Title: Progress with On-The-Fly Neutron Doppler Broadening in MCNP

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Intended for: 2012 ANS Summer Meeting, 2012-06-24/2012-06-28 (Chicago, Illinois, United States)
Web
Progress with

On-The-Fly Neutron Doppler Broadening in MCNP

Forrest Brown (LANL), William Martin (Michigan), Gokhan Yesilyurt (ANL), Scott Wilderman (Michigan)

US DOE NE-UP Project
Abstract

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On-The-Fly Neutron Doppler Broadening in MCNP

Forrest Brown, William Martin, Gokhan Yesilyurt, Scott Wilderman

The University of Michigan, ANL, and LANL have been collaborating on a US-DOE-NE University Programs project “Implementation of On-the-Fly Doppler Broadening in MCNP5 for Multiphysics Simulation of Nuclear Reactors.” This talk describes the project and provides results from the initial implementation of On-The-Fly Doppler broadening (OTF) in MCNP and testing.

The OTF methodology involves high precision fitting of Doppler broadened cross-sections over a wide temperature range (the target for reactor calculations is 250-3200K). The temperature dependent fits are then used within MCNP during the neutron transport, for OTF broadening based on cell temperatures. It is straightforward to extend this capability to cover any temperature range of interest, allowing the Monte Carlo simulation to account for a continuous distribution of temperature ranges throughout the problem geometry.
Introduction - Doppler Broadening
- Importance, Examples, Numerics
- Temperature Variation in Monte Carlo Codes

On-The-Fly Doppler Broadening in MCNP (OTF)
- Methodology
- Union Energy Mesh
- Temperature Fitting
- MCNP Implementation
- Testing

Work-in-Progress
Introduction – Doppler Broadening

**UO₂ Fuel Pin**

- 3.1% Enriched
- 293.6 °K
- .01 eV – 20 MeV

- Neutrons born in MeV range from fission
- Most fissions caused by thermal neutrons
- 1/3 of neutron losses are due to \(^{238}\text{U}\) capture in epithermal energy range during slowing down
Introduction – Doppler Broadening

**UO₂ Fuel Pin**

3.1% Enriched

293.6 °K vs 900 °K

.01 eV – 20 MeV

Keeping same densities, but changing cross-sections:

\[ k_{\text{inf}} (\text{cold}) = 1.34498 \ (8) \]

\[ k_{\text{inf}} (\text{hot}) = 1.31167 \ (8) \]

At higher temperatures, Doppler broadening of resonance cross-sections increases resonance capture
Introduction – Doppler Broadening

- **Target nucleus thermal motion important**
  - Maxwell-Boltzmann energy distribution at temperature $T$, isotropic $\Omega$
  - Detailed kinematics of collisions must include nucleus $E$ & $\Omega$

- **Free-flight, selection of collision isotope, & tallies of overall reactions:**
  Must use effective cross-sections, averaged over $(E, \Omega)$ distribution of nuclides at temperature $T$

$$\sigma_{\text{eff}}(v) = \int \frac{|\vec{v} - \vec{V}|}{v} \sigma(|\vec{v} - \vec{V}|) P(\vec{V}) \, d\vec{V}, \quad P(\vec{V}) = \left( \frac{M}{2\pi kT} \right)^{3/2} e^{-\left(\frac{M}{2kT}\right)v^2}$$

Doppler broadening equation

$v = \text{neutron}, V=\text{nucleus}$

This is a convolution of the cross-section with the target energy or speed distribution. Smears out & smoothes the cross-section, reduces peak values.
### Temperature Range (K) | Field of Study
--- | ---
77 - 293.6 | Cold Neutron Physics
293.6 – 550 | Benchmarking Calculations
550 – 1600 | Reactor Operation
1600 – 3200 | Accident Conditions
• ENDF/B nuclear data is represented by piecewise-linear tabulation of $\sigma(E)$

Typically, a linearization tolerance of 0.1% is used.

$$\sigma_{\text{eff}}(\mathbf{v}) = \int \frac{|\mathbf{v} - \mathbf{\bar{v}}|}{\mathbf{v}} \sigma(\mathbf{v}) P(\mathbf{\bar{v}}) \, d\mathbf{\bar{v}}, \quad P(\mathbf{\bar{v}}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\frac{M}{2kT}v^2}$$

– Red Cullen (NSE, 1976) showed how to exactly perform this convolution of Maxwell Boltzmann PDF with piecewise-linear $\sigma(E)$, called sigma1 method

– NJOY code is similar & adaptively chooses energy points to meet 0.1% accuracy in $\sigma_{\text{eff}}$ at $T$

– $\sigma_{\text{eff}}(E)$ has different E-mesh at different $T$’s

– Very compute-intensive, typically performed prior to Monte Carlo in preparing nuclear data libraries
Introduction – Temperature Variation in Monte Carlo

What if there are 1000s of T's?

Six approaches:

1. Traditional NJOY+MC (exact)
   • NJOY data at specific problem T's
   • Each MC region in MC uses specific pre-broadened data
   • Exact, very cumbersome, very large amount of xsec data

2. Traditional NJOY+MC (approx.)
   • Like (1), but round off T's to nearest 10-20°
   • Approximate, very cumbersome, very large amount of xsec data

3. Stochastic Mixing (approx)
   • NJOY data at a few bounding T's
   • Set up MC input with a mix of hot & cold data for each nuclide, such that average T for the mix matches region T
   • Run MC, will sometimes get "hot" data, sometimes "cold", average is OK
   • Approximate, cumbersome, very large amount of xsec data

4. OTF Sigma1 (Monk)
   • Use only 1 set of NJOY datafiles
   • During MC, use sigma1 method to broaden data as needed
   • Exact, but very expensive, ~10x increase in computer time

5. OTF Using Delta-Track (Serpent)
   • Use only 1 set of NJOY datafiles
   • During MC, use delta-tracking rejection method to broaden data as needed
   • Cannot do pathlength MC estimators or flux at a point estimators
   • Exact, but complex & expensive, ~4x increase in computer time

6. OTF Temp. Fitted Data (MCNP)
   • Use only 1 set of NJOY datafiles
   • Prior to MC, generate OTF datasets to handle temperature variation
   • During MC, Doppler broaden as needed using fitting data
   • Exact, extra data for T-fits, ~1.1x increase in computer time
On-The-Fly Neutron Doppler Broadening

• OTF Methodology (for each nuclide)
  – Create union energy grid for a range of temperatures
  – Create fits for $\sigma_{\text{eff}}(T,E)$, for range of temperatures, on union E-grid
  – MCNP – evaluate $\sigma_{\text{eff}}(T,E)$ OTF during simulation

• Comments
  – Target application, for now: reactors

  – Relies on NJOY methodology
    • Supplements & extends NJOY
    • Methodology consistent with NJOY

  – Fitting $\sigma$ vs temperature (at each $E$)
    • High precision, least squares with singular value decomposition
    • Adaptive (for each $E$, MT, & nuclide)
    • Explicit, direct error checking for fits - fit error < linearization tolerance
    • Threaded parallel, broadening routines called millions of times
    • Over temperature, maintains accuracy consistent with NJOY
• $^{238}$U energy grid, 35-36 eV, various temperatures (ENDF/B-VII.0)

NJOY adapts the energy grid (for each nuclide, at given T) to preserve linearization tolerance

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Number of E pts</th>
<th>Union E-grid:</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.6</td>
<td>157754</td>
<td>Need to determine 1 energy grid (for each nuclide) that preserves linear interpolation tolerance in E over the entire T range</td>
</tr>
<tr>
<td>600</td>
<td>133964</td>
<td></td>
</tr>
<tr>
<td>900</td>
<td>122581</td>
<td></td>
</tr>
<tr>
<td>1200</td>
<td>115361</td>
<td></td>
</tr>
<tr>
<td>2500</td>
<td>99631</td>
<td></td>
</tr>
</tbody>
</table>
OTF Methodology – Union Energy Grid (2)

• For 1 nuclide, determine:
  – **MT numbers** for reactions to be broadened
  – **Energy range** for broadening, \( E_{\text{min}} - E_{\text{max}} \)
    • Up to start of unresolved data, or high-threshold reactions (whichever smaller)
  – **Temperature range** \( T_{\text{min}} - T_{\text{max}} \) & interval \( \Delta T \) for tolerance testing (input)
  – **Base set of** \( \sigma_x(e) \)'s from NJOY at \( T_{\text{base}} \)
    • “\( x \)” = any MT reaction that needs broadening
    • ACE data file from NJOY: Yesilyurt: \( T_{\text{base}} = 0 \) K, Brown: \( T_{\text{base}} = 293.6 \) K
  – **Energy grid** from NJOY at \( T_{\text{min}} \)

• For 1 nuclide & a set of T’s in range, at each T:
  – **Adaptively add E points so that** 0.1% linear tolerance is maintained
    • Exact Doppler broadening from \( T_{\text{base}} \) to T, using sigma1 method
    • Check all broadened MT reaction data for each E interval
    • Subdivide E interval until 0.1% linearization tolerance met for all MT’s
    • Add E points as needed, do not remove E points
  – **Compute-intensive** – millions of calls to sigma1 routine, parallel threads
  – **Typically expands number of E points by** ~10%, for 293-3200 K range
  – **Result:** union E-grid for nuclide, 0.1% linear tolerance over entire \((E,T)\) ranges
Near resonance peaks:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} \frac{a_k}{T^{k/2}}$$

Mid resonance:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} a_k T^{k/2}$$

Wings of resonance:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} b_k T^{k}$$

Combined functional form:

$$\sigma_{T,C,F}(T) \sim \sum_{k=1}^{n} \frac{a_k}{T^{k/2}} + \sum_{k=1}^{n} b_k T^{k/2} + c$$

Functional forms for temperature fitting based on multilevel Adler-Adler model, with expansions for peak, mid-res, wings
OTF Methodology – Fitting vs T (2)

• **For 1 nuclide, determine:**
  - **MT numbers** for reactions to be broadened
  - **Energy range** for broadening, \( E_{\text{min}} - E_{\text{max}} \)
    - Up to start of unresolved data, or high-threshold reactions (whichever smaller)
  - **Temperature range** \( T_{\text{min}} - T_{\text{max}} \) & interval \( \Delta T \) for tolerance testing (input)
  - **Base set of** \( \sigma_x(e) \)'s from NJOY at \( T_{\text{base}} \)
    - “\( x \)” = any MT reaction that needs broadening
    - ACE data file from NJOY: Yesilyurt: \( T_{\text{base}} = 0 \) K, Brown: \( T_{\text{base}} = 293.6 \) K
  - **Union energy grid** for this nuclide & T range
  - **Maximum order for temperature fitting**
    - Adler-Adler based functional form, using powers of \( T^{1/2} \) and \( 1/T^{1/2} \)

• **For 1 nuclide, at each point in the union E grid:**
  - Exact Doppler broadening from \( T_{\text{base}} \) to all \( T \)'s in range, using sigma1 method
  - Least-squares fitting over \( T \)
    - Singular value decomposition, least squares for temperature dependence
    - Fitting order chosen adaptively for each energy & reaction so that fits accurate within 0.1\% for all \( T \)'s and all \( E \)'s in range, for all MT's
  - Coefficients saved in files for MCNP use
OTF Methodology – MCNP OTF

• **At problem setup, read in OTF data for various nuclides**
  – Each OTF nuclide set can have different fit orders & union E-grid & reactions

• **During simulation, if neutron in E-T range of fits**
  – Use OTF data for each nuclide to create on-the-fly Doppler broadened cross-sections at current cell temperature
  – If outside E-T range of OTF data, use standard ACE data
  – Collision physics (exit E & angles) uses standard ACE data

• **Only need to generate OTF datasets once, & then use for any problems**

• **Cost**
  – Extra storage for OTF data
  – Extra computing for evaluating OTF functions (typical <10% runtime)

• **Benefit**
  – Less storage for ACE data (no need for multiple temperatures)
  – Can solve problems with 1000s of T’s or more, no limit
  – Greatly simplifies problem setup
$^{238}$U Capture – NJOY vs OTF at 2000 K

Cross-sections from NJOY & OTF match within linearization tolerance 0.1% at all energies
NJOY vs OTF $^{238}$U Capture Cross-Section

- **NJOY vs OTF at 1000 K**
  (curves with higher peak)

- **NJOY vs OTF at 2000 K**
  (curves with lower peak)

Cross-sections from NJOY & OTF match within linearization tolerance 0.1% at all energies

- 6.67 eV resonance
- 20.9 eV resonance
- 36.6 eV resonance
MCNP Test Results – Doppler Defect Benchmark

- **Doppler Reactivity Benchmark**
  - Compare k-effective for HZP (hot, zero power) and HFP (hot, full power) conditions for a unit fuel cell typical of a PWR
  - **Basic model:**
    - PWR fuel pin cell with reflecting BCs, various enrichments
    - HZP cases: fuel at 600K, clad/moderator at 600K
    - HFP cases: fuel at 900K, clad/moderator at 600K
    - Uniform temperature within each fuel, clad, moderator region.
    - Number densities and dimensions adjusted for the HFP thermal expansion
    - 5M active neutron histories per each of 28 MCNP runs

- **NJOY+MCNP:** NJOY-broadened data at exact temperatures
- **OTF+MCNP:** OTF data for $^{16}\text{O}$, $^{234}\text{U}$, $^{235}\text{U}$, $^{238}\text{U}$ in fuel

- **OTF details**
  - For union E-grid: $T_{\text{base}}=293.6\text{K}$, T range 300-1000K, $\Delta T=100\text{K}$
  - For OTF fitting: 8$^{\text{th}}$ order, T range 300-1000K, $\Delta T=10\text{K}$
  - For general production use, would use larger T range & smaller $\Delta T$'s
## Doppler Defect Benchmark Results

<table>
<thead>
<tr>
<th>Enrichment</th>
<th>Material</th>
<th>Code</th>
<th>HZP</th>
<th>HFP</th>
<th>Doppler Coef.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UO₂ fuel pin</td>
<td></td>
<td>0.66556 (18)</td>
<td>0.65979 (19)</td>
<td>-4.38 (0.20)</td>
</tr>
<tr>
<td>0.711%</td>
<td>NJOY+MCNP</td>
<td></td>
<td>0.66567 (18)</td>
<td>0.66022 (19)</td>
<td>-4.13 (0.20)</td>
</tr>
<tr>
<td></td>
<td>OTF+MCNP</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.60%</td>
<td>NJOY+MCNP</td>
<td></td>
<td>0.96094 (26)</td>
<td>0.95293 (25)</td>
<td>-2.92 (0.13)</td>
</tr>
<tr>
<td></td>
<td>OTF+MCNP</td>
<td></td>
<td>0.96026 (24)</td>
<td>0.95283 (23)</td>
<td>-2.71 (0.13)</td>
</tr>
<tr>
<td>2.40%</td>
<td>NJOY+MCNP</td>
<td></td>
<td>1.09912 (27)</td>
<td>1.08997 (26)</td>
<td>-2.55 (0.10)</td>
</tr>
<tr>
<td></td>
<td>OTF+MCNP</td>
<td></td>
<td>1.09923 (27)</td>
<td>1.08975 (28)</td>
<td>-2.64 (0.10)</td>
</tr>
<tr>
<td>3.10%</td>
<td>NJOY+MCNP</td>
<td></td>
<td>1.17718 (27)</td>
<td>1.16744 (27)</td>
<td>-2.36 (0.09)</td>
</tr>
<tr>
<td></td>
<td>OTF+MCNP</td>
<td></td>
<td>1.17703 (30)</td>
<td>1.16767 (30)</td>
<td>-2.27 (0.10)</td>
</tr>
<tr>
<td>3.90%</td>
<td>NJOY+MCNP</td>
<td></td>
<td>1.23967 (27)</td>
<td>1.22920 (30)</td>
<td>-2.29 (0.09)</td>
</tr>
<tr>
<td></td>
<td>OTF+MCNP</td>
<td></td>
<td>1.23953 (29)</td>
<td>1.22979 (29)</td>
<td>-2.13 (0.09)</td>
</tr>
<tr>
<td>4.50%</td>
<td>NJOY+MCNP</td>
<td></td>
<td>1.27501 (30)</td>
<td>1.26526 (27)</td>
<td>-2.01 (0.09)</td>
</tr>
<tr>
<td></td>
<td>OTF+MCNP</td>
<td></td>
<td>1.27534 (29)</td>
<td>1.26552 (29)</td>
<td>-2.03 (0.09)</td>
</tr>
<tr>
<td>5.00%</td>
<td>NJOY+MCNP</td>
<td></td>
<td>1.29901 (31)</td>
<td>1.28920 (29)</td>
<td>-1.95 (0.08)</td>
</tr>
<tr>
<td></td>
<td>OTF+MCNP</td>
<td></td>
<td>1.29907 (28)</td>
<td>1.28938 (29)</td>
<td>-1.93 (0.08)</td>
</tr>
</tbody>
</table>

\[
\rho = \left( \frac{1}{K_{HZP}} - \frac{1}{K_{HFP}} \right) \times 10^5 / 300 \quad \text{pcm/K}
\]
Results – Fuel Assembly

• Simplified PWR 15 x 15 fuel assembly, with varying temperatures
  
  – From OECD/NEA fuel storage vault benchmark
    • Fuel = 900 K, 600 K, 300 K
    • Clad = 900 K, 600 K, 300 K
    • Water = 600 K, 300 K
    • Outer iron rack = 293.6K

  – Standard NJOY+MCNP5:
    • ACE data at explicit temperatures

  – OTF+MCNP5
    • use 293.6K ACE data for all nuclides
    • OTF data for all nuclides (except iron)

  – MCNP5
    • 20,000 neutrons/cycle,
    • 10 inactive cycles, 1000 active cycle
    • Reflecting BCs
# Results – Fuel Assembly

## k-effective:

<table>
<thead>
<tr>
<th></th>
<th>STD</th>
<th>OTF</th>
</tr>
</thead>
<tbody>
<tr>
<td>STD</td>
<td>1.11599 (15)</td>
<td>1.11592 (15)</td>
</tr>
</tbody>
</table>

### Total fission

<table>
<thead>
<tr>
<th></th>
<th>900K</th>
<th>600K</th>
<th>300K</th>
</tr>
</thead>
<tbody>
<tr>
<td>STD</td>
<td>0.045140 (.08%)</td>
<td>0.161186 (.04%)</td>
<td>0.248782 (.03%)</td>
</tr>
<tr>
<td>OTF</td>
<td>0.045081 (.08%)</td>
<td>0.161329 (.04%)</td>
<td>0.248731 (.03%)</td>
</tr>
</tbody>
</table>

### Total capture in fuel

<table>
<thead>
<tr>
<th></th>
<th>900K</th>
<th>600K</th>
<th>300K</th>
</tr>
</thead>
<tbody>
<tr>
<td>STD</td>
<td>0.027672 (.09%)</td>
<td>0.096276 (.05%)</td>
<td>0.116745 (.04%)</td>
</tr>
<tr>
<td>OTF</td>
<td>0.027667 (.09%)</td>
<td>0.096268 (.05%)</td>
<td>0.116829 (.04%)</td>
</tr>
</tbody>
</table>

### U235 capture in fuel

<table>
<thead>
<tr>
<th></th>
<th>900K</th>
<th>600K</th>
<th>300K</th>
</tr>
</thead>
<tbody>
<tr>
<td>STD</td>
<td>0.008993 (.08%)</td>
<td>0.031910 (.04%)</td>
<td>0.045998 (.03%)</td>
</tr>
<tr>
<td>OTF</td>
<td>0.008983 (.08%)</td>
<td>0.031932 (.04%)</td>
<td>0.045987 (.03%)</td>
</tr>
</tbody>
</table>

### U238 capture in fuel

<table>
<thead>
<tr>
<th></th>
<th>900K</th>
<th>600K</th>
<th>300K</th>
</tr>
</thead>
<tbody>
<tr>
<td>STD</td>
<td>0.018547 (.11%)</td>
<td>0.063887 (.06%)</td>
<td>0.070236 (.05%)</td>
</tr>
<tr>
<td>OTF</td>
<td>0.018551 (.11%)</td>
<td>0.063858 (.06%)</td>
<td>0.070332 (.05%)</td>
</tr>
</tbody>
</table>

### O16 capture in fuel

<table>
<thead>
<tr>
<th></th>
<th>900K</th>
<th>600K</th>
<th>300K</th>
</tr>
</thead>
<tbody>
<tr>
<td>STD</td>
<td>1.15E-04 (.23%)</td>
<td>4.18E-04 (.14%)</td>
<td>4.37E-04 (.13%)</td>
</tr>
<tr>
<td>OTF</td>
<td>1.15E-04 (.23%)</td>
<td>4.16E-04 (.14%)</td>
<td>4.37E-04 (.13%)</td>
</tr>
</tbody>
</table>
OTF Work in Progress

• Better integration & optimization in MCNP

• FIT_OTF fitting program
  – Investigate scaling & Chebychev, for better numerical stability [done]
  – Investigate regression, to vary fit order by energy & reaction [done]

• U. Michigan work
  – Create OTF libraries for all nuclides in ENDF/B-VII.0 [in progress]
  – Test various applications: fuel assemblies, 3D whole core, LWR, HTGR, ...

• Methodology for Unresolved Resonances & S(α,β) data
  – Probable 1st cut – tables with temperature interpolation
  – Possible thesis topic for PhD student

• Implement corrected free-gas scatter model
  – Demonstrated, needs robust implementation

• Easy to extend to any temperature range
  – Need to investigate broadening for high-threshold reactions
References


