

H. bin Zubair*

* NW, DIAM, Delft University of Technology

*Email: h.binzubair@tudelft.nl

Abstract

In this talk we present the construction and performance of a geometric multigrid method for grids having two different layers of refinement. The method is employed to approximately invert the Krylov-preconditioner, i.e., the complex shifted Helmholtz operator, for the indefinite Helmholtz equation. The usual FAC and MLAT based grid coarsening techniques only coarsen the fine layer of the grid. The method presented here, in contrast, coarsens the whole grid simultaneously. Combined with a simple smoother, piece-wise constant restriction and bilinear prolongation, this gives an efficient multigrid method that works very well for the model problems, which are 2d Helmholtz equations with strongly varying coefficients.

Introduction

2d Helmholtz problems arise as simplified models from the 6-particle Schrödinger equation describing photo-induced ionization of the Hydrogen molecule H₂ [1]. The strongly varying spatial dependence in the Helmholtz term causes a singularity at the origin, and the solution also exhibits the so-called evanescent waves at the south and the east edges of the domain. Ensuring sufficient numerical accuracy ($kh < 0.625$) near these edges dictates the use of an over-whelming grid size. We tackle this problem by saturating grid cells only near these boundaries and using a considerably larger mesh size (at least double) elsewhere in the domain. Cell-centered Finite Volume Method is used, and it yields second order discretization accuracy over this local refinement topology. The conservative FVM discretization scheme also takes care of the flux mismatch at the interface of the adjacent grid layers, and works nicely with the presented multigrid method.

1 Model Problems and Discretization on Locally Refined Grids

The 2d helmholtz model problems are given as:

$$[-\Delta - \phi(x, y)] u(x, y) = \frac{1}{e^{x^2+y^2}} \quad (1)$$

The truncated computational domain is $[0, L] \times [0, L]$. The three different problems are characterized by the function $\phi(x, y)$ as well as L . For Model Problem 1 (MP1), we have $\phi(x, y) = \lambda(1/e^{x^2} + 1/e^{y^2}) + K^2$,

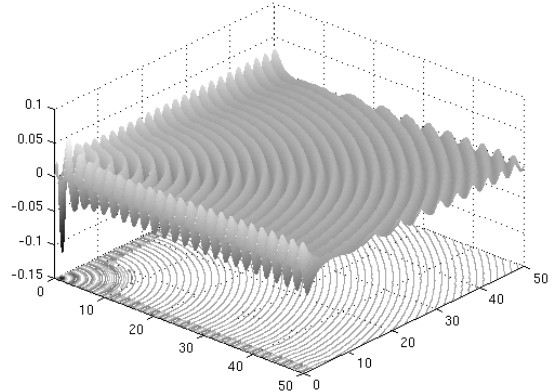


Figure 1: Evanescent waves for MP1 with $\lambda = 5$ and $K = 3$

$L = 50$, and $0 < \lambda < 10$. In MP2 and MP3, L ranges from 50 to 200, while $\phi(x, y) = 1/\min(x, y) + K^2$ for MP2, and $\phi(x, y) = 1/x + 1/y + K^2$ for MP3. For all model problems $K < 5$ and homogeneous Dirichlet boundary conditions are prescribed on the south and the west edge of the domain, while first order Sommerfeld (outgoing) boundary conditions, i.e., $\partial u / \partial n = -\iota K u$ ($\iota = \sqrt{-1}$, n is the outward unit normal) are considered on the east and the north edges. All model problems give evanescent waves (MP1 for $\lambda > 2.73$) at the Dirichlet edges, such as shown in Figure 1.

To avoid the *pollution effect* [2], we impose the condition $kh > 0.625$ as in [3]. This condition imposes a constraint on the maximum mesh size due to the singularity near the origin. The option of using a single constant mesh size throughout the domain is therefore not very viable as it leads to large grids. For example, MP3 for $K = 1$ and $L = 200$ requires a mesh size of 0.095 around the origin. However, on chopping off the L-shaped strip demarked by the lines $y = L/3$ and $x = L/3$, the mesh size requirement in the remaining domain is just 0.616 (which is around 6 times as large). We exploit this feature in this work, by using customized grids, saturated near Dirichlet edges of the domain, and having relatively larger mesh spacing in the remaining part. An example of such a grid is shown in Figure 1.

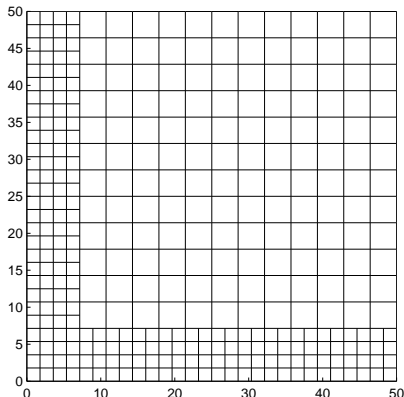


Figure 2: Grid locally refined in the area where evanescent waves are expected

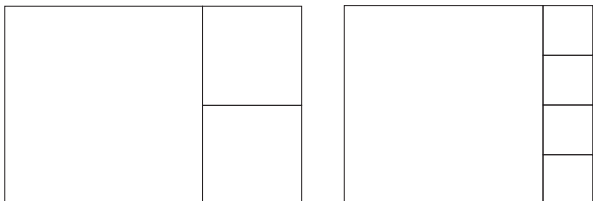


Figure 3: Possible (but not preferred) agglomeration of control volumes across fine-coarse layer interface

2 The Preconditioning Operator

Helmholtz equations with large negative wavenumbers cannot be handled directly by multigrid due to their indefinite spectrum, which implies both positive and negative eigenvalues. One way of solving such a discrete system iteratively, is by using a complex shifted Helmholtz operator (proposed in [3]) as a Krylov preconditioner. This operator is given as:

$$M = -\Delta - (\beta_1 - \iota\beta_2)\phi(x, y) \quad \beta_1, \beta_2 \in \mathbb{R}$$

This operator is discretized using the same boundary conditions as the original Helmholtz operator and can be inverted approximately by multigrid.

3 Multigrid for Locally Refined Grids

We enumerate the grid in L-shaped strips of control volumes (as in [4]), and perform standard coarsening at all levels. Grid coarsening is done by agglomerating neighboring grid cells. This is a 2 cell by 2 cell agglomeration (standard) unless coarsening across a layer interface is involved. In this case control volume agglomeration as depicted in Figure 3 is carried out. This leads to better grid reduction on each level than the coarsening strategies used in the well known FAC and MLAT approaches.

We use ω -Jacobi point based relaxation, piece-wise constant restriction and bilinear prolongation as in

[4]. The restriction and prolongation procedures follow the enumeration order of the grid cells. This multigrid demonstrates excellent convergence properties for the preconditioning operator specified in Section 2.

4 Numerical experiments

In the talk we present the result of numerical experiments based on Bi-CGSTAB preconditioned with the complex shifted Helmholtz operator approximately inverted by our multigrid method. We demonstrate that a careful selection of the discretization grid circumvents the complexity issue associated with extremely large grids for the model problems. Due to the extreme perturbation, especially in MP2 and MP3, we still observe many iterations of the preconditioned Bi-CGSTAB method. However, it can be shown that the number of iterations scale linearly with the largest wave-number involved.

5 Outlook

Although in two dimensions, direct methods can compete with iterative methods (for moderate grid-sizes); they are not an option in three or more dimensions, and therefore, efficient iterative methods are important. The extension of the presented method to 3 or more dimensions is straight forward and can be brought about as Kronecker tensor products. Multigrid preconditioned Krylov stays a good iterative candidate, but further enhancement is necessary to yield realistic compute times for the indefinite Helmholtz equations.

References

- [1] W. Vanroose, F. Martin, T. N. Rescigno, and C. W. McCurdy. Complete photo-induced breakup of the h_2 molecule as a probe of molecular electron correlation. *Science*, 310: 1787–1789, 2005.
- [2] A. Bayliss, C. I. Goldstein, and E. Turkel. On accuracy conditions for the numerical computation of waves. *J. Comput. Phys.*, 59: 396–404, 1985.
- [3] Y.A. Erlangga, C.W. Oosterlee, and C. Vuik. A novel multigrid based preconditioner for heterogeneous helmholtz problems. *SIAM J. Sci. Comput.*, 27: 1471–1492, 2006.
- [4] H. bin Zubair, S. P. MacLachlan, and C.W. Oosterlee. A geometric multigrid method based on L-shaped coarsening for PDEs on stretched grids. Technical report, Delft University of Technology, 2008.