Iterative Schemes for the Neutron Diffusion Equation [1]

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Abstract

In this paper, a second degree iterative method for the solution of the time dependent neutron diffusion equation is studied. In practice, this method is combined with a variational strategy to accelerate its convergence rate with very good results. In addition, these results are compared with those given by other conjugate gradient type iterative methods for nonsymmetric matrices. Particularly the GMRES, BiCGSTAB and TFQMR methods are used.

key words: ITERATIVE METHODS, NEUTRON DIFFUSION EQUATION, SECOND DEGREE METHOD, VARIATIONAL ACCELERATION.

1 Introduction and preliminaries

The time-dependent two energy group neutron diffusion equation is written using standard matrix notation as follows [8]

$$[v^{-1}]\dot{\phi} + \mathcal{L}\phi = (1-\beta)\mathcal{M}\phi + \sum_{k=1}^{K} \lambda_k \mathcal{C}_k \chi \,, \tag{1}$$

$$\dot{\mathcal{C}}_k = \beta_k \mathcal{M}\phi - \lambda_k \mathcal{C}_k ; \; k = 1, \ldots, K \,, \tag{2}$$

where K is the number of delayed neutron precursors,

$$\mathcal{L} = \left[\begin{array}{cc} -\vec{\nabla}(D_1\vec{\nabla}) + \Sigma_{a1} + \Sigma_{12} & 0 \\ -\Sigma_{12} & -\vec{\nabla}(D_2\vec{\nabla}) + \Sigma_{a2} \end{array} \right] , \; [v^{-1}] = \left[\begin{array}{cc} \frac{1}{v_1} & 0 \\ 0 & \frac{1}{v_2} \end{array} \right] ,$$

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and

$$\mathcal{M} = \begin{bmatrix} \nu\Sigma_{f_1} & \nu\Sigma_{f_2} \\ 0 & 0 \end{bmatrix}, \; \phi = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}, \; \chi = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

The boundary conditions for the neutron flux are $\phi|_\Gamma = 0$, where Γ is the reactor boundary. To study the rapid transients of neutronic power and other space and time phenomena related with the neutron flux variations, fast codes for solving these equations are needed. The first step to obtain a numerical solution of these equations consists of choosing a spatial discretization for the equation (1). In [2] and [3] the reactor is divided in cells or nodes, and a nodal collocation method is applied. Moreover, finite difference and finite element methods can be used for this purpose. In this work both the nodal collocation and the finite difference methods are used, yielding the following systems of ordinary differential equations

$$\begin{aligned} [v^{-1}]\dot{\psi} + L\psi &= (1-\beta)M\phi + \sum_{k=1}^{K} \lambda_k X C_k \,, & (3) \\ \dot{C}_k &= \beta_k M\psi - \lambda_k C_k; \; k = 1, \ldots, K \,, & (4) \end{aligned}$$

where L, M, and $[v^{-1}]$ are matrices with the following block structure

$$L = \begin{bmatrix} L_{11} & 0 \\ -L_{21} & L_{22} \end{bmatrix}, \; M = \begin{bmatrix} M_{11} & M_{12} \\ 0 & 0 \end{bmatrix}, \; v^{-1} = \begin{bmatrix} v_1^{-1} & 0 \\ 0 & v_2^{-1} \end{bmatrix}, \; X = \begin{bmatrix} I \\ 0 \end{bmatrix}. \qquad (5)$$

These methods usually lead to symmetric and diagonally dominant blocks L_{11} and L_{22} and to diagonal blocks L_{21}, M_{11} and M_{12}. Indeed, for the finite difference method the blocks L_{11} and L_{22} are symmetric and positive definite matrices (spd). The next step consists of integrating the above ordinary differential equations over a series of time intervals, $[t_n, t_{n+1}]$. Equation (4) is integrated under the assumption that the term $[M_{11}M_{12}]\psi$ varies linearly from t_n to t_{n+1}, obtaining the solution C_k in t_{n+1} expressed as

$$C_k^{n+1} = C_k^n e^{-\lambda_k h} + \beta_k(a_k[M_{11}M_{12}]^n\psi^n + b_k[M_{11}M_{12}]^{n+1}\psi^{n+1}) \,, \qquad (6)$$

where $h = t_{n+1} - t_n$, and the coefficients a_k and b_k are given by

$$a_k = \frac{(1+\lambda_k h)(1-e^{-\lambda_k h})}{\lambda_k^2 h} - \frac{1}{\lambda_k}, \quad b_k = \frac{\lambda_k h - 1 + e^{-\lambda_k h}}{\lambda_k^2 h}.$$

To integrate equation (3) we must take into account that it constitutes a system of stiff differential equations, mainly due to the elements of the diagonal matrix $[v^{-1}]$. This makes necessary to use implicit backward difference methods (BDF) for the integration (see [2]). A stable one-step BDF formula to integrate (3) is given by

$$\frac{[v^{-}1]}{h}\left(\psi^{n+1} - \psi^n\right) + L^{n+1}\psi^{n+1} = (1-\beta)M^{n+1}\psi^{n+1} + \sum_{k=1}^{K} \lambda_k X C_k^{n+1}. \qquad (7)$$

Since the truncation error for this BDF formula is proportional to the integration step h, to keep a good level of accuracy the choice of small time intervals is needed. In this work, to simplify the experimental results presented, we use the one-step BDF method (7). We mention that in [3] the autors present a combined algorithm which makes use of one-, two- and four-step BDF methods. This method allows the choice of bigger integration steps keeping the same level of accuracy. Taking into account equation (6) and the structure of matrices L and M, we rewrite (7) as the system of linear equations

$$\begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \begin{bmatrix} \psi_1^n \\ \psi_2^n \end{bmatrix} + \sum_{k=1}^{K} \lambda_k e^{-\lambda_k h} \begin{bmatrix} C_k^n \\ 0 \end{bmatrix}, \qquad (8)$$

where

$$
\begin{aligned}
T_{11} &= \frac{1}{h}\upsilon_1^{-1} + L_{11}^{n+1} - (1-\beta)M_{11}^{n+1} - \sum_{k=1}^{K}\lambda_k\beta_k b_k M_{11}^{n+1}\ ,\ T_{21} = -L_{21}^{n+1}\ , \\
T_{12} &= -(1-\beta)M_{12}^{n+1} - \sum_{k=1}^{K}\lambda_k\beta_k b_k M_{12}^{n+1}\ ,\ T_{22} = \frac{1}{h}\upsilon_2^{-1} + L_{22}^{n+1}\ , \\
R_{11} &= \frac{1}{h}\upsilon_1^{-1} + \sum_{k=1}^{K}\lambda_k\beta_k a_k M_{11}^{n}\ ,\ R_{12} = \sum_{k=1}^{K}\lambda_k\beta_k a_k M_{12}^{n}\ ,\ R_{22} = \frac{1}{h}\upsilon_2^{-1}\ .
\end{aligned} \tag{9}
$$

Thus, for each time step it is necessary to solve a large and sparse system of linear equations with the following structure:

$$
\begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} E_1 \\ E_2 \end{bmatrix} \tag{10}
$$

where the independent term depends on both the solution in previous time steps and also the backward difference method used. Usually, the blocks on this system conserve the same properties as in matrix L and M in equation (5), namely blocks T_{11} , T_{22} are symmetric and diagonally dominant square matrices (spd matrices for the finite differences case), and blocks T_{12} , T_{21} are diagonal matrices. In [2] the system (10) is solved with a block stationary iterative method with the following structure

$$
\begin{aligned}
T_{11}\psi_1^{\ell+1} &= E_1 - T_{12}(\omega\psi_2^{\ell} + (1-\omega)\psi_2^{\ell-1})\ , \\
T_{22}\psi_2^{\ell+1} &= E_2 - T_{21}(\omega\psi_1^{\ell+1} + (1-\omega)\psi_1^{\ell})\ ,
\end{aligned} \tag{11}
$$

where ω is a relaxation factor. In [3] this iterative method is accelerated with a varitional technique. In both cases very good results were obtained.

The paper is structured as follows. In section 2, a theoretical result concerning the convergence properties of method (11) is stated without proof (which can be found in [1]). In section 3, some experimental results will permit us to compare the presented method with other well known iterative methods for nonsymmetrics matrices. The benchmark choosen for this comparison corresponds to the bidimensional Seed-Blanket reactor. Finally, the main conclusions are given.

2 Second degree method

We are concerned with the problem of solving the nonsingular linear system

$$
T\psi = E. \tag{12}
$$

partitioned in 2×2 blocks as in (10), by means of the iterative scheme (11). A second degree stationary method is defined as follows [9],

$$
\psi^{(n+1)} = G_1\psi^{(n)} + G_0\psi^{(n-1)} + k. \tag{13}
$$

for some matrices G_0 and G_1, generally related with the iteration matrix of a first degree stationary method for solving the system (12). This class of methods are usually studied in the bibliography by means of the following auxiliary system

$$\begin{bmatrix} \psi^{(n)} \\ \psi^{(n+1)} \end{bmatrix} = \begin{bmatrix} 0 & I \\ G_0 & G_1 \end{bmatrix} \begin{bmatrix} \psi^{(n-1)} \\ \psi^{(n)} \end{bmatrix} + \begin{bmatrix} 0 \\ k \end{bmatrix}. \tag{14}$$

The iterative solver (11) corresponds to a second degree method with matrices G_0, G_1 and k defined as

$$G_0 = \begin{bmatrix} 0 & -(1-w)B_{12} \\ 0 & (1-w)wB_{21}B_{12} \end{bmatrix}; \; G_1 = \begin{bmatrix} 0 & -wB_{12} \\ -(1-w)B_{21} & w^2 B_{21}B_{12} \end{bmatrix} \tag{15}$$

$$k = \begin{bmatrix} T_{11}^{-1}E_1 \\ T_{22}^{-1}E_2 - wB_{21}T_{11}^{-1}E_1 \end{bmatrix}$$

where $B_{12} = T_{11}^{-1}T_{12}$ and $B_{21} = T_{22}^{-1}T_{21}$ are the off diagonal block submatrices of the 2×2 block Jacobi matrix B. The next result determines the w values for wich the method converges, under the assumption that the infinity matrix norm of the block Jacobi method lies in the range $0.5 < \|B\|_\infty < 1$.

Theorem 1 ([1],Theorem 9) *Let B be the block Jacobi matrix partitioned in 2×2 blocks obtained from (10). If $0.5 < \|B\|_\infty < 1$ then $\rho(\hat{G}_w) < 1$, provided that*

$$2 - \frac{1}{\|B\|_\infty} < w < \sqrt{\frac{\|B\|_\infty + 1}{2\|B\|_\infty}}$$

.

3 Numerical experiments

In this section we present the results of numerical experiments corresponding to the transient on the bidimensional Seed-Blanket reactor (figure 1). This problem is similar to the TWIGL problem ([5],[6] and [7]). It is modeled with two energy groups, one delayed neutron precursor group, and a quarter core symmetry. The transient consists of decreasing the thermal absorption cross section in region 1 as the ramp function $\Sigma_{a2}(t) = 0.15 - \frac{0.0035}{0.2}t$, $0 \le t \le 0.2$. The kinetic parameters, β and λ, have been modified to accelerate the transient (see [2]).

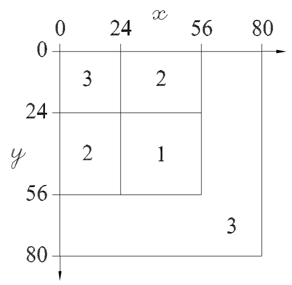

Figure 1: Quadrant of the Seed-Blanket reactor.

The reactor has been discretized using both a five point centered finite differences scheme

Method	Error Test	(RTol,Atol)	$iterations^*$	$time(s)^*$	Power
ASD$(1.55,5,1)$ $JCG(20,5.10^{-6})$	TEST2	$(10^{-5},0.0)$	6	0.045	2.163
ASD$(1.55,5,1)$ $JCG(20,10^{-5})$	TEST2	$(10^{-7},0.0)$	6	0.044	2.094
$BiCGSTAB_{ILU0}$	TEST1	$(5.10^{-5},0.0)$	52	0.320	2.160
	TEST2	$(5.10^{-5},0.0)$	57	0.360	2.160
	TEST1	$(5.10^{-5},10^{-5})$	12	0.077	2.156
	TEST2	$(5.10^{-5},10^{-5})$	20	0.127	2.151
	TEST1	$(5.10^{-5},5.10^{-5})$	2	0.02	1.28
$BiCGSTAB_{ILUT}$	TEST1	$(5.10^{-5},10^{-5})$	13	0.080	2.114
$GMRES(10)_{ILU0}$	TEST2	$(10^{-5},5.10^{-6})$	18	0.18	2.140
$GMRES(20)_{ILU0}$	TEST1	$(10^{-5},5.10^{-6})$	11	0.14	2.153
$GMRES(20)_{ILUT}$	TEST1	$(10^{-5},5.10^{-6})$	14	0.2	2.120
$TFQMR_{ILU0}$	TEST2	$(10^{-10},0.0)$	8	0.05	1.003
	TEST1	$(10^{-5},10^{-6})$	36	0.25	2.159
$TFQMR_{ILUT}$	TEST1	$(10^{-5},10^{-6})$	52	0.34	2.159

Table 1: Performance of the different methods with a spatial discretization NODAL(3). Matrix size 1200 with 14960 nonzero elements. $iterations^*$ and $time(s)^*$ stand for the average number of iterations and CPU time in seconds needed to compute a time step or equivalently to solve a linear system. Power stands for the relative power reached at time 0.2 seconds, for a reference power of 2.160. TEST1 = $||r^i||_2 \leq ||r^0||_2 * Rtol + Atol$, TEST2 = $||d^i||_2 \leq ||d^0||_2 * Rtol + Atol$, where $Rtol, Atol$ are the relative and absolute error tolerance respectively. For the JCG inner solver the maximum number of iterations and error tolerance are indicated between brackets. For GMRES(k), BiCGSTAB and TFQMR the subscript indicates the preconditioner used.

with uniform grid size $h_x = h_y = 3\ cm$, and a nodal collocation method with square nodes $8\ cm$ wide. Roughly speaking, the nodal collocation method tries to expand the solution in each node in terms of a given number of p Legendre polynomials. In the rest of the section we will refer to it as NODAL(p). As in [3], to accelerate the convergence rate of the second degree method (11), we combine it with a variational strategy of the form

$$\psi^{n+1} = \psi^n + \alpha r^n + \beta d^n \tag{16}$$

$$\alpha = \frac{\langle r^n, T^{-1}r^n\rangle\langle d^n, d^n\rangle - \langle d^n, T^{-1}r^n\rangle\langle r^n, d^n\rangle}{\langle r^n, r^n\rangle\langle d^n, d^n\rangle - \langle r^n, d^n\rangle^2},$$

$$\beta = \frac{\langle r^n, r^n\rangle\langle d^n, T^{-1}r^n\rangle - \langle r^n, T^{-1}r^n\rangle\langle r^n, d^n\rangle}{\langle r^n, r^n\rangle\langle d^n, d^n\rangle - \langle r^n, d^n\rangle^2},$$

where $\langle a,b\rangle = a^T T^T T b$ denotes the inner product defined by the spd matrix $T^T T$ (we assume that T is nonsingular), $r^n = E - T\psi^n$ and $d^n = \psi^n - \psi^{n-1}$ are the residual and the previous change in ψ at step n respectively. The parameters α and β are choosen such that $\|r\|_2^2$ is minimized. We will refer to it as ASD(w,r,q) meaning that each r iterations of the second degree method with parameter w, q iterations of the variational technique (16) are performed. We found experimentally that combining five iterations of the second degree method (11) with one of the variational technique was optimal for all the matrices tested. For the w parameter we tried $w = 1.55$ in our experiments, showing that the degree of accuracy in the estimation of this parameter does not seem to be crucial for the performance of the ASD(w,r,q) method. We also note that the second degree method can be

Method	Error Test	(RTol,Atol)	$iterations^*$	$time(s)^*$	Power
ASD$(1.55, 5, 1)$ $JCG(20, 5.10^{-6})$	TEST2	$(10^{-5}, 0.0)$	6	0.24	2.138
$BiCGSTAB_{ILU0}$	TEST1	$(5.10^{-5}, 10^{-5})$	16	0.38	2.132
$BiCGSTAB_{ILUT}$	TEST2	$(5.10^{-5}, 10^{-5})$	12	0.40	2.132
$GMRES(10)_{ILU0}$	TEST1	$(5.10^{-5}, 10^{-5})$	15	0.66	2.127
$GMRES(10)_{ILUT}$	TEST1	$(5.10^{-5}, 10^{-5})$	10	0.50	2.132
$GMRES(20)_{ILUT}$	TEST1	$(5.10^{-5}, 10^{-5})$	10	0.53	2.132
$TFQMR_{ILU0}$	TEST1	$(5.10^{-5}, 10^{-5})$	27	0.65	2.132
$TFQMR_{ILUT}$	TEST1	$(5.10^{-5}, 10^{-5})$	16	0.53	2.132

Table 2: Performance of the different methods with the finite centered differences method. Uniform grid size $h_x = hy = 3\ cm$. Matrix size 5408 with 32032 nonzero elements.

seen as a two stage method, and therefore we make the distinction between inner and outer iterations. For the inner iterations, corresponding to the solution of the diagonal blocks T_{11} and T_{22}, the Jacobi Preconditioned Conjugate Gradient method (JCG) was used. In this section we compare the performance of the ASD(w, r, q) method with the GMRES, TFQMR and BiCGSTAB methods. For these methods, the ILU0 and ILUT (level of fill-in 5, drop tolerance 10^{-2}) were used as preconditioners. The integration time step was fixed to $h = 1.25 \times 10^{-3}$ seconds which implies a number of 160 time steps to simulate all the transient. As reference power, the value of 2.160 was computed for this problem, with a spatial discretization NODAL(4) and a time step integration $h = 6.25 \times 10^{-4}\ s$. The codes were written in FORTRAN 77 and tested on a HP Exemplar S Class.

Table 1 shows the average time and number of iterations needed to solve a time step, and the peak power reached at the end of the transient for differents error tests and tolerances. This table have been obtained with a spatial discretization (NODAL(3)). We see for the ASD$(1.55, 5, 1)$ method that the best execution time is obtained for the case of solving the inner systems with a maximum number of 20 inner iterations (JCG$(20, 5.10^{-6})$). The peak power reached was very good. We note that for this method it is more important to compute the inner iterations with enough accuracy than the outer ones. For instance, if we see for the case of using the JCG$(20, 10^{-5})$, even solving the outer iterations with a relative error tolerance of 10^{-7}, the peak power only grows until 2.094. This fact was observed in all the experiments. The number of outer iterations observed was always 6 (see also Table 2). Moreover, the time needed to simulate the transient was between 40 and 80 per cent smaller than for the others methods compared. For the GMRES, BiCGSTAB and TFQMR methods, we see that taking $Atol = 0.0$, the time spent for the integration was very large. For these methods the best results are obtained when the error test is relaxed, i.e, taking $Atol$ close to $Rtol$. However, we still must keep a minimum level of accuracy. For instance, for the BiCGSTAB with ILU0 preconditioner, if we take $Atol = Rtol = 5.10^{-5}$ we obtain a poor peak power of only 1.28. For these methods the best computation time was obtained whith the ILU0 preconditioner, using TEST1 as the error test. For the BiCGSTAB the time spent was 40 percent larger than for the ASD(1.55,5,1), although it performed better than the GMRES(k) and TFQMR methods. For the GMRES(k), similar conclusions hold. The best performance was obtained for a maximum dimension of the Krylov subspace $k = 20$, but the observed time was 65 percent larger than for the ASD$(1.55, 5, 1)$. For the TFQMR, the first thing to be observed is that checking the error with TEST2 the method loses all the power variation. Therefore we must use always TEST1. The time spent was larger than for the other methods, and 80 percent slower compared with the ASD$(1.55, 5, 1)$

method. The peak power reached for these methods was comparable to that obtained with the ASD$(1.55, 5, 1)$.

For the finite differences spatial discretization method, the results are shown in table 2. We observe that the ASD$(1.55, 5, 1)$ is still between 40 and 50 per cent faster than the other methods considered. Moreover, the peak power reached is slightly better. For the BiCGSTAB the ILU0 preconditioner is again the best choice, but now for the GMRES and TFQMR is the ILUT preconditioner which gives the best results. Besides, the BiCGSTAB still continues being faster than GMRES and TFQMR. On the other hand, comparing the different discretizations used we see that clearly the nodal collocation method obtains the best result in time and peak power. With this method we work with smaller matrices while obtaining a more accurate power estimation. It is worth to note that with NODAL(p) the matrices are denser than those obtained with the finite differences method, and this can explain the differences observed.

The main conclusion of the study is that, independently of the discretization method used, nodal collocation or finite differences, the ASD(w, r, q) obtains the best relation time/accuracy. Comparing the GMRES(k), BiCGSTAB and TFQMR, it is the BiCGSTAB which obtains the best results. For these methods, the ILU0 preconditioner seems to be the best choice, although for the finite differences case the GMRES and TFQMR perform better with the ILUT type. Regarding the spatial discretization type, the nodal collocation method is clearly the best option because it gives the most accurate results while using smaller matrices, which implies a reduction on the computation time.

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