An efficient iterative scheme for the Helmholtz equation with deflation

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Abstract

An efficient iterative solution of the Helmholtz equation is discussed in this document. The linear system obtained from the Helmholtz equation by discretizing by the Finite Difference Method is preconditioned with the shifted Laplace preconditioner [1, 2] and deflation accelerates it with GMRES. Experimental results with a 2-D problem are presented in support of claims, showing that the deflated preconditioned shifted Laplace preconditioner is quite fast and efficient and also mesh-independent. Multigrid deflation vectors are used as columns of the deflation matrix, which are cheap in terms of memory. Furthermore some versions of *ILU* are also combined with GMRES but are less efficient than shifted Laplace precondtitioner.

Keywords: Helmholtz equation, Shifted Laplace preconditioner, Deflation, Krylov space methods.

1 Introduction

The *Helmholtz* equation arises in many physical problems involving steady state (mechanical, acoustical, thermal, electromagnetic) oscillations. The complexity of the physical problem leaves no choices except to solve the equation numerically. The finite difference discretization leads to sparse, complex symmetric coefficient matrices that become indefinite for sufficient large wave number. The size of the problem increases with the wave number as a minimum number of grid points per wavelength is required to represent the physics correctly.

Krylov subspace and *Multigrid* techniques have been succesfully applied in a wide range of applications. For symmetric positive definite problems, the *conjugate gradient* (CG) is the method of choice. For indefinite problems, more general Krylov subspace solvers are to be applied. The fast convergence of these methods requires some form of preconditioning. The straightforward application of multigrid as a preconditioner is hampered by slow convergence causes by eigenmodes corresponding to eigenvalues with a negative real part. To overcome this difficulty, *Shifted-Laplace preconditioners* have been developed [3, 1, 2].

The idea of shifted-Laplace preconditioners is to base the precondioner of the discrete Helmholtz operator with a modified shift (coefficient before the first order term) for with the multigrid preconditioner can be shown to satisfaction. It was shown that the resulting preconditioned GMRES solver has favourable convergence properties in the sense the required number of iterations only depends mildly on the wavenumber. Allowing some damping in the shifted Laplace operator in particalur proves to benefical for speeding up overall convergence. In more recent work [4], the combined use of deflation and the shifted-Laplace precondioner was shown to result in a on more performant solver.

In this paper we study the combined use of the shifted-Laplace precondioner with multigrid deflation. We show that deflation allows to remove unfavourable modes in the spectrum of the precondioned operator. This allows us to that the Krylov solver is close to optimal in the sense that the required number of iterations is almost indepent of the wavenumber. This paper is structured as follows: In Section 2, problem with boundary conditions and domain. In Section 3, iterative solvers and their preconditioning are defined. Particular preconditioner for Helmholtz equation is explained in Subsection 3.2. In Section 3.3 deflation is defined. In Section 4, supporting numercial results are showed. Section 5, further work regarding Fourier analysis of deflated GMRES preconditioned with shifted Laplace preconditioner is projected. Section 6 contains concluding remarks.

2 Problem Description

The Helmholtz equation for the unknown field u in 2-D reads

$$-\Delta u - (1 - \alpha\iota)k^2 u = g \tag{1}$$

where $0 \leq \alpha \ll 1$ the *fraction of damping*, k the *wave number*, ι the imaginary unit i.e $\iota = \sqrt{-1}$ and $g(x, y)$ the *source function*. A relation for the wavenumber k is

$$k(x) = \frac{2\pi}{\lambda} = \frac{\omega}{c(x)},$$

where $\omega = 2\pi f$ with f the *wave frequency*, $\lambda = \frac{c(x)}{f}$ the wavelength and $c(x)$ the speed of sound.

An un-damped problem (with $\alpha = 0$) is considered in the unit square domain $\Omega = (0, 1)\times(0, 1)$. Sommerfeld-like conditions

$$\frac{\partial u}{\partial n} - \iota k u = 0 \quad \text{on } \partial\Omega \tag{2}$$

are imposed on boundaries, where n is the outward direction normal to boundaries. The source function g is chosen as

$$g(x, y) = \delta(x_1 - \frac{1}{2}, x_2 - \frac{1}{2}) \tag{3}$$

which means waves propagates from the center of domain outwards.

Discretization of the problem leads to a linear system

$$Au = g \tag{4}$$

which is complex-valued, sparse, symmetric and indefinite for sufficiently large wavenumber.

3 Preconditioning and Deflation

The GMRES (and other Krylov subspace solvers) converge fast for linear systems with a favorable spectrum. In general, linear systems arised from various physical problems have not a favorable spectrum for respective Krylov solvers. Therefore preconditioning is introduced.

Simply, preconditioning means transforming a linear system by multiplying the preconditioner M^{-1} on left, (or right and split) into one which is favourable for any iterative solver, preserving

			$ILU(0)$	$ILU(0.01)$	
k	**Dim** A	**nz(A)**	Iterations	**Iterations**	**nz(L +U)/nz(A)**
10	289	1377	21	8	3.6536
20	1089	5313	43	13	4.2415
30	2401	11809	71	21	4.4762
40	4201	20865	99	32	4.6116
50	6561	32481	120	49	4.7077

Table 1: An analysis of $ILU(0)$ and $ILU(0.01)$ preconditioners.

the solution. In the extreme case, A itself is the best choice to choose as preconditioner, but it is impracticable, since using A as a preconditioner is as expensive as solving the original system. So the preconditioner must resemble the coefficient matrix A but must be cheaper to solve than A. Many preconditioners are developed and used for various problems, those were obtained by the coefficient matrix of the linear system or by a discrete operator of the related problem. After choosing a preconditioner M for any system $Au = g$, whose inverse is cheap to compute, then the transformed system is

$$M^{-1}Au = M^{-1}g.$$

This is called *left preconditioning*. Also *right* preconditioning

$$AM^{-1}\bar{u} = g,$$

where $\bar{u} = Mu$ and *split preconditioning* if $M = M_1M_2$ then

$$M_1AM_2M_2^{-1}u = M_1b.$$

3.1 ILU Preconditioner for Helmholtz

One simple class of preconditioners is obtained by an *Incomplete LU* factorization of A, where L and U are a lower and upper triangular matrix respectively. There are many ways to obtain approximate ILU factorizations of A, e.g. Zero fill-in ILU and ILU with some tolerance. ILU obtained by restricting the structure of L and U to equal that of A leads to preconditioner, known as $ILU(0)$ which is easy to compute but not so effective for Krylov subspace methods. A more accurate ILU factorization of A is obtained by allowing more fill-in the ILU-factorization. Dropping the elements less than some given value in ILU gives rise to $ILU(tolerance)$.

Amongst the Krylov subspace methods, GMRES [5] is the best choice for Helmhotz problem, as claimed in [3]. Thus all the results are produced by GMRES. Table 1 shows results of GMRES preconditioned with preconditioners $ILU(0)$ and $ILU(tolerance)$ with tolerance (0.01). Results in Table 1 indicate that $ILU(0.01)$ works better than $ILU(0)$ but at the cost of big storage, that is due to more allowed *fill-in*, which is indicated by the number of nonzero elements in factorizations L and U and their ratio to nonzero elements in A. In view of increase in this ratio, for practicle problems, it can be presumed that $ILU(0.01)$ is impracticable.

Further, for Helmholtz problem, Krylov solvers preconditioned with ILU preconditioners are mesh dependent, as examined in [6] and this also follows from Table 1.

In the next section, an other preconditioner called *"Shifted Laplace Preconditioner"* is discussed

3.2 Shifted Laplace Preconditioner

An other way of obtaining a preconditioner is by a related operator. This class of preconditioners for the Helmholtz equation contains the most effective preconditioner, *shifted Laplace preconditioners*. The idea started with the preconditioner obtained by discretizing *Laplace operator* $M = \Delta$, which was used as preconditioner in [7]. Later an additional real term *Shift* was added into the Laplace operator, making this preconditioner resembling more the Helmholtz operator but with an opposite sign as investigated in [8]. Later Laplace operator with an imaginary shift was introduced in [3] and found to be more effective for the Helmholtz equation, and named complex shifted Laplace preconditioner (For details, see [3]).
This is developed by a discretization of the operator

$$M(\beta_1, \beta_2) = -\Delta - (\beta_1 - \iota\beta_2)k^2, \beta_1, \beta_2 \in \mathbb{R}$$

where β_1 and β_2 are real and imaginary shifts respectively. The shifted Laplace preconditioner with both real and imaginary shifts is best when solved by multigrid. Since in this paper, for all results the preconditioner is solved by a direct solver therefore only an imaginary shift is used.

For the notation, $M(0, 0)$ is simply discretized Laplace preconditioner without any shift, $M(-1, 0)$ is preconditioning matrix with real shift , and $M(0, 1)$ is the complex shifted Laplace preconditioner.
The spectral properties of the shifted Laplace operator are elaborated in [9, 4] and it is showed that the spectrum of the discretized Helmholtz operator preconditioned by shifted Laplacian is clustered near one, but some eigenvalues lie at $O(\epsilon/k^2)$. The eigenvalues are bounded above by one but the smallest eigenvalues rush to zero as k increases. This is shown in Figure 1. With increase in wavenumber, iterative scheme encompass some very small eigenvalues, which cause slow convergence. The small eigenvalues are handeled by *deflation*.

3.3 Deflation

The Krylov method to solve linear system is typically adversely affected by a few unfavorable eigenvalues of the coefficient matrix. Deflation is a technique dealing with those undesired eigenvalues. Deflation for SPD systems is used in [10] and [11] with Conjugate Gradient to improve the condition number. Various ideas such as sub-domain deflation are used in [11]. Later this idea was extended to non-symmetric systems in [12]. The basic idea is to deflate the smallest eigenvalues to zero by choosing eigenvectors or approximate Ritz vectors corresponding to those smallest eigenvalues as deflation vectors [10] and [11]. In [12], instead of deflating the small eigenvalues to zero, a deflation preconditioner is discussed which deflates the smallest eigenvalues of discretized preconditoned Helmholtz operator around zero to the maximum eigenvalue (in absolute value for a complex eigenvalue).

Defining deflation for any matrix $Z \in \mathbb{R}^{n \times k}$ of deflating vectors, deflation preconditioner is the projection defined as

$$P = I - AQ \qquad \text{with} \qquad Q = ZE^{-1}Z^T \qquad E = Z^TAZ \tag{5}$$

where E is called the Galerkin or coarse matrix and Z the matrix, whose columns span the deflation subspace, is chosen such that E is non-singular. For A SPD, it is sufficient that $Rank(Z) = k$. Further properties of deflation space for an arbitrary Z are elaborated in detail in [10] and [12].

For the problems with large wavenumber k, the spectrum has more small eigenvalues, and a large deflation matrix Z will be needed to deflate more number of small eigenvalues. A large deflation matrix Z leads to large E, which can be impractal to solve by a direct solver. One may sovle E then iteratively and its iterative solution may lead to scattering of very small eigenvalues. A tight stopping criteria may prevents this. An other idea of deflating eigenvalues to the maximum eigenvalue can be favorable. It is not theoritically established how to choose Z, but an optimal choice for matrix Z in Equation 5 is to set eigenvectors of matrix as columns of deflation matrix Z. This is off course expensive in terms of memory, since it needs to solve E. When choosing Z, one should take care that it should be sparse. In [12], piece-wise constant interpolation is used to construct Z, as in Multigrid. We use multigrid-deflation vectors, which are very sparse and hence cheap.

4 Numerical Results

In this part, numerical results are shown for a 2D Helmholtz problem with a source function emmiting from the center defined in Equation 3. The problem is discretized with first order radiation conditions (Equation 2) on all boundaries. GMRES is used and iterations are terminated if the residual satisfies the relation

$$\frac{\|g - Au^n\|}{\|g\|} \leq 10^{-7}. \tag{6}$$

In Figure 1, the convergence history of GMRES is compared with deflated GMRES with and without shifted Laplace preconditoner for the wavenumber $k = 40$. This is sufficient to show that deflation is still efficient when the scheme is preconditioned with the shifted Laplace preconditioner.

Table 2 gives a comparison of iterations taken by GMRES precondtioned with $ILU(0)$, $ILU(0.01)$ and shifted Laplace preconditioners and deflated GMRES with shifted Laplace preconditioner respectively. Though shifted Laplace preconditioner and $ILU(0.01)$ are comparable for small wavenumber-problem but memory problems with $ILU(0.01)$ can be severe with an increase in wavenumber. On the other hand, the shifted Laplace preconditioner is more diagonally dominant than A with the same sparsity. Deflated GMRES preconditioned by shifted Laplace preconditioner is more attractive, and is mildly dependent on the wavenumber. Further the deflated GMRES preconditioned by $M(0, 1)$ is also mesh independent, which is shown in Figure 2, where for a problem with wavenumber $k = 20$, deflated GMRES preconditioned with $M(0, 1)$ takes 10, 8, and 7 iterations for meshsizez n= 33, 49, and 65 respectively. Figure 2 also shows mesh independent convergence of deflated GMRES without preconditioner.

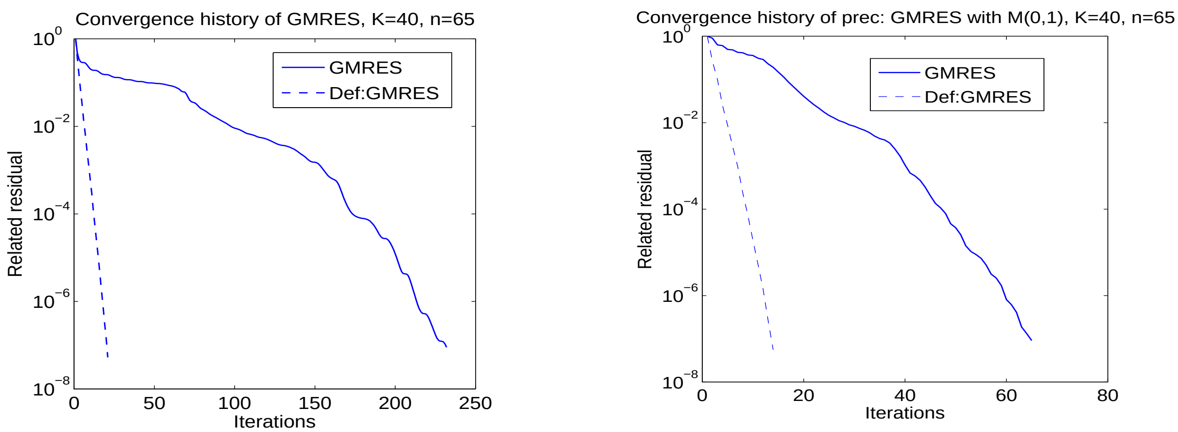

Figure 1: (a) Convergence history of deflated GMRES without preconditioner using MG deflation vectors for K =40. (b)Conv: history of deflated GMRES preconditioned by shifted Laplace preconditioner using MG deflation vectors for K=40.

k	**ILU(0)**	**ILU(0.01)**	**shifted Laplace**	**Deflated shifted Laplace**
10	21	8	10	7
20	43	13	19	9
30	71	21	30	11
40	99	32	40	13
50	120	49	51	15

Table 2: Number of iterations by GMRES with ILU and shifted Laplace preconditioners with different values of wavelength k.

A comparison of the spectrum of the coefficient matrix for wavenumber $k = 10$ and $k = 40$ is shown in Figure 3. The spectrum of discrete Helmholtz operator A is very scattered for wavenumber $k = 10$ and $k = 40$. Though the spectrum of the preconditioned operator is bounded above by one; the eigenvalues rush to zero as k increases, causing slow convergence. The spectrum of $M^{-1}PA$ is clustered around one. Deflation removes the lowest part of spectrum, by deflating smallest eigenvalues to zero, making no contribution of components of corresponding vectors.

5 Further Work

Deflated GMRES preconditioned by complex shifted Laplace preconditioner give impressive results. We plan to analyse this good convergence behaviour. Multigrid deflation vectors are used as columns in the deflation matrix. Analysis for this scheme is proposed by *local Fourier analysis*. This can give nice information about convergence factor/rate and its dependency on wavenumber k and mesh size.

6 Conclusions

For linear systems obtained from a discretization of the Helmholtz equation by the finite difference method, experiments are done with GMRES, GMRES preconditioned by ILU and shifted Laplace preconditioner. The comparison of preconditioners for the Helmholtz equation is carried out. For a small wavenumber k, ILU preconditioners with GMRES work well, but they are no more of use for larger k. For larger k, shifted Laplace preconditioner performs better than ILU. The preconditioned coefficient matrix however still has some eigenvalues near zero, causing GMRES to converge slowly. This problem appears to be more serious for increasing k, but can be fixed by deflation. Multigrid deflation vectors are used as columns of the deflation matrix, which are very sparse. Deflated GMRES preconditioned by shifted Laplace preconditioner is not only wavenumber independent but also is mesh independent.

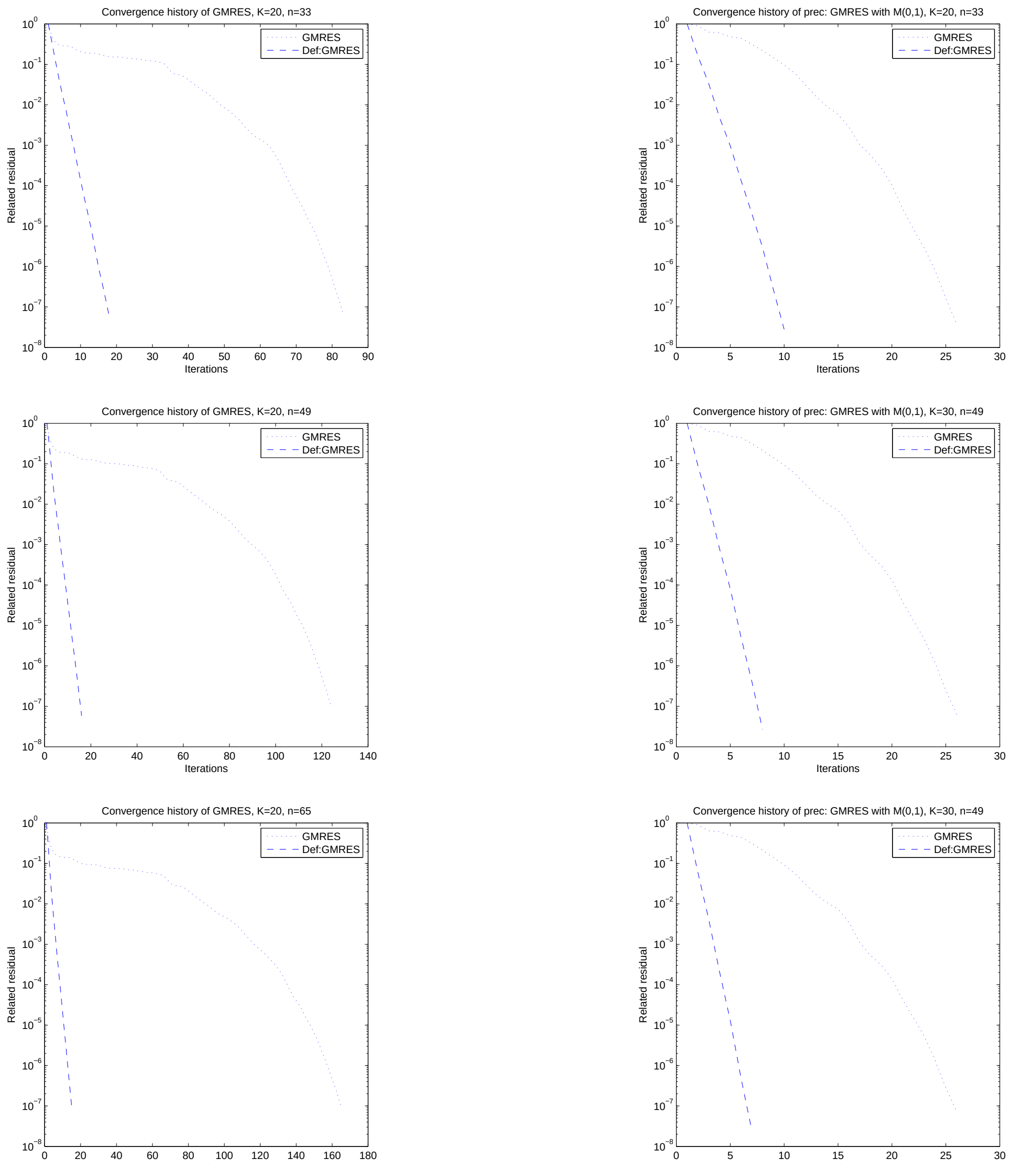

Figure 2: Convergence History of deflated GMRES for $k = 20$ for three different mesh sizes left: without preconditioner, right: with shifted Laplace preconditioner

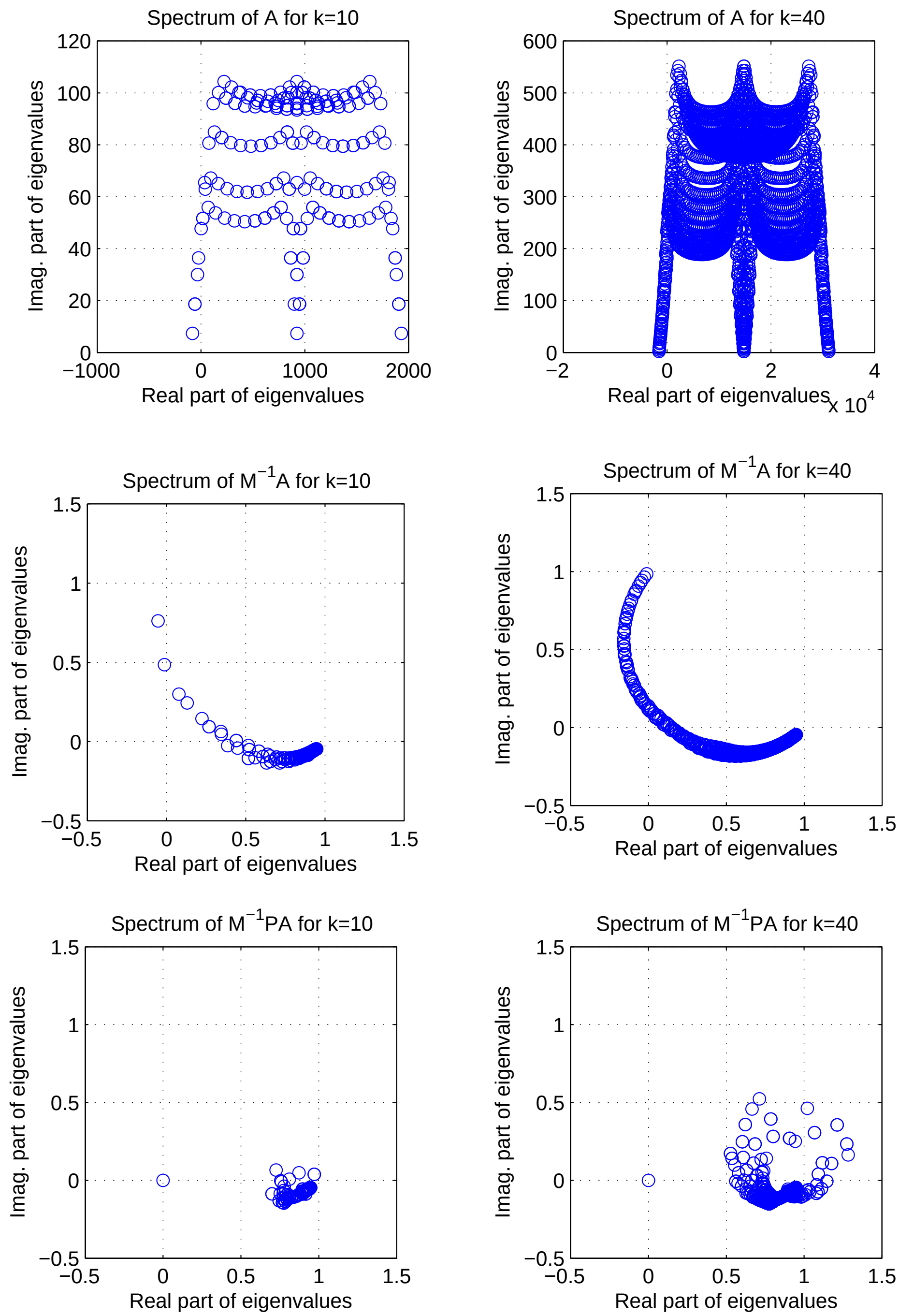

Figure 3: Spectrum of matrices A, $M^{-1}A$ and $M^{-1}PA$ for wavenumber $k = 10$ and $k = 40$

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