Implementation of Iterative Resonance Integral Table (i-RIT), Subgroup Methods in STREAM for High Temperature Reactor Analysis

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Chang Keun Jo
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As one of the generation four nuclear reaction designs, a very high temperature gas-cooled reactor (VHTR) has been in the spotlight with its high safety feature.

For VHTR compact problem, iterative Resonance Integral Table (i-RIT) method has been implemented in STREAM.

For VHTR compact problem, subgroup method has been implemented in STREAM.

The two methods have been tested in STREAM with a newly generated STREAM 190G and 220G libraries.
Methodology

- **i-RIT(b) method**

\[
\Omega \cdot \nabla \psi + \left( \Sigma_a + \lambda \Sigma_p \right) \psi = \frac{1}{4\pi} \lambda \Sigma_p
\]

1. Initial guess
2. Solve MOC
3. Get RI from library
4. Obtain effective \( \Sigma_a \)
5. Update \( \Sigma_a \)
6. Iteration until \( \Sigma_a \) converges

\[
\sigma_{b}^{MOC} = \frac{1}{N_r} \cdot \frac{\Sigma_a \phi}{(1 - \phi)}
\]

\[
\Sigma_a = \sum_{r \in R} N_r \sigma_a^r
\]

\[
\sigma_a^r = \frac{RI(\sigma_{b}^{MOC})/\Delta u}{1 - (RI(\sigma_{b}^{MOC})/\Delta u)/\sigma_{b}^{MOC}}
\]
Methodology

- i-RIT(a) method
  - Method of equivalence XS tabulation

\[
\begin{align*}
\Sigma_{b,c,g}^{MOC} (\sigma_{a,c,r,g,m}) &= \sum_{i} \lambda \Sigma_{p}^{i} + \Sigma_{eq,c,g} (\sigma_{a,c,r,g,m}) \\
\Sigma_{eq,c,g} (\sigma_{a,c,r,g,m}) &= \Sigma_{b,c,g}^{MOC} (\sigma_{a,c,r,g,m}) - \sum_{i} \lambda \Sigma_{p}^{i}
\end{align*}
\]

1. Initial guess
2. Update \( \sigma_{a,k,g}^{(l)} \)
3. Update \( \sigma_{k,g}^{*(l)} \)
4. Update \( \Sigma_{eq,k,g}^{(l+1)} \)
5. Update \( \sigma_{b,k,g}^{(l+1)} \)
6. Iteration until \( \sigma_{b,k,g} \) converges

\[
\mathcal{G}_{eq,c,g} (\sigma_{k,g}^{*(l)}) = G_{eq,c,g} \left( \sigma_{k,g}^{*(l)} \right)
\]

\[
\sigma_{a,k,g}^{(l)} = \frac{R_{a} (\sigma_{b,k,g}^{(l)})}{1 - \frac{R_{a} (\sigma_{b,k,g}^{(l)})}{\sigma_{b,k,g}^{(l)}}}
\]

\[
\sigma_{k,g}^{*(l)} = \frac{R_{a,c,r,g} (\sigma_{a,k,g}^{(l)})}{R_{a,c,r,g,k}}
\]
Methodology

- **Subgroup method**

\[ \phi_k = \frac{\sum_i \lambda_i N_i \sigma_p^i + \Sigma_e}{N_r \sigma_{ak} + \sum_i \lambda_i N_i \sigma_p^i + \Sigma_e} = \frac{\sigma_b}{\sigma_{ak} + \sigma_b} \]

where
\[ \sigma_b = \frac{1}{N_r} \left( \sum_i \lambda_i N_i \sigma_p^i + \Sigma_e \right) \]

\[ \sigma_{bk} = \frac{\sigma_{ak} \phi_k}{(1 - \phi_k)} \]

\[ \sigma_{a,eff} = \frac{\sum_{k=1}^{n} \omega_k \sigma_{ak} \frac{\sigma_{bk}}{\sigma_{ak} + \sigma_{bk}}}{\sum_{k=1}^{n} \omega_k \frac{\sigma_{bk}}{\sigma_{ak} + \sigma_{bk}}} \]

- **Subgroup Parameter Generation in STREAM**
  - Generated in homogeneous 0-D problem
  - Using NJOY code
Problem Description

- **VHTR homogenized compact problem**
  - **Fuel:** UO\(_2\) + Graphite
  - **Moderator:** Graphite
  - **Packing fraction:** 1 ~ 60\% (Total 40 cases)

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<th>Geometry</th>
<th>Radius or Pitch [cm]</th>
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<td>0.6225 (Radius)</td>
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Verification of STREAM Solver Module

Using the same DeCART 190G library

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<th>STREAM (i-RIT(a))</th>
<th>STREAM (Subgroup)</th>
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*MCS solutions have 15~25 pcm of standard deviations
Verification of STREAM Solver Module

- Using the same DeCART 190G library
  - Well-matched between STREAM and DeCART solutions
C-Based 190G STREAM Library Production

- **NJOY 99.364**
  - RECONR: Getting ENDF resonance parameters, and processing XSs in resolved resonance region for some nuclides
  - BROADR: Processing Doppler broadening
  - UNRESR: Processing XSs in unresolved resonance region
  - HEATR: Processing heating XSs and radiation damage XSs
  - THERMR: Processing $S(\alpha,\beta)$ XSs
  - GROUPR: Collasing multi-group XSs from point-wise XSs

- **Post-processing of NJOY output**
  - Merging outputs of each nuclide and generating a multi-group data file

- **RUP, IR parameter**
  - 190G RUP and IR parameters
C-Based 190G Spectrum Correction

- Spectrum Difference between H-based and C-based Problems

![Neutron Spectrum Graph](image-url)
Subgroup Parameter Generation

- 19 background XSs for $^{235}$U and $^{238}$U in STREAM
Subgroup Parameter Generation

- **NJOY-generating Effective XSk**
  - Representing resonance integrals (RIs)
  - Total 56 sets of effective cross sections for each resonance energy group
    - 2 nuclides: $^{235}\text{U}$, $^{238}\text{U}$
    - 2 reactions: Capture, Fission
    - 7 temperatures: 293.6 K, 600 K, 900 K, 1200 K, 1500 K, 1800 K, 2100 K
    - 2 multi-group libraries: 190G, 220G
Subgroup Parameter Generation

- **NJOY-generating Effective XSs**

U-238 Capture at $T = 293.6$ K

![Graph showing effective XSs for U-238 capture](image)
### Determination of Subgroup Level

1. Get continuous energy XS for the resonance energy groups
2. Get the minimum and the maximum XSs in the given energy group
3. Get a difference between the minimum and the maximum
4. Divide the difference into \( N+1 \) in linear scale
5. Generation \( N \) subgroup levels with the same logarithm interval

\[
\sigma_{a,\text{min}}^{sg \subset g} = \sigma_{a,\text{min}}^{sg \subset g} \cdot e^{\frac{n}{N+1} \left(\log\left(\sigma_{a,\text{max}}^{sg \subset g}\right) - \log\left(\sigma_{a,\text{min}}^{sg \subset g}\right)\right)}
\]

in logarithm scale, where \( 1 \leq n \leq N \) and \( N = 7 \)
Subgroup Parameter Generation

**Subgroup Weight Generation**

\[
\sigma_{ak,\text{eff}} \overset{\infty}{=} \frac{\sum_{n=1}^{7} \left( \omega_n \cdot \sigma_{an} \cdot \frac{\sigma_{bk}}{\sigma_{an} + \sigma_{bk}} \right)}{1 - \sum_{n=1}^{7} \left( \omega_n \cdot \frac{\sigma_{an}}{\sigma_{an} + \sigma_{bk}} \right)} 
\]

where \( 1 \leq k \leq 19 \)

\[
\left[ \sigma_{ak,\text{eff}} - \sum_{n=1}^{7} \left( \omega_n \cdot \sigma_{an} \cdot \frac{\sigma_{ak,\text{eff}} + \sigma_{bk}}{\sigma_{an} + \sigma_{bk}} \right) \right]^2 \approx 0 \quad \text{and} \quad \sum_{n=1}^{7} \omega_n \approx 1
\]

\[
\sigma_{a1,\text{eff}} \cdot \frac{\sigma_{a1,\text{eff}} + \sigma_{b1}}{\sigma_{a1} + \sigma_{b1}} \quad \sigma_{a7,\text{eff}} \cdot \frac{\sigma_{a7,\text{eff}} + \sigma_{b1}}{\sigma_{a7} + \sigma_{b1}}
\]

\[
\sigma_{a1,\text{eff}} \cdot \frac{\sigma_{a1,\text{eff}} + \sigma_{b19}}{\sigma_{a1} + \sigma_{b19}} \quad \sigma_{a7,\text{eff}} \cdot \frac{\sigma_{a19,\text{eff}} + \sigma_{b19}}{\sigma_{a7} + \sigma_{b19}}
\]

\[
\begin{bmatrix}
\sigma_{a1,\text{eff}} \\
\sigma_{a2,\text{eff}} \\
\sigma_{a18,\text{eff}} \\
\sigma_{a19,\text{eff}}
\end{bmatrix}
= \begin{bmatrix}
\omega_1 \\
\omega_M \\
\omega_M \\
\omega_M
\end{bmatrix}
\]

\[
\begin{bmatrix}
\sigma_{a1,\text{eff}} \\
\sigma_{a2,\text{eff}} \\
\sigma_{a18,\text{eff}} \\
\sigma_{a19,\text{eff}}
\end{bmatrix}
= \begin{bmatrix}
19 \times 7 \\
7 \times 1 \\
19 \times 1
\end{bmatrix}
\]
Subgroup Parameter Generation

- Subgroup Weight Generation

\[ A^T A W = A^T \Sigma \]

\[
\begin{align*}
\sum_{k=1}^{19} \left( \sigma_{a_1} \cdot \frac{\sigma_{ak,eff} + \sigma_{bk}}{\sigma_{a_1} + \sigma_{bk}} \right)^2 & \quad \text{M} \\
\sum_{k=1}^{19} \left( \sigma_{a_1} \cdot \sigma_{a_7} \cdot \frac{\left( \sigma_{ak,eff} + \sigma_{bk} \right)^2}{\left( \sigma_{a_1} + \sigma_{bk} \right)\left( \sigma_{a_7} + \sigma_{bk} \right)} \right) & \quad \text{K} \\
\sum_{k=1}^{19} \left( \sigma_{a_7} \cdot \sigma_{a_1} \cdot \frac{\left( \sigma_{ak,eff} + \sigma_{bk} \right)^2}{\left( \sigma_{a_7} + \sigma_{bk} \right)\left( \sigma_{a_1} + \sigma_{bk} \right)} \right) & \quad \text{L} \\
\sum_{k=1}^{19} \left( \sigma_{a_7} \cdot \sigma_{ak,eff} + \frac{\sigma_{bk}}{\sigma_{a_7} + \sigma_{bk}} \right)^2 & \quad \text{M} \\
\sum_{k=1}^{19} \left( \sigma_{a_7} \cdot \sigma_{ak,eff} + \frac{\sigma_{bk}}{\sigma_{a_7} + \sigma_{bk}} \right) & \quad \text{M} \\
\sum_{k=1}^{19} \left( \sigma_{a_7} \cdot \sigma_{ak,eff} + \frac{\sigma_{bk}}{\sigma_{a_7} + \sigma_{bk}} \right) & \quad \text{M}
\end{align*}
\]

\[ \begin{bmatrix}
\omega_1 \\
\omega_2 \\
\omega_7
\end{bmatrix} \]

\[ \sigma_{a_1} \sum_{k=1}^{19} \left( \sigma_{ak,eff} \cdot \frac{\sigma_{ak,eff} + \sigma_{bk}}{\sigma_{a_1} + \sigma_{bk}} \right) \]

\[ \sigma_{a_7} \sum_{k=1}^{19} \left( \sigma_{ak,eff} \cdot \frac{\sigma_{ak,eff} + \sigma_{bk}}{\sigma_{a_7} + \sigma_{bk}} \right) \]

\[ \sigma_{a_7} \sum_{k=1}^{19} \left( \sigma_{ak,eff} \cdot \frac{\sigma_{ak,eff} + \sigma_{bk}}{\sigma_{a_7} + \sigma_{bk}} \right) \]}
Subgroup Parameter Generation

- **Subgroup Weight Generation**
  - MATLAB algorithm

\[ \omega_n^{(0)} \text{ initialization} \]

**Start loop** \((i)\)

\[
A^T A W^{(i)} = A^T \lambda^{(i)} \sum \quad \text{where} \quad \lambda^{(i)} = \sum_{n=1}^{N} \omega_n^{(i)}
\]

Least square fitting using \textit{fminsearch} function

\[
W^{(i+1)} = W^{(i)} \div \text{sum}(W^{(i)})
\]

\[
\lambda^{(i+1)} = \sum_{n=1}^{N} \omega_n^{(i+1)}
\]

\[
\sum_{n=1}^{N} \left( \omega_n^{(i+1)} - \omega_n^{(i)} \right)^2 < \text{eps} \quad \Rightarrow \quad \text{break}
\]

**End loop** \((i)\)
\[ \text{Sum}(wgt \times \text{sign} \times \phi) / \text{sum}(wgt \times \phi) - \text{siga(effective)} \]

- **Error Check : 190G Subgroup Weight**

![Graph of U-238 Capture at T = 293.6 K](image-url)
### Numerical Results

- **Using a new STREAM 190G library**

<table>
<thead>
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<th>Packing Fraction [%]</th>
<th>*MCS reference</th>
<th>STREAM (i-RIT(b))</th>
<th>STREAM (Subgroup)</th>
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*MCS solutions have 15~25 pcm of standard deviations*
Numerical Results

- Using a new STREAM 190G library

![Graph showing keff error vs. packing fraction]

- STREAM(i-RIT(b))
- STREAM(subgroup)
Numerical Results

- Using a new STREAM 220G library

190G → 220G

6.476 ~ 6.868 eV : 10 divisions (0.04 eV interval)
19.947 ~ 22.603 eV : 22 divisions (0.12 eV interval)
### Numerical Results

**Using a new STREAM 220G library**

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*MCS solutions have 15~25 pcm of standard deviations*
Numerical Results

- Using a new STREAM 220G library
Conclusions

- i-RIT and subgroup methods were implemented in STREAM and they were verified with the DeCART library.

- For a newly generated 190G STREAM library, both methods showed large keff errors compared to MCS reference keffs.

- For a newly generated 220G STREAM library slicing into resonance peaks, both methods showed improved accuracy.

- Especially, the subgroup method showed very high accuracy with keff errors below 300 pcm.
Future Plan

- Subgroup methods will be tested in STREAM with STREAM’s 72G PWR library.

- Two-term expansion (flux-sigb relation) of the subgroup method will be implemented in STREAM to get higher accuracy.

\[
\phi_k = \frac{\sum_i \lambda_i N_i \sigma_p^i + \Sigma^k}{N_r \sigma_{ak} + \sum_i \lambda_i N_i \sigma_p^i + \Sigma^k} = \frac{\sigma_b}{\sigma_{ak} + \sigma_b}, \quad \text{where} \quad \sigma_b = \frac{1}{N_r} \left( \sum_i \lambda_i N_i \sigma_p^i + \Sigma^k \right)
\]

\[
\sigma_{bk} = \frac{\sigma_{ak} \phi_k}{(1 - \phi_k)}
\]

\[
\sigma_{a,\text{eff}} = \frac{\sum_{k=1}^n \omega_k \sigma_{ak}}{\sum_{k=1}^n \omega_k} \frac{\sigma_{bk}}{\sigma_{ak} + \sigma_{bk}}
\]