditioner is now symmetric positive definite and a few sweeps of a multigrid solver may be used. Later, Laird and Giles [25] add a mass matrix part in the preconditioner while the mass matrix is associated with a negative sign in the original equation, and do not include boundary conditions for this matrix. Recently, Erlangga et al. [26,27] add a complex shift for the mass matrix, still allowing the possibility of a multigrid solve for the the fast inversion of the preconditioner, as shown in an unstructured context by Airaksinen et al. [28]. Bollhöfer et al. [29] present an algebraic multilevel preconditioner in heterogeneous media. Finally, Osei-Kuffuor and Saad [30] combine imaginary diagonal shifts with an algebraic recursive multilevel preconditioner. Recently, deflation has been applied to the Helmholtz equation discretized by an Integral Formulation [31]. The deflation space is composed of the eigenvectors of a coarse grid operator interpolated on the fine grid. It is clearly shown that deflation may improve drastically convergence, and as a by product, demonstrates the weak non normality of the Helmholtz equation [32]. However, the coarse mesh size presented is of the order of 40 percent of the size of the fine mesh, which is not affordable for large problems. Regarding multigrid techniques, a major breakthrough comes from Brandt and Livshits [33–35]. There are at least two reasons for the bad convergence of standard multigrids for the Helmholtz equation. First, standard smoothers diverge due to the non SPD behavior of the operator. Secondly, due to the oscillatory nature of the Helmholtz solution, standard restriction operators put a heavy constraint on the size of the coarse grid. To alleviate the latter major drawbacks, exponential restriction is performed, and only the smooth part of the solution is transfer to the ray grids, where it is solved efficiently. A similar approach is followed in Lee et al. [36] for a first order system least-squares formulation. Kim and Kim [37] use a Gauss Seidel (GS) or Conjugate Gradient for the Normal equation (CGNR) as a smoother. The large coarse grid problem is solved by a domain decomposition method. Elman et al. [38] use GMRES as a smoother in an outer flexible loop for robustness. Another approach is proposed in Vanek et al. [39], where aggregation is first performed to obtain a coarse level. Relying on the free space solution of the Helmholtz equation, a tentative prolongation is then build and smoothed through a polynomial matrix iteration, whose main aim is to minimize the energy of the columns of the prolongation. Oscillatory functions are interpolated with a constant value and with their gradients, as they do not belong exactly to the discrete space. As a final remark on multigrids relying on exponential interpolation, only two dimensional examples with very simple geometries have been shown to illustrate their numerical performances. Domain decomposition methods have also been applied to the Helmholtz equation by Farhat et al. for continuous [40] and discontinuous discretizations [41] relying on plane waves for the Lagrange multiplier space as well as for the primary variable.

It is therefore obvious that plane waves play a special part in the numerical resolution of the Helmholtz equation, as much from an accuracy as from an efficiency viewpoint. The shift produced by the wave number in the Laplacian spectrum implies that Laplacian eigenmodes associated with higher and higher eigenvalues become low energy modes impeding convergence. Furthermore, as noted in [36], though not from an algebraic viewpoint, the density of these modes increases with the wave number, as the Laplacian spectrum is much denser at its upper end. As plane waves do not belong to low order discretization, it may be foreseen that they will approximate well the low energy modes only for low to mid frequencies. The dispersion induced by the discretization will create a larger mismatch as the wave number increases.

In this paper, deflation applied to the Helmholtz equation is presented. Deflation has been shown to possess various computational advantages compared to other algebraic solvers for large unstructured meshes [1–4]. Whereas the multigrid approach gives a sound basis to tackle the problem, the geometric multigrid hierarchy is awkward to treat in an unstructured context with moving bodies, and the algebraic set up is slow. As noted in [38], the wave ray multigrid is "considerably more difficult to implement" than the multigrid proposed in the latter paper, even though it may be more efficient. It was hoped that deflation may achieve this efficiency in a three dimensional context with the ease of implementation of the deflation technique. However, this aim is only partially met. After this introduction, the deflation technique is reviewed in Section 2, and differences between the SPD and the non SPD case are highlighted. The complex deflated GMRES algorithm is recalled. It will be the method of choice for the next section as the Helmholtz equation gives rise to a symmetric complex but non Hermitian matrix. The Helmholtz equation is then presented in Section 3. Deflation applied to the discrete Helmholtz equation is considered. Finally, numerical results are provided in Section 4.

2. Complex deflation

In this section, the complex deflated GMRES used in this paper is presented. First, deflation applied to iterative solvers is succinctly reviewed. The Hermitian case is then recalled, followed by the non Hermitian case. Finally, the complex deflated GMRES is derived.

2.1. Deflation applied to iterative solvers

Deflation is an old and common technique in iterative solvers for eigenvalues [42,43]. In his seminal paper [44], Nicolaides accelerates an iterative solver for symmetric positive definite matrices, the widely utilized preconditioned conjugate gradient (PCG) [45], through a deflation technique (see [1] for other references). In a non symmetric context, Morgan [46] considers deflation to improve the GMRES restart. More recently, deflation has been extended to non symmetric solvers with success in [47,48]. The deflated preconditioned GMRES is at the crossroads of various iterative solvers for large matrices such as multigrid, either geometric or algebraic, domain decomposition, and of course Krylov subspace methods, as all these methods may be interpreted as projection methods [49,5,50]. Even though the core algorithm is constituted by a Krylov iterative solver, its main aim is to remove from the residual eigenvector components that are difficult to remove by standard iterative solvers. Convergence of GMRES for symmetric positive definite matrices can be shown to strongly rely on the con-