Iterative Schemes for the Neutron Diffusion Equation *

R. Bru † D. Ginestar ‡ T. Manteuffel § J. Marín ¶
J. Mas ‖ G. Verdú **

February 6, 2002

Abstract

We study iterative methods for solving linear systems arising in the discretization of the time dependent neutron diffusion equation. These methods are obtained accelerating two different stationary iterative methods, of second degree type, with a variational technique. We have obtained some results concerning the convergence and the selection of the optimal extrapolation factor for some particular matrices. To test their performance, the bidimensional Seed-Blanket transient has been simulated. From the numerical results, compared with the ones obtained with other methods as the restarted GMRES, BiCGSTAB and TFQMR, we can conclude that the proposed methods are competitive for this type of problem.

Key words. iterative methods, neutron diffusion equation, second degree methods, variational acceleration.

AMS subject classifications. 65F10, 65N22, 65C99, 75R50, 35Q35

---

*This work was supported in part by spanish DGI grant BFM2001-2641 and CICYT grant DPI2001-2766-C02-01.

†Departament de Matemàtica Aplicada. Universitat Politècnica de València. E-46071 València, Spain.(rbru@mat.upv.es).

‡Departament de Matemàtica Aplicada. Universitat Politècnica de València. E-46071 València, Spain.(dginesta@mat.upv.es).

§Applied Math Department, Campus Box 526, University of Colorado at Boulder, Boulder, CO 80309-0526. (tmanteuf@colorado.edu).

¶Departament de Matemàtica Aplicada. Universitat Politècnica de València. E-46071 València, Spain. (jmarinma@mat.upv.es).

‖Departament de Matemàtica Aplicada. Universitat Politècnica de València. E-46071 València, Spain. (jmasm@mat.upv.es).

**Departament d'Engenyería Química i Nuclear. Universitat Politècnica de València. E-46071 València, Spain. (gverdu@iqn.upv.es).

1 Introduction and preliminaries

For design and safety reasons, nuclear power plants need fast and accurate plant simulators. Nuclear power plants basically consist of a steam generator system, called the nuclear steam supply system and a turbo generator which converts the steam energy into electricity. The energy used to produce steam comes from basic nuclear reactions induced by neutrons in the nuclear fuel of the reactor core. Plant simulators mainly consist of two different modules which account for the basic physical phenomena taking place in the plant. A neutronic module which simulates the neutron balance in the reactor core, and a thermalhydraulic module which simulates the heat transfer from the fuel to the coolant, and the evaporation and condensation processes. In this paper we will focus on the neutronic module. The balance of neutrons in the reactor core can be approximately modelled by the time-dependent two energy group neutron diffusion equation, which is written using standard matrix notation as follows [1]

$$
\begin{aligned}
[v^{-1}]\dot{\phi} + \mathcal{L}\phi &= (1-\beta)\mathcal{M}\phi + \chi \sum_{k=1}^{K} \lambda_k \mathcal{C}_k \ , && (1)\\
\dot{\mathcal{C}}_k &= \beta_k [\nu\Sigma_{f_1} \nu\Sigma_{f_2}]\phi - \lambda_k \mathcal{C}_k ; \ k = 1, \dots, K \ , && (2)
\end{aligned}
$$

where K is the number of delayed neutron precursors groups considered,

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

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 rapid transients of neutronic power and other space and time phenomena related to 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 [4] and finite element methods [5] can be used for this purpose. After the discretization of the spatial part of the equations, we obtain the following systems of ordinary differential equations

$$
\begin{aligned}
[v^{-1}]\dot{\psi} + L\psi &= (1-\beta)M\psi + X\sum_{k=1}^{K}\lambda_k C_k \ , && (3)\\
\dot{C}_k &= \beta_k[M_{11}M_{12}]\psi - \lambda_k C_k;\ k = 1,\dots,K \ , && (4)
\end{aligned}
$$

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

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

Blocks L_{11} and L_{22} are symmetric positive definite matrices [21] while blocks L_{21}, M_{11} and M_{12} are diagonal.

The next step consists of integrating the above ordinary differential equations over a series of time interval, $[t_n, t_{n+1}]$. 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 at t_{n+1} expressed as

$$
C_k^{n+1} = C_k^n e^{-\lambda_k h} + \beta_k(a_k[M_{11}M_{12}]^n\psi^n + b_k[M_{11}M_{12}]^{n+1}\psi^{n+1}) \ , \qquad (5)
$$

where $h = t_{n+1} - t_n$ is a fixed time step size, 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 $[v^{-1}]$. Hence, for its integration it is convenient to use an implicit backward difference formula (BDF) [6]. A stable one-step BDF to integrate (3) is given by

$$
\frac{[v^{-1}]}{h}\left(\psi^{n+1} - \psi^n\right) + L^{n+1}\psi^{n+1} = (1-\beta)M^{n+1}\psi^{n+1} + X\sum_{k=1}^{K}\lambda_k C_k^{n+1}. \quad (6)
$$

Since the truncation error for this BDF is proportional to the integration step h, to keep a good level of accuracy a small time step is needed. In this work, to simplify the presented results, we use the one-step BDF method (6). We mention that in [3] the authors present a combined algorithm which makes use of one-, two- and four-steps BDF methods. This method allows the choice of bigger integration steps keeping the same level of accuracy.

Taking into account equation (5) and the structure of matrices L and M, we rewrite (6) as the system of linear equations

$$\begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \begin{bmatrix} \psi_1^{n} \\ \psi_2^{n} \end{bmatrix} + \sum_{k=1}^{K} \lambda_k e^{-\lambda_k h} \begin{bmatrix} C_k^n \\ 0 \end{bmatrix} \tag{7}$$

where

$$\begin{aligned} T_{11} &= \frac{1}{h}\upsilon_1^{-1} + L_{11}^{n+1} - (1-\beta)M_{11}^{n+1} - \sum_{k=1}^{K} \lambda_k \beta_k b_k M_{11}^{n+1} \ , \ T_{21} = -L_{21}^{n+1} \ , \\ T_{12} &= -(1-\beta)M_{12}^{n+1} - \sum_{k=1}^{K} \lambda_k \beta_k b_k M_{12}^{n+1} \ , \ T_{22} = \frac{1}{h}\upsilon_2^{-1} + L_{22}^{n+1} \ , \\ R_{11} &= \frac{1}{h}\upsilon_1^{-1} + \sum_{k=1}^{K} \lambda_k \beta_k a_k M_{11}^{n} \ , \ R_{12} = \sum_{k=1}^{K} \lambda_k \beta_k a_k M_{12}^{n} \ , \ R_{22} = \frac{1}{h}\upsilon_2^{-1} \ . \end{aligned} \tag{8}$$

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

$$\begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} , \tag{9}$$

where the right-hand side depends on both the solution in previous time steps and the backward difference method used. Usually, the coefficients matrix of system (9) has similar properties as the matrices L and M in equation (3), namely blocks T_{11} , T_{22} are symmetric positive definite matrices, and blocks T_{12} , T_{21} are diagonal matrices. System (9) will be also denoted as

$$T\psi = e \, . \tag{10}$$

Since the system matrix is large and sparse, an iterative method is recommended to solve it. In [2] the system (9) is solved with the block stationary iterative method,

$$\begin{aligned} T_{11}\psi_1^{\ell+1} &= e_1 - T_{12}(\omega\psi_2^{\ell} + (1-\omega)\psi_2^{\ell-1}) \ , \\ T_{22}\psi_2^{\ell+1} &= e_2 - T_{21}(\omega\psi_1^{\ell+1} + (1-\omega)\psi_1^{\ell}) \ , \end{aligned} \tag{11}$$

where ω is a extrapolation factor. In [3] this iterative method is accelerated with the variational technique given by

$$\psi^{\ell+1} = \psi^{\ell} + \alpha^{\ell} r^{\ell} + \beta^{\ell} d^{\ell}, \tag{12}$$

where $r^{\ell} = E - T\psi^{\ell}$ and $d^{\ell} = \psi^{\ell} - \psi^{\ell-1}$ are the residual and the previous change in ψ at iteration ℓ, respectively. The parameters α^{ℓ} and β^{ℓ} are chosen such that the 2-norm of the residual is minimized. In [7] a multilevel algorithm based on the nodal collocation method which uses (11) accelerated with (12) as relaxation method is presented. In all cases very good results were obtained.

Consider the related system of equations

$$\begin{aligned} T_{11}\psi_1^{\ell+1} &= e_1 - T_{12}(\omega\psi_2^{\ell} + (1-\omega)\psi_2^{\ell-1})\ , \\ T_{22}\psi_2^{\ell+1} &= e_2 - T_{21}(\omega\psi_1^{\ell} + (1-\omega)\psi_1^{\ell-1})\ . \end{aligned} \tag{13}$$

The main difference between methods (11) and (13) is that in (11) the new solution for ψ_1, the more energetic group or fast group, is used as soon as it is available to compute ψ_2, also called the thermal group. Therefore, a fast convergence rate may be expected, as it is observed in practice. In the rest of the paper we will refer to the methods (13) and (11) as methods A and B, respectively. We note that for both methods A and B we should distinguish between inner and outer iterations. The inner iterations correspond to the solution of the linear systems with matrices T_{11} and T_{22}. Since they are symmetric and positive definite, a preconditioned conjugate gradient method is specially recommended.

Our goal is the study of the convergence properties of these methods. Moreover, comparing their performance with other conjugate gradient type methods for nonsymmetric matrices is of particular interest.

The paper is structured as follows. In sections 2 and 3, the methods A and B will be characterized as second degree methods. Some theoretical results concerning their convergence properties are presented. In section 4, the variational technique (12) is studied as a projection method, and a practical implementation is proposed. In section 5, the results of the numerical experiments will permit us to compare the proposed methods with other well known iterative methods for nonsymmetrics matrices, as the restarted GMRES [8], the BiCGSTAB [9] and the TFQMR [10] methods. The benchmark chosen for the comparisons corresponds to the bidimensional Seed-Blanket reactor [3]. Finally, the main conclusions are given in section 6.

2 Second degree method A

Consider the coefficient matrix T of the linear system (10) and the splitting $T = M - N$ with matrices M and N given by,

$$M = \begin{bmatrix} T_{11} & 0 \\ 0 & T_{22} \end{bmatrix}, \; N = \begin{bmatrix} 0 & -T_{12} \\ -T_{21} & 0 \end{bmatrix}.$$

This splitting corresponds to the associated iterative block Jacobi method [11, 12, 13] with iteration matrix,

$$B = M^{-1}N = \begin{bmatrix} 0 & -T_{11}^{-1}T_{12} \\ -T_{22}^{-1}T_{21} & 0 \end{bmatrix} = \begin{bmatrix} 0 & -B_{12} \\ -B_{21} & 0 \end{bmatrix}. \tag{14}$$

Considering the matrices $G_1 = \omega B$, $G_0 = (1-\omega)B$ and the vector $k = M^{-1}e$ we can write the second degree method

$$\psi^{(n+1)} = G_1\psi^{(n)} + G_0\psi^{(n-1)} + k = B(\omega\psi^{(n)} + (1-\omega)\psi^{(n-1)}) + k, \tag{15}$$

that corresponds to the method A (equation (13)). It can easily be checked that if the spectral radius of B, $\rho(B)$, is less than 1 then the method is completely consistent, that is, if the sequence of vectors (15) converges, it converges to the unique solution of (9) (see [12], pp. 64). Note that different second degree methods can be constructed using matrices different from B. For instance, it could be used the block Gauss-Seidel method which iteration matrix for the matrix T is given by

$$\mathcal{L} = \begin{bmatrix} T_{11} & 0 \\ T_{21} & T_{22} \end{bmatrix}^{-1} \begin{bmatrix} 0 & -T_{12} \\ 0 & 0 \end{bmatrix}. \tag{16}$$

In the rest of the section we will consider a general matrix G (usually the iteration matrix of a first degree method), and matrices G_0, G_1 given by

$$G_1 = \omega G \quad , \quad G_0 = (1-\omega)G. \tag{17}$$

Second degree methods are usually studied (c.f. [12], pp. 486) by means of the following auxiliary system

$$\begin{bmatrix} \psi^{(n)} \\ \psi^{(n+1)} \end{bmatrix} = \begin{bmatrix} 0 & I \\ G_0 & G_1 \end{bmatrix} \begin{bmatrix} \psi^{(n-1)} \\ \psi^{(n)} \end{bmatrix} + \begin{bmatrix} 0 \\ k \end{bmatrix}. \tag{18}$$

The method is convergent for all $\psi^{(0)}$ and $\psi^{(1)}$ if and only if $\rho(\hat{G}_\omega) < 1$, where

$$\hat{G}_\omega = \begin{bmatrix} 0 & I \\ G_0 & G_1 \end{bmatrix}. \tag{19}$$

Moreover, denoting by λ the eigenvalues of $\hat{G}_\omega$, we have that $\rho(\hat{G}_\omega) < 1$ if all roots of

$$\det(\lambda^2 I - \lambda G_1 - G_0) = 0, \tag{20}$$

are less than unity in modulus. From equations (17) and (20) it follows that the eigenvalues of $\hat{G}_\omega$ are related to the eigenvalues of G, that we have called μ, by the quadratic equation

$$\lambda^2 - \omega\mu\lambda + (\omega - 1)\mu = 0. \tag{21}$$

Given a quadratic function of the form $x^2 - bx + c = 0$, we recall that its root radius, $\rho(b, c)$, is defined as the maximum of the moduli of its roots. It is well known (see [12]) that if b and c are real, both roots of the quadratic equation $x^2 - bx + c = 0$ are less than one in modulus if and only if $|c| < 1$ and $|b| < 1 + c$.

Theorem 1 *Let G be a matrix with real and positive eigenvalues, and let $\hat{G}_\omega$ be the matrix of equation (19). Then $\rho(\hat{G}_\omega) < 1$ if and only if*

$$\frac{\bar{\mu} - 1}{2\bar{\mu}} < \omega < \frac{\bar{\mu} + 1}{\bar{\mu}} \quad \textit{and} \quad \bar{\mu} < 1\ , \tag{22}$$

where $\bar{\mu}$ is the spectral radius of G.

Proof: The root radius of (21) is less than unity in modulus if and only if both conditions $|c| = |(\omega - 1)\mu| < 1$ and $|b| = |\omega\mu| < 1 + c$, are satisfied for all μ in the spectrum of G. If $\rho(\hat{G}_\omega) < 1$, consider the case $\mu = \bar{\mu}$. From the first condition we deduce the following equivalence

$$|(\omega - 1)\bar{\mu}| < 1 \quad \text{if and only if} \quad 1 - \frac{1}{\bar{\mu}} < \omega < 1 + \frac{1}{\bar{\mu}}.$$

From the second condition it follows

$$-1 - (\omega - 1)\bar{\mu} < \omega\bar{\mu} < 1 + (\omega - 1)\bar{\mu}.$$

Then,

$$\omega > \frac{\bar{\mu} - 1}{2\bar{\mu}} > 1 - \frac{1}{\bar{\mu}}.$$

Therefore, the range for ω is

$$\frac{\bar{\mu} - 1}{2\bar{\mu}} < \omega < 1 + \frac{1}{\bar{\mu}}.$$

Conversely, from equation (22) it follows that,

$$\frac{-(1+\bar{\mu})}{2} < \omega - 1 < 1 \quad \text{if and only if} \quad |c| = |(\omega-1)\mu| \leq |(\omega-1)\bar{\mu}| < 1.$$

On the other hand, to show that $|b| < 1 + c$ we consider two cases,
$(b > 0)$

$$1 + c - |b| = 1 + c - b = 1 - \mu > 0.$$

$(b < 0)$

$$1 + c - |b| = 1 + c + b = 1 - \mu + 2\omega\mu > 0.$$

Therefore $|c| < 1$ and $|b| < 1 + c$ which implies $\rho(\hat{G}_\omega) < 1$. ■

Theorem 2 *Let G be a matrix with real eigenvalues, and let $\hat{G}_\omega$ be the matrix of equation (19). Then $\rho(\hat{G}_\omega) < 1$ if and only if*

$$\frac{\bar{\mu}-1}{2\bar{\mu}} < \omega < \frac{\bar{\mu}+1}{2\bar{\mu}} \quad \textit{and} \quad \bar{\mu} < 1\ ,$$

where $\bar{\mu}$ is the spectral radius of G.

Proof: Considering the cases $\mu = \bar{\mu}$ and $\mu = -\bar{\mu}$, the proof is similar to the one of previous theorem. ■
Next result determines the optimum value of ω, denoted ω_b, which minimizes the spectral radius of $\hat{G}_\omega$.

Theorem 3 *Let G be a matrix with real and positive eigenvalues such that $\bar{\mu} = \rho(G) < 1$, and let $\hat{G}_\omega$ be the matrix of equation (19). If ω_b is defined by*

$$\omega_b = \frac{2}{1+\sqrt{1-\bar{\mu}}}\ , \tag{23}$$

then

$$\rho(\hat{G}_{\omega_b}) = \frac{\omega_b\bar{\mu}}{2}\ , \tag{24}$$

and if $\omega \neq \omega_b$, then

$$\rho(\hat{G}_\omega) > \rho(\hat{G}_{\omega_b})\ .$$

Finally, if $\frac{\bar{\mu}-1}{2\bar{\mu}} < \omega < \omega_b$, then $\rho(\hat{G}_\omega)$ is a strictly decreasing function of ω.

Proof: The proof is based on geometrical considerations, and its technique is similar to that used in [11, Theorem 4.4]. ∎

In the case of G having complex eigenvalues the analysis of the convergence of the method is different. Computing the square of matrix (19) we obtain,

$$\hat{G}_\omega^2 = \begin{bmatrix} (1-\omega)G & \omega G \\ (1-\omega)\omega G^2 & (1-\omega)G + \omega^2 G^2 \end{bmatrix}. \tag{25}$$

The following lemma is from [14].

Lemma 4 *Let A be a matrix in $\mathbb{R}^{n\times n}$. Then $lim_{k\to\infty} A^k = 0$ if and only if $\rho(A) < 1$. Moreover, $\|A^k\|$ is bounded as $k \to \infty$ if and only if $\rho(A) < 1$.*

From Lemma 4 it follows that if $\|\hat{G}_\omega^2\| < 1$ for some matrix norm, then the second degree method converges. The following matrix norm exploits the block structure of the matrix (25), and therefore it will be used later. Given a matrix norm $\|.\|_\alpha$ over the set of all $n \times n$ matrices, consider the $qn \times qn$ matrix M partitioned as

$$M = \begin{bmatrix} M_{11} & M_{12} & \cdots & M_{1q} \\ M_{21} & M_{22} & \cdots & M_{2q} \\ \vdots & \vdots & & \vdots \\ M_{q1} & M_{q2} & \cdots & M_{qq} \end{bmatrix} : M_{ij} \text{ square of order } n.$$

Define

$$\|M\| = \max_{1\le i\le q} \sum_{j=1}^{q} \|M_{ij}\|_\alpha, \tag{26}$$

then, $\|.\|$ is a matrix norm over the set of all $qn \times qn$ matrices [15].

To apply matrix norm (26) to the matrix given in (25) the following expression must be evaluated,

$$\max\left\{\|(1-\omega)G\|_\alpha + \|\omega G\|_\alpha,\ \|(1-\omega)\omega G^2\|_\alpha + \|(1-\omega)G + \omega^2 G^2\|_\alpha\right\}. \tag{27}$$

Theorem 5 *Let G be the iteration matrix of a convergent first degree method, and let $\hat{G}_\omega$ be the matrix of equation (19). If*

$$0 < \omega < \sqrt{\frac{1+\bar{\mu}}{2\bar{\mu}}}$$

then $\rho(\hat{G}_\omega) < 1$, where $\bar{\mu} = \rho(G)$.

Proof: We shall prove that $\|\rho(\hat{G}_\omega)^2\| < 1$ and then $\rho(\hat{G}_\omega) < 1$. Because G is the iteration matrix of a convergent first degree method, then $\bar{\mu} < 1$. Thus, there is a compatible matrix norm $\|.\|_\alpha$ such that $\|G\|_\alpha < 1$.

- $0 < \omega < 1$

  Let β be a real constant such that $\|G\|_\alpha < \beta < 1$. Then, we have for the first term of (27) that $\|(1-\omega)G\|_\alpha + \|\omega G\|_\alpha = (1-\omega+\omega)\|G\|_\alpha < \beta < 1$. And for the second term, $\|(1-\omega)\omega G^2\|_\alpha + \|(1-\omega)G + \omega^2 G^2\|_\alpha \leq \|(1-\omega)\omega G^2\|_\alpha + \|(1-\omega)G\|_\alpha + \|\omega^2 G^2\|_\alpha = ((1-\omega)\omega + \omega^2)\|G^2\|_\alpha + (1-\omega)\|G\|_\alpha = \omega\|G^2\|_\alpha + (1-\omega)\|G\|_\alpha \leq (\omega + 1 - \omega)\|G\|_\alpha < \beta < 1$.

- $1 \leq \omega < \sqrt{\dfrac{1+\bar{\mu}}{2\bar{\mu}}}$

  For the first term we will show that $\|(1-\omega)G\|_\alpha + \|\omega G\|_\alpha < 1$ if $1 \leq \omega < \dfrac{1+\bar{\mu}}{2\bar{\mu}}$. For ω in this range, there exists $\beta \in \mathbb{R}$ such that $1 \leq \omega < \beta < \dfrac{1+\bar{\mu}}{2\bar{\mu}}$. Consider $0 < \alpha < \min(1-\bar{\mu}, \dfrac{1-(2\beta-1)\bar{\mu}}{(2\beta-1)})$. Because $\bar{\mu} < 1$, there exists a compatible matrix norm such that $\bar{\mu} \leq \|G\|_\alpha \leq \bar{\mu} + \alpha < 1$. Therefore, we have $\|(1-\omega)G\|_\alpha + \|\omega G\|_\alpha = (2\omega - 1)\|G\|_\alpha < (2\beta-1)\|G\|_\alpha = \gamma$. Moreover $\alpha < \dfrac{1-(2\beta-1)\bar{\mu}}{(2\beta-1)}$ and then $(2\beta - 1) < \dfrac{1}{\bar{\mu}+\alpha}$. It follows that $\gamma \leq (2\beta-1)(\bar{\mu}+\alpha) < \dfrac{1}{\bar{\mu}+\alpha}(\bar{\mu}+\alpha) = 1$.

  Similarly for the second term there exists $\beta \in \mathbb{R}$ such that $1 \leq \omega < \beta < \sqrt{\dfrac{1+\bar{\mu}}{2\bar{\mu}}}$. Consider now $0 < \alpha < \min(1-\bar{\mu}, \dfrac{1-(2\beta^2-1)\bar{\mu}}{(2\beta^2-1)})$. With an argument similar to the one used in the previous case it follows that $\|\omega(1-\omega)G^2\|_\alpha + \|(1-\omega)G + \omega^2 G^2\|_\alpha \leq \|\omega(1-\omega)G^2\|_\alpha + \|(1-\omega)G\|_\alpha + \|\omega^2 G^2\|_\alpha = (2\omega^2 - \omega)\|G^2\|_\alpha + (\omega - 1)\|G\|_\alpha \leq (2\omega^2 - \omega + \omega - 1)\|G\|_\alpha < (2\beta^2 - 1)\|G\|_\alpha = \gamma$. Moreover $\alpha < \dfrac{1-(2\beta^2-1)\bar{\mu}}{(2\beta^2-1)}$ and then $(2\beta^2 - 1) < \dfrac{1}{\bar{\mu}+\alpha}$ and therefore $\gamma \leq (2\beta^2-1)(\bar{\mu}+\alpha) < \dfrac{1}{\bar{\mu}+\alpha}(\bar{\mu}+\alpha) = 1$.

■

3 Second degree method B

For the method shown in (11), we can also identify a second degree method as in (15) but with the matrices G_0, G_1 and the vector k given by

$$G_0 = \begin{bmatrix} 0 & -(1-\omega)B_{12} \\ 0 & (1-\omega)\omega B_{21}B_{12} \end{bmatrix}, \quad G_1 = \begin{bmatrix} 0 & -\omega B_{12} \\ -(1-\omega)B_{21} & \omega^2 B_{21}B_{12} \end{bmatrix}, \quad (28)$$

and

$$k = \begin{bmatrix} T_{11}^{-1}e_1 \\ T_{22}^{-1}e_2 - \omega B_{21}T_{11}^{-1}e_1 \end{bmatrix},$$

where $B_{12} = T_{11}^{-1}T_{12}$, $B_{21} = T_{22}^{-1}T_{21}$. These matrices can be factorized as,

$$G_0 = \begin{bmatrix} 0 & -B_{12} \\ -(1-\omega)B_{21} & \omega B_{21}B_{12} \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & (1-\omega)I \end{bmatrix} = H_\omega P_0 \;, \qquad (29)$$

$$G_1 = \begin{bmatrix} 0 & -B_{12} \\ -(1-\omega)B_{21} & \omega B_{21}B_{12} \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & \omega I \end{bmatrix} = H_\omega P_1 \,. \qquad (30)$$

Matrix H_ω corresponds to the iteration matrix of the accelerated block Gauss-Seidel method [16] applied to the coefficient matrix T of (9). In fact, considering the splitting

$$T = M_\omega - N_\omega = \begin{bmatrix} T_{11} & 0 \\ \omega T_{21} & T_{22} \end{bmatrix} - \begin{bmatrix} 0 & -T_{12} \\ -(1-\omega)T_{21} & 0 \end{bmatrix}, \qquad (31)$$

it follows that $H_\omega = M_\omega^{-1}N_\omega$. Taking into account that $H_\omega P_0 + H_\omega P_1 = H_\omega$, and

$$k = M^{-1}E = \begin{bmatrix} T_{11}^{-1} & 0 \\ -\omega B_{21}T_{11}^{-1} & T_{22}^{-1} \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \end{bmatrix},$$

it can be checked that the second degree method B is completely consistent if the spectral radius of H_ω is less than one, i.e, the accelerated block Gauss-Seidel method is convergent.

The matrix of the equivalent augmented system $\hat{G}_\omega$ in (18) is now given by

$$\hat{G}_\omega = \begin{bmatrix} 0 & I \\ H_\omega P_0 & H_\omega P_1 \end{bmatrix}, \qquad (32)$$

and its square is given by

$$\hat{G}_\omega^2 = \begin{bmatrix} H_\omega P_0 & H_\omega P_1 \\ H_\omega P_1 H_\omega P_0 & H_\omega P_0 + (H_\omega P_1)^2 \end{bmatrix}. \qquad (33)$$

Theorem 6 *Let H_ω be the iteration matrix of the accelerated block Gauss-Seidel method, with $\|H_\omega\|_\infty < 1$, and let $\hat{G}_\omega$ be the matrix of equation (32). If*

$$2 - \frac{1}{\|H_\omega\|_\infty} < \omega < \frac{\|H_\omega\|_\infty + 1}{2\|H_\omega\|_\infty}\,, \tag{34}$$

then $\rho(\hat{G}_\omega) < 1$.

Proof: Applying the norm (26) to the matrix given in equation (33) it can easily be shown that

$$\max\left\{\|H_\omega P_0\|_\infty + \|H_\omega P_1\|_\infty, \|H_\omega P_1 H_\omega P_0\|_\infty + \|H_\omega P_0 + (H_\omega P_1)^2\|_\infty\right\} < 1\,, \tag{35}$$

for ω ranging in the interval (34). ■

4 Accelerated second degree method

In this section we present a variational method to accelerate the convergence rate of the second degree methods A and B. We recall that at each integration time step it must be solved a nonsymmetric linear system of the form,

$$T\psi = e\,, \tag{36}$$

where the matrix $T \in \mathbb{R}^{n\times n}$. Given two initial approximate solutions ψ^0 and ψ^1, the proposed variational method for solving the system (36) is given by the equation,

$$\psi^{\ell+1} = \psi^\ell + \alpha^\ell r^\ell + \beta^\ell d^\ell \qquad \ell = 1, 2, \ldots \tag{37}$$

where $r^\ell = e - T\psi^\ell$ and $d^\ell = \psi^\ell - \psi^{\ell-1}$ are the residual and the previous change in ψ at iteration ℓ, respectively. The coefficients α^ℓ and β^ℓ are chosen to minimize the $2-$norm of the residual, $\|r^{\ell+1}\|_2$, over the two dimensional space,

$$\mathcal{L}_\ell = span\{Tr^\ell, Td^\ell\}\,. \tag{38}$$

In the next subsection the variational method (37) is studied, and in subsection 4.2, a practical implementation of the accelerated second degree methods A and B is proposed.

4.1 Variational Method

First, we recall some basic concepts about projection methods and optimality Petrov-Galerkin conditions (see for instance [13]). A projection technique extracts an approximate solution to the problem (36) from a subspace of $\mathbb{R}^n$, namely $\mathcal{K}$, by imposing the conditions that the new residual vector has to be orthogonal to another subspace of $\mathbb{R}^n$, $\mathcal{L}$, both of dimension m. When $\mathcal{L}$ equals $\mathcal{K}$ the projection method is called orthogonal, and oblique when they are different. Moreover, for a general projection method the new residual satisfies the relation

$$r^{\ell+1} = r^\ell - TV(W^T TV)^{-1} W^T r^\ell \, , \tag{39}$$

where W and V are bases for $\mathcal{L}$ and $\mathcal{K}$, respectively. If $\mathcal{L} = T\mathcal{K}$, then $W^T TV$ is nonsingular ([13], Proposition 5.1).

In our case, taking the subspaces

$$\mathcal{K}_\ell = span\{r^\ell, d^\ell\} \ \text{ and } \ \mathcal{L}_\ell = span\{Tr^\ell, Td^\ell\} \, , \tag{40}$$

we have, from equation (37), that $\psi^{\ell+1} = \psi^\ell + \delta$ with $\delta \in \mathcal{K}_\ell$, and $r^{\ell+1} = r^\ell - T\delta$, with $T\delta \in \mathcal{L}_\ell$. Therefore, if the orthogonality condition $r^{\ell+1} \perp \mathcal{L}_\ell$ is satisfied, then the new solution $\psi^{\ell+1}$ is optimal in a least squares sense, since the new residual is the vector with minimal 2-norm in the afine space $r^\ell + \mathcal{L}_\ell$.

Forcing orthogonality between the new residual and the subspace $\mathcal{L}_\ell$ leads to the following system of equations:

$$\alpha^\ell \langle Tr^\ell, Tr^\ell \rangle + \beta^\ell \langle Td^\ell, Tr^\ell \rangle = \langle r^\ell, Tr^\ell \rangle \, , \tag{41}$$

$$\alpha^\ell \langle Tr^\ell, Td^\ell \rangle + \beta^\ell \langle Td^\ell, Td^\ell \rangle = \langle r^\ell, Td^\ell \rangle . \tag{42}$$

The solutions of this system are the coefficients,

$$\alpha^\ell = \frac{\langle Tr^\ell, r^\ell \rangle \langle Td^\ell, Td^\ell \rangle - \langle Td^\ell, r^\ell \rangle \langle Tr^\ell, Td^\ell \rangle}{\langle Tr^\ell, Tr^\ell \rangle \langle Td^\ell, Td^\ell \rangle - \langle Tr^\ell, Td^\ell \rangle^2}, \tag{43}$$

$$\beta^\ell = \frac{\langle Tr^\ell, r^\ell \rangle \langle Td^\ell, r^\ell \rangle - \langle Tr^\ell, r^\ell \rangle \langle Tr^\ell, Td^\ell \rangle}{\langle Tr^\ell, Tr^\ell \rangle \langle Td^\ell, Td^\ell \rangle - \langle Tr^\ell, Td^\ell \rangle^2}, \tag{44}$$

where $\langle a, b \rangle = a^T b$ denotes the euclidean inner product. These coefficients have some redundant information. If we write

$$r^{\ell-1} - r^\ell = \alpha^{\ell-1} Tr^{\ell-1} + \beta^{\ell-1} Td^{\ell-1} = Td^\ell, \tag{45}$$

we have that

$$r^{\ell} = r^{\ell-1} - Td^{\ell}. \tag{46}$$

Thus, Td^{ℓ} is just the orthogonal projection onto $\mathcal{L}_{\ell-1}$ of the residual $r^{\ell-1}$. Therefore the $\langle r^{\ell}, Td^{\ell}\rangle$ term is zero, giving the new expressions

$$\begin{aligned}
\alpha^{\ell} &= \frac{\langle Tr^{\ell}, r^{\ell}\rangle\langle Td^{\ell}, Td^{\ell}\rangle}{\langle Tr^{\ell}, Tr^{\ell}\rangle\langle Td^{\ell}, Td^{\ell}\rangle - \langle Tr^{\ell}, Td^{\ell}\rangle^2}, \\
\beta^{\ell} &= \frac{-\langle Tr^{\ell}, r^{\ell}\rangle\langle Tr^{\ell}, Td^{\ell}\rangle}{\langle Tr^{\ell}, Tr^{\ell}\rangle\langle Td^{\ell}, Td^{\ell}\rangle - \langle Tr^{\ell}, Td^{\ell}\rangle^2}.
\end{aligned} \tag{47}$$

These coefficients are well defined if

$$\langle Tr^{\ell}, Tr^{\ell}\rangle\langle Td^{\ell}, Td^{\ell}\rangle - \langle Tr^{\ell}, Td^{\ell}\rangle^2 \neq 0. \tag{48}$$

Note that, by the Cauchy-Schwarz inequality, condition (48) is violated if and only if Tr^{ℓ} and Td^{ℓ} are linearly dependent vectors. A natural question that arises is when Tr^{ℓ} and Td^{ℓ} are linearly dependent vectors. To answer this question let us suppose that $Tr^{\ell} = cTd^{\ell}$ ($r^{\ell} = cd^{\ell}$) with $c \in \mathbb{R}$. In this context, provided that r^{ℓ} is orthogonal to Td^{ℓ}, we have that r^{ℓ} is orthogonal to $\mathcal{L}_{\ell} = span\{Tr^{\ell}, Td^{\ell}\}$. Thus, $\langle r^{\ell}, Tr^{\ell}\rangle = 0$. Suppose now that either T is a definite matrix or the field of values[1] of T, $\mathcal{F}(T)$, does not include 0. Then, $\langle r^{\ell}, Tr^{\ell}\rangle = 0$ if and only if $r^{\ell} = 0$, and therefore $\psi^{\ell} = T^{-1}e$. Moreover, since $Tr^{\ell} = 0 = cTd^{\ell} = c(r^{\ell-1} - r^{\ell})$ then $r^{\ell-1} = r^{\ell}$. Therefore, the solution has been reached at step $\ell - 1$, i.e, $\psi^{\ell-1} = T^{-1}e$. We conclude that, while the system solution has not been reached, the coefficients given in (47) are well defined. We have the following result.

Theorem 7 *Assume that $0 \notin \mathcal{F}(T)$. The coefficients (47) are well defined if and only if $\psi^{\ell-1}$ is not the solution of (36).*

Proof: The sufficient condition has been proved above. To show the necessary condition assume that the coefficients (47) are well defined, and suppose that $\psi^{\ell-1} = T^{-1}e$. Then $r^{\ell-1} = 0$, and it follows that $Td^{\ell} = 0$ in contradiction with (48). ■

The variational method finds solutions of the form

$$\psi^{\ell+1} = \psi^{\ell} + \alpha^{\ell} r^{\ell} + \beta^{\ell} d^{\ell} \equiv \psi^{\ell} + [r^{\ell}\ d^{\ell}]y^{\ell},$$

[1] The field of values of $A \in \mathbb{R}^{n\times n}$ is $\mathcal{F}(A) = \{y^T Ay\ :\ y \in \mathbb{R}^n,\ y^T y = 1\}$ [17].

with

$$y^\ell = \left[\begin{array}{c} \alpha^\ell \\ \beta^\ell \end{array} \right].$$

The vector of coefficients y^ℓ is the argument which minimizes the residual norm,

$$y^\ell = \arg\min_y \|r^\ell - T[r^\ell\ d^\ell]y\|_2 \,. \tag{49}$$

Since T is a nonsingular matrix, the solution for the least squares problem (49) always exists, it is unique and coincides with (47).

Now, we propose an alternative way of computing these coefficients efficiently. Building an orthonormal basis for the subspace of $\mathbb{R}^n$ spanned by the vectors $\{r^\ell, Tr^\ell, Td^\ell\}$ with the standard Gram-Schmidt algorithm we obtain the relation,

$$T[r^\ell\ d^\ell] = QH_{3,2} \tag{50}$$

The columns of Q are the vectors of the orthonormal basis $\{v_1, v_2, v_3\}$ obtained as follows,

$$\begin{aligned} \beta v_1 &= r^\ell \,, & (51) \\ h_{21} v_2 &= Tr^\ell - h_{11} v_1 \,, & (52) \\ h_{32} v_3 &= Td^\ell - h_{12} v_1 - h_{22} v_2 \,, & (53) \end{aligned}$$

and the coefficients β and h_{ij} are given by,

$$\begin{aligned} &\beta = \|r^\ell\|_2 \,, \\ &h_{11} = \langle Tr^\ell, v_1 \rangle,\ h_{21} = \|(Tr^\ell - h_{11} v_1)\|_2 \,, \\ &h_{12} = \langle Td^\ell, v_1 \rangle,\ h_{22} = \langle Td^\ell, v_2 \rangle,\ h_{32} = \|(Td^\ell - h_{12} v_1 - h_{22} v_2)\|_2 \,. \end{aligned}$$

Thus, $H_{3,2}$ is the upper Hessenberg matrix,

$$H_{3,2} = \left[\begin{array}{cc} h_{11} & h_{12} \\ h_{21} & h_{22} \\ 0 & h_{32} \end{array} \right] .$$

Using (50) an equivalent formulation for the least squares problem (49) can be obtained as follows,

$$\begin{aligned} y_\ell &= \arg\min_y \|r^\ell - A[r^\ell\ d^\ell]y\|_2 \\ &= \arg\min_y \|r^\ell - QH_{3,2}y\|_2 \\ &= \arg\min_y \|Q(\beta e_1 - H_{3,2}y)\|_2 \\ &= \arg\min_y \|\beta e_1 - H_{3,2}y\|_2 \,, \end{aligned} \tag{54}$$

where $e_1 = (1,0,0)^T$. The problem has been reduced to obtain the solution of a 3×2 least squares problem which can easily be done. Algorithm 1 implements this method.

Algorithm 1 Variational method.

---

1. **Choose** ψ^0 and d^0. Compute $r^0 := E - T\psi^0$
2. **For** $\ell = 0, 1, 2, \dots$,
   (a) **Compute** $\beta := \|r^\ell\|_2$, $v_1 := r^\ell/\beta$, $w_1 := Tr^\ell$ and $w_2 := Td^\ell$
   (b) **For** $j = 1, 2$
   For $i = 1, \dots, j$
   $h_{ij} := \langle w_j, v_i \rangle$
   $w_j := w_j - h_{ij} v_j$
   $h_{j+1,j} := \|w_j\|_2$
   $v_{j+1} := w_j / h_{j+1,j}$
   (c) **Compute** $y_\ell = \arg\min_y \|\beta e_1 - H_{3,2} y\|_2$
   (d) **Compute** $\psi^{\ell+1} := \psi^\ell + [r^\ell \ d^\ell] y_\ell$, $r^{\ell+1} := r^\ell - QH_{3,2} y_\ell$ and $d^{\ell+1} = \psi^{\ell+1} - \psi^\ell$

4.2 Implementation of the accelerated second degree method

The second degree methods A and B are accelerated using the variational method as follows. Every r iterations of the second degree method A or B, q iterations of the variational method are performed. Algorithm 2 implements the accelerated second degree method B. The accelerated second degree method A is obtained replacing step *4(b)* by

$$T_{22}\psi_2^{l+1} = e_2 - T_{21}(\omega\psi_1^l + (1-\omega)\psi_1^{l-1}) \ .$$

$ASD^*(\omega, r, q)$ and $ASD(\omega, r, q)$ will denote the accelerated second degree method A and B, respectively.

5 Numerical experiments

In this section we present the results of the numerical experiments corresponding to a transient on the bidimensional Seed-Blanket reactor (Figure

Algorithm 2 Accelerated second degree method B, $ASD(\omega, r, q)$.

1. **Choose** ψ_2^0.
2. **Solve** $T_{11}\psi_1^1 = e_1 - T_{12}\psi_2^0$.
3. **Solve** $T_{22}\psi_2^1 = e_2 - T_{21}\psi_1^1$.
4. **For** $\ell = 1, 2, \ldots, r$
   (a) **Solve** $T_{11}\psi_1^{\ell+1} = e_1 - T_{12}(\omega\psi_2^\ell + (1-\omega)\psi_2^{l-1})$.
   (b) **Solve** $T_{22}\psi_2^{\ell+1} = e_2 - T_{21}(\omega\psi_1^{(\ell+1)} + (1-\omega)\psi_1^\ell)$.
   (c) **If** convergence, STOP.
5. **Perform** q iterations of algorithm 1, with $\psi^0 = \psi^{(r+1)}$, $r^0 = E - T\psi^{r+1}$ and $d^0 = \psi^{r+1} - \psi^r$.
6. **To** point 4.

1) where each material region is represented by the numbers 1, 2 and 3, and lenghts are mentioned in cm. It is modelled with two energy groups and one delayed neutron precursor group. Moreover, it presents a quarter core symmetry. The transient consists of decreasing the thermal absorption cross

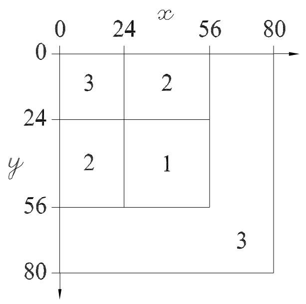

Figure 1: Quadrant of the Seed-Blanket reactor.

section in region 1 as the linear function $\Sigma_{a2}(t) = 0.15 - \frac{0.0035}{0.2}t\ ,\ 0 \le t \le 0.2$. The relative power evolution is shown in Figure 2. This benchmark is widely used in the literature and more details on this problem can be obtained from [18], [19] and [20].

The reactor has been discretized using both a nodal collocation method

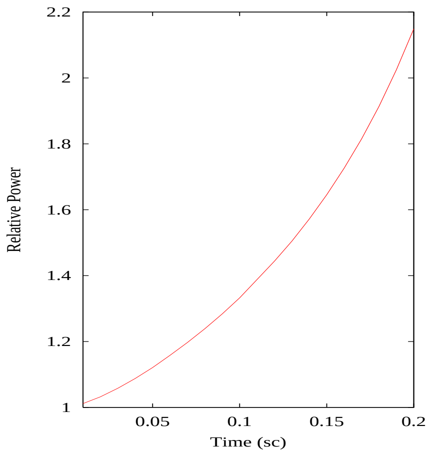

Figure 2: Seed-Blanket transient. Relative power evolution.

Table 1: Matrix size, n, and number of nonzero elements, nnz, of the matrices obtained using the nodal collocation method with 4 polynomials, and the finite differences method.

spatial discretization	n	nnz
Nodal(4)	2000	31920
Finite Differences	50562	302100

using 4 polynomials with square nodes 8 cm wide [21], and a five point centered finite differences scheme with uniform grid size $h_x = h_y = 1\ cm$ (see [13]). Although using a uniform grid size of 3 cm in the finite differences scheme sufices to get a precision comparable to the nodal collocation method for this benchmark, we employed this smaller grid size to check if the results presented still hold for larger problems where iterative methods are specially recommended instead of direct ones. The size and number of nonzero elements of the coefficient matrices are shown in Table 1.

As it has been mentioned above, for the time discretization we have used a one step BDF method. The integration time step was fixed to 1.25 milliseconds needing a total number of 160 time steps to simulate all the transient. At each time step, the solution from the previous one was used as initial solution for solving (9). An approximate solution was considered satisfactory when the initial residual was reduced at least five orders of magnitude. The codes were written in FORTRAN 77 and tested on a single node PA-RISC

Table 2: CPU simulation time for the second degree methods A and B with different values of ω . † indicates that convergence was not attained. Spatial discretization: nodal collocation method.

time (sc)		
ω	method B	method A
0	†	†
0.5	†	†
1	53.93	91.96
1.2	53.78	91.50
1.4	53.60	90.70
1.5	53.24	90.87
1.6	53.45	92.32
1.8	53.96	93.05
2	†	†

Table 3: CPU simulation time for the second degree methods A and B with different values of ω . † indicates that convergence was not attained. Spatial discretization: finite differences method.

time (sc)		
ω	method B	method A
0	†	†
0.5	†	†
1	2200	4217
1.2	2180	4260
1.4	2220	4105
1.5	2100	4217
1.6	2110	4150
1.8	2111	4100
2	†	†

$8000/180MHz$ of a HP Exemplar S Class shared memory multicomputer.

With the numerical experiments we study the following aspects. First, which is the best value of the extrapolation parameter ω, and which of the second degree method, A or B, performs better. Second, we measure the performance improvement when the second degree methods are accelerated with the variational technique presented. And finally, the accelerated second degree methods are compared with standard Krylov subspace methods for nonsymmetric matrices, as BiCGSTAB, GMRES(k) and TFQMR. The use of iterative Krylov methods to solve the non-symmetric linear systems of equations derived from the time dependent neutron diffusion equation is not new in the literature. A comparison between different Krylov methods for the same benchmark problem considered in this paper can be found, for instance, in [20].

In Tables 2 and 3, it is shown that for a value of ω about 1.5 the second degree methods A and B performed the best. In any case, for ω ranging from 1 to 1.8 the performance does not degrade significantly. Thus, determining the exact value for this parameter is not very important. We also note that for values of ω less than 1, the method peformed poorly. Theorem 3 may explain this behavior, although it gives the optimal extrapolation factor for real and positive eigenvalues, which are conditions not warranted for the tested problem. From equation (23) it follows that the optimal factor lies into the range $]1, 2[$, and that the spectral radius of the iteration matrix its a decreasing function of ω on this interval. This behavior is also observed for other stationary methods as the SOR method [11].

Comparing both methods A and B, clearly the second degree method B performed the best since it spent approximately half of the time spent by method A. It is worth the while to note that for the solution of the inner iterations, corresponding to the solution of the linear systems with matrices T_{11} and T_{22} in (11) and (13), the conjugate gradient method preconditioned with point Jacobi was used. Table 4 shows the results of applying different preconditioners for the method B. In all the cases the maximum number of inner iterations was set to 20. Although this scheme could be also thought as a nested iterative method, given that the integration time step is small, the number of inner iterations used is large enough to consider that the systems associated with blocks T_{11} and T_{22} are solved exactly for the tested problems. Furthermore, to obtain an accurate solution for the inner systems is essential for a good performance of the proposed second degree methods.

To accelerate the second degree methods we found experimentally that combining five iterations of the second degree method with one of the variational technique was nearly optimal. Table 5 shows the results for the

Table 4: CPU simulation time for the second degree method B with different choices of the preconditioner for solving the inner iterations. Extrapolation factor $\omega = 1.5$. For ILUT the level of fill-in and threshold are indicated. Spatial discretization: nodal collocation method.

preconditioner	time (sc)
No preconditioning	57.81
Jacobi	53.24
SSOR	110.53
ILU0	76.27
ILUT(5.10^{-2})	108.6
ILUT(5.1)	60.13

Table 5: CPU simulation time for the accelerated second degree method B ($ASD(1.5, r, q)$) with different values of the parameters r and q. Spatial discretization: nodal collocation method.

r	q	time (sc)
1	1	35.85
2	1	34.82
2	2	43.01
3	1	30.50
3	2	43.14
3	3	32.51
4	1	30.93
4	2	44.03
4	3	32.80
4	4	45.18
5	1	29.20

Table 6: Summary: CPU simulation time for the second degree methods A and B, and their accelerated versions $ASD^*(1.5, 5, 1)$ and $ASD(1.5, 5, 1)$, with the nodal collocation and finite differences matrices.

	$Nodal(4)$	Finite Differences
method A	90.7	4100
method B	53.24	2100
$ASD^*(1.5, 5, 1)$	80.1	3600
$ASD(1.5, 5, 1)$	29.2	1667

Table 7: CPU simulation time and average number of matrix-vector products for the BiCGSTAB, GMRES(20) and TFQMR methods. Spatial discretization: nodal collocation method.

method	preconditioner	matvecs	time (sc)
BiCGSTAB	ILU0	39	43.3
	ILUT(5,1)	37	40.3
	ILUT(5,10^{-2})	37	40.3
GMRES(20)	ILU0	58	56.1
	ILUT(5,1)	78	60.7
	ILUT(5,10^{-2})	75	80.7
TFQMR	ILU0	51	67.3
	ILUT(5,1)	102	66.2
	ILUT(5,10^{-2})	84	81.9

$ASD(1.5, r, q)$ method with different values of r and q when the nodal collocation method was used to discretize the equations. The results for $ASD^*(1.5, r, q)$ were similar and they are not presented.

Table 6 summarizes the results for the second degree methods and their accelerated versions. We observe that the simulation time of the second degree methods was reduced considerably in the accelerated cases. Furthermore, as for the unaccelerated versions, the method $ASD^*(1.5, 5, 1)$ performed worse than $ASD(1.5, 5, 1)$.

To compare $ASD(1.5, 5, 1)$ against the GMRES(k), TFQMR and BiCGSTAB methods, the ILU0 and ILUT preconditioners were used. Codes from SPARSKIT collection were used [22]. A level of fill-in of 5 with drop tolerances 1 and 10^{-2} were considered for ILUT. In order to save computation time these preconditioners were computed only once, at the first time step, without any significant loss of performance. The method GMRES(k) was restarted after 20 iterations.

Table 7 shows the CPU time spent by these methods to simulate all the transient when the nodal collocation method was used. The average number of matrix-vector products needed to solve the linear system (9) at each time step is also indicated. From Tables 6 and 7 it can be observed that $ASD(1.5, 5, 1)$ spent about 30 per cent less time than BiCGSTAB. Comparing with GMRES(k) and TFQMR the improvement is even better since $ASD(1.5, 5, 1)$ spent approximately a half of the time use by these methods to simulate the transient. Furthermore, the unaccelerated version also performed better. On the other hand, among the Krylov methods is

Table 8: CPU simulation time and average number of matrix-vector products for the BiCGSTAB, GMRES(20) and TFQMR methods. Spatial discretization: finite differences method.

method	preconditioner	matvecs	time (sc)
BiCGSTAB	ILU0	87	3427
	ILUT(5,1)	119	3620
	ILUT(5,10^{-2})	31	2040
GMRES(20)	ILU0	99	4200
	ILUT(5,1)	121	4410
	ILUT(5,10^{-2})	35	2976
TFQMR	ILU0	90	4500
	ILUT(5,1)	123	4740
	ILUT(5,10^{-2})	89	3600

the BiCGSTAB which shows the best performance. For GMRES(k) and TFQMR the simulation time was very similar. Concerning the preconditioners, for BiCGSTAB and TFQMR the smallest time was obtained preconditioning with ILUT(5,1), while GMRES(k) performed slightly better with ILU0.

Finally, Table 8 shows the results for the finite differences matrices. For these large matrices similar conclusions to the previous ones can be obtained. As for the nodal collocation matrices, the $ASD(1.5, 5, 1)$ method performed the best compared with BiCGSTAB, GMRES(20) and TFQMR. Among the last methods, again BiCGSTAB presents the best behaviour. Concerning the preconditioner, the best results were obtained with ILUT(5,10^{-2}).

6 Conclusions

We have studied two second degree methods for solving linear systems arising in the discretization of the neutron diffusion equation. They have been referred to as second degree methods A and B. With the aim of improving the convergence rate, as it is observed in practice, the method B is obtained from A using the new fast group solution to compute the thermal group as soon it is available. These methods are based on a extrapolation factor ω. The optimal choice of ω has been investigated and some convergence results of the second degree methods have been presented. To accelerate the convergence of the second degree methods a projection method is proposed. This method extracts approximate solutions from a bidimensional space by minimizing the 2-norm of the residual. The accelerated second degree methods A and B have been referred to as $ASD^*(\omega, r, q)$ and $ASD(\omega, r, q)$, respectively. It means that each r iterations of the second degree method with extrapolation parameter ω, q iterations of the projection method are performed. Experimentally it has been observed that taking the values $\omega = 1.5$, $r = 5$ and $q = 1$ is particularly convenient. To evaluate the performance of these methods, they have been compared with other well known Krylov subspace methods for solving nonsymmetric linear systems. In particular, the BiCGSTAB, restarted GMRES and TFQMR have been tested. From the experimental results we conclude the following. The second degree B method performs better than the method A. Accelerating with the projection method results on a considerably reduction on the simulation time. And finally, for the benchmark considered, $ASD(1.5, 5, 1)$ spent the smallest time compared with the BiCGSTAB, GMRES(k) and TFQMR methods.

References

[1] W. M. Stacey, Jr. *Space–Time Nuclear Reactor Kinetics*. Academic Press, New York, 1969.

[2] G. Verdú, D. Ginestar, V. Vidal, and J.L. Muñoz-Cobo. A consistent multidimensional nodal method for transient calculations. *Annals of Nuclear Energy*, 22(6):395–410, 1995.

[3] D. Ginestar, G. Verdú, V. Vidal, R. Bru, J. Marín, and J.L. Muñoz-Cobo. High order backward discretization of the neutron diffusion equation. *Annals of Nuclear Energy*, 25(1–3):47–64, 1998.

[4] V. G. Zimin and H.Ninokata. Acceleration of the outer iterations of the space–dependent neutron kinetics equations solution. *Annals of Nuclear Energy*, 23(17):1407–1424, 1996.

[5] A. Hébert. Application of the Hermite method for finite element reactor calculations. *Nuclear Science and Engineering*, 91:34–58, 1985.

[6] S. Grainville. *The Numerical Solution of Ordinary and Partial Differential Equations*. Academic Press, New York and London, 1988.

[7] D. Ginestar, J. Marín, and G. Verdú. Multilevel methods to solve the neutron diffusion equation. *Applied Mathematical Modelling*, 25:463–477, 2001.

[8] Y. Saad and M. H. Schultz. GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM J. Sci. Statis. Comput.*, 7:856–869, 1986.

[9] H. A. van der Vorst. Bi-CGSTAB: A fast and smoothly converging variant of Bi-CG for the solution of non-symmetric linea systems. *SIAM Journal on Scientific and Statistical Computing*, 12(6):631–644, 1992.

[10] R. W. Freund. A transpose-free quasi-minimal residual algorithm for non-hermitian linear systems. *SIAM J. Sci. Comput.*, 14:470–482, 1993.

[11] R. S. Varga. *Matrix Iterative Analysis*. Prentice–Hall, Englewood Cliffs, NJ, 1962.

[12] D. M. Young. *Iterative Solution of Linear Systems*. Academic Press, New York and London, 1971.

[13] Y. Saad. *Iterative Methods for Sparse Linear Systems*. PWS Publishing Company, Boston, 1996.

[14] J. M. Ortega. *Numerical Analysis, A Second Course*. Academic Press, New York, 1972. Reprinted by SIAM, Philadelphia, 1990.

[15] J. Marín. *Métodos numéricos para la resolución de la ecuación de la difusión neutrónica dependiente del tiempo*. PhD thesis, Departamento de Matemática Aplicada, Universidad Politécnica de Valencia, 2000.

[16] N. M. Missirlis and D. J. Evans. On the convergence of some generalized preconditioned iterative methods. *SIAM Journal on Numerical Analysis*, 18(4):591–596, 1979.

[17] R. A. Horn and C. R. Johnson. *Matrix Analysis*. Cambridge University Press, London, UK, 1985.

[18] J-W. Song and J-K. Kim. An efficient nodal method for transient calculations in light water reactors. *Nuclear Technology*, 103:157–167, 1993.

[19] S. Langenbuch, W. Maurer, and W. Werner. Coarse-mesh flux-expansion method for the analysis of space-time effects in large light water reactor cores. *Nuclear Science and Engineering*, 63:437–456, 1977.

[20] G. S. Chen, J. M Christenson, and D. Y. Yang. Application of the preconditioned transpose-free quasi-minimal residual method for two-group reactor kinetics. *Annals of Nuclear Energy*, 24(5):339–35, 1996.

[21] A. Hébert. Development of the nodal collocation method for solving the neutron diffusion equation. *Annals of Nuclear Energy*, 14(10):527–541, 1987.

[22] Y. Saad. SPARSKIT: A basic tool kit for sparse matrix computations. Technical Report 90–20, Research Institute for Advanced Computer Science, NASA Ames Research Center, Moffet Field, CA, 1990.