Block strategies to compute the lambda modes associated with the neutron diffusion equation

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Abstract: *Given a configuration of a nuclear reactor core, the spatial distribution of the power can be approximated by solving the λ-modes problem associated with the multigroup neutron diffusion equation. It is a partial generalized eigenvalue problem whose dominant eigenvalue characterises the criticality of the reactor and its associated eigenvector represents the distribution of the neutron flux in steady-state. The spatial discretization of the equation is made by using a continuous Galerkin high order finite element method. Usually, the matrices obtained from the discretization are huge and sparse. Moreover, they have a block structure given by the different number of energy groups. In this work, block strategies are developed to optimize the computation of the associated eigenvalue problems. First, different block eigenvalue solvers are studied. On the other hand, the convergence of these iterative methods mainly depends on the initial guess and the preconditioner used. In this sense, different multilevel techniques to accelerate the rate of convergence of this problem are proposed. A large three-dimensional benchmark shows the efficiency of the methodology proposed.*

1 INTRODUCTION

The computation of the dominant λ-modes associated with the neutron diffusion equation has an interest in nuclear engineering to study the criticality of a reactor and also to develop modal methods to integrate the time dependent equation. This equation is an approximation of the neutron transport equation that assumes that the neutron current is proportional to the gradient of the scalar neutron flux with a diffusion coefficient.

The λ-modes problem is discretized to yield a large algebraic generalized eigenvalue problem that has to be solved by using iterative methods to compute its dominant eigenvalues and their corresponding eigenvectors. In this work, a high order finite element method has been used for the spatial discretization of the λ-modes problem.

Krylov subspace methods, such as Arnoldi or Krylov-Schur method, can be applied to solve this non-symmetric eigenvalue problem [10, 12]. However, these iterative methods require reducing the generalized eigenvalue problem to an ordinary problem, and it implies solving many linear systems. Other methods to solve eigenvalue problems associated with nonsymmetric matrices are the gradient type methods, such as the Generalized Davidson method, that do not require solving linear systems involving the full operator. However, if there are clustered or degenerate eigenvalues, these methods may have problems to find all the eigenvalues.

In this work, a hybrid method is proposed that combines two types of solvers, the block inverse-free Arnoldi method (BIFPAM) and the modified generalized block Newton method (MGBNM). The BIFPAM was proposed in [8] for symmetric problems, but the authors nu-

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merically showed that it also converges for this type of neutron problems where the dominant eigenvalues are positive. It does not need to solve linear systems. It improves the traditional steepest descent method by expanding the search direction to a Krylov subspace with the advantage of better approximation properties offered by Krylov subspaces. The MGBNM is a generalization of the modified block Newton method ([7]). It has a quadratic convergence, but it is very sensitive to the initial guess.

The structure of the rest of the paper is as follows. In section 2 the definition of λ-modes problem and the spatial discretization by using a high order finite element method is given. Section 3 briefly describes the eigenvalue solvers. Section 4 presents the multilevel strategy to improve the computational efficiency of the eigenvalue solvers. Section 5 presents the numerical results for the analysis of the methodology in a benchmark problem. Finally, Section 6 collects the main conclusions of the work.

2 THE λ-MODES PROBLEM

Given a configuration of a nuclear reactor core, it is possible to force its criticality dividing the neutron production rate by a positive number, λ, obtaining the known λ-modes problem [9],

$$\mathcal{L}\phi = \frac{1}{\lambda}\mathcal{M}\phi, \tag{1}$$

where $\mathcal{L}$ is the neutron loss operator, $\mathcal{M}$ is the neutron production operator and ϕ the neutron flux.

To solve the problem (1), a spatial discretization of the equations has to be selected. In this work, a high order Galerkin finite element method is used (see [12]) leading to an algebraic eigenvalue problem associated with the discretization of (1) with the following structure,

$$Ax = \lambda Bx\,, \tag{2}$$

where A and B are the matrices that appear from the discretization of $\mathcal{M}$ and $\mathcal{L}$, respectively. The vector x is the algebraic vector of weights associated with the neutron flux. For simplicity, the shape functions used are part of Lagrange finite elements. More details on the spatial discretization used and general boundary conditions can be found in [12]. The finite element method has been implemented using the open-source finite elements library Deal.II [2].

3 BLOCK SOLVERS

In this Section, several well-known eigenvalue solvers to solve the partial eigenvalue problem (2) are described. This list is not intended to be exhaustive, and other eigenvalue solvers appear in the neutron transport computations or the mathematical literature.

In nuclear computations, different strategies have been used to solve the generalized problem obtained from the discretization. First, we can transform the problem as an ordinary eigenvalue problem by using the inverse of B. The inverse of the matrix B is not computed and its product by a vector is applied by solving linear systems. Second, for the special case of the λ-modes and two energy groups, many works define an ordinary eigenvalue problem, but with half of the size of the original problem. Finally, in this work, we aim to apply direct methods for the generalized eigenvalue problem.

For this problem, we are interested in using block methods, that converge the set of eigenvectors in a block, in order to initialize the iterative methods if an initial set of approximated eigenvectors is provided.

Generalized Davidson method Davidson methods take one eigenvector and apply a correction as

$$x^{(i+1)} = x^{(i)} + t^{(i)}, \quad \text{where} \quad (A - \lambda^{(i)}B)t^{(i)} = -(A - \lambda^{(i)}B)x^{(i)}\,. \tag{3}$$

In particular, the generalized Davidson method estimates the correction by solving the problem

$$P_i t^{(i)} = -r^{(i)}, \text{ where } P_i \approx (A - \lambda^{(i)} B). \tag{4}$$

This method, although its convergence is slow, does not need to solve any linear system involving the full operator. This makes that the iterations are very cheap. In this case, the block implementation provided by the library SLEPC is used [6]. As preconditioner for this method, the ILU(0) factorization from the library PETSc is used [1].

Block Inverse-free preconditioned Arnoldi method (BIFPAM) This block method is proposed for symmetric and positive definite matrices [8]. However, we have shown that the convergence is also obtained for neutronic problems where the eigenvalues are positive numbers. Given a set of eigenvectors X_i, the following approximated eigenvectors X_{i+1} are obtained from the first Ritz q-eigenvectors of the small problem

$$Z^T A Z U = Z^T B Z U \Lambda, \text{ as } X_{i+1} = ZU, \tag{5}$$

where Z is a basis of [8]

$$\mathcal{K}_{d_k} := \bigcup_{m=1}^{q} K^i_{d_k,m}(P_{m,i}(A - \lambda_{m,i} B), X_{m,i}).$$

These bases are constructed with the Arnoldi method. It does not solve any linear system and it has a block implementation. However, this method must be preconditioned to improve the convergence. In this work, we test two preconditioners of the linear systems: the ILU(0) preconditioner and the GMG preconditioner [4].

Modified block generalized Newton method (MGBNM) The original method was proposed for ordinary eigenvalue problems and we have proposed two generalizations [4]. In this work, it assumes that a set of eigenvectors X can be decomposed as

$$X = ZQ, \text{ such that } Z^T Z = I_q\,. \tag{6}$$

Now, the Newton's method is applied to solve the non-linear problem

$$F(Z, K) := \begin{pmatrix} AZ - BZK \\ W^T Z - I_q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \text{where } K \equiv Q^{-1} \Lambda Q \tag{7}$$

as

$$Z^{(k+1)} = Z^{(k)} - \Delta Z^{(k)}, \qquad K^{(k+1)} = K^{(k)} - \Delta K^{(k)}, \tag{8}$$

where the corrections are given by solving the q systems

$$\begin{pmatrix} A - \lambda_m^{(i)} B & B\bar{Z}^{(i)} \\ \bar{Z}^{(i)^T} & 0 \end{pmatrix} \begin{pmatrix} \Delta \bar{z}_m^{(i)} \\ -\Delta \lambda_m^{(i)} \end{pmatrix} = \begin{pmatrix} A\bar{z}_m^{(i)} - B\bar{z}_m^{(i)} \lambda_m^{(i)} \\ 0 \end{pmatrix}. \tag{9}$$

This block method has a quadratic convergence, then few linear systems must be solved in the computation. However, a 'good' initial guess must be provided to obtain convergence results. The linear systems are solved by using the GMRES method from the PETSc library [1] preconditioned with the block preconditioner developed for this method in [3].

Hybrid From the convergence histories of the BIFPAM and the MGBNM we have developed a hybrid method based on these methods [4]. We start from a set of sinitial eigenvectors, we then apply the BIFPAM method until a tolerance of 10^{-3} and then, with this solution we apply the MGBNM that has a quadratic convergence to reach the desired tolerance.

4 MULTILEVEL INITIALIZATION

Usually, the computation of the λ-modes for a realistic nuclear reactor requires much time to be solved. In this work, we propose a multilevel initialization to accelerate the convergences of the eigenvalue solvers.

It is well known that the convergence of iterative methods improves if better initial guesses are used. In this sense, it is proposed to use a multi-level method with two meshes: the initial mesh chosen from the spatial discretization, called the fine mesh and a coarse mesh obtained from the initial one considering a lower number of nodes. The solution obtained in the coarse mesh is used to generate an improved initial guess for the solution in the fine mesh.

In the coarse mesh, the materials and their corresponding cross-section must be redefined in each cell with a homogenization method. To solve the coarse eigenvalue problem we use Krylov-Schur method implemented in the library SLEPc [6]. The multi-level method can be summarized in Figure 1.

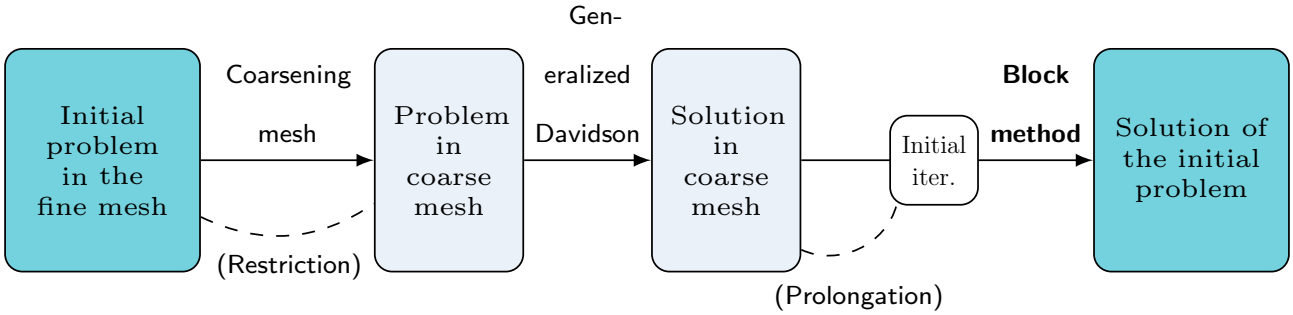


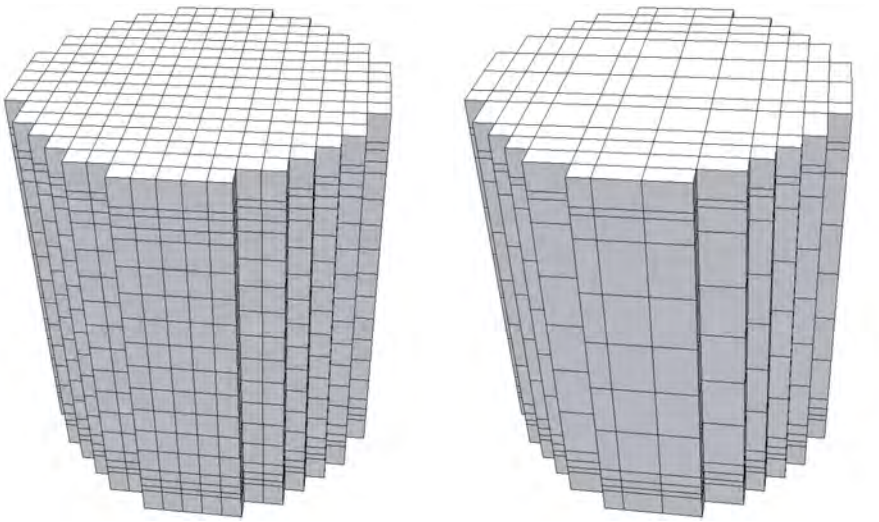
Figure 1: Scheme for the multilevel initialization.

5 NUMERICAL RESULTS

The three-dimensional NEACRP reactor is used to test the methodology described in this work [5]. The block strategies are tested to compute the dominant 4 λ-modes associated with the neutron diffusion equation. The initial mesh to discretize the reactor geometry has 3978 cells. Polynomials of degree 3 are used in the FEM, to have a problem of size 230 120 degrees of freedom. Tolerance for the eigenvalue solvers is set to obtain a residual error lower than 10^{-6}.

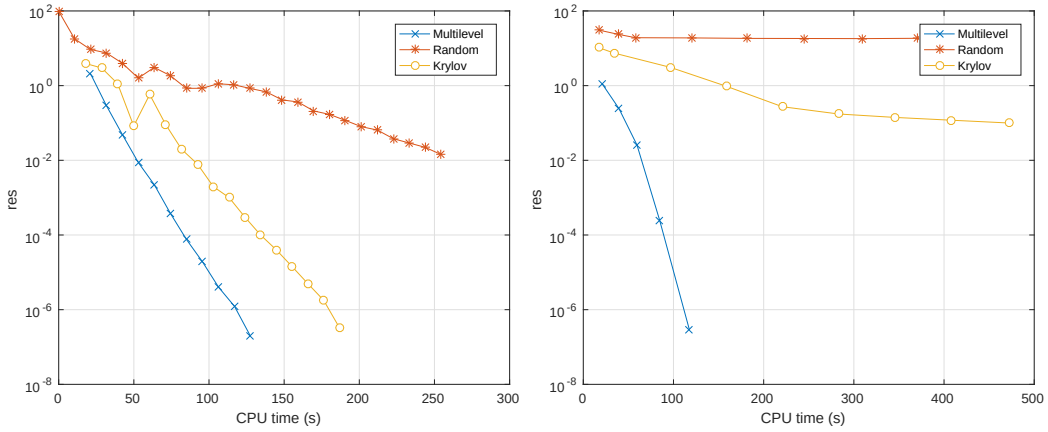
The methodology has been implemented in C++ based on data structures provided by the libraries Deal.II [2] and PETSc [1]. It has been incorporated to the open-source neutronic code `FEMFFUSION` [11]. For the computations, a computer with an Intel® Core™ i7-4790 @3.60GHz×8 processor with 32Gb of RAM running on Ubuntu GNU/Linux 18.04 LTS has been used.

First, multilevel initialization is analysed. It is compared with a Krylov initialization and a Random initialization. In the Krylov initialization, the vectors are obtained from a subspace of Krylov of dimension 10 associated to the matrix $A - \lambda_0^{(0)} B$. The Random initialization generates the q vectors using random numbers in the interval $[-1, 1]$. In both cases, the Gram-Schmidt orthogonalization and the generalized Rayleigh-Ritz process are then applied [4]. In the multilevel initialization, the simplified problem is defined by using a mesh of 1308 cells. Figure 2(a) shows the fine mesh used for the spatial discretization to solve the problem and Figure 2(a) represents the coarse mesh used to apply the multilevel initialization. The tolerance to solve for the simplified problem has been 10^{-3}. Figure 3 shows the convergence histories for the BIFPAM and the MBGNM with the different initializations. Both graphics reflect that the multilevel initialization, although it takes more time to obtain the initial guess, is a better strategy to initialize the block methods.



(a) Fine mesh (n. cells = 3978) (b) Coarse mesh (n. cells =1308)

Figure 2: Meshes for NEACRP reactor.



(a) BIFPAM (b) MGMNM

Figure 3: Convergence histories for the BIFPAM and the MGBNM using different initializations for the computation of the λ-modes of the NEACRP problem.

Now, the performance of the hybrid method is tested. Figure 4 compares the convergence histories of the MGBNM and the BIFPAM with the ILU and GMG preconditioner. It is deduced that the desired tolerance is reached quicker with the MGBNM. However, we would like to highlight that the convergence behaviour of BIFPAM-ILU is very similar to the one of BIFPAM-GMG and when the residual becomes smaller the convergence of the Newton method becomes faster.

Thus, it is proposed the hybrid method that initializes the algorithm with the BIFPAM method until $\text{res}_g = 10^{-2}$ and then, the MGBNM is applied. The BIFPAM has been set with the ILU preconditioner. Figure 5 compares the hybrid scheme with the MGBNM and the BIFPAM with ILU preconditioner. It is showed that the hybrid algorithm is an efficient scheme to compute 4 eigenvalues of the NEACRP problem.

Table 1 shows a comparison of the different eigenvalue solvers for the computation of several sets of eigenvalues of size q. In this computation, a semi-matrix free technique is used to avoid the full assemble of the matrices and then, the ILU preconditioner is substituted by the block Gauss-Seidel preconditioner [13]. All solvers are initialized with the multilevel technique. This

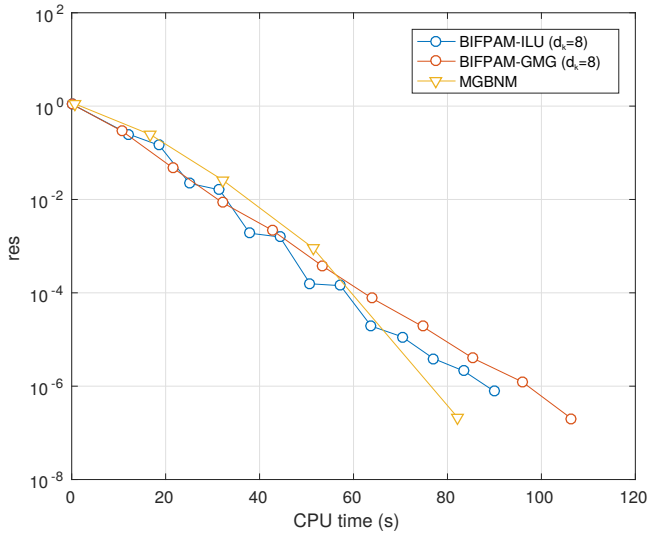


Figure 4: Convergence history for the fourth dominant eigenvalues of the NEACRP problem using the MGBNM and the BIFPAM.

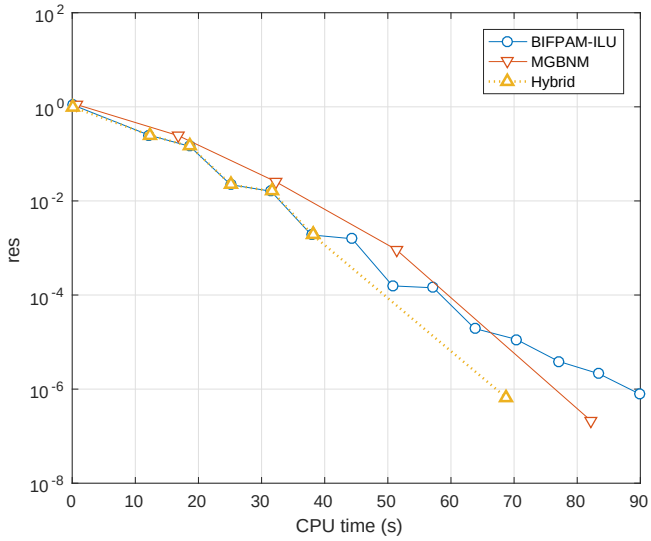


Figure 5: Convergence history of the BIFPAM with ILU preconditioner, the MGBNM and the hybrid method.

Table shows that the fastest results are obtained by applying the hybrid method, although, for a small number of eigenvalues, the BIFPAM is also very efficient.

Table 1: Computational times (s) obtained for the NEACRP reactor using the KSM method, the GDM, the BIFPAM, the MGBNM and the Hybrid method for different set of eigenvalues q.

q	GDM	BIFPAM	MGBNM	Hybrid
1	26	20	43	20
4	92	57	80	53
6	135	131	82	78

6 CONCLUSIONS

This work presents and compares several block eigenvalue solvers to compute a set of λ-modes associated with the neutron diffusion equation. Moreover, different strategies to improve the efficiency of these methods are described. First, numerical results show that the multilevel

initialization improves the efficiency of the methodologies. Regarding the eigenvalue solvers, one can deduce that the hybrid method (that combines the BIFPAM and the MGBNM) reduces the computational time to compute a set of modes in comparison with the BIFPAM, the MGBNM and the block Generalized Davidson.

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