

Different modes associated with the neutron diffusion equation and their computation

A. Carreño*, A. Vidal-Ferrández*, D. Ginestar†, G. Verdú*, M.T. Capilla*

*Instituto de Seguridad Industrial, Radiofísica y Medioambiental,
Universitat Politècnica de València, Camino de Vera, s/n, 46022, Valencia

†Instituto Universitario de Matemática Multidisciplinar,
Universitat Politècnica de València, Camino de Vera, s/n, 46022, Valencia
amcarsan@iqn.upv.es, anvifer2@upv.es, dginesta@mat.upv.es, gverdu@iqn.upv.es, tcapilla@mat.upv.es

Abstract - The λ , γ and α -modes can be defined in neutron diffusion equation to study the characteristics of nuclear reactor. A high order finite element method is used for the discretization of the differential eigenvalue problems. The aim of this work is to study the differences between the modes and analyze two methods to compute the resulting algebraic eigenvalue problem after the spatial discretization. Krylov-Schur method is used to solve these kind of problems. As an alternative to speed-up the calculations for γ and α -modes, a strategy based on the modified block Newton method is proposed. To present numerical results and compare the eigenvalue solvers, a homogeneous reactor and the NEACRP reactor are studied.

I. INTRODUCTION

The time-dependent transport equation can be transformed into several eigenvalue equations forcing the criticality to obtain steady-state equations [1, 2]. If fission terms are modified to have a critical configuration, the λ -modes problem is obtained. If instead of this, the fission and scattering terms are divided by $\gamma > 0$, the resulting eigenvalue problem is known as the γ -modes problem. Finally, if it is assumed an exponential time behavior for the neutron flux, i.e. $\varphi(\mathbf{r}, E, \Omega, t) = e^{\alpha t} \varphi(\mathbf{r}, E, \Omega)$, the α -modes problem is obtained [3]. The dominant λ -modes have been frequently used to study the kinetics in the reactor core with modal methods and to study BWR reactor instabilities [4]. The α -modes have been used to develop monitoring techniques for subcritical systems [5]. There are not many studies on the γ -modes, but, these last modes are interesting because they have the advantage that they are not limited to systems on which fission is included and they are a good option to analyze critical systems, since the γ spectrum will be closest to the critical one [1].

However, due to the complexity of transport equation, the multigroup neutron diffusion equation is used as an approximation. The above modes problems are considered for this approximation. In this work, the energy is divided into two groups: fast and thermal. So, the diffusion equations for λ , γ and α -modes are, respectively,

$$\begin{pmatrix} -\nabla(D_1 \nabla) + \Sigma_{a_1} + \Sigma_{12} & 0 \\ -\Sigma_{12} & -\nabla(D_2 \nabla) + \Sigma_{a_2} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \frac{1}{\lambda} \begin{pmatrix} \nu \Sigma_{f1} & \nu \Sigma_{f2} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad (1)$$

$$\begin{pmatrix} -\nabla(D_1 \nabla) + \Sigma_{a_1} + \Sigma_{12} & 0 \\ 0 & -\nabla(D_2 \nabla) + \Sigma_{a_2} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \frac{1}{\gamma} \begin{pmatrix} \nu \Sigma_{f1} & \nu \Sigma_{f2} \\ \Sigma_{12} & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad (2)$$

$$\begin{pmatrix} \left(\begin{matrix} \nu_1 \nabla(D_1 \nabla) - \nu_1(\Sigma_{a_1} + \Sigma_{12}) & 0 \\ \nu_2 \Sigma_{12} & \nu_2 \nabla(D_2 \nabla) - \nu_2 \Sigma_{a_2} \end{matrix} \right) \\ + (1 - \beta) \begin{pmatrix} \nu_1 \nu \Sigma_{f1} & \nu_1 \nu \Sigma_{f2} \\ 0 & 0 \end{pmatrix} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = \alpha \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \quad (3)$$

If we replace $\beta = 0$ in (3), we obtain the intermediate α -modes, otherwise the prompt α -modes are obtained [3].

All these problems are generalized eigenvalue problems associated with differential operators and the aim of this work is to obtain a set of dominant eigenvalues and their corresponding eigenmodes.

The rest of the paper is organized as follows: In Section II., the high order finite elements method used to discretize equations (1), (2) and (3) is briefly exposed and an algebraic generalized eigenvalue problem is obtained for each one of the mode problems. In Section III., two eigenvalue solvers are analyzed. The first one is the Krylov-Schur method, a Krylov subspace method, typically used for this kind of computations. The second one is an alternative method to speed-up the calculations for γ and α -modes based on Rayleigh-Ritz procedure and modified block Newton method. To test the performance of the method, several benchmarks are studied in Section IV.. Finally, in Section V., the conclusions are summarized.

II. DISCRETIZATION BY FINITE ELEMENTS

For simplicity, the discretization used is shown only for one energy group but the same process can be applied for two or more groups [6].

Let us consider the one energy group λ -modes equation,

$$(-\nabla(D \nabla) + \Sigma_a) \phi = \frac{1}{\lambda} (\nu \Sigma_f) \phi, \quad (4)$$

the weak formulation is obtained by pre-multiplying by a test function φ and integrating over the domain, Ω , defining the reactor core,

$$\int_{\Omega} \varphi (-\nabla(D \nabla) + \Sigma_a) \phi \, dV = \frac{1}{\lambda} \int_{\Omega} \varphi (\nu \Sigma_f) \phi \, dV. \quad (5)$$

Using Gauss Divergence theorem in (5) and simplifying, the following equation is obtained

$$\begin{aligned} & \int_{\Omega} \nabla \varphi \cdot D \nabla \phi \, dV - \int_{\Gamma} \varphi D \nabla \phi \, dS + \int_{\Omega} \Sigma_a \varphi \phi \, dV \\ &= \frac{1}{\lambda} \int_{\Omega} \nu \Sigma_f \varphi \phi \, dV, \end{aligned} \quad (6)$$

where Γ is the boundary of the domain defining the reactor.

It is supposed the domain Ω can be decomposed as $\Omega = \cup_{e=1, \dots, N_r} \Omega_e$, where the cross sections in Ω_e remain constant for all $e = 1, \dots, N_r$, thus, (6) is equivalent to,

$$\begin{aligned} & \sum_{e=1}^{N_r} \left(D \int_{\Omega_e} \nabla \varphi \cdot \nabla \phi \, dV - D \int_{\Gamma_e} \varphi \nabla \phi \, dS + \Sigma_a \int_{\Omega_e} \varphi \phi \, dV \right) \\ &= \frac{1}{\lambda} \sum_{e=1}^{N_r} \nu \Sigma_f \int_{\Omega_e} \varphi \phi \, dV. \end{aligned} \quad (7)$$

The solution ϕ is approximated through usual trial solution as sum of shape functions N_j multiplied by their corresponding nodal values $\tilde{\phi}_j$, as,

$$\phi \approx \sum_{j=1}^p N_j \tilde{\phi}_j. \quad (8)$$

Substituting in (7) and after a condensation process, a generalized algebraic eigenvalue problem of the form

$$\mathbf{A} \tilde{\phi} = \frac{1}{\lambda} \mathbf{B} \tilde{\phi}, \quad (9)$$

is obtained, where the matrix elements are given by

$$\begin{aligned} A_{ij} &= \sum_{e=1}^{N_r} \left(D \int_{\Omega_e} \nabla N_i \cdot \nabla N_j \, dV - D \int_{\Gamma_e} N_i \nabla N_j \, dS \right. \\ &\quad \left. + \Sigma_a \int_{\Omega_e} N_i N_j \, dV \right), \\ B_{ij} &= \sum_{e=1}^{N_r} \nu \Sigma_f \int_{\Omega_e} N_i N_j \, dV. \end{aligned} \quad (10)$$

The same method is applied to γ and α -modes problems.

For two energy groups, the generalized algebraic eigenvalue problem, after the spatial discretization, for each mode takes the form,

$$\begin{pmatrix} A_{11}^{\lambda} & 0 \\ A_{21}^{\lambda} & A_{22}^{\lambda} \end{pmatrix} \begin{pmatrix} \tilde{\phi}_1 \\ \tilde{\phi}_2 \end{pmatrix} = \frac{1}{\lambda} \begin{pmatrix} B_{11}^{\lambda} & B_{12}^{\lambda} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \tilde{\phi}_1 \\ \tilde{\phi}_2 \end{pmatrix}, \quad (11)$$

$$\begin{pmatrix} A_{11}^{\gamma} & 0 \\ 0 & A_{22}^{\gamma} \end{pmatrix} \begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = \frac{1}{\gamma} \begin{pmatrix} B_{11}^{\gamma} & B_{12}^{\gamma} \\ B_{21}^{\gamma} & 0 \end{pmatrix} \begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix}, \quad (12)$$

$$\begin{pmatrix} A_{11}^{\alpha} & A_{12}^{\alpha} \\ A_{21}^{\alpha} & A_{22}^{\alpha} \end{pmatrix} \begin{pmatrix} \tilde{\varphi}_1 \\ \tilde{\varphi}_2 \end{pmatrix} = \alpha \begin{pmatrix} B_{11}^{\alpha} & 0 \\ 0 & B_{22}^{\alpha} \end{pmatrix} \begin{pmatrix} \tilde{\varphi}_1 \\ \tilde{\varphi}_2 \end{pmatrix}. \quad (13)$$

The finite element method used in this work has been implemented using the open source finite elements library Deal.II [7].

III. SOLUTION OF THE EIGENVALUE PROBLEMS

The modes problems (11), (12) and (13) can be reduced to a generic ordinary algebraic eigenvalue problem of the form,

$$Mv = \delta v, \quad (14)$$

that it has to be solved to find a set of dominant eigenvalues and their corresponding eigenfunctions (modes). We denote the number of desired eigenvalues by q .

For λ -modes, due to their block structure, it is possible to reduce the generalized problem to one whose matrices have the half of the size of the initial problem,

$$(A_{11}^{\lambda})^{-1} (B_{11}^{\lambda} - B_{12}^{\lambda} (A_{22}^{\lambda})^{-1} A_{21}^{\lambda}) \tilde{\phi}_1 = \lambda \tilde{\phi}_1. \quad (15)$$

For γ -modes, the problem is reduced to,

$$(\mathbf{A}^{\gamma})^{-1} \mathbf{B}^{\gamma} \tilde{\phi} = \gamma \tilde{\phi}. \quad (16)$$

And for the α -modes the ordinary eigenvalue problem associated is equal to,

$$(\mathbf{A}^{\alpha})^{-1} \mathbf{B}^{\alpha} \tilde{\varphi} = \tilde{\alpha} \tilde{\varphi}, \quad \text{with } \tilde{\alpha} = \frac{1}{\alpha}. \quad (17)$$

All these problems are very large and the matrices involved are sparse, thus the solution of the partial eigenvalue problems is done by using an iterative method based on the matrix-vector product. We have to take into account that the matrix inverses are not computed explicitly. They can be handled implicitly by solving systems of linear equations. These systems are solved using the BiCGStab method, together with a Cuthill-McKee reordering and incomplete LU factorization for preconditioning. Note that, the matrices associated with λ and γ -mode problems are symmetric, so, the rate of convergence to solve the systems in λ and γ problems are faster than for α -modes.

1. Krylov-Schur method

The basic idea of the Krylov-Schur method is to iteratively expand a Krylov subspace (with the Arnoldi process) and contract with a so-called Krylov-Schur decomposition with a matrix in a real Schur form (for more details, see [8]). To solve these problems by Krylov-Schur method the library SLEPc [?] is used.

2. Modified block Newton method

As it will be discussed later, the Krylov-Schur method is expensive from the computational point of view, specially, to compute the γ and α -modes. Thus, an alternative method based on the Block Newton method is studied. We want to remark that previous studies based on Newton method only compute the dominant mode and here we want to obtain several modes.

This method is decomposed in two steps: first, a procedure based on Rayleigh-Ritz method is applied to obtain an initial approximation of eigenvalue problem. Then, the solution is iteratively computed with the Modified block Newton method [9], using as initial iteration the approximation obtained in the first step.

Given a partial eigenvalue problem of the form

$$MV = V\Lambda, \quad (18)$$

where Λ is a diagonal matrix with the desired eigenvalues and V , the matrix in whose columns are their corresponding eigenvectors, it is assumed that the eigenvectors can be factorized as

$$V = ZS, \quad (19)$$

where $Z^T Z = I$, and it is introduced the biorthogonality condition $W^T Z = I$, where W is a fixed matrix, to make it a determinate problem.

Introducing (19) in (18) and denoting,

$$K = S\Lambda S^{-1}, \quad (20)$$

we have the non linear problem (21)

$$F(Z, \Lambda) := \begin{pmatrix} MZ - ZK \\ W^T Z - I_q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (21)$$

From Newton's method, a new iterated solution arises as

$$Z^{(k+1)} = Z^{(k)} - \Delta Z^{(k)}, \quad K^{(k+1)} = K^{(k)} - \Delta K^{(k)}, \quad (22)$$

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

$$\begin{cases} M\Delta Z^{(k)} - \Delta Z^{(k)}K^{(k)} - Z^{(k)}\Delta K^{(k)} = MZ^{(k)} - Z^{(k)}K^{(k)}, \\ W^T \Delta Z^{(k)} = W^T Z^{(k)} - I_q, \end{cases} \quad (23)$$

which is obtained by substituting (22) in (21) and removing the second order terms.

The system of equations in (23) is coupled because $K^{(k)}$ is not necessarily a diagonal matrix. To decouple this system, the Modified Block Newton method applies two previous steps. The first step consists of an orthogonalization to the matrix $Z^{(k)}$ using the modified Gram-Schmidt algorithm. Once $Z^{(k)}$ is an orthonormal matrix, i.e., $Z^{(k)T} Z^{(k)} = I_q$, as a second step, a Rayleigh-Ritz procedure is applied, which consists of obtaining the eigenvectors $S^{(k)}$ and their corresponding eigenvalues $\Lambda^{(k)}$ that satisfy

$$Z^{(k)T} MZ^{(k)} S^{(k)} = S^{(k)} \Lambda^{(k)}. \quad (24)$$

Note that the size of $Z^{(k)T} MZ^{(k)}$ is equal to the number of required eigenvalues. So, the dimension of problem (24) is much smaller than initial eigenvalue problem (18).

Defining $\bar{Z}^{(k)} := Z^{(k)} S^{(k)}$, we have, from (24), that $\Lambda^{(k)}$ is a diagonal matrix whose elements, λ_i are the Ritz values and $\bar{Z}^{(k)}$ are the approximated Ritz eigenvectors, satisfying the equation

$$Z^{(k)T} (M\bar{Z}^{(k)} - \bar{Z}^{(k)} \Lambda^{(k)}) = 0. \quad (25)$$

At each iteration, the matrix W in equation (23) is chosen as the previous approximation for the invariant subspace, that is, $W = \bar{Z}^{(k)}$. Using the definition of $K^{(k)}$ on (20), system (23) is decoupled into the q linear systems

$$\begin{pmatrix} M - \lambda_i^{(k)} & \bar{Z}^{(k)} \\ \bar{Z}^{(k)T} & 0 \end{pmatrix} \begin{pmatrix} \Delta \bar{z}_i^{(k)} \\ -\Delta \lambda_i^{(k)} \end{pmatrix} = \begin{pmatrix} M\bar{z}_i^{(k)} - \bar{z}_i^{(k)} \lambda_i^{(k)} \\ 0 \end{pmatrix} \quad i = 1, \dots, q, \quad (26)$$

where $\Delta \bar{z}_i^{(k)}$ is the i -th column of $\Delta \bar{Z}^{(k)}$. Vectors $Z^{(k+1)}$ are updated according to equation (22) and the eigenvalues $\lambda_i^{(k)}$ are obtained from the small problem (24). The Modified Block Newton method to obtain the γ and α -modes from the solution of λ -modes problem, can be summarized as in Algorithm 1.

Algorithm 1 MBNM

Input: M^δ , δ eigenvalue matrix problem (14), ($\delta = \gamma, \alpha$) and V_λ matrix of λ problem with column eigenvectors.

Output: Λ_δ , diagonal matrix of eigenvalues and V_δ matrix with corresponding column eigenvectors.

- 1: Orthonormalize(V_λ) ▷ MODIFIED GRAM-SCHMIDT
 - 2: Compute $F = V_\lambda^T M^\delta V_\lambda$, ▷ RAYLEIGH-RITZ (Start)
 - 3: Solve the reduced problem $FZ = Z\Lambda_\delta$
 - 4: Compute $V_\delta = V_\lambda Z$ ▷ RAYLEIGH-RITZ (End)
 - 5: **while** V_δ, Λ_δ do not satisfy a termination criterion **do**
 - 6: Compute $\Delta V_\delta = [\Delta v_1^\delta, \dots, \Delta v_q^\delta]$
(Correction determined with the
Newton iteration of Eq. (26))
 - 7: $V_\delta = V_\delta - \Delta V_\delta$
 - 8: Orthonormalize(V_δ) ▷ MODIFIED GRAM-SCHMIDT
 - 9: Compute $F = V_\delta^T M^\delta V_\delta$, ▷ RAYLEIGH-RITZ (Start)
 - 10: Solve the reduced problem $FZ = Z\Lambda_\delta$
 - 11: Compute $V_\delta = V_\delta Z$ ▷ RAYLEIGH-RITZ (End)
 - 12: **end while**
-

IV. RESULTS AND ANALYSIS

To study the performance of the methods exposed above to determine the λ -modes, α -modes and γ -modes, two benchmark reactor problems have been considered.

The computer used has been an Intel® Core™ i7-4790 @3.60GHz×8 processor with 32Gb of RAM running Ubuntu GNU/Linux 16.04 LTS.

1. Homogeneous reactor

First, a 3D prismatic reactor with homogeneous material is considered since it can be solved analytically for all its eigenvalues and compared with the numerical results obtained using the finite element method. The analytical solution is developed in APPENDIX. The dimensions are 300 cm × 300 cm × 450 cm and the material cross sections for the prismatic reactor are displayed in Table I. The velocities are $v_1 = 2.8 \cdot 10^7$ cm/s and $v_2 = 4.4 \cdot 10^7$ cm/s. The number of neutrons produced by fission (ν) has been considered equal to 2.5. The modeling mesh of reactor is composed of 36 cells of size 50 × 50 cm² per 6 planes of height 75cm.

The mean relative error,

$$\bar{\varepsilon} = \frac{1}{V_t} \sum_i \varepsilon_i V_i, \quad \text{where } \varepsilon_i = \frac{|P_i - P_i^*|}{|P_i|}$$

and the eigenvalue error expressed in pcm,

$$\varepsilon_{eig} = 10^5 \left(\frac{|\delta_i - \delta_i^*|}{|\delta_i|} \right),$$

TABLE I. Macroscopic cross section values for the homogeneous reactor.

$D_1(\text{cm}^{-1})$	$D_2(\text{cm}^{-1})$	$\Sigma_{a1}(\text{cm}^{-1})$	$\Sigma_{a2}(\text{cm}^{-1})$	$\Sigma_{12}(\text{cm}^{-1})$	$\nu\Sigma_{f1}(\text{cm}^{-1})$	$\nu\Sigma_{f2}(\text{cm}^{-1})$
1.501	4.329e-01	9.400e-03	8.210e-02	1.685e-02	6.060e-03	1.010e-01

are considered to analyze the numerical results. P_i and P_i^* are the analytical power and the computed power in the i -th cell (cell averages), respectively. V_i is the volume of the cell and V_t is the total volume of the reactor. δ_i and δ_i^* with $\delta = \lambda, \alpha, \gamma$ are the analytical and computed eigenvalues.

Tables II, III and IV show the eigenvalue and power errors between the analytical and numerical solution with different polynomial degree in finite element method (FED), mesh refinement level (Refin.) and number of degree of freedom (DoFs) for λ -modes, γ -modes and α -modes, respectively. Also, in each case, the computational time is displayed.

The method used to solve the ordinary eigenvalue problems (15), (16) and (17) has been Krylov-Schur. The number of eigenvalues requested has been 4, the dimension of Krylov subspace chosen has been 19 and the relative tolerance has been set to 10^{-8} . The tolerance in BiCGStab has been 10^{-9} .

In these Tables it is observed, in general, that good approximations are obtained choosing a finite element degree (FED) equal to 2 and 1 mesh refinement. Although, for γ -modes, the error are very low with FED equal to 1 and 1 refinement. Also, it can be concluded that the errors do not depend on which eigenvalue (first or second) is being calculated. However, the computational times for different kind of modes are not similar, and for λ -modes, they are smaller than for γ and α -modes.

2. NEACRP reactor

The NEACRP benchmark [10] is chosen to compare the different modes and eigenvalue solvers in a more realistic case. The core has a radial dimension of $21.606 \text{ cm} \times 21.606 \text{ cm}$ per assembly. Axially the reactor, with the total height of 427.3 cm, is divided into 18 layers with height (from bottom to top): 30.0 cm, 7.7 cm, 11.0 cm, 15.0 cm, 30.0 cm (10 layers), 12.8 cm (2 layers), 8.0 cm and 30.0 cm. The distribution of the different materials is shown in Figure 1 and Figure 2. The cross sections of materials are displayed in Table V. The boundary condition for the solution is flux vanishing in the outer reflector surface. And the velocities are $v_1 = 2.8 \cdot 10^7 \text{ cm/s}$ and $v_2 = 4.4 \cdot 10^5 \text{ cm/s}$.

In the following computations, the options used for the finite element method to discretize the different eigenvalue problems are: finite element degree equal to 3 and without refinement of the mesh (Refin.=0). For solving the eigenvalue problems, Krylov-Schur method is applied for ordinary modes problems (15), (16) and (17) to obtain 6 eigenvalues, setting the Krylov subspace dimension to 13. The relative tolerance used, in Krylov-Schur and BiCGStab method, is 10^{-8} for λ and γ -modes, and 10^{-13} for α -modes. This difference for α -modes is because matrix A^α is ill-conditioned and to obtain good approximations (with residual errors less than 10^{-5}) in the generalized eigenvalue problem is necessary to request a

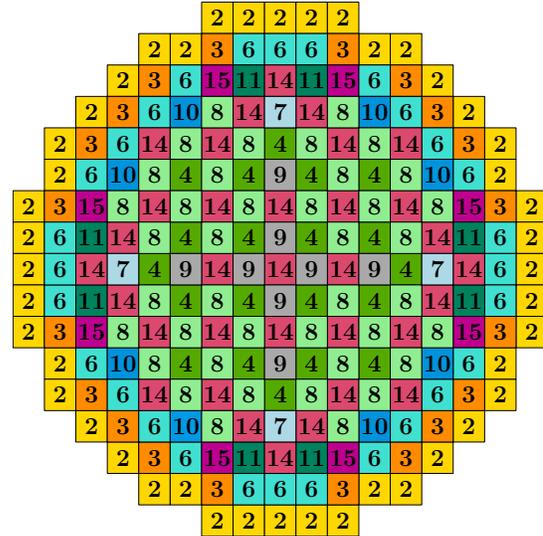


Fig. 1. Top view of NEACRP reactor and distribution of materials.

tolerance equal to 10^{-13} in the ordinary eigenvalue problem.

The results for four eigenvalues together with the number of iterations of Krylov-Schur, the mean of iterations of BiCGStab, the memory consumption of matrices and the CPU time necessary for their calculation, are displayed in Table VI. In this Table, it is observed that reactor is quasi-critical since the dominant λ and γ are near 1, and α is near to 0. The problems are large eigenvalue problems and they need to be solved with iterative methods. If the iterations of BiCGStab are compared, the number for α -modes is much higher to the rest, because A^α is ill-conditioned. The number of iterations required for the Krylov-Schur method to converge for γ -modes is much larger compared with the other modes. The reason is that the spectrum of γ -modes is more clustered.

The radial and axial profiles for the fast flux associated with the first two eigenvalues are represented in Figure 3 for each kind of mode. In this Figure, small differences are observed between different kind of modes due to quasi-criticality of reactor. Furthermore, it is shown that the fast flux for the first modes is positive and has radial and axial symmetry, whereas the second modes are antisymmetric in axial profile and symmetric in the radial one.

The computational time necessary to obtain the different modes with the Krylov-Schur method is very different (the computational time to solve the eigenvalue problem associated to α and γ -modes is much larger than the time for λ -modes). So, it is proposed computing α -modes and γ -modes using an alternative methodology based on modified block Newton method. The MBNM is a sensitive iterative method to ini-

TABLE II. λ -modes and errors for the homogeneous reactor.

FED	Refin.	DoFs	First eigenvalue			Second eigenvalue			CPU Time (s)
			λ_1	ϵ_{eig}	$\bar{\epsilon}$	λ_2	ϵ_{eig}	$\bar{\epsilon}$	
1	1	2197	3.95612	294030	8.26	3.95306	297200	4.94	1
2	0	2197	1.91598	90830	13.67	1.91597	92516	7.48	0.8
2	1	15625	1.00402	0.02	1.5e-3	0.99523	0.7	6.80e-3	4
3	0	6859	1.00402	0.07	1.4e-3	0.99526	3.2	5.41e-3	5
Anal. solut.:			1.00402			0.99523			

TABLE III. γ -modes and errors for the homogeneous reactor.

FED	Refin.	DoFs	First eigenvalue			Second eigenvalue			CPU Time (s)
			γ_1	ϵ_{eig}	$\bar{\epsilon}$	γ_2	ϵ_{eig}	$\bar{\epsilon}$	
1	1	4394	1.0022	5.2	8.95e-8	0.99711	19.4	1.26e-7	0.5
2	0	4394	1.0023	0.07	1.23e-8	0.99730	1.1	4.44e-7	1.2
2	1	31250	1.0023	0.02	4.63e-8	0.99731	0.07	2e-7	11.5
3	0	13718	1.0023	0.02	5.26e-8	0.99731	0.01	4.28e-7	20
Anal. solut.:			1.0023			0.99731			

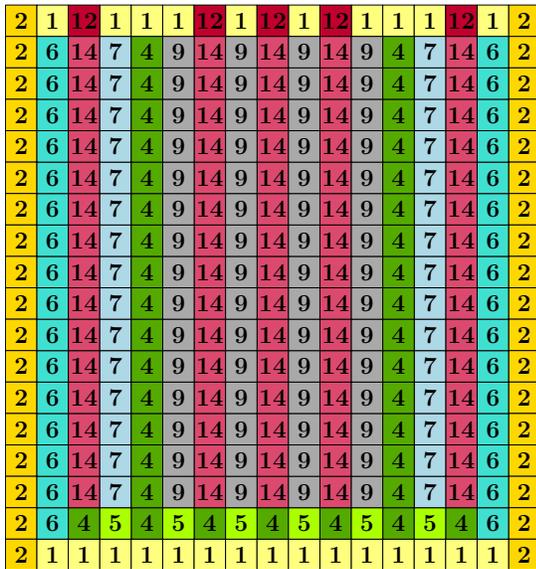


Fig. 2. Profile view of NEACRP reactor and distribution of materials.

tial approximation. As near criticality the eigenfunctions for different kind of modes are similar, it is proposed initiate the MBNM with the solution of λ -modes problem to compute the solution of γ and α eigenvalue problems. The stopping criterion used in these methods is based on the residual of the calculated eigenvalues and eigenvectors in generalized eigenvalue problem,

$$\text{res} = \sqrt{\sum_{k=1, \dots, q} \|A^\delta v_k - B^\delta v_k \delta_k\|_2}, \quad (27)$$

where the v_k are the corresponding k -eigenvectors associated to the eigenvalues $\delta_k = \lambda_k, \gamma_k, \alpha_k$.

The computational times necessary to obtain the γ and α -modes with both methods are shown in Table VII with residual error (res) lower than 10^{-6} . The computational time for λ -modes has been added to CPU time of MBNM shown. It is observed that the MBNM is competitive for computing α and γ modes.

V. CONCLUSIONS

In this work, the λ , α and γ -modes have been considered for neutron diffusion equation. A high order finite element method is used to discretize these equations. A homogeneous reactor is presented to analyze the numerical errors in the discretization method and to compare them between the different modes. A good approximation is obtained with degree of polynomial in finite element equal to 2 and one refinement of the mesh.

According to modes, the γ eigenvalues have the advantage that they are not limited to systems with fissions like the λ -modes. However, it has the limitation that $|\gamma - 1|$ is lower than $|\lambda - 1|$ for the same configuration, this implies that the eigenvalue is less sensitive, and its numerical calculation requires more computational time to reach the convergence than the λ -modes calculations.

Regarding α -eigenvalues, they are best suited for transient analysis, due to the nature of this kind of modes. Nevertheless, as the γ -modes problem, the computational time necessary to obtain the α -modes is larger than for the computation of the λ -modes. The reason is that the matrix obtained in discretization of α -modes problem is ill-conditioned. Solving linear system with this matrix is very expensive and low tolerances in ordinary eigenvalue problem are needed to set to obtain good approximations in the generalized problem.

The Modified block Newton Method has been considered as an alternative to compute the α and γ -modes. As near

TABLE IV. α -modes and errors for the homogeneous reactor.

FED	Refin.	DoFs	First eigenvalue			Second eigenvalue			CPU Time (s)
			α_1	ϵ_{eig}	$\bar{\epsilon}$	α_2	ϵ_{eig}	$\bar{\epsilon}$	
1	1	4394	173.10	2313.7	2.11e-7	-225.19	7183	1.10e-7	0.5
2	0	4394	177.13	41.5	4.65e-7	-210.97	413.5	4.09e-7	1
2	1	31250	177.19	2.6	7.46e-8	-210.16	26.8	5.06e-8	14
3	0	13718	177.20	0.06	2.78e-7	-210.11	3.1	6.95e-8	10
Anal. solut.:			177.20			-210.10			

TABLE V. Macroscopic cross section of the NEACRP reactor.

Mat.	$D_1(\text{cm}^{-1})$	$D_2(\text{cm}^{-1})$	$\Sigma_{a1}(\text{cm}^{-1})$	$\Sigma_{a2}(\text{cm}^{-1})$	$\Sigma_{12}(\text{cm}^{-1})$	$\nu\Sigma_{f1}(\text{cm}^{-1})$	$\nu\Sigma_{f2}(\text{cm}^{-1})$	$\Sigma_{f1}(\text{cm}^{-1})$	$\Sigma_{f2}(\text{cm}^{-1})$
1	5.9263	8.2277e-01	2.6191e-04	1.1477e-02	2.7988e-02	0.0000	0.0000	0.0000	0.0000
2	1.1276	1.6978e-01	1.1878e-03	1.9865e-01	2.3161e-02	0.0000	0.0000	0.0000	0.0000
3	1.1276	1.6978e-01	1.1878e-03	1.9865e-01	2.0081e-02	0.0000	0.0000	0.0000	0.0000
4	1.4624	3.9057e-01	8.4782e-03	6.2649e-02	1.9684e-02	5.0150e-03	8.7684e-02	6.1479e-14	1.1511e-12
5	1.4637	3.9489e-01	8.8239e-03	7.0055e-02	1.9435e-02	5.6085e-03	1.0421e-01	6.9274e-14	1.3681e-12
6	1.4650	3.9855e-01	9.1498e-03	7.6924e-02	1.9195e-02	6.1819e-03	1.1951e-01	7.6810e-14	1.5689e-12
7	1.4641	4.0582e-01	9.0882e-03	7.7758e-02	1.8525e-02	5.5830e-03	1.0286e-01	6.8995e-14	1.3504e-12
8	1.4641	4.0950e-01	9.1752e-03	8.0371e-02	1.8221e-02	5.5741e-03	1.0229e-01	6.8912e-14	1.3429e-12
9	1.4642	4.1317e-01	9.2609e-03	8.2990e-02	1.7919e-02	5.5649e-03	1.0166e-01	6.8816e-14	1.3347e-12
10	1.4653	4.0923e-01	9.4110e-03	8.4530e-02	1.8287e-02	6.1564e-03	1.1804e-01	7.6529e-14	1.5497e-12
11	1.4655	4.1280e-01	9.4969e-03	8.7097e-02	1.7985e-02	6.1474e-03	1.1741e-01	7.6448e-14	1.5414e-12
12	5.5576	8.7000e-01	2.7396e-03	3.7064e-02	2.4796e-02	0.0000	0.0000	0.0000	0.0000
13	5.6027	8.6358e-01	2.4190e-03	3.3753e-02	2.5209e-02	0.0000	0.0000	0.0000	0.0000
14	1.4389	4.0090e-01	1.0956e-02	8.8237e-02	1.6492e-02	4.9121e-03	8.4861e-02	6.0264e-14	1.1141e-12
15	1.4413	4.0669e-01	1.1579e-02	1.0257e-01	1.6053e-02	6.0592e-03	1.1622e-01	7.5334e-14	1.5259e-12

the criticality of reactor, the eigenfunctions are similar, the λ -modes have been used to initiate the Modified block Newton method to compute the γ and α -modes. The numerical results show that this last method computes the solution in a faster way than Krylov-Schur method.

APPENDIX

Analytical solution for λ -modes

A 3D rectangular homogeneous reactor is considered. The λ -modes problem for a tridimensional domain, $\Omega = [0, L_x] \times [0, L_y] \times [0, L_z]$, is defined as

$$-\nabla D_1 \nabla \phi_1 + (\Sigma_{a1} + \Sigma_{12})\phi_1 = \frac{1}{\lambda}(\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2), \quad (\text{A.1})$$

$$-\Sigma_{12}\phi_1 - \nabla D_2 \nabla \phi_2 + \Sigma_{a2}\phi_2 = 0, \quad (\text{A.2})$$

with the boundary conditions

$$\begin{aligned} \phi_g(0, y, z) &= \phi_g(L_x, y, z) = 0, \\ \phi_g(x, 0, z) &= \phi_g(x, L_y, z) = 0, \quad g = 1, 2. \\ \phi_g(x, y, 0) &= \phi_g(x, y, L_z) = 0, \end{aligned}$$

Using the variables separation method, the solution of λ -modes problem is obtained. The thermal and fast group eigenfunctions are, respectively,

$$\phi_2(x, y, z) = k \sin\left(\frac{m\pi}{L_1}x\right) \sin\left(\frac{n\pi}{L_2}y\right) \sin\left(\frac{p\pi}{L_3}z\right). \quad (\text{A.3})$$

$$\phi_1(x, y, z) = \frac{D_2 B_{m,n,p}^2 + \Sigma_{a2}}{\Sigma_{12}} \phi_2(x, y, z). \quad (\text{A.4})$$

with

$$B_{m,n,p}^2 = B_{x,m}^2 + B_{y,n}^2 + B_{z,p}^2. \quad (\text{A.5})$$

and

$$B_{x,m} = \frac{m\pi}{L_x}, \quad B_{y,n} = \frac{n\pi}{L_y}, \quad B_{z,p} = \frac{p\pi}{L_z}. \quad (\text{A.6})$$

Different values of the integer numbers m , n and p correspond to the different eigenvalues and the corresponding eigenfunctions of the reactor.

The eigenvalues λ are of the form,

$$\lambda = \frac{\nu\Sigma_{f1}(D_2 B_{m,n,p}^2 + \Sigma_{a2}) + \nu\Sigma_{f2}\Sigma_{12}}{(D_2 B_{m,n,p}^2 + \Sigma_{a2})(\Sigma_{a1} + \Sigma_{12} + D_1 B_{m,n,p}^2)}$$

Analytical solution for γ -modes

The γ -modes problem for a tridimensional domain, $\Omega = [0, L_x] \times [0, L_y] \times [0, L_z]$, is defined as,

$$-\nabla D_1 \nabla \psi_1 + (\Sigma_{a1} + \Sigma_{12})\psi_1 = \frac{1}{\gamma}(\nu\Sigma_{f1}\psi_1 + \nu\Sigma_{f2}\psi_2), \quad (\text{A.7})$$

$$-\nabla D_2 \nabla \psi_2 + \Sigma_{a2}\psi_2 = \frac{1}{\gamma}\Sigma_{12}\psi_1, \quad (\text{A.8})$$

TABLE VI. Eigenvalues of NEACRP reactor.

	1st	2nd	3rd	4th	its. Krylov-Schur	mean its. BiCGStab	memory consumption	CPU Time (s)
λ -modes	0.99919	0.98792	0.98442	0.98442	16	17.35	406.19Mb	131s
γ -modes	0.99955	0.99332	0.99137	0.99137	40	5.01	388.39Mb	422s
α -modes	-31.2450	-468.709	-612.494	-612.494	6	43.61	493.91Mb	651s

TABLE VII. Computational time(s) using Krylov-Schur and MBNM methods.

Method	Krylov-Schur	MBNM
α -modes	651	563
γ -modes	488	389

with the boundary conditions

$$\begin{aligned}\psi_g(0, y, z) &= \psi_g(L_x, y, z) = 0, \\ \psi_g(x, 0, z) &= \psi_g(x, L_y, z) = 0, \quad g = 1, 2. \\ \psi_g(x, y, 0) &= \psi_g(x, y, L_z) = 0,\end{aligned}$$

The solution of γ -modes problem is obtained using the variables separation method following an analogous process to the λ -modes problem. For this problem we get,

$$\psi_2(x, y, z) = k \sin\left(\frac{m\pi}{L_x}x\right) \sin\left(\frac{n\pi}{L_y}y\right) \sin\left(\frac{p\pi}{L_z}z\right), \quad (\text{A.9})$$

$$\psi_1(x, y, z) = \frac{\gamma(B_{m,n,p}^2 D_2 + \Sigma_{a2})}{\Sigma_{12}} \psi_2(x, y, z), \quad (\text{A.10})$$

with $m, n, p \in \mathbb{N}$.

The eigenvalue γ is a solution of the equation

$$\begin{aligned}\left[D_1 B_{m,n,p}^2 (D_2 B_{m,n,p}^2 + \Sigma_{a2}) + (\Sigma_{a1} + \Sigma_{12})(D_2 B_{m,n,p}^2 + \Sigma_{a2}) \right] \gamma^2 \\ - \left[\nu \Sigma_{f1} (D_2 B_{m,n,p}^2 + \Sigma_{a2}) \right] \gamma - \Sigma_{12} \nu \Sigma_{f2} = 0,\end{aligned}$$

with $B_{m,n,p}^2$ defined in (A.5). In typical reactors, the two solutions of this equation are real and they are sorted by largest magnitude. Different values of m, n, p correspond to the different eigenvalues and eigenfunctions of the reactor.

Analytical solution for α -modes

The α -modes problem for a tridimensional domain, $\Omega = [0, L_x] \times [0, L_y] \times [0, L_z]$, is defined as,

$$\nu_1 (\nabla D_1 \nabla \varphi_1 - (\Sigma_{a1} + \Sigma_{12}) \varphi_1 + \nu \Sigma_{f1} \varphi_1 + \nu \Sigma_{f2} \varphi_2) = \alpha \varphi_1, \quad (\text{A.11})$$

$$\nu_2 (\Sigma_{12} \varphi_1 + \nabla D_2 \nabla \varphi_2 - \Sigma_{a2} \varphi_2) = \alpha \varphi_2, \quad (\text{A.12})$$

with the boundary conditions

$$\begin{aligned}\varphi_g(0, y, z) &= \varphi_g(L_x, y, z) = 0, \\ \varphi_g(x, 0, z) &= \varphi_g(x, L_y, z) = 0, \quad g = 1, 2. \\ \varphi_g(x, y, 0) &= \varphi_g(x, y, L_z) = 0,\end{aligned}$$

Using a similar procedure to the one followed for the other modes, the analytical solution of the α -modes problem is,

$$\varphi_2(x, y, z) = k \sin\left(\frac{m\pi}{L_1}x\right) \sin\left(\frac{n\pi}{L_2}y\right) \sin\left(\frac{p\pi}{L_3}z\right), \quad (\text{A.13})$$

$$\varphi_1(x, y, z) = \frac{B_{m,n,p}^2 \nu_2 D_2 + \nu_2 \Sigma_{a2} + \alpha}{\nu_2 \Sigma_{12}} \varphi_2(x, y, z), \quad (\text{A.14})$$

with $m, n, p \in \mathbb{N}$, where the eigenvalues α are solutions of

$$\alpha^2 + \left[B_{m,n,p}^2 \nu_2 D_2 + \nu_2 \Sigma_{a2} - \nu_1 \nu \Sigma_{f1} + \nu_1 (\Sigma_{a1} + \Sigma_{12}) \right] \alpha + \nu_1 D_1 B_{m,n,p}^2 \left[\alpha + \nu_1 D_1 B_{m,n,p}^2 (B_{m,n,p}^2 \nu_2 D_2 + \nu_2 \Sigma_{a2}) \right] \quad (\text{A.15})$$

$$+ \nu_1 (\Sigma_{a1} + \Sigma_{12}) (B_{m,n,p}^2 \nu_2 D_2 + \nu_2 \Sigma_{a2}) \quad (\text{A.16})$$

$$- (\nu_1 \nu \Sigma_{f1} (B_{m,n,p}^2 \nu_2 D_2 + \nu_2 \Sigma_{a2}) + \nu_2 \Sigma_{12} \nu_1 \nu \Sigma_{f2}) = 0, \quad (\text{A.17})$$

$$- (\nu_1 \nu \Sigma_{f1} (B_{m,n,p}^2 \nu_2 D_2 + \nu_2 \Sigma_{a2}) + \nu_2 \Sigma_{12} \nu_1 \nu \Sigma_{f2}) = 0, \quad (\text{A.18})$$

and $B_{m,n,p}^2$ defined in (A.5). If typical macroscopic cross sections are used, the two solutions of this equation are real numbers. Also, different eigenvalues are obtained changing the value of m, n and p .

ACKNOWLEDGMENTS

This work has been partially supported by Spanish Ministerio de Economía y Competitividad under projects ENE2014-59442-P, MTM2014-58159-P and BES-2015-072901.

REFERENCES

1. J. W. Y. RONEN, D. SHVARTS, "A Comparison of Some Eigenvalues in Reactor Theory," *American Nuclear Society*, **60**, 1, 97–101 (1976).
2. G. VELARDE, C. AHNERT, and J. ARAGONES, "Analysis of the eigenvalue equations in $k, \lambda, \gamma, \alpha$, and β applied to some fast- and thermal-neutron systems," *Nucl. Sci. Eng.*, **66:3** (Jun 1978).
3. G. VERDU, D. GINESTAR, J. ROMAN, and V. VIDAL, "3D alpha modes of a nuclear power reactor," *Journal of nuclear science and technology*, **47**, 5, 501–514 (2010).

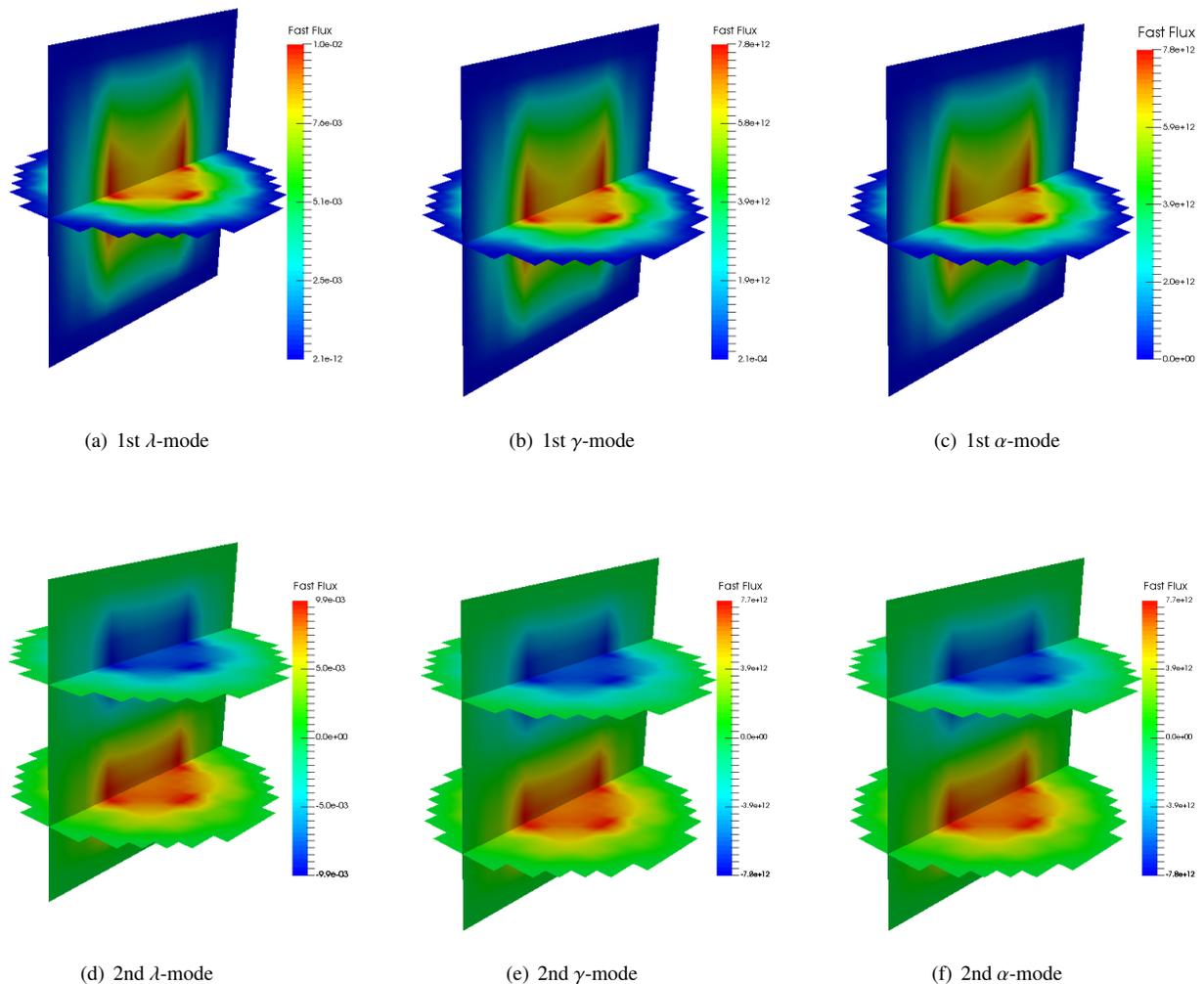


Fig. 3. Radial and axial fast flux profiles for NEACRP reactor.

4. G. VERDÚ, D. GINESTAR, V. VIDAL, and J. MUÑOZ-COBO, “3D λ -modes of the neutron-diffusion equation,” *Annals of Nuclear Energy*, **21**, 7, 405–421 (1994).
5. J. KÓPHÁZI and D. LATHOUWERS, “Three-dimensional transport calculation of multiple alpha modes in subcritical systems,” *Annals of Nuclear Energy*, **50**, 167–174 (2012).
6. A. VIDAL-FERRANDIZ, R. FAYEZ, D. GINESTAR, and G. VERDÚ, “Solution of the Lambda modes problem of a nuclear power reactor using an h - p finite element method,” *Annals of Nuclear Energy*, **72**, 338 – 349 (2014).
7. W. BANGERTH, R. HARTMANN, and G. KANSCHAT, “deal.II – a General Purpose Object Oriented Finite Element Library,” *ACM Trans. Math. Softw.*, **33**, 4, 24/1–24/27 (2007).
8. G. W. STEWART, “A Krylov–Schur algorithm for large eigenproblems,” *SIAM Journal on Matrix Analysis and Applications*, **23**, 3, 601–614 (2002).
9. Y. SAAD, *Iterative methods for sparse linear systems*, SIAM (2003).
10. H. FINNEMANN and A. GALATI, “NEACRP 3-D LWR core transient benchmark, final specification,” *NEACRPL-335 (Revision 1)* (1991).