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Numerical Analysis

Polynomial preconditioning and the Generalized Minimal Residual algorithm solver for the 2-D Boltzmann transport equation

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Abstract

This Note describe a new algorithm to solve the neutron transport equation in 2-D geometry. This algorithm is based on a splitting of the collision operator and an infinite dimensional adaptation of the Generalized Minimal Residual algorithm using a polynomial preconditioning. The theoretical proof of the convergence and numerical results are given here. ***To cite this article: A. Tizaoui, C. R. Acad. Sci. Paris, Ser. I 345 (2007).***

Résumé

Préconditionnement polynomial et algorithme du résidu minimal généralisé appliqués à l'équation de Boltzmann. Dans cette Note on étudie des problèmes liés à l'équation de transport neutronique en géométrie bidimensionnelle plane. On propose un nouvel algorithme utilisant un splitting de l'opérateur de collision et un algorithme du résidu minimal généralisé après préconditionnement polynomial en dimension infinie. On présente des résultats tant théoriques que numériques, et une comparaison entre cet algorithme, de la méthode SOR et l'algorithme du résidu minimal généralisé avec précontionnement diagonal. ***Pour citer cet article : A. Tizaoui, C. R. Acad. Sci. Paris, Ser. I 345 (2007).***

Version française abrégée

Dans cette Note on propose une résolution itérative de l'équation de transport neutronique en géométrie bidimensionnelle plane (1). Il s'agit de décrire l'évolution d'une population de neutrons confinés dans un domaine borné. Sous des hypothèses simplificatrices, on introduit la densité angulaire de neutrons. Cette fonction scalaire vérifie une équation de transport linéaire incluant un opérateur intégral linéaire de collision de noyau positif et borné. C'est une situation classique en physique. Néanmoins, même dans la situation simple du cas monocinétique stationnaire, la résolution numérique de cette équation de transport n'est pas facile du fait du nombre des degrés de liberté nécessaires

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et de la présence du terme modélisant les collisions qui connecte « presque » tous les degrés de liberté entre eux. Ainsi les matrices représentant le système discrétisé sont quasiment pleines, empêchant d'utiliser des méthodes directes de résolution des systèmes linéaires. Une difficulté importante réside dans le fait que l'opérateur de transport n'est pas auto-adjoint. Dans [1], une stratégie de décomposition de l'opérateur de transport, selon une partition des directions angulaires, se ramène à la résolution du système couplé (2). Avec cette décomposition, de nombreuses méthodes itératives de résolution ont été analysées dans [1,2].

Dans cette Note, nous proposons une accélération de l'algorithme du résidu minimal généralisé par un préconditionnement polynomial en dimension infinie pour résoudre (3). Dans un premier lieu, nous démontrons théoriquement que l'estimation de la vitesse de convergence de cet algorithme est meilleure que celle obtenue dans [2]. Ensuite, nous comparons numériquement le nombre d'itérations ainsi que le temps (CPU) nécessaire à la convergence de ce nouvel algorithme avec ceux obtenus dans [1,2] pour différentes valeurs des sections efficaces, de la criticité et du pas d'espace. Nous obtenons une meilleure convergence.

1. Introduction

The evolution of interacting neutrons in a two dimensional domain R is described by a function $\varphi(r,\omega)$ which represents, up to some factor, the flux of neutrons density at the position r with velocity $\omega \in B(0,1)$. The cross section σ accounts for neutron-domain interaction, whereas a kernel $h(r,\omega,\omega')$ describes the collisions between neutrons. At last, a neutron source is represented by a function $f(r,\omega)$. We refer to [3,4] for a more precise introduction.

We consider the following problem: given a source term f, we have to find $\varphi : Q \to \mathbb{R}^+$, a solution of the transport equation [4],

$$\begin{cases} T\varphi(r,\omega) = H\varphi(r,\omega) + f(r,\omega), \quad (r,\omega) \in Q, \\ \varphi \in D(T), \end{cases} \tag{1}$$

where $\omega := (\mu,\eta)$, $r := (x,y)$, $Q = R \times B$, $R =]0,a[\times]0,b[$, $a,b > 0$, $B = \{\omega \in \mathbb{R}^2 :\ \|\omega\|_2 < 1\}$, T is the transport operator defined on $D(T)$ by $T\varphi(r,\omega) = \omega \cdot \nabla_r \varphi(r,\omega) + \sigma(r)\varphi(r,\omega)$, where $D(T) = \{\varphi \in L^2(Q) :\ \omega \cdot \nabla_r \varphi \in L^2(Q)$ and $\varphi_{|\Gamma_-} = 0\}$, $\Gamma_- = \{(r,\omega) \in \partial R \times B :\ \mu n_x + \eta n_y < 0\}$, $n(n_x,n_y)$ the outer normal to ∂B and H is an integral operator of positive kernel h given by

$$H\varphi(r,\omega) = \int_B h(r,\omega,\omega')\varphi(r,\omega')\,\mathrm{d}\omega'.$$

The hypothesis are:

(A_1) $\sigma \in L^\infty(R)$ and $\sigma(r) > 0$ *a.e.* on R.
(A_2) h is positive and bounded.
(A_3) $\exists c \in]0,1[, \forall i \in \{1,2,3,4\}$, $\int_{B_i} h(r,\omega,\omega')\,\mathrm{d}\omega' \leqslant \frac{c\cdot\sigma(r)}{4}$ a.e. on Q, where B_i is the ith quarter of the disk B.
(A_4) $h(r,\omega,\omega') = C(r)\sum_{l=1}^{N_h} \alpha_l(\omega)\alpha_l(\omega')$, $N_h \in \mathbb{N}^*$.

Remark 1.

(1) Assumptions (A_1)–(A_3) ensure the existence and uniqueness of the solution of the problem (1) in $D(T)$ [4].
(2) Assumption (A_4) is not necessary for a theoretical proof of the convergence. However, for numerical reasons, it is used in the splitting of the collision operator.

In the critical case ($c \approx 1$), the standard algorithm becomes extremely slow [1]. Several acceleration methods of the convergence of this algorithm have been introduced and studied. In particular, the diffusion synthetic acceleration (DSA) methods developed in [5], and multigrid algorithms [7]. The main difficulties encountered while studying these methods lead the authors either to consider the discretized equation in the angular variable [5], or the continuous equation with a truncated expansion of h with respect to this angular variable [5,7]. The idea in [1,2] is to introduce and study various algorithms, relying on a splitting of the collision operator, and adapted from the methods of Jacobi, Gauss–Seidel, SOR and the Generalized Minimal Residual, in the infinite dimensional case. The SOR algorithm gives

excellent results, but it needs the computation of its optimal parameter, which in turn can be very slow in the critical case. Let us describe the natural splitting of H which leads to this scheme. Let H_{ij}, $i, j \in \{1, 2, 3, 4\}$, be the integral operators with kernel:

$$h_{ij}(r, \omega, \omega') = h(r, \omega, \omega') \times 1_{Q_i}(r, \omega) \times 1_{Q_j}(r, \omega'), \quad i, j \in \{1, 2, 3, 4\},$$

with $Q_i = R \times B_i$. We deduce that $H_{ij}(\varphi) = H(\varphi \times 1_{Q_j}) \times 1_{Q_i}$. We obtain a splitting of the integral operator H in the form $H = \sum_{i=1}^{4} \sum_{j=1}^{4} H_{ij}$. The solution φ of (1) is given under the form $\varphi = \sum_{i=1}^{4} \varphi_i$, where φ_1, φ_2, φ_3 and φ_4, are the solutions in $D(T)$ of the coupled system:

$$\begin{pmatrix} T - H_{11} & -H_{12} & -H_{13} & -H_{14} \\ -H_{21} & T - H_{22} & -H_{23} & -H_{24} \\ -H_{31} & -H_{32} & T - H_{33} & -H_{34} \\ -H_{41} & -H_{42} & -H_{43} & T - H_{44} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}, \tag{2}$$

where $f_i = f \times 1_{Q_i}$. It is easy to prove that $\varphi_i = \varphi \times 1_{Q_i}$ for $i \in \{1, 2, 3, 4\}$.

Let $\Lambda_{ij} = T^{-1} H_{ij}$, $\tilde{f}_i = T^{-1} f_i$, $i, j \in \{1, 2, 3, 4\}$; $J_{ij} = -(I - \Lambda_{ii})^{-1} \Lambda_{ij}$, $i \neq j$, $\tilde{\varphi} = (\varphi_1, \varphi_2, \varphi_3, \varphi_4)^t$, $\xi = (\xi_1, \xi_2, \xi_3, \xi_4)^t$, $\xi_i = (I - \Lambda_{ii})^{-1} \tilde{f}_i$, $A = (A_{ij})$, $A_{ii} = I$, $A_{ij} = J_{ij}$ for $i \neq j$ and with the use of the diagonal preconditioner, the system (2) can be written:

$$A\tilde{\varphi} = \xi. \tag{3}$$

A polynomial preconditioning technique is proposed in this Note to accelerate the Generalized Minimal Residual algorithm for solving (3). We analyze a theoretical and numerical aspects of this algorithm. One of the advantages of this algorithm is that it gives a good rate of convergence, but it does not need any extra parameter calculation. This algorithm was introduced by Axelsson [6], in the finite dimensional case, and has been proved to converge by providing a linear system matrix with positive definite symmetric part. We denote by $\langle \cdot, \cdot \rangle_\sigma$: $(\varphi, \psi) \to \int_Q \sigma(r) \varphi(r, \omega) \phi(r, \omega) \, \mathrm{d}r \, \mathrm{d}\omega$ the scalar product in $L^2(Q)$. Similarly, $\| \cdot \|_\sigma$ will represent the norm associated to this scalar product.

2. Polynomial preconditioning and the Generalized Minimal Residual algorithm

We decompose the operator A under form $A = I - \Phi$ where $\Phi = (X_{ij})_{1 \leqslant i, j \leqslant 4}$, $X_{ii} = 0$ and $X_{ij} = -J_{ij}$ for $i \neq j$. We need to control the norm of Φ. For this we must control the norms of the operators Λ_{ij} and J_{ij}. We have the following result:

Corollary 2.1. *Under* (A$_1$)–(A$_3$)*, we have* $\| \Lambda_{ij} \|_\sigma \leqslant \frac{c}{4}$ *and* $\| J_{ij} \|_\sigma \leqslant \frac{c}{4-c}$ *for* $i, j \in \{1, 2, 3, 4\}$.

Sketch of proof. Let $\varphi \in D(T)$ solution of $T\varphi = H_{ij}\phi$ with $\phi \in D(T)$. We have

$$\langle T\varphi, \varphi \rangle = \langle \omega \cdot \nabla_r \varphi, \varphi \rangle + \langle \sigma\varphi, \varphi \rangle,$$

where $\langle \cdot, \cdot \rangle$ the standard scalar product. The operator $\omega \cdot \nabla_r \varphi$ is m-accretive with domain $D(T)$ [4], then $\| \varphi \|_\sigma^2 = \langle \varphi, \varphi \rangle_\sigma \leqslant \langle H_{ij}\phi, \varphi \rangle$. Using the Cauchy–Schwarz inequality, we obtain

$$\| \varphi \|_\sigma^2 \leqslant \left[\int_R \int_{B_j} \phi^2(r, \omega') \left(\int_{B_i} h(r, \omega, \omega') \, \mathrm{d}\omega \right) \mathrm{d}\omega' \, \mathrm{d}r \right]^{1/2} \times \left[\int_R \int_{B_j} \varphi^2(r, \omega') \left(\int_{B_i} h(r, \omega, \omega') \, \mathrm{d}\omega \right) \mathrm{d}\omega' \, \mathrm{d}r \right]^{1/2}.$$

Thanks to (A_3), we deduce that $\| \varphi \|_\sigma^2 \leqslant \frac{c}{4} \| \varphi \|_\sigma \| \phi \|_\sigma$. Therefore $\| \varphi \|_\sigma = \| \Lambda_{ij} \phi \|_\sigma \leqslant \frac{c}{4} \| \phi \|_\sigma$, so $\| \Lambda_{ij} \|_\sigma \leqslant \frac{c}{4}$. From this inequality, it is easy to prove $\| J_{ij} \|_\sigma \leqslant \frac{c}{4-c}$.

Using the Corollary 2.1, We easily obtain $\| \Phi \|_\sigma \leqslant \sqrt{3}e < \frac{\sqrt{3}}{3} < 1$, then $A^{-1} = \sum_{n=0}^{\infty} \Phi^n$. Taking the approximation $C_p = \sum_{i=0}^{p} \Phi^i$ of A^{-1}, $p \in \mathbb{N}^*$ as preconditioner and by putting $\tilde{A} = C_p A := (I - \Phi^{p+1})$ and $\tilde{b} = C_p \xi$, the system (3) becomes $\tilde{A}\tilde{\varphi} = \tilde{b}$. We propose to solve this new system by the Generalized Minimal Residual algorithm. This algorithm, minimizing $E(\tilde{\varphi}) = || \tilde{b} - \tilde{A}\tilde{\varphi} ||_\sigma^2$, takes the following form: Let $\tilde{\varphi}$ in $D(T)$, $r^0 = \tilde{b} - \tilde{A}\tilde{\varphi}^0$, $p^0 = r^0$, $q^0 = \tilde{A}p^0$. While $\| r^k \|_\sigma > \varepsilon$

begin
$\alpha^k = \frac{\langle r^k, q^k\rangle_\sigma}{\langle q^k, q^k\rangle_\sigma}$, $\varphi^{k+1} = \varphi^k + \alpha^k p^k$, $r^{k+1} = r^k - \alpha^k q^k$, $\beta^{k+1} = -\frac{\langle \tilde{A} r^{k+1}, q^k\rangle_\sigma}{\langle q^k, q^k\rangle_\sigma}$, $p^{k+1} = r^{k+1} + \beta^{k+1} p^k$, $q^{k+1} = \tilde{A} r^{k+1} + \beta^{k+1} q^k$
end. □

In the following, we propose a theoretical and numerical study of the convergence of this algorithm.

3. Rate of residual decreasing

Applying the elementary analysis of [6], we have the following estimate on the residual term (cf. [2] for the proof).

Proposition 3.1. *Let φ^k be constructed by the preceding algorithm and starting from φ^0. For $k \geqslant 0$, we have*

$$E\big(\tilde{\varphi}^{k+1}\big) \leqslant E\big(\tilde{\varphi}^k\big)\left(1 - \frac{\langle r^k, \tilde{A} r^k\rangle_\sigma}{\langle r^k, r^k\rangle_\sigma} \frac{\langle r^k, \tilde{A} r^k\rangle_\sigma}{\langle \tilde{A} r^k, \tilde{A} r^k\rangle_\sigma}\right). \tag{4}$$

We need to estimate the following quantities $\frac{\langle r^k, \tilde{A} r^k\rangle_\sigma}{\langle r^k, r^k\rangle_\sigma}$ and $\frac{\langle r^k, \tilde{A} r^k\rangle_\sigma}{\langle \tilde{A} r^k, \tilde{A} r^k\rangle_\sigma}$. By using Corollary 2.1, we can prove the following proposition:

Proposition 3.2. *Under assumptions* (A_1)–(A_3)*, the operator $\tilde{A}$ has a positive definite part and satisfies*

$$\langle \tilde{A}\tilde{\varphi}, \tilde{\varphi}\rangle_\sigma \geqslant \big(1 - (\sqrt{3}\,e)^{p+1}\big)\|\tilde{\varphi}\|_\sigma^2 \quad \text{and} \quad \langle \tilde{A}\tilde{\varphi}, \tilde{\varphi}\rangle_\sigma \geqslant \frac{1}{1 + (\sqrt{3}\,e)^{p+1}} \langle \tilde{A}\tilde{\varphi}, \tilde{A}\tilde{\varphi}\rangle_\sigma, \quad \forall \varphi \in D(T). \tag{5}$$

Plugging estimations (5) into the estimation (4), we have the following:

Theorem 3.1. *Under assumptions* (A_1)–(A_3)*, the Generalized Minimal Residual algorithm converges, and the residual decreases at least at the following rate*:

$$E\big(\tilde{\varphi}^{k+1}\big) \leqslant \frac{2(\sqrt{3}\,e)^{p+1}}{1 + (\sqrt{3}\,e)^{p+1}} E\big(\tilde{\varphi}^k\big). \tag{6}$$

Remark 2. The theoretical estimation $\frac{2(\sqrt{3}e)^{p+1}}{1+(\sqrt{3}e)^{p+1}}$ decreases more and more when p is large enough.

4. Numerical results

For the numerical results, we take the same data of φ and f that in [1,2]. For every iterative methods tested there, iterations are stopped when $\|\varphi^{k+1} - \varphi^k\|_1 / \|\varphi^k\|_1$ is less than a prescribed $\varepsilon > 0$. There is two sets of test. We study the behavior with respect to c and to σ. In [2], the numerical results of SOR algorithm gives excellent results than the diagonal Generalized Minimal Residual preconditioning for values of c close to 1 ($\sigma = 50$). However, at fixed the parameter c at 0.98, and turning to the σ dependence, we recover the inverse, so in order to appreciate the gain of this algorithm we compare our algorithm with the diagonal Generalized Minimal Residual preconditioning for values of c, and with SOR for values of σ.

Tables 1 and 2 present, respectively, the iterations number and CPU(s) times, as a function of c, necessary for the convergence corresponding to diagonal Generalized Minimal Residual preconditioning, and to this new algorithm for $p = 1$, and $p = 2$.

Tables 3 and 4, respectively, present, as a function of σ, the iteration number and the CPU(s) time, for the SOR algorithm and our new algorithm, for $p = 1$, and $p = 2$.

From these numerical results (iterations, CPU(s) times), we deduce that our algorithm for $p = 2$ is a very efficient method.

Table 1
Iterations number at fixed $\sigma = 50$

c	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.98
Iter. GMRES D	5	6	7	8	11	10	12	16	24	73
Iter. GMRES P (1)	3	4	5	5	6	6	7	9	13	26
Iter. GMRES P (2)	2	3	4	4	5	5	5	7	9	19

Table 2
CPU time at fixed $\sigma = 50$

c	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.98
Time (s) GMRES D	0.5	0.57	0.50	0.69	0.81	0.88	1.03	1.34	1.94	5.71
Time (s) GMRES P (1)	0.4	0.48	0.42	0.59	0.7	0.8	0.9	1.1	1.54	4.5
Time (s) GMRES P (2)	0.4	0.47	0.4	0.49	0.65	0.7	0.8	0.9	0.99	3.6

Table 3
Iterations number at fixed $c = 0.98$

σ	1	10	20	30	40	50	60	70	80	90	100
Iter. SOR	6	25	40	47	52	59	60	60	60	60	60
Iter. GMRES P (1)	6	19	27	31	35	39	44	48	49	52	53
Iter. GMRES P (2)	3	15	23	30	33	36	40	42	42	42	43

Table 4
CPU time at fixed $c = 0.98$

σ	1	10	20	30	40	50	60	70	80	90	100
Time (s) SOR	0.3	0.4	0.6	0.69	0.6	0.6	0.6	0.6	0.6	0.6	0.6
Time (s) GMRES P (1)	0.2	0.32	0.58	0.6	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Time (s) GMRES P (2)	0.2	0.2	0.4	0.5	0.4	0.4	0.4	0.45	0.4	0.4	0.4

5. Conclusion

The numerical results confirm that our new algorithm converges much more quickly than the algorithms given in [1,2]. An important point is the existence of the theoretical proof of convergence, independent of discretization, made in the general case for the kernel and with the σ parameter which can vanish in some points of the domain. Finally, let us mention that the structure of our scheme, constructed upon an operator splitting, is naturally devised for parallelization. A work is in progress for the acceleration of this algorithm using an adapted DSA method [5], and its comparison with standard DSA.

References

[1] S. Akesbi, Splitting d'opérateur pour l'équation de transport neutronique en géométrie bidimensionnelle plane, ESAIM: M2AN 34 (6) (2000) 1109–1122.
[2] S. Akesbi, E. Maitre, Theoretical and numerical analysis of Minimal Residual Solver for 2D Boltzmann transport equation, J. Comput. Appl. Math. 150 (2003) 357–374.
[3] J. Bussac, P. Reuss, Traité de neutronique, Hermann, Paris, 1978.
[4] R. Dautray, J.-L. Lions, Analyse mathématique et calcul numérique, vol. 9, Masson, Paris, 1987.
[5] K.M. Khattab, E.W. Larsen, Synthetic acceleration methods for linear transport problems with highly anisotropic scattering, Nucl. Sci. Eng. 107 (1991) 217–227.
[6] P. Lascaux, R. Théodor, Analyse numérique matricielle appliquée à l'art de l'ingénieur, vol. 2, Masson, 1987.
[7] T. Manteuffel, S. McCormick, J. Morel, G. Yang, A fast multigrid algorithm for isotropic transport problems. II. With absorption, SIAM J. Sci. Comput. 17 (6) (1996) 1449–1474.