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

– Invited –

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Table of Contents

1. Nuclear Reactor Analysis Methods

Current Status

- Assembly or pincell transport (many-group) + Whole-core diffusion theory (few-group)
  - "Multigroup" cross section library
    - ✓ Space is simplified.
    - ✓ Resonance self-shielding methods : suppositions and heuristics
- Assembly or pincell transport (many-group) + Whole-core transport theory (few-group)
- Whole-core Monte Carlo (continuous-energy) : emerging,
  event-wise first principles,
  but brute force
  - Time and memory
  - Variance
  - "Convergence" and acceleration

1. Nuclear Reactor Analysis Methods

❑ Proposed New Framework

- Local : Continuous-energy MC (with albedo parameterized boundary conditions)

- Global : Homogeneity and Isotropy Restoration (HIRE)-theoretic
  "multigroup" (few-group) transport equations

- Two templates : LWRs
  FNRs

2. HIRE-Theoretic Multigroup Transport Equations

- Continuous-energy neutron transport equation is rigorously derived as:

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

- To obtain corresponding multigroup transport equations, Eq. (1) is integrated over an energy interval $E_g \le E \le E_{g-1}$ leading to:

$$\vec{\Omega}\cdot\nabla\varphi_g(\vec{r},\vec{\Omega})+\sigma_{t,g}(\vec{r},\vec{\Omega})\varphi_g(\vec{r},\vec{\Omega})=\sum_{g'=1}^{G}\int d\Omega'\sigma_{s,gg'}(\vec{r},\vec{\Omega}'\to\vec{\Omega})\varphi_{g'}(\vec{r},\vec{\Omega}') + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\sigma_{f,g'}(\vec{r})\phi_{g'}(\vec{r}), \quad (2)$$

where the standard notations are used.

2. HIRE-Theoretic Multigroup Transport Equations

- Note that the group total cross section in Eq. (2) becomes angle-dependent as:

$$\sigma_{t,g}(\vec{r},\vec{\Omega}) = \frac{\int_{E_g}^{E_{g-1}} dE\sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})}{\int_{E_g}^{E_{g-1}} dE\varphi(\vec{r},E,\vec{\Omega})}. \quad (3)$$

- We note in Eq. (2) that $\sigma_{t,g}$ and $\sigma_{s,gg'}$ become also $\vec{r}$ dependent, even in a homogenized region.

2. HIRE-Theoretic Multigroup Transport Equations

❑ **HIRE theory : On reaction terms in Eq. (2), we perform, over V_m of material region m,**

$$\sigma_{t,g}(\vec{r},\vec{\Omega}) = \frac{\int_{E_g}^{E_{g-1}} dE\sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})}{\int_{E_g}^{E_{g-1}} dE\varphi(\vec{r},E,\vec{\Omega})}, \quad (3)$$

$$\sigma_{t,g}^{m} = \frac{\int_{\vec{r}\in V_m} dV \int d\Omega \int_{E_g}^{E_{g-1}} dE\sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})}{\int_{\vec{r}\in V_m} dV \int d\Omega \int_{E_g}^{E_{g-1}} dE\varphi(\vec{r},E,\vec{\Omega})}, \quad (3a)$$

2. HIRE-Theoretic Multigroup Transport Equations

- **HIRE theory : On reaction terms in Eq. (2), we perform, over V_m of material region m,**

$$\sigma_{t,g}(\vec{r},\vec{\Omega}) = \frac{\int_{E_g}^{E_{g-1}} dE\sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})}{\int_{E_g}^{E_{g-1}} dE\varphi(\vec{r},E,\vec{\Omega})}, \quad (3)$$

$$\sigma_{t,g}^m = \frac{\int_{\vec{r}\in V_m} dV \int d\Omega \int_{E_g}^{E_{g-1}} dE\sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})}{\int_{\vec{r}\in V_m} dV \int d\Omega \int_{E_g}^{E_{g-1}} dE\varphi(\vec{r},E,\vec{\Omega})}, \quad (3a)$$

$$\sigma_{s,gg'}(\vec{r},\vec{\Omega}'\to\vec{\Omega}) = \frac{\int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE'\sigma_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\varphi(\vec{r},E',\vec{\Omega}')}{\int_{E_{g'}}^{E_{g'-1}} dE'\varphi(\vec{r},E',\vec{\Omega}')}, \quad (4)$$

$$\sigma_{s0,gg'}^m = \frac{\int_{\vec{r}\in V_m} dV \int d\Omega \int_{E_g}^{E_{g-1}} dE \int d\Omega' \int_{E_{g'}}^{E_{g'-1}} dE'\sigma_s(\vec{r},E'\to E,\vec{\Omega}'\to\vec{\Omega})\varphi(\vec{r},E',\vec{\Omega}')}{\int_{\vec{r}\in V_m} dV \int d\Omega \int d\Omega' \int_{E_{g'}}^{E_{g'-1}} dE'\varphi(\vec{r},E',\vec{\Omega}')}, \quad (4a)$$

2. HIRE-Theoretic Multigroup Transport Equations

$$\nu\sigma_{f,g'}(\vec{r}) = \frac{\int d\Omega' \int_{E_{g'}}^{E_{g'-1}} dE' \nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')}{\int d\Omega' \int_{E_{g'}}^{E_{g'-1}} dE' \varphi(\vec{r},E',\vec{\Omega}')}. \Rightarrow \tag{5}$$

$$\nu\sigma_{f,g'}^{m} = \frac{\int_{\vec{r}\in V_m} dV \int d\Omega \int d\Omega' \int_{E_{g'}}^{E_{g'-1}} dE' \nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')}{\int_{\vec{r}\in V_m} dV \int d\Omega \int d\Omega' \int_{E_{g'}}^{E_{g'-1}} dE' \varphi(\vec{r},E',\vec{\Omega}')}, \tag{5a}$$

$$\chi_g^m = \frac{\int_{\vec{r}\in V_m} dV \int d\Omega \int_{E_g}^{E_{g-1}} dE \int d\Omega' \sum_{g'=1}^{G} \int_{E_{g'}}^{E_{g'-1}} dE' \chi(E)\nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')}{\int_{\vec{r}\in V_m} dV \int d\Omega \int d\Omega' \sum_{g'=1}^{G} \int_{E_{g'}}^{E_{g'-1}} dE' \nu\sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')}. \tag{6a}$$

- The above multigroup constants are obtained by tallies from the continuous-energy Monte Carlo calculation on a unit problem with albedo boundary condition α.

2. HIRE-Theoretic Multigroup Transport Equations

❑ Multigroup Transport Equations

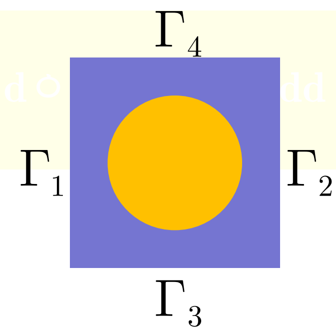
– Eq. (2) becomes, after averaging over each material region and integrating over angle,

$$\frac{1}{V_m}\int_{\partial V_m} dA\vec{n}\cdot\vec{J}(\vec{r})+\sigma_{t,g}^{m}\phi_g^m=\sum_{g'=1}^{G}\sigma_{s0gg'}^{m}\phi_{g'}^{m}+\frac{\chi_g^m}{k_{eff}}\sum_{g'=1}^{G}\nu\sigma_{f,g'}^{m}\phi_{g'}^{m}\ . \qquad (7)$$

where $\vec{J}_g(\vec{r})=\int d\Omega\vec{\Omega}\varphi(\vec{r},\vec{\Omega}),\ \ \phi_g^m=\frac{1}{V_m}\int_{\vec{r}\in V_m} dV\phi_g(\vec{r})\ .$

– Eq. (2) is then recast in the following multigroup equations with cross sections of Eqs. (3a)–(6a):

$$\vec{\Omega}\cdot\nabla\varphi_g(\vec{r},\vec{\Omega})+\sigma_{t,g}^{m}\varphi_g(\vec{r},\vec{\Omega})=\sum_{g'=1}^{G}\sigma_{s0gg'}^{m}\phi_{g'}(\vec{r})+\frac{\chi_g^m}{k_{eff}}\sum_{g'=1}^{G}\nu\sigma_{f,g'}^{m}\phi_{g'}(\vec{r}), \qquad (8)$$



with albedo boundary condition $\varphi_g(\vec{r},\vec{\Omega}')=\alpha_k\varphi_g(\vec{r},\vec{\Omega})\ k=1$ to 4.

- Eq. (8) is the multigroup transport equations, derived in this paper.
- Only σ_{s0} term remains : a byproduct
- Eigenvalue and material region-wise flux distributions, as such obtained with the usual continuity conditions, will show discrepancies compared to those from the continuous-energy calculation. ⇔ PCDF

2. HIRE-Theoretic Multigroup Transport Equations

Partial Current Discontinuity Factor (PCDF)

– To preserve the reference neutron leakages, PCDF is introduced to each outgoing and incoming current with respect to material region surface k (Γ_k, k=1 to 8) as:

$$f_{g,k}^{+}\varphi_g(\vec{r}_k,\vec{\Omega}) \quad \text{for} \quad \vec{\Omega}\cdot\vec{n}_k > 0, \tag{9a}$$

$$f_{g,k}^{-}\varphi_g(\vec{r}_k,\vec{\Omega}) \quad \text{for} \quad \vec{\Omega}\cdot\vec{n}_k < 0, \tag{9b}$$

where $f_{g,k}^{\pm}$ are initially guessed and updated by PCDF iterations.

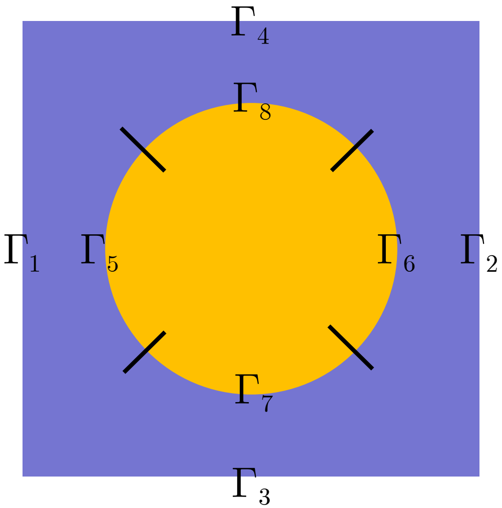


Fig. 1. Surface divisions for PCDFs.

2. HIRE-Theoretic Multigroup Transport Equations

❑ Update of PCDFs

– Partial currents obtained from the multigroup transport solution:

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

$$J_{g,k}^{-} = \int_{\vec{r}\in\Gamma_k} dA \int_{\vec{\Omega}\cdot\vec{n}_k<0} d\Omega \left|\vec{n}_k\cdot\vec{\Omega}\right| \varphi_g(\vec{r},\vec{\Omega}). \quad (10b)$$

– Discontinuity in partial currents:

$$\tilde{J}_{g,k}^{-} = f_{g,k}^{-} J_{g,k}^{-}, \quad (11a)$$

$$\tilde{J}_{g,k}^{+} = f_{g,k}^{+} J_{g,k}^{+}. \quad (11b)$$

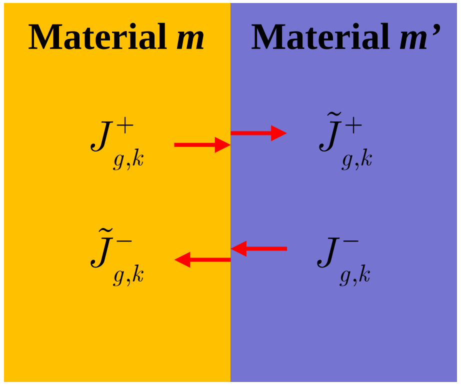


Fig. 2. Leakage corrections based on PCDFs at interface k.

Reference surface net current $J_{g,k}^{ref}$ from the continuous-energy MC calculation

– Conditions on the updated PCDFs:

$$J_{g,k}^{ref} = J_{g,k}^{+} - \tilde{J}_{g,k}^{-} = J_{g,k}^{+} - f_{g,k}^{-} J_{g,k}^{-} \quad \Leftrightarrow \quad f_{g,k}^{-} = \frac{J_{g,k}^{+} - J_{g,k}^{ref}}{J_{g,k}^{-}}, \quad (12a)$$

$$J_{g,k}^{ref} = \tilde{J}_{g,k}^{+} - J_{g,k}^{-} = f_{g,k}^{+} J_{g,k}^{+} - J_{g,k}^{-} \quad \Leftrightarrow \quad f_{g,k}^{+} = \frac{J_{g,k}^{-} + J_{g,k}^{ref}}{J_{g,k}^{+}}. \quad (12b)$$

2. HIRE-Theoretic Multigroup Transport Equations

PCDF Iteration Scheme

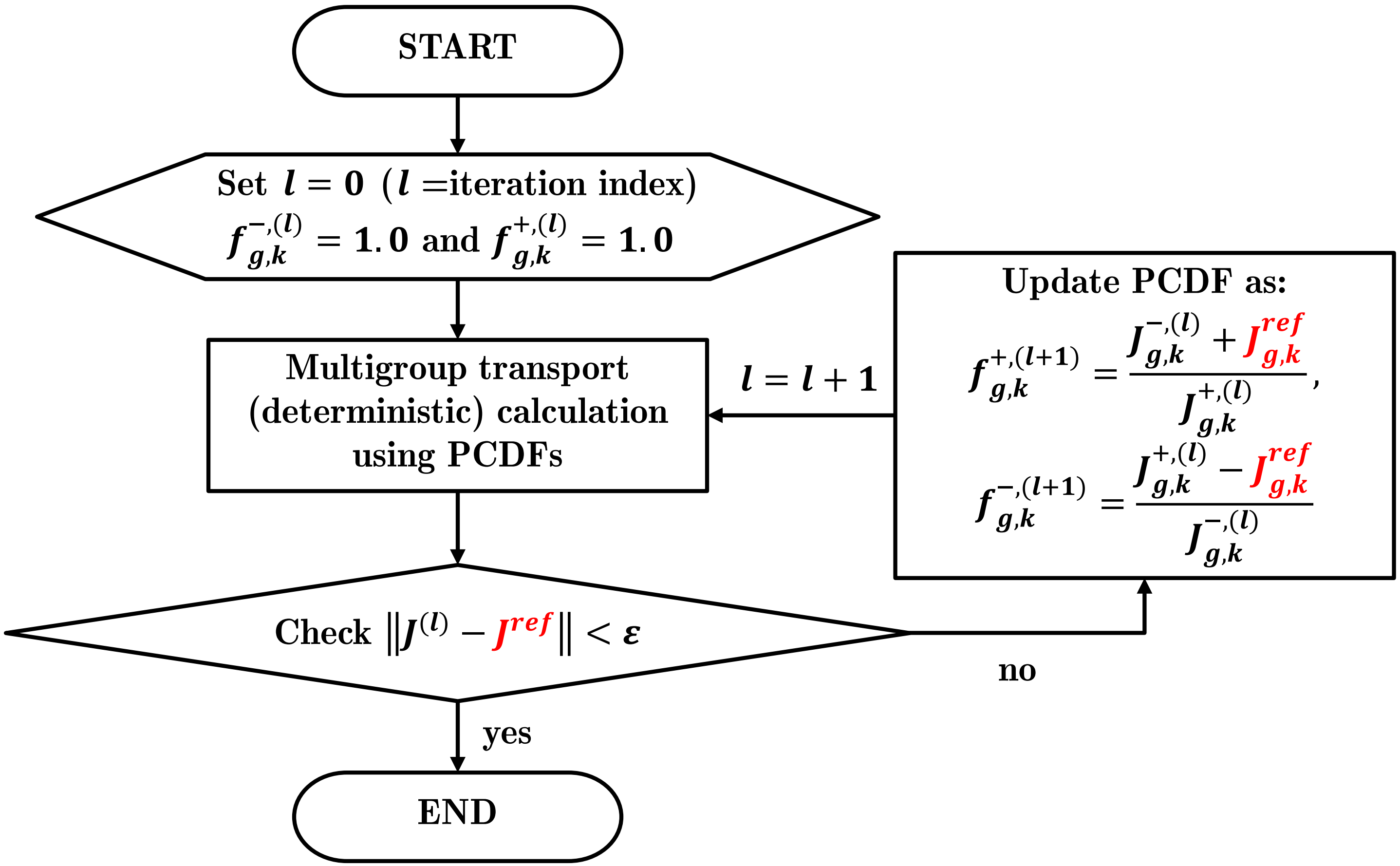


Fig. 3. Flow Chart of PCDF Iteration.

3. New Framework for Reactor Analysis

❑ Spectrum Characteristics of Two Reactor Types

– Spectrum characteristics

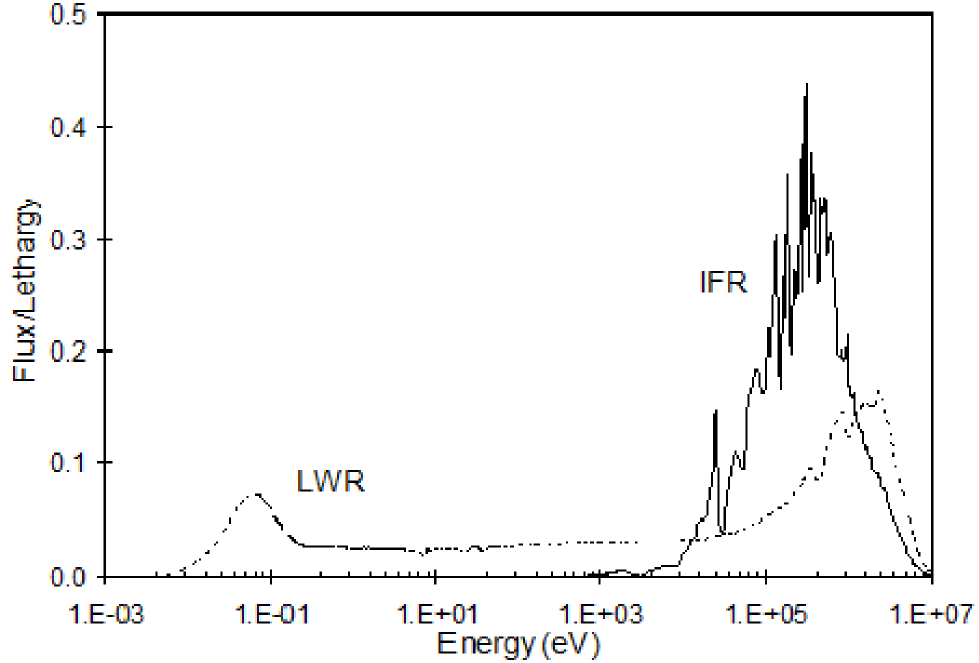


Fig. 4. Comparison of neutron energy spectra.

– Mean free paths

$$\lambda_{LWR} < \lambda_{FNR}$$

3. New Framework for Reactor Analysis

❑ Global/Local Decomposition

– **LWR**

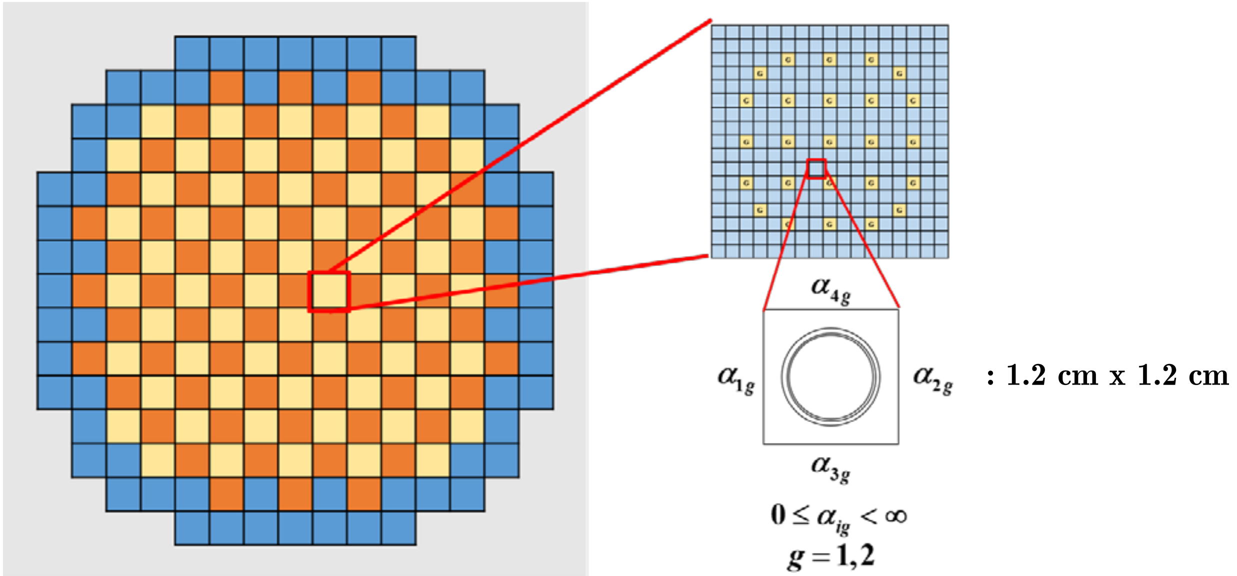


Fig. 5. Unit problem in a light water reactor.

- Local problem : Continuous-energy MC on a square pin-cell (with parameterized albedos)
- Global problem : Two-group

  MOC (2-D), MOC/S_N 2D/1D Fusion (3-D)

  Two-Level p-CMFD acceleration

3. New Framework for Reactor Analysis

– **FNR**

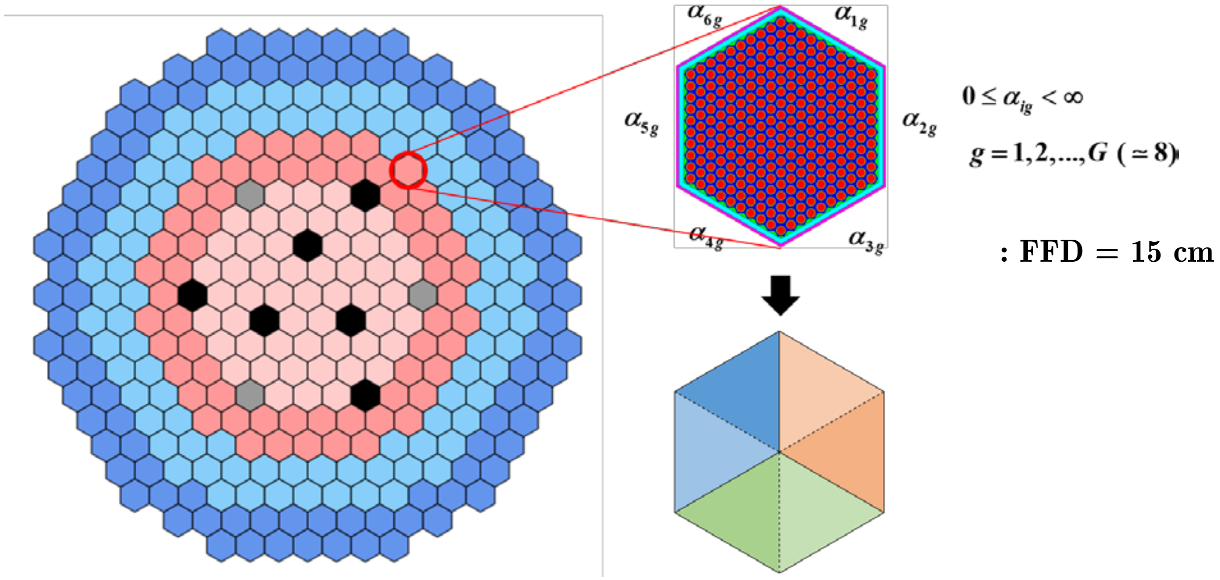


Fig. 6. Unit problem in a fast reactor.

- **Local problem : Continuous-energy MC on a hexagon (with parameterized albedos)**
- **Global problem : Eight (possibly four) - group**

  S_N method (2-D, 3-D) + KBA parallel sweep procedures

  Two-Level p-CMFD acceleration

4. Summary and Concluding Remarks

❑ Summary

- Homogeneity and Isotropy Restoration (HIRE) theory:
  - Provides "multigroup" transport equations with PCDFs
    - ✓ Angle-independent total XS
    - ✓ Material region-wise homogeneous XS (restoration of homogeneity)
    - ✓ In scattering terms, only σ_{s0} term remains in the multigroup transport equations.
  - Partial current discontinuity factors (PCDFs) are introduced to preserve the neutron leakages at material interfaces.

- Global/Local Decomposition Framework
  - Local: Continuous-energy MC: square pin-cell for LWRs
    hexagonal fuel assembly for FNRs
  - Global: HIRE-"multigroup" transport: $G = 2$ for LWRs, $G = 8$ for FNRs

4. Summary and Concluding Remarks

❑ Concluding Remarks

- The volume of integration for material region (V_m) can be chosen as:
  1) A multi-region such as pin-cell homogenization or baffle-reflector homogenization
  2) Resolved regions such as rings in a fuel rod for
     - i) rim effect in depletion
     - ii) fuel temperature feedback effect

- HIRE-multigroup cross sections and PCDFs could be tabulated or functionalized in :
  1) α values (representing the environment)
  2) Burnup
  3) Fuel and moderator temperatures

- The resulting "multigroup" transport equations can be solved by existing numerical methods:
  - MOC, S_N method
  - Sweeping procedures
  - Acceleration methods

5. References

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Thank you!