2021 International Nuclear Atlantic Conference - INAC 2021
Virtual meeting, Brazil, November 29 - December 2, 2021

ISBN: 978-65-594-1256-3

Estimation of Neutral Particle Leakage via the Adjoint Discrete Ordinates Transport Techniques

J. P. Curbelo[1] and R. C. Barros[2]

[1]jpcurbelo@uesc.br, Universidade Estadual de Santa Cruz, UESC, Campus Soane Nazaré de Andrade, Rodovia Jorge Amado, km 16, Bairro Salobrinho, CEP: 45.662-900, Ilhéus, Bahia, Brazil
[2]ricardob@iprj.uerj.br, Instituto Politécnico, IPRJ/UERJ, P.O.Box 97282, 28610-974 Nova Friburgo, RJ, Brazil

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]. This is due to the fact that the adjoint flux can be interpreted as an importance function 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 [2]. Some of recent contributions are related to solving slab–geometry and two–dimensional problems by using spectral nodal methods [2, 3, 4].

In the referenced works, for the sake of computing quantities inside the geometric domain, zero outgoing adjoint flux has been considered as prescribed boundary conditions. This is consistent with the concept of importance since particles leaving the domain do not contribute to the system's particle population. According to [1], to estimate the total leakage from the domain given a monodirectional and monoenergetic incident beam, the homogeneous adjoint transport equation must be solved by considering unit outgoing adjoint flux at the boundary. In this work, we use this basic idea to calculate neutral particle leakage for energy multigroup S_N transport problems. We have used the adjoint spectral Green's function constant–nodal (SGF†–CN) method to numerically solve adjoint S_N transport problems in X, Y–geometry [4]. We present and discuss numerical results to a typical model problem.

2. Methodology

The adjoint problem cannot be considered independently 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] 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 the reciprocity condition

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

In Eq. (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 $\psi^{\dagger}(\boldsymbol{r}, E, \boldsymbol{\Omega}) = 1$, $\boldsymbol{r} \in \Gamma$, $\boldsymbol{n} \cdot \boldsymbol{\Omega} > 0$, respectively. Thus, Eq. (1) appears as

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

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

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

2.1. The adjoint S_N two–dimensional case

We consider a two–dimensional rectangular domain whereon a discretization spatial grid composed of $I \times J$ homogeneous nodes $d_{i,j}$ $(h_{xi}\ cm \times h_{yj}\ cm)$, $i = 1 : I$ and $j = 1 : J$, is set. Therefore, the steady–state adjoint multigroup S_N transport equations with linearly anisotropic scattering in non–multiplying media on $d_{i,j}$ appear as

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

A thorough description of the notation used in Eq. (4) can be found in [4].

In the multigroup and the S_N formulation, Eq. (3) appears as

$$
\begin{aligned}
\mathcal{J}^{\dagger}_{b,g} = & \sum_{g'=1}^{G} Q_{g'} \sum_{i=1}^{NX} \sum_{j=1}^{NY} h_{xi}\, h_{yj}\, \frac{1}{4} \sum_{n=1}^{M} \omega_n \, \overline{\psi}^{\dagger\, b,g}_{ng'}(i,j) + \sum_{i=1}^{I} h_{xi} \sum_{g'=1}^{G} \sum_{n=1}^{M/2} |\eta_n|\, \omega_n \, \widehat{\psi}^{\dagger\, b,g}_{ng'}(i,0) \ f^{B}_{ng'} \\
& + \sum_{j=1}^{J} h_{yj} \sum_{g'=1}^{G} \sum_{n=M/4}^{3M/4} |\mu_n|\, \omega_n \, \widetilde{\psi}^{\dagger\, b,g}_{ng'}(H_x,j) \ f^{R}_{ng'} + \sum_{i=1}^{I} h_{xi} \sum_{g'=1}^{G} \sum_{n=M/2}^{M} |\eta_n|\, \omega_n \, \widehat{\psi}^{\dagger\, b,g}_{ng'}(i,H_y) \ f^{T}_{ng'} \\
& + \sum_{j=1}^{J} h_{yj} \sum_{g'=1}^{G} \left[\sum_{n=1}^{M/4} + \sum_{n=3M/4}^{M} \right] |\mu_n|\, \omega_n \, \widetilde{\psi}^{\dagger\, b,g}_{ng'}(0,j) \ f^{L}_{ng'} \ .
\end{aligned} \tag{5}
$$

Here $\mathcal{J}^{\dagger}_{b,g}$ is the leakage through boundary b in the energy group g; the quantities $\widetilde{\psi}^{\dagger}_{ng'}(x,j)$ and $\widehat{\psi}^{\dagger}_{ng'}(i,y)$ are the group average adjoint angular flux over the spatial coordinate direction y and x within $d_{i,j}$, respectively; $\overline{\psi}^{\dagger}_{ng'}(i,j)$ 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 of 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 of 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 obtain the values of the quantities representing the adjoint flux, we solve Eq. (4) by using the SGF†–CN method [4]. In the next section, we present the numerical results to a typical fixed–source problem by using the adjoint technique, as described in the present work.

3. Results and Discussion

Since the accuracy of the SGF†–CN method has been thoroughly discussed in [4], in this work, we rather present results to the leakage computation by using the adjoint technique compared to the forward problem rather than compare the numerical results with other methods. We have adapted a problem, first solved in [4], which consists of shielding calculations considering 10 energy groups and linearly anisotropic scattering. Figure 1 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 I.

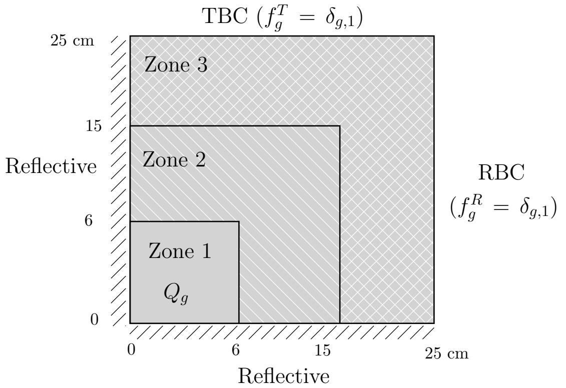

Figure 1: Geometry and material distribution.

Table I: Macroscopic cross sections (cm^{-1}).

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

Now we perform the numerical experiment of estimating the leakage of neutral particles through the right and top boundaries due to the radiation source $Q_g = (1.1 - 0.1\,g)\ cm^{-3}s^{-1}$, $g = 1 : 10$, located at the center of the shielding structure as illustrated in Fig. 1, and prescribed boundary conditions at both the 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., $f^R_{ng'} = \delta_{g,1}\ cm^{-3}s^{-1}$ and $f^T_{ng'} = \delta_{g,1}\ cm^{-3}s^{-1}$. Firstly, we apply the SGF†–CN method to the adjoint problem (4) on a coarse spatial grid composed of 100×100 nodes and the level symmetric S_8 angular quadrature set. Then, the importance maps are substituted in the corresponding terms of Eq. (5) to estimate the group leakages.

Table II 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 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 Eq. (5), to obtain the results in Table II, for each of the 10 energy groups individually, we solved 20 adjoint S_8 problems (10 groups $\times$ 2 adjoint boundary sources). This allows to store the importance maps and perform leakage calculations due to several sources of particles.

Table II: Group leakage estimation for the model problem (SGF†–CN method, spatial grid of 100×100 nodes, S_8 level symmetric model).

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

4. Conclusions

The numerical solution to the adjoint transport equation is used to estimate group leakage in fixed–source problems. 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 certain 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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