Solving Helmholtz Equation Using the Temporal Wave Equation

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Abstract

We consider iterative methods for the Helmholtz equation that are based on the related time domain wave equation. In each iteration, the solution to the wave equation with a time-periodic forcing is computed and filtered in time. For Dirichlet and Neumann problems the iteration corresponds to a linear and coercive operator which, after discretization, is recast as a positive definite linear system of equations that can be solved with the conjugate gradient method.

Keywords: Helmholtz, Wave Equation.

1 Introduction

Designing efficient iterative solvers for the Helmholtz equation is a challenging problem, in particular when the frequency is high. The main difficulties stem from the resolution requirements and the highly indefinite character of the discretized problem. For detailed reviews see the articles by Ernst, Gander, Zhang and Erlangga [6, 7, 9].

Computational costs and memory requirements increase rapidly with the frequency ω. To maintain a fixed accuracy with a p-th order method at frequency ω the number of grid points per wavelength must scale as $\omega^{1/p}$ due to the pollution errors. The total number of degrees of freedom is then proportional to $\omega^{d(1+1/p)}$ in d dimensions. At high frequencies this leads to large scale problems that require parallel high-performance computers. It is thus important that solver implementations work well on such platforms. Moreover, solvers should be based on high order accurate methods, or the extra penalty $\omega^{d/p}$ due to pollution errors can become prohibitive, in particular in 3D.

As discretizations of Helmholtz give rise to indefinite linear systems, the conjugate gradient (CG) method cannot be used and the method of necessity becomes the generalized minimal residual method (GMRES). Without preconditioning, the convergence is, however, very slow and the iteration typically stagnates. Efficient preconditioners tailored to the Helmholtz equation must be used to accelerate the convergence. Many such preconditioners have been developed in the past two decades, for instance the analytic incomplete LU [8], shifted laplacian [5], and sweeping [4] preconditioners, to mention a few. Specialized, and efficient, preconditioners give faster convergence, but they can be harder to reconcile with the need for high order implementations that can use high performance computers to good advantage.

2 Time-domain methods

In this talk I will discuss time-domain methods, which is a less explored type of iterative method for the Helmholtz equation that exploits its connection to the time-dependent wave equation. Specifically, I will consider the *WaveHoltz* method that was developed in [2].

There are many advantages to solving the time dependent wave equation rather than the Helmholtz equation. Algorithms for solving the wave equation are memory lean. They are easy to parallelize and scale well. There are also many provably stable and high order accurate methods available. Compared to discretizations of Helmholtz, time domain methods can therefore more easily deal with large scale high-frequency problems.

In the simplest time-domain method one runs the wave equation for a long time to get a Helmholtz solution. The theoretical underpinning of this approach is the limiting amplitude principle [12] which says that every solution to the wave equation with an oscillatory forcing, in the exterior of a domain with reflecting boundary conditions tends to the Helmholtz solution. However, this method generally does not work for interior problems and becomes very slow for problems with trapping waves.

The Controllability Method (CM) is an alternative approach. It was originally proposed by Bristeau et al. [3] and was further developed by Heikkola et al. [11] as well as Grote and Tang [10]. In CM the solution to the Helmholtz equation is found by solving a convex constrained least-squares minimization problem where the

deviation from time-periodicity is minimized in the classic wave equation energy. The basic iteration step in CM includes the solution of a forward and a backward wave equation over one time-period. In some versions one must also solve a symmetric coercive elliptic (and wave number independent) problem.

3 The WaveHoltz method

The WaveHoltz method is inspired by CM. It only requires a single forward wave equation solve per iteration, and no elliptic solves. For Dirichlet and Neumann problems it leads to a positive definite linear system that can be solved with CG or other Krylov methods. Below we describe the simplest version of the method for the Helmholtz equation. It can also be generalized to other frequency domain wave equations, such as the elastic wave equation and the Maxwell equations [1, 13].

Consider the Helmholtz equation in a bounded open smooth domain Ω,

$$\nabla \cdot (c^2 \nabla u) + \omega^2 u = f, \qquad \text{in } \Omega, \qquad (1)$$

with either Dirichlet or Neumann boundary conditions,

$$u = 0 \quad \text{or} \quad \vec{n} \cdot \nabla u = 0, \qquad \text{on } \partial\Omega.$$

In this formulation no energy leaves the domain and for (1) to be well-posed, ω must not be a resonant frequency, i.e. ω cannot be an eigenvalue of the operator $-\nabla \cdot (c(x)^2 \nabla)$. We assume non-resonance, $f \in L^2(\Omega)$ and $c \in L^\infty(\Omega)$ bounded away from zero, which ensures that there is a unique weak solution $u \in H^1(\Omega)$ to (1).

This energy conserving case is typically the most difficult one for iterative Helmholtz solvers. Moreover, the limiting amplitude principle does not hold, and one can thus not obtain the Helmholtz solution by solving the wave equation over a long time interval.

To motivate the methods, we first note that if u solves (1) then the function

$$w(t, x) := u(x) \cos(\omega t),$$

is a $T = 2\pi/\omega$-periodic (in time) solution to the forced scalar wave equation

$$\begin{aligned} w_{tt} &= \nabla \cdot (c^2(x) \nabla w) - f(x) \cos(\omega t), \qquad (2) \\ w(0, x) &= v_0(x), \quad w_t(0, x) = 0, \end{aligned}$$

where $v_0 = u$. The domain and boundary conditions are the same as in (1). Based on this observation, our approach is to find w instead of u. We could thus look for initial data v_0 such that w is a T-periodic solution to (2). However, there may be several such w, see [10], and we therefore impose the alternative constraint that a certain time-average of w should equal the initial data. More precisely, we introduce the operator Π acting on the initial data $v_0 \in H^1(\Omega)$ as

$$\Pi v_0 = \frac{2}{T} \int_0^T \left(\cos(\omega t) - \frac{1}{4} \right) w(t, \cdot) dt, \qquad (3)$$

where w satisfies the wave equation (2) with initial data $w = v_0$ and $w_t = 0$. The result of Πv_0 can thus be seen as a filtering in time of w around the ω-frequency. By construction, the solution u of Helmholtz is a fixed point of Π,

$$u = \Pi u,$$

and the basic method amounts to solving this equation with the fixed point iteration

$$\boxed{v^{n+1} = \Pi v^n, \qquad v^0 \equiv 0.} \qquad (4)$$

Provided this iteration converges and the fixed point is unique we obtain the Helmholtz solution as $u = \lim_{n \to \infty} v^n$.

Remark 1 *Note that each iteration is inexpensive and that T is reduced by the reciprocal of ω as ω grows. If we assume that the number of degrees of freedom in each dimension scales with ω and that we evolve the wave equation with an explicit method this means that the number of timesteps per iteration is independent of ω. Also note that the iteration is trivial to implement (in parallel or serial) if there is already a time domain wave equation solver in place. The integral in the filtering* (3) *is carried out independently for each degree of freedom and simply amounts to adding up a weighted sum (e.g. a trapezoidal sum) of the solution one timestep at a time. Finally, note that the time-domain iteration allows all the advanced techniques that have been developed for wave equations (e.g. local timestepping, non-conforming discontinuous Galerkin finite elements h- and p-adaptivity etc.) to be transferred to the Helmholtz equation and other time harmonic problems.*

4 Analysis

We will now make a simple analysis of the iteration (4). Consider the Helmholtz solution u and the wave equation solution w with initial data $w = v$, $w_t = 0$ and forcing f. Let ϕ_j and λ_j^2 be the eigenfunctions and corresponding eigenvalues of $-\nabla(c^2(x)\nabla)$. We can then expand the functions

$$u(x) = \sum_{j=0}^{\infty} \hat{u}_j \phi_j(x), \qquad v(x) = \sum_{j=0}^{\infty} \hat{v}_j \phi_j(x),$$

$$w(t,x) = \sum_{j=0}^{\infty} \hat{w}_j(t) \phi_j(x), \qquad f(x) = \sum_{j=0}^{\infty} \hat{f}_j \phi_j(x).$$

The modes of the wave equation solution w can be written explicitly as functions of time,

$$\hat{w}_j(t) = (\hat{v}_j - \hat{u}_j)\cos(\lambda_j t) + \hat{u}_j \cos(\omega t),$$

and the filtering step (3) gives

$$\Pi v = \sum_{j=0}^{\infty} \bar{v}_j \phi_j(x), \qquad \bar{v}_j = \beta(\lambda_j)(\hat{v}_j - \hat{u}_j) + \hat{u}_j,$$

where

$$\beta(\lambda) := \frac{2}{T} \int_0^T \left(\cos(\omega t) - \frac{1}{4} \right) \cos(\lambda t) dt.$$

(Note that $\beta(\omega) = 1$.) Upon defining the linear operator $\mathcal{S}$ by

$$\mathcal{S} \sum_{j=0}^{\infty} \hat{u}_j \phi_j(x) := \sum_{j=0}^{\infty} \beta(\lambda_j) \hat{u}_j \phi_j(x),$$

we can then write the iteration as

$$v^{n+1} = \Pi v^n = \mathcal{S}(v^n - u) + u. \tag{5}$$

The operator $\mathcal{S}$ is self-adjoint and has the same eigenfunctions $\phi_j(x)$ as $-\nabla \cdot (c^2(x)\nabla)$ but with the (real) eigenvalues $\beta(\lambda_j)$. The convergence properties of the iteration depend on these eigenvalues and it is therefore of interest to study the range of the filter transfer function β. Figure 1 shows a plot of β which indicates that the eigenvalues of $\mathcal{S}$ are inside the unit interval, with a few of them being close to 1 (when $\lambda_j \approx \omega$), and most of them being close to zero (when $\lambda_j \gg \omega$). In fact, one can show that $\beta(\lambda) \in [-0.5, 1]$ and

$$\beta(\omega + \varepsilon\omega) \approx 1 - c\varepsilon^2, \qquad |\varepsilon| \ll 1. \tag{6}$$

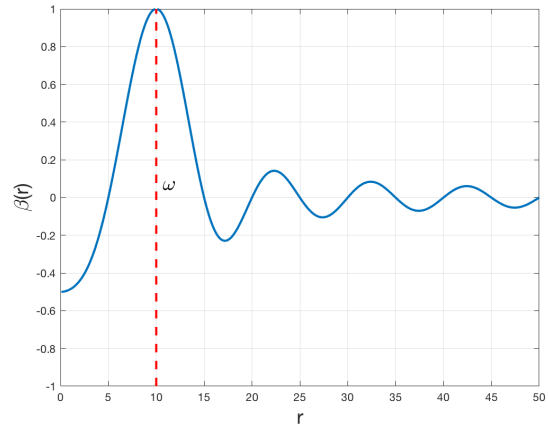

Figure 1: The filter transfer function β for $\omega = 10$.

We can now derive a convergence result. We quantify the non-resonance condition by letting

$$\delta = \inf_j \frac{|\lambda_j - \omega|}{\omega} > 0,$$

be the relative size of the smallest gap between λ_j and the Helmholtz frequency. Then we introduce

$$\rho = \max_j |\beta(\lambda_j)| = \beta(\omega \pm \delta\omega) \approx 1 - c\delta^2,$$

where the last step follows from (6), assuming $\delta \ll 1$. We can rearrange (5) and obtain

$$v^{n+1} - u = \mathcal{S}(v^n - u).$$

Then,

$$\begin{aligned} ||v^{n+1} - u||^2_{L^2(\Omega)} &= \sum_{j=0}^{\infty} \beta(\lambda_j)^2 (\hat{v}_j^n - \hat{u}_j)^2 \\ &\leq \rho^2 \sum_{j=0}^{\infty} (\hat{v}_j^n - \hat{u}_j)^2 \\ &= \rho^2 ||v^n - u||^2_{L^2(\Omega)}, \end{aligned}$$

which shows that v^n converges to u in L^2 with rate $\rho = 1 - O(\delta^2)$. Thus, not surprisingly, the smallest gap, δ, determines the convergence factor. It is straightforward to also get convergence in H^1. In the end we obtain the following theorem, [2].

Theorem 2 *The iteration* (4) *converges in* $H^1(\Omega)$ *for the Dirichlet and Neumann problems away from resonances to a unique fixed point which is the solution of the Helmholtz equation* (1). *The convergence rate is* $1 - O(\delta^2)$.

The iteration operator is an affine operator of the form

$$\Pi v = \mathcal{S}v + b, \qquad b = u - \mathcal{S}u.$$

Setting $\mathcal{A} = I - \mathcal{S}$ we can reformulate the fixed point problem $v = \Pi v$ as a linear equation

$$\mathcal{A}v = b. \tag{7}$$

Further analysis of $\mathcal{S}$ shows that it is a bounded, linear, self-adjoint, compact operator from $H^1(\Omega)$ to $H^1(\Omega)$, whose eigenvalues lie in the interval $[-0.5, \rho]$. Therefore, $\mathcal{A}$ is a bounded, linear, self-adjoint operator from $H^1(\Omega)$ to $H^1(\Omega)$, which is positive and coercive, with eigenvalues in the interval $(1-\rho, 3/2]$. Its condition number is of size $O(1/(1-\rho)) = O(1/\delta^2)$.

Krylov acceleration. We note that $b = \Pi 0$ in (7) and can therefore easily be pre-computed. Furthermore, we can then evaluate the action of $\mathcal{A}$ as

$$\mathcal{A}v = v - \Pi v + b.$$

Thus, we can simply carry out the evaluation of $\mathcal{A}v$ by evolving the wave equation for one period in time with v as the initial data and then subtract the filtered solution from the sum of the initial data and the right hand side b. This makes it possible to replace the simple fixed point iteration (4) with accelerated Krylov methods. Since $\mathcal{A}$ is positive and self-adjoint one can use the conjugate gradient (CG) method.

Although the formulation (7) is mathematically equivalent to the original Helmholtz equation (1) for the interior Dirichlet and Neumann problems away from resonances, there are two striking differences:

- The linear equation (7) is positive definite, not indefinite.
- Since $\mathcal{S}$ is compact, the condition number of $\mathcal{A}$ after discretization is essentially independent of the grid size Δx. This means that, similar to many boundary integral methods, the number of iterations needed for convergence is also virtually independent of Δx.

For CG the number of iterations needed to obtain a fixed accuracy scales as the square root of the condition number of $\mathcal{A}$, i.e. as $1/\delta$. To further understand how δ may depend on the frequency ω, consider the asymptotic distribution of large eigenvalues. By the work of Weyl we know that the eigenvalues of elliptic operators grow asymptotically as $\lambda_j \sim j^{1/d}$ in d dimensions. For large j the eigenvalues thus become more dense in dimensions $j \geq 2$. The average relative gap δ when $\omega \approx \lambda_j$ can be estimated as

$$\delta \approx \frac{\lambda_{j+1} - \lambda_j}{\omega} \sim \omega^{-d}.$$

Thus, for high frequencies, one expects the number of iterations with an (unconditioned) CG method to grow as $O(\omega^d)$. However, in numerical experiments we observe slightly better complexity.

Remark 3 *The iteration count above is for the interior energy conserving case, which is ill-posed for resonant ω. Moreover, when $d \geq 2$ the problem will be closer and closer to resonance as ω grows. To have a physically relevant model at high frequencies some damping may be required, for instance by adding a term $i\omega\eta u$ to* (1)*. In this case, we observe that the number of iterations for the corresponding WaveHoltz method grows as just $O(\omega)$ in all dimensions.*

Impedance case. For open, non energy conserving problems, the Dirichlet or Neumann boundary conditions, are replaced by the impedance condition

$$i\omega u + \vec{n} \cdot \nabla u = 0, \qquad \text{on } \partial\Omega.$$

This is a common situation in practical applications. In this case the boundary conditions in the wave equation (2) should be

$$w_t + \vec{n} \cdot \nabla w = 0, \qquad \text{on } \partial\Omega.$$

Moreover, also the initial data for the time-derivative $u_t(0,x) = v_1(x)$ must be included in the iteration:

$$\begin{bmatrix} v_0 \\ v_1 \end{bmatrix}^{(n+1)} = \Pi \begin{bmatrix} v_0 \\ v_1 \end{bmatrix}^{(n)}, \qquad \begin{bmatrix} v_0 \\ v_1 \end{bmatrix}^{(0)} \equiv 0,$$

where v_1^{n+1} is the time-filter of w_t in the same way as v_0^{n+1} is the time-filter of w in (3). The resulting operator $\mathcal{A}$ is no longer self-adjoint, and GMRES must be used instead of CG to solve (7). For these open problems we observe convergence but do not yet have a complete theory

explaining it. Since the operator in the wave equation in this case does not have a point spectrum, nor an eigen basis, the simple analysis used above fails. However, numerical experiments show that the number of iterations for fixed accuracy generally grows as $O(\omega)$ independent of Δx and dimension d.

We note finally that the convergence rates reported above are all for the unconditioned case. As for frequency domain methods, preconditioners could potentially improve these rates significantly.

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