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Albedo Conditions for Multigroup Anisotropic Scattering Models of Nuclear Reactors

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We report some improvements in the theory of spectral nodal methods for the numerical solution of nuclear reactor problems in the discrete ordinates (S_N) formulation of neutron transport theory. Specifically, we derive exact and numerically stable multigroup S_N albedo conditions that substitute the axially oriented, geometrically thick reflector regions of thermal nuclear reactors in S_N multiplication eigenvalue calculations with arbitrary (Legendre) order of anisotropic scattering. The relevance of our multigroup S_N albedo conditions is indicated by means of numerical experiments with an axial model for a thermal reactor core and is tightened by a possible extension to more realistic multidimensional reactor core models.

KEYWORDS: nuclear reactor analysis, multigroup theory, anisotropic scattering, albedo conditions, discrete ordinates, mathematical model

1. Introduction

We have been working over a decade on the development of numerical methods for the accurate solution of neutron transport problems in the discrete ordinates (S_N) formulation [1]. Target problems in this enterprise have been mostly the stationary nuclear reactor problem of estimating multiplication eigenvalue and thermal power distribution and the shielding problem of estimating the angular distribution of neutrons passing through and emerging from a neutron shield. For solving these S_N problems in slab- and multidimensional rectangular geometry, we have developed a particularly accurate class of nodal methods — spectral nodal methods [2-6]. In slab-geometry, spectral nodal methods display an outstanding feature: they are free from spatial truncation error. That is to say, the numerical solutions generated for S_N local and distributed quantities agree with the analytical S_N ones on corresponding points/regions of the slab domain. Besides, slab geometry is a suitable laboratory for improvements in spectral nodal methods applied to S_N problems in multidimensional rectangular geometry.

In this article, we report some improvements in the theory of spectral nodal methods for the numerical solution of slab-geometry nuclear reactor problems in the S_N formulation. Specifically, we derive exact and numerically stable multigroup S_N albedo conditions that substitute the axially oriented, geometrically thick reflector regions of thermal nuclear reactors in S_N multiplication eigenvalue and thermal power density calculations, with arbitrary (Legendre) order of anisotropic scattering. Here, the word exact is to mean without spatial truncation error. These conditions enable us to increase the computational efficiency of our slab-geometry spectral nodal method for multiplication eigenvalue problems described in Ref. [5]. Moreover, they can be used to both increase the computational efficiency and

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improve the numerical accuracy of slab-geometry S_N computer codes grounded in discretization schemes with spatial approximation [7]. The relevance of our multigroup S_N albedo conditions is indicated by means of numerical experiments with an axial model for a thermal nuclear reactor core and is tightened by a possible extension to more realistic multidimensional reactor core models.

2. Multigroup S_N Albedo Conditions

2.1 Multigroup S_N Equations with Anisotropic Scattering

We start with a discrete ordinates version of a first-order neutron transport equation suitable for a mathematical description of the behavior of neutrons in the axial reflector regions of thermal nuclear reactors. It can be written in the form

$$\mu_m \frac{d}{dz}\psi_{m,g}(z)+\sigma_{t,g}\psi_{m,g}(z)=\sum_{\ell=0}^{L}\frac{2\ell+1}{2}P_\ell(\mu_m)\sum_{g'=1}^{G}\sigma_\ell^{gg'}\sum_{n=1}^{N}P_\ell(\mu_n)\omega_n\psi_{n,g'}(z)$$

$$z \in [z_{int}, z_{up}],\ m = 1 : N,\ g = 1 : G, \tag{1}$$

for the upper reflector, where z_{int} denotes the spatial coordinate of the active core – upper reflector interface and z_{up} denotes the spatial coordinate of the upper boundary of the nuclear reactor core. The remaining notation in the S_N equations (1) is standard [1] and similar equations hold for the lower reflector region. Analytic solution to the S_N equations (1) can be written in the open form [2]

$$\psi_{m,g}(z)=\sum_{i=1}^{GN}\alpha_i\, a_{m,g}(\nu_i)\exp[(z-z_i)/\nu_i],$$

$$z \in [z_{int}, z_{up}],\ m = 1 : N,\ g = 1 : G, \tag{2}$$

where the i-labeled functions on the right hand side of expression (2) are non-trivial elementary solutions to the S_N equations (1). The quantities ν_i, i = 1:GN, denote the spectrum of the multigroup slab-geometry S_N operator associated to equations (1); the quantities $a_{m,g}(\nu_i)$ are the multigroup spectrum-dependent angular components of the elementary solutions; the real numbers z_i are to render non-positive the arguments of the exponentials in solution (2), as described in Ref. [3], and α_i, i = 1:GN, are constants depending upon the interface conditions at z_{int} and on the (zero) incoming conditions at z_{up}. The derivation of the spectrum and of the multigroup spectrum-dependent angular components of the elementary solutions (2) is described in detail in Ref. [2]. We assume here that the elementary solutions form a vector basis for the null space of the multigroup slab-geometry S_N operator associated to equations (1). We note that m from 1 to N/2 is to denote the upwelling directions $\mu_m > 0$ and m from (N/2+1) to N is to denote the downwelling directions $\mu_m < 0$.

2.2 Spectral Green's Function Equations for the Upper Reflector

The spectral Green's function (SGF) method is a spatial discretization method for accurately solving S_N problems defined in slab- or two-dimensional rectangular geometry [4]. In slab-geometry problems, the SGF method generates numerical solutions that are free from

spatial truncation error, because the discretized equations of the SGF method preserve the analytic solution of the S_N equations defined in each mesh cell [5]. So, we consider the entire upper reflector as a single spatial cell and the SGF equations defined in the upper reflector are the multigroup spatial balance equations

$$\frac{\mu_m}{h_{ref}}[\psi_{m,g}(z_{up})-\psi_{m,g}(z_{int})]+\sigma_{t,g}\overline{\psi}^{ref}_{m,g}=\sum_{\ell=0}^{L}\frac{2\ell+1}{2}P_\ell(\mu_m)\sum_{g'=1}^{G}\sigma_\ell^{gg'}\sum_{n=1}^{N}P_\ell(\mu_n)\omega_n\overline{\psi}^{ref}_{n,g'}, \tag{3}$$

and the multigroup SGF auxiliary equations

$$\overline{\psi}^{ref}_{m,g}=\sum_{p=1}^{N/2}\sum_{g''=1}^{G}\theta_{m,g\leftarrow p,g''}\psi_{p,g''}(z_{int})+\sum_{p=N/2+1}^{N}\sum_{g''=1}^{G}\theta_{m,g\leftarrow p,g''}\psi_{p,g''}(z_{up}), \tag{4}$$

m = 1 : N, g = 1 : G.

The quantity on the left hand side of equation (4) is the spatially averaged angular flux over the upper reflector region, h_{ref} is the geometrical thickness of the upper reflector and $\theta_{m,g\leftarrow p,g''}$ are the coefficients of the multigroup SGF auxiliary equations (4). A detailed description for the determination of these coefficients can be found in Ref. [5]. A scaling technique for selecting the real numbers z_i, i = 1:GN, in order to avoid computer overflow exceptions caused by geometrically thick reflectors is provided in Ref. [3].

2.3 Multigroup S_N Albedo Conditions for an Anisotropically Scattering Upper Reflector

Since the upper boundary condition is source-free vacuum, the downwelling neutron flux is zero at z_{up} and so, we may write equations (3-4) for m = N/2+1 : N in the form

$$\frac{|\mu_m|}{h_{ref}}\psi_{m,g}(z_{int})+\sigma_{t,g}\overline{\psi}^{ref}_{m,g}=\sum_{\ell=0}^{L}\frac{2\ell+1}{2}P_\ell(\mu_m)\sum_{g'=1}^{G}\sigma_\ell^{gg'}\sum_{n=1}^{N}P_\ell(\mu_n)\omega_n\overline{\psi}^{ref}_{n,g'}, \tag{5}$$

and

$$\overline{\psi}^{ref}_{m,g}=\sum_{p=1}^{N/2}\sum_{g''=1}^{G}\theta_{m,g\leftarrow p,g''}\psi_{p,g''}(z_{int}),\ m = N/2+1 : N,\ g = 1 : G, \tag{6}$$

respectively. We substitute equations (6) into both sides of equations (5) with appropriate changes in the subscripts (m,g) and, after some algebra, we obtain the multigroup S_N albedo conditions

$$\psi_{m,g}(z_{int})=\sum_{p=1}^{N/2}\sum_{g''=1}^{G}\rho_{m,g\leftarrow p,g''}\psi_{p,g''}(z_{int}),\quad m = N/2+1 : N,\ g = 1 : G, \tag{7}$$

where

$$\rho_{m,g\leftarrow p,g''} \equiv \frac{h_{ref}}{|\mu_m|}(K_{m,g\leftarrow p,g''} - \sigma_{t,g}\theta_{m,g\leftarrow p,g''}),$$

(8)

$$K_{m,g\leftarrow p,g''} \equiv \sum_{n=1}^{N} \omega_n \sum_{g'=1}^{G} (X_{m,g\leftarrow n,g'}\,\theta_{n,g'\leftarrow p,g''})$$

(9)

and

$$X_{m,g\leftarrow n,g'} \equiv \sum_{\ell=0}^{L} \frac{2\ell+1}{2} P_\ell(\mu_m) P_\ell(\mu_n) \sigma_\ell^{gg'}.$$

(10)

Similar multigroup S_N albedo conditions for the lower reflector can be likewise derived. It is noted here that the quantities defined in expressions (8-10) do not depend on the (dominant) solution of the S_N eigenvalue problem. Therefore, the multigroup S_N albedo conditions (7) can be generated and stored for use in S_N computer codes grounded in approximate spatial discretization schemes, e.g. the well-known (and still widely used) ORNL S_N computer code ANISN [8], to improve their accuracy and to increase their efficiency in the solution of multigroup slab-geometry S_N multiplication eigenvalue problems. The improvement in accuracy owes to the replacement of the reflector regions, in which the spatial dependence of angular flux is taken approximately, by exact S_N conditions at fuel-reflector interfaces. The increase in efficiency (time and memory savings) owes to the reduction of the spatial domain, which leads to a decrease in the number of floating point operations for solving the S_N eigenvalue problem, for a fixed space-angle grid imposed on the active core.

3. Numerical Results

We now perform numerical experiments with a ten-layer, two-group thermal reactor core model with anisotropic scattering and no upscattering adapted from the model reported in Ref. [5]. The core model considered here consists of a lower reflector (LR), eight homogeneous, contiguous and disjoint active layers of fissionable material (A_i, i = 1 : 8, where A_1 is the lowermost active layer and A_8 is the uppermost one) and an upper reflector (UR). The size of each layer (in cm) and the material parameters (macroscopic cross sections in cm^{-1}) for the eight active layers can be found in Ref. [5]. We have assumed that scattering is linearly anisotropic (L = 1) in the reflector regions, and we provide in Table 1 the material parameters for the reflectors. Also, we have assumed that all neutrons from fission are yielded within the fast (first) group. Source-free vacuum conditions [1] apply at the top and bottom boundaries of the core. In order to normalize the dominant numerical results generated for the model problem, we have assumed that 200MeV of energy is released on the average per fission reaction in either group and that the core generates 100MW of thermal power.

In order to illustrate how the multigroup S_N albedo conditions (7) and their lower reflector counterpart can improve the accuracy and increase the efficiency of S_N computer codes based on approximate methods of spatial discretization, we performed the following numerical

experiment: we took an upgraded multigroup slab-geometry diamond-difference [1] S_N computer code (developed by the present author some years ago and validated with available results in the open literature), with the option of using the multigroup S_N albedo conditions (7), and

i) we generated S_4 numerical results with the albedo conditions disabled for three spatial grids imposed on the full (ten-layer) spatial domain;

ii) we generated S_4 numerical results with the albedo conditions enabled for corresponding grids imposed on the reduced spatial domain (upper/lower reflectors removed, active core only);

iii) we compared numerical results, computer memory location and execution (CPU) time for the runs in steps i and ii and for corresponding grids.

Table 1 Material parameters (cm^{-1}) for the reflector regions

	LR	UR
$\sigma_{t,1}$	0.2139495	0.2727769
$\sigma_{t,2}$	1.393534	2.0500205
σ_0^{11}	0.1652080	0.2208792
σ_0^{12}	0.0	0.0
σ_0^{21}	0.04797	0.0506087
σ_0^{22}	1.3830772	2.0144887
σ_1^{11}	0.03287	0.06211
σ_1^{12}	0.0	0.0
σ_1^{21}	0.0	0.0
σ_1^{22}	0.18469	0.41553

The spatial grids considered here were so chosen as to mitigate the truncation errors in the numerical results generated by our diamond-difference code. These errors owe to the fact that diamond difference is not a spatial discretization method free from spatial truncation error. In Tables 2 through 5, we present comparative results. In Table 2, we present percent relative deviations for the numerical results generated in steps i and ii for the thermal power generated in some active layers and in Table 3, we present percent relative deviations for the effective multiplication factor (the dominant eigenvalue k_{eff}).

Table 2 Percent relative deviations for thermal power in some active layers

	A_1		A_2		A_4		A_6		A_8	
Grid	Step i	Step ii	Step i	Step ii	Step i	Step ii	Step i	Step ii	Step i	Step ii
$^{\dagger}\Omega_6$	0.134	0.108	0.097	0.061	0.071	0.049	0.112	0.072	0.151	0.129
Ω_5	0.331	0.289	0.264	0.216	0.187	0.134	0.273	0.227	0.355	0.311
Ω_4	0.588	0.522	0.533	0.447	0.389	0.316	0.548	0.466	0.572	0.532

$^{\dagger}\Omega_n$ is to mean 2^n spatial cells per layer.

Table 3 Percent relative deviations for the dominant eigenvalue

	k_{eff}	
Grid	Step i	Step ii
Ω_6	0.003	0.001
Ω_5	0.005	0.002
Ω_4	0.008	0.004

The reference results for the calculation of the relative deviations in Tables 2 and 3 were generated with our SD-SGF computer code [5], which is free from spatial truncation error. Therefore, the reference results considered here are exactly those obtained from the analytical solution of the S_N equations (1), apart from finite arithmetic computational errors and regardless of the spatial grid. We should note that the diamond-difference code and the reference SD-SGF code were written in standard FORTRAN and were executed on an IBM-compatible PC (1.4GHz-clock Pentium 4 Intel processor, 256Mbytes of RAM) running on GNU/Linux, version 0.2. In Table 4, we provide computer memory location for the runs in steps i and ii and in Table 5, we list CPU time for the same runs.

Table 4 Computer memory location

	Memory (Kbyte)	
Grid	Step i	Step ii
Ω_6	71.11	67.85
Ω_5	36.90	33.44
Ω_4	18.56	16.32

Table 5 Execution (CPU) time

	CPU time (second)	
Grid	Step i	Step ii
Ω_6	367	314
Ω_5	189	142
Ω_4	102	77

From Tables 2 through 5, it is apparent that the use of our albedo conditions improved the accuracy (deviations are smaller in step ii) and increased the efficiency (reduced memory requirements and CPU times in step ii) of our diamond-difference computer code.

4. Concluding Remarks

We have outlined the major steps in the derivation of multigroup S_N albedo conditions for primary use in axial models of thermal nuclear reactors with an arbitrary (Legendre) order of anisotropic scattering. These S_N albedo conditions substitute exactly (in a discrete ordinates sense) the axial reflector regions in S_N multiplication eigenvalue calculations. They can be obtained without prior knowledge of the solution of the S_N eigenvalue problem that we are looking for. We remark that our multigroup S_N albedo conditions are expected to improve the numerical accuracy and to increase the computational efficiency of *any* slab-geometry S_N code grounded in spatial discretization methods that are approximate, e.g. the well-known (and still widely used) ORNL computer code ANISN. These overall improvements can be

achieved by removing the axial reflector regions from the spatial domain and by replacing them with our multigroup S_N albedo conditions. In concluding, we note that the material provided here may serve as a basis for improvements in approximate S_N albedo conditions recently developed by Alves Filho and Barros [6] for x,y-geometry nuclear reactor calculations, as they are presently limited to one-speed models with isotropic scattering and, to the best of our perception, they are not numerically stable.

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