Modified Block Newton Method for the Lambda Modes Problem

S. González-Pintor[a], D. Ginestar[b], G. Verdú[a,*]

[a]*Departamento de Ingeniería Química y Nuclear, Universidad Politécnica de Valencia. Camino de Vera, 14. 46022 Valencia. Spain.*
[b]*Instituto de Matemática Multidisciplinar, Universidad Politécnica de Valencia. Camino de Vera, 14. 46022 Valencia. Spain.*

Abstract

To study the behaviour of nuclear power reactors it is necessary to solve the time dependent neutron diffusion equation using either a rectangular mesh for PWR and BWR reactors or a hexagonal mesh for VVER reactors. This problem can be solved by means of a modal method, which uses a set of dominant modes to expand the neutron flux. For the transient calculations using the modal method with a moderate number of modes, these modes must be updated each time step to maintain the accuracy of the solution. The updating modes process is also interesting to study perturbed configuration of the reactor. A Modified Block Newton method is studied to update the modes. The performance of the Newton method has been tested for a steady state perturbation analysis of two 2D hexagonal reactors, a perturbed configuration of the IAEA 3D reactor and two configurations associated with a boron dilution transient in a BWR reactor.

Keywords: Lambda Modes Problem, Block Newton Mehtod, Subspace Tracking Problem, Boron Injection.

1. Introduction

To improve the safety of nuclear power reactors it is necessary to develop fast and accurate plant simulators. In the BWR and PWR the fuel elements

*Corresponding author.
Email addresses: segonpin@isirym.upv.es (S. González-Pintor), dginesta@mat.upv.es (D. Ginestar), gverdu@iqn.upv.es (G. Verdú)

are square prisms and in the VVER reactors the fuel elements are hexagonal prisms. For this reason, it is interesting to develop efficient methods for both rectangular and hexagonal meshes.

Under general assumptions, the neutronic population inside a nuclear power reactor can be modelled by the time dependent neutron diffusion equation in the approximation of two energy groups. This model is of the form (Stacey, 2001),

$$\begin{aligned} \left[v^{-1}\right] \frac{\partial \Phi}{\partial t} + \mathcal{L}\Phi &= (1-\beta)\mathcal{M}\Phi + \sum_{k=1}^{K} \lambda_k \chi \mathcal{C}_k \ , \\ \frac{\partial \mathcal{C}_k}{\partial t} &= \beta_k [\nu\Sigma_{f1} \ \nu\Sigma_{f2}]\Phi - \lambda_k \mathcal{C}_k \ , \ k = 1, \ldots, K \ , \end{aligned} \tag{1}$$

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

$$\mathcal{L} = \begin{bmatrix} -\vec{\nabla}\cdot(D_1\vec{\nabla}) + \Sigma_{a1} + \Sigma_{12} & 0 \\ -\Sigma_{12} & -\vec{\nabla}\cdot(D_2\vec{\nabla}) + \Sigma_{a2} \end{bmatrix} \ ,$$

$$[v^{-1}] = \begin{bmatrix} \frac{1}{v_1} & 0 \\ 0 & \frac{1}{v_2} \end{bmatrix} \ ,$$

and

$$\mathcal{M} = \begin{bmatrix} \nu\Sigma_{f1} & \nu\Sigma_{f2} \\ 0 & 0 \end{bmatrix} \ , \quad \Phi = \begin{bmatrix} \Phi_1 \\ \Phi_2 \end{bmatrix} \ , \quad \chi = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \ .$$

The diffusion constants and cross-sections, D_g, Σ_{12}, Σ_{ag}, $\nu\Sigma_{fg}$, $g = 1, 2$, appearing in these equations depend on the reactor materials, that is, they are position and time dependent functions.

Associated with this problem, there is the following generalised eigenvalue problem,

$$\mathcal{L}\Phi_i = \frac{1}{k_i}\mathcal{M}\Phi_i \ . \tag{2}$$

This problem is known as the Lambda modes problem for a given configuration of the reactor core. The fundamental eigenvalue (the largest one) is called the effective multiplication constant, k-effective, of the reactor core, and this eigenvalue and its corresponding eigenfunction describe the steady state neutron distribution in the core. In this way, the calculation of the stationary neutron flux distribution is the first calculation for any transient analysis.

To solve both problems (1) and (2), a spatial discretization of the equations has to be selected. Once this discretization has been selected, the semidiscrete version of the time dependent neutron diffusion equation is solved. Since the ordinary differential equations resulting from the discretization of diffusion equations are, in general, stiff, implicit methods are necessary. With the aim of reducing the computational cost of implicit methods, we have used a modal method based on expanding the neutron flux in terms of the dominant Lambda modes of the reactor core (Miró et al., 2002).

Starting from a steady state configuration of a nuclear power reactor some situations arise in which the reactor configuration is perturbed. To compute several eigenvalues and their corresponding eigenfunctions for the new configuration of the reactor is quite expensive from the computational point of view. Krylov subspace methods are efficient methods to compute the dominant Lambda modes associated with a given configuration of the reactor, but when the Lambda modes have to be computed from previous perturbed configurations of the reactor other kind of methods that use the information provided by the computed modes in previous steps can be more convenient. In this line, we have studied a Modified Block Newton Method (MBNM) to speed-up the calculations in the updating modes process.

The rest of the paper is organised as follows: In section 2, the spatial discretization used for the Lambda modes problem is briefly exposed. In section 3, to motivate the necessity of efficient method to update the Lambda modes, the modal method for the time discretization of the equations is reviewed. In section 4, the Modified Block Newton algorithm is developed. Section 5, is devoted to test the performance of the MBNM algorithm updating the modes for perturbed configurations of different reactors with hexagonal and rectangular geometries. Finally, the conclusions are summarised in section 6.

2. Spatial discretization

The spatial mesh used to discretize a reactor core is naturally defined by the different compositions of the materials present in the core. Thus, we use a coarse mesh adapted to the fuel bundles composing the core and different strategies are used for the spatial discretization of the equations depending on the core geometry.

2.1. PWR and BWR reactors

In PWR and BWR reactors the fuel assemblies are rectangular prisms. Thus, a rectangular mesh is suitable to describe these prisms. Each one of these prisms is divided into different nodes, and each node, e, is mapped onto a reference domain by means of a change of variables from the real space (x, y, z) to the variables of the reference domain (x', y', z'). Then the neutron flux into each node e is expanded in terms of the ortonormal Legendre polynomials as follows (Verdú et al., 1994),

$$\Phi_e(x', y', z') = \sum_{i=0}^{K} \sum_{j=0}^{K} \sum_{k=0}^{K} \psi_{e,ijk} P_i(x') P_j(y') P_k(z') \ . \tag{3}$$

Continuity over the inner interfaces of the elements for the neutron flux, continuity for the neutron current over the normal directions of these interfaces and, boundary conditions over the external boundary of the reactor are ensured by means of imposing them explicitly, and then, some algebraic manipulations are used to introduce these conditions into weighted equations for each face of the nodes obtaining a set of algebraic equations that constitute the approximation known as the Nodal Collocation method for the Lambda modes problem (Verdú et al., 1994).

2.2. VVER Reactors

The fuel assemblies in VVER reactors are hexagonal prisms. Thus, different strategies from the ones used for rectangular reactors have to be considered. We will study bidimensional reactors discretized using a hexagonal grid ana high order finite element method (Gonzalez-Pintor et al., 2009) that uses a fixed mesh and increases its accuracy by increasing the order of the polynomials expansions. The first step to perform the discretization is to divide each hexagon corresponding to the fuel bundles into six equilateral triangles, denoted by Ω_e. To show the process followed we will consider the neutron diffusion equation in the monoenergetic approximation. This equation without loss of generality can be written as

$$-\vec{\nabla} D(x, y) \cdot \vec{\nabla} \Phi(x, y) + \Sigma_a(x, y) \Phi(x, y) = S(x, y) \ . \tag{4}$$

The boundary conditions considered are albedo boundary conditions

$$D(x, y) \vec{n}(x, y) \cdot \vec{\nabla} \Phi(x, y) + \frac{1}{2} \frac{1 - \beta}{1 + \beta} \Phi(x, y) = 0 \ , \quad (x, y) \in \partial\Omega_\beta \ . \tag{5}$$

The neutron diffusion equation (4) is a stationary condition (Hébert, 2008) for the functional

$$\begin{aligned}\mathcal{F}(\Phi) &= \frac{1}{2}\iint_{\Omega} D(x,y)\vec{\nabla}\Phi(x,y)\cdot\vec{\nabla}\Phi(x,y)dxdy \\ &+ \frac{1}{2}\iint_{\Omega}\Sigma_a(x,y)\Phi^2(x,y)dxdy \\ &- \iint_{\Omega} S(x,y)\Phi(x,y)dxdy \\ &+ \int_{\partial\Omega_\beta}\frac{1}{4}\frac{1-\beta}{1+\beta}\Phi^2(x,y)dl \ , \end{aligned} \tag{6}$$

where $\Phi(x,y)$ is defined in the Sobolev space

$$\mathcal{H}_{\partial\Omega_0}(\Omega) = \left\{h : h \in L^2(\Omega) \ , \ h(x,y) = 0 \ \forall (x,y) \in \partial\Omega_0 \wedge \vec{\nabla}h \in \left[L^2(\Omega)\right]^2\right\} \ . \tag{7}$$

To develop the method, we use a change of variables transforming each one of the triangles, Ω_e, of the mesh into the *Reference domain*, Ω_{REF}, also known in the literature as *the Right Triangle*, which is defined as

$$\Omega_{REF} = \{(x,y)/x \geq 0, y \geq 0, 0 \leq x+y \leq 1\} \ . \tag{8}$$

Denoting by Φ_e the restriction on the neutron flux, Φ, to the element Ω_e of the mesh, it is assumed that it can be approximated by a finite expansion of the form

$$\Phi_e(x',y') = \sum_{i,j=0}^{i+j\leq K} \psi_{e,ij} g_{ij}(x',y') \ , \tag{9}$$

where g_{ij} are elements of a polynomial basis in terms of the coordinates (x',y') of the reference domain. The modified Dubiner's polynomials (Karniadakis et al., 2005) are used for the flux expansions. Some coefficients of the expansions are fixed to assure the continuity of the neutron flux. Details of the definition of the polynomials and the selection of the expansions coefficients can be found in (Gonzalez-Pintor et al., 2009).

2.3. Algebraic Problem

After performing the spatial discretization, the problem (1), can be approximated by the following semidiscrete system of equations

$$\begin{aligned} \left[v^{-1}\right]\dot{\psi} + L\psi &= (1-\beta)M\psi + \sum_{k=1}^{K}\lambda_k X C_k \ , \\ X\dot{C}_k &= \beta_k M\psi - \lambda_k X C_k \ , \end{aligned} \tag{10}$$

where matrices L, M and X have the following block structure

$$L = \begin{bmatrix} L_{11} & 0 \\ -L_{21} & L_{22} \end{bmatrix}, \ M = \begin{bmatrix} M_{11} & M_{12} \\ 0 & 0 \end{bmatrix}, \ X = \begin{bmatrix} I \\ 0 \end{bmatrix};$$

and for the Lambda modes problem (2) we have

$$L\psi_l = \frac{1}{k_l} M\psi_l \ . \tag{11}$$

As the matrix L is nonsymmetric, we also consider the adjoint problem

$$L^{\dagger}\psi_l^{\dagger} = \frac{1}{k_l} M^{\dagger}\psi_l^{\dagger} \ , \tag{12}$$

since the eigenvectors solutions of problems (11) and (12) satisfy the following biorthogonality relationship

$$< \psi_m^{\dagger}, M\psi_n > = < \psi_m^{\dagger}, M\psi_m > \delta_{n,m} = N_m \delta_{n,m} \ . \tag{13}$$

3. Modal method

Different methods have been proposed to solve equations (10). One possibility that makes use of the dominant Lambda modes associated with a given configuration of the reactor core is to use a modal method (Miró et al., 2002). This method assumes that $\psi(t)$ can be expressed approximately as

$$\psi(t) = \sum_{l=1}^{M_d} n_l(t)\psi_l \quad , \tag{14}$$

where ψ_l, $l = 1, \ldots, M_d$ are the dominant Lambda modes of a given configuration of the core. A small amount of the dominant Lambda modes and their

corresponding adjoint modes can be efficiently computed using, for example, the implicit restarted Arnoldi method (Verdú et al., 1999). Multiplying equations (10) by $\psi_m^\dagger$, writing

$$L = L_0 + \delta L \quad , \quad M = M_0 + \delta M \quad ,$$

and making use of expansion (14), we obtain the equations

$$\begin{aligned}
&\sum_{l=1}^{M_d} \langle \psi_m^\dagger, [v^{-1}]\psi_l \rangle \frac{d}{dt} n_l + \sum_{l=1}^{M_d} \frac{1}{k_l} \langle \psi_m^\dagger, M_0 \psi_l \rangle n_l \\
&+ \sum_{l=1}^{M_d} \langle \psi_m^\dagger, \delta L \psi_l \rangle n_l = (1-\beta) \sum_{l=1}^{M_d} \langle \psi_m^\dagger, M_0 \psi_l \rangle n_l \\
&+ (1-\beta) \sum_{l=1}^{M_d} \langle \psi_m^\dagger, \delta M \psi_l \rangle n_l + \sum_{k=1}^{K} \lambda_k \langle \psi_m^\dagger, X C_k \rangle \ , \\
&\frac{d}{dt} \langle \psi_m^\dagger, X C_k \rangle = \beta_k \sum_{l=1}^{M_d} \langle \psi_m^\dagger, M_0 \psi_l \rangle n_l \\
&+ \beta_k \sum_{l=1}^{M_d} \langle \psi_m^\dagger, \delta M \psi_l \rangle n_l - \lambda_k \langle \psi_m^\dagger, X C_k \rangle \ . \qquad (15)
\end{aligned}$$

Using the biorthogonality relationship (13), introducing the notation,

$$\begin{aligned}
\Lambda_{ml} &= \left\langle \psi_m^\dagger, [v^{-1}]\psi_l \right\rangle \ , & A^L_{ml} &= \left\langle \psi_m^\dagger, \delta L \psi_l \right\rangle \ , \\
A^M_{ml} &= \left\langle \psi_m^\dagger, \delta M \psi_l \right\rangle \ , & C_{mk} &= \left\langle \psi_m^\dagger, X C_k \right\rangle ,
\end{aligned}$$

and the mode m reactivity, defined as $\rho_m = (k_m - 1)/k_m$, equations (15) can be expressed as the following matrix equations (see reference (Miró et al., 2002) for full details)

$$\begin{aligned}
\frac{d[n]}{dt} &= [\Lambda]^{-1} \big([\rho - \beta I][N][n] + (1-\beta)[A^M][n] \\
&\quad - [\Lambda]^{-1}[A^L][n] + \sum_{k=1}^{K} \lambda_k [C_k] \big) \ , \\
\frac{d[C_k]}{dt} &= \beta_k [N][n] + \beta_k [A^M][n] - \lambda_k [C_k] \ , \quad k = 1, \ldots \ , K \ . \qquad (16)
\end{aligned}$$

Because of the stiffness of the differential equations (16), to solve this system we have used a high order implicit method (Hindmarsh, 1983).

As initial conditions for the time integration of a transient, we start from a critical configuration of the core. To obtain this critical configuration we solve the Lambda modes problem (11) for a given initial configuration, searching for the fundamental mode. Dividing the fission cross-sections of the initial configuration by the fundamental eigenvalue, k_1, we obtain

$$L_0\psi_1 = M^{Crit}\psi_1 \quad , \tag{17}$$

where M^{Crit} is a matrix whose components are the components of M divided by k_1. Equation (17) together with equation

$$0 = \beta_k M^{Crit}\psi_1 - \lambda_k X C_k \quad , \tag{18}$$

constitute the set of equations defining the steady state associated with the critical configuration.

For realistic transients, the nuclear cross-sections are time dependent functions and to obtain good accuracy using the modal method a large amount of modes are necessary. This is prohibitive from the computational point of view. Thus, instead of this, we use a small number of modes together with an updating modes strategy that is performed at each certain *updating time step* (Miró et al., 2002). In this way, to update the modes it is necessary to develop an efficient strategy that uses the modes computed in the previous steps as starting initial guess to speed-up the computation. A method of this kind is the Block Newton Method, presented in next section. Also, a modes updating methodology is of interest when perturbed configurations of the reactor core are studied.

4. Modified Block Newton Method

With the spatial discretization methods exposed above, the the Lambda modes equation with two groups of energy (2) can be approximated by an algebraic generalised eigenvalue problem with the following block structure

$$\begin{bmatrix} L_{11} & 0 \\ -L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \frac{1}{\lambda} \begin{bmatrix} M_{11} & M_{12} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \ , \tag{19}$$

where ψ_1 is a vector with the unknowns corresponding to the neutron flux for the fast group, and ψ_2 is a vector with the unknowns corresponding to the thermal flux.

To solve this problem, it is reduced to the ordinary eigenvalue problem

$$A\psi_1 = \lambda\psi_1 \ , \tag{20}$$

where the matrix A in equation (20) is defined as

$$A = L_{11}^{-1}\left(M_{11} + M_{12}L_{22}^{-1}L_{21}\right) \ . \tag{21}$$

As it has already mentioned, to update the modes along a transient or for a perturbed configuration of the core it is interesting to take into account that the space spanned by the new modes should be close to the space spanned by the previous ones. For this reason, a Modified Block Newton Method (Lösche, 1998), which has a high order of local convergence, is applied to update the modes using as initial guess the modes obtained in a previous step. In the following, we expose the main ideas of this method.

Given a partial eigenvalue problem of the form

$$AV = V\Lambda \ , \tag{22}$$

where $V \in \mathbb{R}^{n\times q}$ is the matrix of eigenvectors and $\Lambda \in \mathbb{R}^{q\times q}$ is a diagonal matrix whose elements are the dominant eigenvalues. It is assumed that the eigenvectors can be factorized as

$$V = ZS \ , \tag{23}$$

where $Z^{\mathrm{T}}Z = I_q$. Problem (22) can be rewritten as

$$AV = V\Lambda \Rightarrow AZS = ZS\Lambda \Rightarrow AZ = ZS\Lambda S^{-1} \Rightarrow AZ = ZK \ , \tag{24}$$

where matrix K is not necesarily a diagonal matrix. This system is undetermined (Lösche, 1998). To determine the problem we introduce the biorthogonality condition $W^{\mathrm{T}}Z = I_q$, where W is a fixed matrix of rank q. Then the Newton method is used to solve the problem

$$F_W(Z,K) := \left[\begin{array}{c} AZ - ZK \\ W^{\mathrm{T}}Z - I_q \end{array}\right] = \left[\begin{array}{c} 0 \\ 0 \end{array}\right] \ . \tag{25}$$

From Newton's method the new iterated solution arises

$$Z^{(k+1)} = Z^{(k)} - \Delta Z^{(k)} \ , \quad K^{(k+1)} = K^{(k)} - \Delta K^{(k)} \ , \tag{26}$$

where $\Delta Z^{(k)}$ and $\Delta K^{(k)}$ are solutions of the system

$$\begin{aligned} A\Delta Z^{(k)} - \Delta Z^{(k)} K^{(k)} - Z^{(k)} \Delta K^{(k)} &= AZ^{(k)} - Z^{(k)} K^{(k)} \ , \\ W^{\mathrm{T}} \Delta Z^{(k)} &= W^{\mathrm{T}} Z^{(k)} - I_q \ . \end{aligned} \tag{27}$$

The system (27) is coupled because of the off-diagonal elements of $K^{(k)}$.

To avoid this difficulty the Modified Block Newton Method (see Algorithm (3)) applies two previous steps to decouple system (27). The first step consists of an orthogonalisation to the $Z^{(k)}$ matrix (see Algorithm (1)). Once $Z^{(k)}$ is an orthonormal matrix, i.e., ${Z^{(k)}}^{\mathrm{T}} Z^{(k)} = I_q$, as a second step, a

Algorithm 1 Modified Gram-Schmidt Orthogonalisation (Orth)

Require: A set of p independent vectors $v_1, \ldots, v_p$

1: **for** $i = 1$ to k **do**
2: **for** $j = 1$ to $i - 1$ **do**
3: $v_i \leftarrow v_i - \langle v_j, v_i \rangle$
4: **end for**
5: $v_i \leftarrow v_i / \left\| v_i \right\|_2$
6: **end for**

Rayleigh-Ritz procedure is applied, which consists of obtaining the eigenvectors $U^{(k)}$ and their corresponding eigenvalues $R^{(k)}$, of $B^{(k)} = {Z^{(k)}}^T A Z^{(k)}$, in such a way that

$$B^{(k)} U^{(k)} = U^{(k)} R^{(k)} \ . \tag{28}$$

Then, taking into account the definition of $B^{(k)}$ and making use of the orthogonality of matrix $Z^{(k)}$ on equation (28), the following equation is obtained

$${Z^{(k)}}^{\mathrm{T}} A Z^{(k)} U^{(k)} = {Z^{(k)}}^{\mathrm{T}} Z^{(k)} U^{(k)} R^{(k)} \ . \tag{29}$$

Renaming $\tilde{Z}^{(k)} := Z^{(k)} U^{(k)}$ and $\Lambda^{(k)} := R^{(k)}$. From equation (29), we have that $\Lambda^{(k)}$ is a diagonal matrix whose elements, $\lambda_i^{(k)}$ are called the Ritz values and $\tilde{Z}^{(k)}$ are the approximated Ritz eigenvectors, that satisfy the equation

$${Z^{(k)}}^{\mathrm{T}} \left(A \tilde{Z}^{(k)} - \tilde{Z}^{(k)} \Lambda^{(k)} \right) = 0 \ . \tag{30}$$

This Rayleigh-Ritz procedure is implemented in Algorithm (2). At each iteration, the matrix W is chosen as the previous approximation for the

invariant subspace, that is $W = Z^{(k)}$, and system (27) is decoupled into the q linear systems

$$\begin{bmatrix} A - I\lambda_i^{(k)} & Z^{(k)} \\ Z^{(k)^{\mathrm{T}}} & 0 \end{bmatrix} \begin{bmatrix} \Delta z_i^{(k)} \\ -\Delta\lambda_i^{(k)} \end{bmatrix} = \begin{bmatrix} AZ^{(k)} - Z^{(k)}\Lambda^{(k)} \\ 0 \end{bmatrix} \mathbf{e}^i \ , \quad i = 1, \ldots, q \ . \tag{31}$$

where $\mathbf{e}^i$ denotes the i-th coordinate vector, and $\Delta z_i^{(k)}$ is the i-th column of $\Delta Z^{(k)}$.

Algorithm 2 Rayleigh-Ritz procedure (rr)

Require: Initial approximation Z for the desired invariant subspace of A

1: $B \leftarrow Z^T AZ$
2: Calculate $[U, R]$ such that $BU = UR$ for the small matrix B
3: $V \leftarrow ZU$ {Approximated Ritz eigenvectors}
4: $\Lambda \leftarrow R$ {Ritz Values}

The Modified Block Newton Method can be summarized as in Algorithm (3).

Algorithm 3 Modified Block Newton Method (MBNM)

Require: Initial approximation $\tilde{V}^{(0)}$ of the eigenmodes

1: $[Z^{(0)}] \leftarrow \mathtt{orth}(\tilde{V}^{(0)})$
2: $[V^{(0)}, \Lambda^{(0)}] \leftarrow \mathtt{rr}(Z^{(0)}, A)$
3: **while** $V^{(k)}$ does not satisfy a termination criterion **do**
4: $\quad \Delta V^{(k)} = [\Delta v_1^{(k)}, \cdots, \Delta v_p^{(k)}]$ {Correction determined with the Newton iteration of equation (31)}
5: $\quad \tilde{V}^{(k)} \leftarrow V^{(k)} - \Delta V^{(k)}$
6: $\quad Z^k \leftarrow \mathtt{orth}(\tilde{V}^{(k)})$
7: $\quad [V^{(k)}, \Lambda^{(k)}] \leftarrow \mathtt{rr}(Z^{(k)}, A)$
8: $\quad k \leftarrow k + 1$
9: **end while**

5. Numerical Results

The behaviour of the Block Newton method presented above for updating the dominant Lambda modes of a nuclear reactor core is tested with

four different problems, two of them with hexagonal geometry for the fuel assemblies, and the other two with rectangular geometry.

Starting from a steady state configuration of a nuclear power reactor some situations arise in which the reactor configuration is perturbed. Different events justify the study of these perturbations: poisoning by Xenon, insertion of control rods, subcooling of the entry, study of Doppler effect of a nuclear core by means of a uniform perturbation of the core, etc. To test the behaviour of the Modified Block Newton method different perturbations have been defined for different reactors. First, a bidimensional VVER 1000 reactor (Chao and Shatilla, 1995) will be perturbed increasing the second group absortion cross section Σ_{a2} of seven control rods equally distributed over the reactor. This is a symmetric perturbation, where the shape of the modes after the perturbation is close to the one of the initial state, athough the corresponding eigenvalues are quite different.

Similarly, the second problem is a perturbation for a VVER 440 reactor core which is based on a collapsed three dimensional benchmark for a transient in the reactor (Keresztúri, 1992). In this transient the peak of the power distribution performs a large increase in a non-symmetric form and the dominant eigenmodes change their shape along the transient.

The first problem with rectangular geometry considered is a perturbed configuration of the well known three dimensional IAEA reactor (Argone National Laboratory , 1977), which is a PWR reactor. The perturbation is performed by means of the extrusion of a set of control rods and the insertion of another set symmetricaly.

The last example considered corresponds to the compuation of the dominant eigenmodes of two configurations of a three dimensional BWR reactor in a boron ijection transient. This problem shows a strong perturbation for the shape of the dominand modes to be updated, and it is proposed to check the behaviour of Newton method for updating the modes in strong perturbations.

5.1. VVER-1000 problem

The VVER-1000 problem (Chao and Shatilla, 1995) with the geometry shown in Figure 1 is considered. The core has a 1/6 cyclic symmetry, and the assembly pitch is of 23.60 cm. The reflector is not explicitly modelled, but it is assumed to be represented by means of albedos at the boundary of the core.

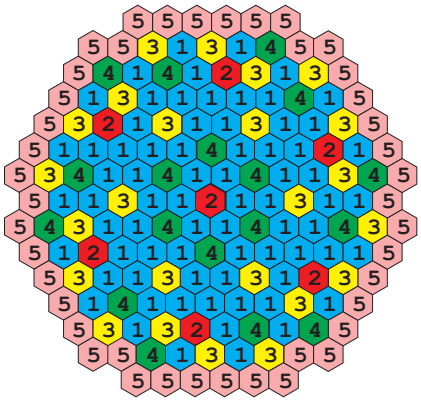


Figure 1: Geometry of the VVER-1000 reactor.

This original configuration will be perturbed increasing the second group absortion macroscopic cross section Σ_{a2} (see Table 1) of material 2 from 0.0810328 to 0.2010328, simulating a perturbation due to the insertion of control rod banks at these positions.

Table 1: Cross sections of the VVER-1000 problem

Mat.	g	D_g	$\Sigma_{a,g}$	$\Sigma_{g,g+1}$	$\nu\Sigma_{f,g}$
1	1	1.38320	0.0083859	0.0164977	0.00481619
	2	0.386277	0.0673049		0.0846154
2	1	1.38299	0.0115490	0.0147315	0.00466953
	2	0.389403	0.0810328		0.0852264
3	1	1.39522	0.0089441	0.0156219	0.00604889
	2	0.386225	0.0844801		0.1194280
4	1	1.39446	0.0119932	0.0140185	0.00591507
	2	0.387723	0.0989670		0.1204970
5	1	1.39506	0.0091160	0.0154981	0.00640256
	2	0.384492	0.0893878		0.1292810

The results for the first seven dominant eigenvalues of the initial configuration, together with the eigenvalues corresponding to the perturbed configuration are shown in Table 2.

Table 2: Eigenvalues of the initial and perturbed configurations of VVER-1000 reactor.

	λ_l	
l	Initial conf.	Perturbed conf.
1	1.006451	0.995906
2	0.994809	0.984379
3	0.994809	0.984379
4	0.973759	0.964955
5	0.973759	0.964955
6	0.955171	0.953445
7	0.948344	0.941234

The shape for the normalised power distribution associated with the fundamental mode and the first subcritical harmonic mode are shown in Figure 2.

The stoping criterion used in the Modified Block Newton method is based on the residual of the calculated eigenvalues and eigenvectors at step k,

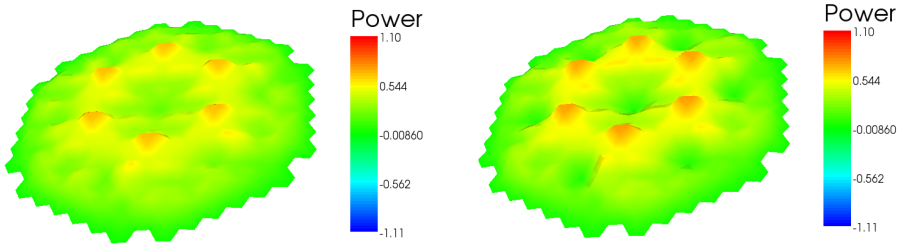
$$Res_k := \left\| AV^k - V^k\Lambda^k \right\|_2 \leq eps \ . \tag{32}$$

The tolerance has been set to $eps = 10^{-6}$. To show the performance of the Newton method along the different steps, in Table 3, we present the value of the residual Res_k for different steps of the Newton Method using eigenvector spaces with different size q, (q is the number of modes). We observe that for this problem three steps of the Modified Block Newton method are enough to achieve the convergence of 7 modes of the perturbed configuration.

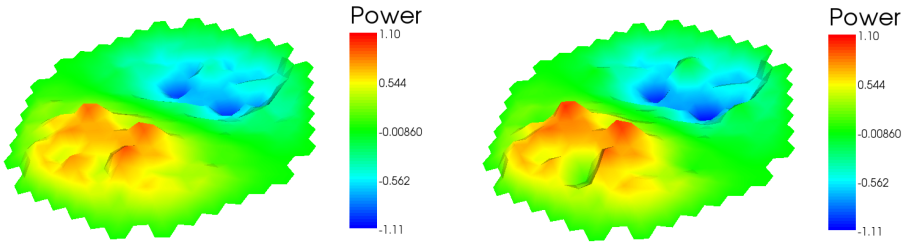
5.2. VVER-440 problem

This problem is based on the 3-dimensional transient benchmark AER-DYN-001 proposed in (Keresztúri, 1992). The nuclear cross section given in the 3D benchmark have been collapsed in a single plane. Materials of the bidimensional reactor have been defined as is shown in Figure 3 and the cross sections of the materials are shown in Table 4.

A perturbed configuration that simulates the movement of two control rods has been defined by means of changing the absorption cross section Σ_{a2} for the material 8 from 0.11887 to 0.016917.



(a) Neutron distribution



(b) First harmonic

Figure 2: Shape of the power distribution associated with the first for two dominant modes of the VVER-1000 problem for the initial configuration (left) and the perturbed one (right).

Table 3: Evolution of the residual in the problem VVER-1000 for different steps of the Newton method and different number of modes.

	Res_k			
q	$k=0$	$k=1$	$k=2$	$k=3$
1	0.043835	0.000628	0.000006	0.000000
2	0.044356	0.000797	0.000005	0.000000
3	0.044396	0.000851	0.000006	0.000000
4	0.044505	0.001341	0.000008	0.000000
5	0.044489	0.001376	0.000008	0.000000
6	0.044494	0.001379	0.000007	0.000000
7	0.047095	0.001305	0.000008	0.000000

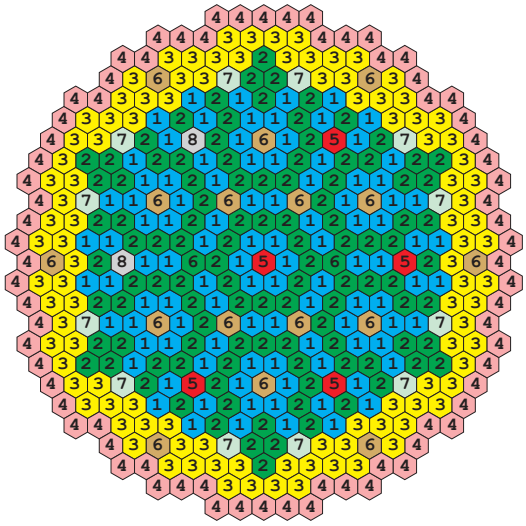


Figure 3: VVER 440 2D

The first 7 dominant Lambda modes of the initial configuration of the reactor have been updated to obtain a set of dominant modes of the perturbed condiguration. The eigenvalues of these modes are shown in Table 5.

The shape for the normalised power distribution associated with the fundamental mode and the first two subcritical modes are shown in Figure 4.

The residual of the calculated eigenvalues and eigenvectors at step k of the Modified Block Newton Method using different numbers of modes, q, is presented at Table 6. We observe that also in this case the modes can be updated with three steps of the Newton method.

5.3. IAEA 3D problem

The IAEA 3-D PWR problem (Argone National Laboratory , 1977) is a standard benchmark problem to measure the performance of neutronic calculation methods. The core is composed by 177 fuel assemblies including 9 fully rodded fuel assemblies and 4 partially rodded fuel assemblies, as it is shown in Figure 5. Radial reflector is modelled by means of 64 assemblies surrounding the core. The fuel assembly pitch is 20cm and the active height of a fuel assembly is 340cm. The thickness of axial reflector is 20cm. Nuclear cross sections for this problem are shown in Table 7.

As it is shown in Figure 5, two configurations are considered for this

Table 4: Cross sections for the 2-D VVER 440 reactor.

Mat.	g	D_g	$\Sigma_{a,g}$	$\Sigma_{g,g+1}$	$\nu\Sigma_{f,g}$
1	1	1.346557	0.008312	0.016976	0.004413
	2	0.370075	0.064282		0.072784
2	1	1.337728	0.008745	0.016000	0.005491
	2	0.367411	0.079145		0.104256
3	1	1.332264	0.009411	0.014974	0.006990
	2	0.363171	0.099536		0.147261
4	1	1.447520	0.000933	0.032215	0.000000
	2	0.251741	0.033037		0.000000
5	1	1.231711	0.012120	0.020782	0.001345
	2	0.240027	0.118846		0.027352
6	1	1.337727	0.008747	0.015996	0.005492
	2	0.367479	0.079153		0.104316
7	1	1.346561	0.008317	0.016968	0.004416
	2	0.370177	0.064282		0.072846
8	1	1.231640	0.012123	0.020785	0.001342
	2	0.239942	0.118870		0.027299

problem, CONF.1 is the initial configuartion and CONF.2 is the perturbed one. In the perturbed configuration the control rods of fully inserted assemblies have been extracted 40cm, and the control rods of partially rodded assemblies are inserted 40cm. Table 8, shows the three dominant eigenvalues obtained for both configurations.

The axial and radial profiles of the normalised power distribution associated with the fundamental mode and the first harmonic mode are shown in Figure 6.

The evolution of the residual of the calculated eigenvalues and eigenvec-

Table 5: Eigenvalues for the initial and perturbed configuartions of reactor VVER 440.

	λ_l	
l	Initial conf.	Perturbed conf.
1	1.005186	1.011159
2	0.998421	1.001079
3	0.998420	1.000791
4	0.984674	0.988257
5	0.984675	0.985502
6	0.967776	0.967903
7	0.964815	0.965150

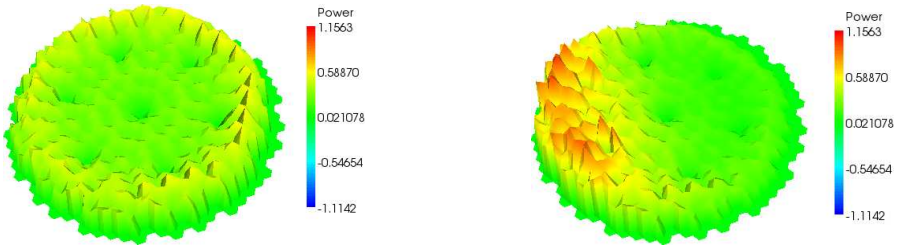
Table 6: Residual evolution for different steps of the Newton method for different number of modes of reactor VVER-440.

	Res_k			
q	$k=0$	$k=1$	$k=2$	$k=3$
1	0.015864	0.002868	0.000292	0.000000
2	0.015866	0.002868	0.000292	0.000000
3	0.023867	0.000599	0.000000	0.000000
4	0.025380	0.000398	0.000000	0.000000
5	0.025380	0.000546	0.000000	0.000000
6	0.025380	0.000546	0.000000	0.000000
7	0.025630	0.000546	0.000000	0.000000

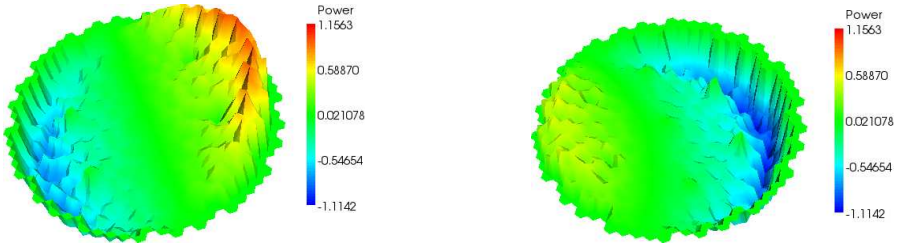
tors at step k of the Modified Block Newton Method using different number of modes q, is presented at Table 9. We can see that only 3 steps of the Newton's method are enough to reach the convergence, as in the previous problems.

5.4. Boron Injection in a BWR

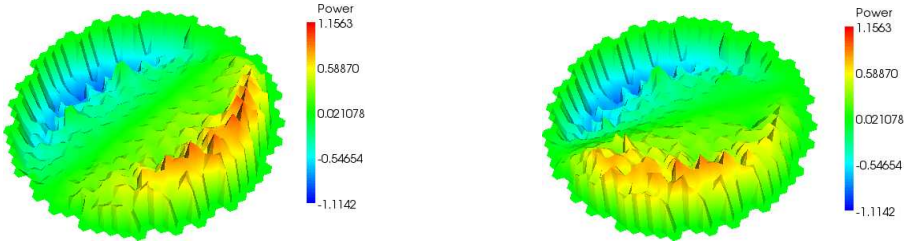
An interesting transient is found in the BWR reactors when the SLCS (standby liquid control system) injects water with a high proportion of boron dissolved (Tinoco, 2010). This system is expected to work when the temperature of suppression pool is enough high after the closure of the MSIV (Main



(a) Neutron distribution



(b) First harmonic



(c) Second harmonic

Figure 4: Shape of the normalised power distribution associated with the first three dominant modes of the initial configuration (left) and perturbed configuration (right) of reactor VVER-440.

Steam Isolation Valve) and with a ATWS (Anticipated Transient Without Scram). In this situation, the reactor can increase its power and an instability event can occur. The Lambda Modes are eigenfunctions, which have been successfully used to describe the instable events in BWRs (Miró et al., 2002).

An initial configuration of a typical BWR reactor is considered and a perturbed configuration is proposed due to the injection of water with a proportion of boron dissolved of 1500 ppm. This consists of a strong perturbation of the reactor core. The first three dominant eigenvalues associated with the reactor before the poisoning are shown in Table 10, together with the three

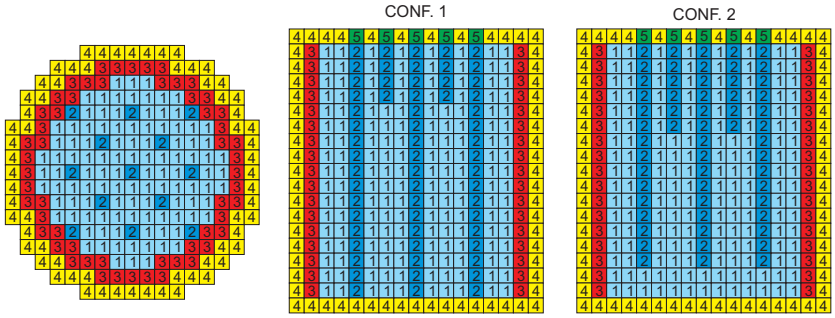


Figure 5: Geometry of the 3D IAEA without reflector problem.

Table 7: Cross sections of 3D IAEA problem.

Mat.	g	D_g	$\Sigma_{a,g}$	$\Sigma_{g,g+1}$	$\nu\Sigma_{f,g}$
1	1	1.500	0.010	0.020	0.000
	2	0.400	0.085		0.135
2	1	1.500	0.010	0.020	0.000
	2	0.400	0.130		0.135
3	1	1.500	0.010	0.020	0.000
	2	0.400	0.080		0.135
4	1	2.000	0.000	0.040	0.000
	2	0.300	0.010		0.000
5	1	2.000	0.000	0.040	0.000
	2	0.300	0.055		0.000

dominant eigenvalues associated with the reactor perturbed by boron.

The profiles of the normalised power distribution associated with the fundamental mode and the first subcritical mode are shown in Figure 7.

The evolution of the residual of the calculated eigenvalues and eigenvectors at different steps of the Block Newton method for different number of modes q, is presented in Table 11. We can see that even with a strong perturbation, as the one induced by Boron in the BWR reactor, a small number

Table 8: First three dominant eigenvalues of 3D IAEA reactor.

	λ_l	
l	Initial conf.	Perturbed conf.
1	1.028857	1.027907
2	1.016490	1.015933
3	1.016490	1.015933

Table 9: Residual for different steps of Newton's method to update the modes of 3D IAEA reactor.

	Res_k			
q	$k=0$	$k=1$	$k=2$	$k=3$
1	0.012160	0.000090	0.000001	0.000000
2	0.012160	0.000119	0.000001	0.000000
3	0.019517	0.000246	0.000002	0.000000

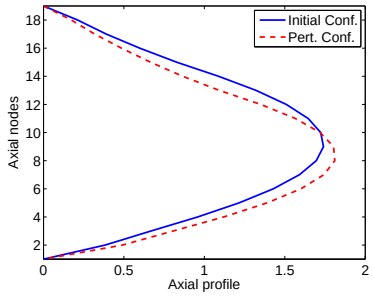
Table 10: Eigenvalues associated with the two configurations of the BWR reactor.

	λ_l	
l	Without Boron	With Boron
1	1.000487	0.937197
2	0.989536	0.919430
3	0.989396	0.919146

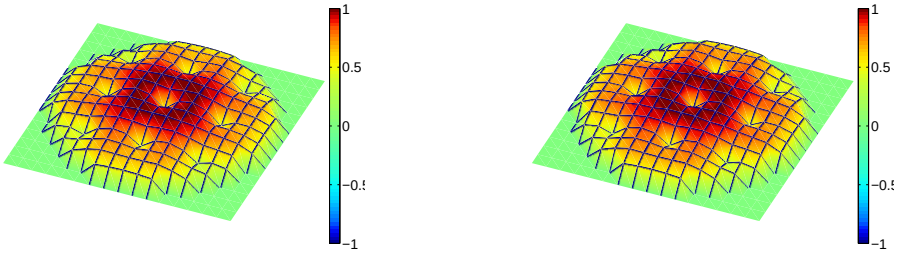
of steps of the Newton method are enough to update the modes.

6. Conclusions

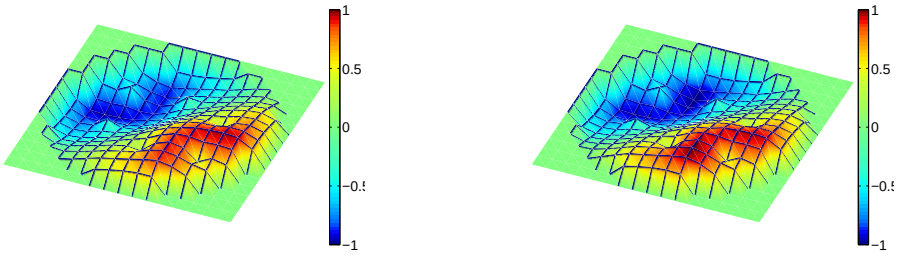
The Lambda Modes of a reactor for a given configuration of the core are used to integrate the time dependent neutron diffusion equation, using modal methods. To compute a large amount of Lambda modes is a prohibitive task from the computational point of view and to obtain accurate results with a small amount of modes a modes updating strategy is needed. Also to



(a) Axial profile for the fundamental mode of the two configurations of the 3D IAEA reactor.



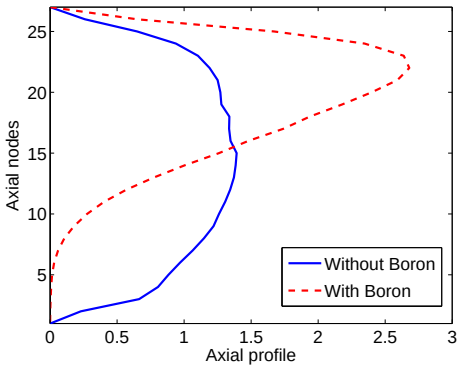
(b) Radial profile of the fundamental mode for the initial configuration (left) and the perturbed configuration (right) of the 3D IAEA reactor.



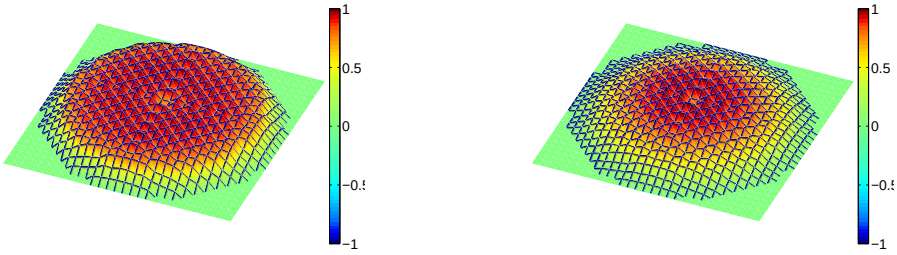
(c) Radial profile for the first subcritical mode of the initial configuration (left) and the perturbed configuration (right) of the 3D IAEA reactor.

Figure 6: Shape of the normalized power distribution of the first two dominant Lambda modes of the initial and the perturbed configuration of 3D IAEA reactor.

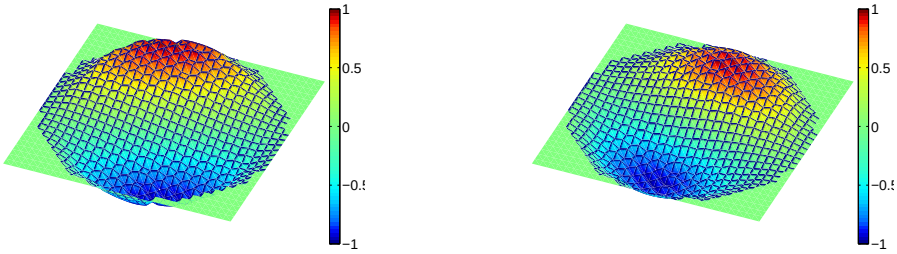
update the modes of a reactor core can be useful in perturbative calculations. Because the calculation of the Lambda modes is an expensive task, efficient



(a) Axial profiles of the fundamental mode for the initial and the perturbed configuration.



(b) Radial profile of the fundamental mode for the initial configuration (left) and the perturbed configuration (right).



(c) Radial profile of the first subcritical mode for the initial configuration (left) and the perturbed configuration (right).

Figure 7: Shape of the normalized power distribution of the first two dominant Lambda modes of the initial and the perturbed configuration of BWR reactor.

Table 11: Residual evolution for different steps of the Newton method to update the modes of the BWR reactor.

	Res_k			
q	$k=0$	$k=1$	$k=2$	$k=3$
1	0.023849	0.015123	0.000627	0.000008
2	0.031375	0.022050	0.003632	0.000098
3	0.031956	0.023237	0.004542	0.000082
	Res_k			
q	$k=4$	$k=5$	$k=6$	$k=7$
1	0.000000	0.000000	0.000000	0.000000
2	0.000040	0.000011	0.000001	0.000000
3	0.000000	0.000000	0.000000	0.000000

methods to update the Lambda modes using the information provided by previous calculations are necessary to improve the improve the utility of modal and perturbative methods.

Once an initial set of Lambda modes has been obtained, the update of these modes we have used a Modified Block Newton Method, which has a local cubic convergence (Lösche, 1998). BY studying different benchmark problems, we have shown that this method is robust to deal with problems that have degenerate or clustered eigenvalues, and it has fast convergence in such a way that the number of steps needed to update the modes is not very dependent on the kind of perturbation considered and the number of modes to be updated. For these reasons it seems to be interesting to take advantage of the convergence properties of this kind of updating methods when perturbed configurations of a reactor core have to be studied.

7. Acknowledgements

This work has been partially supported by the Spanish Ministerio de Educación y Ciencia under projects ENE2008-02669 and MTM2007-64477-AR07, the Generalitat Valenciana under project ACOMP/2009/058, and the Universidad Politécnica de Valencia under project PAID-05-09-4285.

References

Benchmark Problem Book, ANL-7416, Suppl. 2, Argonne National Laboratory (1977)

Y.A. Chao and Y.A. Shatilla, Conformal mapping and hexagonal nodal methods-II: implementation in the ANC-H Code, Nuclear Science and Engineering 121 (1995) 210–225.

S. González-Pintor, D. Ginestar, G. Verdú, High order finite element method for the lambda modes problem on hexagonal geometry, Annals of Nuclear Energy 36 (9) (2009) 1450–1462.

A. Hébert, A Raviart-Thomas-Schneider solution of the diffusion equation in hexagonal geometry, Annals of Nuclear Energy 35 (3) (2008) 363–376.

A. Hindmarsh, ODEPACK, a systematized collection of ode solvers, in: R. e. a. Stepleman (Ed.), Scientific Computing, North-Holland, Amsterdam, Netherlands; New York, U.S.A., 1983, pp. 55–64.

G. E. Karniadakis, S. J. Sherwin, Spectral/hp Element Methods for Computational Fluid Dynamics, Oxford University Press, 2005.

A. Keresztúri, M. Telbisz, A three dimensional hexagonal kinetic benchmark problem, in: Procedings of 2nd AER Symposium, (1992). (`http://aerbench.kfki.hu/`).

R. Lösche, H. Schwetlick, G. Timmermann, A modified block newton iteration for approximating an invariant subspace of a symmetric matrix, Linear Algebra and its Applications 275-276 (1998) 381–400.

R. Miró, D. Ginestar, G. Verdú, D. Hennig, A nodal modal method for the neutron diffusion equation. application to BWR instabilities analysis, Annals of Nuclear Energy 29 (10) (2002) 1171–1194.

W. M. Stacey, Nuclear Reactor Physics, John Wiley & Sons Inc, 2001.

H. Tinoco, P. Buchwald, W. Frid, Numerical simulation of boron injection in a BWR, Nuclear Engineering and Design 240 (2) (2010) 221–234.

G. Verdú, D. Ginestar, V. Vidal, J. Muñoz-Cobo, 3D λ-modes of the neutron-diffusion equation, Annals of Nuclear Energy 21 (7) (1994) 405–421.

G. Verdu, R. Miro, D. Ginestar, V. Vidal, The implicit restarted arnoldi method, an efficient alternative to solve the neutron diffusion equation, Annals of Nuclear Energy 26 (7) (1999) 579–593.