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BENCHMARK

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A Heterogeneous Medium Analytical Benchmark

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Abstract

A benchmark, called benchmark **BLUE**, has been developed for one-group neutral particle (neutron or photon) transport in a one-dimensional sub-critical heterogeneous plane parallel medium with surface illumination. General anisotropic scattering is accommodated through the Green's Function Method (GFM). Numerical Fourier transform inversion is used to generate the required Green's functions which are kernels to coupled integral equations that give the exiting angular fluxes. The interior scalar flux is then obtained through quadrature. A compound iterative procedure for quadrature order and slab surface source convergence provides highly accurate benchmark quality (4- to 5- places of accuracy) results

Introduction

Assurance that particle transport methods are efficiently implemented and that current codes are adequately maintained is a major challenge facing today's power reactor and weapons communities. As used here, an analytical benchmark refers to highly accurate evaluations of analytical representations of solutions to the neutral particle transport equation. The primary advantage of an analytical benchmark is that its numerical evaluation occurs at the level of the solution rather than at the level of the integro-differential Boltzmann equation itself. Numerical evaluation generally occurs after the transport equation has been solved theoretically to obtain a solution representation continuous in the independent variables thus, in principle, avoiding discretization error altogether. Because of the requirement of an analytical solution however, only relatively limited transport scenarios can be treated. To some this may seem to be a major disadvantage of analytical benchmarks. To the code developer however, simplicity by no means diminishes the usefulness of these benchmarks since transport codes *must* perform adequately for simple as well as comprehensive transport scenarios. Thus, comparisons to analytical benchmarks always provide diagnostic information about any comprehensive transport code by either uncovering errors or assessing performance. As will be demonstrated with this benchmark, the nature of transport problems that can be treated has become progressively more advanced since analytical benchmarks in neutron transport theory first appeared in 1953¹.

The benchmark considered, in this presentation, is for **1-D** steady state monenergetic (one-group) neutral particle transport in an anisotropically scattering heterogeneous medium. A new Fourier transform inversion, to be employed in the Green's Function Method (GFM), generates the required analytical solution representation. This method effectively specifies the Green's function for a 1-D plane parallel medium, which when integrated over appropriate (unknown) boundary sources, gives the solution representation for the angular flux within a finite medium. The resulting integral equations are solved for the unknown boundary fluxes which then allows the determination of the interior fluxes via quadrature. A heterogeneous medium is accommodated through iteration on the boundary fluxes.

I. The Green's Function Method: Theory

A. Neutron transport equation in a slab: Placzek's Lemma

Only the transport of neutrons will be consider in the remainder of this presentation; however, the analysis remains valid for photon transport in the gray approximation and for electron transport for screened-Rutherford scattering with appropriate redefinition of the interaction parameters.

In general, we are interested in the solution to the following 1-D monoenergetic neutron transport equation:

$$\left[\mu \frac{\partial}{\partial x} + 1 \right] \Psi(x, \mu) = \frac{\omega}{2} \sum_{l=0}^L \omega_l P_l(\mu) \Psi_l(x) \quad (1a)$$

where the flux moments are defined as

$$\Psi_l(x) = \int_{-1}^1 d\mu P_l(\mu) \Psi(x, \mu). \quad (1b)$$

The flux Ψ is to be determined for neutrons at the position x travelling in the direction μ resulting from sources at the slab boundaries for a slab of thickness a . General anisotropic scattering is assumed through a truncated (at L) Legendre polynomial (P_l) series expansion (with coefficient ω_l) of the differential scattering cross section. The number of secondaries per collision is ω and all distances are measured in terms of the total mean free path. Equation (1a) is to be solved with known fluxes illuminating the slab surfaces

$$\Psi(0, \mu) = F_L(\mu), \quad \mu > 0, \quad \Psi(a, \mu) = F_R(-\mu), \quad \mu < 0. \quad (1c)$$

From the well-known lemma of G. Placzek¹, the boundary conditions can be replaced by an equivalent volume source

$$S(x, \mu) \equiv \mu \Psi(0, \mu) \delta(x) - \mu \Psi(a, \mu) \delta(x - a). \quad (2b)$$

to give the following transport equation: to be solved:

$$\left[\mu \frac{\partial}{\partial x} + 1 \right] \Psi(x, \mu) = \frac{\omega}{2} \sum_{l=0}^L \omega_l P_l(\mu) \Psi_l(x) + S(x, \mu)$$

B. Solution representation via Green's functions

A solution representation is obtained by first expressing the Green's function in plane-parallel geometry as the solution to the following transport equation:

$$\left[\mu \frac{\partial}{\partial x} + 1 \right] G(x, \mu; \mu_0) = \frac{\omega}{2} \sum_{l=0}^L \omega_l P_l(\mu) G_l(x; \mu_0) + \delta(\mu - \mu_0) \delta(x) \quad (3)$$

with moments $G_l(x; \mu_0)$ subject to the finiteness condition $\lim_{|x| \rightarrow \infty} G(x, \mu; \mu_0) < \infty$. Then multiplying eqs(3) by the source $S(x - x', \mu')$ and integrating over all x' and μ' gives a representation of the solution in terms of the Green's function

$$\Psi(x, \mu) = \int_{-1}^1 d\mu' \int_{-\infty}^{\infty} dx' S(x - x', \mu') G(x', \mu; \mu'). \quad (4)$$

By substitution of S from eq(2b) along with the decomposition of the Green's function into collided (G_c) and uncollided components, performing the integrations over the delta functions and replacing x by 0^+ and a^- , eq(4) becomes

$$\begin{aligned} \Psi(0^+, -\mu) = & e^{-a/\mu} F_R(\mu) + \int_0^1 d\mu' \mu' F_L(\mu') G_c(0^+, -\mu; \mu') + \int_0^1 d\mu' \mu' F_R(\mu') G_c(a, \mu; \mu') - \\ & - \int_0^1 d\mu' \mu' G_c(0^+, -\mu; -\mu') \Psi(0^+, -\mu') - \int_0^1 d\mu' \mu' G_c(a, \mu; -\mu') \Psi(a^-, \mu') \end{aligned} \quad (5a)$$

$$\begin{aligned} \Psi(a^-, \mu) = & e^{-a/\mu} F_L(\mu) + \int_0^1 d\mu' \mu' F_L(\mu') G_c(a, \mu; \mu') + \int_0^1 d\mu' \mu' F_R(\mu') G_c(0^+, -\mu; \mu') - \\ & - \int_0^1 d\mu' \mu' G_c(a, \mu; -\mu') \Psi(0^+, -\mu') - \int_0^1 d\mu' \mu' G_c(0^+, -\mu; -\mu') \Psi(a^-, \mu'). \end{aligned} \quad (5b)$$

The corresponding scalar flux is obtained by integration over μ .

Once the Green's function has been determined, eqs(5) are solved as coupled integral equations for the exiting fluxes. Thus, to this point, the two numerical methods associated with the Green's function method are the determination of the Green's function and the solution to two coupled integral equations.

For future convenience in treating heterogeneous slab geometry, the incoming flux at $x=0$ will be assumed to contain a monodirectional component which is separated from a diffuse component

$$F_L(\mu) = \alpha_L \delta(\mu - \mu_0) + \tilde{F}_L(\mu).$$

When substituted into eqs(5), we obtain the following modified integral equations:

$$\begin{aligned}\Psi_c(0^+,-\mu) &= e^{-a/\mu} F_R(\mu) + \alpha_L \mu_0 \left[G_c(0^+,-\mu;\mu_0) - e^{-a/\mu_0} G_c(a,\mu;-\mu_0) \right] + \\ &+ \int_0^1 d\mu' \mu' \tilde{F}_L(\mu') G_c(0^+,-\mu;\mu') + \int_0^1 d\mu' \mu' F_R(\mu') G_c(a,\mu;\mu') - \\ &- \int_0^1 d\mu' \mu' G_c(0^+,-\mu;-\mu') \Psi_c(0^+,-\mu') - \int_0^1 d\mu' \mu' G_c(a,\mu;-\mu') \Psi_c(a^+,\mu')\end{aligned}\quad (6a)$$

$$\begin{aligned}\Psi_c(a^+,\mu) &= e^{-a/\mu} \tilde{F}_L(\mu) + \alpha_L \mu_0 \left[G_c(a,\mu;\mu_0) - e^{-a/\mu_0} G_c(0^+,-\mu;-\mu_0) \right] + \\ &+ \int_0^1 d\mu' \mu' \tilde{F}_L(\mu') G_c(a,\mu;\mu') + \int_0^1 d\mu' \mu' F_R(\mu') G_c(0^+,-\mu;\mu') - \\ &- \int_0^1 d\mu' \mu' G_c(a,\mu;-\mu') \Psi_c(0^+,-\mu') - \int_0^1 d\mu' \mu' G_c(0^+,-\mu;-\mu') \Psi_c(a^+,\mu')\end{aligned}\quad (6b)$$

where $\Psi_c(x, \mu)$ is the collided component in the decomposition

$$\Psi(x, \mu) = \alpha_L e^{-x/\mu_0} \delta(\mu - \mu_0) + \Psi_c(x, \mu).$$

C. Determination of the Green's function: Theory

When eq(3) is operated on by a Fourier transform, there results

$$(1 + ik\mu) G(k, \mu; \mu_0) = \frac{\omega}{2} \sum_{l=0}^L \omega_l P_l(\mu) G_l(k; \mu_0) + \delta(\mu - \mu_0), \quad (7a)$$

where the transformed moments are

$$G_l(k; \mu_0) \equiv \int_{-\infty}^{\infty} dx e^{-ikx} G_l(x; \mu_0) \quad (7b)$$

and the Fourier transform of the flux is defined by

$$G(k, \mu; \mu_0) \equiv \int_{-\infty}^{\infty} dx e^{-ikx} G(x, \mu; \mu_0). \quad (7c)$$

Note, that in this presentation, the transformed Green's function is implied when the argument is either k or z . Once the image functions are known explicitly, the angular and scalar Green's functions are determined from their respective inversions as

$$G(x, \mu; \mu_0) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} G(k, \mu; \mu_0), \quad G(x; \mu_0) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} G(k; \mu_0).$$

Since the image functions are much too complicated for the inversions to be performed analytically in terms of special functions, a numerical inversion will be employed.

When eq(7a) is divided through by $(1 + ik\mu)$ and projected over the Legendre polynomials, the following closed system of equations is obtained for the transformed moments:

$$G_j(k; \mu_0) = \omega \sum_{l=0}^L \omega_l L_{jl}(k) G_l(k; \mu_0) + \frac{P_j(\mu_0)}{1 + ik\mu_0} \quad (8a)$$

for $0 \leq j \leq L$ with the matrix elements defined as

$$L_{jl}(k) = \frac{1}{2} \int_{-1}^1 d\mu \frac{P_j(\mu) P_l(\mu)}{1 + ik\mu}. \quad (8b)$$

In principle, eq(8a) can be solved for the transformed moments through matrix inversion. While this approach has proven to generally result in an accurate numerical algorithm for low order scattering ($L < 5$), theoretically it is less than satisfying since the transform of the moments is not explicitly expressed. For this reason, an alternative formulation will be followed to obtain an explicit moment representation through the solution of a recursion relation.

A recurrence relation satisfied by the moments can be obtained by projection of eq(10a) over the Legendre polynomials

$$zh_l G_l(k; \mu_0) + (l+1)G_{l+1}(k; \mu_0) + lG_{l-1}(k; \mu_0) = z(2l+1)P_l(\mu_0) \quad (9)$$

where

$$z \equiv 1/ik \text{ and } h_l \equiv 2l+1-\omega\omega_l.$$

From a rather involved derivation making use of Chandrasekhar polynomials of the first (g_l) and second (ρ_l) kinds² and an auxiliary transport solution for isotropic source emission, the following new representation of the transform of the l -th moment is obtained³:

$$G_l^L(k; \mu_0) \equiv G_l^L(-z; \mu_0) = \frac{z}{z+\mu_0} \left\{ \frac{P_l(\mu_0)}{\Lambda_L(z)} - \omega [\rho_l(-z)g_l(-z, \mu_0) - g_l(-z)h_l(-z, \mu_0)] \right\} \quad (10)$$

where

$$\begin{aligned} f_L(-z; \mu_0) &\equiv g_L(-z, \mu_0)G_0(-z) - h_L(-z, \mu_0), \quad G_0(z) \equiv \frac{\hat{g}_L(z)}{\Lambda_L(z)} \\ \hat{g}_L(z) &\equiv (L+1)[\rho_{L+1}(z)Q_L(z) - \rho_L(z)Q_{L+1}(z)], \quad \Lambda_L(z) \equiv (L+1)[g_{L+1}(z)Q_L(z) - g_L(z)Q_{L+1}(z)] \\ g_L(z, \mu) &\equiv \sum_{l=0}^L \omega_l P_l(\mu)g_l(z), \quad h_L(z, \mu) \equiv \sum_{l=0}^L \omega_l P_l(\mu)\rho_l(z). \end{aligned}$$

Q_L is the Legendre function of the second kind of order L and the Chandrasekhar polynomials of the first and second kinds satisfy the following recursion relations:

$$-zh_l g_l(z) + (l+1)g_{l+1}(z) + lg_{l-1}(z) = 0, \quad g_0(z) \equiv 1 \quad (11a)$$

$$-zh_l \rho_l(z) + (l+1)\rho_{l+1}(z) + l\rho_{l-1}(z) = 0, \quad \rho_0(z) \equiv 0, \quad \rho_1(z) \equiv 1. \quad (11b)$$

A superscript L on the moment G_l indicating scattering order has been included for clarity of the expressions to follow.

While eq(10) is explicit, it is mainly of theoretical interest and is not particularly useful for numerical evaluation. The numerical difficulty is a direct result of the polynomial nature of the subtracted terms which readily leads to catastrophic roundoff error. Thus, an alternative representation has been sought. After some extensive algebra, we find

$$G^L(k, \mu; \mu_0) = G^0(k; \mu, \mu_0) + \frac{\omega}{2} \left[\frac{z}{z+\mu} \left[\frac{z}{z+\mu_0} \right] \sum_{l=1}^L \omega_l \left[\frac{\xi_l(-z, \mu)}{\Lambda_l(-z)} \right] \left[\frac{\xi_l(-z, \mu_0)}{\Lambda_{l-1}(-z)} \right] \right] \quad (12a)$$

where $G^0(k; \mu, \mu_0)$ is the transformed solution for isotropic scattering

$$\begin{aligned} G^0(k, \mu; \mu_0) &= \left[\frac{z}{z+\mu_0} \right] \delta(\mu - \mu_0) + \frac{\omega}{2} \left[\frac{z}{z+\mu} \right] \left[\frac{z}{z+\mu_0} \right] + \\ &+ \frac{\omega}{2} \left[\frac{z}{z+\mu} \right] \left[\frac{z}{z+\mu_0} \right] \left[\frac{-\omega z Q_0(-z)}{1 + \omega z Q_0(-z)} \right]. \end{aligned} \quad (12b)$$

The transformed scalar flux is found simply by integration

$$G^L(k, \mu_0) = G^0(k; \mu_0) - \omega \left[\frac{z^2}{z+\mu_0} \right] \sum_{l=1}^L \omega_l \left[\frac{Q_l(-z)}{\Lambda_l(-z)} \right] \left[\frac{\xi_l(-z, \mu_0)}{\Lambda_{l-1}(-z)} \right] \quad (13a)$$

with

$$G^0(k; \mu_0) = \left[\frac{z}{z + \mu_0} \right] + \left[\frac{z}{z + \mu_0} \right] \frac{\omega Q_0(-z)}{1 + \omega Q_0(-z)}. \quad (13b)$$

To the author's knowledge, these image functions have never before been published.

II. The Green's Function Method: Numerical Implementation

A. Numerical Fourier Transform Inversion

The evaluation of the following improper integral constitutes the numerical Fourier inversion:

$$f(x) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} \bar{f}(k); \quad (14)$$

k is a real variable. For clarity, the image function has been defined with an overbar. Integrals of this type are well known to be difficult to numerically evaluate because of the infinite integration range compounded by the unending oscillations of the integrand. Needless to say, special care must be exercised.

By noting that $\text{Re}[f(k)]$ and $\text{Im}[f(k)]$ are even and odd functions of k respectively, the inversion integral can be rewritten in the form

$$f(x) \equiv \frac{1}{\pi} \int_0^{\infty} dk \{ \text{Re}[\bar{f}(k)] \cos(kx) - \text{Im}[\bar{f}(k)] \sin(kx) \}. \quad (15)$$

From a change of variable and reformulation of the improper integral as an infinite series, there results for $x \neq 0$

$$f(x) \equiv \frac{1}{\pi x} \sum_{j=0}^{\infty} (-1)^j \int_0^{\pi} du \{ \text{Re}[\bar{f}((u + j\pi)/x)] \cos(u) - \text{Im}[\bar{f}((u + j\pi)/x)] \sin(u) \}. \quad (16)$$

The integrals in each term are to be evaluated by a shifted Gauss/Legendre (GL) quadrature of order m_b . The convergence of the infinite series is accelerated through the Wynn-epsilon algorithm⁴ which is the primary reason that this procedure can be used at all.

For $x = 0$, a change of variables gives

$$f(0) = \frac{2}{\pi} \int_{-1}^1 dt \frac{1}{(1-t)^2} \text{Re} \left[\bar{f} \left(\frac{1+t}{1-t} \right) \right]. \quad (17)$$

This integral is evaluated as a GL-quadrature on the interval $[-1, 1]$. The apparent singularity is effectively ignored since its influence is negated by the attenuation of $\bar{f}(k)$ as k approaches infinity. This expression is numerically advantageous since it does not involve an infinite series evaluation. For this reason, an algorithm has been crafted around eq(17) to evaluate the angular Green's function for $x \neq 0$ as will be discussed.

B. Fourier inversion for the angular and scalar Green's functions

The Green's function determination (collide only) is partitioned into 4 components depending on the sign of the independent variables x and μ . These components correspond to the 4 quadrants $++, +-, -+, --$ for x and μ respectively. In particular, to determine the exiting angular fluxes, only the Green's functions in quadrants 1 and 4 are required. This approach provides a distinct numerical advantage in which the relatively straightforward Green's function evaluation at $x = 0$ can be utilized as will now be demonstrated.

The infinite medium Green's function solution can be reformulated as two half-space problems connected at the interface ($x = 0$) by a source condition. Assuming that the Green's function at $x = 0$ is known results in the following integral equation between the Green's functions of quadrants 1 and 4:

$$G_c(-x, -\mu; \mu_0) = e^{-x/\mu} \Theta(x/\mu) G_c(0^-, -\mu; \mu_0) + \\ + \int_0^1 d\mu' \mu' G_c(0^-, -\mu'; \mu_0) G_c(x, \mu; \mu') - \int_0^1 d\mu' \mu' G_c(0^-, \mu'; \mu_0) G_c(-x, -\mu; \mu'). \quad (18)$$

For completeness, the representation of the Green's function at $x = 0$ is repeated here

$$G_c(0^-, \mu; \mu_0) = \frac{2}{\pi} \int_{-1}^1 dt \frac{1}{(1-t)^2} \operatorname{Re} \left[\bar{G}_c \left(\frac{1+t}{1-t}, \mu; \mu_0 \right) \right].$$

Thus, with the knowledge of $G_c(0^-, \mu; \mu_0)$ and $G_c(x, \mu; \mu')$ (in the first quadrant), eq(32) can be solved for $G_c(-x, -\mu; \mu')$ (in the fourth quadrant). By approximating the integrals in terms of a shifted GL-quadrature of order L_m , eq(18) can be recast as a matrix equation

$$\begin{aligned} \sum_{l=1}^{L_m} [\delta_{j,l} + \omega_l \mu_l G_c(0^-, \mu_l; \mu_j)] G_4(\mu_j) = \\ = e^{-x/\mu} G_c(0^-, -\mu; \mu_j) + \sum_{l=1}^{L_m} \omega_l \mu_l G_1(\mu_l) G_c(0^-, -\mu_l; \mu_j) \end{aligned} \quad (19)$$

where

$$G_1(\mu_j) \equiv G_c(x, \mu; \mu_j) \quad G_4(\mu_j) \equiv G_c(-x, -\mu; \mu_j)$$

Note that x and μ are just parameters in this formulation.

Similarly for the scalar flux, from integration of eq(18) over μ , there results

$$\begin{aligned} G_c(-x; \mu_0) = \int_0^1 d\mu e^{-x/\mu} G_c(0^-; \mu_0) + \\ + \int_0^1 d\mu' \mu' G_c(0^-, -\mu'; \mu_0) G_c(x; \mu') - \int_0^1 d\mu' \mu' G_c(0^-, \mu'; \mu_0) G_c(-x; \mu'). \end{aligned} \quad (20)$$

Therefore, from a knowledge of $G_c(0^-, \mu; \mu_0)$ and $G_c(x; \mu')$, $G_c(-x; \mu')$ is obtained as the solution of

$$\begin{aligned} \sum_{l=1}^{L_m} [\delta_{j,l} + \omega_l \mu_l G_c(0^-, \mu_l; \mu_j)] G_2(\mu_l) = \\ = \sum_{l=1}^{L_m} \omega_l e^{-x/\mu_l} G_c(0^-; \mu_j) + \sum_{l=1}^{L_m} \omega_l \mu_l G_c(0^-, \mu_l; \mu_j) G_1(\mu_l) \end{aligned} \quad (21)$$

with

$$G_1(\mu_j) \equiv G_c(x; \mu_j) \quad G_2(\mu_j) \equiv G_c(-x; \mu_j)$$

C. Solution for the exiting angular and scalar fluxes

1. Exiting angular fluxes

Rather than solve the coupled integral equations [eqs(9)] directly for the exiting angular fluxes, they can be manipulated into two uncoupled integral equations. If $r_{\pm}(\mu)$ is defined as

$$r_{\pm}(\mu) \equiv \Psi_c(0^+, -\mu) \pm \Psi_c(a^-, \mu), \quad (22)$$

eqs(9a) and (9b) can be added and subtracted to give

$$\begin{aligned} r_{\pm}(\mu) = e^{-a/\mu} [\tilde{F}_L(\mu) \pm F_R(\mu)] + \int_0^1 d\mu' \mu' [\tilde{F}_L(\mu') \pm F_R(\mu')] [G_c(0^+, -\mu; \mu') \pm G_c(a, \mu; \mu')] + \\ + \alpha_L \mu_0 \left\{ [G_c(0^+, -\mu; \mu_0) \pm G_c(a, \mu; \mu_0)] - e^{-a/\mu_0} [G_c(a, -\mu; \mu_0) \pm G_c(0^+, \mu; -\mu_0)] \right\} - \quad (23) \\ - \int_0^1 d\mu' \mu' [G_c(0^+, -\mu; -\mu') \pm G_c(a, \mu; -\mu')] r_{\pm}(\mu') \end{aligned}$$

When the integrals are approximated by a GL-quadrature and μ is evaluated at the abscissa, the following matrix equations result:

$$\begin{aligned}
& \sum_{l=1}^{L_m} \left\{ \delta_{l,j} + \omega_l \mu_l \left[G_c(0^+, -\mu_j; -\mu_l) \pm G_c(a, \mu_j; -\mu_l) \right] \right\} r_{\pm j} = \\
& = e^{-a/\mu_j} \left[\tilde{F}_L(\mu_j) \pm F_R(\mu_j) \right] + \sum_{l=1}^{L_m} \omega_l \mu_l \left[\tilde{F}_L(\mu_l) \pm F_R(\mu_l) \right] \left[G_c(0^+, -\mu_j; \mu_l) \pm G_c(a, \mu_j; \mu_l) \right] + \\
& + \alpha_L \mu_0 \left\{ \left[G_c(0^+, -\mu_j; \mu_0) \pm G_c(a, \mu_j; \mu_0) \right] - e^{-a/\mu_0} \left[G_c(a, -\mu_j; \mu_0) \pm G_c(0^+, \mu_j; -\mu_0) \right] \right\}.
\end{aligned} \tag{24a}$$

Finally, the fluxes are recovered from

$$\Psi_c(0^+, -\mu_j) = \frac{r_{+j} + r_{-j}}{2}, \quad \Psi_c(a, -\mu_j) = \frac{r_{+j} - r_{-j}}{2} \tag{24b}$$

2. Interior scalar flux

The interior scalar flux is obtained from eq(6a) as

$$\begin{aligned}
\Psi(x) = & \alpha_L \mu_0 \left[G(x; \mu_0) - e^{-a/\mu_0} G(a - x; -\mu_0) \right] + \\
& + \int_0^1 d\mu' \mu' \left[\tilde{F}_L(\mu') G(x; \mu') + F_R(\mu') G(a - x; \mu') \right] - \\
& - \int_0^1 d\mu' \mu' \left[G(x; -\mu') \Psi_c(0^+, -\mu') + G(a - x; -\mu') \Psi_c(a, \mu') \right].
\end{aligned} \tag{25}$$

A reduction in numerical effort is achieved for uniform spatial edit intervals by evaluating $\Psi(x)$ and $\Psi(a - x)$ simultaneously. Since

$$\begin{aligned}
\Psi(a - x) = & \alpha_L \mu_0 \left[G(a - x; \mu_0) - e^{-a/\mu_0} G(x; -\mu_0) \right] + \\
& + \int_0^1 d\mu' \mu' \left[\tilde{F}_L(\mu') G(a - x; \mu') + F_R(\mu') G(x; \mu') \right] - \\
& - \int_0^1 d\mu' \mu' \left[G(a - x; -\mu') \Psi_c(0^+, -\mu') + G(x; -\mu') \Psi_c(a, \mu') \right]
\end{aligned} \tag{26}$$

and if

$$q_{\pm}(x) \equiv \Psi(x) \pm \Psi(a - x),$$

then adding and subtracting eqs(25) and (26) gives

$$\begin{aligned}
q_{\pm}(x) = & \alpha_L \mu_0 \left\{ \left[G(x; \mu_0) \pm G(a - x; \mu_0) \right] - e^{-a/\mu_0} \left[G(a - x; -\mu_0) \pm G(x; -\mu_0) \right] \right\} + \\
& + \int_0^1 d\mu' \mu' \left[\left[\tilde{F}_L(\mu') \pm F_R(\mu') \right] G(x; \mu') \pm G(a - x; \mu') \right] - \\
& - \int_0^1 d\mu' \mu' \left[G(x; -\mu') \pm G(a - x; -\mu') r_{\pm}(\mu') \right].
\end{aligned} \tag{27a}$$

Therefore

$$\Psi(x) = \frac{[q_+(x) + q_-(x)]}{2}, \quad \Psi(a - x) = \frac{[q_+(x) - q_-(x)]}{2}$$

and the evaluation of $\Psi(x)$ is required at only half the number of edit points for uniform spatial edit intervals.

3. Auxiliary functions

Several auxiliary functions are required in order to evaluate the integrands for the Fourier inversions for the angular and scalar fluxes. In the evaluation of eqs(12) and (13), both the Legendre function of the second kind and the Chandrasekhar g -polynomial are necessary. The Legendre function of the second kind for a complex variable z is evaluated via the usual recurrence relation. The recurrence is

run in the forward direction for $|z| < 1$ and in the backward direction for $|z| > 1$. The g -polynomial is obtained from eq(11a) run in the forward direction. Note that the ρ -polynomial is not required and is mainly of theoretical interest.

III. Computational Strategies

A. Evaluation of Fourier transforms

In order to make the BLUE analytical benchmark as efficient as possible, special treatment of the evaluation of eqs(12) and (13) is required for the Fourier inversion. In particular, for a given quadrature order and position x , all complex quantities independent of μ and μ_0 need be calculated only once for each desired edit and stored. Thus, the necessary Q_l and g_l need be determined once per x saving a significant amount of computational effort given the heavy reliance on iteration required for benchmark quality results.

B. Global L_2 and L_{∞} relative errors

One possible measure of error used to specify the accuracy of a benchmark is the global L_2 error. Global, here, refers to a macroscopic error over either the angular or spatial edit grids. The L_2 -error over an edit grid between iterations is defined as

$$e_2 \equiv \left\{ \frac{1}{M} \sum_{i=1}^M \left[\frac{[f^k(y_i) - f^{k-1}(y_i)]}{f^k(y_i)} \right]^2 \right\}^{1/2} \quad (28)$$

where k indicates the k^{th} iterate and the summation is over either the angular or spatial edit grids. This expression holds for both inner slab and outer quadrature iterations, which are to be discussed in the following sections.

In addition to the L_2 error, L_{∞} , called the maximum relative error for the angular or scalar fluxes between iterations, is defined as the maximum relative error occurring over the angular or spatial edit grids respectively. The maximum relative error is more conservative than the L_2 relative error.

C. Outer quadrature iteration

As is evident, an analytical benchmark requires numerical evaluation as does any solution to the transport equation. Both the determination of the Green's functions and the exiting fluxes requires numerical quadrature. The difference, however, between an analytical benchmark and a corresponding numerical transport solution, say as given by an SN algorithm, is that errors associated with an analytical benchmark are more easily controlled than those resulting from spatial and angular discretizations.

To ensure benchmark quality results, a compound iterative strategy is followed. The desired benchmark solution is recalculated by increasing the quadrature order used to determine the Green's functions and the exiting fluxes until convergence. This is the first of two iteration schemes and is called the outer quadrature iteration. In this iteration, the quadrature order L_m [i.e., in eqs(19),(21) and (24a)] is advanced until the exiting angular fluxes on the angular edit grid have converge to the desired relative error. Upon angular flux convergence, the interior scalar flux is then determined with increasing quadrature order until convergence on the spatial edit grid. Convergence as used here is the agreement between two consecutive approximations to within a specified global L_2 relative or L_{∞} error as defined above.

D. Inner slab iteration

The theory and numerical implementation discussed in sections I and II have been concerned with a single homogeneous medium. An iterative strategy has been devised to treat a heterogeneous medium consisting of contiguous homogeneous slabs. The slabs are connected through the boundary conditions

\tilde{F}_L, F_R . For a particular slab, the incoming flux at $x = 0$ is the transmitted flux from the adjacent slab say to the left, and at $x = a$ the reflected flux from the adjacent slab to the right. Similarly, the exiting fluxes from the slab of interest are the sources for the adjacent slabs. Since only the boundary conditions at the slabs bordering on a vacuum are known, an iterative procedure, called the slab inner iteration, has been devised to determine the unknown interior surface sources. The slab inner iteration is performed within

each quadrature iteration. At each step of the inner iteration, the boundary conditions are updated. In general, the inner iteration need not be taken to convergence since the quadrature order has not yet converged. For a full benchmark calculation, a maximum of 30 inner slab iterations is allowed.

IV. Benchmark Demonstrations

A. Multiple slabs demonstration

The a multiple slab benchmark was run for slabs with the following material properties:

Slab	α	ω	g	L
1	1.0	0.95	0.8	10
2	0.1	0.15	0.1	3
3	4.0	0.90	0.6	8
4	2.0	0.30	0.7	7

Where a Henyey-Greenstein (H-G) scattering kernel of order L has been assumed ($\omega=g^1$). Table 1 shows the scalar flux within the four slabs for two cases for a normally incident source on the left boundary of slab e. The first case is for an error of 10^{-5} while the second case is for a relatively large quadrature order (45) and is expected to be correct to all digits shown. In general, the accuracy of the first case is as expected in comparison to the second. A slight discrepancy in the last place at the first and last slab boundaries (almost within the desired relative error) can be observed in the first case however. This discrepancy is eliminated with higher quadrature order.

B. Benchmark Comparisons with ONEDANT and MCNP

A deep penetration problem for a 150mfp thick homogeneous slab was chosen for comparison purposes. This problem stresses a numerical method because the neutrons experience 23 orders of attenuation from surface to surface. The slab is assumed to be primarily scattering with $\omega=0.9$ and to have a mildly forward peaked H-G kernel with $g = 0.6$ and $L = 10$. A unit source is normally incident on the left surface. For the analytical benchmark calculation, the medium was divided into 5 regions for efficiency of convergence. Apparently, the benchmark could not handle 23 orders of attenuation directly. Since an iterative procedure for the surface sources is used, partitioning the slab requires convergence on the smaller interior slabs only which is less demanding than on the entire slab. **ONEDANT** calculations were performed for several numerical configurations. In particular, the medium was divided into 15000 mesh cells each of thickness $\Delta x=0.01$ mfp and standard quadrature sets of double Gauss (DG) for $N=96$ and $N=200$ were used. Also, cases using Lobatto sets were run. In addition, several new features were introduced to make the comparisons more meaningful. Specifically, the angular edit grid was added to the quadrature set with (near) zero weights in order to avoid the need to interpolate between quadrature angles. Also an attempt was made to standardize the source direction to be perpendicular ($\mu = 1$) to the free surface. Thus, $\mu = 1$ was input with zero weight and the source was, for some cases, specified to be at this quadrature point. Finally, both the diamond difference (DD) and linear discontinuous (LD) spatial differencing schemes were tested.

Tables 2a,b,c show angular exiting and scalar flux comparisons where the ANB column is the analytical benchmark. All digits shown are believed to be correct. The column labeled SLD200⁺ is the result for Lobatto quadrature with LD and with edit angles added at zero weight. Except for the grazing angle ($\mu = 0$), the agreement with ANB is excellent. Even better agreement is observed for column SLD200^{*} using a standard double-Gauss quadrature with the source introduced at $\mu = 1$. Both LD-ONEDANT results seem to have some difficulty at $\mu = 0$ the causes of which are under currently investigation. For a DD approximation DGN=96 and the source perpendicular given in column SDD96^{*} the discrepancy seems to have disappeared. Column RDD96 is included to show the standard **ONEDANT** result with linear interpolation between quadrature directions to get the edit directions and for the source at the SN direction closest to 1. The accuracy is greatly reduced for this case. Similar agreement is observed for the transmitted flux; however, flux fix-up caused oscillations for some cases at $\mu = 1$ and no value was available. **MCNP** calculations, run for almost 2 weeks, are also include in the tables. At best only 3 digits of accuracy are obtained for the **MCNP** angular fluxes. This most likely results from degradation of the flux tally which is, in effect, a current in an angular bin divided by an average direction. There is some uncertainty concerning the appropriate direction to use as the divisor.

Table 4c shows the interior scalar flux comparison. Again excellent agreement is observed for the SLD200[†] and SLD200^{*} cases except near the surfaces.

References

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**Table 1: Four-Slab Demonstration
Scalar Flux**

<i>x</i>	err = 1.0e-05	Quad Order = 45
slab= 1		
0.00000E+00	1.34659E+00	1.34660E+00
2.00000E-01	1.45854E+00	1.45855E+00
4.00000E-01	1.51248E+00	1.51248E+00
6.00000E-01	1.53920E+00	1.53920E+00
8.00000E-01	1.54489E+00	1.54489E+00
1.00000E+00	1.50835E+00	1.50836E+00
slab= 2		
1.00000E+00	1.50837E+00	1.50836E+00
1.02000E+00	1.47672E+00	1.47672E+00
1.04000E+00	1.45601E+00	1.45599E+00
1.06000E+00	1.44165E+00	1.44162E+00
1.08000E+00	1.43386E+00	1.43387E+00
1.10000E+00	1.43881E+00	1.43881E+00
slab= 3		
1.10000E+00	1.43881E+00	1.43881E+00
1.90000E+00	1.38505E+00	1.38505E+00
2.70000E+00	1.14057E+00	1.14057E+00
3.50000E+00	8.78584E-01	8.78584E-01
4.30000E+00	6.32282E-01	6.32282E-01
5.10000E+00	3.72041E-01	3.72043E-01
slab= 4		
5.10000E+00	3.72045E-01	3.72043E-01
5.50000E+00	2.11853E-01	2.11853E-01
5.90000E+00	1.34346E-01	1.34346E-01
6.30000E+00	8.77821E-02	8.77822E-02
6.70000E+00	5.81507E-02	5.81507E-02
7.10000E+00	3.81154E-02	3.81155E-02

Table 2: Deep Penetration Problem: $\alpha=150\text{mfp}$, $L=10$, $\omega=0.9$

Table 2a: Reflection

μ	ANB	SLD200 ⁺	RDD96	SDD96*	SLD200*	MCNP*
-1.0	0.439438	0.439436	0.438841	0.439438	0.439438	--
-0.8	0.468676	0.468674	0.468577	0.468676	0.468676	0.4680
-0.6	0.491836	0.491832	0.492291	0.491836	0.491836	0.4922
-0.4	0.518433	0.518425	0.518452	0.518435	0.518435	0.5179
-0.2	0.499727	0.499710	0.500071	0.499727	0.499727	0.4995
0.0	0.395614	0.396395	0.397550	0.395614	0.396862	--

*Source at $\mu_0=1$

+Lobatto quadrature

Table 2b: Transmission $\times 10^{23}$

μ	ANB	SLD200 ⁺	RDD96	SDD96*	SLD200*	MCNP*
0.0	1.18640	1.18868	1.19038	--	1.19007	--
0.2	1.93253	1.93246	1.93095	1.93243	1.93253	1.9363
0.4	2.62817	2.62813	2.62631	2.62803	2.62815	2.6330
0.6	3.42320	3.42316	3.42091	3.42302	3.42318	3.4267
0.8	4.39503	4.39498	4.39195	4.39479	4.39499	4.4017
1.0	5.63563	5.63555	5.62665	5.63535	5.63555	--

Table 2c: Scalar Flux

x	ANB	SLD200 ⁺	RDD96	SDD96*	SLD200*	MCNP*
0.05	1.54580	1.54569	1.54664	1.54568	1.54569	--
0.95	1.66667	1.66666	1.66715	1.66666	1.66666	--
10.0	1.00460-01	1.00460	1.00384	1.00460	1.00460	1.0048
50.0	8.33981-08	8.33982	8.33326	8.33969	8.33983	8.3422
100.0	2.08521-15	2.08521	2.08354	2.08514	2.08521	2.0864
149.95	3.40420-23	3.40392	3.40115	3.40377	3.40392	--