New Multigroup Transport Equations Derived via Homogeneity and Isotropy Restoration (HIRE) Theory

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1. Introduction (1/3)

- 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.

1. Introduction (2/3)

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

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

- Previous studies on angle-dependency of the group total cross section
  - Removal of angle-dependency
    - Consistent P approximation
    - Extended (BHS) transport approximation: outflow/inflow approximations
  - Angle-dependency is expanded in Legendre functions and retained in LHS.
    - Anisotropic media approach
  - Angle-dependent portion is moved to RHS and expanded in spherical harmonics and added to the scattering term.
    - Generalized energy condensation (GEC) scheme

1. Introduction (3/3)

- **Homogeneity and Isotropy Restoration (HIRE) Theory in this presentation:**
  - **Homogeneity in material region**
  - **Angle-independence in total XS**
  - **Preservation of region-wise reaction rate**

  are achieved in the derivation of multigroup transport equations by the device of partial current discontinuity factor (PCDF).

2. Methodology: Problems of Multigroup XS (1/7)

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

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

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

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

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

2. Methodology: Problems of Multigroup XS (2/7)

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

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

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

- 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. Methodology: HIRE Theory (3/7)

❑ Multigroup Transport Equations

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

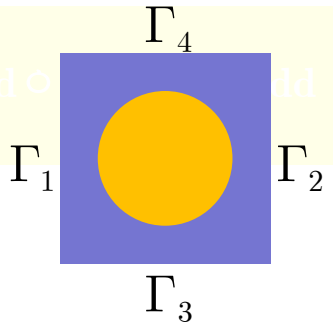
$$\frac{1}{V_m}\int_{\partial V_m} dA\vec{n}\cdot\vec{J}(\vec{r}) + \sigma^m_{t,g}\phi^m_g = \sum_{g'=1}^{G}\sigma^m_{s0gg'}\phi^m_{g'} + \frac{\chi^m_g}{k_{eff}}\sum_{g'=1}^{G}\nu\sigma^m_{f,g'}\phi^m_{g'} \quad , \qquad (7)$$

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

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

$$\vec{\Omega}\cdot\nabla\varphi_g(\vec{r},\vec{\Omega}) + \sigma^m_{t,g}\varphi_g(\vec{r},\vec{\Omega}) = \sum_{g'=1}^{G}\sigma^m_{s0gg'}\phi_{g'}(\vec{r}) + \frac{\chi^m_g}{k_{eff}}\sum_{g'=1}^{G}\nu\sigma^m_{f,g'}\phi_{g'}(\vec{r}) \quad , \qquad (8)$$

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. Methodology: HIRE Theory (4/7)

❑ 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 $f^{\pm}_{g,k}$ are initially guessed and updated by PCDF iterations.

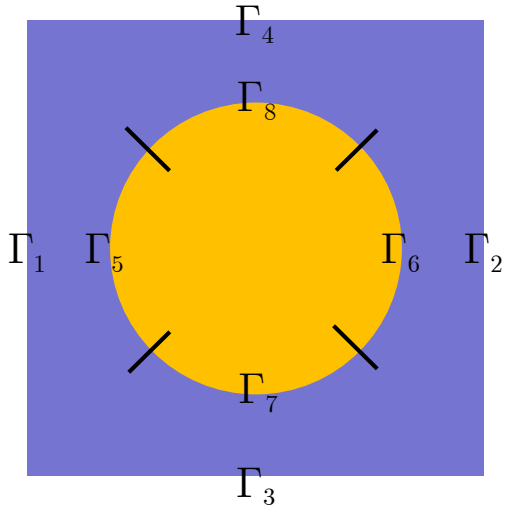


Fig. 1. Surface divisions for PCDFs.

2. Methodology: HIRE Theory (5/7)

❑ 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:

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

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

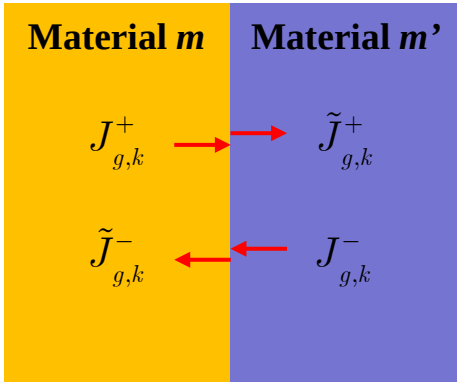


Fig. 2. Leakage corrections based on PCDFs at interface *k*.

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. Methodology: HIRE Theory (6/7)

❑ PCDF iteration scheme

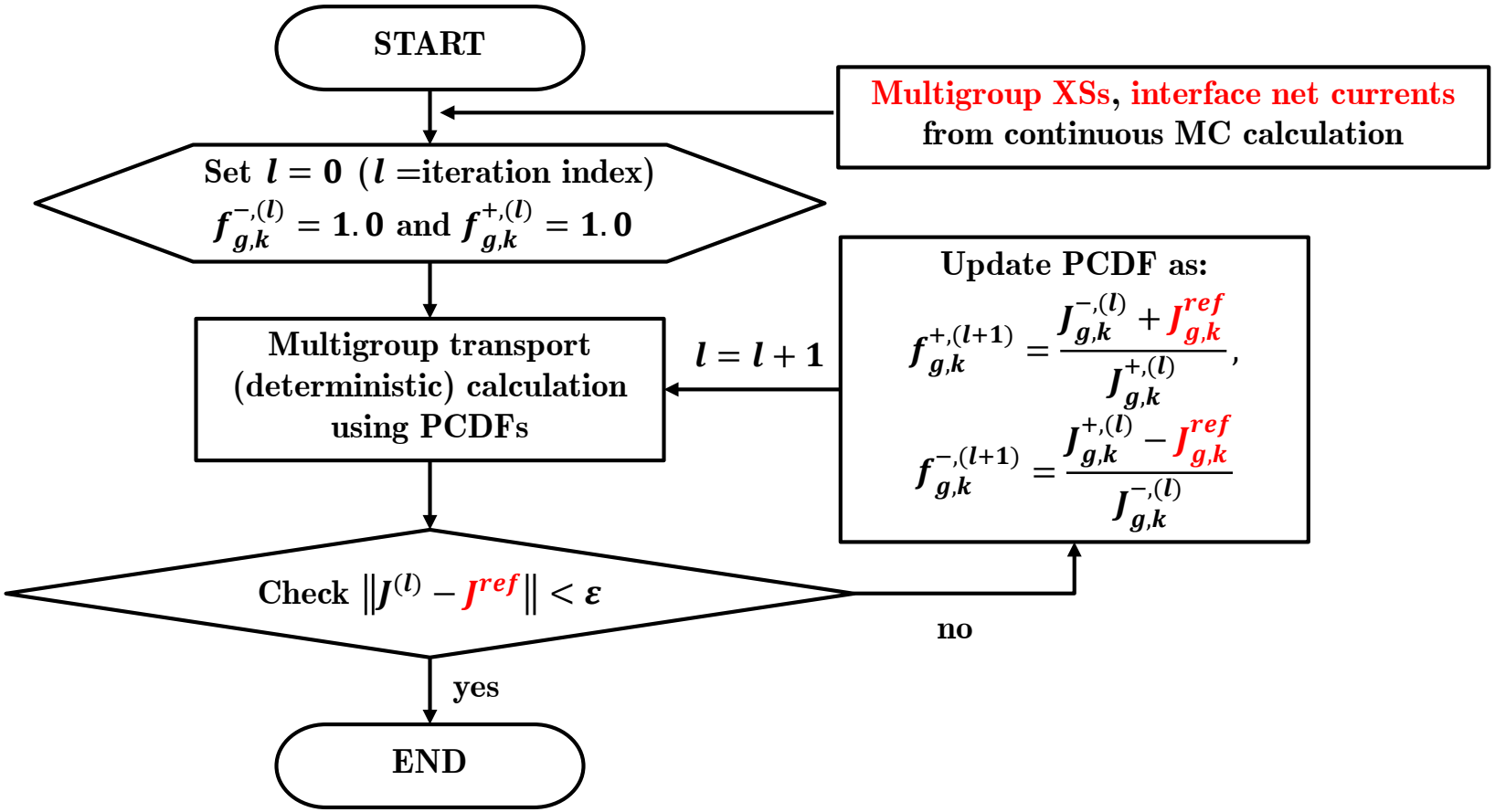


Fig. 3. Flow Chart of PCDF Iteration.

2. Methodology: HIRE Theory (7/7)

❑ JFNK Method with Exponential Transformation

1) $\vec{F}(\vec{f}) = \left(F^{\pm}_{g,k}(\vec{f})\right)_{g=1..G,\,k=1..8} = 0,$

where

$$F^{\pm}_{g,k}(\vec{f}) = \frac{J^{\mp}_{g,k}(\vec{f}) + J^{ref}_{g,k}}{J^{\pm}_{g,k}(\vec{f})} - f^{\pm}_{g,k},$$

$$\vec{f} = \left(f^{\pm}_{g,k}\right)_{g=1..G,\,k=1..8}.$$

2) Since $\vec{f} > 0,$

$$\vec{G}(\vec{x}) \equiv \vec{F}(\exp(\vec{x})) = 0.$$

Then, the PCDFs become $\exp(\vec{x})$.

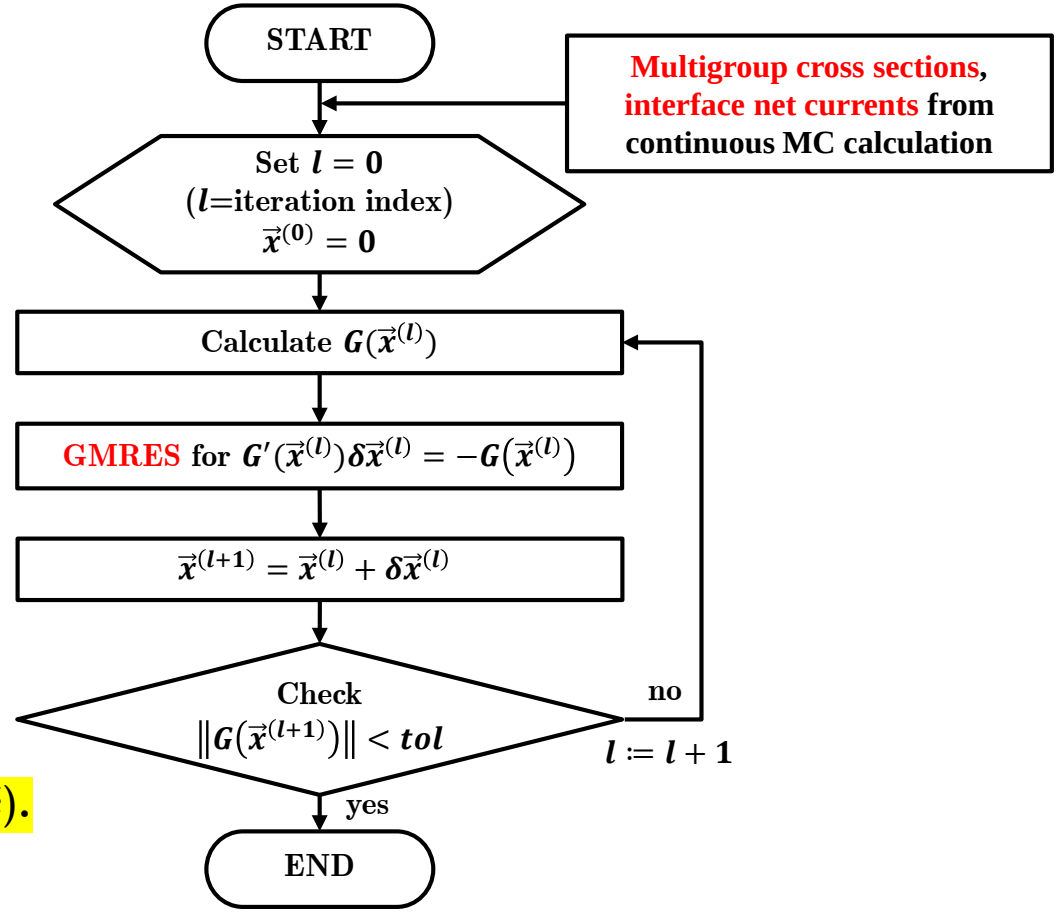


Fig. 4. PCDF Iteration with the JFNK method.

3. Numerical Results (1/11)

❑ Pin Specifications

- Pin pitch = 1.26 cm
- Fuel radius = 0.4095 cm
- UO_2: 10.2 g/cc with U-235 enrichment 3.3 w/o
- Moderator: 800 ppm boron concentration
- Divisions of surfaces for application of PCDFs

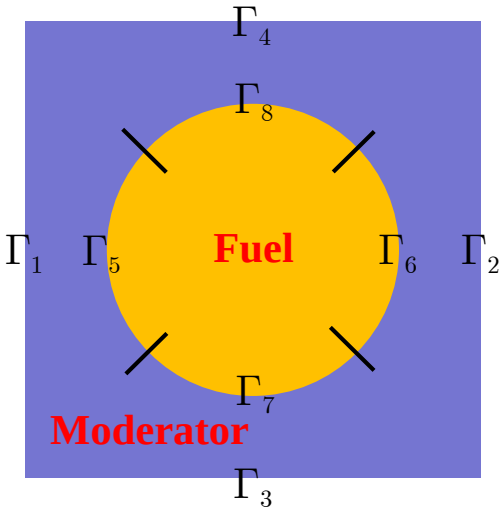


Fig. 5. 2-D UO_2 Pin Geometry.

❑ Test of HIRE theory with PCDF iteration

Step 1. Continuous-energy MC calculations

Step 2. Generation of region-averaged multigroup XS and net currents on region interfaces

Step 3. PCDF iteration with multigroup method of characteristics (MOC) calculation

3. Numerical Results (2/11)

❑ Test Problems

- Test Problem 1: One pin-cell problem (reflective BC)
- Test Problem 2: One pin-cell problem (albedo BC)
- Test Problem 3: 2 × 2 pin-cell problem (3 fuel pins and 1 moderator) (reflective BC)
- Test Problem 4: 4 × 4 pin-cell problem (fuel and baffle) (albedo BC)
- Test Problem 5: One pin-cell problem (rim effect in depletion)

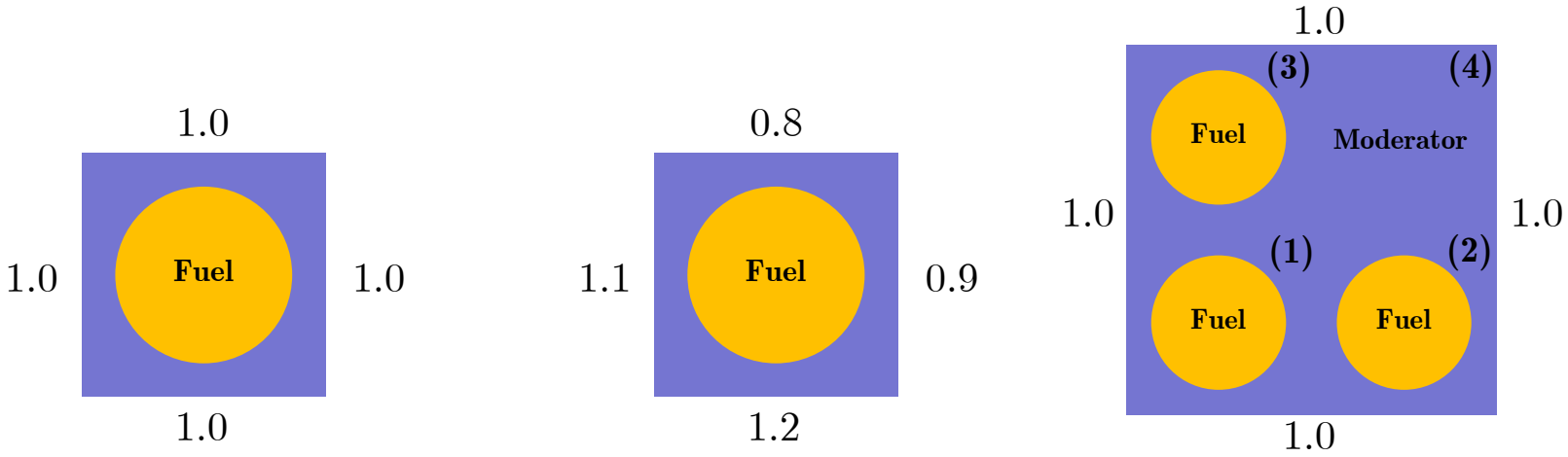


Fig. 6. Geometry of Test Problems 1~3
(#.# are albedo values at surfaces).

3. Numerical Results (3/11)

❑ Calculational Conditions

– **Continuous-energy Monte Carlo calculation: McBOX**

- **No. of inactive cycles: 100**
- **No. of active cycles: 200**
- **No. of histories per cycles: 5,000,000**
- **Energy group boundary: 0.625 eV**

– **Two-group MOC calculation : CRX3**

- **Mesh division: 4 rings with 8 sectors in a pin cell**
- **Angular mesh: 8 azimuthal/3 polar angles per quadrant**
- **No. of rays per cell per angle: 50**
- **Stopping criteria: 1.0e-7 for fission source and k_{eff}**

– **PCDF iteration**

- **Stopping criterion: 1.0e-7 for surface net current**

3. Numerical Results (4/11)

❑ Numerical Results: Two-Group Cross Sections

Table I. Two-group cross sections [cm^{-1}] for test problem 2

Region	Group	σ_t	$\nu\sigma_t$	$\sigma_{s0,*\rightarrow1}$	$\sigma_{s0,*\rightarrow2}$
Fuel	1	4.0702E-01	2.3291E-02	3.7740E-01	6.7072E-04
	2	7.6754E-01	6.9308E-01	4.0395E-04	3.9355E-01
Moderator	1	8.7733E-01	0.0000E+00	8.3570E-01	4.0810E-02
	2	1.9473E+00	0.0000E+00	4.6988E-04	1.9066E+00

- **Group cross sections in Test Problem 1 and 3 are slightly different from those in Table I, even for the same material, due to the differing leakages.**

3. Numerical Results (5/11)

❑ Numerical Results: PCDFs

Table II. PCDFs for test problem 2

Group	f_1^-	f_2^-	f_3^-	f_4^-
1	0.99904	0.99768	0.99511	0.99184
2	0.99773	0.99808	0.99270	0.99015
Group	f_5^+	f_6^+	f_7^+	f_8^+
1	1.00576	1.00521	1.00606	1.00550
2	0.99630	0.99653	0.99405	0.99696
Group	f_5^-	f_6^-	f_7^-	f_8^-
1	0.99432	0.99388	0.99449	0.99288
2	1.00253	1.00289	1.00370	1.00282

– **PCDF are not symmetric, because of the boundary conditions.**

3. Numerical Results (6/11)

❑ Numerical Results: Multiplication Factor

Table III. Multiplication factor from PCDF iteration

Problem	k_{eff}^{ref}	k_{eff}^{HIRE}	Δk_{eff} (pcm)	Number of fixed-point iterations /MOC calculations	Number of JFNK iterations /MOC calculations
1	1.283819 (±2.6 pcm)*	1.283823	0.4	987/988	2/23
2	1.125992 (±2.6 pcm)*	1.125990	-0.2	825/826	4/60
3	1.199928 (±2.8 pcm)*	1.199925	-0.3	847/848	4/124

* Standard deviation of the reference MC calculation.

- **Note that the multiplication factors of the PCDF iteration converge to those in the reference calculations for all three test problems.**

3. Numerical Results (7/11)

❑ Numerical Results: Flux Error

Table IV. Maximum relative error in region-averaged flux

Problem	Group 1 (%)	Std.* of Group 1 (%)	Group 2 (%)	Std.* of Group 2 (%)
1	2.64E-05	1.25E-03	1.33E-04	2.84E-03
2	7.63E-05	2.03E-03	1.07E-03	4.46E-03
3	5.82E-02	4.59E-03	1.63E-03	4.60E-03

*Std.: standard deviation of the region-averaged flux in the reference MC calculation

- **Three test problems have maximum errors of less than 0.06%.**
  - **Hence, the converged PCDFs give accurate region-averaged fluxes in the multigroup transport calculation.**
- **Tables III and IV reveal that the HIRE theory generates group constants (cross sections and PCDFs) that can reproduce the multiplication factor and region-averaged reaction rates of the continuous-energy MC transport calculation.**

3. Numerical Results (8/11)

- **Test Problem 5: Sub-pin level depletion (rim effect) (via MC code McBOX)**
  - **10 equally spaced concentric rings in fuel region**
  - **Continuous-energy nuclear data library : ENDF/B-VII.0 at 600K**
  - **Decay constant and yield data : ORIGEN2 library**
  - **Matrix exponential calculation : Chebyshev rational approximation method (CRAM)**
  - **Power : 100 kW (520 full power days)**

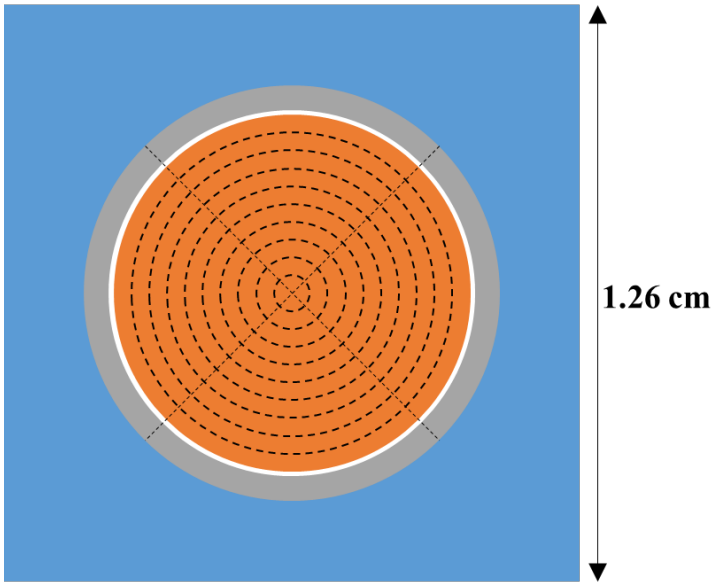


Fig. 7. UO2 pin-cell problem; axial length with 100 cm (all reflective boundary conditions)

Table V. Materials and radii of concentric rings

Material Region Index	Radii of Concentric Rings [cm]	Material
1	0.03922	UO_2
2	0.07844	UO_2
3	0.11765	UO_2
4	0.15687	UO_2
5	0.19609	UO_2
6	0.23531	UO_2
7	0.27453	UO_2
8	0.31374	UO_2
9	0.35296	UO_2
10	0.39218	UO_2
11	0.40005	Helium
12	0.45720	Cladding
13	-	Moderator

3. Numerical Results (9/11)

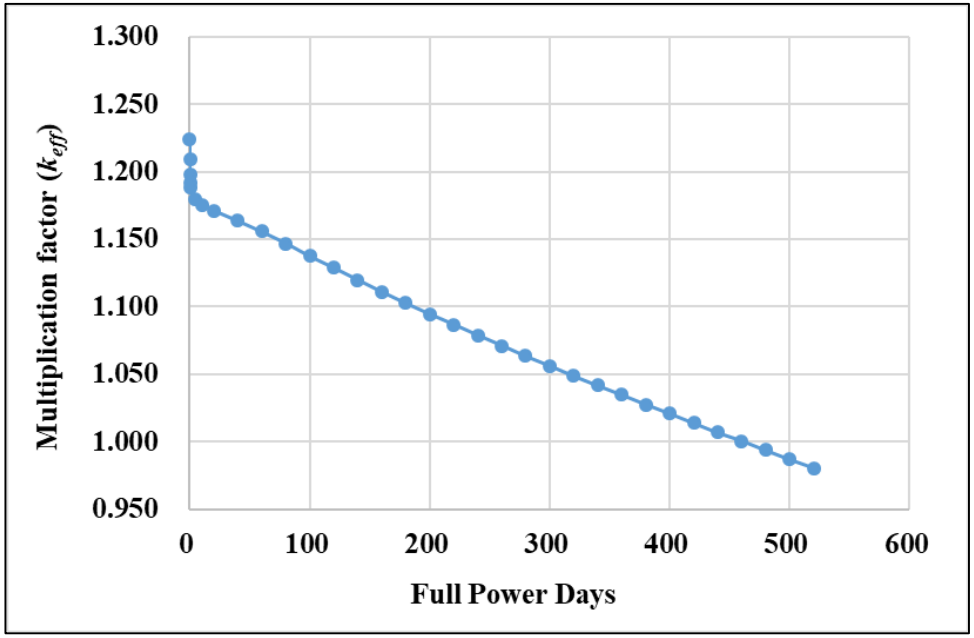


Fig. 8. Multiplication factors versus full power days.

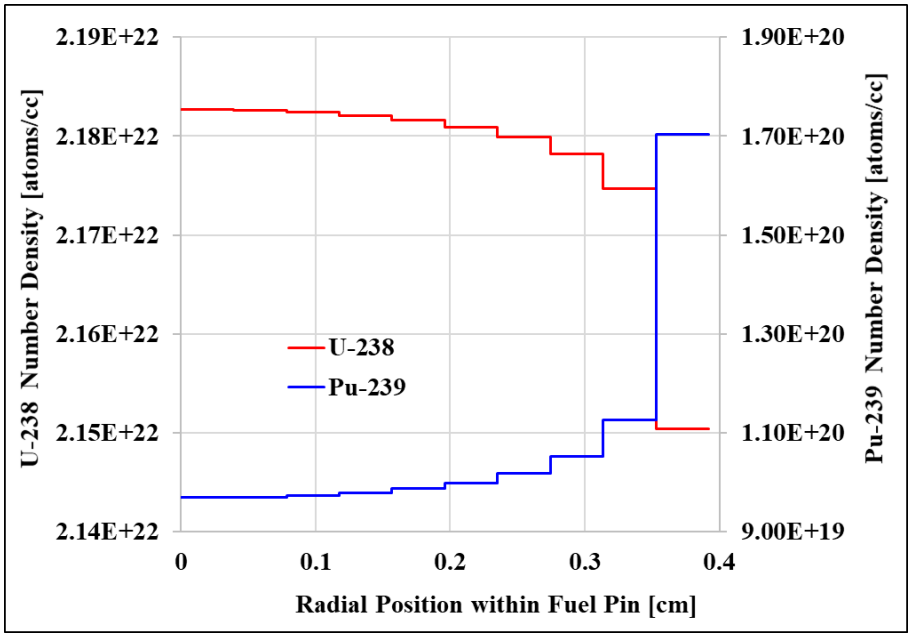


Fig. 9. Number densities of U-238 (left y-axis) and Pu-239 (right y-axis) versus radial position within the fuel pin at 520 full power days.

– The rim effect is observed in a high burnup UO_2 fuel (at 520 full power days).

3. Numerical Results (10/11)

- **Application of two-group HIRE theory to high burnup UO_2 fuel pin**
  - Continuous-energy MC simulation (McBOX) to tally two-group cross sections (collision estimator) and surface net currents (surface-crossing estimator)
    - No. of inactive cycles : 50
    - No. of active cycles : 200
    - No. of histories per cycles : 5,000,000
    - Energy group boundary : 1 eV
  - Two-group MOC calculation for PCDF iteration (multigroup MOC code CRX3)
    - Mesh division : 13 rings with 8 azimuthal sectors in a pin cell
    - Angular mesh : 8 azimuthal/3 polar angles per quadrant
    - No. of ray per cell per angle: 150
    - Stopping criteria : 1.0e-8 for fission source and k_{eff}
    - Stopping criterion for PCDF iteration : 1.0e-6 for surface net current

Table VI. Multiplication factor from PCDF iteration with JFNK method

k_{eff}^{MC}	k_{eff}^{MOC}	Δk_{eff} (pcm)	Number of PCDF iterations	Number of MOC calculations	Computing times for PCDF iterations
0.980556 (2.2 pcm)*	0.980552	-0.434 pcm	3	146	8.42 sec**

*Standard deviation of the continuous-energy MC simulation
**Intel® Core™ i7-7700K processor

3. Numerical Results (11/11)

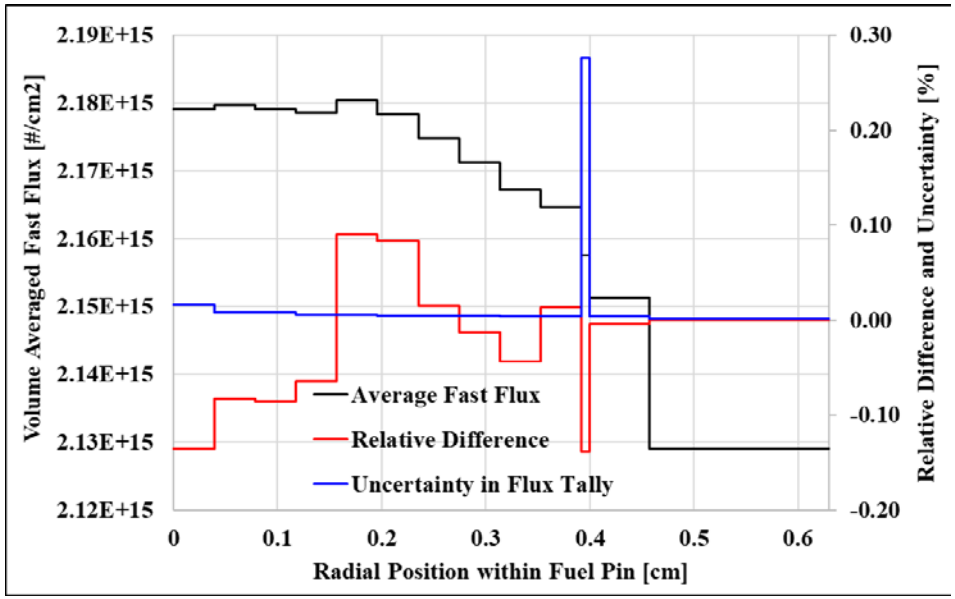


Fig. 10. Region-wise volume averaged fast scalar flux distributions (left axis), their relative difference distributions (right axis), and uncertainty distributions in fast flux(right axis).

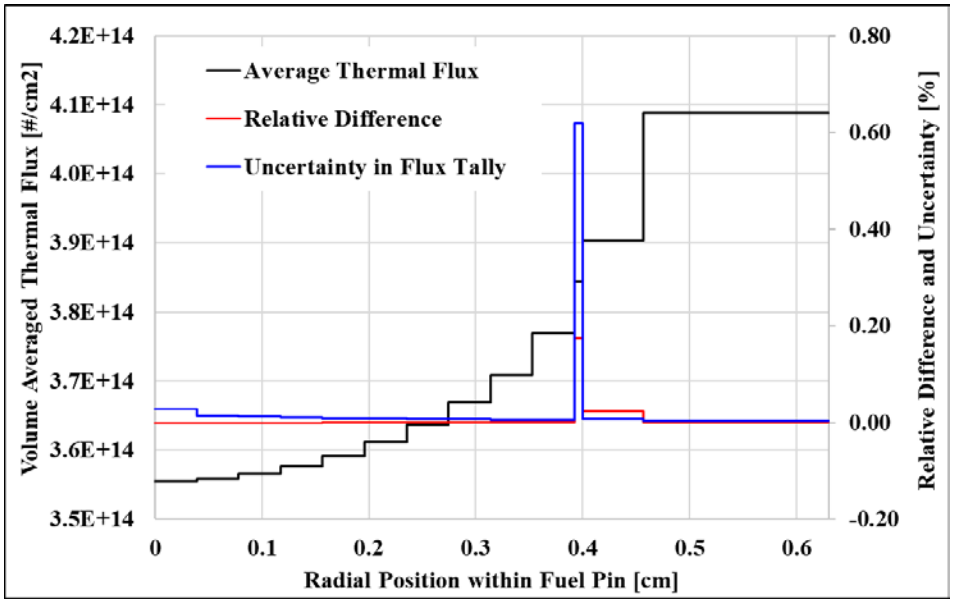


Fig. 11. Region-wise volume averaged thermal scalar flux distributions (left axis), their relative difference distributions (right axis), and uncertainty distributions in thermal flux (right axis).

- Relative differences in flux distributions less than 0.2%.
- Uncertainty errors in HIRE-theoretic group constants (cross sections and net currents)
  - Small fast net current (near to zero) at the innermost region
  - Inefficient collision estimator at helium gap

4. Summary and Concluding Remarks (1/2)

❑ Summary

– **Homogeneity and Isotropy Restoration (HIRE) theory:**

- **Provides multigroup transport equations with**
  - ✓ **Material region-wise homogeneous XS (restoration of homogeneity)**
  - ✓ **Angle-independent total XS (restoration of isotropy)**
  - ✓ **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.**

– **For the test problems, HIRE theory with PCDF iteration via JFNK gives accurate results very fast, compared to the MC reference values:**

- **Multiplication factor with errors < 1 pcm.**
- **Region-averaged flux with errors $< 0.07\%$.**

4. Summary and Concluding Remarks (2/2)

❑ Concluding Remarks

– The volume of integration for material region can be chosen:

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

4. Summary and Concluding Remarks (2/2)

❑ Concluding Remarks

- The volume of integration for material region can be chosen:
  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

- Multigroup cross sections and PCDFs could be tabulated or functionalized in :
  i) α values
  ii) Burnup
  iii) Fuel and moderator temperatures

4. Summary and Concluding Remarks (2/2)

❑ Concluding Remarks

- The volume of integration for material region can be chosen:
  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

- Multigroup cross sections and PCDFs could be tabulated or functionalized in :
  i) α values
  ii) Burnup
  iii) Fuel and moderator temperatures

- Need a study for "representativeness" of a unit problem, depending on the reactor types: a square pin cell, a super-hexagon of fuel assemblies
- …….. for the choice of few-group G (2 – 10)), depending on the reactor types.
- The few-group HIRE equations can be solved efficiently in Two-Level p-CMFD acceleration framework.

5. References

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Thank you!