Development of Multigroup Cross Section Generation Code MC$^2$-3 for Fast Reactor Analysis

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Background

- Under the Nuclear Energy Advanced Modeling and Simulation (NEAMS) of U.S. DOE, an integrated, advanced neutronics code system is being developed to allow the high fidelity description of a nuclear reactor and simplify the multi-step design process
  - Development of UNIC with unstructured finite element mesh capabilities on a large scale of parallel computation environment
  - Integration with thermal-hydraulics and structural mechanics calculations

- As part of this effort, an advanced multigroup cross section generation code named MC²-3 is being developed
  - The ANL multigroup generation code system, ETOE-2 / MC²-2 / SDX, has been successfully used for fast reactor analysis
  - Recent studies with the ENDF/B-VII.0 data identified some improvement needs of MC²-2
    - Increased importance of resolved resonances in the ENDF/B-VII.0 data due to the extended upper energy cutoff and significantly increased number of resolved resonances required the use of RABANL for a rigorous treatment of resolved resonances
    - Use of RABANL is limited to the relatively low energy range where the isotropic source approximation is valid
ETOE-2 / MC²-2 / SDX

- **ETOE-2**
  - Generate MC² libraries by processing ENDF/B data, including ultrafine group smooth cross sections (2,082 groups with constant lethargy from 20 MeV to 0.4 eV)
  - Screen out wide resonances to smooth cross sections
  - Convert the resolved resonances in the Reich-Moore formalism to those in the multipole formalism

- **MC²-2**
  - Self-shield unresolved and resolved resonances using the generalized resonance integral method based on the narrow resonance (NR) approximation
  - Perform the consistent P1 or B1 transport spectrum calculations
    - Multigroup method for above resolved resonance energy range
    - Continuous slowing down method for the resolved resonance energy range
  - RABANL option for the hyperfine group slowing-down calculation based on isotropic elastic scattering (applicable below ~tens keV)

- **SDX**
  - Perform the 1D integral transport calculation to account for the local heterogeneity effects
**MC²-2/SDX vs. MC²-3**

**ETOE-2 / MC²-2 / SDX**

- **ETOE-2**
  - Generation of MC² Library Files (Screening out Wide Resonances)

- **MC²-2**
  - Unresolved Resonance (Analytic integration)
  - Resolved Resonance (Analytic integration)
  - Ultrafine Group Solver (Multigroup above RRR*, CDS** for RRR and below)
  - Hyperfine Group Solver (RABANL) (Required for ENDF/B-VII)
  - Collapse to Broad-group Cross Sections

- **SDX**
  - 1D Transport Solver (Intermediate groups)

**ETOE-2 / MC²-3**

- **ETOE-2**
  - Generation of MC² Library Files (No Screening)

- **MC²-3**
  - Unresolved Resonance (Analytic integration)
  - Resolved Resonance (Numerical integration with pointwise cross sections)
  - Ultrafine Group Solver (Multigroup for entire energy range)
  - Hyperfine Group Solver (Optional)
  - 1D Transport Solver (Hyperfine, ultrafine, or broad groups)
  - Collapse to Broad-group Cross Sections

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* RRR: resolved resonance energy range
** CDS: continuous slowing-down

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Changes and Improvements in MC$^2$-3

- Numerical integration of resolved resonances with pointwise cross sections based on the NR approximation
  - Reconstruction of pointwise cross sections with Doppler broadening
  - Optionally, use of PENDF files from NJOY
- Multigroup spectrum calculation with the consistent $P_1$ transport equation for the entire energy range
- New capability of treating anisotropic inelastic scattering
- Self-shielding of resonance-like cross sections above the resonance energy for intermediate-weight nuclides (Fe, Cr, Ni, etc.)
- 1D transport calculation with ultrafine (2082) or user-defined groups (SDX capability)
- 1D hyperfine (> ~100,000) group transport calculation
  - MOC solver with higher-order anisotropic scattering in the LS and CMS (up to ~1 MeV)

$$\sigma_{st}^l(g \rightarrow g') = \frac{1}{\psi_{lg}} \int_{u_{g-1}}^{u_g} du' \int_{u_{g-1}}^{u_g} du \psi_j(u)\sigma_{ij}^l(u)e^{-(u'-u)}P_i(\mu_i^l)\sum_{n=0}^{N} (2n+1)f_{n}^j(u)P_n(\mu_c^l)$$

- Inline cross section generation as a module of UNIC
  - Standalone version for conventional multi-step analyses
- FORTRAN 90/95 memory structure
Critical Experiments

- \( \Delta k \) in pcm from Monte Carlo results

![Graph showing \( \Delta k \) in pcm from Monte Carlo results for various models. The graph includes data points for MCC-2 and MCC-3, with different models labeled on the x-axis such as Flattop-25, Flattop-23, Godiva, and others. The y-axis represents \( k \) in pcm ranging from -1000 to 1000. The x-axis includes labels for Flattop-25, Flattop-23, Godiva, and other models.]
# C/E of Fission Reaction Rate Ratios for LANL Assemblies

<table>
<thead>
<tr>
<th>Assembly</th>
<th>Data</th>
<th>( \sigma_{f}^{U\text{235}} / \sigma_{f}^{U\text{238}} )</th>
<th>( \sigma_{f}^{Np\text{237}} / \sigma_{f}^{U\text{235}} )</th>
<th>( \sigma_{f}^{U\text{233}} / \sigma_{f}^{U\text{235}} )</th>
<th>( \sigma_{f}^{Pu\text{239}} / \sigma_{f}^{U\text{235}} )</th>
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</thead>
<tbody>
<tr>
<td>GODIVA</td>
<td>Experiment</td>
<td>0.1643±0.0018</td>
<td>0.8516±0.013</td>
<td>1.59±0.03</td>
<td>1.4152±0.025</td>
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<tr>
<td></td>
<td>C/E</td>
<td>MCNP</td>
<td>0.960</td>
<td>0.975</td>
<td>0.987</td>
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<td></td>
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<td>MC(^2)-3 (^a)</td>
<td>0.958</td>
<td>0.974</td>
<td>0.987</td>
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<td>JEZEBEL</td>
<td>Experiment</td>
<td>0.2133±0.0023</td>
<td>0.9835±0.016</td>
<td>1.578±0.027</td>
<td>1.4609±0.013</td>
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<td>C/E</td>
<td>MCNP</td>
<td>0.978</td>
<td>0.988</td>
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<td>MC(^2)-3</td>
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<td>0.987</td>
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<td>JEZEBEL</td>
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<td>-23</td>
<td>C/E</td>
<td>MCNP</td>
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<td>0.984</td>
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<td></td>
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<td>MC(^2)-3</td>
<td>0.988</td>
<td>0.998</td>
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<tr>
<td>FLATTOP</td>
<td>Experiment</td>
<td>0.1492±0.0016</td>
<td>0.7804±0.01</td>
<td>1.608±0.003</td>
<td>1.3847±0.012</td>
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<tr>
<td>-25</td>
<td>C/E</td>
<td>MCNP</td>
<td>0.968</td>
<td>0.988</td>
<td>0.975</td>
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<tr>
<td></td>
<td></td>
<td>MC(^2)-3</td>
<td>0.966</td>
<td>0.988</td>
<td>0.975</td>
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<tr>
<td>FLATTOP</td>
<td>Experiment</td>
<td>0.1799±0.0021</td>
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<td>-Pu</td>
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<td>0.984</td>
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<td>MC(^2)-3</td>
<td>0.970</td>
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<td>-23</td>
<td>C/E</td>
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<td>0.997</td>
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<td></td>
<td></td>
<td>MC(^2)-3</td>
<td>0.976</td>
<td>0.998</td>
<td></td>
</tr>
</tbody>
</table>
C/E of Fission Reaction Rate Ratios for LANL Assemblies

- **U-238 / U-235**
  - MC2-3
  - MCNP

- **Pu-239 / U-235**
  - MC2-3
  - MCNP

- **Np-237 / U-235**
  - MC2-3
  - MCNP

- **U-233 / U-235**
  - MC2-3
  - MCNP

Groups:
- Godiva
- Flattop-25
- Jezebel
- Jezebel-23
- Flattop-Pu
- Flattop-23
Hyperfine-Group Spectrum Calculation

- Inner core composition of ZPR-6/6A
Ultrafine and Hyperfine Group Spectrum Calculation with Anisotropic Scattering Sources

![Graph showing normalized flux vs. energy (eV) for different calculations.]

- **UFG Calc. w/ Anisotropic Scattering**
- **HFG Calc. w/ Anisotropic Scattering**
- **HFG Calc. w/o Anisotropic Scattering**
ZPPR-15A Critical Experiments

<table>
<thead>
<tr>
<th>Loading</th>
<th>Experiment</th>
<th>VIM</th>
<th>MC$^2$-2</th>
<th>MC$^2$-3</th>
</tr>
</thead>
<tbody>
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<td>15</td>
<td>1.00046</td>
<td>0.99985</td>
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<td>-245</td>
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<tr>
<td>16</td>
<td>0.99627</td>
<td>0.99571</td>
<td>-393</td>
<td>-244</td>
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<tr>
<td>20</td>
<td>0.99853</td>
<td>0.99742</td>
<td>-316</td>
<td>-192</td>
</tr>
</tbody>
</table>

* Uncertainty: Experiment < ±0.0018, VIM < ±0.00020
ZPR-6 Critical Experiments

A full core heterogeneous reactor calculations with explicit fuel plate representation

- 50,000,000 vertices (~equivalent to 200 million PARTISN finite difference cells)
- 200+ angles with $P_5$ anisotropic scattering
- 9, 33, 70, and 230 groups
- No thermal-hydraulics considerations (i.e. clean comparison with MCNP/VIM)
UNIC Results with MC²-3 Cross Sections

- Homogeneous cell cross sections with MC²-3 without the heterogeneity effect of fuel drawers

<table>
<thead>
<tr>
<th>Energy Group</th>
<th>K-effective</th>
<th>Δk pcm</th>
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<tbody>
<tr>
<td>9</td>
<td>0.99513</td>
<td>113</td>
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<tr>
<td>33</td>
<td>0.99373</td>
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<td>116</td>
<td>0.99355</td>
<td>-45</td>
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<tr>
<td>230</td>
<td>0.99344</td>
<td>-56</td>
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</tbody>
</table>

VIM : 0.99400 ±0.00020

- Cell-averaged cross sections with the 1D slab transport calculation of MC²-3 to account for the heterogeneity effect of fuel drawers

<table>
<thead>
<tr>
<th>Energy Group</th>
<th>K-effective</th>
<th>Δk pcm</th>
</tr>
</thead>
<tbody>
<tr>
<td>VIM</td>
<td>0.99981</td>
<td>±0.00025</td>
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</table>

<table>
<thead>
<tr>
<th>Energy Group</th>
<th>K-effective</th>
<th>Δk pcm</th>
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<tbody>
<tr>
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<td>26</td>
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<td>33</td>
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<td>116</td>
<td>0.99965</td>
<td>-16</td>
</tr>
<tr>
<td>230</td>
<td>0.99966</td>
<td>-15</td>
</tr>
</tbody>
</table>
Summary

- New multigroup cross section generation code MC$^2$-3 has been developed with improved methods
- Verification tests with LANL, ZPR-6, ZPPR-15A, ZPPR-21, and BFS critical experiments showed more rigorous and accurate solutions compared to MC$^2$-2 / SDX
- 1D hyperfine-group transport calculation capability with higher-order anisotropic scattering sources is near completion
- Initial integration of MC$^2$-3 into UNIC for inline cross section generation was accomplished
- Development of efficient algorithms for inline multigroup cross section generation is in progress