On-The-Fly Interpolation for Thermal Scattering in MCS

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1. Introduction

The on-the-fly Doppler broadening has been actively studied in the Monte Carlo community for multi-physics simulation. The multipole based on-the-fly broadening method for resolved resonance energy has been studied and implemented in MCS [1-2].

The makxsf [3] is often used to generate the thermal scattering data. Makxsf pre-processes the thermal scattering data by interpolating the two data sets at lower and higher temperature [4].

The OTF interpolation capability for thermal scattering data has been implemented into MCS with the same interpolation assumption as used in makxsf. In this paper, the implemented method will be verified against three benchmark problems containing light water and graphite.

2. Method

When applying On-The-Fly(OTF) interpolation, MCS reads two thermal data sets, at lower and higher temperature data, D_{low} and D_{high}, than the target temperature. The cross section at the target temperature T ($T_{low} < T < T_{high}$) is interpolated as shown in Eqs. (1-2) by assuming a linear relation.

$$f = \frac{T_{high} - T}{T_{high} - T_{low}} , \tag{1}$$

$$\sigma_T = f\sigma_{T\_low} + (1-f)\sigma_{T\_high} . \tag{2}$$

Algorithm OTF interpolation collision kernel

```
f = (T_high – T)/(T_high – T_low)
seed0 = get_random_seed
[E_low, uvw_low] = collision_kernel (D_low)
change_seed(seed0)
[E_high, uvw_high] = collision kernel (D_high)

E_out = 1/(f/E_low + (1-f)/E_high)
if  (GetRN() < f)
   uvw_out = uvw_low
else
   uvw_out = uvw_high
end if
```

Fig. 1. Algorithm of OTF interpolation collision kernel.

When sampling outgoing information, the outgoing direction vector uvw_{out} can be assumed to have a linear relation with outgoing energy sampled from lower and higher temperature data: uvw_{low} and uvw_{high}. However, the outgoing energy should be interpolated as shown in Eq. (3) since outgoing energy is inversely proportional to the temperature [4].

$$E_{out} = \left(\frac{f}{E_{low}} - \frac{1-f}{E_{high}} \right) . \tag{3}$$

The same random number must be used for the sampling of outgoing information from lower and higher data since the outgoing energy and angle is sampled with random number. The OTF interpolation can be easily implemented by using existing routine as shown in Fig. 1.

3. Results

Three problems were tested to verifiy the accuracy of the OTF interpolation and to demonstrate its efficiency. All simulations were performed on a Linux cluster (Intel Xeon 3250 @ 3.00GHz) using the ENDF-VII.0 library.

3.1 INDC Pin

The half-inch pin in the INDC (USA)-107 benchmark problem was selected to test thermal scattering of light water since it shows large differences depending on thermal scattering data while it has very simple geometry and material composition [5] as shown in Fig. 2. The original benchmark temperature is 293.6K, but the temperature was changed to 600K for the interpolation test and Makxsf.

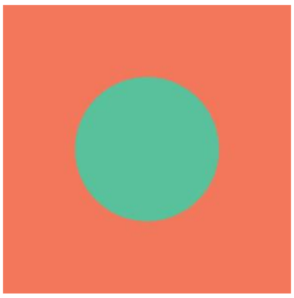

Fig. 2. INDC benchmark half-inch pin.

Three cases were simulated to verify the OTF interpolation. All cases use the same cross section data but different thermal scattering data.

- NJOY: with 600K data processed by NJOY
- Makxsf: with 600K data interpolated using 550K and 650K data by Makxsf
- OTF: OTF interpolation using 550K and 650K data

The true reference here is the NJOY data. However, the OTF interpolation must follow the results of Makxsf since it uses the same approximation. As shown in Table I, OTF and Makxsf agree very well while both methods underestimate about 15 pcm in comparison to NJOY. An overhead of about 14% is observed in the OTF results since this benchmark is a very simple problem which contains only 2 nuclides in water and 2 nuclides in the fuel. The overhead will decreases when applying it to a realistic problem.

Table I: Simlation results of INDC half-pitch pin

Case	k_{eff}	SD	Diff. (pcm)	Time
NJOY	1.00757	0.00001	-	1.00
Makxsf	1.00743	0.00001	-14	1.01
OTF	1.00741	0.00001	-16	1.14

Fig. 3. shows the flux spectrum comparison result. The OTF result matches well with the result of Makxsf, and both results are slightly different from the reference NJOY result.

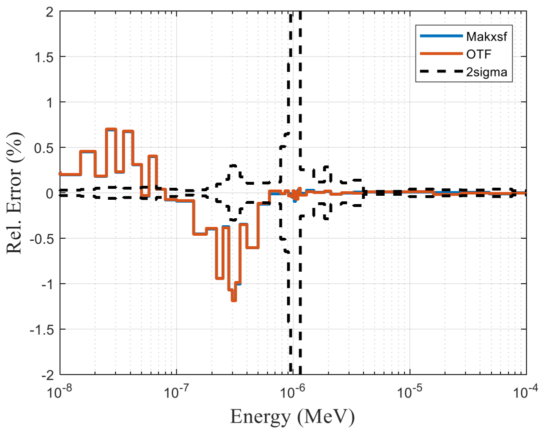

Fig. 3. Flux spectrum relative error of INDC half-pitch pin in moderator region.

3.2 VERA-1C

The VERA benchmark hot zero power beginning of cycle pin-cell problem 1C was selected to test OTF interpolation [6]. Fig. 4 shows the VERA-1C pin geometry. The fuel temperature is 900K and the cooland temperature is 600K.

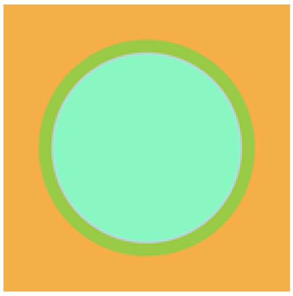

Fig. 4. VERA-1C pin.

Here again, three cases were simulated using same ACE files but thermal data.

- NJOY: with 600K data processed by NJOY
- Makxsf: with 600K data interpolated using 550K and 650K data by Makxsf
- OTF: OTF interpolation using 550K and 650K data

Table II shows the multiplication factor of three cases, and the OTF result matches well with Makxsf and NJOY within statistical uncertainty. Fig. 5 shows the flux spectrum error in the moderator range. OTF result agrees well with Makxsf.

Table II: Simlation results of VERA-1C pin

Case	k_{eff}	SD	Diff. (pcm)	Time
NJOY	1.17402	0.00012	-	1.00
Makxsf	1.17414	0.00011	12	0.99
OTF	1.17402	0.00013	0	1.01

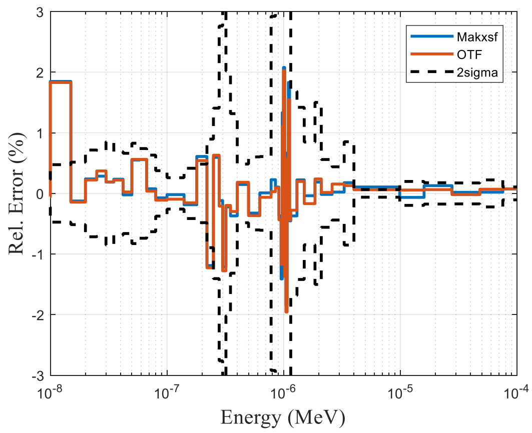

Fig. 5. Flux spectrum relative error of VERA-1C pin in moderator region.

3.3 PMR-200

The PMR-200 compact with 23.5% packing fraction unit cell was selected to test thermal scattering of graphite [7]. Fig. 6 shows the configureation of the PMR-200 compact.

Three cases were simulated to verify the OTF interpolation. All cases use the same cross section data but different thermal scattering data.

- NJOY: with 1000K data processed by NJOY
- Makxsf: with 1000K data interpolated using 800K and 1200K data by Makxsf
- OTF: OTF interpolation using 800K and 1200K data

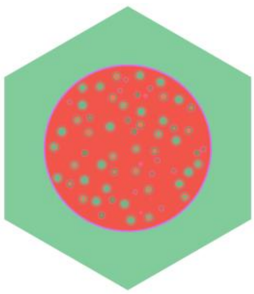

Fig. 6. PMR-200 unit cell with 23.5 packing fraction compact.

Table III and Fig. 7 show the simulation result and spectrum comparison. Here again, OTF and Makxsf agree with each other very well.

Table III: Simlation results of PMR-200 compact

Case	k_{eff}	SD	Diff. (pcm)	Time
NJOY	1.28546	0.00004	-	1.00
Makxsf	1.28551	0.00004	5	1.00
OTF	1.28555	0.00004	9	1.02

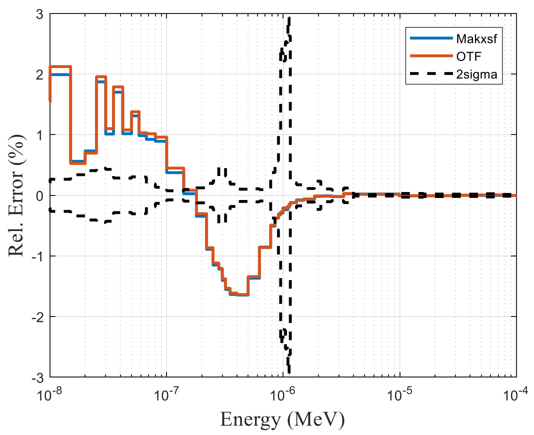

Fig. 7. Flux spectrum relative error of PMR-200 compact in moderator region.

4. Conclusions

The OTF interpolation module for thermal scattering cross section has been implemented in MCS. The OTF capability has also been tested and verified against INDC benchmark, VERA benchmark, and PMR-200 benchmark cases, which contain light water and graphite. The OTF and makxsf agree very well, as expected.

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