A transport theoretic approximation method for the monoenergetic neutron transport equation

1982 J. Phys. A: Math. Gen. 15 L487

(http://iopscience.iop.org/0305-4470/15/9/010)

J. Phys. A: Math. Gen. 15 (1982) L487–L493. Printed in Great Britain

LETTER TO THE EDITOR

A transport theoretic approximation method for the monoenergetic neutron transport equation

A Sengupta

Nuclear Engineering and Technology Programme, Indian Institute of Technology, Kanpur, India

Received 15 March 1982

Abstract. This letter introduces the basic features of a proposed transport theoretic approximation of the one-speed neutron transport equation. The method utilises the exact results of Case, and retains the use of the eigenfunctions $\phi_{0\pm}(\mu)$ together with a properly constructed rational approximation $\bar{\phi}_\nu(\mu)$ of the singular eigenfunction $\phi_\nu(\mu)$ as the complete set of basis functions. A major contribution of this work is the adaption of Case's orthogonality relations to this basis, $\{\phi_{0\pm}(\mu), \bar{\phi}_\nu(\mu)\}$, for obtaining the desired solution.

In this letter, we present the basic features of a novel scheme for obtaining an approximate solution of the one-speed neutron transport equation utilising the standard exact results of Case and Zweifel (1967). While a detailed report will be published separately, it is our opinion that the method is of sufficient interest and generality to merit a short communication here.

We are concerned with the solution of the one-speed equation

$$\mu \frac{\partial\psi(x,\mu)}{\partial x} + \psi(x,\mu) = \frac{c}{2}\int_{-1}^{1} \psi(x,\mu')\,\mathrm{d}\mu' \tag{1}$$

for full- and half-range boundary conditions. For this, we use Case's solution in standard notation (Case and Zweifel 1967)

$$\psi(x,\mu) = a_{0+}\exp(-x/\nu_0)\phi_{0+}(\mu) + a_{0-}\exp(x/\nu_0)\phi_{0-}(\mu) + \int_{-1}^{1} A(\nu)\exp(-x/\nu)\phi_\nu(\mu)\,\mathrm{d}\nu \tag{2a}$$

and

$$\psi(x,\mu) = a_{0+}\exp(-x/\nu_0)\phi_{0+}(\mu) + \int_{0}^{1} A(\nu)\exp(-x/\nu)\phi_\nu(\mu)\,\mathrm{d}\nu \qquad \mu \geqslant 0 \qquad x \geqslant 0 \tag{2b}$$

for the full- and half-range problems, respectively. Here ν_0 satisfies

$$\frac{c\nu_0}{2}\ln\frac{\nu_0+1}{\nu_0-1} = 1 \tag{3}$$

0305-4470/82/090487+07\$02.00

and the Case eigenfunctions are

$$\phi_{0\pm}(\mu)=\frac{c\nu_0}{2}\frac{1}{\nu_0\mp\mu} \tag{4}$$

$$\phi_\nu(\mu)=\frac{c\nu}{2}P\frac{1}{\nu-\mu}+\lambda(\nu)\delta(\nu-\mu). \tag{5}$$

The necessary and sufficient conditions for the determination of the constants $a_{0\pm}$ and $A(\nu)$ are the orthogonality integrals (Case and Zweifel 1967)

$$\int_{-1}^{1}\mu\phi_{0\pm}^2(\mu)\,\mathrm{d}\mu=N_{0\pm} \tag{6a}$$

$$\int_{-1}^{1}\mu\phi_\nu(\mu)\phi_{\nu'}(\mu)\,\mathrm{d}\mu=N(\nu)\delta(\nu-\nu')\qquad \nu,\nu'\in(-1,1) \tag{6b}$$

where

$$N_{0\pm}=\pm\frac{c\nu_0^3}{2}\left(\frac{c}{\nu_0^2-1}-\frac{1}{\nu_0^2}\right)$$

$$N(\nu)=\nu\left[\left(1-\frac{c\nu}{2}\ln\frac{1+\nu}{1-\nu}\right)^2+\frac{c^2\pi^2\nu^2}{4}\right]$$

for the full-range problem, and when $\nu,\nu'\in(0,1)$,

$$\int_0^1 W(\mu)\phi_{0+}(\mu)\phi_\nu(\mu)\,\mathrm{d}\mu=0 \tag{7a}$$

$$\int_0^1 W(\mu)\phi_{0-}(\mu)\phi_\nu(\mu)\,\mathrm{d}\mu=c\nu\nu_0X(-\nu_0)\phi_{0-}(\nu) \tag{7b}$$

$$\int_0^1 W(\mu)\phi_{0+}(\mu)\phi_{-\nu}(\mu)\,\mathrm{d}\mu=\tfrac{1}{4}c^2\nu\nu_0X(-\nu) \tag{7c}$$

$$\int_0^1 W(\mu)\phi_\nu(\mu)\phi_{\nu'}(\mu)\,\mathrm{d}\mu=W(\nu)(N(\nu)/\nu)\delta(\nu-\nu') \tag{7d}$$

$$\int_0^1 W(\mu)\phi_{0\pm}(\mu)\phi_{0+}(\mu)\,\mathrm{d}\mu=\mp(\tfrac{1}{2}c\nu_0)^2X(\pm\nu_0) \tag{7e}$$

for the half-range case. Here (Case and Zweifel 1967)

$$X(-\mu)=\frac{1}{\mu+1/X(0)}\Omega(-\mu) \tag{8}$$

$$\Omega(-\mu)=1-\frac{c\nu_0^2}{2}\mu\int_0^1\frac{1-t^2X^2(0)}{(\nu_0^2-t^2)(\mu+t)\Omega(-t)}\,\mathrm{d}t \tag{9}$$

with

$$X(0)=1/(\nu_0\sqrt{1-c})$$

and

$$W(\mu)=\frac{c\mu}{2(1-c)}\frac{1}{(\nu_0+\mu)X(-\mu)}. \tag{10}$$

Also,

$$X(\nu_0) = -\left(\frac{\nu_0^2(1-c)-1}{2a_{0m}(1-c)\nu_0^2(\nu_0^2-1)}\right)^{1/2}$$

$$X(-\nu_0) = a_{0m}X(\nu_0)$$

where

$$a_{0m} = -\exp(-2z_0/\nu_0),$$

z_0 being the extrapolated end point.

Our solution procedure starts by recognising (Ganguly and Sengupta 1980) that one should, strictly speaking, use the exact ν_0 and $\phi_{0\pm}(\mu)$ in the asymptotic part of the solutions (2). Unlike in Ganguly and Sengupta (1980), however, we do not replace the transient integral by utilising the roots of the P_N approximation, nor use modified Marshak boundary conditions to obtain the coefficients in the solution. Instead, we reason as follows.

(i) The discretisation of $\nu \in (-1, 1)$ (or $\nu \in (0, 1)$) should be done such that these roots, ν_j, $j = 1, 2, \ldots$ are consistent with the particular choice of ν_0. The P_N approximation has this desirable property, as all its $N+1$ ν_j are solutions of a polynomial equation of degree $N+1$, $g_{N+1}(\nu) = 0$. In contrast, by requiring the asymptotic ν_0 to satisfy equation (3) and the transient ν_j the equation $g_{N+1}(\nu) = 0$, the TP_N procedure (Ganguly and Sengupta 1980) violates this property.

(ii) The natural basis functions for the solution of the transport equation are the Case eigenfunctions $\phi_{0+}(\mu)$, $\phi_{0-}(\mu)$, $\phi_\nu(\mu)$. Any other basis such as the $\{P_n(\mu)\}_{n=0}^N$ (as in the P_N case), or a combination $\{\phi_{0+}(\mu), \phi_{0-}(\mu), \{P_n(\mu)\}\}$ (as in the TP_N case), is likely to be unsatisfactory.

(iii) By the very nature of the eigenfunctions, a rational function approximation is expected to be superior to a standard polynomial approximation.

In view of the above, let $\bar{\phi}_\nu(\mu)$, an approximation of $\phi_\nu(\mu)$, have the form

$$\bar{\phi}_\nu(\mu) = \sum_{l=0}^{L} a_l(\nu)\pi_l(\mu) + R_L(\nu, \mu) \tag{11}$$

where $\{\pi_l(\mu)\}_{l=0}^\infty$ is a complete set of orthogonal polynomials, and $R_L(\nu, \mu)$ is the remainder, or error, in representing $\phi_\nu(\mu)$ by a finite linear combination of the $\pi_l(\mu)$. This remainder is expressed as a rational function, i.e. as

$$R_L(\nu, \mu) = \frac{\sum_{n=L+1}^N a_n(\nu)\pi_n(\mu)}{\sum_{m=0}^M b_m(\nu)\pi_m(\mu)} \qquad b_0 = 1.$$

Alternatively, we can also write

$$\bar{\phi}_\nu(\mu) = \frac{\sum_{n=0}^N a_n(\nu)\pi_n(\mu)}{\sum_{m=0}^M b_m(\nu)\pi_m(\mu)} \qquad b_0 = 1. \tag{12}$$

For the present problem we can choose the $\pi_n(\mu)$ to be either the Legendre or Chebyshev polynomials and observe that it is necessary to have $\bar{\phi}_{-\nu}(\mu) = \bar{\phi}_\nu(-\mu)$. If now the polynomial expansion of $\phi_\nu(\mu)$ is of the form

$$\phi_\nu(\mu) = \sum_{n=0}^\infty g_n(\nu)\pi_n(\mu) \tag{13}$$

it is possible to find the a_n and b_n in terms of the (known) $g_n(\nu)$. For example if

$\pi_n(\mu) = T_n(\mu)$, we get for equation (12)

$$a_0 = g_0 + \tfrac{1}{2} \sum_{j=1}^{\infty} b_j g_j \tag{14}$$

$$a_i = g_i + \tfrac{1}{2} b_i g_0 + \tfrac{1}{2} \sum_{j=1}^{\infty} b_j (g_{i+j} + g_{|i-j|}) \qquad i = 1, 2, \ldots, M+N \ldots,$$

$a_i = 0$, $i > N$ and $b_j = 0$, $j > M$, as the set of equations for determining the a_i and b_i. The first $N+1$ equations relate a_i to b_j, while the next M homogeneous equations solve for b_j. Note that the corresponding equations when $\pi_n(\mu) = P_n(\mu)$ are more difficult to obtain as, unlike in the Chebyshev case, there is no simple relation for the product $P_n(\mu)P_m(\mu)$. However, unlike in the P_n case, integration of (13) over μ with $\pi_n(\mu) = T_n(\mu)$ produces the infinite series

$$2(g_0/2 - g_2/3 - g_4/15 - g_6/35 - \cdots)$$

where

$$g_0(\nu) = [2/\pi(1-\nu^2)^{1/2}]\lambda(\nu), \qquad g_1(\nu) = \nu(g_0 - c),$$

$$g_{n+1}(\nu) + g_{n-1}(\nu) = 2\nu g_n(\nu),$$

and the condition $\int_{-1}^{1} \phi_\nu(\mu)\, d\mu = 1$ is not as simply satisfied. Though this is the standard procedure for obtaining a rational fraction approximation to a given function, one of the principal contributions of this work is to use the constraints imposed by the orthogonality conditions, i.e. equations (6) and (7), in addition to equation (14), for obtaining the parameters $\{a_i\}$ and $\{b_i\}$.

In accordance with the above, for the full-range case, equation (6a) is automatically satisfied, and for (6b) we write

$$\int_{-1}^{1} \mu \phi_{0+}(\mu) \bar{\phi}_\nu(\mu)\, d\mu = 0 \tag{15}$$

$$\int_{-1}^{1} \mu \phi_{0-}(\mu) \bar{\phi}_\nu(\mu)\, d\mu = 0 \tag{16}$$

$$\int_{-1}^{1} \mu \bar{\phi}_\nu(\mu) \bar{\phi}_{\nu'}(\mu)\, d\mu = N(\nu)\delta(\nu - \nu') \tag{17}$$

any other combination of the eigenfunctions being contained in the above. In order to discretise the interval $(-1, 1)$ from the above integrals, it is necessary to replace $\delta(\nu - \nu')$ by a suitable representation, which in the present case we obtain from its expansion in terms of the complete set $\{\phi_{0+}, \phi_{0-}, \phi_\nu\}$, i.e. from the Green function jump condition

$$\frac{1}{\nu}\delta(\nu - \nu') = \frac{1}{N_{0+}}(\phi_{0+}(\nu')\phi_{0+}(\nu) - \phi_{0-}(\nu')\phi_{0-}(\nu)) + \int_{-1}^{1} \frac{1}{N(\mu)} \phi_\mu(\nu')\phi_\mu(\nu)\, d\mu$$

by neglecting the transient integral†. Therefore

$$\delta(\nu - \nu') \Rightarrow \frac{\nu}{N_{0+}}(\phi_{0+}(\nu')\phi_{0+}(\nu) - \phi_{0-}(\nu')\phi_{0-}(\nu)). \tag{18}$$

† This is the simplest possibility. Other more realistic representations of the delta function from the jump condition are possible.

The three orthogonality—or constraint—integrals are now evaluated using equation (4) and the assumed form of $\bar{\phi}_\nu(\mu)$, expression (18), with $\nu=\nu'$, being employed on the right-hand side of (17). The number of parameters retained in $\bar{\phi}_\nu(\mu)$ is taken to be both necessary and sufficient for a unique solution to be obtained in terms of $g_n(\nu)$ from the orthogonality constraints and the first $N+1$ non-homogeneous equations of the set (14). This implies that $\bar{\phi}_\nu(\mu)$ contains only $a_0, a_1, \ldots, a_N$ and b_1, b_2, b_3. Finally the normalisation,

$$\int_{-1}^{1} \bar{\phi}_\nu(\mu)\, \mathrm{d}\mu = 1$$

yields the required discretisation of $\nu \in (-1, 1)$, consistent with the choice of ν_0 satisfying equation (3) and with all the orthogonality conditions needed for a complete solution of the problem.

In the case of a half-range problem, a simple but remarkably accurate expression for $W(\mu)$ is first developed for use in the orthogonality relations (7). From equations (8) and (10), we write for $W(\mu)$

$$\bar{W}(\mu)=\frac{c}{2\Omega(1-c)}\,\frac{\mu\nu_0\sqrt{1-c}+\mu^2}{\nu_0+\mu} \tag{19}$$

where Ω is taken to be a constant. With this $\bar{W}(\mu)$, equations (7e) are evaluated to give

$$\frac{c}{2\Omega(1-c)}(\tfrac{1}{2}c\nu_0)^2(\alpha C_1+C_2)=-(\tfrac{1}{2}c\nu_0)^2X(\nu_0)$$

and

$$\frac{c}{2\Omega(1-c)}(\tfrac{1}{2}c\nu_0)^2(\alpha D_1+D_2)=(\tfrac{1}{2}c\nu_0)^2X(-\nu_0)$$

where

$$C_1=\frac{1}{2\nu_0(\nu_0-1)}-\frac{1}{2c\nu_0^2} \qquad C_2=\frac{1}{2(\nu_0-1)}+\frac{1}{2c\nu_0}-\ln\frac{\nu_0}{\nu_0-1}$$

$$D_1=\frac{1}{2c\nu_0^2}-\frac{1}{2\nu_0(\nu_0+1)} \qquad D_2=\frac{1}{2(\nu_0+1)}-\frac{3}{2c\nu_0}+\ln\frac{\nu_0}{\nu_0-1}.$$

If Ω is very nearly constant, which is assumed to be the case in equation (19), then the solutions of the above two equations for Ω, Ω_+ and Ω_- respectively say, will be nearly the same. Calculations show that for $c=0.2$, $\Omega_+=0.980237$, $\Omega_-=0.983046$; $c=0.5$, $\Omega_+=0.959663$, $\Omega_-=0.959432$ and for $c=0.9$, $\Omega_+=0.938081$, $\Omega_-=0.937203$. To take care of this weak dependence of Ω on μ to a satifactory degree, we use the average of Ω_+ and Ω_-, i.e. let

$$\Omega=\tfrac{1}{2}(\Omega_++\Omega_-) \tag{20}$$

in equation (19). As an independent check on the utility of this $\bar{W}(\mu)$ in evaluating integrals of the type (7), we calculated

$$\int_0^1 \bar{W}(\mu)\phi_{0+}(\mu)\, \mathrm{d}\mu$$

to be

$$(c^2\nu_0)[4\Omega(1-c)]^{-1}(\alpha F_1+F_2)$$

where

$$F_n=\int_0^1\frac{\mu^n}{\nu_0^2-\mu^2}\,d\mu$$

$$=-\left(\frac{1}{n-1}+\frac{\nu_0^2}{n-3}+\frac{\nu_0^4}{n-5}+\ldots\right)+\begin{cases}\nu_0^{n-2}/c & n\text{ even}\\ \nu_0\ln[\nu_0/\nu_0^2-1)^{1/2}] & n\text{ odd}\end{cases}$$

and compared it with the exact value $\frac{1}{2}c\nu_0$. The ratio of the approximate to exact integrals for different c are 0.999874, 0.999594, 0.999530, 0.999693 and 0.999832 for $c=0.2$, 0.4, 0.6, 0.8 and 0.9 respectively. Thus the very good accuracy of $\bar{W}(\mu)$ is verified.

With this constant Ω, it is also possible to obtain a first iterant of $\Omega(-\mu)$ from equation (9) to be

$$\Omega(-\mu)=1-\tfrac{1}{2}c\nu_0^2\omega\mu/\Omega \tag{21}$$

where

$$\omega=\alpha_1\ln\frac{1+\nu_0}{\nu_0}+\alpha_2\ln\frac{\nu_0-1}{\nu_0}+\alpha_3\ln\frac{1+\mu}{\mu}$$

$$\alpha_1=\frac{c}{2\nu_0(\nu_0-\mu)(1-c)}\qquad\alpha_2=\frac{c}{2\nu_0(\nu_0+\mu)(1-c)}$$

$$\alpha_3=X^2(0)-\frac{c}{(1-c)(\nu_0^2-\mu^2)}.$$

Because successive iterations on equation (9) converge extremely rapidly (Case and Zweifel 1967), equation (21) with equation (20), yields an $X(-\mu)$ from equation (8) that differs by no more than 1–2% from its true value for all magnitudes of μ and c. In comparison, the X function calculated from equation (20) in place of (21), has a maximum error of about 4%. The above, therefore, constitutes an extremely reliable approximation to Case's W and X functions.

Having obtained $X(\mu)$ and $W(\mu)$, we evaluate the integrals in (7a)–(7d) with the proper form of $\bar{\phi}_\nu(\mu)$ (as in the full range case), and for $\delta(\nu-\nu')$ use the asymptotic component of the boundary condition for the albedo problem, i.e.

$$\delta(\nu-\nu')\Rightarrow-\frac{\bar{W}(\nu')}{X(\nu_0)}\frac{1}{(c\nu_0/2)^2}\phi_{0+}(\nu)\qquad\nu=\nu'\geqslant 0.$$

A procedure completely similar to the full-range case then gives the constants in $\bar{\phi}_\nu(\mu)$ and the discretisation of the range $0\leqslant\nu\leqslant 1$. The solution of equation (1) can now be written as a linear superposition over all the roots, for the general case, as for example by

$$\psi(x,\mu)=a_{0+}\exp(-x\,|\,\nu_0)\phi_{0+}(\mu)+a_{0-}\exp(x\,|\,\nu_0)\phi_{0-}(\mu)$$
$$+\sum_j A(\nu_j)\exp(-x/\nu_j)\bar{\phi}_{\nu_j}(\mu),$$

and the coefficients evaluated from the boundary conditions and use of the orthogonality relations satisfied by the set $\{\phi_0\pm(\mu),\bar{\phi}_{\nu_j}(\mu)\}$ constructed above.

In concluding, we summarise as follows. We have succeeded in using $\phi_{0\pm}(\mu)$ and a properly constructed rational approximation $\bar{\phi}_\nu(\mu)$ to $\phi_\nu(\mu)$ as the basis functions for the solution of equation (1). These functions satisfy all the necessary orthogonality relations (with a suitable definition of the δ function) needed for a complete solution of the one-speed equation, and yield the exact asymptotic solution in all cases. This justifies the use of the exact asymptotic form of $\delta(\nu-\nu')$ in the orthogonality integrals above. The possibility of such a general solution procedure that does not use singular eigenfunctions has become more significant now with the recent demonstration (Sengupta 1982) that the solution of the energy dependent transport equation can be expressed in terms of the solutions of the one-speed and slowing down equations.

References

Case K M and Zweifel P F 1967 *Linear Transport Theory* (Reading, Mass.: Addison Wesley)
Ganguly K and Sengupta A 1980 *Nucl. Sci. Eng.* **74** 1
Sengupta A 1982 *Solution of the Energy Dependent Neutron Transport Equation in Plane Geometry by Separation of Variables*, Nucl. Sci. Eng. to appear