TECHNICAL REPORT HG CP 94–00820–CICT–3.1

Conjugate Gradient Method with Circulant Block-Factorization Preconditioners for 3D Elliptic Problems

Ivan Lirkov Svetozar Margenov
BAS, Sofia, Bulgaria

Abstract

This report follows the research plan of the HIPERGEOS Project COP–94 00820.

The numerical solution of large scale elliptic boundary value problems is discussed in this report. We analyze the circulant block-factorization preconditioners when solving elliptic problems by Preconditioned Conjugate Gradient (PCG) method. Both methods, the conjugate gradient and the inversion of the circulant matrices using Fast Fourier Transform (FFT) are highly parallelizable.

An estimate of the relative condition number for a model 3D Dirichlet boundary value problem is derived. A set of numerical test is presented at the end of the report. The obtained results are in good agreement with the theory.

Our next goal is to implement the studied here circulant block-factorization algorithms as a basic preconditioning solver for 3D elasticity problems.

1 Introduction

In this report we are concerned with the numerical solution of linear boundary value problems of elliptic type. After discretization, such problems are reduced to find the solution of linear systems of the form $Ax = b$. We shall only consider the case where A is symmetric and positive definite. In practice, large problems of this class are often solved by iterative methods, such as the conjugate gradient method. At each step of these iterative methods only the product of A with a given vector v is needed. Such methods are therefore ideally suited to exploit the sparsity of A.

Typically, the rate of convergence of these methods depends on the condition number $\kappa(A)$ of the coefficient matrix A: the smaller $\kappa(A)$ is, the faster convergence. Unfortunately, for elliptic problems of second order, usually $\kappa(A) = \mathcal{O}(n^2)$, where n is the number of mesh points in each coordinate direction, and hence grows rapidly with n. To somewhat facilitate this problem, these methods are almost always used with a preconditioner M. The preconditioner is chosen with two criteria in mind: to minimize $\kappa(M^{-1}A)$ and to allow efficient computation of the product $M^{-1}v$ for a given vector v. These two goals are often conflicting ones and much research has been done into devising preconditioners that strike a delicate balance between both.

One of the most popular and the most successful class of preconditioners is the class of incomplete LU (ILU) factorizations, see e.g. [7].

One potential problem with the ILU preconditioners is that it have limited degree of parallelism. Some attempts to modify the method and to devise other more parallel methods often result in a deterioration of the convergence rate.

In [1], R. Chan and T. F. Chan proposed another class of preconditioners which is based on averaging coefficients of A to form a block-circulant approximation (see also [8, 10, 15]). Circulant preconditioners for Toeplitz systems have been proposed first by Olkin [14] and Strang [15]. Their properties and practicality have been studied by Strang [15], Chan & Jin [2], Chan & Olkin [5], etc. The usage of the block-circulant approximations is motivated by their fast inversion based on the FFT (see [6, 12]). In addition, the recent research on circulant preconditioners for Toeplitz systems [4, 3, 9, 10] shows good results for favorable clustering of eigenvalues of the preconditioned system. The block–circulant preconditioners are highly parallelizable, see, e.g., [12, 13], but they are substantially sensitive with respect to a possible high variation of the coefficients of the elliptic operator.

The sensitivity of the block–circulant approximations with respect to a high variation of the problem coefficients was relaxed in the circulant block–factorization (CBF) preconditioners ([11]). This preconditioning technique incorporates the circulant approximations into the framework of the LU block–factorization. The computational efficiency and parallelization of the resulting algorithm is as high as of the block circulant one ([1, 13]).

The goal of the present report is to study the convergence rate of the circulant block–factorization preconditioners for 3D elliptic problems. The relative condition number $\kappa(M^{-1}A)$ is estimated with $\mathcal{O}(n)$ which is the same as for the 2D elliptic problems. The presented numerical tests demonstrate the features of the circulant block–factorization preconditioners for 3D elliptic problems.

2 The 2D elliptic problem and the circulant preconditioners

We consider the following 2D elliptic problem:

$$-(a(x,y)u_x)_x - (b(x,y)u_y)_y = f(x,y) \tag{1}$$

on the unit square $[0,1] \times [0,1]$ with Dirichlet boundary condition. Let the domain be discretized by an uniform grid with n grid points in each coordinate direction, denoted by x_i and y_j. Consider the usual five-point centered difference approximation. This discretization leads to a system of linear algebraic equations

$$Ax = b.$$

If the grid points are ordered along, e.g., the x-direction first, the matrix A admits a block-tridiagonal structure where the diagonal blocks are tridiagonal matrices and the off-diagonal blocks are diagonal matrices. The matrix A can be written in the following form

$$A = tridiag(-A_{i,i-1}, A_{i,i}, -A_{i,i+1}) \qquad i = 1, 2, \dots, n,$$

where

$$\begin{aligned} A_{i,i} &= tridiag(-a_{j,j-1}, a_{j,j}, -a_{j,j+1}), \quad j = (i-1)n+1, \dots, in, \quad i = 1, 2, \dots, n, \\ A_{i,i+1} &= diag(a_{j,j+n}), \quad j = (i-1)n+1, \dots, in, \quad i = 1, \dots, n-1, \\ A_{i,i-1} &= diag(a_{j,j-n}), \quad j = (i-1)n+1, \dots, in, \quad i = 2, \dots, n. \end{aligned}$$

Let us remind that a circulant matrix C has the form $(C_{k,j}) = \left(c_{(j-k) \bmod m}\right)$, where m is the size of C. Let us also denote for any given coefficients $(c_0, c_1, \dots, c_{m-1})$ by $C = (c_0, c_1, \dots, c_{m-1})$ the circulant matrix

$$\begin{bmatrix} c_0 & c_1 & c_2 & \dots & c_{m-1} \\ c_{m-1} & c_0 & c_1 & \dots & c_{m-2} \\ \vdots & \vdots & \vdots & & \vdots \\ c_1 & c_2 & \dots & c_{m-1} & c_0 \end{bmatrix}.$$

Any circulant matrix can be factorized as

$$C = F \Lambda F^*, \tag{2}$$

where Λ is a diagonal matrix containing the eigenvalues of C, and F is the Fourier matrix

$$F = \frac{1}{\sqrt{m}} \left\{ e^{2\pi \frac{jk}{m} \mathbf{i}} \right\}_{0 \le j,k \le m-1}.$$

Here $\mathbf{i}$ stands for the imaginary unit.

Let us denote

$$\begin{aligned} \bar{a} &= \tfrac{1}{n^2} \textstyle\sum_{i=1}^{n-1} \sum_{j=(i-1)n+1}^{in} a_{j,j+n} \\ \bar{b} &= \tfrac{1}{n^2} \textstyle\sum_{i=1}^{n} \sum_{j=(i-1)n+1}^{in-1} a_{j,j+1} \end{aligned}$$

$$\begin{aligned} C_0 &= (2\bar{a} + 2\bar{b} + 2\rho n^{-2}, -\bar{b}, 0, \dots 0, -\bar{b}) \\ C_1 &= -\bar{a} I = (-\bar{a}, 0, \dots 0) \end{aligned}$$

where ρ is a positive constant independent of n. Then the *block-circulant preconditioner* can be written in the following form

$$C_B = (C_0, C_1, 0, \dots 0, C_1). \tag{3}$$

The general form of the *circulant block-factorization preconditioner* is defined by

$$C_F = tridiag(-C_{i,i-1}, C_{i,i}, -C_{i,i+1}) \qquad i = 1, 2, \dots, n, \tag{4}$$

where $C_{i,j} = Circulant(A_{i,j})$ is a circulant approximation of the corresponding block $A_{i,j}$.

3 The 3D elliptic problem and the circulant block-factorization preconditioners

We consider the following 3D elliptic problem:

$$-(a(x,y,z)u_x)_x - (b(x,y,z)u_y)_y - (c(x,y,z)u_z)_z = f(x,y,z) \tag{5}$$

on the unit cube $[0,1] \times [0,1] \times [0,1]$ with Dirichlet boundary condition. Let the domain be discretized by an uniform grid with n grid points in each coordinate direction, denoted by x_i, y_j and z_k. Consider the usual seven-point centered difference approximation. This discretization leads to a system of linear algebraic equations

$$Ax = b.$$

If the grid points are ordered along, the x- and y-direction first, the matrix A admits a block-tridiagonal structure. The diagonal blocks are block-tridiagonal matrices and the off-diagonal blocks are diagonal matrices. The matrix A can be written in the following form

$$A = tridiag(-A_{i,i-1}, A_{i,i}, -A_{i,i+1}) \qquad i = 1, 2, \ldots, n,$$

where $A_{i,i}$ are block-tridiagonal matrices which corresponds to one z-plane.

We use now the general form of the circulant block-factorization preconditioning matrix M for the matrix A by

$$M = tridiag(-C_{i,i-1}, C_{i,i}, -C_{i,i+1}) \qquad i = 1, 2, \ldots n,$$

where $C_{i,j} = Circulant(A_{i,j})$ is block-circulant approximation of the corresponding block $A_{i,j}$. An estimate of the relative condition number of the CBF preconditioner for a model problem is derived in the next theorem.

Theorem 1 *The preconditioning matrix M_0 defined by the CBF algorithm for the 3D model problem with Laplace operator, i.e., when $a(x,y,z) = b(x,y,z) = c(x,y,z) = 1$, gives a relative condition number estimated by*

$$\kappa(M_0^{-1}A_0) \leq 4n. \tag{6}$$

Proof: For the model problem we have a matrix $A_0 = tridiag(-I, A_{i,i}, -I)$ where the diagonal blocks are $A_{i,i} = tridiag(-I, tridiag(-1,6,-1), -I)$. Then the preconditioning matrix M_0 has the form $M_0 = tridiag(-I, C_{i,i}, -I)$ where the diagonal blocks are block-circulant $C_{i,i} = ((6,-1,0,\ldots 0,-1), -I, 0, \ldots 0, -I)$. Let us consider the matrices $G = tridiag(-1,2,-1)$ and $H = (2,-1,0,\ldots 0,-1)$. Then

$$\begin{aligned} A_0 &= I \otimes I \otimes G + I \otimes G \otimes I + G \otimes I \otimes I, \\ M_0 &= I \otimes I \otimes H + I \otimes H \otimes I + G \otimes I \otimes I, \end{aligned}$$

where $\otimes$ stands for the Kronecker product.

We next estimate the condition number $\kappa(M_0^{-1}A_0)$. Let x be an arbitrary n^3-vector and y be an arbitrary n-vector. We use the estimates from [11]

$$\begin{aligned} y^T(G+\frac{1}{2n^2}I)y &\geq \frac{1}{2}y^T(H+\frac{1}{2n^2}I)y, &(7)\\ y^T(G+\frac{1}{2n^2}I)y &\leq 2ny^T(H+\frac{1}{2n^2}I)y, &(8)\\ \lambda(G) &\leq \frac{1}{n^2}. \end{aligned}$$

Then we get that $G-\frac{1}{n^2}I$ is positive definite. We can rewrite matrices A_0 and M_0 as

$$\begin{aligned} A_0 &= I\otimes I\otimes(G+\frac{1}{2n^2}I)+I\otimes(G+\frac{1}{2n^2}I)\otimes I+(G-\frac{1}{n^2}I)\otimes I\otimes I,\\ M_0 &= I\otimes I\otimes(H+\frac{1}{2n^2}I)+I\otimes(H+\frac{1}{2n^2}I)\otimes I+(G-\frac{1}{n^2}I)\otimes I\otimes I. \end{aligned}$$

Then from (7) and (8) we obtain

$$\frac{1}{2}\leq\frac{x^TA_0x}{x^TM_0x}\leq 2n$$

and

$$\kappa(M_0^{-1}A_0)\leq 4n.$$

■

4 Numerical tests

In this section, we compare the convergence rate of the CBF preconditioner for the 3D problem and for the 2D problem. The 3D test problem we used is

$$\begin{aligned} \frac{\partial}{\partial x}\left[(1+\frac{\epsilon}{2}\sin(2\pi(x+y+z)))\frac{\partial u}{\partial x}\right] &+ \frac{\partial}{\partial y}\left[(1+\frac{\epsilon}{2}\sin(2\pi(x+y+z)))\frac{\partial u}{\partial y}\right]+\\ \frac{\partial}{\partial z}\left[(1+\epsilon e^{x+y+z})\frac{\partial u}{\partial z}\right] &= f(x,y,z) \end{aligned}$$

on $\Omega_3=[0,1]\times[0,1]\times[0,1]$, where ϵ is a parameter. The 2D problem we use for comparison is

$$\frac{\partial}{\partial x}\left[(1+\frac{\epsilon}{2}\sin(2\pi(x+y)))\frac{\partial u}{\partial x}\right]+\frac{\partial}{\partial y}\left[(1+\epsilon e^{x+y})\frac{\partial u}{\partial y}\right]=f(x,y)$$

on $\Omega_2=[0,1]\times[0,1]$. The computations are done with double precision on a SUN SPARC station 20. The iteration stopping criterion is $\|r^{N_{it}}\|/\|r^0\|<10^{-6}$, where r^j stands for the residual at the jth iteration step of the preconditioned conjugate gradient method.

The Tables show the number of iterations as a measure of the convergence rate of the preconditioner. The preconditioner is characterized by the estimate $\kappa(M^{-1}A) = \mathcal{O}(n)$, or the expected number of the iterations have to grow as $N_{it} = \mathcal{O}(\sqrt{n})$. The presented data demonstrate a slightly slower growth of N_{it} with n, but in general the obtained results are in a good agreement with the theory.

The Table 1 shows the number of iterations for 3D problem. In the Table 2 the number of iterations for 2D problem demonstrate similar behavior as for the 3D test problem.

Table 1: Number of iterations for CBF preconditioner for 3D problem.

n	$\varepsilon = 0$	$\varepsilon = 0.01$	$\varepsilon = 0.1$	$\varepsilon = 1$
8	10	10	10	12
16	12	13	13	15
32	15	15	16	19
64	17	19	21	26

Table 2: Number of iterations for CBF preconditioner for 2D problem.

n	$\varepsilon = 0$	$\varepsilon = 0.01$	$\varepsilon = 0.1$	$\varepsilon = 1$
8	10	10	10	9
16	13	13	12	11
32	17	17	16	15
64	21	21	19	20

5 Summary

We are concerned with the numerical solution of elliptic linear boundary value problems. After discretization, such problems reduce to the solution of linear systems. We use a preconditioner based on a block-circulant approximation of the blocks of the initial matrix. We exploit the fast inversion of block-circulant matrices. The computation and the inversion of these circulant block-factorization preconditioners are highly parallelizable on a wide variety of architectures.

References

[1] R.H. Chan and T.F. Chan. Circulant preconditioners for elliptic problems. *J. Num. Lin. Alg. Appl.*, 1:77–101, Mar. 1992.

[2] R.H. Chan and X. Jin. A family of block preconditioners for block systems. *SIAM J.Sci.Stat.Comp.*, 13(5):1218–1235, Sep. 1992.

[3] R.H. Chan and G. Strang. Toeplitz equations by conjugate gradients with circulant preconditioner. *SIAM J.Sci.Stat.Comp.*, 10:104–119, 1989.

[4] T.F. Chan. An optimal circulant preconditioner for toeplitz systems. *SIAM J.Sci. Stat.Comp.*, 9:766–771, Jul. 1988.

[5] T.F. Chan and J.A. Olkin. Preconditioners for toeplitz-block matrices. Presented at SIAM Conference on Linear Algebra in San Francisco, 1990.

[6] P.J. Davis. *Circulant matrices.* Johns Wiley, New York, 1979.

[7] G.H. Golub and C.F. Van Loan. *Matrix Computations.* Johns Hopkins Univ.Press, Baltimore, 2nd edition, 1989.

[8] S. Holmgren and K. Otto. Iterative solution methods for block-tridiagonal systems of equations. *SIAM J. Matr. Anal. Appl.*, 13:863–886, 1992.

[9] T. Huckle. Circulant and skewcirculant matrices for solving toeplitz matrix problems. *SIAM J.Matr.Anal.Appl.*, 13:767–777, 1992.

[10] T. Huckle. Some aspects of circulant preconditioners. *SIAM J. Sci. Comput.*, 14:531–541, 1993.

[11] I. Lirkov, S. Margenov, and P.S. Vassilevski. Circulant block-factorization preconditioners for elliptic problems. *Computing*, 53(1):59–74, 1994.

[12] C. Van Loan. *Computational frameworks for the fast Fourier transform.* SIAM, Philadelphia, 1992.

[13] S.D. Margenov and I.T. Lirkov. Preconditioned conjugate gradient iterative algorithms for transputer based systems. In K.Boyanov, editor, *Parallel and distributed processing*, pages 406–415, Sofia, 1993.

[14] J.A. Olkin. *Linear and nonlinear deconvolution problems.* PhD thesis, Rice University, TX, 1986.

[15] G. Strang. A proposal for toeplitz matrix calculations. *Stud. Appl.Math.*, 74:171–176, 1986.