# A Proposed New Framework for Nuclear Reactor Physics Analysis with Transport Calculation

- Invited -

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### 1. Introduction

It is a common understanding that the two-group diffusion nodal methods are commonly utilized in the whole-core reactor physics calculations in light water reactors, with prior multigroup (50-100) lattice (transport) calculations usually with reflective boundary conditions [1-3]. In fast breeder (spectrum) reactors, the methods are less established and still evolving [4-7]. They typically require spectrum calculations to prepare many group ( > 2000) cross sections, and then used in the first-order form or even-parity form of the multigroup (> 30) transport equations [6]. In the preparation of the multigroup cross sections to be used in the deterministic lattice calculations both in light water reactors and in fast spectrum reactors, the various resonance self-shielding methods are called for, that are fraught with many heuristics.

On the other hand, with the advancement of computer technology, the use of continuous-energy Monte Carlo simulation is contemplated in the whole-core analysis including depletion and kinetics problems. However, due to the tremendous amount of memory requirement and computing time [8], its routine use will be quite away into the future, although there are active research activities in this direction, e.g., in Ref. [9,10] and references therein.

In light of these circumstances, this paper proposes a new framework for nuclear reactor analysis. The key two elements are:

i) local problems defined for a set of "non reflective" boundary conditions are analyzed by continuous-energy Monte Carlo simulations, and transformed into HIREtheoretic multigroup (2-10 groups) transport equations, and

ii) the global multigroup transport equations are solved by appropriate numerical (deterministic) methods in transport theory, such as discrete ordinate  $(S_N)$  methods and the method of characteristics (MOC), including appropriate acceleration schemes, such as p-CMFD.

#### 2. Elements of HIRE Theory and Its PCDFs

The homogeneity and isotropy restoration (HIRE) theory has been proposed for a consistent derivation of the multigroup transport equations from the continuousenergy transport equation [11, 12]. The HIRE theory maintains angle-independence in the group total cross section and homogeneity in a material region. In addition, only the isotropic moment scattering term remains in the multigroup transport equations. The key idea in the HIRE theory is to replace the traditional definition of the multigroup cross sections, e.g., the group total cross section

$$\sigma_{t,g}(\vec{r},\vec{\Omega}) = \frac{\int_{E_g} dE \ \sigma_t(\vec{r},E)\psi(\vec{r},E,\vec{\Omega})}{\int_{E_g} dE \ \psi(\vec{r},E,\vec{\Omega})} , \qquad (1)$$

by, in a material region  $V_m$ ,

$$\sigma_{t,g}^{m} = \frac{\int_{\vec{r} \in V_{m}} dV \int d\vec{\Omega} \int_{E_{g}} dE \sigma_{t}(\vec{r}, E) \psi(\vec{r}, E, \vec{\Omega})}{\int_{\vec{r} \in V_{m}} dV \int d\vec{\Omega} \int_{E_{g}} dE \psi(\vec{r}, E, \vec{\Omega})} , \qquad (2)$$

and similarly, the group scattering cross section  $\sigma_{s,gg'}(\vec{r},\vec{\Omega}'\rightarrow\vec{\Omega})$  becomes  $\sigma^m_{s0,gg'}$  in  $V_m$ , and  $v\sigma_{f,g'}(\vec{r})$  becomes  $v\sigma^m_{f,g'}$  in  $V_m$ .

Note that how to treat the angle-dependence in  $\sigma_{t,g}(\vec{r},\vec{\Omega})$  in Eq. (1) causes an inconvenience in all computational methods known today. Namely, the consistent P approximation, the inflow- and outflow approximations, and others have been proposed and used, but only with varying degrees of success. Another difficulty that is not well recognized in Eq. (1) is that the group cross sections become space-dependent even in a region that is originally homogeneous.

For a simple illustration of the HIRE theory, let us consider a typical two-dimensional UO2 pin-cell problem (or a three-dimensional "box" if axial heterogeneity is significant) with an albedo boundary condition given as

$$\psi(\vec{r}, E, \vec{\Omega}') = \alpha_k \psi(\vec{r}, E, \vec{\Omega}), \tag{3}$$
  
for  $\vec{r} \in \Gamma_k$ ,  $E \in E_o$ ,  $\vec{\Omega} \cdot \vec{n}_k > 0$ ,

shown in Fig. 1. Then, this unit problem will be submitted to the continuous-energy Monte Carlo calculation.



Fig. 1. Configuration of a 2-D UO2 pin-cell problem;  $\Gamma_k$  denotes the surface with index *k*.

The continuous-energy transport equation can then be recast in the following multigroup transport equations:

$$\begin{split} \vec{\Omega} \cdot \nabla \psi_{g}(\vec{r}, \vec{\Omega}) + \sigma_{l,g}^{m} \psi_{g}(\vec{r}, \vec{\Omega}) &= \\ \int d\vec{\Omega}' \sum_{g'=1}^{G} \sigma_{s0,gg'}^{m} \psi_{g'}(\vec{r}, \vec{\Omega}') + \\ \frac{\chi_{g}^{m}}{k_{eff}} \int d\vec{\Omega}' \sum_{g'=1}^{G} v \sigma_{f,g'}^{m} \psi_{g'}(\vec{r}, \vec{\Omega}') , \end{split}$$

$$(4)$$

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

In the HIRE theory, the partial-current discontinuity factor (PCDF) is introduced and it plays a crucial role. To preserve the region-wise neutron leakage, the PCDF is applied at a region interface, as in Fig. 2. The PCDFs are iteratively determined using the Jacobian-Free Newton-Krylov (JFNK) method. See the details in Ref. 11.



Fig. 2. Leakage corrections based on the PCDFs at interface k.

#### 3. New Framework

Figure 3 shows in comparison the typical neutron energy spectra in a light water reactor and a fast neutron reactor, taken from [13]. Due to the nuclear reaction characteristics, the neutron mean free paths are quite different depending on the reactor types ( $\lambda_{LWR} < \lambda_{FBR}$ ).

Therefore, a square fuel pin cell (typically  $1.26 \text{ cm} \times 1.26 \text{ cm}$ ) is taken as a unit problem in light water

reactors, while a hexagonal fuel assembly (flat-to-flat distance of  $\sim 15$  cm) as a unit problem in fast reactors.



Fig. 3. Comparison of neutron energy spectra

#### 3.1 Light Water Reactors



Fig. 4. Unit problem in a light water reactor.

In light water reactors, the tally volume  $V_m$  in a unit problem can be the whole pin cell if the pin cell is to be homogenized, or the fuel pin can be divided into several rings if the rim effect or radial temperature feedback effect is to be considered. The albedo values can be i) zero if outside is vacuum, or ii) one if reflective, or iii) greater (smaller) than one if more (less) neutrons are incoming than outgoing (Fig. 4). Thus, the albedo values reflect the environmental or neighboring effect on the pin cell. It is recommended that  $\partial V_m$  not cross the fuel (fissionable material) region to minimize the effect on the variance.

Then the unit problems will "tile" (or form) the whole-core (usually one-quarter of the core), that will be then submitted to the multigroup transport (HIRE-theoretic) analysis, with 2D MOC calculation (in the case of two-dimensional problems) or 2D/1D (MOC/SN) fusion method calculation (in the case of three-dimensional problems), with two-level (spatial) p-CMFD acceleration [14].

3.2 Fast Reactors



Fig. 5. Unit problem in a fast reactor.

In fast reactors, the unit problem is chosen as a hexagonal fuel assembly. The tally volume Vm in a unit problem can be chosen as a triangle (six right triangles in a hexagon), but the PCDFs will be defined only on the sides of the rhomboid. There are three rhomboids in a hexagon (two triangles with similar colors form a rhomboid in Fig. 5). This is to avoid the potential numerical difficulty at the center of the hexagon if the PCDFs are defined on every triangles. The whole-core or one-third of the core will be submitted to the HIREtheoretic multigroup transport analysis, with 2D or 3D SN method calculations using the weighted diamond difference (WDD) scheme extended or step characteristic (ESC) scheme [15].

Since the WDD and ESC schemes are sweep procedures, it will be interesting to study the applicability of the Koch-Baker-Alcouffe (KBA) algorithm that are developed and popular in orthogonal geometries [16, 17]. It will be also useful to apply the two-level (spatial and possibly spectral) p-CMFD acceleration [14] in this hexagonal / rhombic prism geometry.

## 4. Summary and Concluding Remarks

This paper proposed a new framework for nuclear reactor analysis based on :

(i) the whole-core problem is decomposed into several unit problems,

(ii) each unit problem is characterized by environmental or neighboring conditions with albedo values,

(iii) a unit problem is analyzed by the continuousenergy Monte Carlo simulation, resulting in the homogeneity and isotropy restoration (HIRE)-theoretic multigroup (2 groups in the case of thermal reactors and less than 10 groups in the case of fast reactors) transport equations,  $(\mathrm{iv})$  step (iii) is repeated for a set of albedo boundary conditions, and

(v) the multigroup transport equations are solved for the whole-core, incorporating the partial current discontinuity factors (PCDFs) between the unit problems and between the subregions as appropriate. For computational efficiency, the two-level p-CMFD acceleration, as an example, and the KBA algorithm could be utilized.

The experience of the author and his co-workers indicates that only a few group representation that is allowed in the HIRE-theory can be a viable and effective approach in the reactor design analysis.

For the practical application of the new framework, a study for tabulation or functionalization of the HIRE parameters (multigroup cross sections and PCDFs) in terms of albedo, depletion, and temperature is needed for a set of typical unit problems (this could be assisted by multi-variate linear interpolation methods or by various artificial intelligence techniques).

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