# Homogeneity and Isotropy Restoration Theory for Derivation of Multigroup Transport Equations

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## 1. Introduction

While the continuous-energy neutron transport equation is derived straightforwardly and rigorously, the multigroup transport equation currently in use involves several approximations during its derivation [1,2].

In this paper, we propose a new way of deriving multigroup transport equation that maintains angle-independence in the total cross section and homogeneity in the material region (originally each material region is usually homogeneous). As a byproduct, only isotropic scattering term remains, which also relieves the computational burden significantly.

In this Homogeneity and Isotropy REstoration (HIRE) theory, we introduce a discontinuity factor in the form of partial current discontinuity factor (PCDF) at material interface. The theory is tested on a simple problem – a typical pin cell in a reactor core – with expected results, providing a proof of the principle.

## 2. Methodology

The continuous-energy neutron transport equation can be rigorously derived as:

$$\vec{\Omega}\cdot\nabla\varphi(\vec{r},E,\vec{\Omega})+\sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})= \int dE'\int d\vec{\Omega}'\ \sigma_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\varphi(\vec{r},E',\vec{\Omega}')+ \frac{\chi(E)}{k_{eff}}\int dE'\int d\vec{\Omega}'\ \nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\,. \quad (1)$$

To obtain corresponding multigroup transport equations, we integrate Eq. (1) over an energy interval $E_g \le E \le E_{g-1}$ as:

$$\vec{\Omega}\cdot\nabla\varphi_g(\vec{r},\vec{\Omega})+\sigma_{t,g}(\vec{r},\vec{\Omega})\varphi_g(\vec{r},\vec{\Omega})= \sum_{g'=1}^{G}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\vec{\Omega})\sigma_{sl,gg'}(\vec{r})\phi_{lg'}^{m}(\vec{r})+ \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\sigma_{f,g'}(\vec{r})\phi_{g'}(\vec{r})\ ;\ g=1\text{ to }G, \quad (2)$$

where the standard notations are used.

Note that, in Eq. (2), the group total cross section in the left hand side becomes angular dependent, because

$$\sigma_{t,g}(\vec{r},\vec{\Omega})=\frac{\int_{E_g}dE\ \sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})}{\int_{E_g}dE\ \varphi(\vec{r},E,\vec{\Omega})}\,. \quad (3)$$

This causes inconvenience in all computational methods known today. This is an unresolved problem and there have been several attempts [3-5] but with limited success.

In this paper, we describe homogeneity and isotropy restoration (HIRE) theory that leads to material region-averaged, angle-independent and group condensed total collision cross section, in contrast to Eq. (3).

For the sake of simplicity, let us consider a typical two-dimensional $UO_2$ pin-cell problem shown in Fig. 1. The continuous-energy Monte Carlo (MC) calculation is performed to solve Eq. (1) with albedo boundary conditions given as :

$$\varphi(\vec{r},E,\vec{\Omega}')=\alpha_k\varphi(\vec{r},E,\vec{\Omega})\ \text{for}\ \vec{r}\in\Gamma_k,\ \vec{\Omega}\cdot\vec{n}_k>0, \quad \text{and}\ \vec{\Omega}'=\text{albedo direction to}\ \vec{\Omega}\ \text{for}\ k=1\ \text{to}\ 4\ , \quad (4)$$

where $\vec{n}_k$ is the outgoing normal direction of surface $k$.

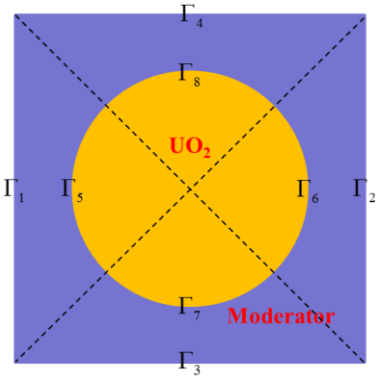


Fig. 1. Configuration of a 2-D $UO_2$ pin-cell problem; $\Gamma_k$ denotes the surface with index $k$.

From the continuous-energy MC calculation, the material region-averaged, angle-independent, and group condensed cross sections for each material region are obtained as:

$$\sigma_{t,g}^{m}=\frac{\int_{\vec{r}\in V_m}dV\int d\vec{\Omega}\int_{E_g}dE\sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})}{\int_{\vec{r}\in V_m}dV\int d\vec{\Omega}\int_{E_g}dE\varphi(\vec{r},E,\vec{\Omega})}\,, \quad (5)$$

$$\sigma_{s0,gg'}^{m}=\left[\int_{\vec{r}\in V_m}dV\int d\vec{\Omega}\int_{E_g}dE\int d\vec{\Omega}'\int_{E_{g'}}dE'\times \sigma_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\varphi(\vec{r},E',\vec{\Omega}')\right]\Big/ \left[\int_{\vec{r}\in V_m}dV\int d\vec{\Omega}\int d\vec{\Omega}'\int_{E_{g'}}dE'\ \varphi(\vec{r},E',\vec{\Omega}')\right], \quad (6)$$

$$\nu\sigma^m_{f,g'} = \left[\int_{\vec{r}\in V_m} dV \int d\vec{\Omega} \int d\vec{\Omega}' \int_{E_{g'}} dE' \times \nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\right] \Big/ \left[\int_{\vec{r}\in V_m} dV \int d\vec{\Omega} \int d\vec{\Omega}' \int_{E_{g'}} dE' \, \varphi(\vec{r},E',\vec{\Omega}')\right], \quad (7)$$

$$\chi^m_g = \left[\int_{\vec{r}\in V_m} dV \int d\vec{\Omega} \int d\vec{\Omega}' \int_{E_g} dE \int dE' \times \chi(E)\nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\right] \Big/ \left[\int_{\vec{r}\in V_m} dV \int d\vec{\Omega} \int d\vec{\Omega}' \int dE' \times \nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\right], \quad (8)$$

where $V_m$ is the volume of the material index $m$.

Then, the multigroup transport equation is constructed as:

$$\vec{\Omega}\cdot\nabla\varphi_g(\vec{r},\vec{\Omega}) + \sigma^m_{t,g}\varphi_g(\vec{r},\vec{\Omega}) = \int d\vec{\Omega}' \sum_{g'=1}^{G} \sigma^m_{s0,gg'}\varphi_{g'}(\vec{r},\vec{\Omega}') + \frac{\chi^m_g}{k_{eff}} \int d\vec{\Omega}' \sum_{g'=1}^{G} \nu\sigma^m_{f,g'}\varphi_{g'}(\vec{r},\vec{\Omega}') \;, \quad (9)$$

with $\varphi_g(\vec{r},\vec{\Omega}') = \alpha_k\varphi_g(\vec{r},\vec{\Omega})$ for $\vec{r}\in\Gamma_k$ , $\vec{\Omega}\cdot\vec{n}_k > 0$, and $\vec{\Omega}'$ = albedo direction to $\vec{\Omega}$ for $k$ = 1 to 4.

Note in Eq. (9) that only the zeroth-moment scattering remained in the scattering term.

Eq. (9) alone as such cannot preserve the eigenvalue and the material region-wise flux distributions of Eq. (1) due to discrepancies of the neutron leakages at the surfaces. To preserve the neutron leakages, the partial current discontinuity factor (PCDF) is introduced to each outgoing and incoming direction with respect to material $m$ at surface $k$ ($k$ = 5 to 8) as shown in Eqs. (10a) and (10b), with an illustration in Fig. 2.

$$\tilde{J}^+_{g,k} = f^+_{g,k}J^+_{g,k},$$
$$\text{with } J^+_{g,k} = \int_{\vec{r}\in\Gamma_k} dA \int_{\vec{\Omega}\cdot\vec{n}_k>0} d\vec{\Omega} \left|\vec{n}_k\cdot\vec{\Omega}_k\right| \varphi_g(\vec{r},\vec{\Omega}) \;, \quad (10a)$$

$$\tilde{J}^-_{g,k} = f^-_{g,k}J^-_{g,k},$$
$$\text{with } J^-_{g,k} = \int_{\vec{r}\in\Gamma_k} dA \int_{\vec{\Omega}\cdot\vec{n}_k<0} d\vec{\Omega} \left|\vec{n}_k\cdot\vec{\Omega}\right|_k \varphi_g(\vec{r},\vec{\Omega}) \;, \quad (10b)$$

where $f^+_{g,k}$ and $f^-_{g,k}$ are PCDF values are obtained as :

$$f^+_{g,k} = \frac{J^-_{g,k} - J^{ref}_{g,k}}{J^+_{g,k}} \;, \quad (11a)$$

$$f^-_{g,k} = \frac{J^+_{g,k} - J^{ref}_{g,k}}{J^-_{g,k}} \;, \quad (11b)$$

with

$$J^{ref}_{g,k} = \int_{\vec{r}\in\Gamma_k} dA \int d\vec{\Omega} \int_{E_g} dE \; \vec{n}_k\cdot\vec{\Omega}\varphi(\vec{r},E,\vec{\Omega}) \;. \quad (12)$$

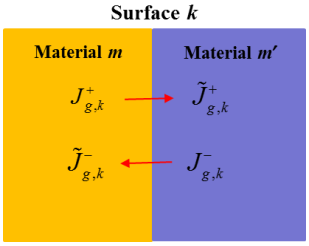


Fig. 2. Leakage corrections based on the PCDFs at surface $k$.

Similar PCDFs were considered before [6,7], but for different reasons from those of this paper. Ref. [6] introduced PCDF in the baffle-reflector homogenization in a diffusion nodal method, while Ref. [7] considered PCDF in the conventional multigroup transport or $SP_3$ solution method with homogenization.

At the beginning, the PCDFs are set as unity and they are updated by solving the multigroup transport calculation iteratively as in Fig. 3, where $l$ is the PCDF iteration index imposed on the multigroup transport solution of Eq. (9).

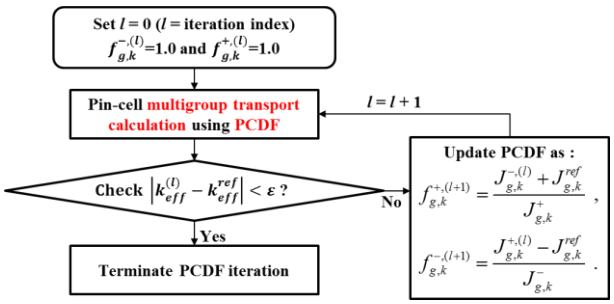


Fig. 3. PCDF iteration until the eigenvalue obtained from the multigroup transport calculation converges.

To accelerate the convergence of the PCDF iteration, the secant method can be applied as:

$$\tilde{f}^{\pm,(l+1)}_{g,k} = \left(\frac{k^{ref}_{eff} - k^{(l)}_{eff}}{k^{(l)}_{eff} - k^{(l-1)}_{eff}}\right)\left(f^{\pm,(l)}_{g,k} - f^{\pm,(l-1)}_{g,k}\right) + f^{\pm,(l)}_{g,k} \;, \quad (13)$$

where $\tilde{f}^{\pm,(l+1)}_{g,k}$ values are the accelerated PCDF values.

## 3. Numerical Results

The geometry of the pin-cell test problem is shown in Fig. 1. The pin pitch is 1.26 cm, where the fuel radius is 0.4095 cm. The fuel is $UO_2$ with 10.2 g/cc, 3.3 w/o U235, while the moderator is 1.0 g/cc with 800 ppm boron concentration. In this test problem, reflective boundary condition is applied to all boundary surfaces. Then, we try to reproduce the material region-wise continuous-energy MC solution from the one-group MC calculation (for this calculation in the 2nd box in Fig. 3, we can use $G$ > 1 and/or deterministic methods) using the HIRE theory.

The continuous-energy MC calculation is performed with 20 inactive cycles, 200 active cycles with 4,000,000 histories per cycle to generate one-group cross section for each material. $k_{eff}^{ref}$ is obtained as 1.28384 with the sample standard deviation of 2.0 pcm. The one-group MC calculation is performed with 20 inactive cycles, 200 active cycles with 1,000,000 histories per cycle.

Table I shows the one-group cross sections obtained by the HIRE theory, while Fig. 4 shows PCDFs for surfaces 5 to 8 (as denoted in Fig. 1) as iteration proceeds. Although the stochastic errors in net currents from the continuous-energy MC calculation cause some variations in PCDFs for symmetric surfaces during iteration, $f^+$ and $f^-$ converge to around 1.0056 and around 0.9944, respectively, at the end of iteration. Figs. 5 and 6 show the errors of the eigenvalue and the material region-wise flux obtained from the one-group MC calculation. After 2 PCDF iterations, the errors are significantly reduced.

Table I. One-group cross sections [$cm^{-1}$] for the pin-cell test problem

| | $\sigma_t$ | $\sigma_{s0}$ | $\nu\sigma_f$ |
|---|---|---|---|
| Fuel | 4.6351E-01 | 3.8184E-01 | 1.2487E-01 |
| Moderator | 1.0736E+00 | 1.0658E+00 | 0.0000E+00 |

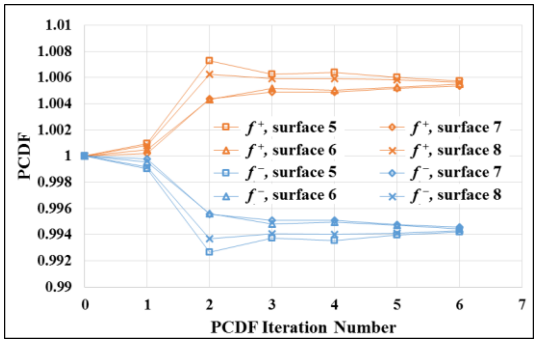


Fig. 4. PCDFs of surfaces 5 to 8 as iteration proceeds; $f^+$ and $f^-$ are PCDFs for the outgoing and incoming partial currents with respect to fuel region, respectively.

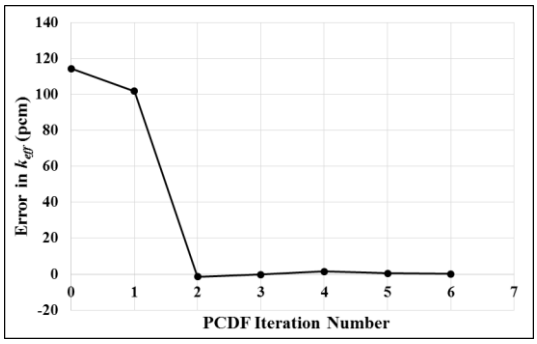


Fig. 5. Error of the eigenvalue from one-group MC calculation.

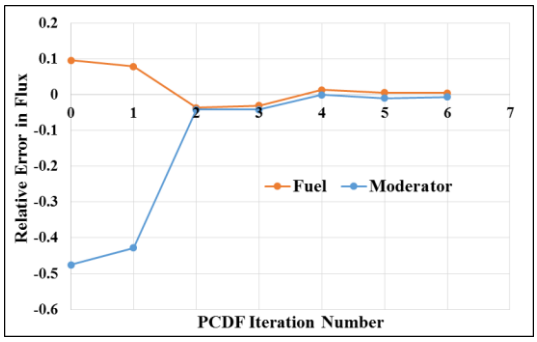


Fig. 6. Error of the material region-wise flux from one-group MC calculation.

## 4. Conclusions

The homogeneity and isotropy restoration (HIRE) theory described in this paper removes the angle dependency of the group condensed total cross section in the multigroup transport equation. For a pin-cell problem with all reflective boundary conditions, the method has been successfully tested. It is noted again that the multigroup transport equatikon thus derived can be solved by a deterministic method well-known in the literature or by a simple MC method.

As an additional remark, the integration volume in Eqs. (5) – (8) could be a multi-region volume such as the pin cell or the baffle-reflector for homogenization, or a sub-region volume such as a ring in a fuel rod for rim effect analysis.

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