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Abstract

The numerical solution of systems of convection-diffusion equations is considered. The problem is described by a system of second order partial differential equations. This system is discretized by Courant-elements. The Preconditioned Conjugate Gradient iterative method is used for solving of the large-scale linear algebraic systems arising after the Finite Element method discretization of the problem. Discrete Helmholtz preconditioner is applied to obtain a mesh independent superlinear convergence of the iterative method. A parallel algorithm is invented for the proposed preconditioner.

Key words: conjugate gradient method, preconditioning, superlinear convergence, mesh independence, numerical experiments.

1 Introduction

The conjugate gradient method is a widespread and efficient way of solving nonsymmetric linear algebraic systems arising from discretized elliptic problems, see the book [2] where an extensive summary is given on the convergence of the CGM. When for elliptic problems the discretization parameter h tends to 0, the required number of iterations for prescribed accuracy tends to ∞. The remedy is suitable preconditioning [2], which sometimes relies on Hilbert space theory [6], [11]. Moreover, it has been shown in [6] that the preconditioned CGM can be competitive with multigrid methods.

The CGM for nonsymmetric equations in Hilbert space has been studied in [4], [5]: in the latter superlinear convergence has been proved in Hilbert space and, based on this, mesh independence of the superlinear estimate has been derived for FEM discretizations of elliptic Dirichlet problems. The mesh independent superlinear convergence results have been extended from a single equation to systems in a recent paper [8] in the framework of normal operators in

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Hilbert space. An important advantage of the obtained preconditioning method for systems is that one can define decoupled preconditioners, hence the size of the auxiliary systems remains as small as for a single equation, moreover, parallelization of the auxiliary systems is available.

The main goal of this paper is to summarize the theoretical result for systems of convection-diffusion equations and to illustrate the efficiency of the preconditioned conjugate gradient method with Matlab for smaller problems and flash the possibility of an MPI parallel code using multiple processors.

The following type of systems are considered

$$\left.\begin{aligned} &-\operatorname{div}(K_i \nabla u_i) + \mathbf{b}_i \cdot \nabla u_i + \sum_{j=1}^{l} V_{ij} u_j = g_i \\ &u_{i|\partial\Omega} = 0 \end{aligned}\right\} \qquad (i = 1, \ldots, l) \tag{1}$$

under the following

Assumptions BVP.

(i) the bounded domain $\Omega \subset \mathbf{R}^N$ is C^2-diffeomorphic to a convex domain;

(ii) for all $i, j = 1, \ldots, l$, $K_i \in C^1(\overline{\Omega})$, $V_{ij} \in L^\infty(\Omega)$ and $\mathbf{b}_i \in C^1(\overline{\Omega})^N$;

(iii) there is $m > 0$ such that $K_i \geq m$ holds for all $i = 1, \ldots, l$;

(iv) letting $V = \{V_{ij}\}_{i,j=1}^{l}$, the coercivity property

$$\lambda_{\min}\left(V + V^T\right) - \max_i \operatorname{div} \mathbf{b}_i \geq 0 \tag{2}$$

holds pointwise on Ω, where $\lambda_{\min}$ denotes the smallest eigenvalue;

(v) $g_i \in L^2(\Omega)$.

Remark 1 *The applicable algorithms have been used for test equations defined on a very simple domain and only for two-dimensional problems, i. e. $N = 2$. Considering constant $\mathbf{b}_i$ is another simplifier factor, therefore no numerical integration is needed and the coercivity property (iv) has a simpler form*

$$\lambda_{min}\left(V + V^T\right) \geq 0. \tag{3}$$

Systems of the form (1) arise e. g. from the time discretization and Newton linearization of nonlinear reaction-convection-diffusion systems which occur frequently in meteorological air-pollution models. We can write the considered system in a short vector form using the corresponding n-tuples:

$$\left.\begin{aligned} &L\mathbf{u} \equiv -\operatorname{div}(\mathbf{K}\nabla\mathbf{u}) + \mathbf{b} \cdot \nabla\mathbf{u} + V\mathbf{u} = \mathbf{g} \\ &\mathbf{u}_{|\partial\Omega} = \mathbf{0} \end{aligned}\right\} \tag{4}$$

where

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_l \end{pmatrix}, \ \mathbf{g} = \begin{pmatrix} g_1 \\ g_2 \\ \vdots \\ g_l \end{pmatrix}, \ \operatorname{div}(\mathbf{K}\nabla\mathbf{u}) = \begin{pmatrix} \operatorname{div}(K_1\,\nabla u_1) \\ \operatorname{div}(K_2\,\nabla u_2) \\ \vdots \\ \operatorname{div}(K_l\,\nabla u_l) \end{pmatrix}, \ \mathbf{b}\cdot\nabla\mathbf{u} = \begin{pmatrix} \mathbf{b}_1\cdot\nabla u_1 \\ \mathbf{b}_2\cdot\nabla u_2 \\ \vdots \\ \mathbf{b}_l\cdot\nabla u_l \end{pmatrix}.$$

The FEM discretization of (4) leads to a linear algebraic system

$$\mathbf{L}_h\mathbf{c} = \mathbf{g}_h.$$

This can be solved by the CGM using a preconditioner. In this paper we consider symmetric Helmholtz preconditioners

$$S_i u_i := -\operatorname{div}(K_i\nabla u_i) + \eta_i u_i \qquad (i = 1, \dots, l) \tag{5}$$

where $\eta_i \in C(\overline{\Omega})$, $\eta_i \geq 0$ are suitable functions. The n-tuple of elliptic operators S and the corresponding matrix $\mathbf{S}_h$ can be defined in the same way as previously, so the preconditioned form of the discretized equation is

$$\mathbf{S}_h^{-1}\mathbf{L}_h\mathbf{c} = \mathbf{f}_h \equiv \mathbf{S}_h^{-1}\mathbf{g}_h. \tag{6}$$

2 The Preconditioned Conjugate Gradient Algorithms

Now let us consider the operator equation

$$Lu = g \tag{7}$$

with an unbounded linear operator $L : D \to H$ defined on a dense domain D, and with some $g \in H$, where H is an infinite dimensional complex separable Hilbert space. We have the following

Assumptions A.

(i) The operator L is decomposed in $L = S + Q$ on its domain D where S is a self-adjoint operator in H.

(ii) S is a strongly positive operator, i.e. there exists $p > 0$ such that

$$\langle Su, u\rangle \geq p\|u\|^2 \qquad (u \in D). \tag{8}$$

(iii) There exists $\varrho > 0$ such that $\Re\,\langle Lu, u\rangle \geq \varrho\,\langle Su, u\rangle$ $(u \in D)$.

(iv) The operator Q can be extended to the energy space H_S, and then $S^{-1}Q$ is assumed to be a compact normal operator on H_S.

The energy space H_S is the completion of the domain D under the energy inner product

$$\langle u, v \rangle_S := \langle Su, v \rangle ,$$

the corresponding norm $\|u\|_S = \sqrt{\langle u, u \rangle_S}$.

The generalized conjugate gradient, least square (GCG-LS) method is defined in [1]. The full version of the GCG-LS method constructs a sequence of search directions d_k and simultaneously a sequence of approximate solutions u_k. To construct the search directions, the definition also involves an integer $s \in \mathbf{N}$, further, we let $s_k = \min\{k, s\}$ $(k \geq 0)$. Not all the previous search directions are used to construct d_{k+1}, but every previous d_k are used for the construction of the new approximative solution u_{k+1}, whereas the truncated algorithm uses only the above-mentioned $s+1$ directions. In particular, if $s = 0$ (GCG-LS(0)) then u_{k+1} is the linear combination of the previous approximate solution u_k and the previous search direction d_k. The algorithm of the full version for the preconditioned operator equation

$$S^{-1}Lu = f \equiv S^{-1}g \tag{9}$$

in H_S is as follows:

$$\begin{cases}
(1) & \text{Let } u_0 \in D \text{ be arbitrary, let } r_0 \text{ be the solution of } Sr_0 = Lu_0 - g; \\
 & d_0 = -r_0; \text{ and } z_0 \text{ be the solution of } Sz_0 = Ld_0; \\
 & \quad \text{for any } k \in \mathbf{N}: \text{ when } u_k, d_k, r_k, z_k \text{ are obtained, let} \\
(2a) & \text{the numbers } \alpha_{k-j}^{(k)} \quad (j = 0, \dots, k) \quad \text{be the solution of} \\
 & \sum_{j=0}^{k} \alpha_{k-j}^{(k)} \langle Sz_{k-j}, z_{k-l} \rangle = - \langle r_k, Sz_{k-l} \rangle \qquad (0 \leq l \leq k); \\
(2b) & u_{k+1} = u_k + \sum_{j=0}^{k} \alpha_{k-j}^{(k)} d_{k-j}; \\
(2c) & r_{k+1} = r_k + \sum_{j=0}^{k} \alpha_{k-j}^{(k)} z_{k-j}; \\
(2d) & \beta_{k-j}^{(k)} = \langle Lr_{k+1}, z_{k-j} \rangle / \|z_{k-j}\|_S^2 \quad (j = 0, \dots, s_k); \\
(2e) & d_{k+1} = -r_{k+1} + \sum_{j=0}^{s_k} \beta_{k-j}^{(k)} d_{k-j}; \\
(2f) & z_{k+1} \text{ be the solution of } Sz_{k+1} = Ld_{k+1}.
\end{cases} \tag{10}$$

When symmetric part preconditioning is used, i. e. $S = (L + L^*)/2$, a more simple truncated algorithm is applicable, namely the so-called GCG-LS(0) (see [4] for details), where only the previous search direction d_k and auxiliary vector z_k are used, so the previous ones do not have to be stored.

$$
\begin{cases}
(1) & \text{Let } u_0 \in D \text{ be arbitrary, and let} \\
& r_0 \text{ be the solution of } Sr_0 = Lu_0 - g; \quad d_0 = -r_0; \\
& \quad \text{for any } k \in \mathbb{N}: \text{ when } u_k,\, d_k,\, r_k \text{ are obtained, let} \\
(2a) & z_k \text{ be the solution of } Sz_k = Ld_k, \\
& \quad \gamma_k = \langle Sz_k, z_k \rangle, \quad \alpha_k = -\frac{1}{\gamma_k} \langle r_k, Sz_k \rangle; \\
(2b) & u_{k+1} = u_k + \alpha_k d_k; \\
(2c) & r_{k+1} = r_k + \alpha_k z_k; \\
(2d) & \beta_k = \frac{1}{\gamma_k} \langle Lr_{k+1}, z_k \rangle; \\
(2e) & d_{k+1} = -r_{k+1} + \beta_k d_k.
\end{cases} \tag{11}
$$

Assumptions A imply that the operator of the preconditioned equation $S^{-1}L$ has the form $I+S^{-1}Q$, which is a compact perturbation of the identity operator, hence the following convergence result (see in [5], [8]) is applicable.

Theorem 2.1 *Let Assumptions A hold. Then the conjugate gradient method applied for equation* (9) *yields for all* $k \in \mathbf{N}$

$$\left(\frac{\|e_k\|_L}{\|e_0\|_L} \right)^{1/k} \leq \frac{2}{\varrho} \left(\frac{1}{k} \sum_{i=1}^{k} \left| \lambda_i(S^{-1}Q) \right| \right) \to 0 \quad \text{as } k \to \infty \tag{12}$$

where $e_k = u_k - u^*$ *is the error vector and* $\lambda_k(S^{-1}Q)$ $(k \in \mathbf{N})$ *are the ordered eigenvalues of the operator* $S^{-1}Q$.

3 Convergence results in $H_0^1(\Omega)^l$

Let us consider the Hilbert space $H = L^2(\Omega)^l$ with the inner product

$$\langle u, v \rangle = \int_\Omega \sum_{i=1}^{l} u_i \overline{v}_i$$

and define the operators L and S corresponding with (4) on the dense domain

$$D(L) = D(S) = D := \left(H^2(\Omega) \cap H_0^1(\Omega) \right)^l$$

Now we would like to use the convergence theorem for this problem in the space $L^2(\Omega)^l$ by verifying that L and S satisfy Assumptions A. First, we prove Theorem 2.1 using the truncated algorithm when S is the symmetric part of L. Then we consider the full version (10) and prove Theorem 2.1 for problems with constant coefficients when the normality of the preconditioned operator in the corresponding Sobolev space can be ensured.

First symmetric part preconditioning is considered, that is $S = (L + L^*)/2$. Since $Q = L - S$ is antisymmetric, it can be shown easily, that the operator $S^{-1}Q$ is antisymmetric in H_S, therefore it is normal automatically. Since we have for $\mathbf{u}, \mathbf{v} \in D$

$$\langle L\mathbf{u}, \mathbf{v}\rangle = \int_\Omega \left(\sum_{i=1}^{l} \left(K_i \nabla u_i \cdot \overline{\nabla} v_i + (\mathbf{b}_i \cdot \nabla u_i)\overline{v}_i \right) + \sum_{i,j=1}^{l} V_{ij} u_j \overline{v}_i \right), \tag{13}$$

Using the divergence theorem and the boundary conditions

$$\int_\Omega (\operatorname{div} \mathbf{b}) u\overline{v} = \int_{\partial\Omega} (\mathbf{b} \cdot \nu) u\overline{v} \, \mathrm{d}\sigma - \int_\Omega \nabla(u\overline{v})\mathbf{b} = -\int_\Omega \nabla(u\overline{v})\mathbf{b} =$$

$$= -\int_\Omega (\mathbf{b} \cdot \nabla u)\overline{v} - \int_\Omega u(\mathbf{b} \cdot \nabla \overline{v}),$$

therefore we have the following form of S:

$$\langle S\mathbf{u}, \mathbf{v}\rangle = \int_\Omega \left(\sum_{i=1}^{l} \left(K_i \nabla u_i \cdot \overline{\nabla} v_i - \frac{1}{2}(\operatorname{div} \mathbf{b}_i) u_i \overline{v}_i \right) + \frac{1}{2} \sum_{i,j=1}^{l} (V_{ij} + V_{ji}) u_j \overline{v}_i \right). \tag{14}$$

The operator S itself falls into the type (5) iff

$$V_{ij} = -V_{ji} \quad (i \neq j) \quad \text{and} \quad \eta_i = V_{ii} - \frac{1}{2}(\operatorname{div} \mathbf{b}_i). \tag{15}$$

Proposition 1 *Under Assumptions BVP and* (15), *Assumptions A are satisfied, therefore the preconditioned truncated CGM for system* (1) *converges superlinearly in the space* $H_0^1(\Omega)^l$ *according to the estimate* (12) *with the parameter* $\varrho = 1$.

Using the truncated algorithm can be beneficial, but it is a significant restriction not having the freedom to choose the coefficients η_i of S in (5). For convection term dominated problems large values choosen for η_i might compensate the large $\mathbf{b}$. Now let us consider the preconditioner operator (5) with arbitrary nonnegative parameters η_i.

Proposition 2 *Assume that* $K_i \equiv K \in \mathbf{R}$, $\eta_i \equiv \eta \in \mathbf{R}$ *and* $\mathbf{b}_i \equiv \mathbf{b} \in \mathbf{R}^N$ *are constants,* $V \in \mathbf{R}^{l \times l}$ *is a normal matrix and suppose that Assumptions BVP hold. Then the full version of the preconditioned conjugate gradient algorithm* (10) *for system* (1) *with the preconditioning operator* (5) *converges superlinearly in the space* $H_0^1(\Omega)^l$ *according to the estimate* (12).

The proofs for Proposition 1, 2 can be found in [8]. It is also possible to give estimations for the value of ϱ in Proposition 2 using the Sobolev inequality. Another important property, that one can give similar upper bounds in the case of the discretized systems. It means that the upper bound for a matrix equations consists of the eigenvalues of an operator, that is the upper bound is independent from the given FEM subspace V_h, therefore it is independent from the mesh parameter h.

Besides the mesh independent superlinear convergence result, the advantage of the preconditioning method (5) is that the elliptic operators are decoupled, that is the corresponding matrix $\mathbf{S}_h$ is symmetric block-diagonal, hence auxiliary equations for the discretized system like $\mathbf{S}_h \mathbf{z}_h = \mathbf{L}_h \mathbf{d}_h$ (step (2f) in algorithm (10)) can be divided into l parts and they can be solved simultaneously.

4 Numerical results

Several numerical tests has been done with simple two-dimensional test equations. The domain D is the unit square and $K_i = 1$ that is the case of Laplacian is considered for the principal part of (1). Let the convection term be a constant vector, therefore $\operatorname{div} \mathbf{b}_i = 0$. Let

$$\mathbf{b} = \mathbf{b}_i = (1, 0), \qquad V = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

For the sake of better lucidity, we write out the system according to these parameters:

$$\left.\begin{aligned} -\Delta u_1 + \tfrac{\partial u_1}{\partial x} + u_2 = g_1 \\ -\Delta u_2 + \tfrac{\partial u_2}{\partial x} - u_1 = g_2 \end{aligned}\right\} \tag{16}$$

These parameters are satisfied the assuptions of the Propositions ($\eta_i = 0$ have to be used for the truncated algorithm), but lots of other cases have been checked and we have managed to verify the superlinear convergence property even in the cases when either V is not normal or the $\mathbf{b}_i$ are different.

Table 1: Results for system (16).

	1/h					
	truncated algorithm			full algorithm, $\beta_i = 8$		
Itr.	32	64	128	32	64	128
1	0.0774	0.0776	0.0776	0.0636	0.0638	0.0638
2	0.0777	0.0780	0.0780	0.0624	0.0626	0.0626
3	0.0802	0.0805	0.0805	0.0642	0.0644	0.0644
4	0.0777	0.0780	0.0781	0.0643	0.0645	0.0646
5	0.0720	0.0723	0.0724	0.0616	0.0618	0.0619
6	0.0663	0.0666	0.0667	0.0579	0.0581	0.0582
7	0.0617	0.0620	0.0621	0.0542	0.0545	0.0546
8	0.0587	0.0590	0.0590	0.0511	0.0514	0.0515
9	0.0574	0.0576	0.0577	0.0489	0.0491	0.0491
10	0.0564	0.0567	0.0568	0.0482	0.0483	0.0483
11	0.0545	0.0552	0.0564	0.0497	0.0522	0.0554

The tables contain the values of

$$\left(\frac{\|e_k\|_L}{\|e_0\|_L}\right)^{1/k},$$

therefore the numbers have to tend to zero in every column according to the estimate in (12). Considering the rows, one can also verify the mesh independent convergence property.

Using a parallel implementation for such problems is not necessary since the matrix of the auxiliary equations has only two blocks in its diagonal. But if we have more than 20 equations, it has turned out, that much better results can be achieved using multiple processors. In [8] a simplified meteorological model problem consist of 10 equations has been investigated. We have compared the computational time of the direct solution of the equation and the preconditioned conjugate gradient method.

Table 2: Computational time for a larger system

1/h	creating $\mathbf{S}_h, \mathbf{L}_h$	Cholesky	iteration	direct solution	CGM
8	0.0470	0.0470	0.5780	0.0150	0.6250
16	0.1090	0.0620	1.2350	0.3130	1.2970
32	0.4220	0.1880	3.9680	9.5780	5.8480
64	1.9070	2.3600	17.8120	177.7030	20.1720

The predictable result was that the PCG algorithm is much more faster even without parallelization, when the mesh parameter is small enough, that is the size of the matrices is large. A Matlab code was invented previously for testing small problems, and the Cholesky decomposition was used at the solution of the auxiliary equations instead of the obvious potential of a parallel implementation. The results of the experiments with parallel algorithms will appear in a joint work with János Karátson and Ivan Lirkov, which has been submitted to the Sixth International Conference on Numerical Methods and Application for publication.

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References

[1] Axelsson, O.: A generalized conjugate gradient least square method. Numer. Math. **51** (1987), 209–227.

[2] Axelsson, O.: Iterative Solution Methods. Cambridge University Press, 1994.

[3] Axelsson, O., Karátson J.: On the rate of convergence of the conjugate gradient method for linear operators in Hilbert space. Numer. Funct. Anal. **23** (2002), No. 3-4, 285–302.

[4] Axelsson, O., Karátson J.: Symmetric part preconditioning for the conjugate gradient method in Hilbert space. Numer. Funct. Anal. **24** (2003), No. 5-6, 455–474.

[5] Axelsson, O., Karátson J.: Superlinearly convergent CG methods via equivalent preconditioning for nonsymmetric elliptic operators. Numer. Math. **99** (2004), No. 2, 197-223.

[6] Faber, V., Manteuffel, T., Parter, S.V.: On the theory of equivalent operators and application to the numerical solution of uniformly elliptic partial differential equations. Adv. in Appl. Math., **11** (1990), 109–163.

[7] Karátson J.: Superlinear PCG algorithms: symmetric part preconditioning and boundary conditions. submitted

[8] Karátson J., Kurics T.: Superlinearly convergent PCG algorithms for some nonsymmetric elliptic systems. submitted

[9] Manteuffel, T., Otto, J.: Optimal equivalent preconditioners. SIAM J. Numer. Anal. **30** (1993), 790–812.

[10] Manteuffel, T., Parter, S. V.: Preconditioning and boundary conditions. SIAM J. Numer. Anal. **27** (1990), no. 3, 656–694.

[11] Winter, R.: Some superlinear convergence results for the conjugate gradient method. SIAM J. Numer. Anal. **17** (1980), 14-17.

[12] Zlatev, Z.: Computer treatment of large air pollution models. Kluwer Academic Publishers, Dordrecht-Boston-London, 1995.