On-The-Fly Interpolation for Thermal Scattering in MCS

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Reactor Physics General II (301)

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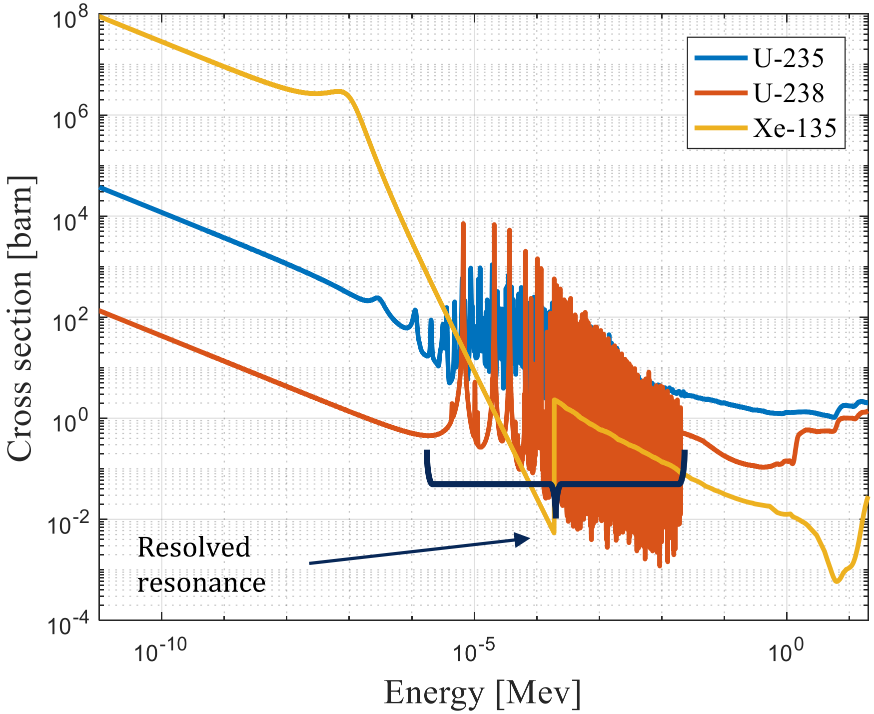
Overview

Overview

- **Resolved resonance energy range**
  - **Windows Multipole**
  - **Target Motion Sampling**
  - **Interpolation**
  - **SIGMA1**
  - **Gauss-Hermite**

Doppler Broadened Cross-section

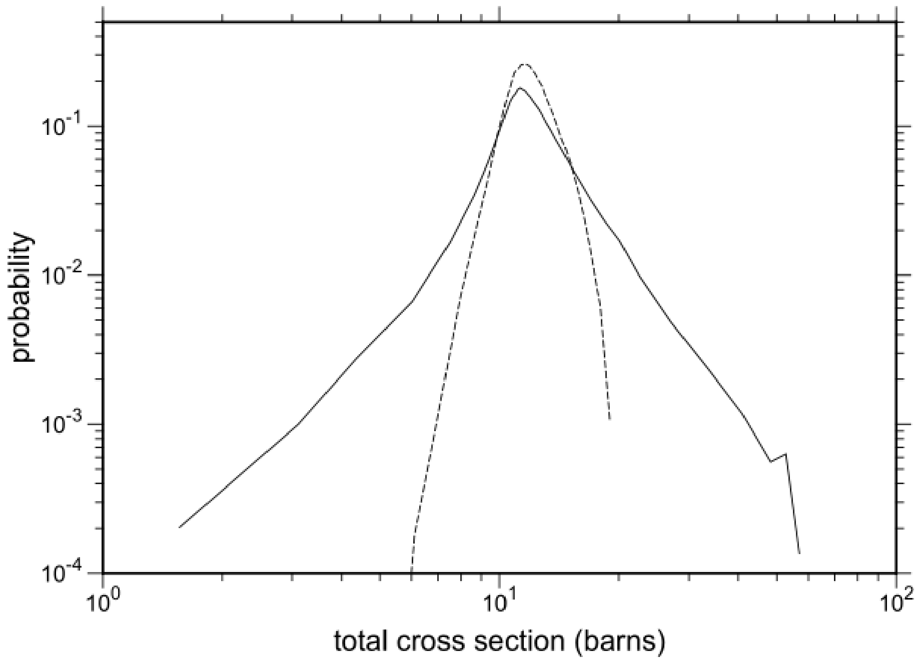
$$\bar{\sigma}(v) = \frac{\alpha^{1/2}}{\pi^{1/2} v^2} \int_0^\infty \sigma(V) V^2 \left\{ e^{-\alpha(V-v)^2} - e^{-\alpha(V+v)^2} \right\} dV$$



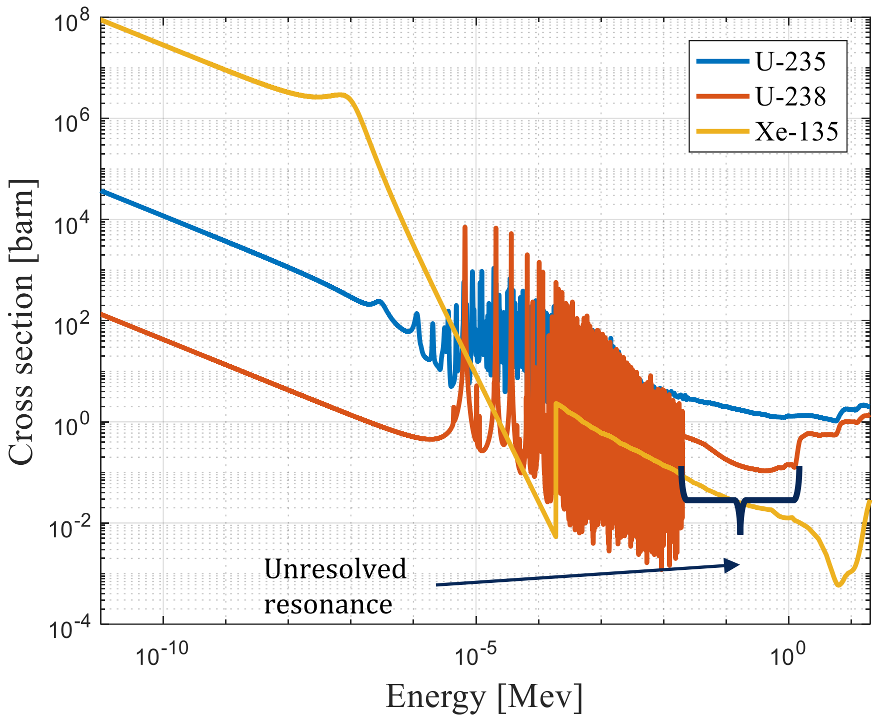
Overview

- **In the unresolved energy range**
  - **Average and variance of resonance parameters are given**
  - **Interpolation**
  - **Sampling Resonance Parameter**

Probability distribution for total cross section at 20 keV (solid) and 140keV (dashed) of ^{238}U



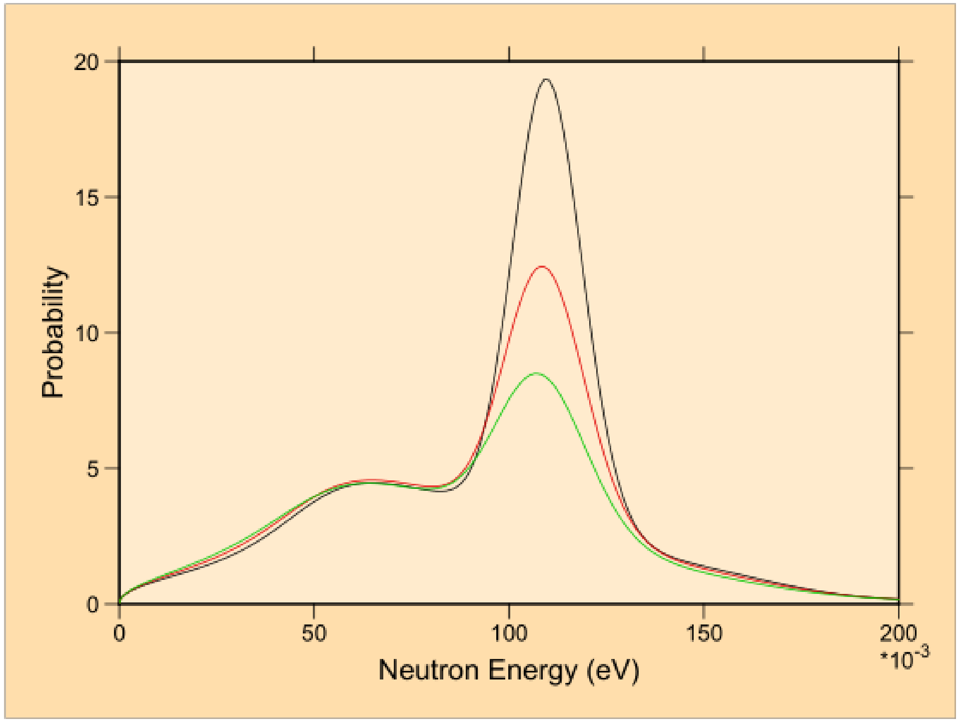
Absorption cross section of ^{235}U, ^{238}U and ^{135}Xe



Overview

- **Thermal Scattering (bond scattering)**
  - **Interpolation**
    - Makxsf (from MCNP)
    - LEAPR (NJOY)

Distribution of outgoing energy with incident energy of 0.115 eV for H in H_2O. (black = 51.3 deg, red = 60 deg, green = 68 deg)



Overview

- **MCS OTF cross-section treatment**

- **Unresolved resonance energy range**
  - **Windows multipole**
  - **SIGMA1 (ongoing)**
  - **Interpolation**

- **Probability-table**
  - **Interpolation**

- **Thermal scattering**
  - **Interpolation**

On-The-Fly Interpolation

On-The-Fly Interpolation

- **MCS follows Makxsf interpolation scheme**

- **Makxsf is utility program for manipulating cross-section library for MCNP5**
  - **Doppler broadening for resolved resonance data by SIGMA1 kernel**
  - **Interpolation of unresolved resonance probability-table data**
  - **Interpolation of S(α,β) thermal scattering data**

- **Interpolation scheme used for Unresolved resonance range**
  - **ACE format outgoing information is not temperature dependent**
  - **Log-lin interpolation for cross-section**

$$\sigma(T) = f \cdot \sigma(T_{low}) + (1 - f) \cdot \sigma(T_{high}) \qquad f = \frac{\ln(T_{high}) - \ln(\mathrm{T})}{\ln(T_{high}) - \ln(T_{low})}$$

On-The-Fly Interpolation

- **Interpolation scheme used for Thermal Scattering Data**
  - **Lin-lin interpolation for cross-section**
  - **Lin-Lin interpolation for outgoing angle**
  - **Reverse lin-lin interpolation for outgoing energy**
    - Outgoing energy distribution is reversely proportional to temperature

$$f = \frac{T_{high} - T}{T_{high} - T_{low}} \qquad E_{out} = \left(\frac{f}{E_{low}} - \frac{1-f}{E_{high}} \right)^{-1}$$

  - **The energy and angle are depends on**
    - Incoming energy
    - Random number (0, 1]
  - **Grid will be different for different temperature**

On-The-Fly Interpolation

- **OTF interpolation can be implemented by using existing kernel**

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})
$E_{out} = 1/(f/E_{low} + (1\text{-}f)/E_{high})$
if (GetRN() < f)
  $uvw_{out} = uvw_{low}$
else
$uvw_{out} = uvw_{high}$
end if

Verification

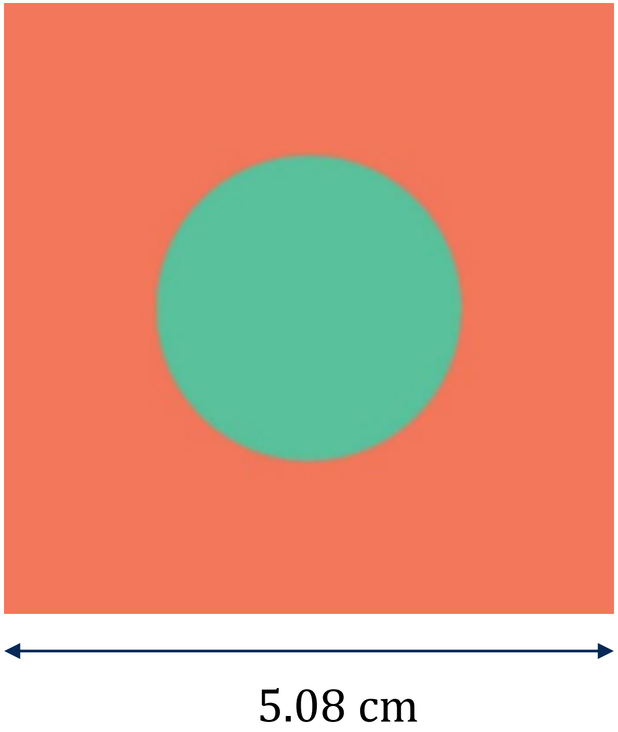
INDC Benchmark
VERA-1C
PMR Compact

INDC Benchmark

▪ INDC Benchmark

- Pin cell benchmark designed to test thermal scattering capability
- Pure water with density of 1g/cm^3
- Temperatures of all regions are 293.6K

Case	ZA	Density (#/barn-cm)
1/2″ pin	92235	4.6614E-04
	92238	4.7099E-02
1/4″ pin	92235	1.6653E-03
	92238	4.5915E-02
1/8″ pin	92235	3.3589E-02
	92238	1.4395E-02

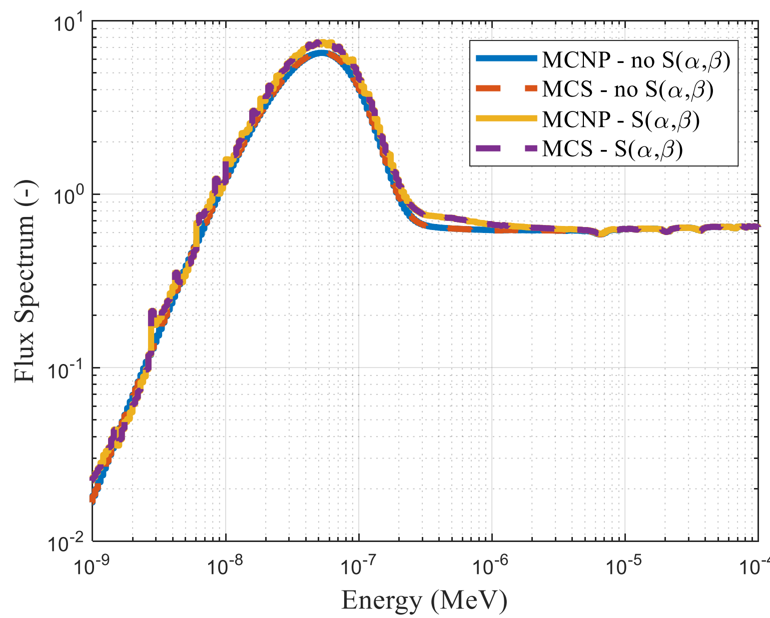


D.E. Cullen, R.N. Blomquist, C. Dean, et al., "How Accurate Can We Calculate Thermal Systems?," INDC(USA)-107, International Nuclear Data Committee, 2004

▪ Verification of MCS S(α,β)

Case	MCNP	SD	MCS	SD	Diff. (pcm)
1/2″ no S(α,β)	1.01649	0.00004	1.01658	0.00004	-9
1/2″ S(α,β)	0.96812	0.00004	0.96806	0.00004	6
1/4″ pin no S(α,β)	1.01320	0.00016	1.01359	0.00017	-39
1/4″ pin S(α,β)	0.92197	0.00017	0.92214	0.00019	-17
1/8″ pin no S(α,β)	1.01320	0.00021	1.01327	0.00024	-7
1/8″ pin S(α,β)	0.90950	0.00021	0.90895	0.00023	55

Flux Spectrum of ½″ pin



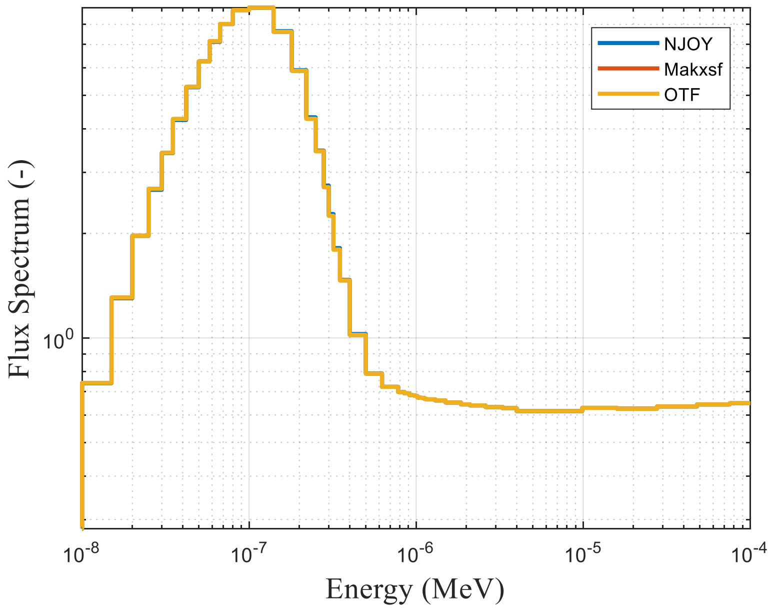
INDC Benchmark

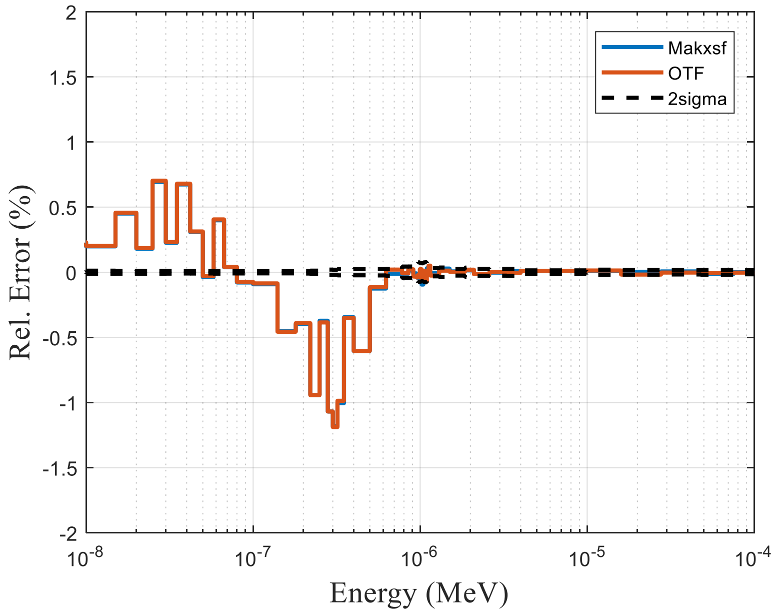
- **For the Test the temperature has changed to 600K**
  - **Since thermal scattering data of light water exist from 293.6K**
- **Three cases (half inch problem)**
  - **NJOY: 600K thermal scattering data processed by NJOY**
  - **Mkaxsf: 600K data interpolated using 550K and 650K by makxsf**
  - **OTF: OTF interpolation using 550K and 650K data**
- **# of nuclides = 4**

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**

INDC Benchmark

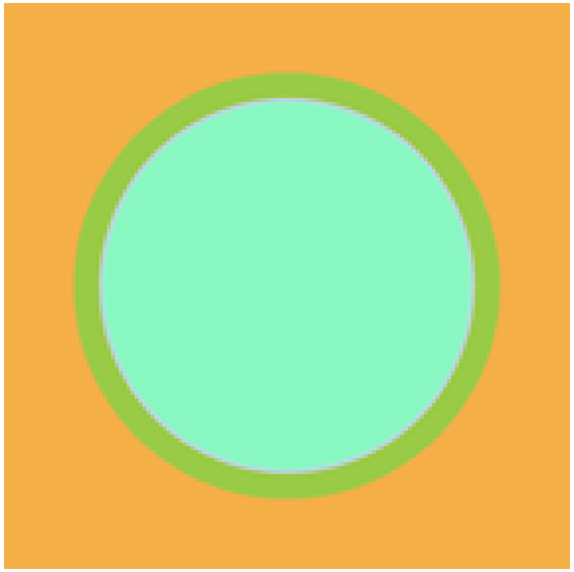
- **Relative error of flux spectrum and 2sigma standard deviation**





VERA-1C Benchmark

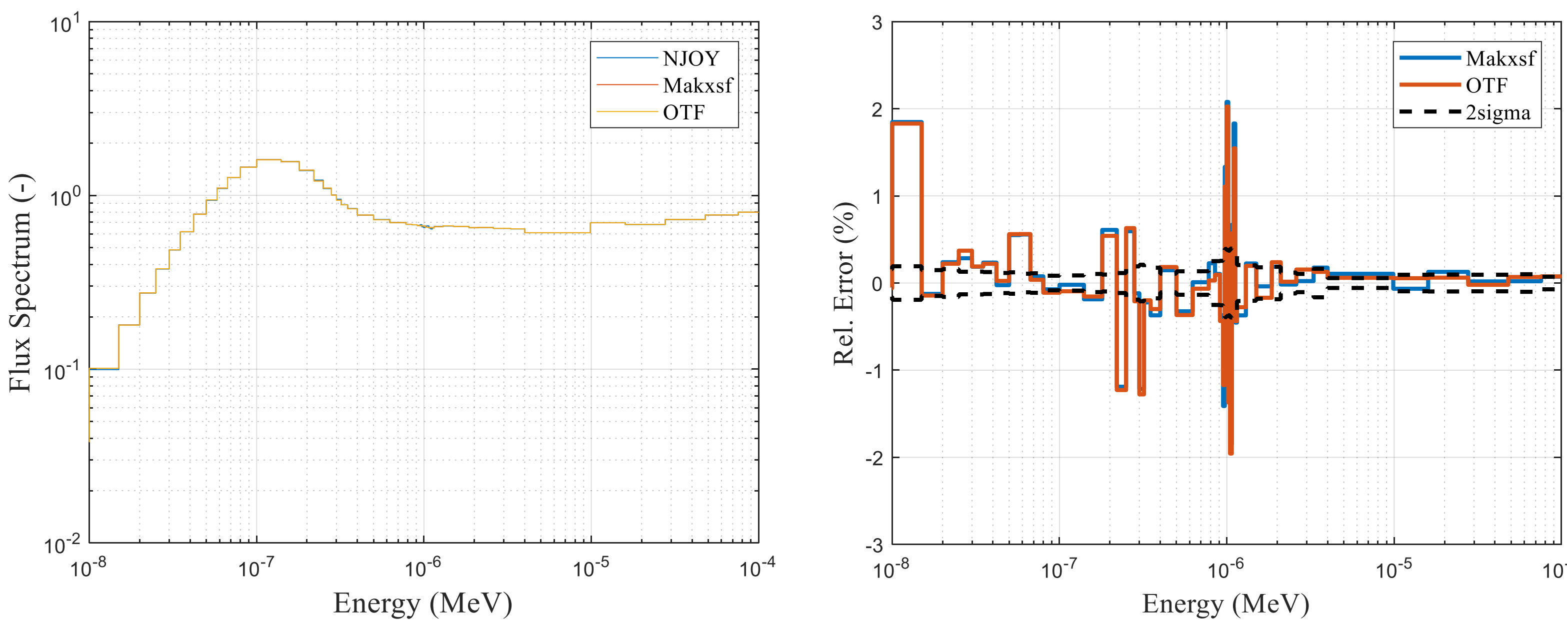
- VERA-1C benchmark
  - Fuel temperature is 900K
  - Others are 600K
  - # of nuclides = 40
  - All nuclides are treated with same ACE files but lwtr thermal scattering data
    - NJOY: with 600K data processed by NJOY
    - Makxsf: with 600K data interpolated using 550K and 650K data by Makxsf
    - OTF: OTF interpolation using 550K and 650K data



VERA-1C Benchmark

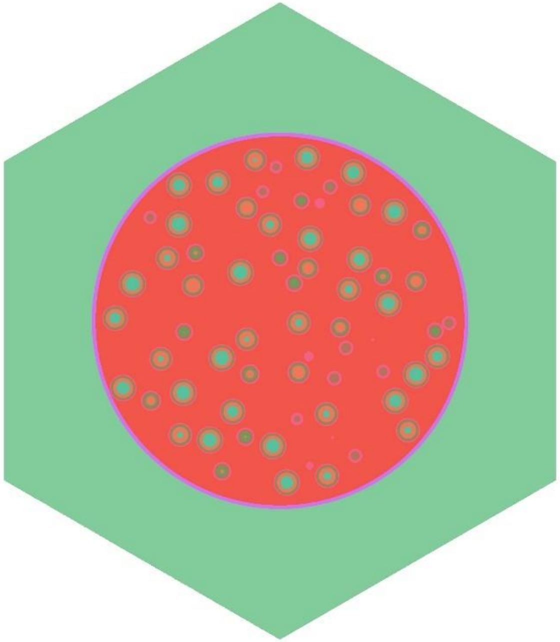
Case	k_{eff}	SD	Diff. (pcm)	Time
NJOY	1.17402	0.00012	-	1.00
Makxsf	1.17414	0.00011	12	0.99
OTF	1.17402	0.00013	0	1.01

Relative error of flux spectrum in coolant region



PMR-200 Compact

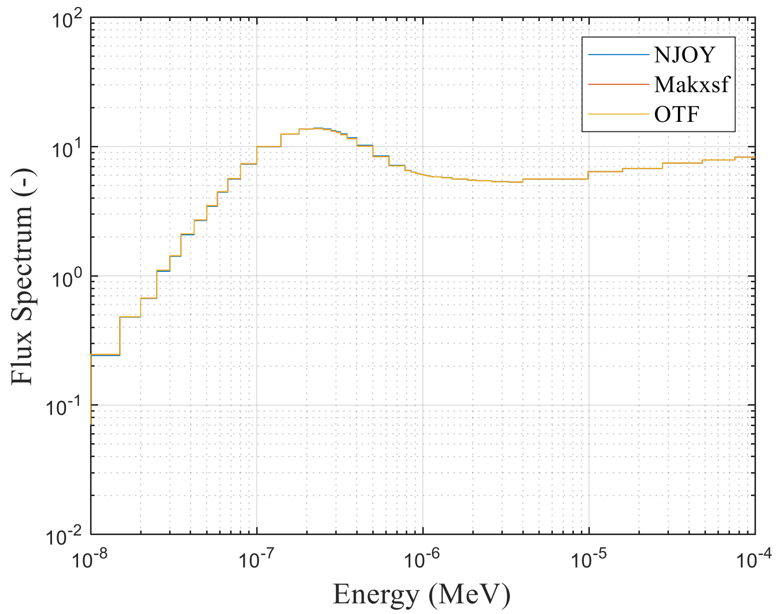
- **PMR-200 compact with 23.5% packing fraction**
  - **1000K is used for all regions**
  - **All nuclides are treated with same ACE files but graphite thermal scattering data**
    - **NJOY: with 1000K data processed by NJOY**
    - **Makxsf: with 1000K data interpolated using 800K and 1200K data by Makxsf**
    - **OTF: OTF interpolation using 800K and 1200K data**

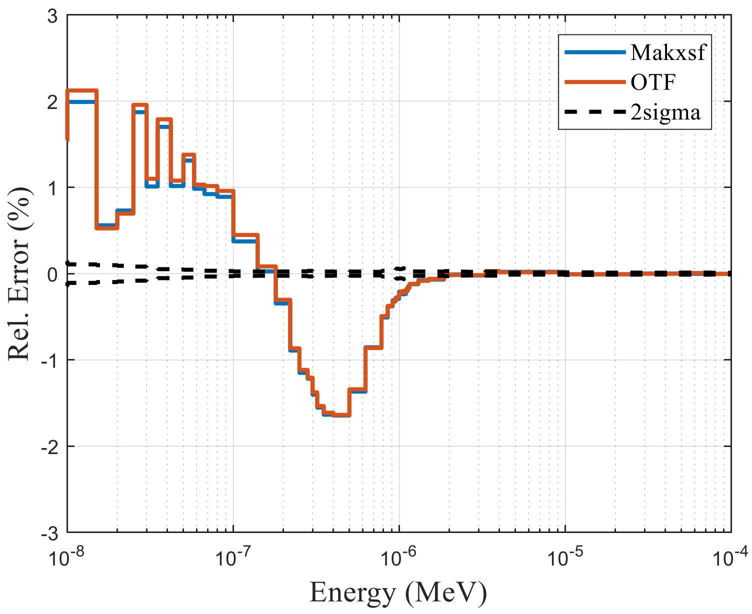


PMR-200 Compact

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

Relative error of flux spectrum in coolant region



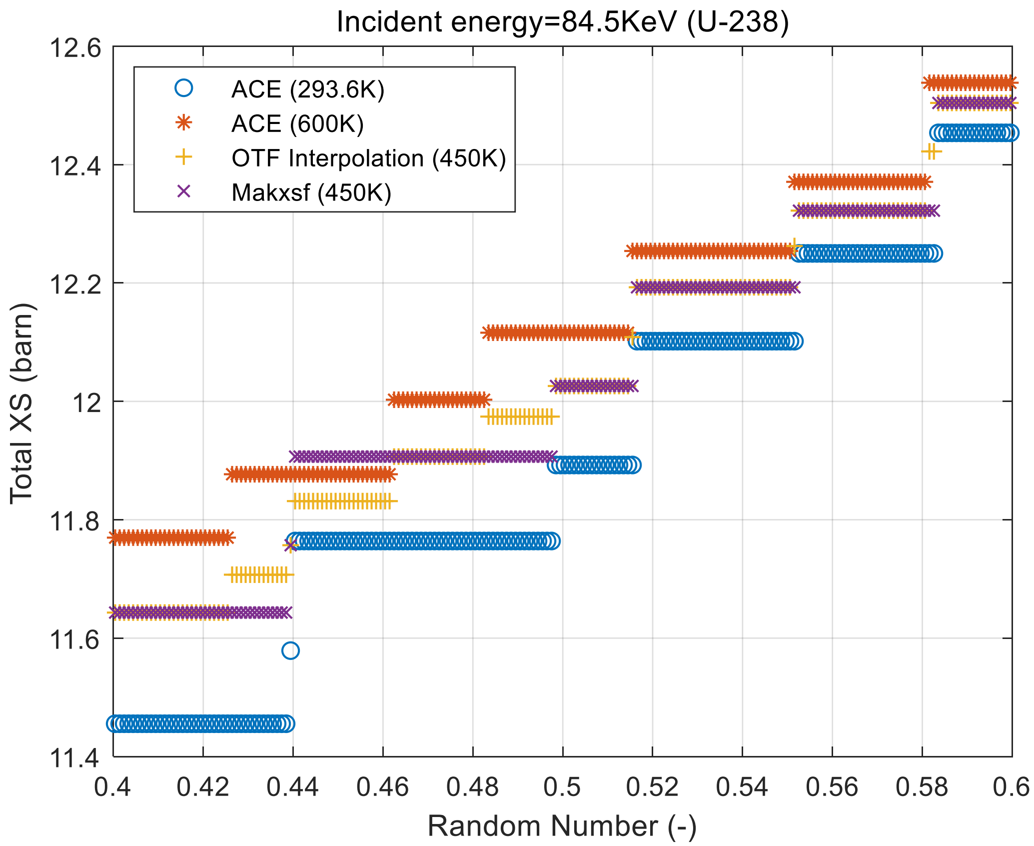


On-The-Fly Interpolation For Probability-Table

OTF Interpolation

- **Log-lin interpolation scheme**

$$\sigma(T) = f \cdot \sigma(T_{low}) + (1 - f) \cdot \sigma(T_{high}) \qquad f = \frac{\ln(T_{high}) - \ln(\mathrm{T})}{\ln(T_{high}) - \ln(T_{low})}$$



OTF Interpolation

Algorithm OTF interpolation of ptable

$f = (\ln(T_{high}) - \ln(T))/(\ln(T_{high}) - \ln(T_{low}))$
seed0 = get_random_seed
XS_{low} = get_xs (D_{low})
change_seed(seed0)
XS_{high} = get_xs (D_{high})
$XS = \mathrm{f}\ XS_{low} + (1\text{-}f)XS_{high})$

Summary

- **On-The-Fly Interpolation Function is implemented**
  - **Thermal scattering**
    - Lin-lin for cross-section
    - Lin-lin for outgoing angle
    - Reverse lin-lin for outgoing energy
  - **Probability-table**
    - Log-lin for cross-section
  - **Cross-sections**
    - Sqrt-lin for cross-section

- **OTF function is tested on**
  - **INDC pin, VERA-1C, PMR-200 compact**

- **OTF XS matches well with Makxsf while the computing cost is negligible**

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