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A One Group-One-Dimensional Transport Benchmark in Cylindrical Geometry

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B.D. Ganapol

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B.D. Ganapol[+]
Department of Aerospace and Mechanical Engineering
University of Arizona
Ganapol@cowboy.ame.arizona.edu

I. INTRODUCTION

When the control rod channels are azimuthally homogenized, the pebble bed modular reactor (PBMR), to a first approximation, can be considered as a multi-region long cylindrical system. Thus, a 1D radially heterogeneous cylindrical model is appropriate as a scooping tool. This is the ultimate case for which the following transport benchmark is designed. In what follows, the scalar flux from the neutron transport equation will be specified for a heterogeneous 1D cylinder. The homogeneous case is then considered in order to develop a new numerical transport algorithm that will eventually be applied to a multi-region cylindrical PBMR transport simulation. The method to be presented is based on the integral transport formulation. This is in contrast to a popular approach in which the solution of a pseudo-transport equation provides a pseudo-angular flux that when integrated gives the correct scalar flux[1,2]. The new method is simply a direct discretization of the integral equation for the scalar flux with subsequent convergence acceleration and does not involve any sophisticated mathematical treatment such as Caseology, which is the basis of the pseudo-solution approach. Besides providing a useful benchmark, for which few exist in cylindrical geometry, the intent of this work is to demonstrate that a relatively unsophisticated formulation can also lead to highly accurate results. In other words, complex mathematical formulations, while quite elegant, are not necessary to precondition the solution representation so that it will yield high accuracy.

II The Integral Transport Equation

From the derivation in ref. 1, the integral transport equation in cylindrical geometry is

$$I(r) = \frac{1}{4\pi}\int_0^R dt t c(t) \int_0^1 \frac{d\mu}{\mu^2}\begin{bmatrix} K_0(r/\mu) I_0(t/\mu)\Theta(r-t)+ \\ +K_0(t/\mu) I_0(r/\mu)\Theta(t-r)\end{bmatrix}\begin{bmatrix} I(t)+ \\ +q(t)\end{bmatrix}$$

(1a)

where the scalar flux is $\psi(r) = I(r) + F$ and

$$q(r) \equiv \frac{1}{4\pi}\left[Q_0(r) - (1-c(r))F\right]. \tag{1b}$$

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$Q_0(r)$ represents a volume source and F represents an isotropic source on the outer surface. $c(t)$ is a variable number of secondaries within a medium of constant total cross section. For the special case of a single homogeneous medium with a uniform source represented by $Q_0 \equiv (1-c)Q$ for convenience, Eq.(1a) becomes

$$\begin{aligned} I(r) &= (1-c)[Q-F]\int_0^1 \frac{d\mu}{\mu^2} K(r,\mu) + \\ &+ c\int_0^1 \frac{d\mu}{\mu^2}\int_0^R dt t K(r,\mu,t) I(t) \end{aligned} \tag{2}$$

where

$$K(r,\mu,t) \equiv \begin{bmatrix} K_0(r/\mu) I_0(t/\mu)\Theta(r-t)+ \\ +K_0(t/\mu) I_0(r/\mu)\Theta(t-r)\end{bmatrix}$$

$$K(r,\mu) \equiv \int_0^R dt t K(r,\mu,t)$$

and I_0 and K_0 are modified Bessel functions of zero order. By performing the first integral $K(r,\mu)$ analytically[3], Eq.(2) becomes

$$\begin{aligned} I(r) &= \\ &= (1-c)[Q-F]\begin{bmatrix} 1- \\ -R\int_0^1 \frac{d\mu}{\mu} I_0(r/\mu) K_1(R/\mu)\end{bmatrix} + \\ &+ c\int_0^1 \frac{d\mu}{\mu^2}\int_0^R dt t K(r,\mu,t) I(t) \end{aligned} \tag{3}$$

where K_1 is the modified Bessel function of order 1.

III Numerical Formulation

To begin, the second integral in the second term in Eq.(3) is rewritten as

$$\int_0^R dt t K(r,\mu,t) I(t) = \sum_{k=1}^{n} \int_{r_k}^{r_{k+1}} dt t K(r,\mu,t) I(t) \tag{4}$$

where the interval $[0,R]$ has been partitioned into n subintervals $[r_k, r_{k+1}]$. The resulting integrals are reformulated using the integral mean value theorem as

$$\int_{r_k}^{r_{k+1}} dt tK(r,\mu,t) I(t) = I(\xi_k) \int_{r_k}^{r_{k+1}} dt tK(r,\mu,t)$$

where there is at least one value of ξ_k in the interval $[r_k, r_{k+1}]$ that makes this expression exact, however it is generally unknown and will be approximated as the interval midpoint

$$\xi_k = r_{k+1/2} \equiv \left[\frac{r_k + r_{k+1}}{2}\right].$$

Now Eq.(3) for $r_j \le r \le r_{j+1}$ becomes,

$$I(r) = (1-c)[Q-F]\left[1 - R\int_0^1 \frac{d\mu}{\mu} I_0(r/\mu) K_1(R/\mu)\right] +$$
$$+cI_{j+1/2}\int_0^1 \frac{d\mu}{\mu}\begin{bmatrix}\mu - r_j K_0(r/\mu) I_1(r_j/\mu) - \\ -r_{j+1} I_0(r/\mu) K_1(r_{j+1}/\mu)\end{bmatrix} +$$
$$+c\sum_{\substack{k=1\\k\ne j}}^{n} I_{k+1/2}\int_0^1 \frac{d\mu}{\mu}\begin{Bmatrix} K_0(r/\mu)\begin{bmatrix} r_k^+ I_1(r_k^+/\mu) - \\ -r_k I_1(r_k/\mu)\end{bmatrix}\Theta(r-r_k) - \\ -I_0(r/\mu)\begin{bmatrix} r_{k+1}K_1(r_{k+1}/\mu) - \\ -r_k^- K_1(r_k^-/\mu)\end{bmatrix}\Theta(r_{k+1}-r)\end{Bmatrix}.$$

(5)
where

$$r_k^+ \equiv \min(r_{k+1}, r) \quad r_k^- \equiv \max(r_k, r)$$

by performing the residual integration analytically. Letting $r = r_{j+1/2}$ gives for Eq.(5)

$$\left(1 - cf_{jj}\right) I_{j+1/2} = q_{c,j+1/2} + c\sum_{\substack{k=1\\k\ne j}}^{n} f_{jk} I_{k+1/2} \qquad (6a)$$

With

$$f_{jj} \equiv \int_0^1 \frac{d\mu}{\mu}\begin{bmatrix}\mu - r_j K_0(r_{j+1/2}/\mu) I_1(r_j/\mu) - \\ -r_{j+1} I_0(r_{j+1/2}/\mu) K_1(r_{j+1}/\mu)\end{bmatrix} \qquad (6b)$$

and for $k \ne j$

$$f_{jk} \equiv$$
$$\int_0^1 \frac{d\mu}{\mu}\begin{Bmatrix} K_0(r_{j+1/2}/\mu)\begin{bmatrix} r_k I_1(r_k/\mu) - \\ -r_k I_1(r_k/\mu)\end{bmatrix}\Theta(r-r_k) - \\ -I_0(r_{j+1/2}/\mu)\begin{bmatrix} r_{k+1}K_1(r_{k+1}/\mu) - \\ -r_k K_1(r_k/\mu)\end{bmatrix}\Theta(r_{k+1}-r)\end{Bmatrix}$$

(6c)
and

$$q_{c,j+1/2} \equiv$$
$$\equiv (1-c)[Q-F]\begin{bmatrix}1 - \\ -R\int_0^1 \frac{d\mu}{\mu} I_0(r_{j+1/2}/\mu) K_1(R/\mu)\end{bmatrix}. \qquad (6d)$$

Equations (6a) can now be inverted for $I_{k+1/2}$ with a subsequent acceleration.

To obtain the cell edge scalar fluxes, let $r = r_j$ with $I_j \equiv I(r_j)$ in Eq.(5) to give

$$I_j = (1-c)[Q-F]\left[1 - R\int_0^1 \frac{d\mu}{\mu} I_0(r_j/\mu) K_1(R/\mu)\right] +$$
$$+cI_{j+1/2}\int_0^1 \frac{d\mu}{\mu}\begin{bmatrix}\mu - r_j K_0(r_j/\mu) I_1(r_j/\mu) - \\ -r_{j+1} I_0(r_j/\mu) K_1(r_{j+1}/\mu)\end{bmatrix} +$$
$$+c\sum_{\substack{k=1\\k\ne j}}^{n} I_{k+1/2}\int_0^1 \frac{d\mu}{\mu}\begin{Bmatrix} K_0(r_j/\mu)\begin{bmatrix} r_{k+1} I_1(r_{k+1}/\mu) - \\ -r_k I_1(r_k/\mu)\end{bmatrix}\Theta(r-r_k) - \\ -I_0(r_j/\mu)\begin{bmatrix} r_{k+1}K_1(r_{k+1}/\mu) - \\ -r_k K_1(r_k/\mu)\end{bmatrix}\Theta(r_{k+1}-r)\end{Bmatrix}.$$

(7)

IV Numerical Implementation

A. Evaluation of the Matrix and Source Elements

The matrix elements and source elements contain integrals of the form

$$INT \equiv \int_0^1 \frac{d\mu}{\mu^\alpha} f(a/\mu), \quad \alpha = 0,1. \qquad (8)$$

These integrals are evaluated with a shifted Legendre/Gauss quadrature of order *N*. As will be indicated below, an acceleration of the flux values with *N* will be an integral part of the solution.

B. Acceleration of the Inner Iterations

There exist several possibilities for obtaining the scalar flux at the interval midpoints $I_{i+1/2}$. Direct or iterative inversions can be applied to Eqs.(6a). Since the number of intervals may be on the order of 1000, direct inversion may not be the most efficient choice. For this reason, iterative inversion will be the choice.

Equation (6a) can be written as

$$I^{l}_{j+1/2} = q_{c,j+1/2} + c\sum_{k=1}^{n} f_{jk} I^{l-1}_{k+1/2} \qquad (9)$$

where l is the iteration index. The inner iteration is initiated with a zero scalar flux and is accelerated with the Wynn epsilon (Wε) acceleration[4].

C. Acceleration

For all numerical demonstration, the flux distributions to be determined will be for $Q = 1$ and $F = 0$.

For the spatial discretization acceleration, 11 uniformly spaced positions ($r_j = jR/10$, $j = 0,1,...10$) will be edited and interrogated for convergence. To provide a sequence of solutions at the edit points, the following sequence of mesh spacings will be used in the solution of Eq.(6a):

$$h_i \equiv \frac{1}{2^i}, \quad i = 0,1,....11 .$$

Three separate accelerations are applied to accelerate the solution at the edit-points to the limit of zero mesh spacing. The first acceleration is the Wε and is applied to the original sequence. The second acceleration, also applied to the original sequence, is the Romberg acceleration, where the diagonal of the tableau is interrogated[5]. The final acceleration is the Wε acceleration applied to the diagonal of the Romberg tableau. The most converged acceleration results from the separate three accelerations are used as the flux. A Wε acceleration in the quadrature order is also applied to converge the integrals given by Eq.(8) toward convergence.

V Demonstration

Results found in Ref. 2 provide the ultimate comparison of the newly developed benchmark. Four cases will be considered. These include c = 0.3(0.2)0.9 for R = 1. Flux results for desired error of ε =1x10^{-6} and starting at quadrature order of N_0 = 20 are presented in Table 1. The incorrect digits are in bold and underlined. Only a total of 4 digits of 44 benchmark values are inaccurate as compared to the Siewert benchmark, which is quite remarkable given that the solution comes from a full spatial/angular discretization. The time of the computation, on a 2.4GHz Dell INSPIRON™, for the entire table is also indicated. All digits can be obtained at the expense of computational time if the starting quadrature N_0 is increased.

Discussion

The first attempt at the development of a transport benchmark to be applied to the PBMR effort at INL has been detailed. Both fixed sources and criticality (not presented here) have been considered. The numerical solution is entirely novel since it applies a "mining" of lower order solutions (of fixed quadrature and spatial discretization) to extrapolate to higher order solutions (infinite quadrature and zero spatial discretization) using convergence acceleration. Only a homogeneous medium has been considered in preparation for the more relevant heterogeneous cylindrical benchmark, which is the subject of a future effort. Also the future effort will treat the multigroup approximation.

Table 1 Flux Comparison to Siewert's Benchmark
For R=1: $\varepsilon = 10^{-6}$ N_0 = 20
T = 62.7s

r/R:*c*	**0.3**	**0.5**	**0.7**	**0.9**
0.00000E+00	3.64405E-01	4.57065E-01	5.9660**8**E-01	8.24677E-01
1.00000E-01	3.66325E-01	4.58897E-01	5.98138E-01	8.25431E-01
2.00000E-01	3.72157E-01	4.64449E-01	6.02766E-01	8.27704E-01
3.00000E-01	3.82121E-01	4.73895E-01	6.10603E-01	8.31533E-01
4.00000E-01	3.96622E-01	4.87552E-01	6.21852E-01	8.36986E-01
5.00000E-01	4.16309E-01	5.05927E-01	6.36839E-01	8.44173E-01
6.00000E-01	4.42206E-01	5.29816E-01	6.56077E-01	8.53271E-01
7.00000E-01	4.75976E-01	5.60510E-01	6.80397E-01	8.64571E-01
8.00000E-01	5.20597E-01	6.00306E-01	7.1129**0**E-01	8.78607E-01
9.00000E-01	5.8259**7**E-01	6.5424**6**E-01	7.5204**9**E-01	8.96589E-01
1.00000E+00	6.94369E-01	7.47538E-01	8.19470E-01	9.24929E-01

References

1. R.M. Westfall and D.R. Metcalf, *NSE*, **52**, 1(1973).
2. C.E. Siewert and J.R. Thomas, Jr., *NSE*, **87**, 107(1984).
3. I. Stegan and M. Abramowitz, *Handbook of Mathematical Functions*, Dover Publications, NY, (1965).
4. G.A. Baker and P. Graves-Morris, *Pádé Approximants*, Cambridge University Press, NY, (1996).
5. W.H. Press, et. al., Romberg Integration, §4.3 in *Numerical Recipes in FORTRAN: The Art of Scientific Computing, 2nd ed.* Cambridge, UK: Cambridge University Press, (1992).