Business from technology

TMS On-the-fly Temperature Treatment in Serpent

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Effects of thermal motion on neutron transport

- On reaction probabilities:
  - “Doppler-broadening” of
    - resolved and
    - unresolved resonances
  - Increase in potential scattering at low energies.
  - Special case: bound atoms with $S(\alpha, \beta)$ tables.
- On collision dynamics:
  - Secondary particle distributions of elastic scattering.
  - Secondary particle distributions of bound-atom scattering.
- Traditionally,
  - Red effects are pre-calculated and
  - Blue effects are taken into account during the transport calculation.

On-the-fly temperature treatment – Background

- With pre-calculated data
  - 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 between 1–30 GB per temperature appearing in the system, depending on the optimization mode and the accuracy of the library.
- Covering the 500–1200 K temperature range of a PWR in HFP conditions requires numerous temperatures.
  $\rightarrow$ **Problem!**
  Solution: On-the-fly temperature treatment.

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.
- To make this possible, a rejection sampling scheme (next slide) based on a temperature majorant $\Sigma_{\mathrm{maj}}(E)$ cross section must be used in the neutron tracking.
- The same idea has been used for many years in PRIZMA Monte Carlo code [1].

[1] 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.

Previous publications in short (1/3)

- Introduction to the TMS method (Explicit Treatment of Thermal Motion) in an NSE article [2].
  - The basic idea is introduced.
  - Just proof-of-concept, no practical calculations.
- First practical results in PHYSOR2012 [3].
  - A very early implementation based on a multigroup majorant $\rightarrow$ results obsolete.

[2] T. Viitanen and J. Leppänen, "Explicit treatment of thermal motion in continuous-energy Monte Carlo tracking routines", *Nucl. Sci. Eng.*, **171**, 165-173 (2012).

[3] T. Viitanen and J. Leppänen, "Explicit temperature treatment in Monte Carlo neutron tracking routines – First results." In proc. PHYSOR 2012, Knoxville, TN, Apr. 15-20, (2012).

Previous publications in short (2/3)

- Optimization of TMS by increasing the sampling efficiency discussed in articles [4, 5, 6]
  1. Changing to a continuous-energy majorant cross section.
  2. Elevating the temperature of basis cross sections above 0 K.
  3. Reducing the conservativity of the majorant.
     - (This affects also the efficiency of DBRC!)

[4] T. Viitanen and J. Leppänen, "Optimizing the implementation of the target motion sampling temperature treatment technique – How fast can it get?", In proc. M&C 2013, Sun Valley, ID, May 5-9, (2013).

[5] T. Viitanen and J. Leppänen, "Target motion sampling temperature treatment technique with elevated basis cross section temperatures.", *Nucl. Sci. Eng.*, **177**, 77-89 (2014).

[6] T. Viitanen and J. Leppänen, "Temperature majorant cross sections in Monte Carlo neutron neutron tracking", *Nucl. Sci. Eng.*, Accepted for publication on Aug 31. 2014.

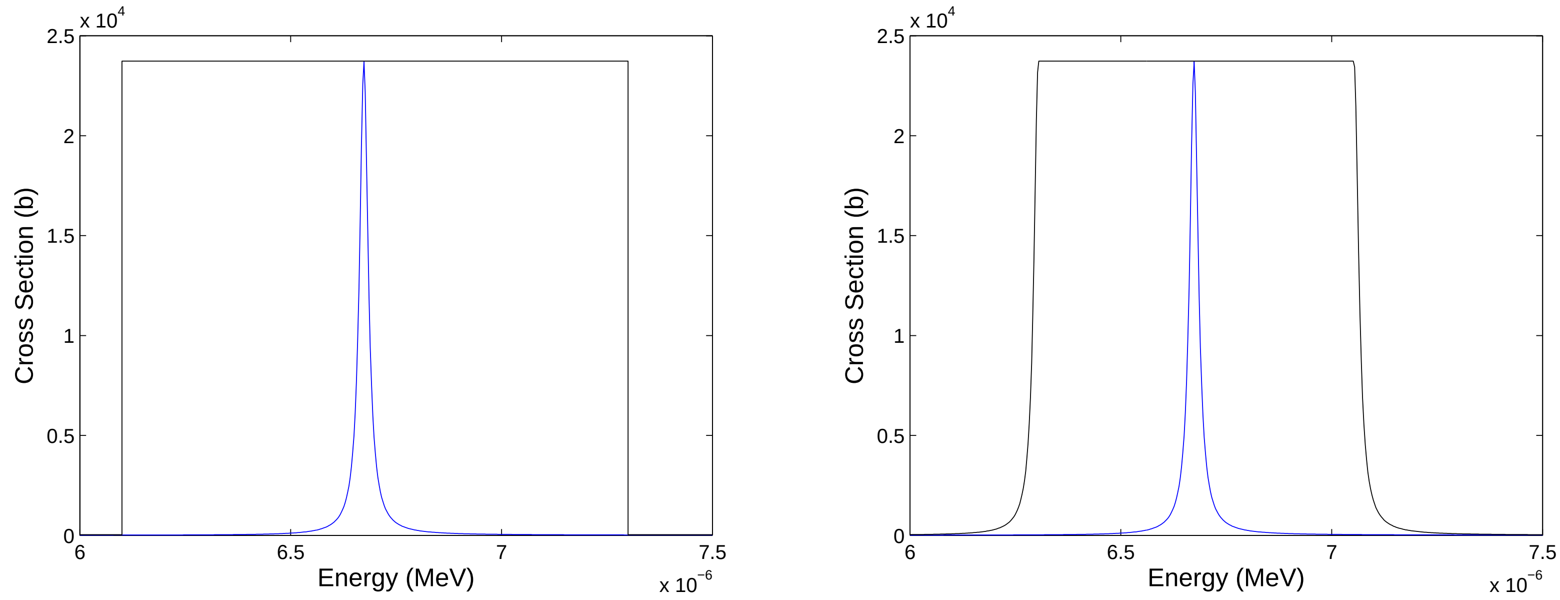


Figure 1: Changing from a multi-group (left) to a continuous-energy (right) removes unnecessary conservativity by making the shape of the majorant xs conform better to the total cross section.

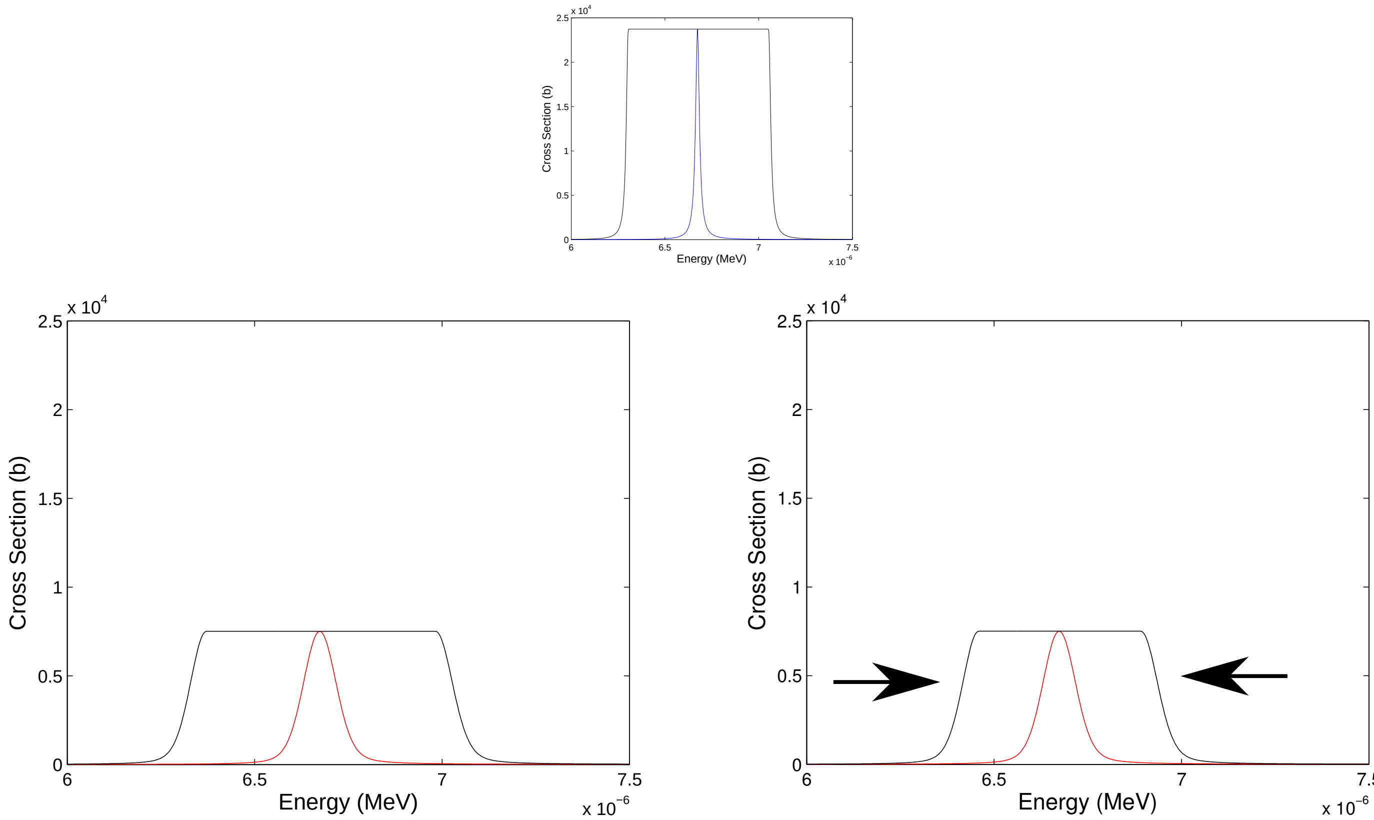
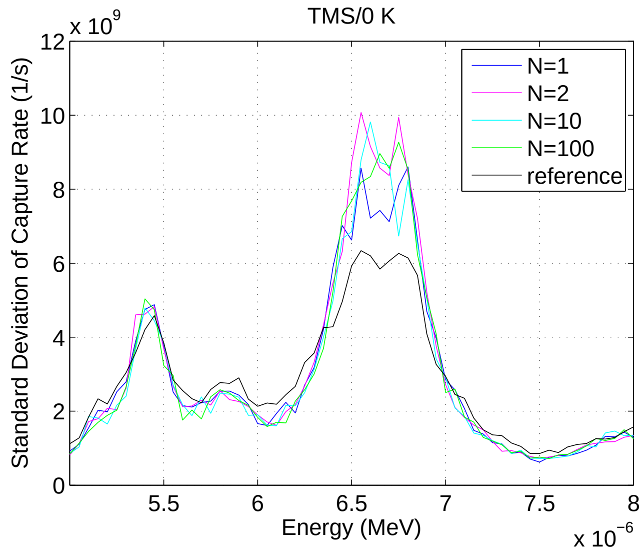


Figure 2: It is also possible to reduce the difference between the majorant and total xs by increasing the basis temperature of the total cross section (left) and by fine-tuning the cut-off conditions in the majorant generation (right).

Previous publications in short (3/3)

- Effects of TMS on reaction rate estimators were studied in [7]
  - TMS has no practical effect on the variances of estimators.
  - Exception: the variances are increased near very strong resonances.



[7] T. Viitanen and J. Leppänen, "Effect of the Target Motion Sampling Temperature Treatment Method on the Statistics and Performance", *Ann. Nucl. Energy*, accepted, in-press.

Performance of TMS in Serpent 2.1.17

	PWR-Gd	PWR-BU
Number of neutron histories	10^9	5×10^8
Reference		
k_{eff}	1.15523	0.93453
Δk_{eff} (pcm)	2	2
Transport time (h)	5.2	2.7
Memory requirement (GB)	3.4	91.2
FOM, Total Capture Rate ($\frac{1}{\mathrm{s}}$)	4.1E+04	5.4E+04
FOM, Capture Rate Around 6.7 eV ($\frac{1}{\mathrm{s}}$)	9.2E+02	8.7E+02
TMS		
$k_{\mathrm{TMS}} - k_{\mathrm{NJOY}}$ (pcm)	3 ± 3	1 ± 3
Abs. / Rel. Transport time (h/-)	6.4 / 1.24	33.2 / 12.33
Abs. / Rel. Memory requirement (GB/-)	2.5 / 0.72	34.0 / 0.37
TMS Sampling efficiency (%)	53.2	52.3
Abs. / Rel. FOM, Tot. Capt. ($\frac{1}{\mathrm{s}}$/-)	3.1E+04 / 0.75	3.9E+03 / 0.07
Abs. / Rel. FOM, Capt. 6.7 eV ($\frac{1}{\mathrm{s}}$/-)	4.9E+02 / 0.53	4.8E+01 / 0.06

Effects of thermal motion on neutron transport (with TMS)

- On reaction probabilities:
  - "Doppler-broadening" of
    - ∗ resolved and
    - ∗ unresolved resonances
  - Increase in potential scattering at low energies
  - Special case: bound atoms with $S(\alpha, \beta)$ tables
- On collision dynamics:
  - Secondary particle distributions of elastic scattering.
  - Secondary particle distributions of bound-atom scattering.
- With the current TMS methodology,
  - Red effects must still be pre-calculated
  - Blue effects can be taken into account on-the-fly.

Howto?

- TMS is only available in Serpent 2.
- Standard temperature treatment in multi-physics interface and fuel temperature feedback features.
- Manual use is similar to the Doppler pre-processor:
  - TMP = Use pre-processor
  - TMS = Use TMS treatment between smallest and largest nuclide temperature

```
mat fuel1  6.7402E-02 tmp 669
92235.06c  9.3472E-04
92238.06c  2.1523E-02
 8016.06c  4.4935E-02
```

```
mat fuel1  6.7402E-02 tms 669
92235.06c  9.3472E-04
92238.06c  2.1523E-02
 8016.06c  4.4935E-02
```

Conclusions and future work

- TMS method is now fully functional in Serpent 2.
- It is about as fast as it gets, as long as all the nuclides are treated as temperature dependent.
  - Using a temperature independent lumped model for less-important fission products will be the next significant optimization step.
- TMS can be extended to unresolved energy region. (not yet demonstrated)
- Extension of the TMS idea to $S(\alpha, \beta)$ turned out to be very complicated $\rightarrow$ Thermal scattering has to be handled by other means (not yet implemented, unfortunately)

Thank you for your attention!

Questions?

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References

[1] 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).

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