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Comparison of power series solutions to the stationary monoenergetic neutron transport equation for slabs

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Abstract. A perturbation expansion of the neutron flux in powers of the total cross-section or an ordinary power series expansion with respect to the space coordinate inserted into the transport equation lead to the same system of linear equations for the expansion coefficients. Two different truncation methods are compared, and after showing the asymptotic behaviour of the flux expansion coefficients, various asymptotic approximation methods are formulated, which permit to reduce the truncation error by several orders of magnitude.

1. Introduction

The following investigations were initiated by some work on phonon transport in a slab-shaped insulator containing small amounts of impurities [1, 2]. The problem could be described by a linear transport equation being equivalent to the one-speed neutron transport equation for an absorption-free material with isotropic scattering. Whereas in [1] the problem was treated by a simple approximation of the scattering integral, applicable for weakly anisotropic flux, in some later unpublished work [3], the problem was tackled by expanding the particle flux into powers of the collision cross-section, the latter being considered a small quantity, and truncating this at order 2. Both methods led to solutions which were shown to be relatively accurate for small optical thicknesses and, against expectation, also for large ones.

Whereas in a few recent publications perturbation expansions into powers of the inverse optical depth were successfully used mainly for the treatment of neutron transport problems in large systems [4–7], a corresponding expansion into powers of the collision cross-section or equivalently the optical thickness was used in this work like in [3], first. It proved to be identical to a spatial power series expansion of the flux, a procedure that has evidently been used by other authors before (e.g. 8–10). However only in [10], for more general problems in radiative and neutron transfer the same treatment of the angular variable was chosen. The aim of the present investigation is to present first two power series approximations with different truncation and to show then especially the asymptotic behaviour of the flux expansion coefficients which will be used for improved approximations, afterwards.

2. Formulation of the power series method

In one-dimensional slab geometry the monoenergetic stationary neutron transport equation may be written in case of linearly anisotropic scattering as follows:

$$\pm \mu \frac{\partial \phi^\pm}{\partial x} + \Sigma \phi^\pm = \frac{c_0}{2} \Sigma \int_0^1 (\phi^+ + \phi^-) d\mu' \pm \mu \frac{3c_1}{2} \Sigma \int_0^1 (\phi^+ - \phi^-) \mu' d\mu'. \quad (2.1)$$

The meaning of the symbols in (2.1) being:

$$\begin{aligned} \mu \in [0, 1] & \text{ modulus of projection of angular unit vector on x-axis} \\ \phi^+(x, \mu) = \phi(x, \mu) & \text{ angular flux (upper sign in equation (2.1))} \\ \phi^-(x, \mu) = \phi(x, -\mu) & \text{ angular flux (lower sign in equation (2.1))} \\ \Sigma & \text{ total cross-section} \\ c_l & \text{ moments of scattering and fission kernel.} \end{aligned}$$

Equation (2.1) shall be solved in a homogeneous slab with half-thickness d and the boundary conditions:

$$\begin{aligned} \phi^+(x = -d, \mu) &= S^+(\mu) \\ \phi^-(x = d, \mu) &= S^-(\mu). \end{aligned} \quad (2.2)$$

The flux is expanded into the power series:

$$\phi^\pm(x, \mu) \approx \sum_{v=0}^N \frac{(\Sigma x)^v}{v!} f_v^\pm(\mu). \quad (2.3)$$

Insertion of this truncated expansion into (2.1) and sorting out coefficients of equal powers in Σx leads to the following recurrence relation:

$$f_{v+1}^\pm = \mp \frac{1}{\mu} \left(f_v^\pm - \frac{c_0}{2} \int_0^1 (f_v^+ + f_v^-) d\mu' - \frac{3c_1}{2} (\mp \mu) \int_0^1 (f_v^- - f_v^+) \mu' d\mu' \right). \quad (2.4)$$

With the definitions:

$$A_v = \int_0^1 (f_v^+ + f_v^-) d\mu' \quad (2.5a)$$

$$B_v = \int_0^1 (f_v^- - f_v^+) \mu' d\mu' \quad (2.5b)$$

f_v^\pm can be expressed in terms of f_0^\pm and the above coefficients:

$$f_v^\pm = \left(\mp \frac{1}{\mu} \right)^v \left(f_0^\pm - \frac{c_0}{2} \sum_{n=0}^{v-1} A_n (\mp \mu)^n - \frac{3c_1}{2} \sum_{n=0}^{v-1} B_n (\mp \mu)^{n+1} \right) \quad (2.6)$$

where $f_0^\pm(\mu)$ remains to be determined by the boundary conditions.

The coefficients A_v and B_v represent simply the expansion coefficients of integrated flux and current respectively, since with (2.3) and (2.5)

$$F_0(x) = \int_0^1 (\phi^+(x, \mu) + \phi^-(x, \mu)) d\mu \approx \sum_{v=0}^N \frac{(\Sigma x)^v}{v!} A_v, \quad (2.7a)$$

$$F_1(x) = \int_0^1 (\phi^+(x, \mu) - \phi^-(x, \mu)) \mu d\mu \approx - \sum_{v=0}^N \frac{(\Sigma x)^v}{v!} B_v. \quad (2.7b)$$

Insertion of (2.6) into (2.3) yields after satisfying the boundary conditions and some rearrangement for $0 \leq v \leq N$:

$$\begin{aligned}
 f_v^\pm = & \left(\mp \frac{1}{\mu} \right)^v \left\{ \frac{c_0}{2} \sum_{n=v}^N A_n (\mp \mu)^n + \frac{3c_1}{2} \sum_{n=v}^N B_n (\mp \mu)^{n+1} \right. \\
 & + \left(\sum_{m=0}^N \frac{\theta^m}{m! \mu^m} \right)^{-1} \left[S^\pm - \sum_{n=0}^N \left(\frac{c_0}{2} A_n (\mp \mu)^n + \frac{3c_1}{2} B_n (\mp \mu)^{n+1} \right) \right. \\
 & \left. \left. \times \sum_{l=0}^n \frac{\theta^l}{l! \mu^l} \right] \right\} \tag{2.8}
 \end{aligned}$$

where

$$\theta = \Sigma d. \tag{2.9}$$

Making use of (2.8) in (2.5) would yield a system of equations for the coefficients A_v and B_v . Some special features of these equations may be visualized more easily, however, when using (2.6) instead of (2.8). Obviously, it is necessary to distinguish between even and odd v . (2.6) in (2.5) gives:

$$A_{2k} = \int_0^1 \frac{d\mu}{\mu^{2k}} \left[f_0^+ + f_0^- - c_0 \sum_{l=0}^{k-1} A_{2l} \mu^{2l} - 3c_1 \sum_{l=0}^{k-1} B_{2l+1} \mu^{2l+2} \right] \tag{2.10a}$$

$$A_{2k+1} = \int_0^1 \frac{d\mu}{\mu^{2k+1}} \left[f_0^- - f_0^+ - c_0 \sum_{l=0}^{k-1} A_{2l+1} \mu^{2l+1} - 3c_1 \sum_{l=0}^k B_{2l} \mu^{2l+1} \right] \tag{2.10b}$$

$$B_{2k+2} = \int_0^1 \frac{d\mu}{\mu^{2k+1}} \left[f_0^- - f_0^+ - c_0 \sum_{l=0}^k A_{2l+1} \mu^{2l+1} - 3c_1 \sum_{l=0}^k B_{2l} \mu^{2l+1} \right] \tag{2.10c}$$

$$B_{2k+1} = \int_0^1 \frac{d\mu}{\mu_{2k}} \left[f_0^+ + f_0^- - c_0 \sum_{l=0}^k A_{2l} \mu^{2l} - 3c_1 \sum_{l=0}^{k-1} B_{2l+1} \mu^{2l+2} \right] \tag{2.10d}$$

Taking the difference between (2.10a) and (2.10d) yields:

$$B_{2k+1} = A_{2k} (1 - c_0) \tag{2.11a}$$

and similarly from (2.10b, c)

$$B_{2k+2} = A_{2k+1} (1 - c_0). \tag{2.11b}$$

These relations permit to substitute the coefficients B_v in the equations for A_v . Formally, this can be done also for B_0 by introduction of a dummy coefficient

$$B_0 = (1 - c_0) A_{-1}. \tag{2.11c}$$

The final equations result from (2.10a, b) after insertion of f_0^\pm from (2.8) and the coefficients B_v from (2.11). In these equations certain exponential-like integrals occur, being defined as

$$J_n^N(\theta) = \int_0^1 d\mu \mu^{-(n+2)} \left(\sum_{m=0}^N \frac{\theta^m}{m! \mu^m} \right)^{-1}. \tag{2.12}$$

With this, one obtains

$$\begin{aligned}
 & \sum_{l=0}^{k-1} A_{2l} \left\{ c_0 \sum_{m=0}^{2l} \frac{\theta^m}{m!} J_{2(k-l-1)+m}^N + 3c_1(1 - c_0) \sum_{m=0}^{2l+1} \frac{\theta^m}{m!} J_{2(k-l-2)+m}^N \right\} \\
 & + \sum_{l=k}^{[N/2]} A_{2l} \left\{ \delta_{k,l} + c_0 \left(-\frac{1}{2(l-k)+1} + \sum_{m=0}^{2l} \frac{\theta^m}{m!} J_{2(k-l-1)+m}^N \right) \right\} \\
 & + \sum_{l=k}^{[(N-1)/2]} A_{2l} \left\{ 3c_1(1 - c_0) \left(-\frac{1}{2(l-k)+3} + \sum_{m=0}^{2l+1} \frac{\theta^m}{m!} J_{2(k-l-2)+m}^N \right) \right\} \\
 & = \int_0^1 d\mu (S^+ + S^-) \mu^{-2k} \left(\sum_{m=0}^N \frac{\theta^m}{\mu^m m!} \right)^{-1} \quad 0 \leq k \leq \left[\frac{N}{2} \right] \tag{2.13a}
 \end{aligned}$$

and

$$\begin{aligned}
 & \sum_{l=-1}^{k-1} A_{2l+1} \left\{ c_0 \sum_{m=0}^{2l+1} \frac{\theta^m}{m!} J_{2(k-l-1)+m}^N + 3c_1(1 - c_0) \sum_{m=0}^{2l+2} \frac{\theta^m}{m!} J_{2(k-l-2)+m}^N \right\} \\
 & + \sum_{l=k}^{[(N-1)/2]} A_{2l+1} \left\{ \delta_{k,l} + c_0 \left(-\frac{1}{2(l-k)+1} + \sum_{m=0}^{2l+1} \frac{\theta^m}{m!} J_{2(k-l-1)+m}^N \right) \right\} \\
 & + \sum_{l=k}^{[(N-2)/2]} A_{2l+1} \left\{ 3c_1(1 - c_0) \left(-\frac{1}{2(l-k)+3} + \sum_{m=0}^{2l+2} \frac{\theta^m}{m!} J_{2(k-l-2)+m}^N \right) \right\} \\
 & = \int_0^1 d\mu \mu^{-(2k+1)} \left(\sum_{m=0}^N \frac{\theta^m}{\mu^m m!} \right)^{-1} \quad -1 \leq k \leq \left[\frac{N-1}{2} \right]. \tag{2.13b}
 \end{aligned}$$

In these equations, the expressions $[N/2]$ etc. stand for the integer part of the numbers in brackets. Moreover, it is understood that a sum vanishes if the lower index exceeds the upper. $\delta_{k,l}$ is the usual Kronecker symbol.

If the boundary sources S^\pm are expanded into power series of μ , the integrals on the right-hand sides of (2.13) can be expressed in terms of the functions J_n^N , as well.

After determination of the quasi-exponential integrals, which is performed via a partial fraction decomposition, the matrix elements are calculated by a recurrence procedure. Then, equations (2.13) can be solved for the coefficients A_ν . In practical computation, the coefficient B_0 was kept back in the equations, because the case $c_0 = 1$ would have required special treatment, otherwise. With the coefficients A_ν and B_ν the fluxes and the current may be calculated for every point in the slab. Numerical results will be given in Section 5. In the following, the above expounded method will be referred to as the Consistent Approximation (CA).

3. The limit $N \rightarrow \infty$ and the Inconsistent Approximation (IA)

If this limit is taken, the number N may simply be replaced by ∞ in all equations. Furthermore, the quasi-exponential integrals converge towards:

$$\lim_{N \rightarrow \infty} J_n^N(\theta) \rightarrow J_n(\theta) = \int_0^1 \mu^{-(n+2)} e^{-\theta/\mu} d\mu = \int_1^\infty \xi^n e^{-\theta\xi} d\xi. \tag{3.1}$$

The functions $J_n(\theta)$, elsewhere [11] denoted by α_n , are related to the usual exponential

integrals as follows:

$$J_{-n}(\theta) = E_n(\theta) = \int_1^\infty \xi^{-n} e^{-\theta\xi} d\xi. \tag{3.2}$$

Of course, the infinite system of equations resulting thus from (2.13) cannot be solved directly, it is possible, however, to make further approximations in order to obtain finite systems.

The most simple assumption is to truncate the flux expansion at some order M , i.e. to put

$$A_\nu = 0 \quad \text{for } \nu > M. \tag{3.3}$$

The resulting equations are essentially those of (2.13) with N substituted by M in the summation limits if J_n^N and the truncated exponential power series are replaced by J_n and $\exp(-\theta/\mu)$ respectively. Because this method can be obtained from the CA by this substitution procedure, it is called Inconsistent Approximation (IA). It must be noted that it satisfies the boundary conditions exactly as well as the CA.

Finally the fluxes and currents for the IA-method can be calculated according to (2.3) and (2.7) with N replaced by M . The main advantage of the IA- over the CA-method is the ease by which the functions J_n may be calculated even for high order, where the partial fraction expansions in the calculations for J_n^N lead to large numerical errors. As a matter of fact, the IA is obtained certainly for isotropic and most probably also for anisotropic scattering if expansion (2.7a) and truncation (3.3) is inserted into the integral form of the transport equation [8, 9]. Therefore, this approximation may be considered to be consistent with integral transport theory where it has been used earlier at least in [9]. There, a relatively slow convergence was reported for the power series method, a result which is confirmed by our own calculations. Numerical results can be found in Section 5.

4. The asymptotic behaviour of the flux expansion coefficients and its use for approximation methods

In order to show this behaviour, a modified version of the limiting form of equations (2.13) shall be used, which is obtained therefrom by help of the recurrence relations (A.1, A.4) and equation (A.6). In addition, a power series expansion

$$S^\pm = \sum_{i=0}^I (\mp 1)^i S_i^\pm \mu^i \tag{4.1}$$

is inserted into equations (2.13), too. For the sake of simplicity, all coefficients being due to anisotropic scattering are omitted, because no relevant additional contributions arise from them. One obtains after some rearrangement:

$$\begin{aligned} & \sum_{l=0}^\infty A_{2l} c_0 \frac{\theta^{2l}}{(2l)!} \left(J_{2k-2} + \frac{2l}{2(k-l)-1} (J_{2k-2} - J_{2l-1}) \right) \\ & + A_{2k} + \sum_{l=k}^\infty A_{2l} \frac{c_0}{2(k-l)-1} = \sum_{i=0}^I ((-1)^i S_i^+ + S_i^-) J_{2(k-1)-i} \quad 0 \leq k \leq \infty, \end{aligned} \tag{4.2a}$$

$$\begin{aligned} & \sum_{l=-1}^{\infty} A_{2l+1} c_0 \frac{\theta^{2l+1}}{(2l+1)!} \left(J_{2k-1} + \frac{2l+1}{2(k-l)-1} (J_{2k-1} - J_{2l}) \right) \\ & + A_{2k+1} + \sum_{l=k}^{\infty} A_{2l+1} \frac{c_0}{2(k-l)-1} = \sum_{i=0}^I (S_i^- - (-1)^i S_i^+) J_{2k-1-i} \\ & \qquad \qquad \qquad -1 \leq k \leq \infty. \end{aligned} \quad (4.2b)$$

In the second equation, the following convention was adopted:

$$\frac{\theta^v}{v!} = 0 \quad \text{for } v < 0.$$

Because of the asymptotic behaviour of the functions J_ν for large ν (A.3), the leading term on the right side of (4.2a) is of order J_{2k-2} . Dividing this equation by J_{2k-2} and neglecting terms of order $(2k-2)^{-1}$ yields:

$$\frac{A_{2k}}{J_{2k-2}} + c_0 \sum_{l=0}^{\infty} A_{2l} \frac{\theta^{2l}}{(2l)!} \left(1 + \frac{2l}{2(k-l)-1} \right) \approx S_0^+ + S_0^-. \quad (4.3)$$

Because the sum in (4.3) must be bounded, one can show that in the limit of $k \rightarrow \infty$:

$$\begin{aligned} \lim_{k \rightarrow \infty} \frac{A_{2k}}{J_{2k-2}} &= a_e = S_0^+ + S_0^- - c_0 \sum_{l=0}^{\infty} A_{2l} \frac{\theta^{2l}}{(2l)!} \\ &= S_0^+ + S_0^- - \frac{c_0}{2} (F_0(d) + F_0(-d)). \end{aligned} \quad (4.4a)$$

Similarly, for the asymptotic form of odd coefficients results:

$$\begin{aligned} \lim_{k \rightarrow \infty} \frac{A_{2k+1}}{J_{2k-1}} &= a_u = S_0^- - S_0^+ - c_0 \sum_{l=0}^{\infty} A_{2l+1} \frac{\theta^{2l+1}}{(2l+1)!} \\ &= S_0^- - S_0^+ - \frac{c_0}{2} (F_0(d) - F_0(-d)). \end{aligned} \quad (4.4b)$$

With these relations and (A.3) the first asymptotic approximation for the coefficients A_ν is defined:

$$\tilde{A}_{2k} = a_e \frac{(2k-2)!}{\theta^{2k-1}} \quad (4.5a)$$

$$\tilde{A}_{2k+1} = a_u \frac{(2k-1)!}{\theta^{2k}}. \quad (4.5b)$$

A higher order approximation is obtained if (4.4a) is subtracted from the quotient of (4.2a) and J_{2k-2} . After neglecting terms of order smaller than $(2k-2)^{-1}$, there results:

$$\frac{A_{2k}}{J_{2k-2}} - a_e \approx -c_0 \sum_{l=1}^{\infty} A_{2l} \frac{\theta^{2l-1}}{(2l-1)!} \frac{\theta}{2(k-l)-1} + \frac{\theta}{2k-2} (S_1^- - S_1^+). \quad (4.6)$$

The order of magnitude of the sum in (4.6) can be estimated by inserting (4.5a). One obtains:

$$\frac{A_{2k}}{J_{2k-2}} - a_e \approx -c_0 a_e \frac{1}{2k-2} \sum_{l=0}^{k-2} \frac{1}{2l+1} + o\left(\frac{1}{2k-2}\right)$$

Therefore, the following second order asymptotic formula results:

$$\tilde{A}_{2k}^2 = a_{e,1} \frac{(2k-2)!}{\theta^{2k-1}} \left(1 - \frac{c_0 \theta}{2k-2} \sum_{l=0}^{k-2} \frac{1}{2l+1}\right) + a_{e,2} \frac{(2k-3)!}{\theta^{2k-2}} \tag{4.7a}$$

and similarly for odd v :

$$\tilde{A}_{2k+1}^2 = a_{u,1} \frac{(2k-1)!}{\theta^{2k}} \left(1 - \frac{c_0 \theta}{2k-1} \sum_{l=0}^{k-2} \frac{1}{2l+1}\right) + a_{u,2} \frac{(2k-2)!}{\theta^{2k-1}}. \tag{4.7b}$$

The leading asymptotic terms (4.5a, b) have an interesting physical meaning, since they contribute significantly to the transient part of the flux at the surfaces $x = \pm d$ of the slab. Admitting $\tilde{A}_0 = 0$ and using (4.5) for $k \geq 1$ in (2.7a) results in

$$\tilde{F}_0(x) = \frac{a_e - a_u}{2} \theta \left(1 + \frac{x}{d}\right) \ln\left(1 + \frac{x}{d}\right) + \frac{a_e + a_u}{2} \theta \left(1 - \frac{x}{d}\right) \ln\left(1 - \frac{x}{d}\right) + a_u \theta \frac{x}{d} \tag{4.8}$$

This looks very similar to the transient solution for the Milne problem [12].

With this, a number of asymptotic approximation methods can be created. Their common feature is that for $v > M$ the expansion coefficients are given by (4.5) or (4.7), and that additional equations must be formulated for the determination of the unknown coefficients a_e, a_u etc. The salient point of these methods is that they cause a drastic reduction of the truncation error of the first $M + 2$ equations, since the residual series in these equations may be summed up with fairly high accuracy. For a better understanding of this statement, the formal equations of such an approximation corresponding to (4.2) with anisotropic scattering are given in the following:

For $0 \leq k \leq K_e = [M/2]$

$$\sum_{l=0}^{\infty} A_{2l} G_{k,l} \approx \sum_{l=0}^{K_e} A_{2l} G_{k,l} + \sum_{l=K_e+1}^{\infty} \tilde{A}_{2l} G_{k,l} \approx Q_k \tag{4.9a}$$

and for $-1 \leq k \leq K_u = [(M-1)/2]$

$$\sum_{l=-1}^{\infty} A_{2l+1} H_{k,l} \approx \sum_{l=-1}^{K_u} A_{2l+1} H_{k,l} + \sum_{l=K_u+1}^{\infty} \tilde{A}_{2l+1} H_{k,l} \approx R_k. \tag{4.9b}$$

The infinite residual sums in (4.9) should not be calculated by a direct numerical addition, because they converge slowly. They can be decomposed, however, into a number of finite and infinite series for which either analytical summation formulae exist or numerical addition shows good convergence. Yet, it is not possible to give here all the resulting formulae, because a great deal of different cases have to be distinguished and the expressions become too voluminous. The same applies also to the formulae for the calculation of the flux- and current distributions especially in case of the second order asymptotic approximation.

Three different asymptotic methods have been investigated numerically. Their characteristics are distinguished in the following:

First Asymptotic Approximation AA1

This method is based on the first order approximations (4.5). The additional equations required are simply those of order $M + 1$ and $M + 2$, respectively.

Second Asymptotic Approximation AA2

Again expressions (4.5) are applied, but here together with the asymptotic equations (4.4).

Improved Asymptotic Approximation IAA

Only in this method the second order approximations (4.7) are used. Since in (4.7) four free coefficients occur, the equations of order $M + 1$ and $M + 2$ together with (4.4) are chosen to give the required number of conditions.

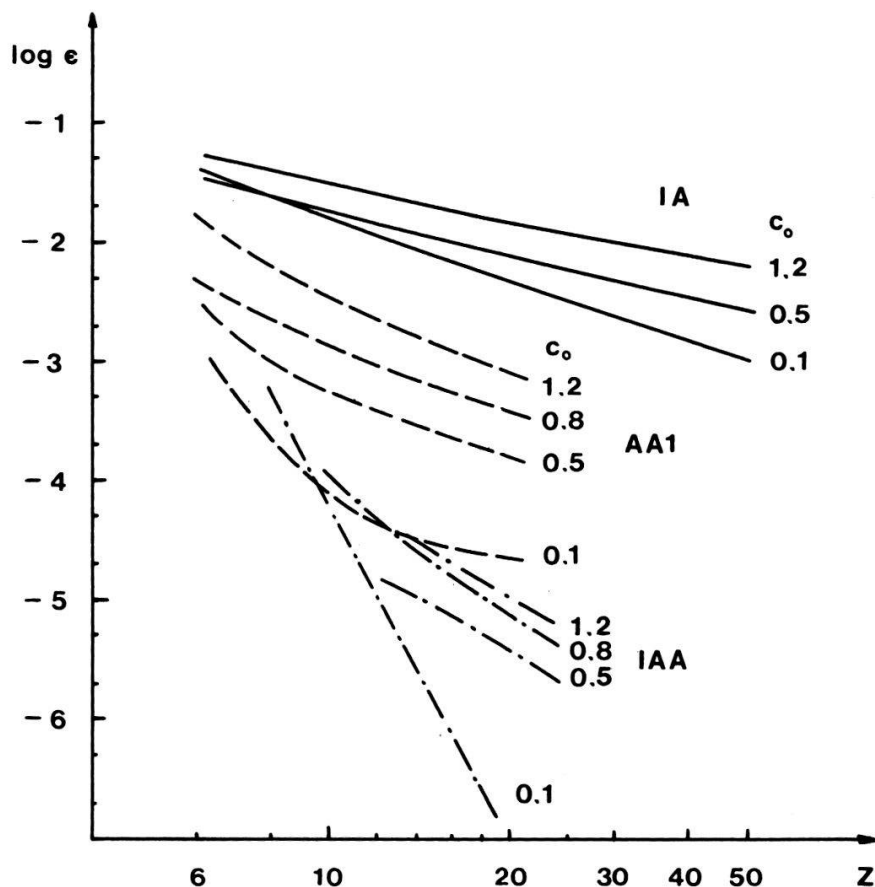


Figure 1
 Comparison of the relative error ϵ of the flux $F_0(d)$ at the vacuum-sided surface of a slab with half-thickness $\theta = \Sigma d = 0.5$ and $c_1 = 0$ for various approximation methods and values of the parameter c_0 . Z = total approximation order.

5. Numerical results

In the graphs, relative errors of the flux $F_0(x = d)$ as functions of the approximation order Z are given for several examples with different c_0 , c_1 , and θ , whereas the boundary conditions are the same in all cases, i.e. $S^+ = 1, S^- = 0$.

The number Z is given by the total order of the equation system which has to be solved. The exact values for $F_0(d)$ were obtained by an extrapolation of the results of the IAA for $Z \rightarrow \infty$. In order to test these limit values, they were compared with those of similar extrapolations of the IA- and CA-calculations and in addition with results given in the literature [13, 14].

In Figs. 1 and 2 the approximations IA, AA1, and IAA are compared. No results of the CA- and AA2-methods are included, because the former is roughly equivalent to the IA and the latter slightly less accurate than the AA1. The results show the high gain of precision and convergence speed obtained by means of the IAA over the IA and also the AA1. But, of course, no low order calculations can be done with this IAA-method. Moreover, an increase of the error with growing c_0 or θ is observed, whereas the scattering coefficient c_1 causes no significant effect. All methods are applicable to slab problems with half-thickness d smaller than a few mean free paths, for the asymptotic methods, however, the loss of accuracy with increasing θ is more pronounced.

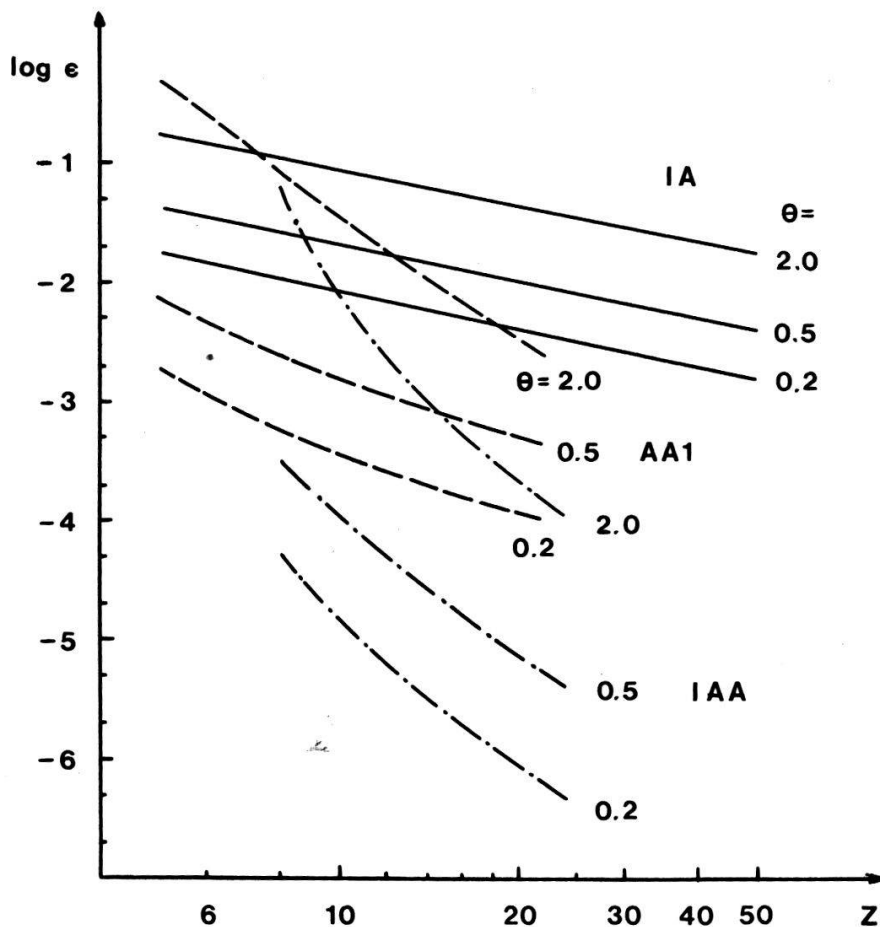


Figure 2

Comparison of the same quantity and methods as in Figure 1 but for $c_0 = 0.8, c_1 = 0.25$, and three different values of θ .

Finally, a particularity of the CA-method should be mentioned yet, i.e. the highly symmetrical alternating convergence of the fluxes $F_0(x = \pm d)$ with increasing order. Thus, a considerable gain of accuracy can be obtained by conveniently averaging the results of adjacent approximations with different parity in Z .

6. Generalizations

It is possible to show that all methods can be generalized to layered slabs, multi-energy groups, higher-order scattering, and source- as well as criticality problems. Optically thick slabs would have to be treated by subdivision. It must be noted, however, that these generalizations entail certain modifications. Thus, in multizone problems the equations for odd and even coefficients get coupled, and for source problems the asymptotic equations contain additional terms. The straightforward application of the methods to optically thick slabs would obviously lead to very large systems of linear equations with essentially full matrices. For a treatment of such problems, it is therefore necessary to investigate whether far-off-diagonal matrix elements can be eliminated or possibly suppressed.

Appendix

The exponential integrals J_n as defined in (3.1) obey the following recurrence relations [11]

$$J_n(x) = \frac{n}{x} J_{n-1}(x) + \frac{e^{-x}}{x} \quad (\text{A.1})$$

so that

$$J_n(x) = \frac{n!}{x^{n+1}} e^{-x} \sum_{v=0}^n \frac{x^v}{v!}. \quad (\text{A.2})$$

This converges for large n towards

$$J_n(x) \xrightarrow{n \gg 1} \frac{n!}{x^{n+1}}. \quad (\text{A.3})$$

For negative n the usual exponential integrals (3.2) are obtained, where (A.1) is usually written as:

$$E_n(x) = \frac{1}{n-1} (e^{-x} - xE_{n-1}(x)) \quad n \geq 2. \quad (\text{A.4})$$

The functions E_n can be determined, therefore, from e^{-x} and $E_1(x)$, where

$$E_1(x) = -\left(\ln x + \gamma + \sum_{v=1}^{\infty} \frac{(-1)^v x^v}{v! v} \right) \quad x > 0 \quad (\text{A.5})$$

$\gamma = 0.5772156649 \dots$ (Euler's constant).

For the derivation of (4.2) the following relation is needed:

$$\sum_{n=0}^N \frac{\theta^n}{n!} J_{n+M} = \frac{\theta}{M+1} \frac{\theta^N}{N!} (J_{N+M+1} - J_N) \quad N \geq 0, M \neq -1. \quad (\text{A.6})$$

It results from (A.1), (A.2), (A.4), and the summation formula:

$$\sum_{n=0}^N \frac{n!}{(M+n)!} = \frac{(N+1)!}{(M-1)(M+N)!} \left[\binom{M+N}{N+1} - 1 \right] \quad M \geq 2 \quad (\text{A.7})$$

which can be proved by induction.

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