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A Laplace transform method for energy multigroup hybrid discrete ordinates slab lattice calculations

C. F. Segatto(1), M. T. Vilhena(1) and R. C. Barros(2)(*)

(1) *Universidade Federal do Rio Grande do Sul - Av. Bento Gonalves 9500 91509-900 Porto Alegre, RS, Brazil*
(2) *Universidade do Estado do Rio de Janeiro - Rua Alberto Rangel s/n 28630-050 Nova Friburgo, RJ - Brazil*

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Summary. — In typical lattice cells where a highly absorbing, small fuel element is embedded in the moderator, a large weakly absorbing medium, high-order transport methods become unnecessary. In this work we describe a hybrid discrete ordinates (S_N) method for energy multigroup slab lattice calculations. This hybrid S_N method combines the convenience of a low-order S_N method in the moderator with a high-order S_N method in the fuel. The idea is based on the fact that in weakly absorbing media whose physical size is several neutron mean free paths in extent, even the S_2 method (P_1 approximation), leads to an accurate result. We use special fuel-moderator interface conditions and the Laplace transform (LTS_N) analytical numerical method to calculate the two-energy group neutron flux distributions and the thermal disadvantage factor. We present numerical results for a range of typical model problems.

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1. – Introduction

In typical lattice cells where a highly absorbing, small fuel element is embedded in the moderator, a large weakly absorbing medium, high-order transport methods become unnecessary. This situation was noted by Leslie [1] who devised techniques for grafting diffusion theory onto transport theory. Later, Nanneh and Williams [2] developed a diffusion-transport theory hybrid method for calculating neutron flux distributions in slab lattices. Further Segatto [3] offered a hybrid discrete ordinates (S_N) Laplace transform method for one-speed slab lattice calculations. In this paper we extend this hybrid S_N method to energy multigroup slab lattice calculations. This hybrid multigroup S_N method combines the convenience of a low-order S_N method in the moderator with a high-order S_N method

(*) E-mail: rcbarros@pq.cnpq.br

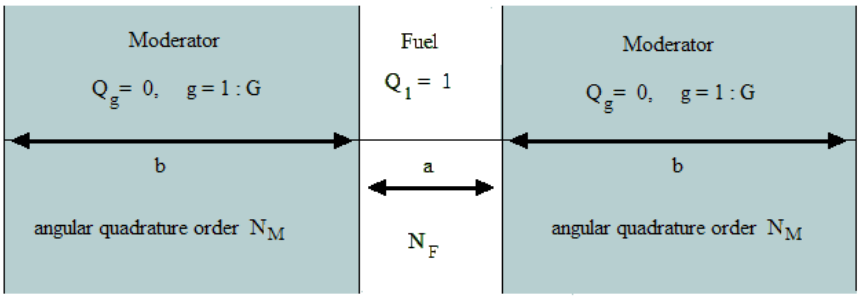

Fig. 1. – Unit cell of slab lattice, $N_F \geq N_M$.

in the fuel. The idea is based on the fact that in weakly absorbing media whose physical size is several neutron mean free paths in extent, even the S_2 method (P_1 approximation) leads to an accurate result [4]. We use special fuel-moderator interface conditions and the Laplace transform (LTS_N) analytical numerical method to calculate the neutron flux distribution and the thermal disadvantage factor [5], which is defined as the ratio of the average scalar flux in the moderator region to the average scalar flux in the fuel rod. At this point we give an outline of the remainder of this paper. In sect. **2** we present the general theory. In sect. **3** we give numerical results for a range of typical lattices. A number of concluding remarks and suggestions for future work are given in sect. **4**.

2. – General theory

Let us consider the energy multigroup S_N equations in slab geometry with isotropic scattering

$$\mu_m \frac{\mathrm{d}}{\mathrm{d}x}\psi_{m,g}(x) + \sigma_{tg}(x)\psi_{m,g}(x) = \frac{1}{2}\sum_{g'=1}^{G}\sigma_{sg'\to g}(x)\sum_{n=1}^{N}\psi_{n,g'}(x)w_n + Q_g(x), \tag{1}$$

$m = 1 : N$, $g = 1 : G$. Here the notation is standard for a given angular quadrature set [6], where G is the number of energy groups. To describe the technique, we consider the slab lattice represented in fig. 1. In eq. (1) if x belongs to the fuel region of thickness a, then we assume the interior neutron source as uniform $Q_1 = 1$, $Q_g = 0$ for $g \neq 1$ and $N = N_F$; if x belongs to the moderator region of thickness b, then we set the group neutron interior source $Q_g = 0$ for $g = 1 : G$ and $N = N_M$, with $N_F \geq N_M$. Periodic or reflective boundary conditions apply in accordance with the domain we consider within the slab lattice. At this point we remark that we assume in this model that the prompt fission neutrons are released in the fast energy group ($g = 1$) in the fuel pin and they are brought down to lower energy groups as they migrate to the moderator region. This is the reason why we set $Q_1 = 1$ in the fuel region, *i.e.* to model the prompt fission neutrons.

To describe the present hybrid S_N method, which we refer to as the LTS_{N_F,N_M} method, we apply the Laplace transform in space to eq. (1) in the fuel and moderator regions, as represented in fig. 1. It is well known that the S_N equations (1) are equivalent to the one-dimensional P_{N-1} equations [7]. Therefore, Barros [8] considered special fuel-moderator interface conditions for the neutrons migrating from the fuel region to

the moderator, by considering P_{N_F-1} expansion of the angular flux to evaluate the angular flux in the $N_M/2$ discrete directions entering the moderator. A similar procedure applies when neutrons leave behind the moderator, to evaluate the angular flux in the $N_F/2$ discrete directions entering the fuel region. To apply the multigroup LTS_{N_F,N_M} method, as described in this paper, we use an alternate special fuel-moderator interface conditions based on an approximate angular flux interpolation analytical method [9], that we describe further in this section. As it is, eq. (1) can be written in matrix form as

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathbf{\Psi}(x) - \mathbf{A}\mathbf{\Psi}(x) = \mathbf{S}, \tag{2}$$

where we have defined the $N \times G$ dimensional vectors

$$\mathbf{\Psi}(x) = (\psi_{1,1}, \psi_{2,1}, \ldots, \psi_{N,1}, \psi_{1,2}, \psi_{2,2}, \ldots, \psi_{N,2}, \ldots\ldots\ldots, \psi_{1,G}, \psi_{2,G}, \ldots, \psi_{N,G})^T, \tag{3}$$

and

$$\boldsymbol{S} = \left(\frac{Q_1}{\mu_1}, \frac{Q_1}{\mu_2}, \ldots, \frac{Q_1}{\mu_N}, \frac{Q_2}{\mu_1}, \frac{Q_2}{\mu_2}, \ldots, \frac{Q_2}{\mu_N}, \ldots\ldots\ldots, \frac{Q_G}{\mu_1}, \frac{Q_G}{\mu_2}, \ldots, \frac{Q_G}{\mu_N}\right)^T, \tag{4}$$

for $N = N_F$ or $N = N_M$ with $N_F \geq N_M$, Q_1 is the fast group fission neutron interior source in the fuel pin as shown in fig. 1. Therefore, we apply the Laplace transform in eq. (2) to obtain the analytical general solution, that appears as

$$\mathbf{\Psi}(x) = \mathbf{B}(x)\mathbf{\Theta} + \mathbf{H}, \tag{5}$$

with

$$\mathbf{B}(x) = \mathbf{X}\mathbf{E}(x). \tag{6}$$

Here $\mathbf{E}(x)$ is a diagonal matrix whose entries are

$$e_{i,j}(x) = \begin{cases} \exp[\lambda_i x], & \text{if } \lambda_i < 0, \\ \exp[\lambda_i (x-\ell)], & \text{if } \lambda_i > 0, \end{cases} \tag{7}$$

where $\ell = a$ or b, cf. fig. 1. The constants λ_i, $i = 1 : G \times N_F$ or N_M, are the eigenvalues of matrix $\mathbf{A}$; $\mathbf{X}$ is a matrix whose columns are eigenvectors of $\mathbf{A}$; and $\mathbf{H}$ is the particular solution vector which is determined by solving the system

$$-\mathbf{A}\mathbf{H} = \mathbf{S}. \tag{8}$$

In order to describe the special interface conditions that we use in the present LTS_{N_F,N_M} method, we consider the multigroup slab-geometry neutron transport equation with isotropic scattering

$$\mu\frac{\partial\psi_g(x,\mu)}{\partial x} + \sigma_{tg}\psi(x,\mu) = \frac{1}{2}\sum_{g'=1}^{G}\sigma_{sg'\to g}(x)\int_{-1}^{+1}\psi_{g'}(x,\mu')\mathrm{d}\mu' + Q_g(x), \quad g = 1 : G, \tag{9}$$

where x belongs to the fuel or moderator region in the repeating slab lattice. Now we approximate the integral term of the scattering source by appropriate Gauss-Legendre angular quadrature. Then, by considering that the angular quadrature order is distinct in the fuel and in the moderator regions, we solve the resulting approximate transport equation analytically to evaluate the angular fluxes at the fuel-moderator interface in the necessary discrete angular directions. In other words, for x in the moderator region, the macroscopic cross-sections in eq. (9) are the total and scattering cross-sections of the moderator and $Q_g = 0$, $g = 1 : G$, as in fig. 1. Therefore, we first approximate the integral term by the Gauss-Legendre quadrature with $N = N_M$

$$\int_{-1}^{+1} \psi_g(x, \mu') \mathrm{d}\mu' = \sum_{n=1}^{N_M} \psi_{n,g}(x) w_n, \quad g = 1 : G, \tag{10}$$

where $\psi_{n,g}(x)$ is the LTS_{N_M} solution [10], and then we solve the resulting transport equation so approximated to evaluate the neutron angular flux in the $N_F/2$ angular directions entering the fuel region. A similar procedure is carried out for x in the fuel region, where the macroscopic cross-sections in eq. (9) are the total and scattering cross-sections of the fuel and $Q_g = 0$ unless $g = 1$, for which we set $Q_1 = 1$, as shown in fig. 1.

3. – Numerical results

To illustrate the accuracy of the LTS_{N_F,N_M} hybrid method, we consider two typical model problems. Model problem No. 1 is a one-speed model ($G = 1$) and corresponds to enriched uranium-water lattice, whose dimensions and material parameters are given in table I [2]. Table II shows the disadvantage factor for this monoenergetic problem, as generated by neutron diffusion theory, DIFTRAN numerical method [2], Gauss-Legendre S_{16} and the present hybrid $\mathrm{LTS}_{16,2}$ method. Comparing these results, we see that the present hybrid method leads to accurate solutions for the disadvantage factor and for such thin lattices, diffusion theory is clearly inadequate.

Model problem No. 2 is a two-group model ($G = 2$) whose dimensions and material parameters are also given in table I. Table III shows the thermal disadvantage factor for this energy-dependent problem, as generated by the present hybrid LTS_{N_F,N_M} method, where we fixed $N_F = 20$ with $N_M = 2 : 20$. From these results, we see that the present hybrid method leads to accurate solutions for the thermal disadvantage factor yielding maximum relative deviation with respect to the non-hybrid result $\mathrm{LTS}_{20,20}$ that did not exceed 2% for the $\mathrm{LTS}_{20,2}$ hybrid method. Moreover, fig. 2 shows how the fast flux ($g = 1$) profile is depressed in the highly diffusive moderator region using the $\mathrm{LTS}_{20,4}$ method. Figure 3 shows the thermal flux ($g = 2$) profile in the highly absorbing fuel region also using the $\mathrm{LTS}_{20,4}$ hybrid method.

4. – Concluding remarks

We described a hybrid discrete ordinates (S_N) method for energy multigroup slab lattice calculations. This hybrid S_N method combines the convenience of a low-order S_N method in the moderator with a high-order S_N method in the fuel. We use special fuel-moderator interface conditions based on an approximate angular flux interpolation analytical method and the Laplace transform (LTS_N) [9] numerical method to calculate the group neutron flux distribution and the disadvantage factor.

TABLE I. – *Data for model problems.*

Data	Enriched U + Water(*) (one-speed model)	Two-energy group model(**)
Total cross-section of fuel (cm^{-1})	1.648	$\sigma_{t1} = 1.4, \quad \sigma_{t2} = 1.2$
Scattering cross-section of fuel (cm^{-1})	0.7278	$\sigma_{s11} = 0.99, \quad \sigma_{s12} = 0.30$ $\sigma_{s21} = 0.10, \quad \sigma_{s22} = 0.75$
Total cross-section of moderator (cm^{-1})	3.691	$\sigma_{t1} = 1.0, \quad \sigma_{t2} = 1.2$
Scattering cross-section of moderator (cm^{-1})	3.6713	$\sigma_{s11} = 0.90, \quad \sigma_{s12} = 0.70$ $\sigma_{s21} = 0.05, \quad \sigma_{s22} = 0.80$
a (cm)	0.1016	2.5098
b (cm)	various	15.7326

(*) Model problem 1.

(**) Model problem 2.

TABLE II. – *Numerical results to model problem No.* 1. *b/a = ratio of moderator length to fuel length.*

	Disadvantage factor			
b/a	Diffusion theory(*)	DIFTRAN(*)	S_{16}	LTS_{N_F,N_M} $N_F = 16, \quad N_M = 2$
3	1.032	1.116	1.112	1.096 (1.4%)(**)
4	1.039	1.125	1.125	1.109 (1.4%)
5	1.048	1.133	1.137	1.121 (1.4%)
6	1.056	1.142	1.149	1.132 (1.5%)
7	1.065	1.151	1.160	1.142 (1.6%)
8	1.074	1.160	1.170	1.152 (1.5%)

(*) See [2].

(**) Relative deviation with respect to the S_{16} result.

TABLE III. – *Numerical results to model problem No. 2.*

Hybrid angular quadratures Fuel S_{20} and Moderator S_2–S_{20}	Thermal disadvantage factor
$LTS_{20,2}$	1.074923 (1.73%)(*)
$LTS_{20,4}$	1.060138 (0.15%)
$LTS_{20,6}$	1.059213 (0.06%)
$LTS_{20,8}$	1.058898 (0.03%)
$LTS_{20,10}$	1.058753 (0.02%)
$LTS_{20,12}$	1.058674 (0.01%)
$LTS_{20,14}$	1.058625 (0.007%)
$LTS_{20,16}$	1.058593 (0.004%)
$LTS_{20,18}$	1.058571 (0.002%)
$LTS_{20,20}$	1.058555

(*) Relative deviation with respect to the non-hybrid $LTS_{20,20}$ result.

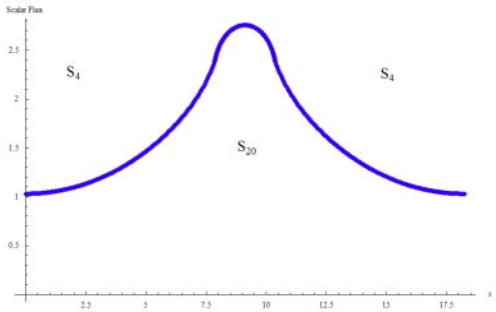

Fig. 2. – Fast group flux profile ($g = 1$) for model problem No. 2.

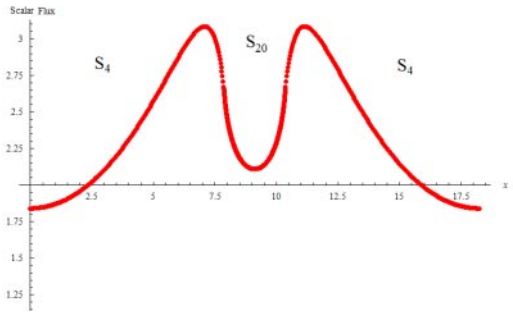

Fig. 3. – Thermal group flux profile ($g = 2$) for model problem No. 2.

TABLE IV. – *Numerical results to model problem No.* 2 *as generated by using Wynn-epsilon acceleration technique* [11].

Hybrid angular quadratures Fuel S_{20} and Moderator S_2–S_{20}	Thermal disadvantage factor
$LTS_{20,2}$	1.074923(*) (1.55%)(**)
$LTS_{20,4}$	1.060138 (0.15%)
$LTS_{20,6}$	1.059151 (0.06%)
$LTS_{20,8}$	1.058736 (0.02%)
$LTS_{20,10}$	1.058625 (0.01%)
$LTS_{20,12}$	1.058556 (0.005%)
$LTS_{20,14}$	1.058532 (0.003%)
$LTS_{20,16}$	1.058513 (0.001%)
$LTS_{20,18}$	1.058505 (0.0005%)

(*) Wynn-epsilon acceleration technique [11].

(**) Relative deviation with respect to the non-hybrid $LTS_{20,20}$ result displayed in table III.

Based on the numerical results shown in sect. **3**, we conclude that the present hybrid S_N method generates accurate numerical results. It seems clear that the special fuel-moderator interface conditions based on the approximate angular interpolation of the neutron flux lead to more accurate results than the continuity interface conditions based on P_N expansion [12]. Table IV shows the numerical results generated by Barry Ganapol (University of Arizona, Tucson, USA) and presented at the 21st International Conference on Transport Theory (21 ICTT) to test problem No. 2. It seems that the LTS_{N_F,N_M} with the Wynn-epsilon technique [13] should be suitable to applications involving hybrid S_N methods as described in this paper, since it generated numerical results for the thermal disadvantage factor [11] with smaller relative deviations.

To conclude we remark that the main goal of the present work with isotropic scattering approximation and slab geometry is to analyze the numerical results generated by the hybrid LTS_N method in energy multigroup calculations. As future work, we intend to consider linearly anisotropic scattering approximation since scattering in the fuel region is definitely not isotropic, and such an approximation in the moderador may be also poor in some cases. Bearing in mind that the LTS_N method is not an approximate numerical technique for problems in curvilinear geometry, we intend to solve more realistic fuel cell problems by the suitable Hankel Transform (HTS_N) [14] approach in cylindrical geometry.

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