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BRAZILIAN JOURNAL OF RADIATION SCIENCES
10-03A (2022) 01-12

The adjoint transport problem applied to estimate neutral particle leakage in the discrete ordinates formulation

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ABSTRACT

In source–detector problems, neutron leakage is a quantity of interest that could lead to improve shielding structures, thus reducing the dose received by humans. In this work, we apply an adjoint technique with spectral nodal methods to compute neutron leakage in multigroup one– and two–dimensional problems in the discrete ordinates (S_N) formulation. The use of the adjoint technique to calculate the leakages due to various source distributions is very convenient as it is possible to run adjoint problems and store the neutron importance maps. Here we solve the homogeneous adjoint S_N transport equation by considering unit outgoing adjoint flux at the boundary. In order to numerically solve slab– and X,Y–geometry problems, we use spectral nodal methods that have been widely applied and discussed in the literature. Numerical results are given to illustrate the present adjoint technique to estimate the neutron leakage for each energy group in source–detector problems. For all the test problems, the results obtained by the adjoint technique as described in this paper do agree with the results obtained by solving the analogous forward problem.

Keywords: **neutron leakage, adjoint transport problem, discrete ordinates, spectral nodal method, energy multigroup**

ISSN: 2319-0612
DOI: https://doi.org/10.15392/2319-0612.2022.1850
Submitted: 2022-12-16
Accepted: 2022-11-26

1. INTRODUCTION

It is well known that the linear Boltzmann transport operator is non self–adjoint and the solution of the adjoint transport equation can play a very useful role in the simulation of a wide variety of nuclear engineering problems [1; 2]. In fact, the adjoint flux can be interpreted as a function of importance that quantifies the relative contribution of neutral particles to a desired physical quantity, such as the detector response for problems in non–multiplying media.

During the last decades, the adjoint technique has been extensively applied along with deterministic methods for discrete–ordinates (S_N) calculations. Two classes of problems have been solved within this scope: source–detector problems and the estimation of interior neutron source distribution [3]. Some of recent contributions are related to solving slab–geometry and two–dimensional problems by using spectral nodal methods [3; 4; 5; 6]. In the referenced works, for the sake of computing quantities inside the structural domain, zero outgoing adjoint flux has been considered as prescribed boundary conditions. This is consistent with the concept of importance since particle leakage through the boundaries does not contribute to the system's particle population.

On the other hand, in shielding calculations, leakage of particles is a desired quantity to determine the dose received by people in the vicinity of a shielding structure containing radioactive material. With an appropriate choice of adjoint boundary condition, the numerical solution of the adjoint transport equation would be more efficient than solving the forward problem. For external detector locations, measuring the importance of outgoing particles, the adjoint boundary conditions require modification [2]. According to Reference [2], in order to estimate the total leakage from the domain, given a unidirectional and monoenergetic incident beam, the homogeneous adjoint transport equation must be solved by considering unit outgoing adjoint flux at the boundaries. In such cases, particles exiting the domain will be more important to the detector than any other interior particle. To the best of our knowledge, this methodology has not been applied to S_N transport problems.

In this work, we use this basic idea in spectral nodal methods to calculate neutral particle leakage for energy multigroup adjoint S_N transport problems in slab– and X, Y–geometry. We consider the homogeneous adjoint S_N problem and unit adjoint flux in the exiting directions as boundary conditions. The remainder of this paper is structured as follows. In Section 2, the adjoint S_N equations are presented, and the methodology used for estimating the group leakage is described. Numerical results to two model problems are presented and discussed in Section 3 and Section 4 offers a number of general concluding remarks and suggestions for future work.

2. MATERIALS AND METHODS

The adjoint problem should not be considered independent of the forward transport problem. Thus, the proper identification of the adjoint source and adjoint boundary conditions in addition to the "importance" meaning of the adjoint flux make possible to determine physically significant quantities. In source–detector problems, it can be proven [1; 2] that the solutions to the forward and adjoint transport problems, i. e., the neutral particle angular flux (ψ) and the adjoint angular flux ($\psi^\dagger$), respectively, are related by the reciprocity condition

$$\langle \psi, Q^\dagger \rangle = \langle \psi^\dagger, Q \rangle - \int_\Gamma d\Gamma \int_0^\infty dE \int_{4\pi} d\Omega \; \boldsymbol{n}\cdot\boldsymbol{\Omega} \; \psi^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega})\,\psi(\boldsymbol{r},E,\boldsymbol{\Omega}), \qquad \boldsymbol{r}\in\Gamma. \tag{1}$$

In Equation (1), the second term on the right–hand side is the bilinear concomitant, $Q^\dagger$ is the adjoint source, Q is the source of particles, $\langle\cdot,\cdot\rangle$ represents the integration over the independent variables, and Γ is the boundary surface of the domain.

Let us now consider the homogeneous adjoint problem and unit adjoint flux in the exiting directions all over the boundary, i. e., $Q^\dagger = 0$ and $\psi^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega}) = 1$, $\boldsymbol{r}\in\Gamma$, $\boldsymbol{n}\cdot\boldsymbol{\Omega} > \boldsymbol{0}$, respectively. Thus, Equation (1) appears as

$$0 = \langle \psi^\dagger, Q \rangle + \int_\Gamma d\Gamma \int_0^\infty dE \int_{\boldsymbol{n}\cdot\boldsymbol{\Omega}<\boldsymbol{0}} d\Omega \; |\boldsymbol{n}\cdot\boldsymbol{\Omega}| \; \psi^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega})\,\psi(\boldsymbol{r},E,\boldsymbol{\Omega})$$
$$- \int_\Gamma d\Gamma \int_0^\infty dE \int_{\boldsymbol{n}\cdot\boldsymbol{\Omega}>\boldsymbol{0}} d\Omega \; \boldsymbol{n}\cdot\boldsymbol{\Omega} \; \psi(\boldsymbol{r},E,\boldsymbol{\Omega}) \;, \quad \boldsymbol{r}\in\Gamma. \tag{2}$$

We note at this point that the third term on the right–hand side in Equation (2) is the total leakage $J^\dagger$ through the surface Γ, which can be written as

$$J^\dagger = \langle \psi^\dagger, Q \rangle + \int_\Gamma d\Gamma \int_0^\infty dE \int_{\boldsymbol{n}\cdot\boldsymbol{\Omega}<0} d\Omega \; |\boldsymbol{n}\cdot\boldsymbol{\Omega}| \; \psi^\dagger(\boldsymbol{r},E,\boldsymbol{\Omega}) \; \psi(\boldsymbol{r},E,\boldsymbol{\Omega}) \;, \; \; r\in\Gamma \;. \tag{3}$$

2.1. The adjoint S_N in slab geometry

Here we consider steady–state problems in slab geometry and non–multiplying media. For this purpose, let us consider a multilayer slab $D1$ of thickness H, as represented in Figure 1. Each region Υ_j has width h_j and constant material parameters, $j = 1 : J$, where J is the total number of regions. Now we write the energy multigroup, slab–geometry adjoint S_N equations in Υ_j, considering arbitrary $L'th$ order of scattering anisotropy, provided $L < N$ [1]

$$-\mu_m \frac{d}{dx}\psi^{\dagger}_{mg}(x) + \Sigma^{j}_{Tg}\,\psi^{\dagger}_{mg}(x) = \sum_{l=0}^{L}\frac{2l+1}{2}\,P_l(\mu_m)\sum_{g'=1}^{G}\Sigma^{(l)\,j}_{S\,g\to g'}\sum_{n=1}^{N}P_l(\mu_n)\,\omega_n\,\psi^{\dagger}_{ng'}(x)$$

$$g = 1{:}G, \qquad m = 1{:}N, \qquad j = 1{:}J, \qquad x \in \Upsilon\,. \tag{4}$$

The notation in Equation (4) is standard [1; 2; 5].

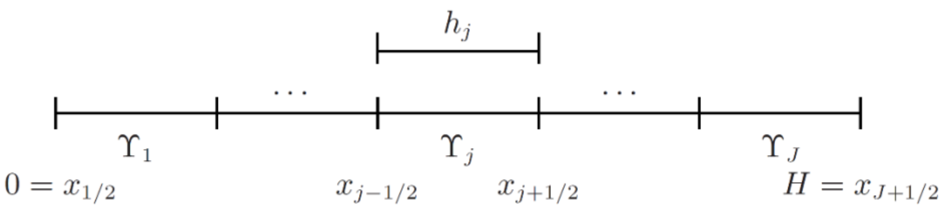

Figure 1: *Spatial grid on slab* $D1$: $0 \leq x \leq H$.

Source: Reference [5]

For slab–geometry S_N, according to Equation (3), the particle leakage through boundary b ($x_{1/2}$ or $x_{J+1/2}$) for the energy group g can be written as

$$\mathcal{J}^{\dagger}_{b,g} = \int_0^H dx \sum_{g'=1}^{G} Q_{g'}(x) \sum_{n=1}^{N}\omega_n\,\psi^{\dagger\,b,g}_{n\,g'}(x)$$

$$+\sum_{g'=1}^{G}\sum_{n=1}^{N/2}\mu_n\,\omega_n\,\psi^{\dagger\,b,g}_{n\,g'}(0)\,f_{n\,g'}(0) + \sum_{g'=1}^{G}\sum_{n=\frac{N}{2}+1}^{N}|\mu_n|\,\omega_n\,\psi^{\dagger\,b,g}_{n\,g'}(H)\,f_{n\,g'}(H)\,, \tag{5}$$

where the quantity $\psi^{\dagger\,b,g}_{n\,g'}(x)$ is the adjoint flux generated by using boundary conditions consisting of a unit adjoint flux for the energy group of interest g in the exiting directions at boundary b and equal to zero for all the other energy groups and boundary. Moreover, the quantities Q and f represent the interior sources of particles and the prescribed incident flux of particles on the boundaries, respectively.

To obtain the adjoint flux, Equation (4) must be solved. In this work, we use the adjoint spectral Green's function (SGF†) method [3] with the adjoint partial one–region block inversion scheme that generates numerical solutions that are completely free from spatial truncation errors. Therefore, it is possible to perform an analytical reconstruction inside the homogenized regions by considering the numerical coarse–mesh solution for the region–edge adjoint angular fluxes.

2.2. The adjoint S_N in X, Y– geometry

In this subsection, we consider a two–dimensional rectangular domain $D2$ whereon a discretization spatial grid composed of $I \times J$ homogeneous nodes $d_{i,j}$ (h_{xi} cm × h_{yj} cm), $i = 1 : I$ and $j = 1 : J$ is set, viz Figure 2. The material parameters are uniform within $d_{i,j}$.

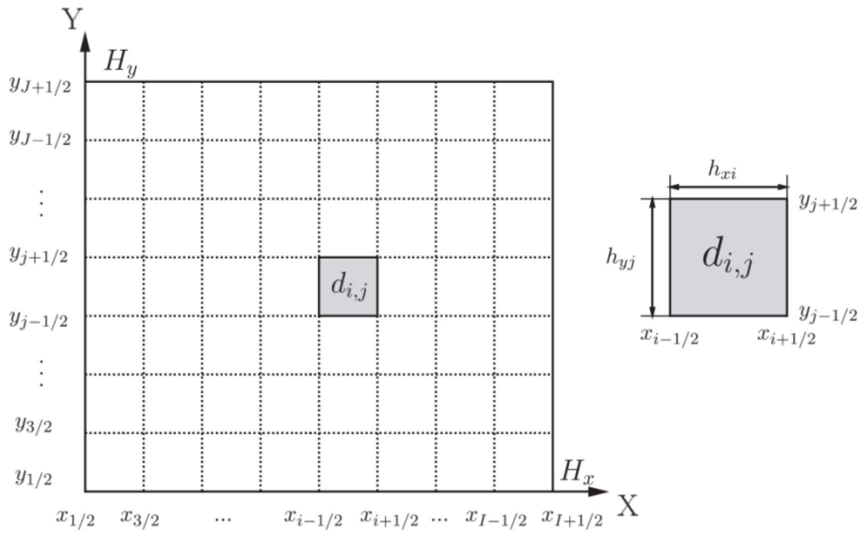

Figure 2: *Rectangular spatial grid on the domain $D2$.*

Source: Reference [6]

Therefore, the steady–state adjoint multigroup S_N transport equations with linearly anisotropic scattering in non–multiplying media on $d_{i,j}$ appear as

$$
\begin{aligned}
&- \mu_m \frac{\partial}{\partial x}\psi^{\dagger}_{mg}(x,y) \;-\; \eta_m \frac{\partial}{\partial y}\psi^{\dagger}_{mg}(x,y) \;+ \Sigma^{i,j}_{Tg}\,\psi^{\dagger}_{mg}(x,y) \\
&= \frac{1}{4}\sum_{g'=1}^{G}\sum_{n=1}^{M}\left[\Sigma^{(0)i,j}_{S\,g\to g'} + 3\,\Sigma^{(1)i,j}_{S\,g\to g'}(\mu_m\mu_n + \eta_m\eta_n)\right]\,\omega_n\,\psi^{\dagger}_{ng'}(x,y)\;, \\
&g = 1{:}\,G, \qquad m = 1{:}\,M, \qquad i = 1{:}\,I, \qquad j = 1{:}\,J, \qquad (x,y) \in d_{i,j}\,.
\end{aligned} \tag{6}
$$

A detailed description of the notation used in Equation (6) can be found in [6; 7]. In addition, for multigroup S_N formulations, Equation (3) appears as

$$
\begin{aligned}
\mathcal{J}^{\dagger}_{b,g} \;=\; &\sum_{g'=1}^{G} Q_{g'} \sum_{i=1}^{NX}\sum_{j=1}^{NY} h_{xi}\,h_{yj}\,\frac{1}{4}\sum_{n=1}^{M}\omega_n\,\bar{\psi}^{\dagger\,b,g}_{n\,g',i,j} \;+\; \sum_{i=1}^{I} h_{xi} \sum_{g'=1}^{G}\sum_{n=1}^{M/2} |\eta_n|\,\omega_n\,\hat{\psi}^{\dagger\,b,g}_{n\,g',i}\,(0)\,f^{B}_{n\,g'} \\
&+ \sum_{j=1}^{J} h_{yj} \sum_{g'=1}^{G}\sum_{n=M/4}^{3M/4} |\mu_n|\,\omega_n\,\tilde{\psi}^{\dagger\,b,g}_{n\,g',j}\,(H_x)\,f^{R}_{n\,g'} + \sum_{i=1}^{I} h_{xi} \sum_{g'=1}^{G}\sum_{n=M/2}^{M} |\eta_n|\,\omega_n\,\hat{\psi}^{\dagger\,b,g}_{n\,g',i}\,(H_y)\,f^{T}_{n\,g'} \\
&+ \sum_{j=1}^{J} h_{yj} \sum_{g'=1}^{G}\left[\sum_{n=1}^{M/4} + \sum_{n=3M/4}^{M}\right] |\mu_n|\,\omega_n\,\tilde{\psi}^{\dagger\,b,g}_{n\,g',j}\,(0)\,f^{L}_{n\,g'} \quad .
\end{aligned} \tag{7}
$$

Here $\mathcal{J}^{\dagger}_{b,g}$ is the leakage through boundary b in the energy group g; the quantities $\tilde{\psi}^{\dagger}_{n\,g',j}\,(x)$ and $\hat{\psi}^{\dagger}_{n\,g',i}\,(y)$ are the group average adjoint angular flux over the spatial coordinate direction y and x within $d_{i,j}$, respectively; $\bar{\psi}^{\dagger}_{n\,g',i,j}$ is the group node–average adjoint angular flux in $d_{i,j}$; and the superscript b,g indicates that the adjoint fluxes are calculated by considering boundary conditions that consist of unit outgoing adjoint angular flux only for the energy group g on boundary b; otherwise, it is set equal to zero. The first term on the right–hand side represents the leakage due to a source of particles Q located in a given region discretized with a rectangular grid composed of $NX \times NY$ nodes. The second through the fourth terms on the right–hand side refer to the leakage due to prescribed incident flux of particles (f) at the bottom (B), right (R), top (T) and left (L) boundaries, respectively.

To numerically solve the adjoint transport problem in Equation (6), we use the adjoint spectral Green's function–constant nodal (SGF†–CN) method [6] with the adjoint partial one–node block inversion iterative scheme. The SGF†–CN method has been successfully applied to fixed–source multigroup adjoint S_N problems in X,Y–geometry [6]. Only the terms referred to as the transverse leakage in the adjoint transverse–integrated S_N nodal equations are approximated by constants, as the scattering source terms are treated analytically in the spectral nodal class of numerical methods. The SGF†–CN method is less sensitive to the spatial discretization grid for coarse–mesh calculations and offers running time economy when compared with the conventional fine–mesh methods [6].

3. RESULTS AND DISCUSSION

In this section, we present numerical results to two typical problems by using the adjoint technique, as described in the present work. Since the algebraic expressions, methodology and accuracy of the SGF† [3] and SGF†–CN [6] methods have been thoroughly discussed in the literature, in this work we present results to the leakage computation by using the adjoint technique compared to the forward problem rather than comparing the numerical results with other methods.

3.1. Model–Problem № 1

Let us first consider a six–group problem with triplet scattering order ($L = 3$). The problem consists of a 30 cm–thick water slab which is bombarded on the left boundary ($x = 0$) by a uniform isotropic source (f^L) with energy range in the first group and vacuum condition for the right boundary. This problem presents strong upscattering and the details about the material cross sections can be found in References [8; 9]. Here, we also consider two interior radiation sources $Q_g^1 = \delta_{1,g}$ cm^{-3}s^{-1} and $Q_g^2 = 2\delta_{1,g}$ cm^{-3}s^{-1} located in the regions $7.5 \leq x \leq 15.0$ cm and $15.0 \leq x \leq 22.5$ cm, respectively. Here $\delta_{1,g}$ is the Kronecker delta.

To model the adjoint transport problem (Equation (4)), we used the S_{16} Gauss–Legendre angular quadrature set [1]. First, we solved the S_N adjoint problem by using the SGF† on a spatial grid consisting of one node per region. Then, the importance maps were substituted into the corresponding terms of Equation (5) to estimate the group leakages.

In Table 1 we list the numerical results for the group leakages through the left and right boundaries ($\mathcal{J}_{L,g}^\dagger$ and $\mathcal{J}_{R,g}^\dagger$, respectively) due to interior and boundary sources of particles. In all cases, the results generated by the present adjoint technique, and the ones obtained from solving the forward problem under similar conditions do agree up to the sixth decimal place. We remark that, as can be inferred from Equation (5), to obtain the results displayed in Table 1, for each of the 6 energy groups individually, we solved 12 adjoint S_{16} problems (6 groups × 2 adjoint boundary sources). This allows to store the importance maps and perform leakage calculations *a posteriori* due to several distributions and intensities of sources of particles.

Table 1: Group leakage estimation for Model–Problem № 1 (SGF† method, spatial grid of one node per region, S_{16} Gauss–Legendre model).

		f^L [a]	Q_g^1 [b]	Q_g^2 [c]	Total leakage
$g = 1$	$\mathcal{J}_{L,g}^{\dagger}$ [d]	1.439510e−02	1.496967e−04	4.486395e−08	1.454484e−02
	$\mathcal{J}_{R,g}^{\dagger}$ [e]	1.462414e−15	4.486395e−08	1.496967e−04	1.497416e−04
$g = 2$	$\mathcal{J}_{L,g}^{\dagger}$	4.996340e−02	7.243481e−02	3.793162e−03	1.261914e−01
	$\mathcal{J}_{R,g}^{\dagger}$	5.495680e−07	3.793162e−03	7.243481e−02	7.622852e−02
$g = 3$	$\mathcal{J}_{L,g}^{\dagger}$	8.152687e−02	1.655983e−01	8.698544e−03	2.558237e−01
	$\mathcal{J}_{R,g}^{\dagger}$	1.260303e−06	8.698544e−03	1.655983e−01	1.742981e−01
$g = 4$	$\mathcal{J}_{L,g}^{\dagger}$	8.511066e−03	1.619353e−02	8.505659e−04	2.555516e−02
	$\mathcal{J}_{R,g}^{\dagger}$	1.232356e−07	8.505659e−04	1.619353e−02	1.704422e−02
$g = 5$	$\mathcal{J}_{L,g}^{\dagger}$	1.635878e−04	2.832014e−04	1.487287e−05	4.616621e−04
	$\mathcal{J}_{R,g}^{\dagger}$	2.154878e−09	1.487287e−05	2.832014e−04	2.980764e−04
$g = 6$	$\mathcal{J}_{L,g}^{\dagger}$	1.919790e−06	2.686348e−06	1.410225e−07	4.747161e−06
	$\mathcal{J}_{R,g}^{\dagger}$	2.043220e−11	1.410225e−07	2.686348e−06	2.827391e−06

[a] f^L: Uniform isotropic flux on the left boundary ($x = 0$)

[b, c] Q_g^1, Q_g^2 : Interior radiation sources located in regions $7.5 \leq x \leq 15.0$ cm and $15.0 \leq x \leq 22.5$ cm

[d, e] $\mathcal{J}_{L,g}^{\dagger}$, $\mathcal{J}_{R,g}^{\dagger}$: Group leakages through the left and right boundaries

3.2. Model–Problem № 2

For the sake of solving a two–dimensional test problem, we have adapted one, first solved in [6], which consists of shielding calculations considering 10 energy groups and linearly anisotropic scattering. Figure 3 represents one–fourth of the whole shielding structure and the macroscopic cross sections (cm^{-1}) of each material zone ($z = 1:3$) are listed in Table 2.

Table 2: Macroscopic cross sections (cm^{-1}) for Model–Problem № 2 .

$\Sigma_{T\,g,z} = \left(\frac{z+20}{21}\right)^5 \left(\frac{g}{10} - 0.15\,\delta_{5,g} - 0.15\,\delta_{10,g}\right), \quad g = 1:10$
$\Sigma^{(l)i,j}_{S\,g'\to g,z} = \left(\frac{z+20}{21}\right)\left(\frac{g'}{100(g-g'+1)}\right)\left(0.7 - \frac{g+g'}{200}\right)^l, \quad g = 1:10, \quad g' = 1:g, \quad l = 0:1$

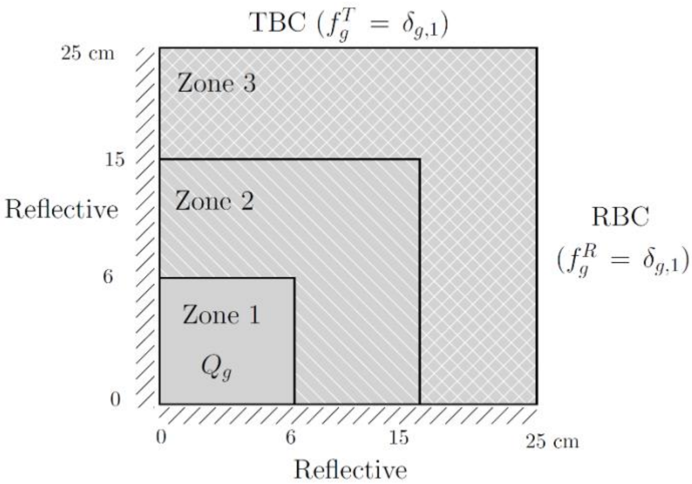

Figure 3: *Geometry and material distribution for Model–Problem № 2.*

Source: Authors

Now we perform the numerical experiment of estimating the leakage of neutral particles through the right and top boundaries due to the radiation source $Q_g = (1.1 - 0.1g)$ cm^{-3}s^{-1}, $g = 1:10$, located at the center of the shielding structure as illustrated in Figure 3, and prescribed boundary conditions at both right and top boundaries. For the forward boundary conditions, we consider unit isotropic incident distributions of radiation only in the first energy group, i.e., $f^R_{n\,g} = \delta_{1,g}$ cm^{-2}s^{-1} and

$f^{T}_{n\,g} = \delta_{1,g}$ cm^{-2}s^{-1}. Here, we apply the SGF†–CN method to the adjoint problem (6) on a coarse spatial grid composed of 100×100 nodes and the level symmetric S_8 angular quadrature set to obtain the importance values to be substituted into the corresponding terms of Equation (7).

Table 3 displays the results for the group leakage through the right and top boundaries ($\mathcal{J}^{\dagger}_{R,g}$ and $\mathcal{J}^{\dagger}_{T,g}$, respectively) due to three distinct sources of particles. For all the cases, the results obtained by the adjoint technique as described in this paper do agree with the forward results up to the sixth decimal place. To obtain such results, we solved 20 adjoint S_8 problems (10 groups × 2 adjoint boundary sources).

Table 3: Group leakage estimation for Model–Problem № 2 (SGF†–CN method, spatial grid of 100×100 nodes, S_8 level symmetric model).

		Q [a]	f^{R} [b]	f^{T} [c]	Total ($\mathcal{J}^{\dagger}_{R,g}/\mathcal{J}^{\dagger}_{T,g}$)
$g = 1$	$\mathcal{J}^{\dagger}_{R,g}$ [d]	1.353066e+00	1.006632e–01	1.523427e+00	2.977156e+00
	$\mathcal{J}^{\dagger}_{T,g}$ [e]	1.353066e+00	1.523427e+00	1.006632e–01	
$g = 2$	$\mathcal{J}^{\dagger}_{R,g}$	7.086908e–02	1.325590e–01	7.119480e–01	9.153760e–01
	$\mathcal{J}^{\dagger}_{T,g}$	7.086908e–02	7.119480e–01	1.325590e–01	
$g = 5$	$\mathcal{J}^{\dagger}_{R,g}$	7.192876e–03	2.257181e–01	3.040443e–01	5.369552e–01
	$\mathcal{J}^{\dagger}_{T,g}$	7.192876e–03	3.040443e–01	2.257181e–01	
$g = 9$	$\mathcal{J}^{\dagger}_{R,g}$	1.217799e–03	1.319387e–01	4.763744e–02	1.807940e–01
	$\mathcal{J}^{\dagger}_{T,g}$	2.844500e–03	1.502993e–01	1.740780e–01	
$g = 10$	$\mathcal{J}^{\dagger}_{R,g}$	1.192818e–03	1.239188e–01	3.187136e–02	1.569830e–01
	$\mathcal{J}^{\dagger}_{T,g}$	1.217799e–03	4.763744e–02	1.319387e–01	

[a] Q: Radiation source located at the center of the shielding structure

[b, c] f^{R}, f^{T}: Unit isotropic incident distributions of radiation at right and top boundaries

[d, e] $\mathcal{J}^{\dagger}_{R,g}$, $\mathcal{J}^{\dagger}_{T,g}$: Group leakages through the right and top boundaries

4. CONCLUSION

The numerical solution to the adjoint transport equation is used in this work to estimate group leakage in S_N fixed–source problems. The SGF† and SGF†–CN methods generate coarse–mesh solutions to numerically obtain the importance map distributions in slab– and X, Y–geometry S_N problems, respectively. We remark that the application of the present adjoint technique generated numerical results for the group leakage that agreed with the forward results up to the sixth decimal places for all the numerical experiments we performed. The methodology presented here can be applied in the context of storage of radioactive sources and nuclear waste. Depending on the Radiation Safety Standards, shielding structures can be properly designed to guarantee the minimum required leakage values. We intend to apply this technique to inverse problems to estimate interior and/or boundary sources, given information about the group leakage through the boundaries of a given shielding structure.

ACKNOWLEDGMENTS

The authors acknowledge the partial financial support of Conselho Nacional de Desenvolvimento Científico e Tecnológico – Brasil (CNPq) and Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro – Brasil (FAPERJ).

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