PHYSOR 2020: Transition to a Scalable Nuclear Future
Cambridge, United Kingdom, March 29th-April 2nd, 2020

INTEGRAL TRANSPORT CORRECTION TO DIFFUSION CALCULATIONS USING pCMFD SCHEME

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ABSTRACT

The Ronen method is implemented and studied numerically in two-group one-dimensional homogeneous slab configuration. Since slow convergence is observed for the scalar flux especially near the vacuum boundary, new methods for accelerating the convergence are reported. For example, the use of the integral flux intermediate values as new boundary conditions in each iteration and iterative updating of the extrapolated boundary using the corrected local diffusion coefficients. Moreover, the pCMFD scheme is implemented and its performances are compared with those of standard CMFD scheme.

KEYWORDS: neutron diffusion ; integral transport ; non-linear transport correction ; CMFD ; pCMFD

1. INTRODUCTION

The distribution of the neutron flux in the reactor core is described by the neutron transport equation. Transport calculations on a full core scale can be a highly intensive computational task. To overcome this difficulty, faster (but less accurate) multigroup neutron diffusion solvers are often used. However, future Gen-IV reactor designs are characterized by strong heterogeneity in the core and modern calculation schemes evolve towards best-estimate codes, aiming at high accuracy. Hence, the accuracy of diffusion calculations is investigated. A crucial issue in obtaining an accurate diffusion calculation is the formulation of the diffusion coefficient. The calculation of this parameter should be based on physical insights from the full transport equation such that the resulting (transport corrected) diffusion approximation can capture the transport phenomena of interest.

The CMFD has been largely used in nodal diffusion codes as a technique for storage reduction, allowing the separate resolution of many two nodes problems in an iterative scheme [1,2]. Recently,

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multi-dimensional transport codes have used it as acceleration technique and the convergence of different implementations was studied in simple homogeneous slab problems [3, 4].

The use of a coarse mesh for the discretization of the problem is generally causing considerable error by truncation applied on the finite difference approximations of the derivative terms. On the other hand, it yields very fast calculations. The CMFD method recovers corrective terms by exploiting functional relations between the (scalar) flux and the current density, which appear in the neutron balance equation. The balance equation is solved for the flux, so that local models seek more accurate estimates of the current in order to derive these corrections. In principle, the corrective terms can be computed with a different physics other than diffusion, which is always solved at the coarse level. This facilitates its application to accelerate complex multi-dimensional transport codes. This acceleration is actually implemented by rebalancing the scalar flux, with the optional use of some relaxation [5]. Hence, a non-linear iterative scheme arises between the CMFD solver and the computation of the local corrections, which use the latest estimates of the flux available from the diffusion solver.

Second-order SPN equations can be solved by ordinary diffusion codes [6]. Yamamoto et al. [7] noticed numerical instabilities when correcting pseudo-currents obtained solely by the second-order moments of the expanded SP3 flux. This is because this quantity is generally smaller than the scalar flux (0-th moment) and can change its sign. They propose to modify the balance equation for the second moment in order to fix this numerical behavior. The modification consists of a shift with a positive quantity of the second moment so that their difference between neighboring quantities is unchanged, and their sum becomes positive and arbitrarily large.

In case partial currents can be computed, the pCMFD method [8] can be used to determine two distinct corrective terms per positive and negative partial currents, instead of having a single degree of freedom per cell surface. Another version of the CMFD called artificial diffusion [3, 9] redefines the diffusion coefficient as the sum of the original value and a complement derived from the current difference, which is still considered as proportional to the flux gradient. This scheme can potentially lead to negative diffusion constants.

The CMFD (and its variants) was also chosen for the implementation of the RM, where an integral transport operator estimated higher order currents to calculate the correction terms. Contrary to the previous implementations, no operator was inverted to get a new higher order solution of the flux. This offers indeed a fast estimate of the higher order current.

2. THE RONEN METHOD

In 2004, Ronen [10] suggested to derive corrected diffusion coefficients using Fick's law and more accurate estimations of the neutron currents by means of integral transport operators, whereas the neutron flux is resolved by diffusion theory. Denoting the integral transport and diffusion currents by $\boldsymbol{J}(\boldsymbol{r}, E)$ and $\boldsymbol{J}^D(\boldsymbol{r}, E)$, respectively, the Ronen idea is based on adapting the diffusion coefficient such that

$$\boldsymbol{J}^D(\boldsymbol{r}, E) = -D(\boldsymbol{r}, E)\boldsymbol{\nabla}\phi(\boldsymbol{r}, E) = \boldsymbol{J}(\boldsymbol{r}, E) \ . \tag{1}$$

Since these accurate estimates of the currents are based on a known flux distribution, it was also

suggested to execute new diffusion calculations, thus updating iteratively the diffusion coefficients in the global calculation according to

$$D^{(k+1)}(\boldsymbol{r}, E) = -\frac{|\boldsymbol{J}^{(k)}(\boldsymbol{r}, E)|}{|\boldsymbol{\nabla}\phi^{(k)}(\boldsymbol{r}, E)|} \ , \tag{2}$$

where k is the iteration index.

The motivation for this method was to overcome the inherent limitation of Fick's law requiring smooth flux gradients and thus weakly absorbing medium. Nevertheless, isotropic scattering remained as a basic postulate. For example, in a one-dimensional homogeneous slab with void boundary conditions, Eq. (2) takes the following form [10]

$$D^{(k+1)}(x, E) = -\frac{\frac{1}{2}\int_0^a dx' E_2[\sigma(E)|x - x'|]\text{sign}(x - x')q^{(k)}(x', E)}{\partial\phi^{(k)}(x, E)/\partial x} \ , \tag{3}$$

where the source term $q^{(k)}(x', E)$ is calculated using the multigroup diffusion model with available diffusion coefficients, and the updated diffusion coefficients $D^{(k+1)}(x, E)$ are evaluated using the integral expression for the transport current.

In 2011, Tomatis and Dall'Osso [11] provided a numerical demonstration in a simple slab problem. They adopted the Coarse Mesh Finite Differences method (CMFD) for taking into account the new currents estimated by the integral transport operator in the diffusion solver. This technique can avoid indeterminate divisions in case of vanishing flux gradients. It was observed that the RM could drive the flux distribution closer to the transport reference solution. As expected, the largest errors were located near the boundary, where the transport effects are most pronounced, slowly decreasing even after many iterations.

3. NUMERICAL IMPLEMENTATION

The CMFD neutron balance equation for a k_{eff}-eigenvalue problem on a one-dimensional mesh, shown in Fig. 1, is

$$J_{i+1/2,g} - J_{i-1/2,g} + \sigma_{i,g}\phi_{i,g} = q_{i,g} \ , \tag{4}$$

where J denotes the accurate net current at the cell surface, σ denotes the total cross section, the subscript g denotes the energy group, and q is the isotropic neutron source defined as

$$q_{i,g} = \sum_{g'=1}^{G} \sigma_{s,0,i,g\leftarrow g'}\phi_{i,g'} + \frac{\chi_g}{2k_{\text{eff}}} \sum_{g'=1}^{G} \nu\sigma_{f,i,g'}\phi_{i,g'} \ , \tag{5}$$

where σ_0 is the isotropic scattering cross section, χ is the fission spectrum, k_{eff} is the eigenvalue, ν is the average number of neutrons emitted per thermal fission, and σ_f is the fission cross section.

The accurate net current and partial current in the case of isotropic scattering are calculated using

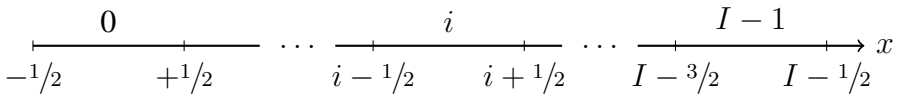

Figure 1: Notation of the one-dimensional mesh.

the following expressions derived from the integral neutron transport equation [11–13]

$$\begin{aligned} J^{+}_{i+1/2,g} &= \frac{1}{2}E_3[\tau_g(x_{-1/2},x_{i+1/2})]\phi_{x_{-1/2},g} \\ &\quad + \frac{1}{2}\sum_{j=0}^{i}\frac{q_{j,g}}{\sigma_{j,g}}\left\{E_3\left[\tau_g(x_{j+1/2},x_{i+1/2})\right]-E_3\left[\tau_g(x_{j-1/2},x_{i+1/2})\right]\right\} \\ J^{-}_{i+1/2,g} &= \frac{1}{2}E_3[\tau_g(x_{i+1/2},x_{I-1/2})]\phi_{x_{I-1/2},g} \\ &\quad + \frac{1}{2}\sum_{j=i+1}^{I-1}\frac{q_{j,g}}{\sigma_{j,g}}\left\{E_3\left[\tau_g(x_{i+1/2},x_{j-1/2})\right]-E_3\left[\tau_g(x_{i+1/2},x_{j+1/2})\right]\right\} \ , \end{aligned} \tag{6}$$

where $\tau_g(x',x) \equiv \int_{x'}^{x}\sigma_g(x'')dx''$ is the optical length and the net current is $J_{i+1/2,g} = J^{+}_{i+1/2,g} - J^{-}_{i+1/2,g}$.

3.1. CMFD IMPLEMENTATION

In standard CMFD implementation, correction terms, e.g., $\delta J_{i+1/2,g}$, are added to the diffusion current $J^{\mathrm{D}}_{i+1/2,g}$, such that it is driven towards the accurate net current $J_{i+1/2,g}$. The accurate net current is calculated by the integral expression given in Eq. 6 and using the scalar flux for evaluating the emission source $q_{i,g}$. The diffusion current is evaluated according to

$$J^{\mathrm{D}}_{i+1/2,g} \cong -D_{i+1/2,g}\frac{\phi_{i+1,g}-\phi_{i,g}}{(\Delta_{i+1}+\Delta_i)/2} \ , \tag{7}$$

where integer and rational subscripts indicate node-averaged and interface quantities, respectively, and

$$D_{i+1/2,g} = \frac{\Delta_i D_{i,g} + \Delta_{i+1}D_{i+1,g}}{\Delta_i + \Delta_{i+1}} \ . \tag{8}$$

Once the accurate net current and the diffusion current are calculated using the most recent flux values, the correction terms on cell interfaces can be calculated. The discretized form of the current $\delta J_{i+1/2,g}$ must involve the neighboring flux as well, but its representation is changed into a drift-advection term to avoid of possible undefined division by zeros in case of flat flux [1, 11]

$$\delta J_{i+1/2,g} = -\delta D_{i+1/2,g}\frac{\phi_{i+1,g}+\phi_{i,g}}{(\Delta_{i+1}+\Delta_i)/2} = J_{i+1/2,g} - J^{\mathrm{D}}_{i+1/2,g} \ . \tag{9}$$

3.2. pCMFD IMPLEMENTATION

The partial currents in any point x in a slab are defined according to

$$J^{\pm}(x) \cong \frac{\phi(x)}{4} \pm \frac{J^{\mathrm{D}}(x)}{2} \ , \tag{10}$$

where J^{D} denotes the diffusion current. The partial currents correction factors are defined on cell surface according to

$$J^{\pm}_{i+1/2} = \frac{1}{4}\phi_{i+1/2} \pm \frac{1}{2}J^{\mathrm{D}}_{i+1/2} \pm \frac{1}{2}\delta J^{\pm}_{i+1/2} \ , \tag{11}$$

where

$$\phi_{i+1/2} = \frac{\Delta_i\phi_i + \Delta_{i+1}\phi_{i+1}}{\Delta_i + \Delta_{i+1}} \, . \tag{12}$$

Substituting [3, 9]

$$\frac{1}{2}\delta J^{+}_{i+1/2} \equiv -\delta D^{+}_{i+1/2}\phi_i \, , \quad \frac{1}{2}\delta J^{-}_{i+1/2} \equiv -\delta D^{-}_{i+1/2}\phi_{i+1} \ , \tag{13}$$

yields

$$J^{+}_{i+1/2} = \frac{1}{4}\phi_{i+1/2} + \frac{1}{2}J^{\mathrm{D}}_{i+1/2} - \delta D^{+}_{i+1/2}\phi_i \tag{14}$$

$$J^{-}_{i+1/2} = \frac{1}{4}\phi_{i+1/2} - \frac{1}{2}J^{\mathrm{D}}_{i+1/2} + \delta D^{-}_{i+1/2}\phi_{i+1} \ . \tag{15}$$

Solving for the partial current correction factors gives

$$\delta D^{+}_{i+1/2} = \frac{\frac{1}{4}\phi_{i+1/2} + \frac{1}{2}J^{\mathrm{D}}_{i+1/2} - J^{+}_{i+1/2}}{\phi_i} \, , \quad \delta D^{-}_{i+1/2} = \frac{-\frac{1}{4}\phi_{i+1/2} + \frac{1}{2}J^{\mathrm{D}}_{i+1/2} + J^{-}_{i+1/2}}{\phi_{i+1}} \ . \tag{16}$$

In case the diffusion current is accurate, e.g., in a weak absorbing medium and several mfp's from the boundary or a strong absorber, the correction factors $\delta D^{\pm}$ vanish and Eq. (16) reduces to Eq. (10), as expected, which implies for the net (accurate) current

$$J_{i+1/2} = J^{+}_{i+1/2} - J^{-}_{i+1/2} = J^{\mathrm{D}}_{i+1/2} \ . \tag{17}$$

4. RESULTS

5. CONCLUSIONS

Present your summary and conclusions here.

NOMENCLATURE

- RM - Ronen Method
- CMFD - Coarse Mesh Finite Difference
- pCMFD - partial current CMFD

ACKNOWLEDGEMENTS

Acknowledge the help of colleagues and sources of funding, as appropriate.

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