Temperature and density distributions in multi-physics calculations

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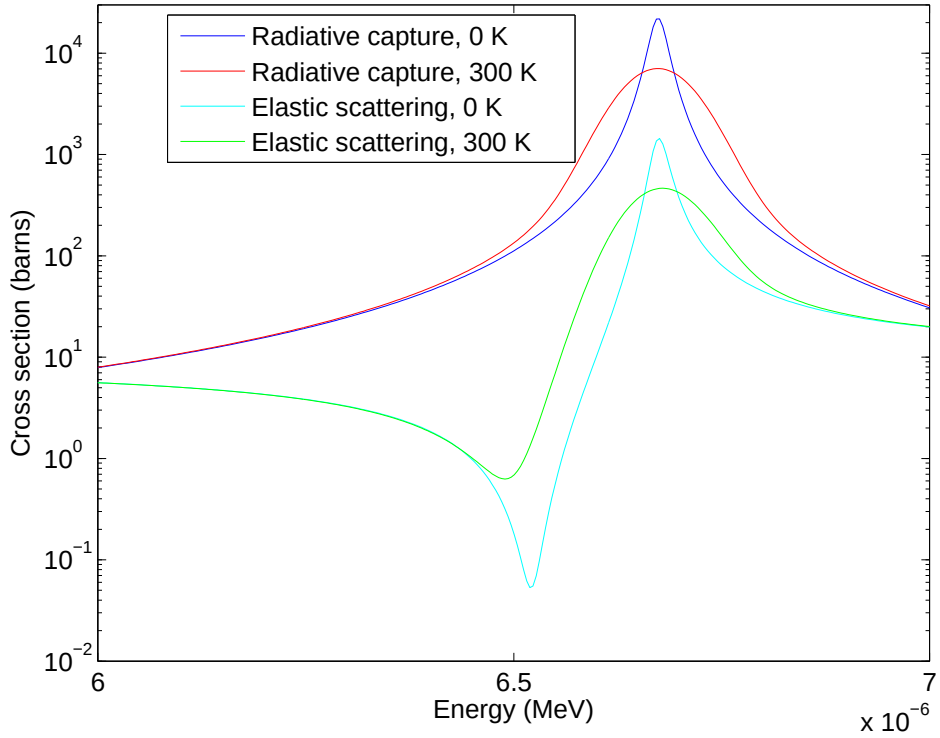
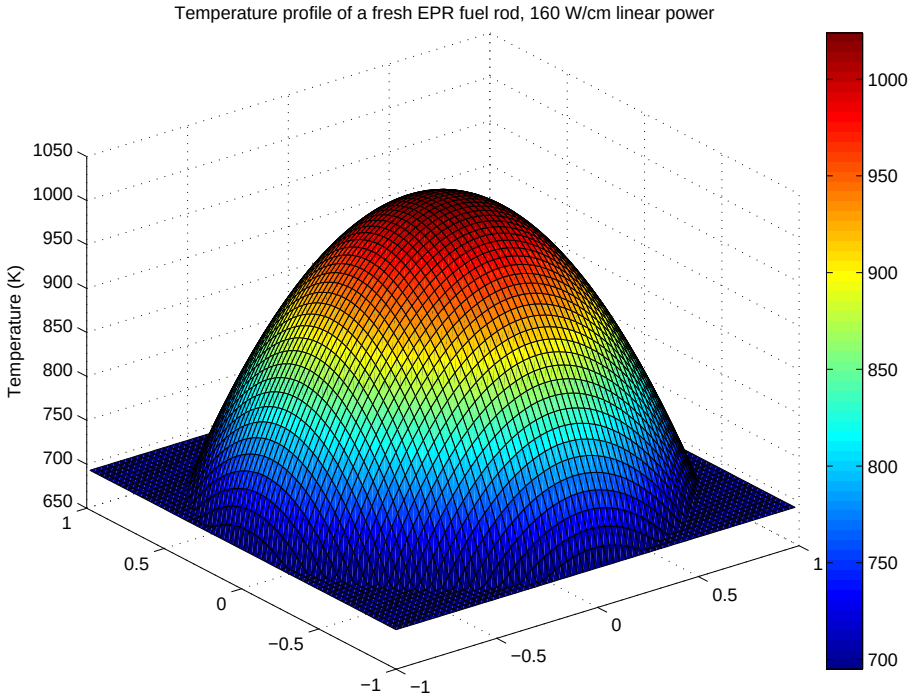
Outline

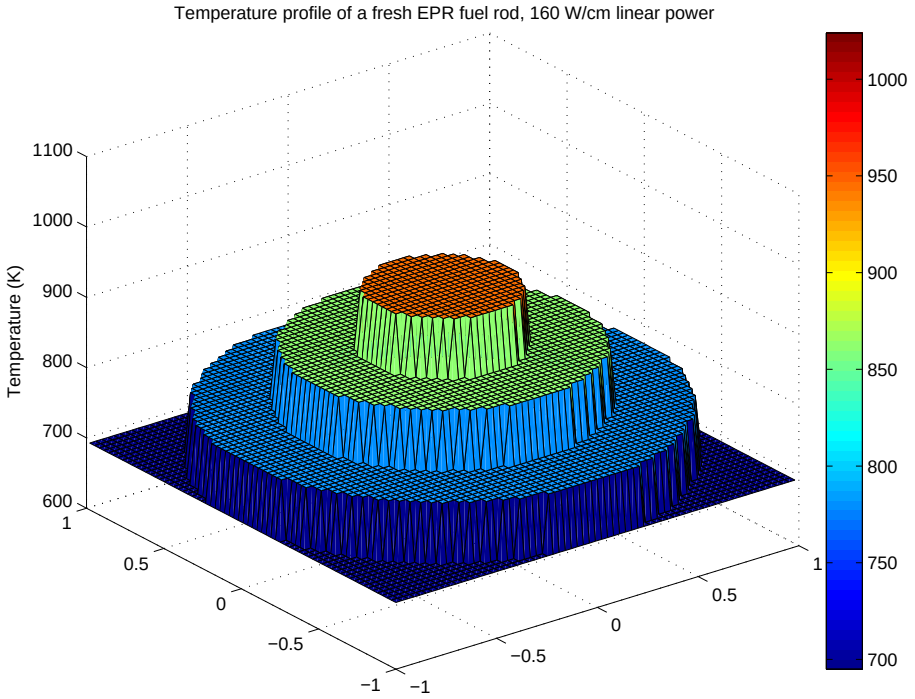
- Introduction
- Treating temperature and density distributions in Serpent
- Input options
- Performance

Introduction

- Temperature affects the neutron transport through:
  - Reaction probabilities (Doppler-broadening)
  - Scattering kinematics
  - Densities
  - (Material dimensions)
- In HFP conditions, densities and temperatures are distributed quantities.




Temperature profile of a fresh EPR fuel rod, 160 W/cm linear power
Temperature (K)
1050
1000
950
900
850
800
750
700
650
1
0.5
0
−0.5
−1
−1
−0.5
0
0.5
1
1000
950
900
850
800
750
700


Temperature profile of a fresh EPR fuel rod, 160 W/cm linear power
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1100
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900
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750
700

Rejection sampling and density/temperature distributions

- In Woodcock Delta-tracking, path lengths are sampled based on a majorant cross section Σ_{maj} and collisions are accepted with probability

$$P_{\mathrm{acc}} = \frac{\Sigma_{\mathrm{tot}}(E, \mathbf{r})}{\Sigma_{\mathrm{maj}}(E)} \tag{1}$$

- Basic requirement for majorant:

$$\Sigma_{\mathrm{tot}}(E, \mathbf{r}) \leq \Sigma_{\mathrm{maj}}(E) \forall E, \mathbf{r} \tag{2}$$

- The idea can be extended also to the modeling of density and temperature distributions, as it is done in the multi-physics interface of Serpent.
  - Modeling of density distribution has been described in Reference [1].
  - Temperature distributions are modeled with TMS [2].

[1] Leppänen, J. “Modeling of nonuniform density distributions in the Serpent 2 Monte Carlo code.” Nucl. Sci. Eng., 174, pp. 318-325 (2013).

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

Density distributions

- When applied in the modeling of density distributions, majorant cross section of a material corresponds to the largest atomic density $N(\mathbf{r})$ within the material, i.e.

$$N(\mathbf{r})\sigma_{\mathrm{tot}}(E) \leq \Sigma_{\mathrm{maj}}(E) \forall E, N \tag{3}$$

- Collision points are accepted with probability

$$P = \frac{N(\mathbf{r})\sigma_{\mathrm{tot}}(E)}{\Sigma_{\mathrm{maj}}(E)} \tag{4}$$

- Local densities $N(\mathbf{r})$ can also be defined as fractions of the maximum density $N(\mathbf{r}) = f(\mathbf{r})N_{\mathrm{max}}$
- In Serpent, density fields can be defined on a mesh, as pointwise averages or using user-defined functional dependence.

Temperature distributions of free atoms

- In TMS, thermal motion is handled by sampling the thermal motion of the target at each collision site and making a coordinate transform to target-at-rest frame.
- The majorant cross section is, again, defined as the maximum total cross section within a material

$$g(E) \max_{E_\mathrm{r} \in [E_\mathrm{min}(E), E_\mathrm{max}(E)]} \Sigma_\mathrm{tot}(E_\mathrm{r}, T_\mathrm{base}) \leq \Sigma_{\mathrm{maj},n}(E) \tag{5}$$

- Collision points are accepted at probability

$$P = \frac{g(E)\Sigma_{\mathrm{tot},n}(E_\mathrm{r}, T_\mathrm{base} < T(\mathbf{r}))}{\Sigma_{\mathrm{maj},n}(E)} \tag{6}$$

E_r corresponding to the target-at-rest energy.

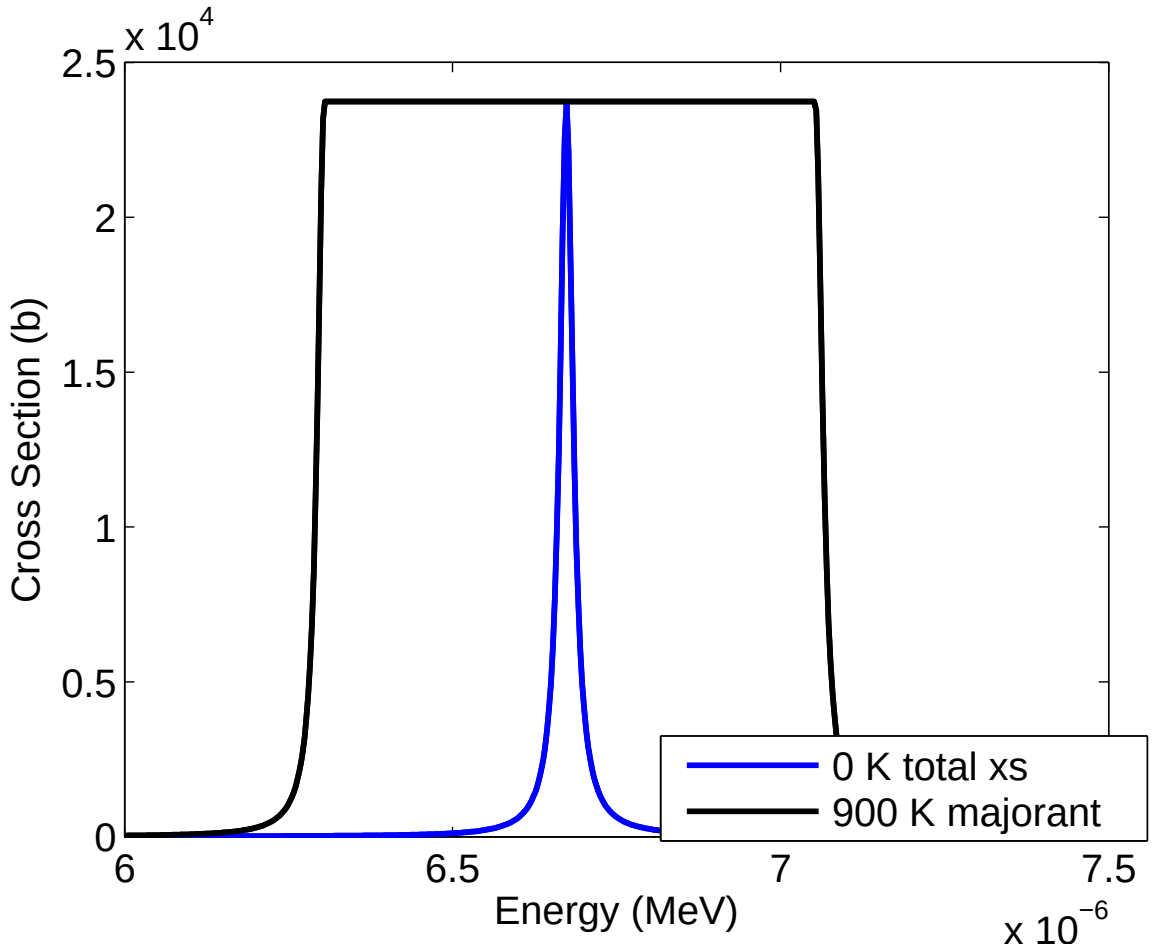

Figure 1: Majorant cross section equals the maximum total cross section within the range of thermal motion. (=range of possible target-at-rest energies)

Temperature distributions of bound atoms

- If also the thermal scattering effects emerging from molecular bonds need to be taken into account, the TMS tracking scheme is further complicated.
- With thermal scattering reactions, the majorant cross section looks like this:

$$\begin{aligned}\Sigma_{\mathrm{maj},n}(E) &= g(E) \max_{E_\mathrm{r}\in[E_\mathrm{min}(E),E_\mathrm{max}(E)]} \left(\Sigma_{\mathrm{tot},n}(E_\mathrm{r},T_\mathrm{base}) - \Sigma_{\mathrm{s},n}(E_\mathrm{r},T_\mathrm{base})\right) \\ &+ \max_{T\in[T_\mathrm{min},T_\mathrm{max}]} \sum_{i=1}^{NTS_n} \Sigma_{i,n}(E,T) \end{aligned} \tag{7}$$

- Serpent interpolates the thermal scattering data on-the-fly using `makxsf` methodology
- More information on Tuesday 11:25 @ Columbine

Why on earth do we voluntarily add extra collisions in transport?

- Transport does not stop at every surface in Woodcock Delta-tracking (geometry-related):

  $\rightarrow$ Reduced computational effort and memory access when transporting in detailed geometries.

- When modeling density/temperature distributions with rejection sampling techniques, the density and temperature fields can be independent of material boundaries.

  $\rightarrow$ Facilitates coupled calculations.

  $\rightarrow$ Enables modeling of continuous distributions as-is.

Input instructions

- Usually, it is practical to model complicated temperature- and density distributions via the multi-physics interface (Ville's talk)
- Temperature distributions can be modeled also without the interface by adding keywords in the material definitions.
  - May save memory!

```
mat fuel_400K -10.0 tms 400
92235.03c 0.05
92238.03c 0.95
8016.03c 2.0
```

```
mat fuel_500K -10.0 tms 500
92235.03c 0.02
92238.03c 0.98
8016.03c 2.0
```

Input insctructions: thermal scattering

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

Effects on performance

- Modeling density distributions with rejection sampling has some effect on the performance
  - Mesh-based input and functional fit are faster with 10 % overhead (strongly problem-dependent!)
  - Pointwise average is slower with 30 % overhead
- TMS transport slows down the calculation somewhat, mainly because macroscopic material cross sections cannot be pre-calculated.
  - Overhead is about 20 % in fresh fuel problems
  - Overhead increases up to 12x in problems with burned fuel
  - Introducing thermal scattering data in TMS transport does not affect the performance in practice.
  - With TMS transport the memory requirement does not depend on the temperature distributions.

When to use the rejection techniques?

- In problems with just a few temperatures or densities, writing the distributions in the ordinary input is the most efficient:
  - Cross sections can be Doppler-broadened using the `tmp` card without any loss in efficiency as long as the memory is sufficient.
  - Thermal scattering data can be inteprolated in pre-processing phase.
- In serious multi-physics modeling, for instance when coupling Serpent with external solvers, the multi-physics interface (which utilizes TMS) should be used.
  - The small increase in CPU time is usually well-worth the savings in workload and memory requirement of the calculations.

Thank you for your attention!

Questions?

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References

[1] Leppänen, J. “Modeling of nonuniform density distributions in the Serpent 2 Monte Carlo code.” Nucl. Sci. Eng., 174, pp. 318-325 (2013).

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