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P_N Synthetic Acceleration for the Source Iteration Scheme in Slab Geometry Discrete Ordinates Transport Calculations

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1. Introduction

The essence of the neutron transport theory is based on the study of the balance between production and removal of particles which migrate in a given material medium. This phenomenon is mathematically modeled by the linear Boltzmann transport equation [1] and has important applications, e.g., in radiological protection; nuclear reactor physics; in the industry in non-destructive testing; in medicine with boron neutron capture therapy, just to mention a few.
Numerical solutions to fixed-source discrete ordinates (S_N) neutron transport problems can be obtained iteratively by the classical source iteration (SI) scheme implemented in the conventional fine-mesh Diamond Difference (DD) method [1]. The SI scheme shows slow convergence rates for scattering dominated slabs with several mean free paths in extent and it is well known that synthetic acceleration (SA) techniques are very efficient for SI schemes [2]. In this work, it is described an acceleration strategy for the SI scheme in slab geometry based on the coarse-mesh solution of the P_N equations as initial guess for the fine-mesh scattering source. We refer to this methodology as the P_NSA scheme.
The application of the P_N method, also known in the literature as the spherical harmonics method, was introduced by R. E. Marshak [3] and J. C. Mark [4] in neutron transport calculations. The methodology, as presented in this summary, is completely free from spatial truncation errors and is described in detail in [5] and [6].

2. Methodology

In the P_N method, adopted in this work for modeling the physical phenomenon of neutron transport, all macroscopic cross sections of the medium are known, the regime is stationary, the domain is a slab and neutrons are monoenergetic, i. e., neutrons do not change their kinetic energy upon collision with the nuclei of atoms of the material medium. In fact this is a good approximation when the non-multiplying scattering media are composed of heavy atoms. This phenomenon can be modeled mathematically by the P_N equations [5] which can be written as

$$\begin{gathered}(\ell+1)\phi'_{\ell+1}(x)+\ell\phi'_{\ell-1}(x)+(2\ell+1)\sigma_\ell(x)\phi_\ell(x)=Q(x)\delta_{\ell,0}\,,\ \ell=0{:}N,\\ \sigma_\ell(x)\equiv\sigma_T(x)-\sigma_{s\ell}(x)\,,\ 0\le x\le X.\end{gathered}\tag{1}$$

where $\phi_\ell(x)$, $\ell=0{:}N$, are the dependent variables defined as angular moments of order ℓ [5], $\sigma_T(x)$ is the total macroscopic cross section at position x; $\sigma_{s\ell}(x)$ is the ℓ-th component of the differential macroscopic scattering cross section at position x; $Q(x)$ is an isotropic interior source at position x; $\delta_{\ell,0}$ is the Kronecker delta, i. e., it is equal to unity for $\ell=0$ and it is equal to zero otherwise; N is the degree of P_N approximation [4]; X is the length of the one-dimensional domain and $\phi'(x)$ is a simplified notation for the first-order ordinary derivative with respect to x, i. e., $\phi'(x)=\frac{d\phi(x)}{dx}$. Moreover, $\phi_0(x)$ is defined as neutron scalar flux and $\phi_1(x)$ is the total neutron current. The other angular moments do not have special definitions [5].
The analytical solution for Eq. (1) is determined by a simplified algorithm proposed in [5] for odd degrees N and arbitrary degrees of scattering anisotropy $L\le N$. In this work we describe an acceleration technique

based on an improved initial guess for the scattering source distribution within the slab.
Consider at this point, for example, a heterogeneous one-dimensional domain with N_R regions. The number of material zones in a one-dimensional domain is always less than or equal to the number of regions N_R. Material parameters $\sigma_\ell(x)$, $\ell = 0{:}\,N$, and interior source Q are uniform within each region of the domain. Thus, the system of equations, as represented in Eq. (1), inside a region r, appears as

$$(\ell+1)\phi'_{\ell+1}(x) + \ell\phi'_{\ell-1}(x) + (2\ell+1)\sigma_\ell\phi_\ell(x) = Q\delta_{\ell,0}\,,\ \ell = 0{:}\,N,$$
$$\sigma_\ell \equiv \sigma_T - \sigma_{s\ell}\,, x \in [0, h_r]\,, r = 1{:}\,N_R\,. \tag{2}$$

As can be seen in Eq. (2), the position x belongs to the interval $[0, h_r]$, where h_r represents the thickness of region r.
Equation (2) constitutes a system of N + 1 first-order linear ordinary differential equations with constant coefficients whose general solution is composed by the sum of a homogeneous solution with a particular solution [5]. To obtain the homogeneous component of the local general solution for $\phi_0(x)$, and also the local solutions for the other angular moments, it is necessary to solve the following homogeneous system:

$$\boldsymbol{\phi}' = \boldsymbol{A}\boldsymbol{\phi}\,, \tag{3}$$

where $\boldsymbol{\phi}'$ represents the column vector with the $N+1$ derivates and $\boldsymbol{\phi}$ is the column vector with the $N+1$ angular moments. The local homogeneous system (3) is solved by performing a spectral decomposition of matrix $\boldsymbol{A}$ [5]. The general solution for the local system (2), i. e., sum of the solution of the homogeneous system (3) with the particular component, can be written as

$$\phi_\ell(x) = \sum_{k=0}^{N} C_k a_\ell(\nu_k) e^{\nu_k x} + \frac{Q}{\sigma_a}\delta_{\ell,0}\,, \ell = 0{:}\,N, x \in [0, h_r], r = 1{:}\,N_R\,, \tag{4}$$

where ν_k, $k = 0{:}\,N$, are the $N+1$ eigenvalues of matrix $\boldsymbol{A}$; $a_\ell(\nu_k)$, $\ell = 0{:}\,N$, is the ℓ-th component of eigenvector of matrix $\boldsymbol{A}$ associated to the eigenvalue ν_k and C_k, $k = 0{:}\,N$, are the $N+1$ constants per region. To determine these $N+1$ constants per region it is necessary to establish boundary conditions and interfaces conditions that yield a system with $(N+1)N_R$ algebraic linear equations in $(N+1)N_R$ unknowns, which are the constants that need to be calculated. In this work, only prescribed boundary conditions are adopted. To approximate the prescribed incidence boundary conditions in the P_N method, Mark type of boundary conditions is considered [5].
To use the boundary conditions of the Mark type, the roots of the $N+1$ degree Legendre polynomial are firstly obtained, which appear in positive and negative pairs and have the following format: $\frac{N+1}{2}$ positive roots equal to the absolute values of the other $\frac{N+1}{2}$ negative roots. At the left end of the domain, i. e., at $x = 0$, the following set of equations [5] is used:

$$\sum_{k=0}^{N}\sum_{\ell=0}^{N} \frac{2\ell+1}{2} P_\ell(\mu_n) a_\ell(\nu_k)\, C_k = I_E - \frac{Q}{2\sigma_a}\,, \mu_n > 0, n = 1{:}\frac{N+1}{2}, \tag{5}$$

where I_E is the isotropic prescribed flux incident on the left boundary and μ_n is the n-th positive root. To the right end of the domain, i. e., at $x = h_{N_R}$, the set of equations used is given by [5]

$$\sum_{k=0}^{N}\sum_{\ell=0}^{N} \frac{2\ell+1}{2} P_\ell(\mu_n) a_\ell(\nu_k) e^{\nu_k h_{N_R}}\, C_k = I_D - \frac{Q}{2\sigma_a}\,, \mu_n < 0, n = 1{:}\frac{N+1}{2}, \tag{6}$$

where I_D is the isotropic prescribed flux incident on the right boundary and, in this case, μ_n is the n-th negative root. In this way, a total of $N+1$ contour equations are obtained: $(N+1)/2$ on the left contour and $(N+1)/2$ on the right contour.

For a heterogeneous domain, i. e., consisting of more than one region, it is necessary to complete the system with additional $(N+1)(N_R-1)$ equations, which are obtained from the continuity of all angular moments in the N_R-1 interfaces of the one-dimensional domain, i. e.,

$$\phi_\ell^r(h_r) = \phi_\ell^{r+1}(0), r = 1:(N_R-1), \ell = 0:N\,. \tag{7}$$

The local general solution (4) is substituted into Eq. (7) and then $(N+1)(N_R-1)$ equations are obtained. Therefore, through the methodology, as outlined above, a system with $(N+1)N_R$ algebraic linear equations in $(N+1)N_R$ unknowns is built. Once these constants are determined, the angular moments can be calculated at any position in the domain using Eq. (4).

In this work it is considered the steady-state, one-speed, fixed source S_N problem with isotropic scattering in slab geometry [1]

$$\mu_m \frac{d}{dx}\psi_m(x) + \sigma_T(x)\psi_m(x) = \frac{1}{2}\sigma_s(x)\sum_{n=1}^{N}\psi_n(x)\omega_n + \frac{Q(x)}{2}, 0 < x < X, m = 1:N, \tag{8}$$

with the boundary conditions $\psi_m(0) = I_E$, $\mu_m > 0$ and $\psi_m(X) = I_D$, $\mu_m < 0$. Here I_E and I_D are prescribed incident fluxes on the outer boundaries of the slab of thickness X; $\psi_m(x) = \psi(x,\mu_m)$ is the angular flux of particles traveling in direction μ_m; ω_n is the angular weight for direction μ_n; σ_T is the total cross section; σ_s is the isotropic component of the differential scattering cross section and Q is the interior source.

Furthermore, considering a discretization spatial grid set up on a given slab of thickness X composed of J fine cells, each discretization cell has thickness h_j, constant cross sections $\sigma_{T,j}$ and $\sigma_{s,j}$ and constant source Q_j and considering $\bar{\psi}_{m,j} = \frac{\psi_{m,j+1/2}+\psi_{m,j-1/2}}{2}$, $m = 1:N$, $j = 1:J$, the standard SI scheme used in the DD method is based on transport sweeps on the slab.

$$\psi_{m,j\pm1/2} = \frac{\left(\frac{|\mu_m|}{h_j} - \frac{\sigma_{T,j}}{2}\right)\psi_{m,j\mp1/2} + \frac{\sigma_{s,j}}{2}\sum_{n=1}^{N}\bar{\psi}_{n,j}\omega_n + Q_j}{\frac{|\mu_m|}{h_j} + \frac{\sigma_{T,j}}{2}}, \tag{9}$$

$$\mu_m > 0: j = 1:J, m = 1:\frac{N}{2}\ and\ \mu_m < 0: j = J:1, m = \left(\frac{N}{2}+1\right):N.$$

For an improved initial guess $\sum_{n=1}^{N}\bar{\psi}_{n,j}\omega_n = \bar{\phi}_j = \frac{1}{h_j}\int_{x_j-1/2}^{x_j+1/2}\phi_0(x)dx$, calculated using Eq. (4), Eq. (9) is used to sweep from left to right ($\mu_m > 0$, upper signs) and from right to left ($\mu_m < 0$, lower signs) to estimate the cell-edge angular fluxes. Then, the scattering source is updated before proceeding to the transport sweeps again, until a preassigned stopping criterion is satisfied.

3. Results and Discussion

It is considered a homogeneous slab of thickness 100 cm with $\sigma_T = 1.0\,cm^{-1}$ and isotropic scattering. Prescribed boundary conditions = 1,000 apply at $x = 0$ and $x = 100$ cm, i. e., I_E = I_D = 1,000 in the boundary conditions equations with Gauss-Legendre S_{32} angular quadrature set.

To solve this problem, it was used the DD method on a fine spatial grid composed of 2,000 uniform nodes and a stopping criterion requiring that the sum of all absolute deviation between two consecutive estimates of the node-edge scalar flux does not exceed 10^{-5}.

As can be seen in Table I, by increasing the scattering macroscopic cross section (σ_s), and thus reducing the

absorption cross section, the non-accelerated SI scheme shows slow convergence rate compared to the accelerated SI scheme with P_NSA. As expected, by increasing the degree N in P_NSA, the number of iterations to convergence is reduced.

Table I – Number of iterations and CPU time for each method with different σ_s.

Method	Scattering Macroscopic Cross Section σ_s (cm^{-1})			
	0.8	0.9	0.97	0.995
SI	70 (2.5 s)	144 (5.0 s)	476 (16 s)	2707 (90.0 s)
P_5SA	53 (2.1 s)	104 (3.7 s)	326 (11.0 s)	1700 (56.5 s)
P_{15}SA	46 (1.9 s)	89 (3.6 s)	273 (9.4 s)	1381 (45.9 s)
P_{31}SA	39 (1.9 s)	74 (3.2 s)	210 (7.6 s)	896 (30.2 s)

4. Conclusions

Based on the numerical results presented in the previous section, it can be concluded that the coarse-mesh P_NSA strategy is very efficient, as it accelerates the SI scheme by reducing the number of iterations to convergence and shortened the CPU execution time. This is more significant in problems with low absorption as can be seen in the fifth column of Table I. As future work, it is intended to apply this acceleration scheme for multidimensional S_N transport calculations.

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