

Integral Transport Correction to Diffusion Calculations Using the pCMFD Scheme

R. Gross^a, D. Tomatis^b, E. Gilad^{a,*}

^a*The Unit of Nuclear Engineering, Ben-Gurion University of the Negev, Beer-Sheva
8410501, Israel*

^b*CEA, DEN, Service d'études des réacteurs et de mathématiques appliquées (SERMA),
Université Paris-Saclay, F-91191, Gif-sur-Yvette, France*

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 techniques for accelerating the convergence are investigated. For example, we use integral flux intermediate values as new boundary conditions at each iteration and we update iteratively the extrapolated boundary using the corrected local diffusion coefficient. 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
5 less accurate) multigroup neutron diffusion solvers are often used. Indeed, 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 for these new configurations. Hence, the accuracy of diffusion calculations is investigated. A crucial issue in obtaining an accurate
10 diffusion calculation is the formulation of the diffusion coefficient. The calculation of this parameter should be based on physical insights from the full

*Corresponding author

Email address: `gilade@bgu.ac.il` (E. Gilad)

transport equation, such that the resulting (transport-corrected) diffusion approximation can capture the transport phenomena of interest.

The main hypothesis of this research, called the Ronen Method (RM) (Ronen, 2004; Tomatis and Dall’Osso, 2011), is based on iterative calculations of the multigroup diffusion coefficients, driven by accurate relations between the neutron current density and the neutron flux as derived from the integral transport equation. The iterative scheme calculates new flux distributions using a diffusion solver but with a (spatially) modified diffusion coefficient according to the current calculated using the integral transport equation. Alternatively, the Coarse Mesh Finite Differences (CMFD) scheme can be enforced in the discretized form of the diffusion equation to reproduce the transport current by means of a drift term. The implementation of one its variants, the partial current formulation of the CMFD (pCMFD), is studied in this work.

2. Coarse Mesh Finite Differences

The CMFD has been largely used in nodal diffusion codes as a technique for storage reduction, allowing for separate resolution of many two nodes problems in an iterative scheme (Smith, 1983; Lawrence, 1986). Recently, multi-dimensional transport codes have used it as acceleration technique and the convergence of different implementations was studied in simple homogeneous slab problems (Jarrett et al., 2016; Shen et al., 2019).

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 (Park et al., 2017). 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 (Larsen et al., 1993). Yamamoto et Al. (Yamamoto et al., 2016) noticed numerical

instabilities when correcting pseudo-currents obtained solely by the second-order moments of the expanded SP_3 flux. This is because this quantity is generally smaller than the scalar flux (0-th moment) and can change its sign. They proposed to modify the balance equation for the second moment in order to fix this numerical behavior. The modification consisted 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.

When partial currents can be computed, the pCMFD method (Cho et al., 2003) 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 (Zhu et al., 2016; Jarrett et al., 2016) 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 scheme 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 approximation of the flux solution. Thereafter, this offered a fast and more accurate estimate of the current too.

3. The Ronen Method

In 2004, Ronen (Ronen, 2004) 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 was resolved by diffusion theory. Denoting the integral transport and diffusion currents by $\mathbf{J}(\mathbf{r}, E)$ and $\mathbf{J}^D(\mathbf{r}, E)$, respectively, the Ronen idea is based on adapting the diffusion coefficient such that

$$\mathbf{J}^D(\mathbf{r}, E) = -D(\mathbf{r}, E)\nabla\phi(\mathbf{r}, E) \cong \mathbf{J}(\mathbf{r}, E). \quad (1)$$

Since these accurate estimates of the currents were 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

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

where k is the iteration index. The use of a tensor notation is needed for the diffusion coefficient in general multidimensional problems (Boffi and Trombetti, 1972).

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 (Ronen, 2004)

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

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

In 2011, Tomatis and Dall'Osso (Tomatis and Dall'Osso, 2011) provided a numerical demonstration of the simple slab problem. They chose the CMFD scheme in the diffusion solver for taking into account the new currents estimated by the integral transport operator. This technique can avoid indeterminate divisions in case of vanishing flux gradients and reproduces the transport effects under a drift term. 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 more pronounced, slowly decreasing even after many iterations.

4. Numerical Implementation

The neutron balance equation for a k -eigenvalue problem integrated in the i -th element of a one-dimensional mesh is (see Fig. 1)

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

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

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

where σ_0 is the isotropic scattering cross section, χ is the fission spectrum, k_{eff} is the effective multiplication factor (the eigenvalue), ν is the average

number of neutrons emitted per thermal fission, and σ_f is the fission cross section. Integer and rational subscripts indicate node-averaged and interface quantities, respectively.

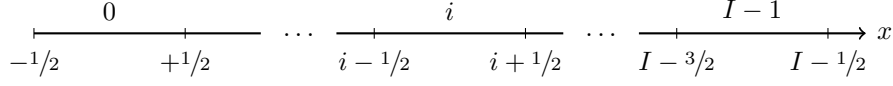


Figure 1: Notation of the one-dimensional mesh.

The partial currents in the case of isotropic scattering are calculated using the following expressions derived from the integral neutron transport equation (Tomatis and Dall’Osso, 2011; Tomatis et al., 2019; Gross et al., 2020):

$$J_{i+1/2,g}^+ = \frac{1}{2} E_3 [\tau_g(x_{-1/2}, x_{i+1/2})] \phi_{x_{-1/2},g} + \frac{1}{2} \sum_{j=0}^i \frac{q_{j,g}}{\sigma_{j,g}} \{ E_3 [\tau_g(x_{j+1/2}, x_{i+1/2})] - E_3 [\tau_g(x_{j-1/2}, x_{i+1/2})] \} \quad (6a)$$

$$J_{i+1/2,g}^- = \frac{1}{2} E_3 [\tau_g(x_{i+1/2}, x_{I-1/2})] \phi_{x_{I-1/2},g} + \frac{1}{2} \sum_{j=i+1}^{I-1} \frac{q_{j,g}}{\sigma_{j,g}} \{ E_3 [\tau_g(x_{i+1/2}, x_{j-1/2})] - E_3 [\tau_g(x_{i+1/2}, x_{j+1/2})] \}, \quad (6b)$$

where $\tau_g(x', x) \equiv \int_{x'}^x \sigma_g(x'') dx''$ is the optical length. The net current is $J_{i+1/2,g} = J_{i+1/2,g}^+ - J_{i+1/2,g}^-$, $\forall i$. Only the zeroth moment of the angular flux, that is the scalar flux yet occurring after its expansion in angle on spherical harmonics, is used at the boundary to include the contribution of possible incoming currents. Eqs. (6) are expected to yield more accurate estimates of the currents even when using a flux distribution obtained from diffusion theory. This is the main assumption of the Ronen Method.

4.1. CMFD Implementation

In classic CMFD implementation, the term $\delta J_{i+1/2,g}$ is added to the diffusion current $J_{i+1/2,g}^D$ in order to reproduce the net current $J_{i+1/2,g}$ used in Eq. (4). Currents are only computed on the surface elements of a coarse mesh in space to save memory and runtime (Smith, 1983). Besides, the net current can be determined from some other expression which is physically or numerically more accurate. Therefore, this new term acts as a correction

for the diffusion current. The diffusion current is generally approximated by discretizing Fick's law, and by finite differences, according to

$$J_{i+1/2,g}^D \cong -D_{i+1/2,g} \frac{\phi_{i+1,g} - \phi_{i,g}}{(\Delta_{i+1} + \Delta_i)/2}, \quad (7)$$

135 where the diffusion coefficient at the interface is volume-averaged as

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

About the RM, more accurate estimates of the net current come from the integral expressions of Eqs. (6), still using the scalar flux in the emission source $q_{i,g}$. In linearly anisotropic problems, the net current can also be considered to compute the source. Once the diffusion currents and the net
140 currents by integral transport are calculated using the most recent flux values, the correction terms can be obtained on the cell interfaces. The discretized form of the terms $\delta J_{i+1/2,g}$ reproduce a centered drift-advection term to avoid possible indeterminate division by zeros in case of flat flux (Smith, 1983; Tomatis and Dall'Osso, 2011):

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

145 for $i = 0, \dots, I-2$. The division by the spatial differences can be removed because the definition of δD is arbitrary. By retrieving the net current from Eq. (9) and substitution in Eq. (4) with the source from Eq. (5) yields the CMFD balance equation. Finally, using Eqs. (7), (9) and rearranging, the flux follows by solving a system of linear equations:

$$\begin{aligned} & \left(\frac{-D_{i-1/2,g} + \delta D_{i-1/2,g}}{\Delta_{i-1} + \Delta_i} \right) \phi_{i-1,g} \\ & + \left(\frac{D_{i+1/2,g} - \delta D_{i+1/2,g}}{\Delta_{i+1} + \Delta_i} + \frac{D_{i-1/2,g} + \delta D_{i-1/2,g}}{\Delta_i + \Delta_{i-1}} + \frac{\sigma_{i,g}}{2} \right) \phi_{i,g} \\ & + \left(\frac{-D_{i+1/2,g} - \delta D_{i+1/2,g}}{\Delta_{i+1} + \Delta_i} \right) \phi_{i+1,g} = \frac{1}{2} q_{i,g}, \end{aligned} \quad (10)$$

150 for $0 < i < I-1$.

Boundary conditions applies on the diffusion current as usual by means of an extrapolated length ζ , i.e., $\zeta J^D \cong D\phi$. The constant ζ can follow from Mark or Marshak approximations, or others derived again from transport theory (Meghreblian and Holmes, 1960). About the correction terms instead,
155 it is simply $\delta J = -\delta D\phi$ with the boundary flux approximated at first order by the cell-averaged value. The introduction of these closures in the equations for $i = 0$ and $i = I-1$ is straightforward.

4.2. pCMFD Implementation

The CMFD introduces in the numerical scheme a free parameter per cell surface through the correction term to adjust the diffusive solution locally. Since separate calculations of the partial currents are possible, two free parameters could be used in the discretized form of the diffusion equation. This idea leads to the development of the pCMFD scheme (Cho and Lee, 2003).

Two corrective terms are then introduced: $J = J^+ - J^- = J^D + \delta J^+ + \delta J^-$. An upwind definition with respect to the direction of flight of neutrons is used for the corrections (Jarrett et al., 2016; Zhu et al., 2016):

$$\delta J_{i+1/2}^+ = -\delta D_{i+1/2}^+ \phi_i \quad \text{and} \quad \delta J_{i+1/2}^- = -\delta D_{i+1/2}^- \phi_{i+1}. \quad (11)$$

It can be noted that the signs before the correction terms are arbitrary, with no need to follow a specific physical meaning. The current by diffusion is distributed on the partial currents in equal parts in order to compute the new corrective coefficients δD^\pm ,

$$J_{i+1/2}^+ - \frac{1}{2} J_{i+1/2}^D = -\delta D_{i+1/2}^+ \phi_i, \quad (12a)$$

$$J_{i+1/2}^- + \frac{1}{2} J_{i+1/2}^D = +\delta D_{i+1/2}^- \phi_{i+1}, \quad (12b)$$

still for $i = 0, \dots, I-2$. The same substitutions indicated in section 4.1 lead to the pCMFD balance equation, where after introducing Eqs. 7 and 11 for the currents it is in the i -th cell

$$\begin{aligned} & \left(-\tilde{D}_{i-1/2,g} + \delta D_{i-1/2,g}^+ \right) \phi_{i-1,g} \\ & + \left(\tilde{D}_{i+1/2,g} - \delta D_{i+1/2,g}^+ + \tilde{D}_{i-1/2,g} + \delta D_{i-1/2,g}^- + \sigma_{i,g} \right) \phi_{i,g} \\ & + \left(-\tilde{D}_{i+1/2,g} - \delta D_{i+1/2,g}^- \right) \phi_{i+1,g} = q_{i,g}, \end{aligned} \quad (13)$$

with $\tilde{D}_{i+1/2,g} = 2D_{i+1/2,g}/(\Delta_{i+1} + \Delta_i)$. The diffusion current is not halved at the boundary, using only Eq. (12b) or Eq. (12a) at the left and at the right boundaries, respectively. Indeed, the implementation of CMFD can be upgraded to support the pCMFD scheme with minimal changes.

In a weakly absorbing medium and several mean free paths away from the boundary or a strong absorber, all correction factors δD^\pm are expected to vanish and the net current must be fully reproduced by the diffusion current. Of course, this must be verified by the classic CMFD scheme too.

5. Results

xy

180 6. Conclusions

Present your summary and conclusions here.

References

- Boffi, V.C., Trombetti, T., 1972. Tensorial formulation of neutron diffusion theory. *Meccanica* 7, 131–140.
- 185 Cho, N.Z., Lee, G.S., 2003. Comparison of CMFD and p-CMFD acceleration methods for neutron transport calculations. *Proc. of Korean Nuclear Society, Gyeongju, Korea* .
- Cho, N.Z., Lee, G.S., Park, C.J., 2003. Partial current based CMFD acceleration of the 2D/1D fusion method for 3D whole-core transport calculations, in: *Transactions of the American Nuclear Society*, p. 594.
- 190 Gross, R., Tomatis, D., Gilad, E., 2020. High-accuracy neutron diffusion calculations based on integral transport theory. *The European Physical Journal - Plus (EPJ Plus)* Submitted.
- Jarrett, M., Kochunas, B., Zhu, A., Downar, T., 2016. Analysis of stabilization techniques for CMFD acceleration of neutron transport problems. *Nuclear Science and Engineering* 184, 208–227.
- 195 Larsen, E.W., Morel, J.E., McGhee, J.M., 1993. Asymptotic derivation of the simplified Pn equations, in: *Proceedings of the Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications*, p. 718.
- 200 Lawrence, R.D., 1986. Progress in nodal methods for the solution of the neutron diffusion and transport equations. *Progress in Nuclear Energy* 17, 271–301. URL: <http://www.sciencedirect.com/science/article/pii/014919708690034X>, doi:[https://doi.org/10.1016/0149-1970\(86\)90034-X](https://doi.org/10.1016/0149-1970(86)90034-X).
- 205 Meghreblian, R.V., Holmes, D.K., 1960. *Reactor analysis*. McGraw-Hill.
- Park, C.J., Park, M.g., Hong, S.G., 2017. Convergence analysis of partial current based coarse mesh finite difference method (p-CMFD) with two parameter relaxation, in: *Proceedings of the International Conference on Mathematics & Computational Methods Applied to Nuclear Science and Engineering M&C 2017, Jeju, Korea*.
- 210

- Ronen, Y., 2004. Accurate relations between the neutron current densities and the neutron fluxes. *Nuclear Science and Engineering* 146, 245–247. URL: <https://doi.org/10.13182/NSE04-A2407>, doi:10.13182/NSE04-A2407, arXiv:<https://doi.org/10.13182/NSE04-A2407>.
- Shen, Q., Xu, Y., Downar, T., 2019. Stability analysis of the CMFD scheme with linear prolongation. *Annals of Nuclear Energy* 129, 298–307.
- Smith, K.S., 1983. Nodal method storage reduction by nonlinear iteration. *Transactions of the American Nuclear Society* 44, 265–266.
- Tomatis, D., Dall’Osso, A., 2011. Application of a numerical transport correction in diffusion calculations, in: *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2011)*, Rio de Janeiro, RJ, Brazil, May 8-12, 2011.
- Tomatis, D., Gross, R., Gilad, E., 2019. On the Ronen method in simple 1-D problems, in: *The 26th International Conference on Transport Theory (ICTT-26)*, Paris, France, September 23-27, 2019.
- Yamamoto, A., Sakamoto, T., Endo, T., 2016. A CMFD acceleration method for SP3 advanced nodal method. *Nuclear Science and Engineering* 184, 168–173.
- Zhu, A., Jarrett, M., Xu, Y., Kochunas, B., Larsen, E., Downar, T., 2016. An optimally diffusive coarse mesh finite difference method to accelerate neutron transport calculations. *Annals of Nuclear Energy* 95, 116–124.