Optimized Eigenvalue Solvers for the Neutron Transport Equation

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Abstract. A discrete ordinates method has been developed to approximate the neutron transport equation for the computation of the lambda modes of a given configuration of a nuclear reactor core. This method is based on discrete ordinates method for the angular discretization, resulting in a very large and sparse algebraic generalized eigenvalue problem. The computation of the dominant eigenvalue of this problem and its corresponding eigenfunction has been done with a matrix-free implementation using both, the power iteration method and the Krylov-Schur method. The performance of these methods has been compared solving different benchmark problems with different dominant ratios.

Keywords: Neutron Transport, Discrete Ordinates, Eigenvalues.

1 Introduction

Neutron transport simulations of nuclear systems are an important goal to ensure the efficient and safe operation of nuclear reactors. The steady-state neutron transport equation [4] predicts the quantity of neutrons in every region of the reactor and thus, the number of fissions and nuclear reactions. The neutron transport equation for three-dimensional problems is an equation defined in a support space of dimension 7, and this makes that high-fidelity simulations using this equation can only be done using super computers.

Different approximations have been successfully used for deterministic neutron transport. They eliminate the energy dependence of the equations by means of the a multi-group approximation and use a special treatment to eliminate the dependence on the direction of flight of the incident neutrons. The angular discretization of the neutron transport equation chosen in this work has been the Discrete Ordinates method (S_N), which is a collocation method based on a

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quadrature set of points for the unit sphere, [4], obtaining equations depending only on the spatial variables. A high-order discontinuous Galerkin finite element method has been used for the spatial discretization. Finally, a large algebraic generalized eigenvalue problem with rank deficient matrices must be solved.

The eigenvalue problem arising from the different approximations to the deterministic neutron transport equations is classically solved with the power iteration method. However, Krylov methods are becoming increasingly popular. These methods permit to solve the eigenvalue problem faster when the power iteration convergence decreases due to high dominance ratios. They also permit to compute more eigenvalues than the largest one. We study the advantage of using a Krylov subspace method such as the Krylov-Schur method for these generalized eigenproblems, compared to the use of simpler solvers as the power iteration method.

The rest of the paper is organized as follows. Section 2 describes the angular discretization method employed. Then, Section 3 briefly reviews the power iteration method and the Krylov-Schur methodology to solve the resulting algebraic eigenvalue problem. In Section 4 some numerical results are given for one-dimensional problems in order to check which is the optimal quadrature order in the S_N method and the performance of the eigenvalue solvers. Lastly, the main conclusions of the work are summarized in Section 5.

2 The Discrete Ordinates Method

The energy multigroup neutron transport equation, which describes the neutron position and energy, can be written as

$$\mathcal{L}_g \psi_g = \sum_{g'=1}^{G} \left(\mathcal{S}_{g,g'} + \frac{1}{\lambda} \chi_g \mathcal{F}_{g'} \right) \psi_{g'}, \qquad g = 1, \ldots, G \tag{1}$$

where ψ_g is the angular neutron flux of energy group g. $\mathcal{L}_g$ is the transport operator, $\mathcal{S}_{g,g'}$ is the scattering operator and $\mathcal{F}_{g'}$ is the fission source operator. They are defined as

$$\mathcal{L}_g \psi_g = \Omega \cdot \nabla \psi_g + \Sigma_{t,\,g} \psi_g \,, \tag{2}$$

$$\mathcal{S}_{g,g'} \psi_{g'} = \int_{(4\pi)} \Sigma_{s,\,gg'} \psi_{g'} \mathrm{d}\Omega' \,, \tag{3}$$

$$\mathcal{F}_{g'} \psi_{g'} = \frac{1}{4\pi} \nu_{g'} \Sigma_{f,g'} \int_{(4\pi)} \psi_{g'} \mathrm{d}\Omega' \,, \tag{4}$$

where $\Sigma_{t,\,g}$, $\Sigma_{s,\,gg'}$ and $\Sigma_{f,g'}$ are the total, scattering and fission cross sections. ν_g is the average number of neutrons produced per fission. Finally, Ω is the unitary solid angle.

This equation is discretized in the angular variable by means of a collocation method on a set of quadrature points of the unit sphere, $\{\Omega_n\}_{n=1}^{N'}$ with their

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respective weights $\{\omega_n\}_{n=1}^{N'}$. This method is referred as the *Discrete Ordinates* method, S_N [4].

At this point, the scattering cross section is expanded into a series of Legendre polynomials as

$$\Sigma_{s,\,gg'}(\mathbf{r},\,\Omega'\cdot\Omega)=\sum_{l=0}^{L}\frac{l+1}{4\pi}\Sigma_{s,\,gg',l}(\mathbf{r})P_l(\Omega'\cdot\Omega) \tag{5}$$

where the expansion is usually truncated at $L=0$, assuming isotropic scattering.

The addition theorem of the spherical harmonics gives an expression for $P_l(\Omega'\cdot\Omega)$ as a function of Y_l^m and Y_l^{m*}. Making use of this expression an the orthogonality properties of the spherical harmonics, the scattering source (3) becomes

$$\mathcal{S}_{g,g'}\psi_{g'}=\sum_{l=0}^{L}\Sigma_{s,\,gg',l}\sum_{m=-l}^{l}Y_l^m\phi_{g',\,ml} \tag{6}$$

where $\phi_{g',\,ml}$ is the flux moment. The scattering source term calculation is performed projecting it in the spherical harmonics basis. So the projector moment-to-direction operator is expressed as follows

$$\psi(\mathbf{r},\,\Omega)=\mathcal{M}\phi(\mathbf{r})=\sum_{l=0}^{L}\sum_{m=-l}^{l}Y_l^m(\Omega)\phi_{ml}(\mathbf{r}) \tag{7}$$

and the direction-to-moment operator is

$$\phi_{ml}(\mathbf{r})=\mathcal{D}\psi(\mathbf{r},\,\Omega)=\int_{(4\pi)}d\Omega\,Y_l^{m*}(\Omega)\psi(\mathbf{r},\,\Omega) \tag{8}$$

where generally $\mathcal{L}\neq\mathcal{M}^{-1}$.

Using the angular discrete ordinates quadrature set the discrete ordinates equation is written as

$$\mathcal{L}_{g,n}\psi_{g,n}=\mathcal{M}_n\sum_{g'=1}^{G}\mathcal{S}_{g,g'}\mathcal{D}\psi_{g'}+\frac{\chi_g}{\lambda}\sum_{g'=1}^{G}\mathcal{F}_{g'}\phi_{g'}^0\,, \tag{9}$$
$$g=1,\,\ldots,\,G,\qquad n=1,\,\ldots,\,N',$$

where

$$\psi_{g,n}(\mathbf{r})=\psi(\mathbf{r},\,\Omega_n) \tag{10}$$

and the transport and fission operators are redefined by

$$\mathcal{L}_{g,\,m}\psi_{g,\,n}=\Omega\cdot\nabla\psi_{g,\,n}+\Sigma_{t,\,g}\psi_{g,\,n}\,,$$
$$\mathcal{F}_{g'}\psi_{g'}=\frac{1}{4\pi}\nu_{g'}\Sigma_{f,g'}\psi_{g'}\mathrm{d}\Omega'\,,$$

The angular discretization to the boundary conditions is applied in a straightforward way, because it we can be applied for the specific set of directions used.

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3 Eigenvalue Calculation

The following algebraic generalized eigenvalue problem is obtained from equation (9).

$$\mathbf{L}\Psi = \mathbf{MSD}\Psi + \frac{1}{\lambda}\mathbf{XFD}\Psi \tag{11}$$

where each matrix is the result of the energetic, angular and spatial discretization of neutron transport operators. Equation (11) can be arranged into an ordinary eigenvalue problem of the form

$$\mathbf{A}\Phi = \lambda\Phi\,, \tag{12}$$

where $\mathbf{A} = \mathbf{DH}^{-1}\mathbf{XF}$, $\mathbf{H} = \mathbf{L}-\mathbf{MSD}$ and $\Phi = \mathbf{D}\Psi$. In particular, the solution of the system involving $\mathbf{H}$ is performed as $\mathbf{H}^{-1}v = (\mathbf{I} - \mathbf{L^{-1}MSD})^{-1}\mathbf{L}^{-1}v$, which greatly reduces the number of iterations needed to solve the system, where $\mathbf{L}^{-1}$ is the most costly operation known as the *transport sweep*.

It must be said that all the matrices involved in this computation are large and sparse. They can have more than hundreds of millions of rows and columns. Then, we cannot explicitly compute the inverse of any of these matrices. Moreover all of these matrices are computed on the fly using a matrix-free scheme [3].

To solve the ordinary eigenvalue problem (12) only the multiplication by the matrix $\mathbf{A}$ is available. Each multiplication is usually called an outer iteration and the total number of outer iterations is defined as O.

The matrices $\mathbf{L}$, $\mathbf{M}$ and $\mathbf{D}$ are block diagonal where each block corresponds to the transport equation for a particular energy group. If a problem does no have up-scattering, the $\mathbf{S}$ is block lower triangular. In that case, the action of the operator $\mathbf{H}$ on a vector is calculated by block forward substitution for each group from high to low energy in a sequence. Each forward substitution requires solving the spatially discretized S_N equations for a single energy group, which is called the source problem [7]. This source problem is usually solved by using an iterative method. The iterations used to solve each source problem are called inner iterations, and the total number of inner iterations used to solve the source problems for every energy group and for every outer iteration is denoted by I. It is worth to notice that each inner iteration performs exactly one transport sweep, so we can expect the computational time to be proportional to the number of transport sweeps, and thus, proportional to the number of inner iterations I.

3.1 Power Iteration method

The power iteration method to solve the eigenvalue problem (12) reads as the iterative procedure

$$\Phi^{i+1} = \frac{1}{\lambda^{(i)}}\mathbf{A}\Phi^{i}, \tag{13}$$

where the fundamental eigenvalue is updated at each iteration according to the Rayleigh quotient

$$\lambda^{(i+1)} = \lambda^{(i)}\frac{\Phi^{(i)T}XF\Phi^{(i+1)}}{\Phi^{(i)T}XF\Phi^{(i)}}\,, \tag{14}$$

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where $\Phi^{(i)} = D\Psi^{(i)}$. It has been observed that using Rayleigh quotient for the eigenvalue can usually improve the efficiency of the power iteration method by providing a better estimate (earlier) of the eigenvalue.

Power iteration will converge to the eigenvalue of largest magnitude, k_{eff}. If more than one eigenvalue is requested a deflation technique should be used. In other words, it can be computed one harmonic at a time while decontaminating the subspace of the computed eigenvalue. However, the deflation technique has a very slow convergence. The convergence rate is determined by the dominance ratio $\delta = |\lambda_2|/|\lambda_1|$, where λ_2 is the next largest eigenvalue in magnitude [7]. Convergence of the power iteration method slows as $\delta \to 1.0$.

3.2 Krylov-Schur method

The Krylov-Schur method is an Arnoldi method which uses an implicit restart based on a Krylov-Schur decomposition [6]. This technique permits to solve more than one eigenvalue without an excessive extra computational cost. In this work, the Krylov-Schur method algorithm has been implemented using the eigenvalue problem library SLEPc [1]. The Arnoldi method is based on the creation of a Krylov subspace of dimension m,

$$\mathcal{K}_m(A, \Phi^{(0)}) = \text{span}\{\Phi^{(0)},\ \mathbf{A}\Phi^{(0)}, \ldots,\ \mathbf{A}^{m-1}\Phi^{(0)}\}. \tag{15}$$

If V_m is a basis of the Krylov subspace of dimension m the method is based on the Krylov decomposition of order m,

$$AV_m = V_m B_m + v_{m+1} b*_{m+1}, \tag{16}$$

in which matrix B_m is not restricted to be an upper Hessenberg matrix and b_{m+1} is an arbitrary vector.

Krylov decompositions are invariant under (orthogonal) similarity transformations, so that

$$AV_m Q = V_m Q(Q^T B_m Q) + v_{m+1} b_{m+1}^T Q,$$

with $Q^T Q = I$, is also a Krylov decomposition. In particular, one can choose Q in such way that $S_m = Q^T B_m Q$ is in a (real) Schur form, that is, upper (quasi-)triangular with the eigenvalues in the 1×1 or 2×2 diagonal blocks. This particular class of relation, called Krylov-Schur decomposition, can be written in block form as

$$A\begin{pmatrix}\tilde{V}_1 & \tilde{V}_2\end{pmatrix} = \begin{pmatrix}\tilde{V}_1 & \tilde{V}_2\end{pmatrix}\begin{pmatrix}S_{11} & S_{12} \\ 0 & S_{22}\end{pmatrix} + v_{m+1}\begin{pmatrix}\tilde{b}_1^T & \tilde{b}_2^T\end{pmatrix},$$

and has the nice feature that it can be truncated, resulting into a smaller Krylov-Schur decomposition,

$$A\tilde{V}_1 = \tilde{V}_1 S_{11} + v_{m+1}\tilde{b}_1^T,$$

that can be extended again to order m.

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4 Numerical Results

4.1 Seven-Region Heterogeneous Slab

A seven-region one-dimensional slab is solved in order to show the capability of the discrete ordinate method to approximate accurately the neutron transport equation. Figure 1 shows the geometry definition of this problem and Table 1 displays the one energy group cross sections. This benchmark was defined and solved using the Green's Function Method (GFM) in [2].

Table 2 shows a comparison for different quadrature orders of the discrete ordinates method of the first 4 eigenvalues of the 1D heterogenoeus slab problem and their error. The eigenvalue error is defined in pcm $\Delta\lambda = 10^5 \left|\lambda - \lambda_{\text{ref}}\right|$ where λ_{ref} is the reference eigenvalue extracted from [2].

Figure 2 shows the neutron flux distribution for the fundamental eigenvalue using S_4, S_{16} and S_{64}. In Figure 3, we can observe an exponential convergence of all the eigenvalues with the quadrature order, N, in the discrete ordinates method.

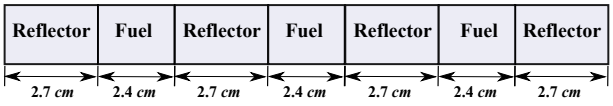

Fig. 1: Geometry of the seven region heterogeneous slab.

Table 1: Eigenvalues results for the 1D heterogeneous slab.

Material	$\nu\boldsymbol{\Sigma_f}(\text{cm}^{-1})$	$\boldsymbol{\Sigma_s}$ (cm^{-1})	$\boldsymbol{\Sigma_t}$ (cm^{-1})
Fuel	0.178	0.334	0.416667
Reflector	0.000	0.334	0.370370

Table 2: Eigenvalues results for the 1D heterogeneous slab.

	$\mathbf{k_{eff}}$	$\boldsymbol{\Delta k_{eff}}$	λ_2	$\boldsymbol{\Delta\lambda_2}$	λ_3	$\boldsymbol{\Delta\lambda_3}$	λ_4	$\boldsymbol{\Delta\lambda_4}$
$\mathbf{S_4}$	1.15885	1476	0.74012	1841	0.53128	2049	0.16603	4602
$\mathbf{S_{16}}$	1.17319	42	0.75808	45	0.55139	38	0.21053	152
$\mathbf{S_{64}}$	1.17359	2	0.75850	3	0.55175	2	0.21200	5
GFM	1.17361		0.75853		0.55177		0.21205	

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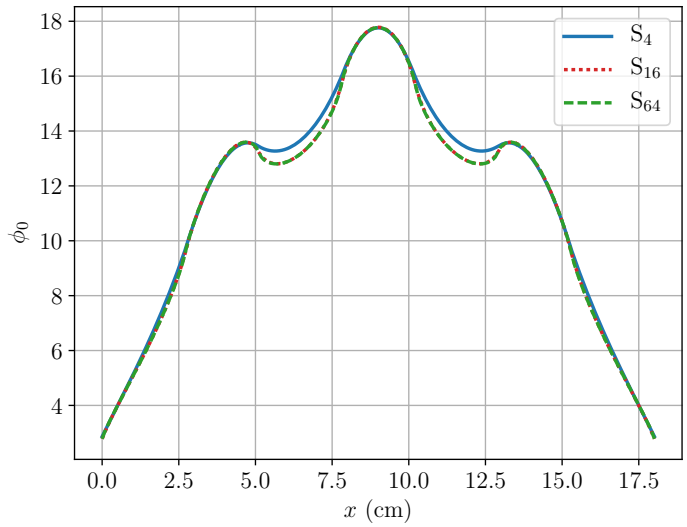

Fig. 2: Scalar neutron flux solution for the fundamental eigenvalue.

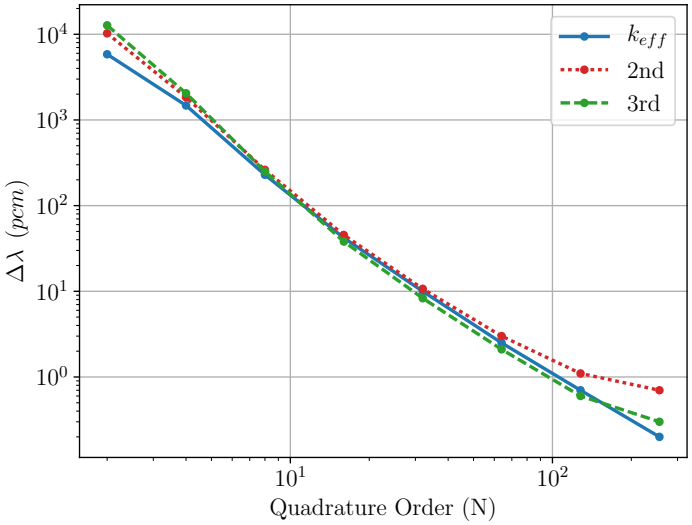

Fig. 3: Eigenvalue errors for the 1D heterogeneous slab.

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4.2 MOX Fuel Slab

The second numerical example studied corresponds to a one-dimensional mixed oxide (MOX) problem, derived from the C5G7 benchmark [5]. The MOX fuel geometry is defined in Figure 4. The assemblies definition and the materials of each assembly are described in Figures 5a and 5b. Seven group cross section data are given in reference [5]. In this work, up-scattering has been neglected and different problems with different dominance ratios, δ, have been defined changing the pin size from 1.26 cm to 1.50 cm and 2.00 cm giving δ =0.895, 0.945 and 0.975, respectively.

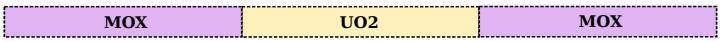
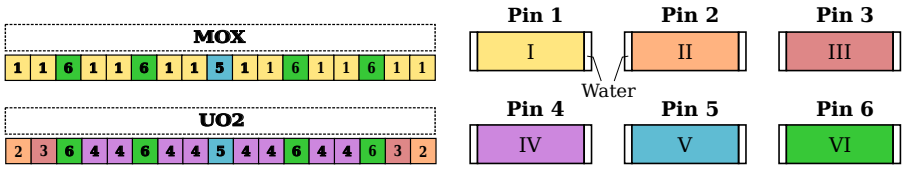


Fig. 4: MOX fuel benchmark definition.



(a) Assemblies definition. (b) Pin definition.

Fig. 5: MOX fuel benchmark materials definition

Table 3 shows the number of outer, O, and inner iterations, I, using the eigenvalue solvers for the different problems with different dominance ratio that have been defined. It can be seen that for problems with a high dominance ratio Krylov-Schur method can be from 1.5 to 6 times faster than the usual power iteration method. Note that high dominance ratios are needed to outperform power iteration with Krylov-Schur method. Also, for these high dominance ratio problems the Krylov subspace dimension, m, must be high to achieve a better performance.

Figure 6 displays the linear dependence of the CPU time with the number of inner iterations, as expected. In other words, the algorithm spends most of the computational resources in the inner iterations, due to the application of a transport sweep per inner iteration.

It is important to mention here that neglecting the upscattering makes the problem easier for the Krylov-Schur method. This is due to the fact that the product by $\mathbf{H}^{-1}$ is only calculated approximately, and the Arnoldi method is more sensible to the error in this approximation than the power iteration. The

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Table 3: Performance results in the MOX Fuel Slab

δ	**Method**	m	O	I	**Time (s)**
0.895	Power Iteration	-	31	2410	14.0
	Krylov-Schur	3	25	3771	22.5
	Krylov-Schur	5	14	2129	11.9
	Krylov-Schur	10	10	1509	9.1
0.945	Power Iteration	-	100	7447	44.8
	Krylov-Schur	3	31	4542	36.8
	Krylov-Schur	5	17	2484	14.0
	Krylov-Schur	10	20	2914	16.7
0.975	Power Iteration	-	191	14264	85.0
	Krylov-Schur	3	53	7876	52.2
	Krylov-Schur	5	23	3364	19.3
	Krylov-Schur	10	17	2484	14.0

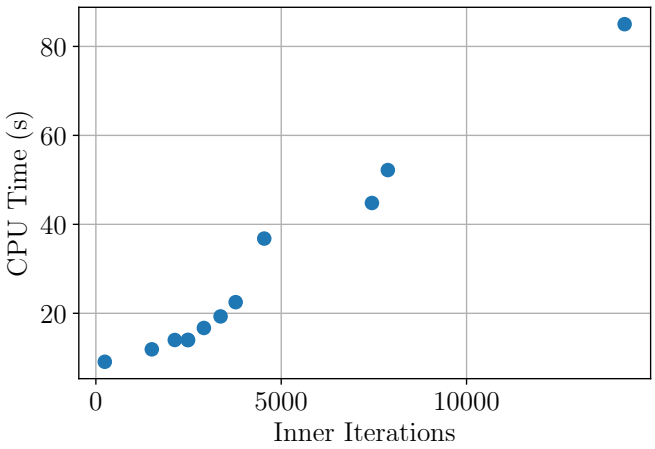

Fig. 6: Dependence of CPU time with the number of inner iterations

reason is that the system has to be solved accurately in order to have a Krylov basis, which is essential for the convergence of the Krylov method to the right solution, while solving this system in an approximate manner requires more iterations of the Power Iteration method, but does not affect its final accuracy. Neglecting the up-scattering we solve the system using just one block Gauss-Seidel iteration because of the block lower triangular structure of $\mathbf{H}$, thus neglecting this effect that will be considered in future works.

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5 Conclusions

In this work, a S_N method has been presented to solve the eigenvalue problem associated to the steady-state neutron transport equation. The generalized algebraic eigenvalue problem resulting from the energy, angles and spatial discretization is sparse and large. Then, it was implemented using a matrix-free methodology. Two eigenvalue solvers have been considered, the usual power iteration method and the Krylov-Schur method and the performance of both methods have been evaluated solving different problems with different dominance ratios. From the obtained results in can be concluded that only for problems with high dominance ratios, $\delta > 0.85$, without up-scattering it is worth to use the Krylov subspace method. Also, this method is a good alternative if more than one eigenvalue must be computed. Otherwise it is better to use the simpler power iteration method to compute the dominant eigenvalue and its corresponding eigenfunction for a reactor core.

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