Business from technology

On-the-fly Temperature Treatment in Serpent

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Serpent User Group Meeting, Berkeley, USA

November 6–8, 2013

TMS Temperature Treatment Method – Background

- With conventional transport methods relying on pre-broadened cross sections
  - Cross sections need to be prepared beforehand at each temperature appearing in the system.
  - XS data needs to be stored at each temperature in the node memory.
- Memory consumption in burnup problems is $\sim 1\,\mathrm{GB}$ per temperature appearing in the system *at minimum*
  - In higher optimization modes and with high-resolution xs libraries the consumption can be even 10–30 GB per temperature.

Modelling the 300–1200 K (–3000 K) temperature range of a PWR in HFP conditions requires numerous temperatures.

Different on-the-fly temperature treatment methods

- Simply on-the-fly Doppler-broaden from 0 K point-wise cross sections using

$$\Sigma_{\mathrm{eff}}(E,T) = \frac{1}{v}\int \mathbf{V}_{\mathrm{rel}}\Sigma(\mathbf{V}_{\mathrm{rel}}, 0\ \mathrm{K}) f_{\mathrm{MB}}(\mathbf{V}_{\mathrm{rel}}, T) d\mathbf{V}_{\mathrm{rel}} \tag{1}$$

  - Calculationally expensive [1]
- Pre-generate cross sections at numerous temperatures and interpolate on-the-fly.
  - The cross sections need to be tabulated in 10–20 K intervals for good accuracy [2].

[1] C. DEAN, R. PERRY, R. NEAL, A. KYRIELEIS, “Validation of Run-time Doppler Broadening in MONK with JEFF3.1,” Journal of the Korean Physical Society, Vol. 59, No.2, pp.1162-1165, (2011).

[2] T. H. TRUMBULL, “Treatment of Nuclear Data for Transport Problems Containing Detailed Temperature Distributions,” Nucl. Technology, 156, pp. 75 (2006).

Different on-the-fly temperature treatment methods

- Stochastic mixing: Instead of actually having materal at T in the system, take proportion p of material at $T_1 < T$ and proportion (1-p) at $T_2 > T$.
  - Simple and easy to implement, but approximate.
- MCNP method: Pre-calculate numerous series expansion coefficients beforehand and perform fast Doppler-broadening on-the-fly based on the Adler-Adler formalism.
  - Fast (in MCNP increase in CPU time only about 1.1)
  - The coefficients take about 3-15 GB of additional memory [3].

[3] G. YESILYURT, W. R. MARTIN, and F. B. BROWN, "On-the-Fly Doppler Broadening for Monte Carlo Codes," Proc. M&C 2009, Saratoga Springs, NY, May 3–7 (2009).

Different on-the-fly temperature treatment methods

- (Coming soon:) Forget-Xu-Smith method. Perform quick on-the-fly Doppler-broadening based on the multipole presentation.
  - Minimal memory requirement (only 100s of MB)
  - Preliminary results show good performance [4].

[4] B. FORGET, S. XU and K. SMITH, “Direct Doppler Broadening in Monte Carlo Simulations using the Multipole Representation”, Annals of Nuclear Energy, accepted (2013).

Target Motion Sampling (TMS) technique

Basic idea: **“There are no effective cross sections, just 0 K cross sections and thermal motion of target nuclei”**

- The effect of thermal motion can be taken into account by sampling velocities at collision points and using 0 K cross sections in target-at-rest frame.
- However, to make this possible, a rejection sampling scheme (next slide) based on a temperature majorant $\Sigma_{\mathrm{maj}}(E)$ must be used.
- Later on it was noticed that the basis temperature of the cross sections can be $T_{\mathrm{base}} \geq 0\ \mathrm{K}$.
- A very similar method has been used for many years in PRIZMA Monte Carlo code [5].

[5] V.N. OGIBIN, A.I. ORLOV, “Majorized Cross-section Method for Tracking Neutrons in Moving Media”, J. Nuclear Science and Technology, Methods and Codes for Mathematical Physics Series, 2(16), pp.6–9 (1984).

TMS Temperature Treatment Method — Tracking scheme

1. Sample path length l based on a majorant cross section $\Sigma_{\mathrm{maj}}(E)$
   $\rightarrow$ New collision point candidate $\mathbf{x_{i+1}} = \mathbf{x_i} + l\mathbf{\Omega}$
2. Sample target nuclide n: $P_n = \dfrac{\Sigma_{\mathrm{maj},n}(E)}{\Sigma_{\mathrm{maj}}(E)} = \dfrac{\Sigma_{\mathrm{maj},n}(E)}{\sum_n \Sigma_{\mathrm{maj},n}(E)}$.
3. Sample target velocity from distribution $f_n(V_{\mathrm{t}}, \mu) = \dfrac{v'}{2v} f_{\mathrm{MB}}\Big(T(\mathbf{x_{i+1}}) - T_{\mathrm{base}}, A_n, V_{\mathrm{t}}\Big)$,
   where v' is the relative (target-at-rest) velocity
   $\rightarrow$ Target-at-rest energy E'
4. Rejection sampling with criterion $\xi < \dfrac{g_n(E, T(\mathbf{x_{i+1}}) - T_{\mathrm{base}})\Sigma_{\mathrm{tot},n}(E', T_{\mathrm{base}})}{\Sigma_{\mathrm{maj},n}(E)}$.
   - If sample is rejected, return to 1.
   - If sample is accepted, sample reactions in target-at-rest frame (E'). Continue accordingly.

Properties

- The method is fully accurate, nowadays works also with detectors.
- XS data needs to be stored in one temperature only.
- The performance of the TMS method is affected by:
  - Difference between nuclide maximum and xs temperatures
  - Number of nuclides in TMS materials.
  - Neutron spectrum
- Worst performance in heavy water or graphite moderated systems with high temperature difference at non-zero burnup. (HTGR)

Howto?

- TMS is only available in Serpent 2.
- TMS is *not* capable of adjusting the temperature of
  - $S(\alpha, \beta)$ (thermal scattering of moderators)
  - Probability tables (ures region)
- Usage is similar to the Doppler pre-processor:
  - TMP = Use pre-processor
  - ETTM (Explicit Treatment of Target Motion) = Use TMS treatment

```
mat fuel1  6.7402E-02 tmp 667
92235.06c  9.3472E-04
92238.06c  2.1523E-02
 8016.06c  4.4935E-02
```

```
mat fuel1  6.7402E-02 ettm 667
92235.06c  9.3472E-04
92238.06c  2.1523E-02
 8016.06c  4.4935E-02
```

Demonstration

- A Serpent calculation in optimization mode 4 is used as the reference.
  $\rightarrow$ "unfair" (but practical) comparison

Arbitrary temperature distributions

- TMS is also capable of modelling arbitrary, continuous temperature distributions.
- If you are interested:
  - Modify GetTemp() to return the desired temperatures.
  - Ensure that the temperature does not exceed the temperature of the majorant.

Conclusions

- TMS on-the-fly temperature treatment can be used to save memory in calculations involving detailed temperature distributions.
- The usage of TMS increases the CPU time requirement.
- The accuracy of the method is only limited by the xs reconstruction tolerance.
  $\rightarrow$ More reliable than the Doppler pre-processor of Serpent!

Thank you for your attention!

Questions?

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References

[1] T. Viitanen and J. Leppänen, "Explicit Treatment of Thermal Motion in Continous-energy Monte Carlo Tracking Routines," *Nuc. Sci. Eng.*, 171 (2012) 165-173.

[2] T. Viitanen and J. Leppänen, "Optimizing the Implementation of the Explicit Treatment of Thermal Motion — How Fast Can It Get?" *Proc. M&C 2013*, Sun Valley, ID, May 5–9, 2013.

[3] T. Viitanen and J. Leppänen, "Target Motion Sampling Temperature Treatment Technique with Elevated Basis Cross Section Temperatures", *Nuc. Sci. Eng.*, Accepted for publication on Aug 25, 2013.

[4] T. Viitanen and J. Leppänen, "Explicit Temperature Treatment in Monte Carlo Neutron Tracking Routines – First Results.", *In Proc.* PHYSOR-2012, Knoxville, TN, 15-20 April, 2012.

[5] V.N. OGIBIN, A.I. ORLOV, "Majorized Cross-section Method for Tracking Neutrons in Moving Media", J. Nuclear Science and Technology, Methods and Codes for Mathematical Physics Series, 2(16), pp.6–9 (1984).