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Acceleration of external iterations using Chebyshev extrapolation in neutron diffusion theory

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Andrey Silva Pontes
Institution: Federal University of Western Pará, Institute of Engineering and Geosciences – Santarém, PA, Brazil
Higher degree of formation: Bachelor of Science and Technology.
E-mail: re.andrey.pontes@gmail.com

Lenilson Moreira Araujo
Institution: Federal University of Western Pará, Institute of Educational Sciences – Santarém, PA, Brazil.
Higher degree of training: Doctor of Nuclear Engineering.
E-mail: lenilson.moreira1@gmail.com

ABSTRACT
This research aims to analyze, compare, and validate the performance of Chebyshev polynomials applied to the acceleration of convergence of external iterations through extrapolation of the fission source. To solve the system of equations generated from the discretization via finite element method of the neutron diffusion equation, Crout's method was applied. Chebyshev's extrapolation method was implemented in the FORTRAN programming language. To validate this method, we used the IAEA and Homogeneous Reactor benchmarks, both two-dimensional defined at 2 and 3 energy groups, respectively. The results obtained from the tests with different mesh refinements demonstrate the effectiveness of the acceleration of the external iterations when different values are considered for the Chebyshev iterations, especially when compared to extrapolation via over-relaxation.

Keywords: Chebyshev, IAEA-2D, homogeneous reactor, neutron diffusion, source extrapolation.

1 INTRODUCTION

Benchmarks are an important tool for modeling reactor cores before a project is executed. In addition, the computational methods employed to solve these problems can be performed in the most severe conditions, simulating phenomena that occur in the most diverse areas of nuclear engineering. Given the above, we have that it is possible to simulate and analyze the distribution of neutrons as well as their rate of variation, within a control volume.

To this end, one can solve the equation of neutron diffusion to multigroups of energy numerically to obtain the eigenvalue corresponding to the criticality state of the reactor. Several methods can be used for the purpose of accelerating the convergence process to obtain the solution of this equation and calculate both the effective multiplication factor and the neutron flux within a reactor.

Thus, this research aims to compare and analyze the behavior of Chebyshev acceleration and over-relaxation acceleration applied to the fission source, focusing mainly on the number of partitions used in each mesh and the runtime that is intrinsically related to the number of iterations.

2 THEORETICAL FRAMEWORKS

2.1 DISCRETIZATION OF THE NEUTRON DIFFUSION EQUATION

The neutron diffusion equation is an elliptical-type partial derivative equation (EDP) that describes the variation in neutron density in a control volume and represents the balance between neutron loss and production within that volume (Roza, 2013). For the development of the numerical analysis of the neutron diffusion equation we used the classical Finite Element Method (FEM) (Liu & Rincon, 2013) a to treat the spatial dependence of the problem in order to obtain its numerical solution. The equation of neutron diffusion in two-dimensional Cartesian geometry, in its multigroup form, is given by

$$-\nabla \cdot D_g(r)\nabla\Phi_g(r) + \Sigma_{r,g}(r)\Phi_g(r) = \sum_{g'\neq g}^{G} \Sigma_{s,g',g}(r)\Phi_{g'}(r) + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(r)\Phi_{g'}(r), \qquad (1.a)$$

$$g = 1, \dots, G,$$

$$\forall\, r = (x, y) \in \Omega \subset \mathbb{R}^2$$

Where all terms are defined in the usual way as in (Duderstadt & Hamilton, 1976).

Through from the principle of orthogonality of functions (Galerkin method) the neutron diffusion equation is transformed into an abstract variational problem. This variational form is discretized into subregions that are here called elements, as follows.

$$\sum_{e=1}^{Ne}\left[\int_{\Omega_e} D_g^e \nabla N^{eT}\Phi_g^e \nabla N^e d_\Omega + \int_{\Omega_e} \Sigma_{r,g}^e N^{eT}\Phi_g^e N^e d_\Omega - \int_{\partial\Omega} D_g^e q_g^e N^e ds\right] = \sum_{e=1}^{Ne}\left[\int_{\Omega_e}\left(\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}^e N^{eT}\Phi_{g'}^e + \sum_{g'\neq g}\Sigma_{s,g',g}^e N^{eT}\Phi_{g'}^e\right)N^e d_\Omega\right], \qquad (1.b)$$

$$g = 1, \dots, G,$$

$$\forall\, e \subset \in \Omega \subset \mathbb{R}^2$$

For the construction of this variational formulation the neutron flux is established as being a linear combination within each of the elements that make up the spatial domain of the problem. All the detail of the process of discretization of the neutron diffusion equation by the finite element method

can be found in (Pessoa et al., 2018). These procedures convert the EDP into a large algebraic linear system. To solve this system, a direct method was used to solve this system, described in item 3, section 3.1.

2.2 THE EIGENVALUE k_{eff}

Or eigenvalue that can be determined by relating the number of fissions of one generation to the number of fissions of the previous generation. Beingk_{eff}

$$\begin{cases} k_{eff} = 1 & Crítico \\ k_{eff} < 1 & Subcrítico \\ k_{eff} > 1 & Supercrítico \end{cases}$$

Starting from this Physical definition, it is essential that there is the balance of the chain reactions inside the reactor core. The proportion of neutron production and loss must then be maintained so that the chain reaction is self-sustaining.

The eigenvalue k_{eff} can be obtained by the relation

$$k_{eff}^{i+1} = k_{eff}^{i} \frac{\int F_{i+1}\, dV}{\int F_i\, dV}\,. \qquad (2a)$$

Where is the iteration index, is the effective neutron multiplication factor and is the fission source given by$ik_{eff}^{i}F_i$

F_i

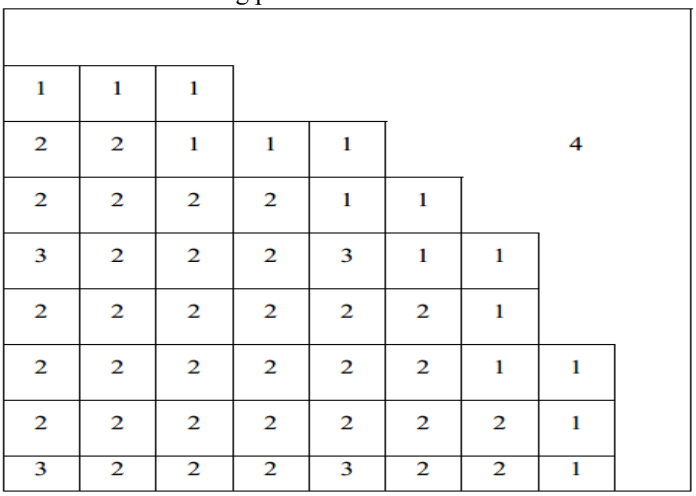
$$= \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(r)\Phi_{g'}^{i}(r). \qquad (2b)$$

The effectiveness of computational calculation seeks the convergence of flow and eigenvalue for as few iterations as possible. However, in more severe problems, making the method converge can be difficult. Because of its relevance, the validation of techniques that aim to accelerate this process is of great importance. Therefore, it is of paramount importance to study methods that seek to accelerate convergence, reducing the number of iterations necessary to obtain a certain level of precision for the flow distribution and flow. In this article, the methodology we use to accelerate the iterative process is set forth in item 3, sections 3.2, 3.3 and 3.4.$\Phi_g^i k_{eff}^i k_{eff} \Phi_g$

2.3 BENCHMARKS

IAEA – 2D. This benchmark has been a very important problem for evaluating the performance of methods in the area of reactor physics (Omara, Amin & Khalaf, 2015). This is a problem modeled on two energy groups. In its two-dimensional configuration this reactor is formed by 177 fuel elements of dimension 20 x 20 cm². The core data are available in the cited reference.

Figure 1- 1/4 radial loading pattern of the IAEA-2D benchmark core.



Homogeneous Reactor. For the Homogeneous benchmark (Han, Dulla & Ravetto, 2009), the dimensions considered are 160 × 140 cm². The test model is the 3 energy groups, and the nuclear data are available in the cited reference.

3 METHODOLOGIES

The methods tested during the simulations were implemented in Fortran 90. For the resolution of the linear system generated by discretization of Eq. (1a) via the finite element method, the direct Crout method, described in section 3.1, was used. For comparative analysis of the acceleration of external iterations, we used the methods of acceleration by over-relaxation and Chebyshev extrapolation, described in sections, sections 3.2 and 3.3, respectively.

3.1 CROUT'S ALGORITHM

The linear system derived from the method of the elements has the form. To solve it, it was used $A\boldsymbol{\Phi_g} = b$the direct Crout method which is a particular case of LU factorization. To avoid excessive storage of arrays, the solution is stored in the vector (Liu & Rincon, 2013)b . Considering the matrix decomposed in the form of Eq. (3), one must then stipulate the solution .$\boldsymbol{\Phi_g} = (\Phi_g^1, \Phi_g^2, \dots, \Phi_g^n)$

$$A\boldsymbol{\Phi_g} = (U^T DU)\boldsymbol{\Phi_g} = b \quad (3)$$

Where A is a symmetric matrix, U is the upper triangular matrix and D is the matrix of the diagonal elements. Crout's algorithm can be implemented according to the structure below

Crout algorithm
1: ***do*** $j = 2,3,\ldots,n$
2: ***do*** $i = 2,3,\ldots,j-1$
3: $A_{ij} = A_{ij} - \sum_{k=1}^{i-1} A_{ki}A_{kj}$
4: ***end do***
5: ***do*** $i = 1,2,\ldots,j-1$
6: $T = A_{ij}$
7: $A_{ij} = T \,/\, A_{ii}$
8: $A_{jj} = A_{jj} - TA_{ij}$
9: ***end do***
11: ***end do***
12: ***do*** $j = 2,3,\ldots,n$
13: $b_j = b_j - \sum_{i=1}^{j-1} A_{ij}b_i$
14: ***end do***
15: ***do*** $j = 1,2,\ldots,n$
16: $b_j = b_j \,/\, A_{jj}$
17: ***end do***
18: ***do*** $j = n, n-1,\ldots,2$
19: ***do*** $i = 1,2,\ldots,j-1$
20: $b_i = b_i - A_{ij}b_j$
21: ***end do***
22: ***end do***

3.2 ACCELERATION OF EXTERNAL ITERATIONS USING OVER-RELAXATION

To accelerate the convergence of external iterations, the method of over-relaxation extrapolation is used to improve iterations in flow (Lewis & Miller, 1984). The over-relaxation applied to the source of fission caused by neutrons is described by

$$\tilde{F}_{i+1} = \omega_f\left(F_i - \tilde{F}_i\right) + \tilde{F}_i \quad (4)$$

Where, is the source of unextrapolated fission, obtained by Eq. (2b), is the extrapolated term and is the over-relaxation parameter for the source.$F\tilde{F}_i\omega_f$

For extrapolation by over-relaxation, we have that, where for every value greater than 1, we have over-relaxation. If, then$1 \leq \omega < 2\omega = 1$

$$\tilde{F}_{i+1} = F_i \quad (5)$$

3.3 ACCELERATION OF EXTERNAL ITERATIONS USING CHEBYSHEV EXTRAPOLATION OF A PARAMETER

Chebyshev's method (Alvim, 2007) to a variable parameter uses a linear combination of fission sources in the iterations and, through the relation$pp + 1$

$$\tilde{F}_{p+1} = F_{p+1} \cdot \theta^{(p+1)} + \tilde{F}_p \cdot \left(1 - \theta^{(p+1)}\right). \quad (6)$$

Where is the source of fission without extrapolation obtained by Eq. (2b), is the extrapolated term. Chebyshev extrapolation is then applied over the course of iterations in order to increase the speed of eigenvalue convergence. $F_{p+1}\tilde{F}_p Lk_{eff}$ For this, one must choose those that minimize the residues of the source vector, in this case the fission source, in relation to the fundamental eigenvector, in this case the solution vector, after the Chebyshev iteration.$\theta^{(p)}\Phi_g L - ésima$

The reason for dominance is defined by

$$\sigma = \frac{\lambda_2}{\lambda_1} < 1. \quad (8)$$

Where

$$\frac{\lambda_2}{\lambda_1} = \frac{k_{eff}^{(p+1)}}{k_{eff}^{(p)}}.$$

The aforementioned minimization process leads to

$$\theta^{(p+1)} = \frac{1}{1 - \left(\frac{\sigma}{2}\right)\left[\xi_{(p+1)} + 1\right]} \quad , \quad p = 0, \ldots, L-1 \quad (9)$$

Being

$$\xi_{(p+1)} = cos\left[\frac{\pi}{2L}(2p+1)\right] \quad p = 0, \ldots, L-1. \quad (10)$$

The number of Chebyshev iterations must be pre-fixed. With values of very large, the values of will also have high magnitude. That is, and will have contrary signs and same order of magnitude, thus propagating errors in the source calculated by extrapolation, when approaching. One can avoid

this setback by defining a small number of iterations using extrapolation repeatedly.$LL\theta^{(p)}\theta^{(p)}(1-\theta^{(p)})\ F_{p+1}\ F_pL$

3.4 SCHEMA FOR ACCELERATING EXTERNAL ITERATIONS

Eq is used. (2a) to update the eigenvalue every iteration. However, to speed up external iterations, the extrapolated sources defined by Eq. (4) or by Eq. (6). In addition, the extrapolated sources are also considered during the construction of the vector from the linear system corresponding to Eq. (3).$k_{eff}^{i}ib$

4 RESULTS AND DISCUSSIONS

We got the results of the test problems considering meshes with four and five distinct amounts of elements. Tables 1 and 2 present the solutions for the cases without applying acceleration methods at the source. For the cases with acceleration, presented in tables 3 and 4, the number of Chebyshev iterations 3, 5, 7 and 15 was used. For acceleration by extrapolation, tables 5 and 6, we define the parameter as the optimal value of 1.40 (Pontes & Araujo, 2018). $L\ \omega_f$Or Total number of iterations present in all tables refers to the sum of the internal and external flow iterations. In all simulations, the tolerance parameters and for the internal and external iterations were used, respectively. The reference values of the IAEA-2D benchmark were extracted from the master's thesis (Dias, F.C., 1999).$\varepsilon_1 = 10^{-6}\varepsilon_2 = 10^{-9}$

Table 1- Results for the IAEA benchmark without acceleration of external iterations.

IAEA – 2D			
Number of Elements	Total Iterations	k_{eff}	Time(s)
289	690	1,03105	5
1156	714	1,02982	38
2061	711	1,02966	253
4624	693	1,02961	1018
7225	687	1,02959	3199

Table 2- Results for the Homougeneous Reactor benchmark without acceleration of external iterations.

Homogeneous Reactor			
Number of Elements	Total Iterations	k_{eff}	Time(s)
224	107	0,90193	1
896	105	0,90205	15
2016	105	0,90207	136
3584	101	0,90207	678

Table 3- Results for the IAEA benchmark accelerating the convergence of external iterations by Chebyshev extrapolation.

As L = 3			
Number of Elements	Total Iterations	k_{eff}	Time(s)
289	390	1,03105	3
1156	366	1,02982	27

2061	405	1,02966	185
4624	351	1,02961	785
7225	351	1,02959	2674
Like L = 5			
289	339	1,03105	3
1156	369	1,02982	26
2061	402	1,02966	177
4624	312	1,02961	750
7225	378	1,02959	2743
As L = 7			
289	354	1,03105	3
1156	351	1,02982	26
2061	384	1,02966	181
4624	396	1,02961	800
7225	342	1,02959	2671
As L = 15			
289	381	1,03105	3
1156	405	1,02982	28
2061	399	1,02966	179
4624	402	1,02961	807
7225	402	1,02959	2780

Table 4 - Results for the Homougeneous Reactor benchmark accelerating the convergence of external iterations by Chebyshev extrapolation.

As L = 3			
Number of Elements	Total Iterations	k_{eff}	Time(s)
224	1547	0,90193	9
896	105	0,90205	12
2016	93	0,90207	92
3584	106	0,90207	474
Like L = 5			
224	237	0,90193	2
896	98	0,90205	12
2016	100	0,90207	94
3584	117	0,90207	424
As L = 7			
224	864	0,90193	7
896	95	0,90205	12
2016	73	0,90207	94
3584	95	0,90207	247
As L = 15			
224	131	0,90193	1
896	130	0,90205	14
2016	138	0,90207	106
3584	133	0,90207	504

Table 5 - Results for the IAEA benchmark accelerating the convergence of external iterations using over-relaxation.

$\omega_f = 1.4$			
Number of Elements	Total Iterations	k_{eff}	Time(s)
289	473	1,03105	3
1156	584	1,02982	31
2061	601	1,02966	201
4624	445	1,02961	897
7225	453	1,02959	2932

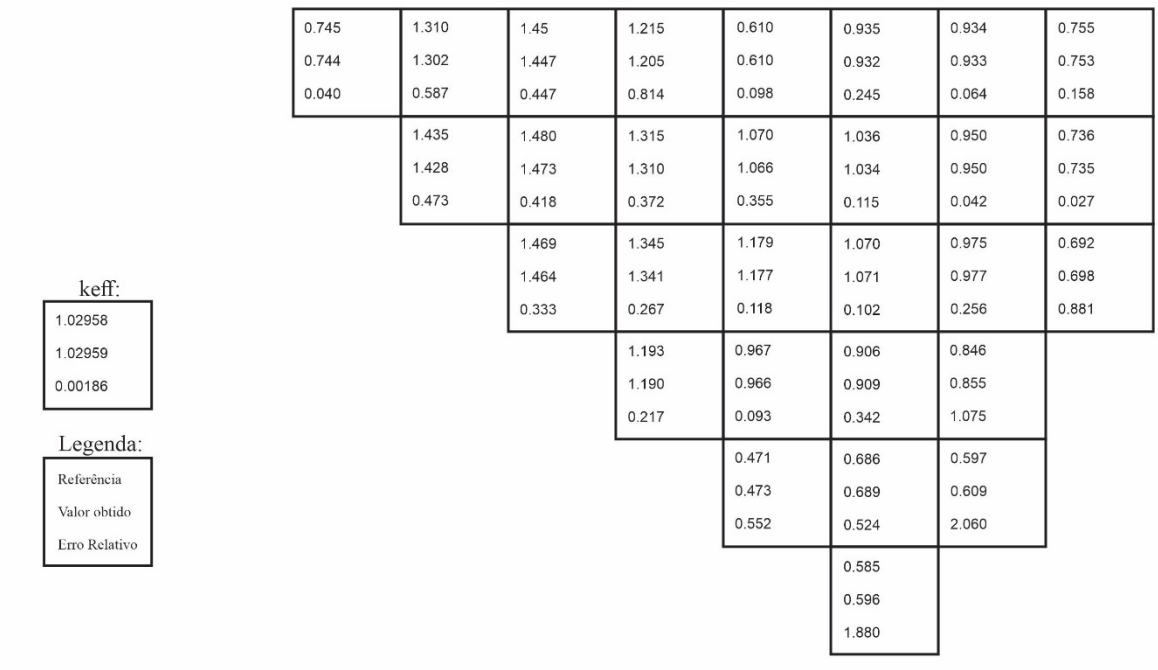
Table 6 - Results for the Homogeneous Reactor benchmark accelerating the convergence of external iterations using over-relaxation.

$\omega_f = 1.4$			
Number of Elements	Total Iterations	k_{eff}	Time(s)
224	84	0,90205	2
896	80	0,90207	13
2016	80	0,90207	120
3584	81	0,90205	660

Checking tables 3 and 4, we noticed that the acceleration of external iterations via Chebyshev extrapolation demonstrated better performance when the number of Chebyshev iterations is equal to 5 in most meshes for the IAEA-2D benchmark. For the benchmark Homogeneous Reactor L equal to 7 is the one that provided better performance in the acceleration of external iterations. However, it was found that as the mesh L=7 is refined, it proves to be the optimal value for both benchmarks.*L*

Comparing now these results with the method of acceleration of external iterations via over-relaxation, shown in tables 5 and 6, we realize that, even so, Chebyshev extrapolation is more efficient and, of course, the acceleration method also becomes advantageous compared to cases without acceleration. The results presented in Figure 2 were obtained using a mesh with 7225 elements using Chebyshev extrapolation with L=7. The results obtained reveal that employing methods of acceleration of iterations to obtain a faster convergence does not interfere significantly in the numerical result of the Eq. (1), as can be seen in Figure 2, and also provides benefits with regard to computational calculation time.

Figure 2- Comparison of the eigenvalue and the normalized power density for 1/8 of the core of the IAEA-2D benchmark.



5 CONCLUSIONS

The yield of the acceleration methods of the external iterations, based on the numerical simulations performed, reveals that the optimal value for the number of Chebyshev iterations is for both benchmarks. Comparing then with the method of extrapolation by over-relaxation, which is a particular case of Chebysev extrapolation with a fixed parameter, we realize that Chebysev extrapolation continues with better performance. Finally, in all cases where we employed the acceleration methods for the external iterations, numerical solutions were obtained more quickly. However, without suffering significant disturbances from acceleration methods, thus minimizing the computational cost substantially. $LL = 7$

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