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

ISBN: 978-65-594-1256-3

Nyström method applied to the non-homogeneous transport equation

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1. Introduction

The Nyström method was proposed by Evert Johannes Nyström as a method to solve integral equations and consist of applying a numerical quadrature on the integral operators, producing an algebraic linear system. As the transport equation is an integro-differential equation, before applying the Nyström method is necessary to establish an equivalent integral formulation. This formulation is obtained by integrating the equation along its characteristic lines. This integral method has been successfully applied in calculating the numerical solutions of the transport problem [1][2][3][4].

In this work, we present a numerical methodology to solve the transport problem with semi-reflective boundary conditionsin in a non-homogeneous domain, based on the Nyström method. This methodology consists of solving an equivalent problem in a homogeneous domain obtained by a change of variable. Following its integral form is derived, analytical and computational techniques are applied to deal with the singularities of the integral operators which is finally approaching using the Nyström method. In order to validate our methodology we simulate a multiregion problem initially studied by Reed [5] but the numerical results for scalar flux were tabulated by Garcia and Siewert [6].

The problem considered here is given by

$$
\begin{aligned}
\mu\frac{\partial}{\partial x}\Psi(x,\mu) \quad &+ \quad \sigma_t(x)\Psi(x,\mu) = \frac{\sigma_s(x)}{2}\int_{-1}^{1}\Psi(x,\mu')d\mu' + S(x), && (1)\\
\Psi(0,\mu) \quad &= \quad \rho_0(\mu)\Psi(0,-\mu) + (1-\rho_0(\mu))B_0(\mu), \quad \mu > 0, && (2)\\
\Psi(L,\mu) \quad &= \quad \rho_L(\mu)\Psi(L,-\mu) + (1-\rho_L(\mu))B_L(\mu), \quad \mu < 0, && (3)
\end{aligned}
$$

where $\Psi(x,\mu)$ is the angular flux, $0 \leq x \leq L$ is the spatial variable and μ is the cosine of the angle formed between the direction of propagation and the axis x. The functions $\sigma_t(x)$ and $\sigma_s(x)$ represent the total macroscopic cross section and scattering macroscopic cross section with $\sigma_t(x) > \sigma_s(x)$ and $\sigma_t(x) > 0$ and $\sigma_s(x) > 0$. The function $S(x)$ is the isotropic internal source. In the boundary conditions, $B_0(\mu)$ and $B_L(\mu)$ represent the contribution of the boundary and $0 \leq \rho_0(\mu), \rho_L(\mu) \leq 1$ are the reflection coefficients. The scalar flux is given by

$$
\Phi(x) = \frac{1}{2}\int_{-1}^{1}\Psi(x,\mu)d\mu = \frac{1}{2}\int_{0}^{1}\left[\Psi(x,-\mu)+\Psi(x,\mu)\right]d\mu. \tag{4}
$$

2. Methodology

We start our methodology by proposing a change of variable to the transport problem in a non-homogeneous domain to obtain an equivalent problem in a homogeneous domain. The change of variable considered here is defined by $y(x) = \int_0^x \sigma_t(\tau)d\tau$.

Now, we define $\bar{\Psi}(y(x),\mu) = \Psi(x,\mu)$, $\bar{\Phi}(y(x)) = \Phi(x)$, $\bar{\sigma}_s(y(x)) = \sigma_s(x)$, and $\bar{\sigma}_t(y(x)) = \sigma_t(x)$ and rewrite the transport equation Eq. 1 using the change of variable as

$$\mu\frac{\partial}{\partial y}\bar{\Psi}(y,\mu) + \bar{\Psi}(y,\mu) = \frac{\bar{\sigma}_s(y)}{2\bar{\sigma}_t(y)}\int_{-1}^{1}\bar{\Psi}(y,\mu')d\mu' + \frac{\bar{S}(y)}{\bar{\sigma}_t(y)}, \tag{5}$$

subjected to the boundary conditions given by Eq. 2 and Eq. 3. The integral formulation of this new problem is determined from the auxiliary problem given by $\mu\frac{\partial}{\partial y}\bar{\Psi}(y,\mu) + \bar{\Psi}(y,\mu) = \bar{Q}(y)$, where $\bar{Q}(y) = \frac{\bar{\sigma}_s(y)}{\bar{\sigma}_t(y)}\bar{\Phi}(y) + \frac{\bar{S}(y)}{\bar{\sigma}_t(y)}$ and solve it by integrating factor method. The solution of this equation produces expressions for $\bar{\Psi}(y,\mu)$ and $\bar{\Psi}(y,-\mu)$ in terms of the scalar flux $\bar{\Phi}(y)$. Then, we replace these two expressions in equation for the scalar flux to obtain the integral formulation $\bar{\Phi}(y) = (L_g\bar{Q})(y) + (L_b\bar{B})(y)$. Here, the integral operator L_g is defined by $L_g\bar{Q}(y) = \int_0^L \bar{k}(y,\tau)\bar{Q}(\tau)d\tau$, where the kernel $\bar{k}(y,\tau)$ is expressed by

$$\begin{aligned}\bar{k}(y,\tau) = \frac{1}{2}\int_0^1 \Bigg[&\frac{\rho_L(-\mu)e^{-\frac{1}{\mu}(2L-\tau-y)} + \rho_0(\mu)\rho_L(-\mu)e^{-\frac{1}{\mu}(2L+\tau-y)}}{\mu\left(1-\rho_0(\mu)\rho_L(-\mu)e^{-\frac{2L}{\mu}}\right)} \\ &\frac{+\rho_0(\mu)e^{-\frac{1}{\mu}(y+\tau)} + \rho_0(\mu)\rho_L(-\mu)e^{-\frac{1}{\mu}(2L-\tau+y)}}{\mu\left(1-\rho_0(\mu)\rho_L(-\mu)e^{-\frac{2L}{\mu}}\right)} + \frac{e^{-\frac{1}{\mu}|\tau-y|}}{\mu}\Bigg]d\mu.\end{aligned} \tag{6}$$

Also, the function $L_b\bar{B}(y)$ is such that

$$\begin{aligned}L_b\bar{B}(y) = \int_0^1 \Bigg[&\frac{(1-\rho_L(-\mu))B_L(-\mu)e^{-\frac{1}{\mu}(L-y)} + (1-\rho_0(\mu))B_0(\mu)\rho_L(-\mu)e^{-\frac{1}{\mu}(2L-y)}}{2(1-\rho_0(\mu)\rho_L(-\mu)e^{-\frac{2L}{\mu}})} \\ &+\frac{(1-\rho_0(\mu)B_0(\mu))e^{-\frac{y}{\mu}} + (1-\rho_L(-\mu))B_L(-\mu)\rho_0(\mu)e^{-\frac{1}{\mu}(y+L)}}{2(1-\rho_0(\mu)\rho_L(-\mu)e^{-\frac{2L}{\mu}})}\Bigg]d\mu.\end{aligned} \tag{7}$$

We observe that the kernel $\bar{k}(y,\mu)$ has an integrable singularity on the diagonal $\tau = y$. This singularity is removed by applying the singularity subtraction technique, i.e,

$$\bar{\Phi}(y) = \int_0^L \bar{k}(y,\tau)\left(\bar{\Phi}(\tau)\frac{\bar{\sigma}_s(\tau)}{\bar{\sigma}_t(\tau)} - \bar{\Phi}(y)\frac{\bar{\sigma}_s(y)}{\bar{\sigma}_t(y)}\right)d\tau + \bar{\Phi}(y)\frac{\bar{\sigma}_s(y)}{\bar{\sigma}_t(y)}\bar{R}(y) + \bar{g}(y), \tag{8}$$

where $\bar{R}(y) = \int_0^L \bar{k}(y,\tau)d\tau$ and $\bar{g}(y) = L_g\left(\frac{\bar{S}(y)}{\bar{\sigma}_t(y)}\right) + \left(L_b\bar{B}\right)(y)$.

Finally, we apply the Nyström method in the first integral of the equation Eq. 8, that is, we approximate this integral using a numerical quadrature and we evaluate the scalar flux on the mesh points to obtain the discrete problem

$$\bar{\Phi}(y_i) \approx \sum_{\substack{j=1 \\ j\neq i}}^{N} w(\tau_j)\bar{k}(y_i,\tau_j)\left[\bar{\Phi}(\tau_j)\frac{\bar{\sigma}_s(\tau_j)}{\bar{\sigma}_t(\tau_j)} - \bar{\Phi}(y_i)\frac{\bar{\sigma}_s(y_i)}{\bar{\sigma}_t(y_i)}\right] + \bar{\Phi}(y_i)\frac{\bar{\sigma}_s(y_i)}{\bar{\sigma}_t(y_i)}\bar{R}(y_i) + \bar{g}(y_i), \tag{9}$$

where $\{w(\tau_j)\}_{j=1}^{N}$ are the quadrature weights and $\{\tau\}_{j=1}^{N}$ the nodes.

3. Results and Discussion

In order to check the efficiency of our methodology we presented in this section the numerical results for a multilayer slab problem with four regions that was initially proposed by Reed [5] and also studied by Garcia and Siewert [6]. In the simulations we used an Intel Core i7 computer, the algorithms were implemented in C language and routines of GNU scientific library were used. The multiregion problem introduced by Reed [5] is described as a slab with four regions wich parameters for each region are presented in the Table I.

Table I: Parameters of the multiregion problem presented by Reed [5].

Region	1	2	3	4
$\sigma_a(x)$	50.0	5.0	0.0	0.1
$\sigma_t(x)$	50.0	5.0	0.0	1.0
$\sigma_s(x)$	0.0	0.0	0.0	0.9
Thickness	2.0	1.0	2.0	3.0

In addition to the parameters in Table I in the first region of this problem is located a source of magnitude 50.0 and in the region 5.0cm $< x <$ 6.0cm a source of magnitude 1.0. Since the region 3 is vacumm and has no source can be omitted in the simulation. So we denoted 3.0cm $< x <$ 4.0cm as region 3 and 4.0cm $< x <$ 6.0cm as region 4. In the simulation we compare our numerical results determined by Boole's rule with the dates presented in work by Garcia and Siewert [6].

In Table II we compare our numerical results for the multiregion problem with the solution tabulated by Garcia and Siewert [6]. In region 1 where we have high absorption and source, the precision of the numerical results is good even for a small number of points, for the other regions the same precision was obtained with 8001 points in the mesh.

4. Conclusions

In this work, we presented a numerical methodology for solving the transport problem in a non-homogeneous domain. The main idea here is to apply a change of variable in the original problem in order to determine an equivalent problem in a homogeneous domain whose integral formulation is solved numerically by the Nyström method. This methodology proved to be efficient in the calculation the scalar flux of the multiregion problem. In the simulations, the solution presented the same accuracy when compared with the literature.

Table II: Numerical results for the multiregion problem

x	F_N	N=501	N=1001	N=2001	N=4001	N=8001	N=16001
0.00	1.000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.00	1.000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
1.90	0.9995	0.999506	0.999506	0.999506	0.999506	0.999506	0.999506
1.95	0.9902	0.990160	0.990160	0.990160	0.990159	0.990160	0.990160
1.99	0.8372	0.837237	0.837238	0.837236	0.837235	0.837236	0.837236
2.00	0.5010	0.500987	0.500994	0.500994	0.500994	0.500993	0.500992
2.05	0.2602	0.260179	0.260193	0.260195	0.260197	0.260193	0.260192
2.09	0.1798	0.179772	0.179791	0.179795	0.179799	0.179791	0.179791
2.10	0.1651	0.165078	0.165099	0.165104	0.165108	0.165100	0.165099
2.50	0.03009	0.029777	0.030069	0.030163	0.030221	0.030100	0.030087
2.90	0.3520	0.347189	0.351781	0.353107	0.353859	0.352104	0.351897
2.95	0.5650	0.558971	0.565194	0.566461	0.567155	0.565140	0.564881
2.99	0.9151	0.912207	0.917572	0.916301	0.915367	0.915223	0.915088
5.00	1.106	1.111896	1.112269	1.106784	1.102728	1.106423	1.106585
5.10	1.441	1.477071	1.446442	1.438398	1.432682	1.441043	1.441883
5.50	1.941	1.954956	1.950887	1.937182	1.932284	1.940790	1.941560
6.00	1.634	1.611912	1.645807	1.630513	1.629035	1.633780	1.634231
7.00	0.7085	0.708400	0.710421	0.708037	0.706999	0.708492	0.708614
8.00	0.2225	0.220057	0.223027	0.222216	0.222085	0.222489	0.222524

Acknowledgments

L. Lazzari was supported by a doctoral fellowship of the CNPQ (Brazil).

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