Temperature treatment capabilites in Serpent 2(.1.24)

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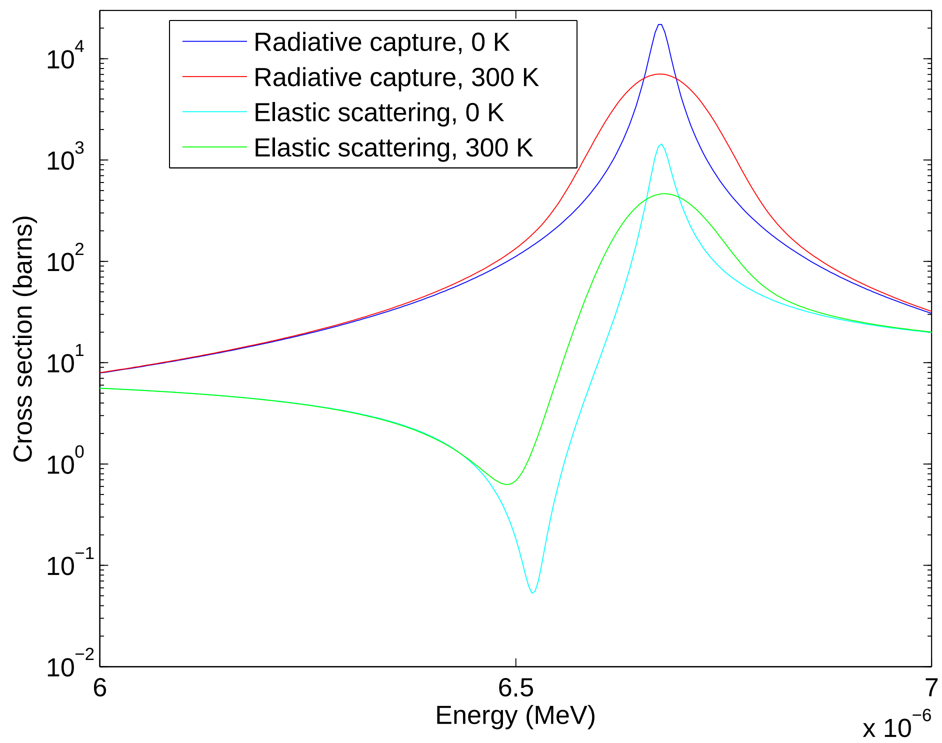
Introduction

- Temperature affects the neutron transport through:
  - Reaction probabilities (Doppler-broadening)
  - Scattering kinematics
  - (Indirectly: material dimensions and densities)



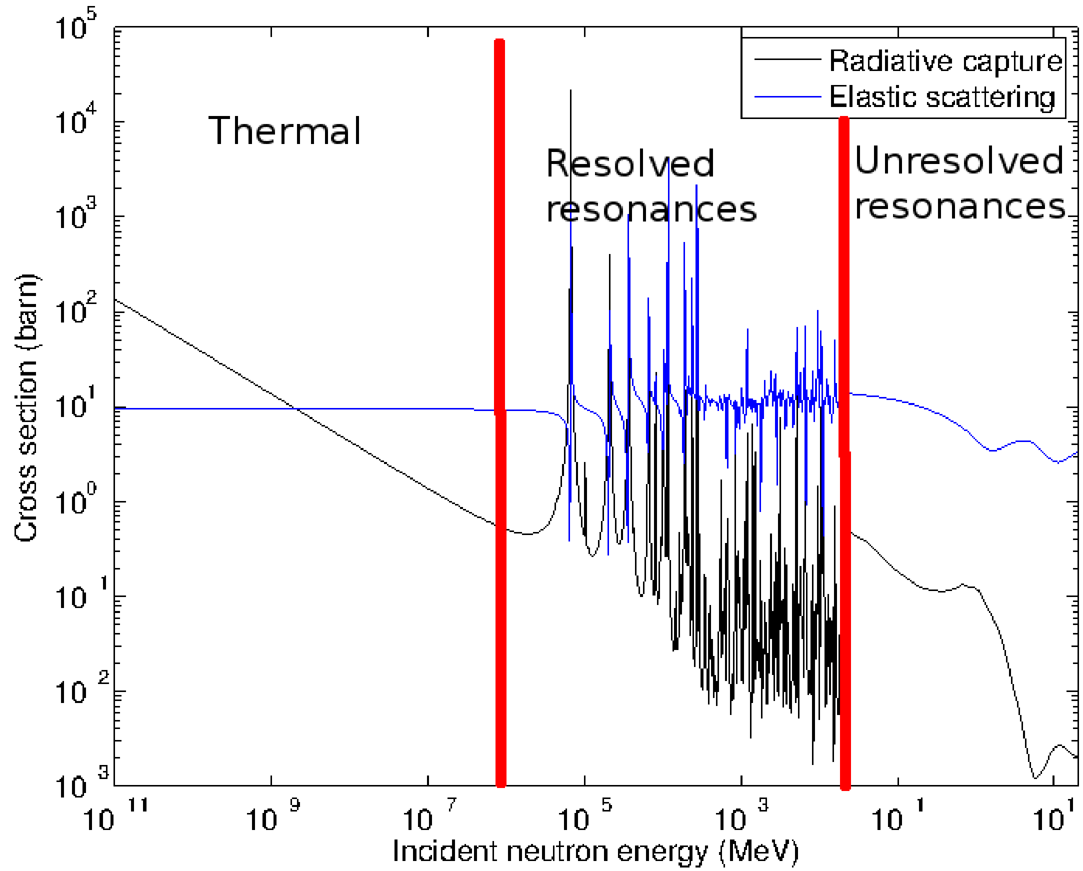


Figure 1: Thermal motion needs to be treated using different techniques in different energy regions.

Energy region of Resolved Resonances

Energy region of Resolved Resonances (RR)

- Serpent has two options for temperature adjustment within RR region:
  - Doppler-preprocessor (pre-calculation)
  - Target Motion Sampling, TMS (on-the-fly calculation)

RR: Doppler-preprocessor

- Performs straightforward, analytical Doppler-broadening based on Solbrig's kernel

$$\sigma_{\mathrm{eff}}(v,T,A_n) = \frac{\gamma}{v^2\sqrt{\pi}}\int_0^\infty v'^2\sigma(v')\left(e^{-\gamma^2(v-v')^2} - e^{-\gamma^2(v+v')^2}\right)dv' \qquad (1)$$

- Unlike codes based on SIGMA1 method, does not optimize the energy grid.

$\rightarrow$ Accuracy of the xs is unknown after the broadening.

- Works just fine in practice, but differences to NJOY based reference can be seen in very accurate analyses.

- Data is stored in memory at each T

RR: Target Motion Sampling (TMS) (1/2)

- On-the-fly temperature treatment specifically developed for Serpent.
- In a nutshell:
  1. Path lenghts are sampled based on a majorant cross section Σ_{maj}.
  2. Target nuclide and its thermal motion are sampled at each collision site.
     $\rightarrow$ Target-at-rest energy E'.
  3. Collision points are accepted according to

$$\xi < \frac{\sigma_{\mathrm{tot}}(E')}{\sigma_{\mathrm{maj}}(E)} \tag{2}$$

  4. Reaction sampling is done in target-at-rest frame .

[1] T. Viitanen, “Development of a stochastic temperature treatment technique for Monte Carlo neutron tracking”, Doctoral dissertation (2015).

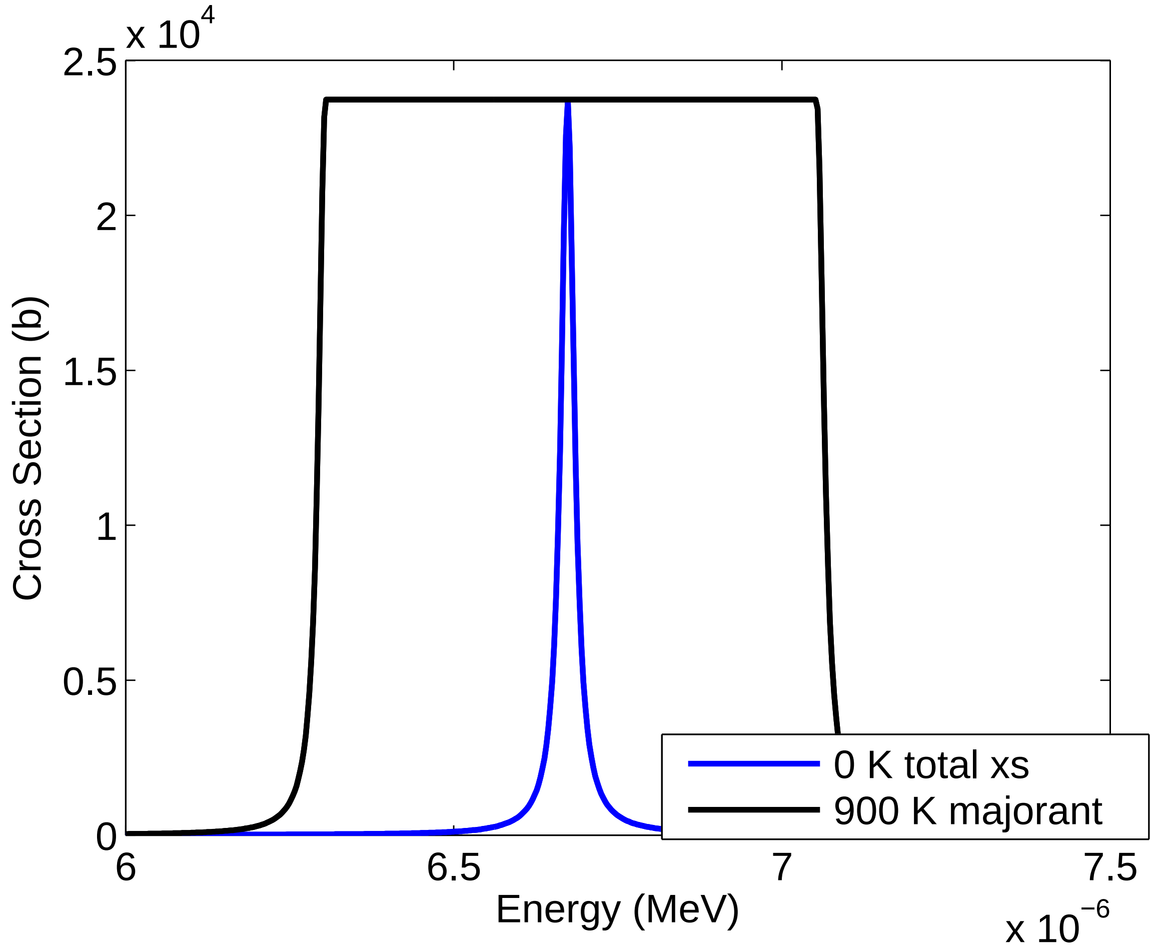


Figure 2: Majorant cross section equals the maximum total cross section within the range of thermal motion. (=range of possible target-at-rest energies)

RR: Target Motion Sampling (TMS) (2/2)

- XS data is first Doppler-broadened to $T_{\min,n}$ using the pre-processor (performance $\uparrow$).
- T is adjusted between $T_{\min,n}$ and $T_{\max,n}$ (majorant temperature) using TMS.
- Data is stored at one temperature only.
- Can model continuous T distributions (multi-physics interface and internal solvers)
- Burnup calculations slow down significantly, since macroscopic material cross sections cannot be pre-calculated.

RR: Summary

	Pre-processor	TMS
Use	`tmp XXX`	`tms XXX` or interface
Overhead in transport	1.000	1.2-12.0
XS memory requirement	$2-30$ GB per T	$2-30$ GB
Accuracy	$<$ original xs	$=$ original xs

- Thus, both techniques should usually provide the same results, but:
  - Using the pre-processor is significantly faster in burnup calculations and
  - TMS may save memory.

Thermal scattering of bound nuclei, “S(α, β)”

Thermal Scattering of bound nuclides (TS)

- The scattering kinematics and scattering cross sections of bound nuclides are strongly affected by the chemical bonds at thermal energies.
- The temperature dependence of bound-atom scattering is described in $S(\alpha, \beta)$ law.
  - Available in ENDF format in 50, 100 or 200 K intervals.
  - Can also be generated using LEAPR/NJOY, but...

For example, incoherent inelastic scattering:

$$\sigma(E \rightarrow E', \mathbf{\Omega} \cdot \mathbf{\Omega}', T) = \frac{\sigma_{\mathrm{b}}}{2kT} \sqrt{\frac{E'}{E}} e^{-\frac{\beta}{2}} S(\alpha, \beta, T) \quad (3)$$

- In ACE format, the $S(\alpha, \beta)$ data is processed into “elastic” and “inelastic” cross sections and associated secondary particle tables.

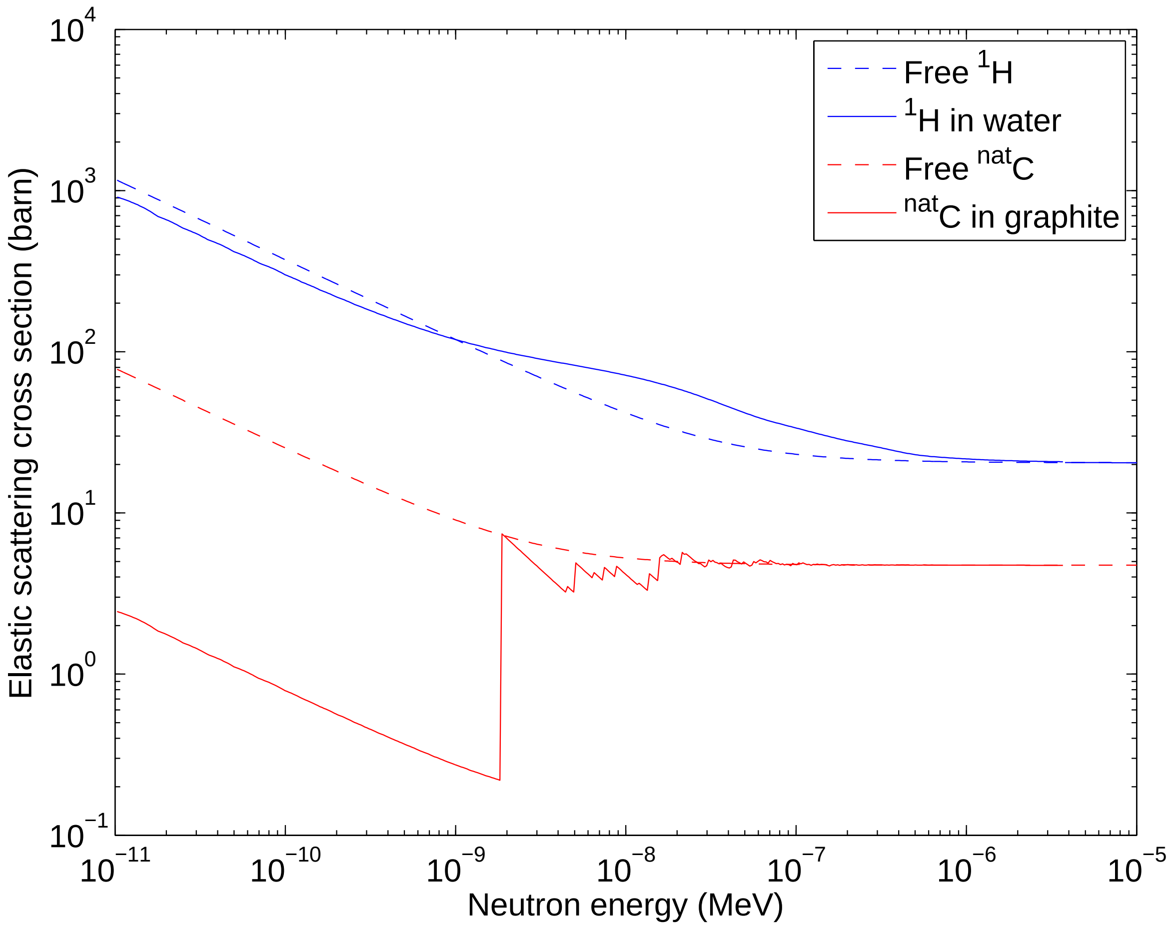
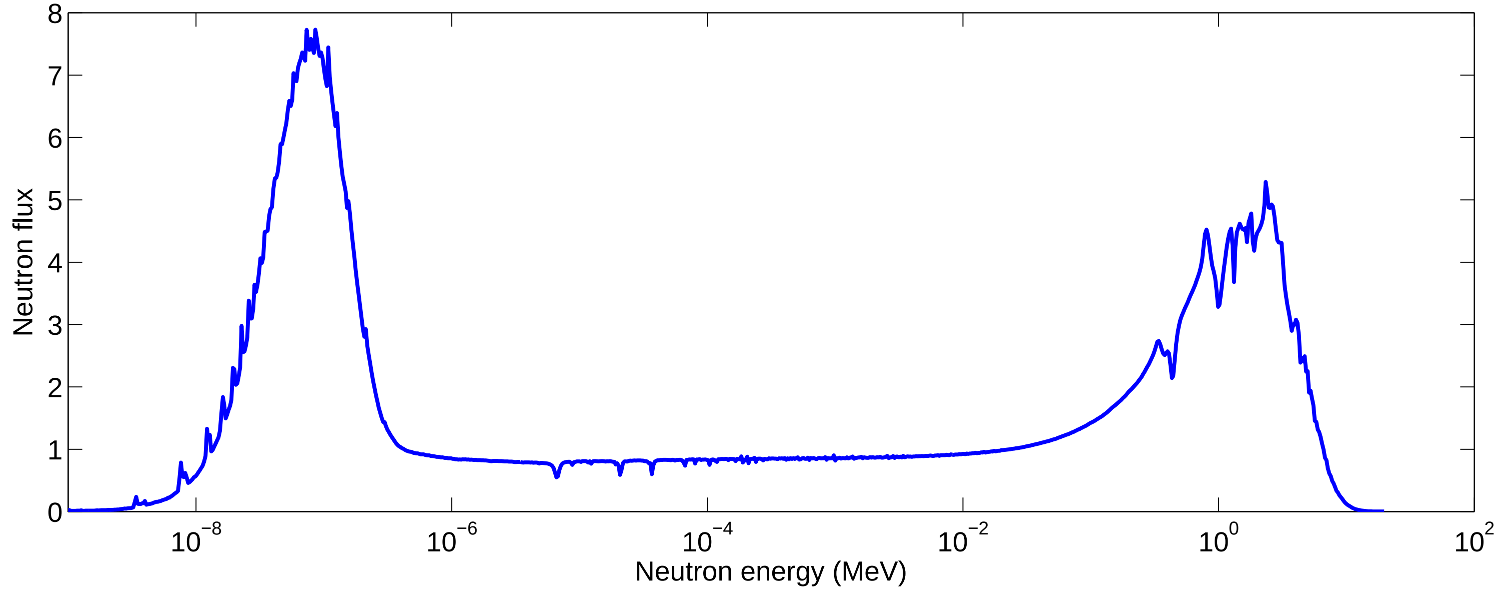


Figure 3: The integral scattering cross sections of H in light water and C in graphite are strongly affected by the molecular bonds and lattice structure.

TS: Thermal scattering in Serpent

- Serpent has always supported the discrete-in-energy thermal scattering, described in ACE data (`iwt=0` or `iwt=1` in NJOY)
  - However, the new continuous-in-energy formalism (`iwt=2`) is not yet supported.



TS: Interpolation of thermal scattering data

- Since the $S(\alpha,\beta)$ data is only available at certain temperatures and the scattering properties change quite significantly between the temperatures, the data should be interpolated somehow.
- Interpolation of $S(\alpha,\beta)$ data using functional fits has been studied recently by A. Pavlou [3]
  - \+ Minimal memory requirement
  - \- Only studied for incoherent inelastic scattering
  - \- Cannot be directly based on ACE data

[2] A. Pavlou and Wei Ji, “On-the-fly sampling of temperature-dependent thermal neutron scattering data for Monte Carlo simulations”, *Ann. Nucl. Energy*, **71**, pp. 411-426, (2014).

TS: Interpolation of thermal scattering data

- MAKXSF is an auxiliary ACE processing code distributed with MCNP.
  - Newest versions perform Doppler-broadening using SIGMA1 and
  - interpolation of thermal scattering data in ACE files using methodology from legacy code “DOPPLER”
- The TS interpolation methodology of MAKXSF has been implemented in Serpent 2.1.24.
  - Both pre-processing and on-the-fly capabilities are available.
  - Cross sections and secondary cosines are interpolated linearly in temperature.
  - Secondary energies are interpolated using a reciprocal law.
  - (old stochastic mixing approach still available)

TS: Howto?

```
mat water1 -1.00 tmp 524 moder lwtr1 1001
1001.03c 2.0
8016.03c 1.0
therm lwtr1 lwj3.09t % .09t = library for exactly 524 K
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

mat water2 -1.00 tmp 550 moder lwtr2 1001
1001.03c 2.0
8016.03c 1.0
therm lwtr2 550.0 lwj3.09t lwj3.11t % .09t = 524 K, .09t = 574 K
% thermstoch lwtr2 550.0 lwj3.09t lwj3.11t % old interpolation
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

mat water -1.00 tms 550 moder lwtr3 1001
1001.03c 2.0
8016.03c 1.0
therm lwtr3 0 lwj3.09t lwj3.11t lwj3.13t lwj3.14t
```

Summary & future prospects

- Serpent 2.1.24 has temperature treatment capabilities for:
  - The resonance region and thermal region of free atoms (pre-processor + TMS)
  - Bound-atom scattering (pre-processor & on-the-fly MAKXSF)
- Techniques are efficient and accurate enough for practical use.
- There are plans to expand TMS to the energy region of unresolved resonances.

Thank you for your attention!

Questions?

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References

[1] G. Yesilyurt, W.R. Martin and F.B. Brown, “On-the-fly Doppler broadening for Monte Carlo codes”, Nucl.Sci.Eng., 171, 239–257 (2012).

[2] B. Forget, S. Xu and K. Smith, “Direct Doppler broadening in Monte Carlo simulations using the multipole representation”, Ann. Nucl. Energy, **64**, 78–85, (2014).

[3] A. Pavlou and Wei Ji, “On-the-fly sampling of temperature-dependent thermal neutron scattering data for Monte Carlo simulations”, *Ann. Nucl. Energy*, **71**, pp. 411-426, (2014).

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

[5] 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).

[6] 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).

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

[8] 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.

[9] 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.