A WKB Based Preconditioner for the 1D Helmholtz Wave Equation

D. L. Green[1,a),*], E. D'Azevedo[1], D. B. Batchelor[1,3], N. Bertelli[2], C. Lau[1], R. L. Barnett[1,4] and J. F. Caneses Marin[1]

[1]*Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, TN, 37831, USA*
[2]*Princeton Plasma Physics Laboratory, 100 Stellarator Road Princeton, NJ, 08540, USA*
[3]*DIDITCO Inc., 4063 Alta Vista Way, Knoxville, TN 37919, USA*
[4]*University of Newcastle, University Drive, Callaghan NSW 2308, Australia*

[a)]Corresponding author: greendl1@ornl.gov

Abstract. Frequency-domain full-wave solutions to the cold-plasma problem have become ubiquitous in the study of radio frequency power in fusion plasmas. However, recent efforts at extreme levels of geometric fidelity have revealed fundamental limits in the problem size that can be solved by typical sparse direct solver based methods. These limits are of particular importance in the 3D study of RF launchers, where the number of degrees of freedom required can exceed 100 million. In such cases, it would be advantageous to solve the system via iterative means, but due to the large null space of the curl-curl operator, the convergence properties of algorithms like GMRES are poor. Here we present a physics-based preconditioner in the form of a WKB solution and demonstrate the iterative solution to the frequency-domain Helmholtz problem in 1D for several cases ranging from satisfying the WKB approximation to strongly violating it.

INTRODUCTION

Numerical simulation has been utilized to investigate the geometric effects of linear propagation of plasma waves for many years. Here we focus on so-called "full-wave" simulations [e.g., 1, 2, 3, 4] where the full effects of refraction, diffraction and reflection are retained (as opposed to methods such as ray-tracing [e.g., 5, 6] where some of these effects are not accounted for). For magnetically confined fusion plasmas, where mega-watts of radio-frequency (RF) power are launched from antenna structures at the periphery of the confined plasma, it is convenient to examine the wave propagation of the launched frequency such that Maxwell's equations are reduced to their time-harmonic form as

$$\nabla \times \nabla \times \mathbf{E} - k^2 \left(\mathbf{E} + \frac{i}{\omega \epsilon_0} \sigma \cdot \mathbf{E} \right) = i \omega \mu_0 \mathbf{J}_A \tag{1}$$

where $k = \frac{\omega}{c}$, and $\omega = 2\pi f$ is the angular frequency of the driving antenna frequency f, c is the speed of light, $\mathbf{E}$ is the wave electric field, μ_0 is the permeability of free space and $\mathbf{J}_A$ is a volumetric current source distribution representative of an applied antenna current. Full-wave codes have proven to be useful in the quantitative prediction of wave propagation and absorption. However, expanding this predictive capability to include geometric details of the plasma facing components and wave modes of multiple spatial scales (fast and slow waves in the same simulation) requires a significant increase in the number of degrees of freedom (DoF). As the number of DoF grows beyond tens of millions, large-scale parallel computing is required. Discretization of the time harmonic (frequency domain) representation of Equation 1, either by finite-difference or finite-element, yields a sparse matrix which must be inverted, and is typically

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achieved via sparse direct solvers. However, a well-known problem [7, 8] is that distributed (parallel across compute nodes) sparse direct solvers do not scale well to large problems. Iterative methods, on the other hand, would enable the very large DoF problems required to simulate the multiple spatial wave scales together with the high geometric fidelity of modern ICRF and LH antenna structures within large simulation volumes (in 3D). While iterative approaches to the inclusion of kinetic effects in full-wave calculations have seen some attention [9, 10, 1], the underlying cold-plasma solvers have always used a direct method. This use of a direct method is because unpreconditoned iterative methods fail for this sign-indefinite problem [11]. Recent work by [12] presents the idea of using a time-domain solution as a preconditioner, but the cost is still high (but scalable). Approaches in the applied math community have focused on a reduced form of Equation 1, where assuming $\frac{\partial}{\partial y} = \frac{\partial}{\partial z} = 0$ and material with diagonal dielectric, but spatially varying (hence the $k(x)$ in Equation 2 below) medium decouples the vector components and leaves a scalar Helmholtz equation

$$\frac{\partial^2 E_i}{\partial x^2} + k^2(x) E_i = f_i(x). \tag{2}$$

where the i subscript represents either the $i = y$ or $i = z$ component. Since Equation 2 retains the same difficulty to iterative solution as Equation 1, it is a good problem for prototyping preconditioners (as we do here). For the 1D Helmholtz problem of Equation 2, the Shifted Laplacian approach has demonstrated success [13] but has not yet been generalized to back to the coupled vector Maxwell's form of Equation 1. There has also been work on overlapping Schwarz type domain decomposition preconditioners (e.g., [14]), but their performance has yet to be made robust for fusion relevant problems. Here we investigate the use of a Wentzel—Kramers—Brillouin (WKB) approximate solution method on Helmholtz (Equation 2), which does have potential to generalize to the Maxwell problem (Equation 1). We also note that working in 1D drops the gradient of a divergence piece of the curl-curl operator $\nabla \times \nabla \times \mathbf{E} = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E}$, but that even this system encompasses a significant portion of the convergence difficulties and that extension to the multi-D system will be future work.

METHOD

Here we apply the GMRES [15] iterative solver to the linear system emitted from Equation 2 when discretized by second order finite difference. Our approach is to use a left preconditioner in the form of an approximate WKB solution to the same problem. The challenge here is that for the WKB method to be applicable as a preconditioner, it needs to be for the inhomogeneous problem ($f_i(x) \neq 0$) such that either the preconditioner matrix can be constructed explicitly (via solving the WKB problem for $f_i(x)$ being a series of delta functions, one at every grid point) or, as we do here, to allow $f(x)$ to be the residual of the present iterate internal to the GMRES solver. We implement the second approach by providing a function handle which accepts $f_i(x)$ and returns E_i (calculated via WKB below) to the GMRES implementation (here the Matlab `gmres` command). The WKB solution to the homogeneous Helmholtz equation, which is written as

$$E_1, E_2 = \frac{1}{\sqrt{k(x)}} \exp\left(\pm i \int_0^x k(s)\,\mathrm{ds}\right) \tag{3}$$

and by the method of variation of parameters the WKB solution for the inhomogeneous equation is

$$E(x) = C_1 E_1(x) + C_2 E_2(x) + \frac{1}{2i} \int_0^x \left(E_1(x) E_2(s) - E_1(s) E_2(x)\right) f(s)\,\mathrm{ds} \tag{4}$$

where

$$C_1 = \frac{-E_2(0)E'(0) + E_2'(0)E(0)}{W(0)}, \quad C_2 = \frac{+E_1(0)E'(0) - E_1'(0)E(0)}{W(0)} \tag{5}$$

Where $W(0) = +E_1(0)E_2'(0) - E_1'(0)E_2(0)$ and we specify the boundary conditions $E(0)$ and $E'(0) = \frac{\partial E}{\partial x}$ at the $x = 0$ (left) boundary of the domain.

RESULTS

With the WKB solution above, we manufacture an $f(x)$ to match an analytic solution of $E(x) = \exp(2.3ikx)$ on a domain $x \in \{0, \pi\}$ with Dirichlet and Neumann boundary conditions on the left boundary as specified by the analytic solution, i.e., $E(0) = 1$ and $E'(0) = 2.3ik$. Figure 1 shows application of our above inhomogeneous WKB solver for a uniform $k(x) = 10$ case where we would expect the WKB approximation to yield an accurate answer. Indeed the left panels of Figure 1 show this. In the right panel of Figure 1 we demonstrate that for both unpreconditioned

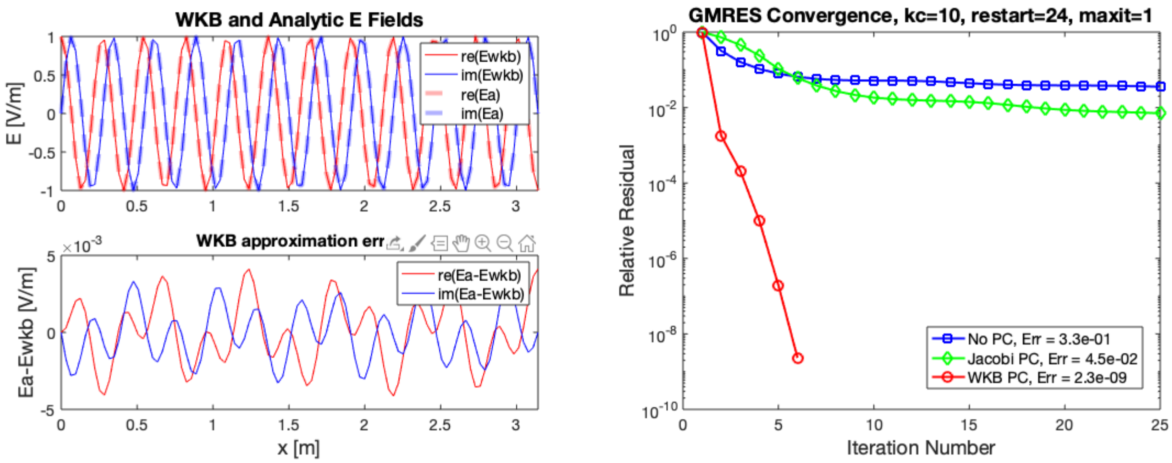

FIGURE 1. Left Top: Analytic and WKB solutions. Left Bottom: Difference between the analytic solution and WKB approximation. Right: Convergence of the preconditioned and unpreconditioned GMRES iteration. The RMS difference between the converged result and the known analytic solution is indicated by the Err values in the legend.

(blue/squares) and Jacobi preconditing (green/diamonds), the iterative solve via GMRES of a first order finite difference discretization (with 100 grid points) on of Equation 2 fails to converge at a useful rate. In the same figure we overlay the convergence curve for using the WKB solution (red/circles) of Equation 4 which shows successful convergence to the correct solution as indicated by the included RMS difference between the converged and known analytic solution. Next, we choose an analytic E field which varies in k fast enough that there is significant error in the WKB approximation, i.e., a Gaussian multiplier on k near the center of the domain. The left panels of Figure 2 show a significant error in the WKB approximation. However, the application of both preconditioner approaches still demonstrates rapid convergence (right panel of Figure 2). In a final test for this paper we increase the k and the

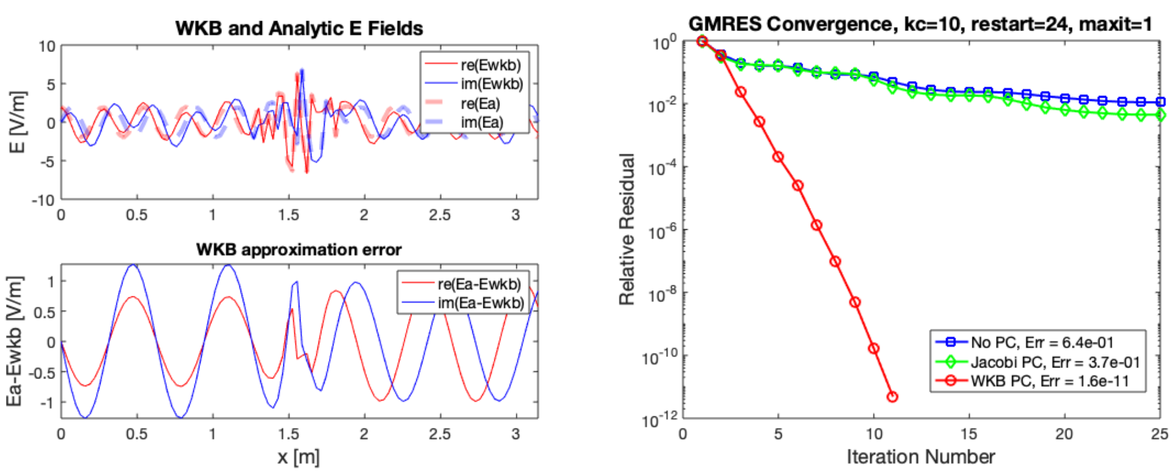

FIGURE 2. As in Figure 1 except for an analytic solution of $E_a(x) = \exp\left(2.3ik(x)x\right)P_2(x)$ where $k(x) = 10P_1(x)$, $M(x) = \exp(\frac{-(x-\pi/2)^2}{2\sigma^2})$, $\sigma = 0.1$, $A_1 = 2$, $A_2 = 5$, $P_1(x) = A_1M(x) + 1$, $P_2(x) = \left(A_2M(x) + 1\right) + 1$.

gridpoints by a factor of 10. As shown in Figure 3, the WKB error is large, but preconditioned convergence is still achieved.

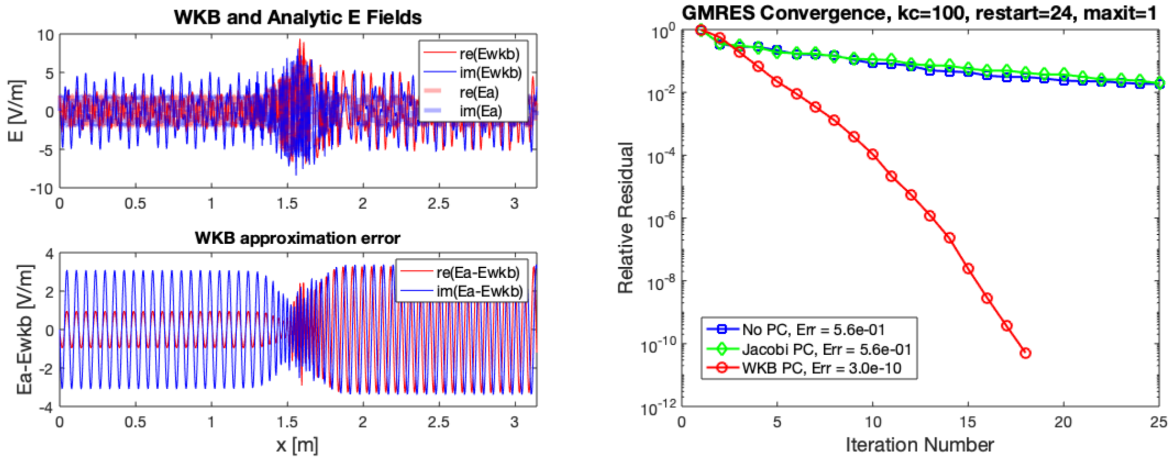

FIGURE 3. As in Figure 3 except with $k(x) = 100P_1(x)$ an 1000 grid points.

DISCUSSION AND FUTURE WORK

We have presented an iterative solution of a simple finite difference discretization for the 1D Helmholtz wave equation which employs the inhomogenuous WKB approximation as the preconditioner to the GMRES method. The preconditioner was demonstrated to work effectively for cases including where the preconditioner is not an accurate representation of the solution. This approach may prove to be of use in enabling full-wave plasma simulation in 3D at the extreme geometric resolutions and large domain sizes required for the accurate design of fusion ICRF and LH antenna systems by enabling iterative solution methods which exhibit desirable scaling properties. Future work will involve extension to multiple dimensions where the gradient of a divergence piece of the curl curl operator are present, replacing a prescribed k field with that calculation from a cold-plasma dispersion relation, and examining the preconditioners performance around resonances and cutoffs.

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