Assessment of numerical methods for the evaluation of higher-order harmonics in diffusion theory

ASSESSMENT OF NUMERICAL METHODS FOR THE EVALUATION OF HIGHER-ORDER HARMONICS IN DIFFUSION THEORY

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ABSTRACT

The knowledge of higher-order harmonics besides the fundamental mode is important and useful in the prediction of the spatial behaviour of nuclear reactors. Previous works have evidenced that the information on higher-order modes is of great relevance in the interpretation of flux tilts in large cores. In order to assess the performance of the methods that are available to evaluate such modes in nuclear systems, simple configurations that allow for an analytical solution are analyzed, and the iteration process of filtered power, sub-space iteration and implicitly restarted Arnoldi methods are compared and discussed. The drawbacks of the filtered power method are highlighted. The implicitly restarted Arnoldi method is then chosen as the best approach for the analysis of a full-core realistic configuration, based on the C5G7 benchmark.

KEYWORDS: eigenvalue problem, higher-order modes, eigenvalue separation, eigenvalue degeneracy

1. INTRODUCTION

The power distribution in reflected large-size Light-Water Reactors (LWR) is very sensitive to a number of small perturbations generated by several independent, sometimes random, effects, which can either mutually cancel out or pile-up, depending on the actual configuration of the core and on the uncertainties locally affecting the water amount through its density and/or the inter-assembly gap size. Such non-predicted very small inhomogeneity in the water distribution can be the consequence of concomitant effects of an assembly bowing, a pump operating in the edge of the uncertainty range, the alignment or the misalignment of groups of assemblies due to the loading mode. This inhomogeneity dramatically affects the local water thermalization capability and produces either an increase or a decrease of the fission efficiency that impacts the overall core power distribution. The effect conventionally identified as "power tilt" is expected to be very high, at least at zero and low power in stainless steel reflected cores, due to the flux flattening induced by the heavy reflector [1].

The presence of a large power tilt at zero power can engender problems at the reactor start-up. The difficulties could be even more important if very sensitive devices are not available to retrieve

accurate assembly-wise power maps to assess the core conformity. Replacement solutions exist but their efficiency remains quite theoretical and has to be confirmed in experimental practice [2].

As can be expected, the power asymmetry is strongly reduced when the system goes to full power, due to the larger effectiveness of thermal feedback, although, generally, it does not vanish completely. Moreover, its reduction vs. the power level is not linear, and it shows to be quite sensitive to the burn-up and the depletion mode [3]. Accordingly, the behavior of a tilted core vs. power and lifetime is a challenge to safety and it must be accurately evaluated and accounted for in the safety demonstration; consequently, the operation may be penalized and/or suitable margins on the onset parameters may need to be enforced. Moreover, predicting the behavior of a tilted core is quite hard because most of conventional design computation chains adopt symmetry assumptions that do not fit with the actual physical conditions.

In previous works it has been demonstrated that such intriguing behavior can be physically explained investigating the change in the coupling of the core which, as it is well known, depends on its size and on the reflector efficiency. The dominance ratio (determined by the difference between two successive eigenvalues) and the contribution of higher harmonics to the tilted flux are attractive and pertinent indicators for such an investigation [4].

Unfortunately the power method adopted in these works to evaluate higher modes did not allow a sufficient in-depth analysis because it fails computing harmonics higher than the second one for symmetrical systems. Similar problems show up also for low-tilt situations, because the orthogonalisation is not effective enough to clean out the lower modes [3]. A solution has been suggested to bypass the problem: it amounts to introducing a spurious tilt through a change in the water density somewhere, thus allowing to separate the eigenvalues and to operate by the power method; however the solution looks quite artificial and the physics is distorted.

The present paper aims at investigating methodologies other than the power method to address the problem of evaluating the higher-order modes of the diffusion equations, for stability analysis [5], for on-line power distribution reconstruction [6] and for the above mentioned "power tilt" problems [7].

The most popular method to compute higher-order eigenpairs is a modification of the traditional power method, known as Filtered Power Method (FPM) or Subtraction Method, which exploits the bi-orthogonality relation to eliminate the contribution of lower-order harmonics to find the higher-order ones. Although valuable analytical [8] and numerical [9] considerations suggesting to look for better methods were presented decades ago, there still is a lot of work under way trying to improve the FPM by means of some artifices and precautions [10–12].

However, it is known that the power method can converge only on the fundamental eigenfunction associated to the largest eigenvalue of the problem. Therefore, approaches based on the power method may have a basic theoretical and computational short-come that justifies the studies of different approaches, based on more efficient and rational algorithms that are proved to converge also for the higher harmonics evaluation.

In this work the attention is focused on two well-known methods that were developed about twenty

years ago for reactor physics applications and that are believed to be excellent compromises among accuracy, stability, simplicity and compatibility with current neutronics codes, i.e. the Implicitly Restarted Arnoldi [13] method (IRA) and the Sub-Space Iteration [14] method (SSI). In the literature one can find plenty of other methods dealing with eigenvalue problems in neutronics, e.g. Jacobi-Davidson [15], modified block Newton iterations or different versions of the Krylov subspace method family [16]. However, the two above methods constitute an already big progress, in spite of their simplicity, with respect to more complicated recent algorithms.

Scrupulous examinations are carried out to assess IRA and SSI main features and performances with respect to FPM and to investigate their major issues in perspective of commercial code implementation. After this study, the most promising method is applied to a reference core based on the C5G7 benchmark [17], in order to evaluate its main spatial modes and the eigenvalue separation behaviour when different kinds of reflector materials are adopted.

2. NUMERICAL METHODS

In this section, the main features of the existing algorithms is briefly outlined.

2.1. Standard Power Iteration Approach

The simplest idea to retrieve higher-order modes is to filter the solution of the standard Power Method at each iteration by projection on the adjoint eigenfunction of a certain order, thus eliminating the contribution of lower-order harmonics. This method is commonly known as Filtered Power Method, Elimination Method or Subtraction Method.

A very deep analysis of FPM was performed in the 80's by Vondy and Fowler [9], who presented relevant considerations about the difficulty in assessing the local convergence, the detrimental effect of degeneracies on convergence, and the influence of the initialization that requires the presence of the components of the searched eigenfunctions. In addition to these drawbacks, one should also consider the following issues:

- the convergence rate scales with the dominance ratio, meaning that for low eigenvalue separation (EVS) there can be convergence troubles: the solution may not converge because of the numerical noise;
- the method requires a double calculation, because also the adjoint problem needs to be solved, thus increasing the computational burden;
- the algorithm is not suited for parallel computing, since each iteration requires the knowledge of the previous direct and adjoint eigenfunctions.

  Recently, some researchers tried to implement some additional constraints that could help FPM convergence, like imposing innovative boundary conditions [10,11] to split it in parallel subproblems according to their symmetry classes, in order to increase artificially the EVS reducing the computational domain, or operating separately on phase-space subregions [12]. These solutions however cannot overcome completely the problem, since it is the basic algorithm to be unstable and inefficient. Moreover, the innovative boundary conditions can be applied only to symmetric domains, therefore in very particular cases and in the absence of depletion effects.

2.2. Other Numerical Methods

In the following, a brief explanation of the methods analysed in this work is presented, trying as much as possible to avoid technical and mathematical details in favour of a more physical interpretation. For the detailed algorithms, see for instance [13,14].

2.2.1. Sub-Space Iteration method

The SSI method [14] is based on the idea that the original eigenvalue problem can be formulated as an eigen-problem on a reduced domain, exploiting the fact that the fission mechanism is the physical driver to establish an equilibrium condition, thus allowing for the solution of the mathematically homogeneous problem. Therefore, looking for fission source eigenfunctions in the fissile regions helps to avoid the explicit construction of the fission matrix $\hat{P}$, leading in addition to a reduction of the domain to the multiplicative region. The eigenvalues of $\hat{P}$ are found by means of a Rayleigh-Ritz projection. Once convergence is reached, a source problem is solved for all the domain, finding the eigenvectors of the original problem.

2.2.2. Implicitly Restarted Arnoldi Algorithm

The IRA method is a combination of an original idea by W. E. Arnoldi [18], with implicitly QR-shifts restarts [19]. The basic idea is similar to the one of the classic power method, since the operator whose spectrum is under investigation is iteratively applied to a guess initial vector; however, thanks to a Gram-Schmidt stabilized procedure [19], it is possible to generate an orthonormal basis starting from the Krylov subspace constructed by the successive operator-vector products.

From a physical point of view, unlike the power method in which the neutron population distribution inherits the information of the previous generation, IRA allows a faster convergence since present neutrons inherit information from all the previous generations, with the further speed-up of the implicit shifts, that damps the undesired components of the spectrum, enhancing the convergence towards the searched ones.

3. ASSESSMENT OF THE PERFORMANCE OF THE NUMERICAL METHODS

In the following, an assessment of the numerical methods illustrated in the previous section is carried out for simplified configurations that allow for a direct analytical approach.

3.1. Two-group Diffusion Equation for a Square Domain

In order to perform the numerical assessment, the two-group diffusion equations in a homogeneous, square domain is discretised adopting the finite difference scheme.

The main reasons to choose such a simple configuration to test the performances of the algorithms can be summarized as follows:

- availability of the analytic solution, that can be used to benchmark the results;

- presence of spatial (i.e. material and geometrical) symmetry to trigger the spectrum degeneracies;
- absence of symmetry in the discretised operator because of the two-group energy model, that makes the matrix structure more general.

To perform a thorough analysis, the size of the reference reactor is changed in order to cover a wide range of values of EVS.

The eigenvalue sequence for the homogeneous square in two energy group model is given by:

$$k_{m,n} = \frac{k_\infty}{(1 + L_1^2 B_{m,n}^2)(1 + L_2^2 B_{m,n}^2)}, \tag{1}$$

where k_∞ is the multiplication factor for the infinite medium, L_1 is the fast diffusion length, L_2 the thermal diffusion length, and $B_{m,n}$ is the geometrical buckling for a square of edge a:

$$B_{n,m}^2 = B_n^2 + B_m^2 = \left(\frac{\pi}{a}\right)^2 \left(n^2 + m^2\right). \tag{2}$$

A direct inspection of Eq. (2) shows that the same buckling can be obtained permuting the indexes n and m, causing what is known as *degeneracy*, whereas the same eigenvalue is associated to more than one eigenfunction. As shown in the literature [20], it is possible to link the definition of eigenvalue separation to the spatial scale of the domain by using Eq. (1) into the following definition,

$$\begin{aligned} S_{i+1} &= \frac{1}{k_{i+1}} - \frac{1}{k_i} \\ &= \frac{1}{k_\infty}\left[(1 + L_1^2 B_{i+1}^2)(1 + L_2^2 B_{i+1}^2) - (1 + L_1^2 B_i^2)(1 + L_1^2 B_i^2)\right] \\ &= \frac{1}{k_\infty}\left[(B_{i+1}^2 - B_i^2)(L_1^2 + L_2^2) + (B_{i+1}^4 - B_i^4)(L_1^2 L_2^2)\right]. \end{aligned} \tag{3}$$

This simple example shows that, restricting to a two-group model, S_{i+1} scales like the inverse of the fourth power of the size of the square, measured in terms of the group diffusion length (a/L). As a matter of fact, if one group is considered, S_{i+1} would be inversely proportional to the square of a, i.e. the spatial scaling depends on the energy grid. In any case, it is clear that, changing the size of the domain, the eigenvalue separation can be largely affected. In particular, Eq. (3) underlines the fact that when two or more eigenvalues are equal the EVS vanishes.

3.2. Space Convergence

First of all, grid independence and space convergence studies are performed in order to choose an appropriate number of spatial nodes for computational time and accuracy. It has been verified that 100 points per side (10^4 grid points) are sufficient to achieve a good agreement with the analytical solution for all the cases analysed (a=100, 200 and 300 cm).

3.3. Convergence Criteria

To assess the convergence of the eigenvalue problem, a double check on both the eigenvalues and the eigenvectors is needed. In FPM, the global convergence is verified computing the relative or

Table 1: Two-group data adopted to perform the study.

Parameter		Value
Fast absorption [cm^{-1}]	Σ_{a1}	9.78E-4
Thermal absorption [cm^{-1}]	Σ_{a2}	5.56E-3
Fast fission [cm^{-1}]	$\nu\Sigma_{f1}$	0
Thermal fission [cm^{-1}]	$\nu\Sigma_{f2}$	1.222E-2
Slowing down [cm^{-1}]	$\Sigma_{1\to2}$	3.08E-3
Fast diffusion coefficient [cm]	D_1	0.9416
Thermal diffusion coefficient [cm]	D_2	0.8150

absolute error on the eigenvalue with respect to the previous iteration, while the local convergence may be performed in different ways, involving the relative difference between the eigenvector absolute values or the norm of the residual of the eigen-problem.

The SSI check on convergence is similar, but it is performed on the eigenvalues of the matrix obtained after the Rayleigh-Ritz projection. When convergence is reached, the eigenpairs of the original problem can be computed solving the source problem on the whole domain. The IRA, on the other hand, allows to define a very convenient indicator, the so-called Ritz estimate [21], that is an equivalent but computationally cheaper indicator of the eigen-problem residual.

It is evident that to compare these methods their convergence criteria should be the same, in order to see how they respond to the same target accuracy. Therefore, the following convergence criteria are defined:

$$\left|\left|\hat{L}\phi_n - \frac{1}{k_n}\hat{F}\phi_n\right|\right|_2 < \varepsilon,\ n = 1, ..., N_{ev} \tag{4}$$

$$|k_n - k_{exact}| < \Delta k,\ n = 1, ..., N_{ev}, \tag{5}$$

where N_{ev} is the number of eigenvalues evaluated. The numbering of the eigenmodes in the following results is introduced for their identification without any relation to their space behaviour.

Figure 1 shows the behaviour of the residuals as a function of the number of iterations, i.e. number of single source calculations performed. It can be noticed that the SSI convergence criterion is good to assess the convergence of both eigenvalues and eigenvectors, since for a high number of iterations it oscillates in a stable way around machine precision. Figure 2 reports a comparison between Ritz estimates and residuals, showing that the former are good estimates until the numerical cancellation errors make them useless, forcing the user to rely on the residuals norm.

In Figure 3 it is possible to see that the convergence for IRA is faster than for the other methods, and after the resolution of the degeneracy, responsible for one single big oscillation, it stabilizes. SSI shows a convergence rate similar to FPM, without any serious problem related to the coupled eigenfunctions, except for the oscillating decreasing behaviour of the residuals before convergence is reached. On the other hand, the degeneracies are an issue for the FPM convergence, which is

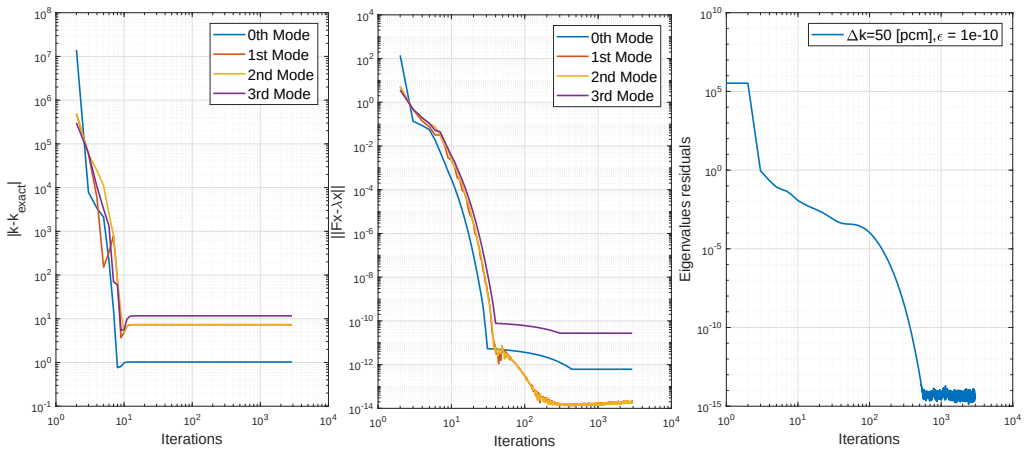

Figure 1: Comparison between integral (left) and local (center) convergence with respect to the convergence on the subspace iterations for the construction of the fission source appropriate for each eigenvectors (right).

not reached for higher-order modes. It is interesting to notice that the limited number of directions spanned by IRA and SSI limits their maximum accuracy, while FPM is able to find the fundamental harmonic with machine precision. If one increases the subspace sizes for IRA and SSI, the accuracy would improve. It should be mentioned that some oscillations due to numerical noise could appear in both IRA and SSI when the residuals stabilize on the lowest achievable tolerance. As a general conclusion, it can be stated that convergence for higher-order harmonics is a very delicate aspect, therefore very narrow tolerances need to be prescribed, especially when looking for the eigenpairs of a decoupled system.

3.4. Sub-Space Size Independence

After having set a number $N = 10^4$ of points as optimum for all the three domains, the effect of sub-space dimension on the number of iterations of SSI and restarts of IRA is studied, setting a fixed tolerance on the norm of the eigen-problem residual and on the absolute difference between exact and calculated eigenvalues. It must be remarked that both methods, as the power method and its versions, require an initial guess able to excite also the higher-order contributions; in this work a uniform random guess is adopted to be fair towards all methods. Because of this, the relation between sub-space dimension and numbers of iterations (SSI) or restarts (IRA) are affected by uncertainty and it may change according to the initial guess and to the eigenvalue separation, which depends on the reactor spatial scale, as proved by Eq. (3).

Figure 4 shows the different behaviour of SSI and IRA with respect to the subspace spanned. IRA proves to be better, requiring fewer restarts and being independent on the eigenvalue separation beyond a certain threshold value. A simple inspection of these graphs shows *ictu oculi* that the number of static source calculations in SSI is higher because of the higher number of iterations needed with respect to the number of IRA restarts, implying that (neglecting the small contributions to the total computational costs of QR-shifts for IRA and of eigenvalue computations for SSI) IRA

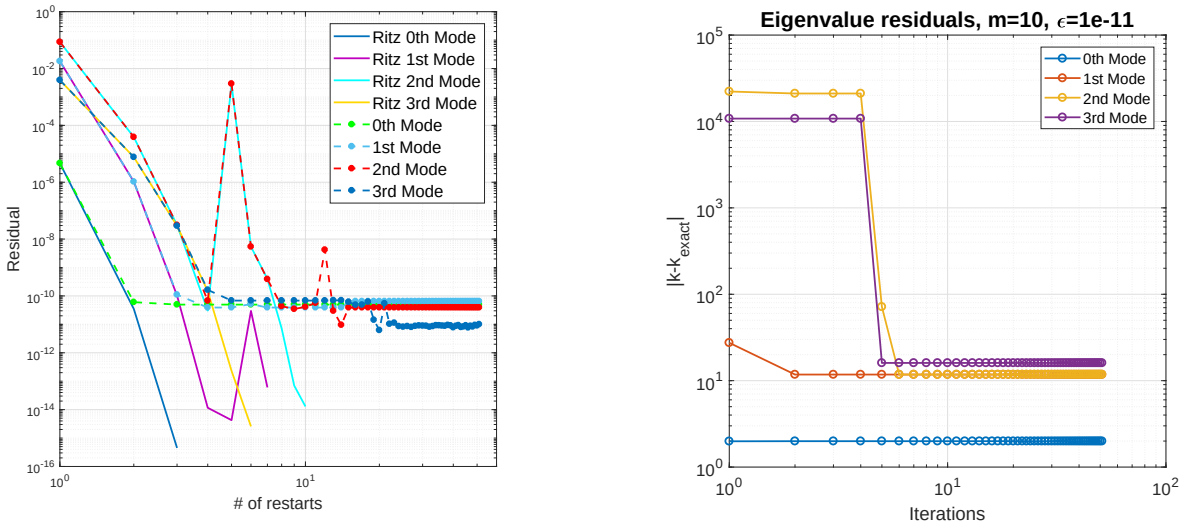

Figure 2: Comparison between Ritz estimate and residuals defined as in Eq. (5) (left) and eigenvalues residuals (right).

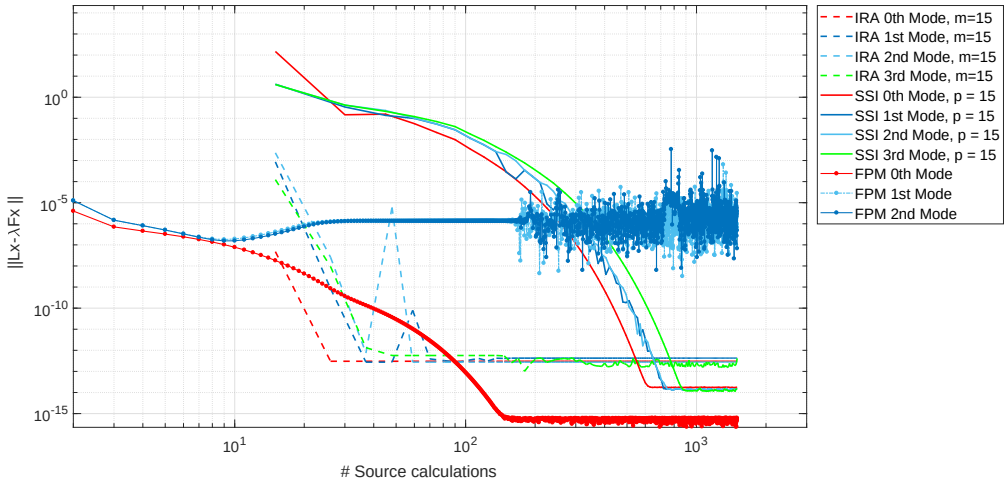

Figure 3: Comparison of residuals of IRA, SSI and FPM, for a calculation performed on a square with edge 300 cm. Since a number $p = 15$ of iterations is performed to start the calculations in both IRA and SSI, their residuals reported after these p calculations.

is faster. However, SSI is more suitable for parallel computing, since it is possible to evaluate the dominant directions independently.

3.5. Tolerance Influence

Tables 2 through 4 show the general trend of the algorithms for different convergence criteria. Both IRA and SSI converge, while FPM does not manage to converge to the second eigenpair, as shown

Figure 4: Number of iterations for SSI (left) and number of restarts for IRA (right).

in Figure 3. Decreasing the target tolerance ε, IRA does not change the residuals order of magnitudes, since it converges after one iteration to machine precision, while SSI progressively improves the eigenvectors convergence, consistently with Figure 1. Finally, the last row shows the number of source calculations needed to accomplish the convergence. It can be seen that, for a sufficient dimension of the Krylov subspace, m, IRA does not need to be restarted; therefore, the number of calculations for the m-step Arnoldi factorization, followed by the $(m - N_{ev})$-step factorization, is minimized. The other two methods need more iterations to achieve a lower tolerance, although SSI is faster and more precise. In particular, SSI seems to be very sensitive to the inner solver accuracy δ, since the number of calculations sharply increases, as can be seen comparing Table 3 and 4, even if the accuracy of the final results is the same.

Table 2: Comparison of methods for fixed convergence criteria, where δ is the linear solver precision (NC: convergence not reached).

$\varepsilon = 10^{-8}$	IRA		SSI		FPM	
$\Delta k = 50$ [pcm]	m=30		p=15			
$\delta = 10^{-10}$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$
Mode 0	1.026	3.72E-13	1.026	5.51E-12	21.4	6.22E-09
Mode 1	7.317	2.08E-13	7.317	6.88E-10	39.21	4.47E-09
Mode 2	7.317	2.12E-13	7.317	6.20E-10	NC	NC
Mode 3	11.668	3.99E-13	11.668	7.45E-09	NC	NC
Source calculations	56		480		NC	

3.6. Statistical Analysis of the Effect of the Initial Guess

Since both SSI and IRA require an initial random guess to excite all the higher-order harmonics, a statistical analysis is carried out to investigate the influence of the random initial guess on the performances and on the accuracy of the results. It is believed that this is an important aspect to be examined, because the FPM is known to be strongly dependent on the initial guess provided [9].

Table 3: Comparison of methods for fixed convergence criteria, where δ is the linear solver precision.

$\varepsilon = 10^{-10}$	IRA		SSI		FPM	
$\Delta k = 50$ [pcm]	m=30		p=15			
$\delta = 10^{-10}$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$
Mode 0	1.026	3.77E-13	1.026	5.00E-13	1.99	8.80E-11
Mode 1	7.317	2.82E-13	7.317	3.89E-12	12.2	7.50E-11
Mode 2	7.317	2.36E-13	7.317	1.95E-12	NC	NC
Mode 3	11.668	1.53E-13	11.668	7.21E-11	NC	NC
Source calculations	56		630		NC	

Table 4: Comparison of methods for fixed convergence criteria, where δ is the linear solver precision.

$\varepsilon = 10^{-10}$	IRA		SSI		FPM	
$\Delta k = 50$ [pcm]	m=30		p=15			
$\delta = 10^{-8}$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$	$\lvert k - k_{ex}\rvert$	$\lvert\lvert Lx - \lambda Fx\rvert\rvert$
Mode 0	1.026	3.40E-11	1.026	4.64E-12	1.99	8.27E-11
Mode 1	7.317	2.03E-11	7.317	8.94E-10	11.77	5.59E-11
Mode 2	7.317	2.40E-11	7.317	2.57E-11	11.65	5.19E-11
Mode 3	11.668	4.42E-11	11.668	4.87E-12	NC	NC
Source calculations	56		1485		NC	

The analysis is restricted to the 300 cm edge domain, using a limited number of directions, since with a sufficient subspace size the performances and the accuracy of the algorithms are practically unchanged. The analysis is focused on three aspects: i) the total number of source calculations required to match the target tolerances ($\Delta k = 50$ pcm and $\varepsilon = 10^{-10}$), ii) the accuracy on the residual and iii) the accuracy with respect to the analytic eigenvalues.

The histograms shown in Figure 5 are generated running the algorithms with different initial random vectors until the relative standard deviation on the average number of source calculations is lower than 0.20%. The number of SSI iterations is more statistically dispersed and always larger than for IRA. Hence, IRA proves to be less sensitive to random guesses than SSI. However, its peculiar behavior deserves some more investigations. When looking at the residuals statistical dispersion, IRA proves again to behave better showing a smaller dispersion and, in average, higher

Figure 5: Statistical distribution of the source calculations for SSI (for 3890 runs) and IRA (for 2039 runs).

accuracy.

4. APPLICATION TO A MODIFIED C5G7 CONFIGURATION

A recent investigation showed that heavy, stainless steel reflected large thermal reactors are affected by a flux tilt effect higher than in water reflected cores [3]. The analysis conducted so far showed that the EVS could be linked to the flux tilt, at least for fresh cores in Hot Zero Power (HZP) conditions. As a matter of fact, when feedback and depletion phenomena are considered, EVS seems to lose its importance, because of higher-order effects that can be evaluated only considering the dominant system modes, which are hard to be evaluated with FPM implemented in standard codes. To investigate such effects, an evaluation of the C5G7 [17] higher-order harmonics is carried out,

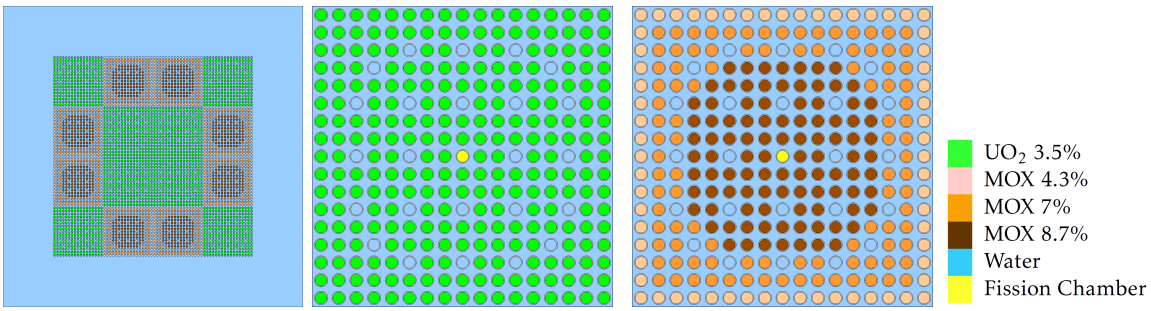

Figure 6: Geometrical configuration of the C5G7 core adopted in the simulation (left), uranium oxide fuel element (center), mixed oxide (MOX) fuel element (right) . The reflector is either water or stainless steel.

adopting the 6-group diffusion model, discretised with a finite element approach using the MATLAB pdetoolbox, which allows to solve eigenproblems using ARPACK routines. The Monte Carlo code SERPENT-2 [22] is adopted to generate the 6-group nuclear data. To account for feedback effects, different average temperatures in the different regions of the core are imposed. The reference core is slightly modified eliminating the aluminium layer that, in the specifications of the benchmark [23], had the purpose to simulate the Full Power (FP) reduced moderation conditions.

The HZP condition are represented assuming a temperature of 550 K for the whole domain. The FP conditions are represented by a temperature of 900 K for the pellet, 600 K for the cladding and 560 K for the reflector and the coolant.

The presence of the heavy reflector increases the value of k_{eff} of the system and, as Table 5 shows, the overall decoupling degree, as underlined by the slightly higher EVS.

Table 5: Eigenvalues for the first eight modes of C5G7 core with two kinds of reflector, in HZP conditions.

HZP	Stainless steel reflected C5G7		Water reflected C5G7	
	k_n	EVS	k_n	EVS
Mode 0	1.1531612	-	1.1358780	-
Mode 1	1.0050644	0.12778	0.96848731	0.15216
Mode 2	1.0050620	0	0.96848680	0
Mode 3	0.89550955	0.12173	0.85388233	0.13857
Mode 4	0.84022123	0.07347	0.79866534	0.08097
Mode 5	0.80535260	0.05153	0.76993643	0.04672
Mode 6	0.73011185	0.12796	0.69904709	0.13171
Mode 7	0.73011004	0	0.69904	0

In Table 6 the results for FP conditions are reported. As expected, the value of k_{eff} is reduced. The table shows that also the difference between the EVS for stainless steel and water reflector systems is reduced.

Table 6: Eigenvalues for the first eight modes of C5G7 core with two kinds of reflector, in FP conditions.

FP	Stainless steel reflected C5G7		Water reflected C5G7	
	k_n	EVS	k_n	EVS
Mode 0	1.1376518	-	1.1200937	-
Mode 1	0.98821405	0.13292	0.95172436	0.15794
Mode 2	0.98821169	0	0.95172383	0
Mode 3	0.87877035	0.12602	0.83728210	0.14361
Mode 4	0.82353652	0.07632	0.78260819	0.08343
Mode 5	0.78765979	0.05530	0.75326450	0.04977
Mode 6	0.71346748	0.13202	0.68310756	0.13634
Mode 7	0.71346575	0	0.68310638	0

5. CONCLUSIONS

An assessment of different methods for the evaluation of higher-order modes in nuclear systems is carried out. The comparison among filtered power, sub-space iteration and implicitly restarted Arnoldi methods has been carried out, analysing the number of source calculations performed, the residual behaviour and the influence of the initial guess.

The most promising method turns out to be IRA, because it is faster and more stable. Furthermore, it allows a certain operational flexibility: in fact, according to the memory storage capabilities, it is possible to speed-up the calculation reducing the number of restarts. In addition, its implementation in already existing codes should not be an issue thanks to the ARPACK library [13,21], that could be wrapped in deterministic solvers. Its main drawback is connected to the fact that IRA inherently requires series calculations, thus possibly limiting its parallelization options. On the other hand, the sub-space iteration method allows to perform the p-source calculations independently, guaranteeing a theoretical speed-up of order p, and to reduce the calculation domain to fissile regions, thus minimizing the cost of each iteration.

In conclusion, the implicitly restarted Arnoldi method is a more accurate and efficient algorithm, although the sub-space iteration method still deserves to be explored and tested with modern multiprocessors machines.

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