How accurately can we calculate neutrons slowing down in water

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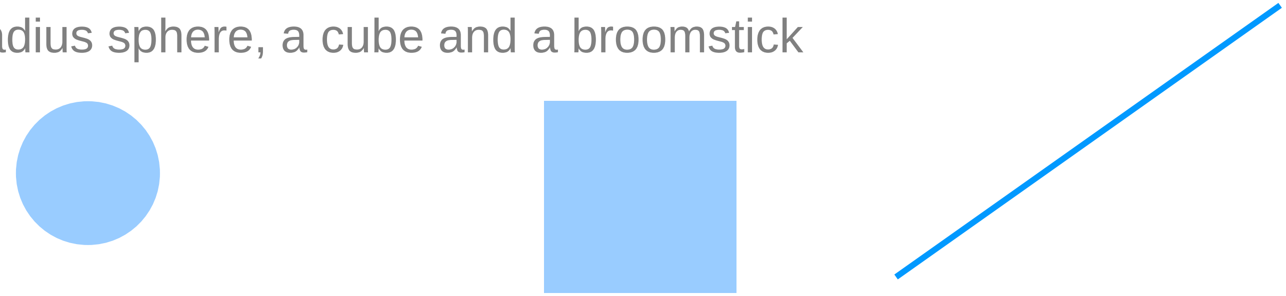
The Tools

- A 30 cm radius sphere, a cube and a broomstick



- 2 atoms of H1 and one of O16
- ONLY ENDF/B-VI release 8 nuclear data, at 293.6 K to start with
- A time independent, isotropic point source at the centre of the sphere, monoenergetic with an energy of 14.1 Mev

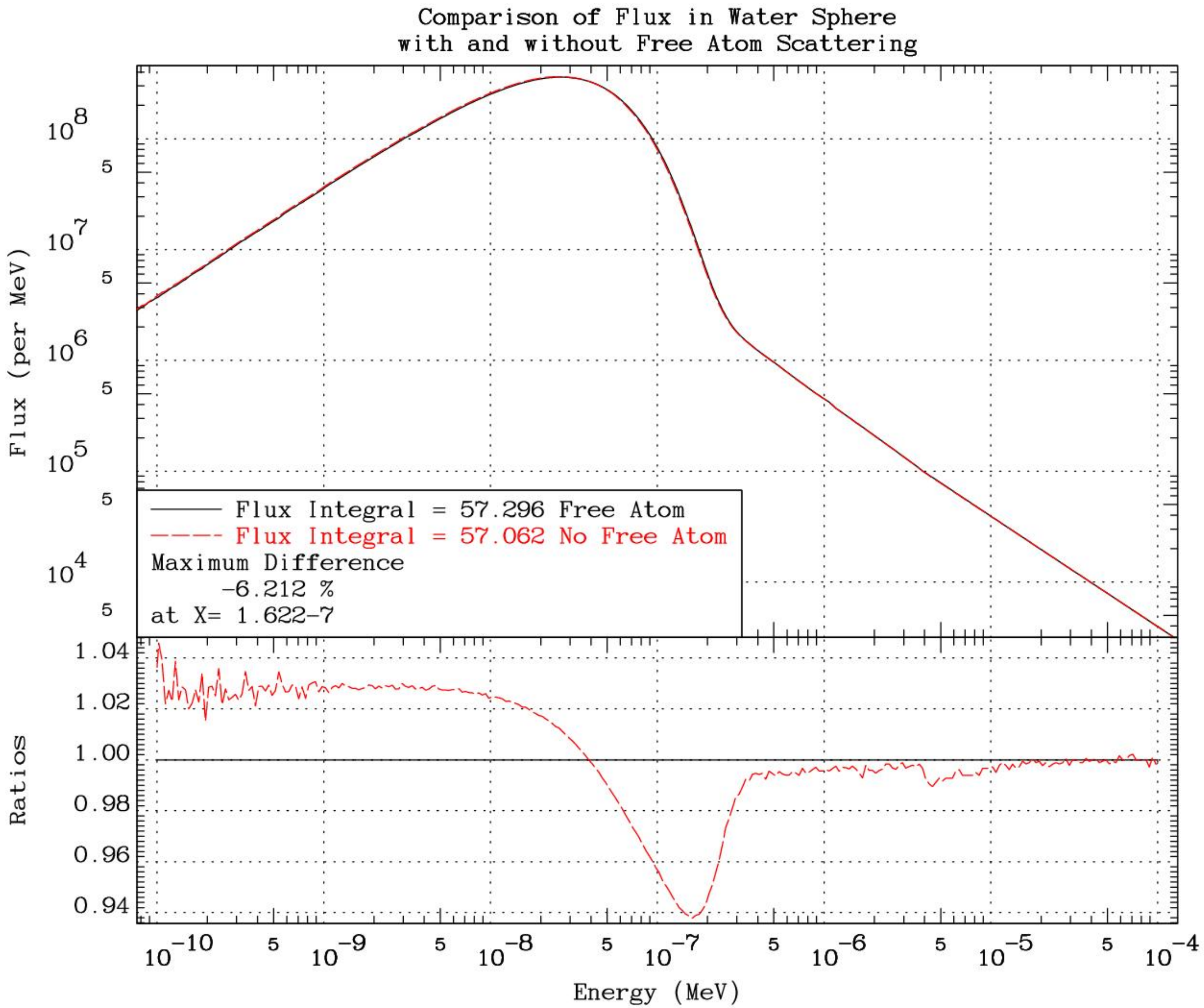
- The today state-of-the-art Monte Carlo codes: COG, MCNP5, MCNPX, MCNP5-Bob, MERCURY, TART and TRIPOLI

- Calculate two separate cases, one using free atom scattering data and the other using bound, thermal scattering law data
- at least 100 Millions (10^8) source neutrons
- Tally both scalar flux within the source, and leakage from the surface
- Use 616 tally bins, equally spaced in lethargy, 50 per decade from 10^{-5} eV up to 20 MeV

Trivial, everybody thought … but we started with up to 80% differences in the calculated flux ....

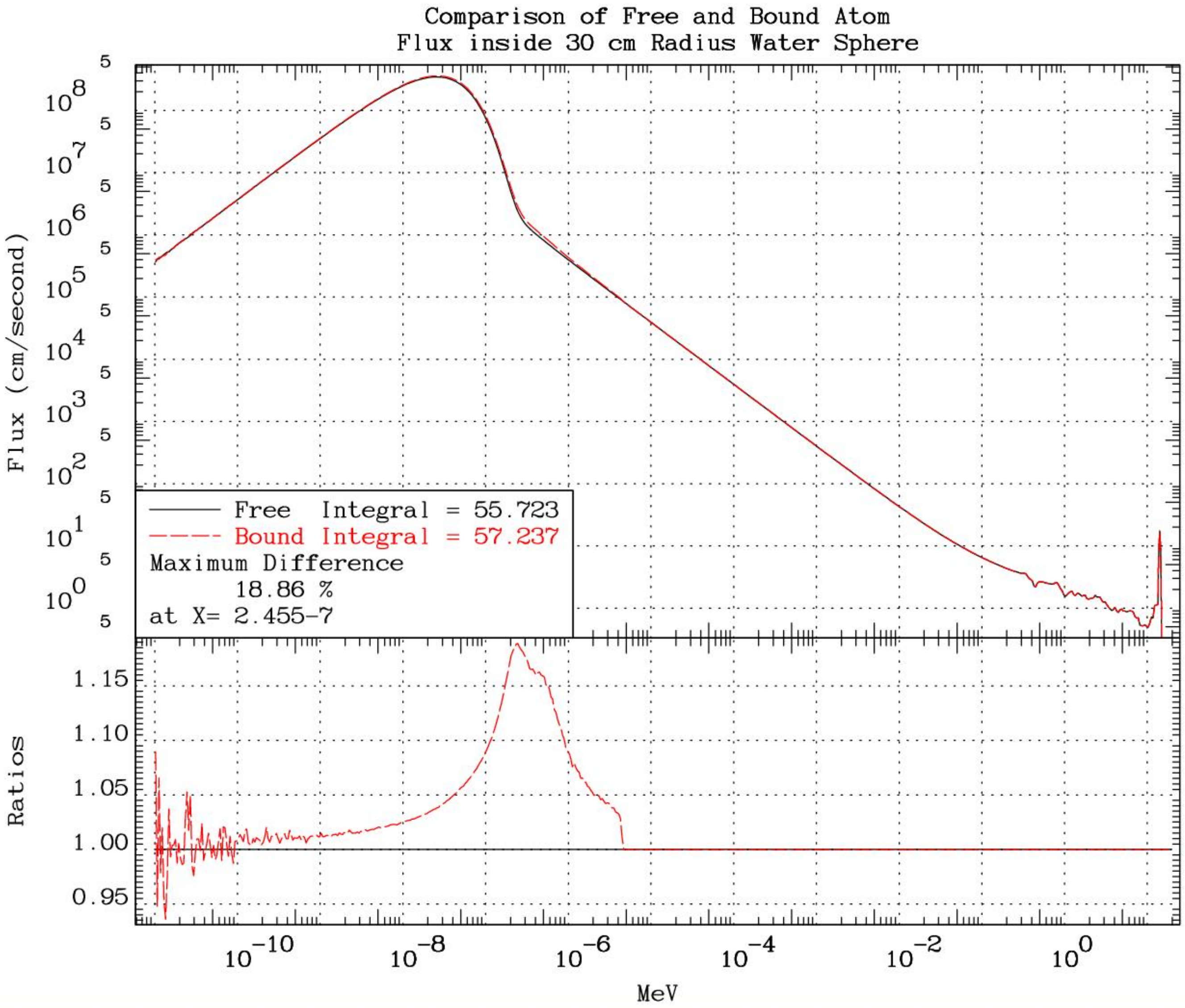
Is Thermal Scattering Important ? free data

Spectral shift



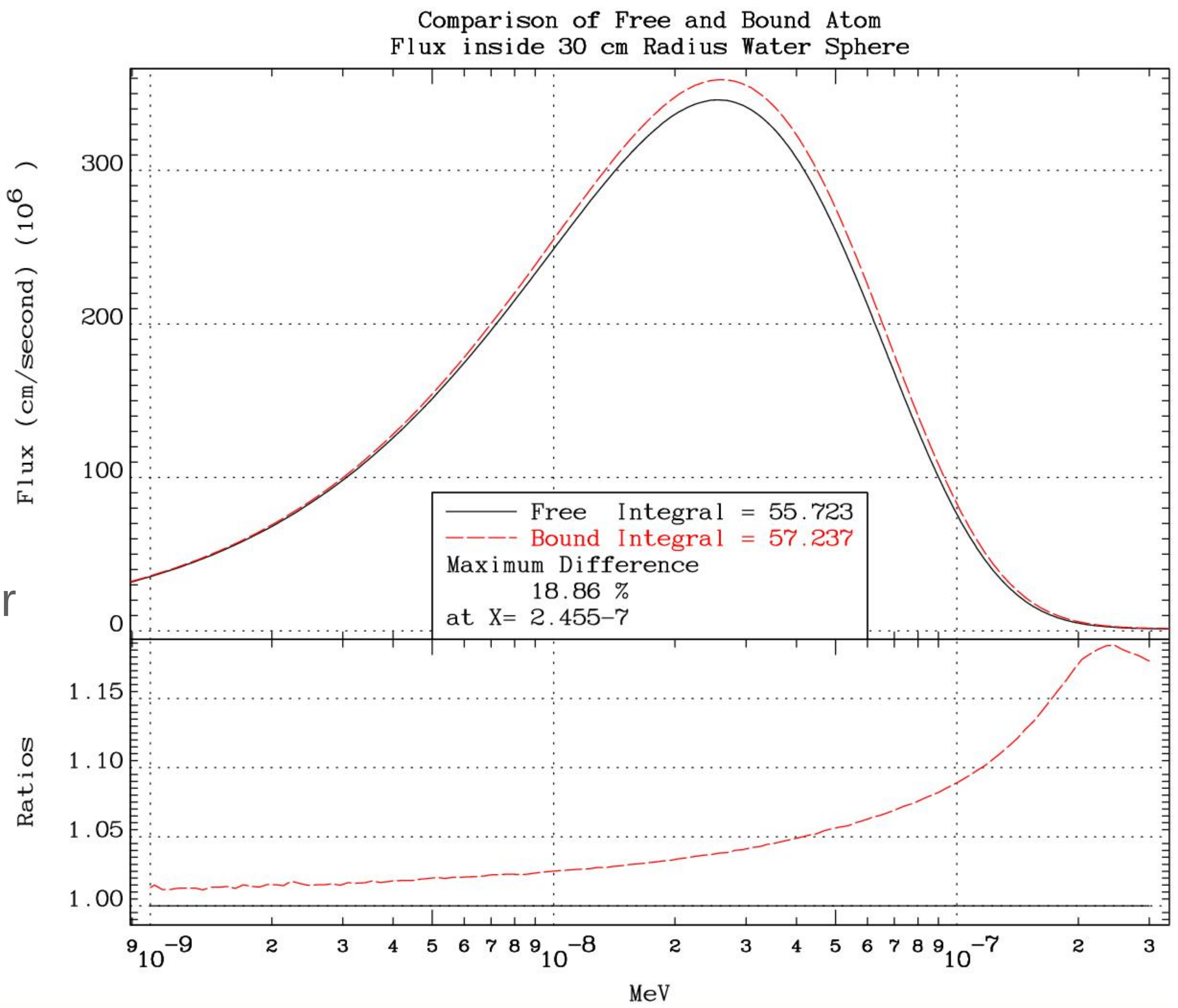
Why study Free and Bound Data Results?

Thermal laws only extend up to 10 eV



Log scaling is often deceptive

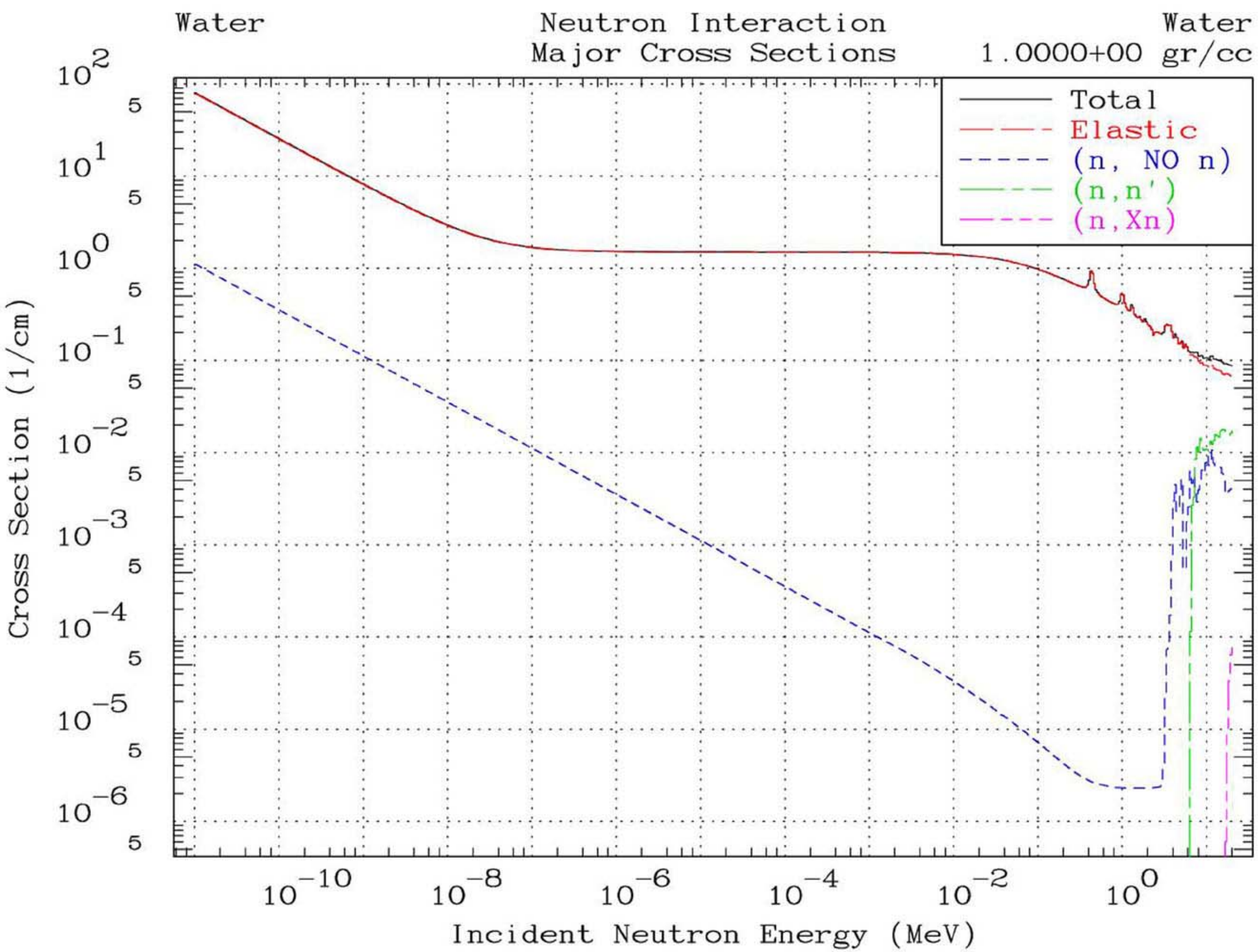
Bound data shifts the thermal spectrum to higher energy



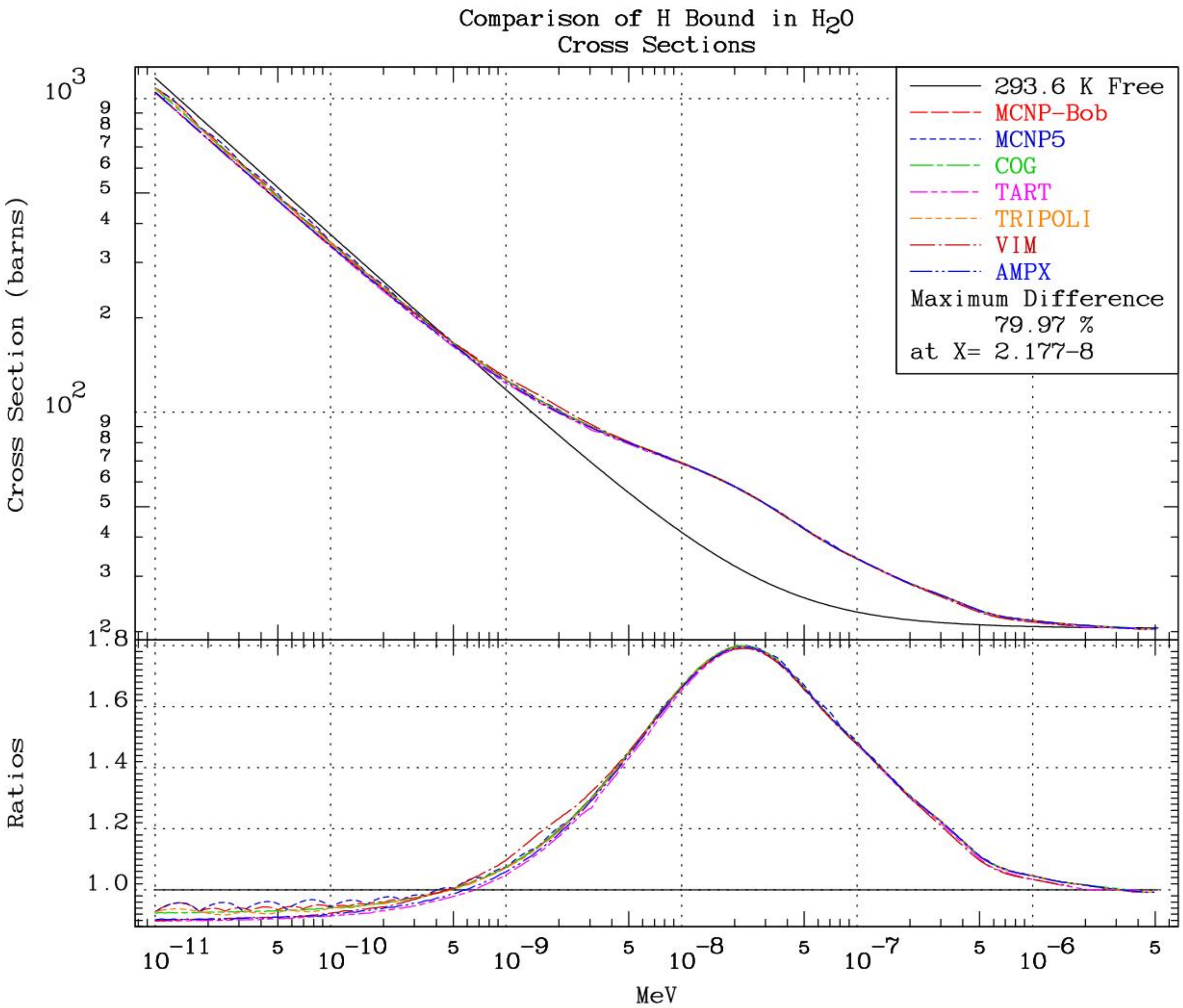
Overview of water cross section

MFPs
14 Mev: 10 cm
 > 1 eV: 0.67 cm
 10-5 eV: 0.012

Ø 30 cm sphere
3 MFPs
40 MFPs
2500 MFPs



H bound in H_2O cross section, at 293.6 K

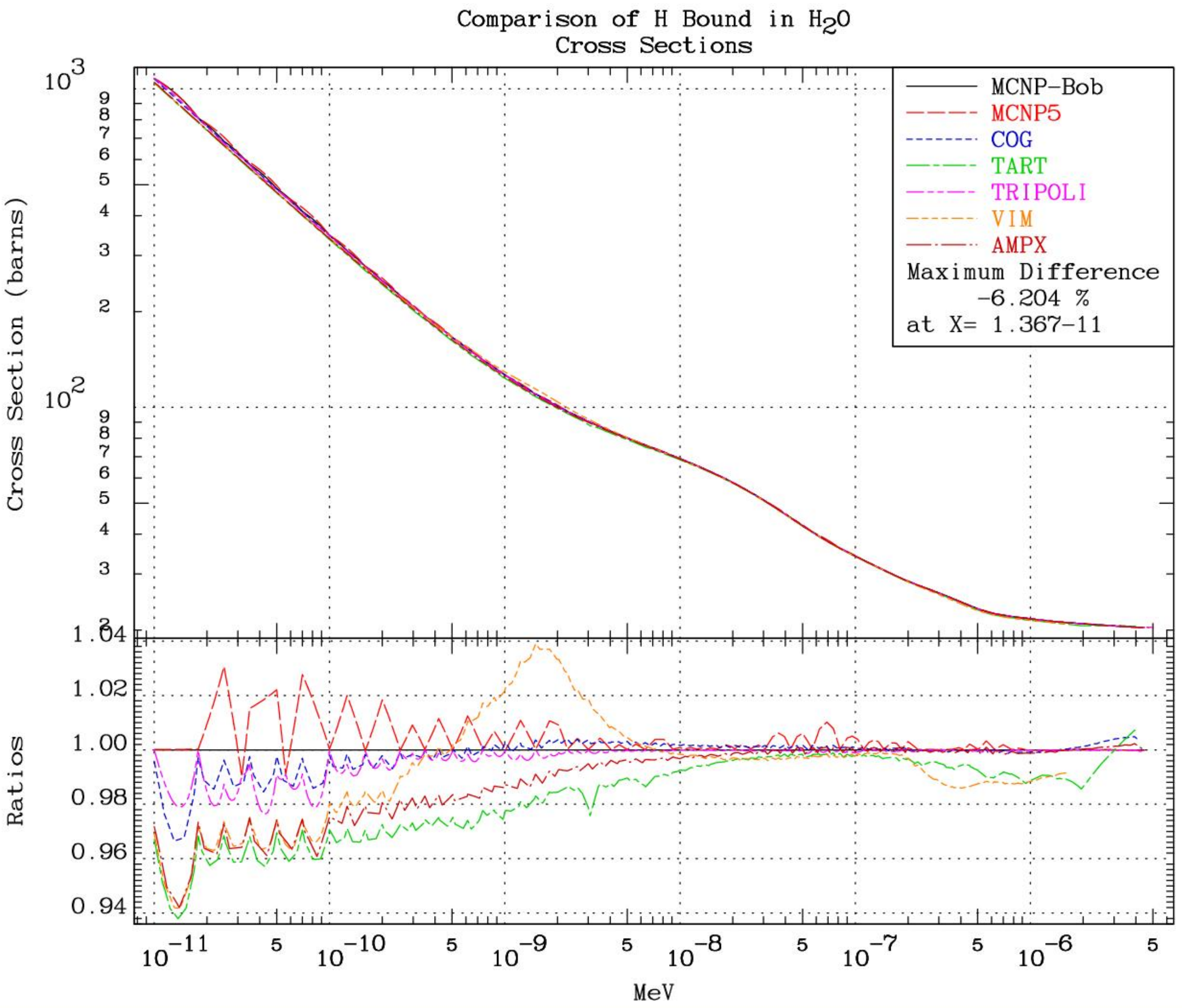


Bound data is 80% higher than the free near the thermal peak

Energy grid scallops effect

Thermr
e-grid(117)
NJOY99.161
up to the job

Processing
"dials"



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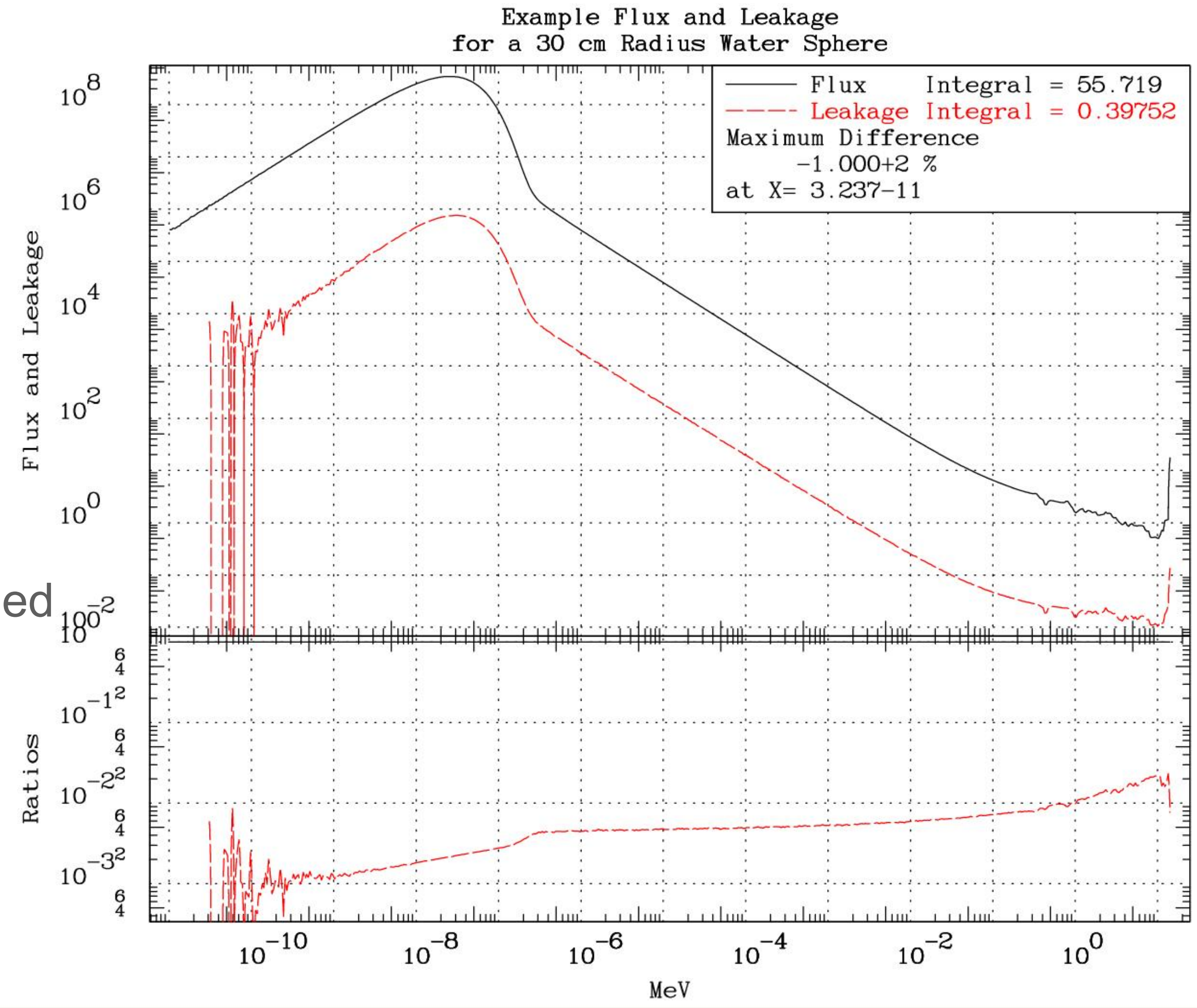
What is important and what is not important

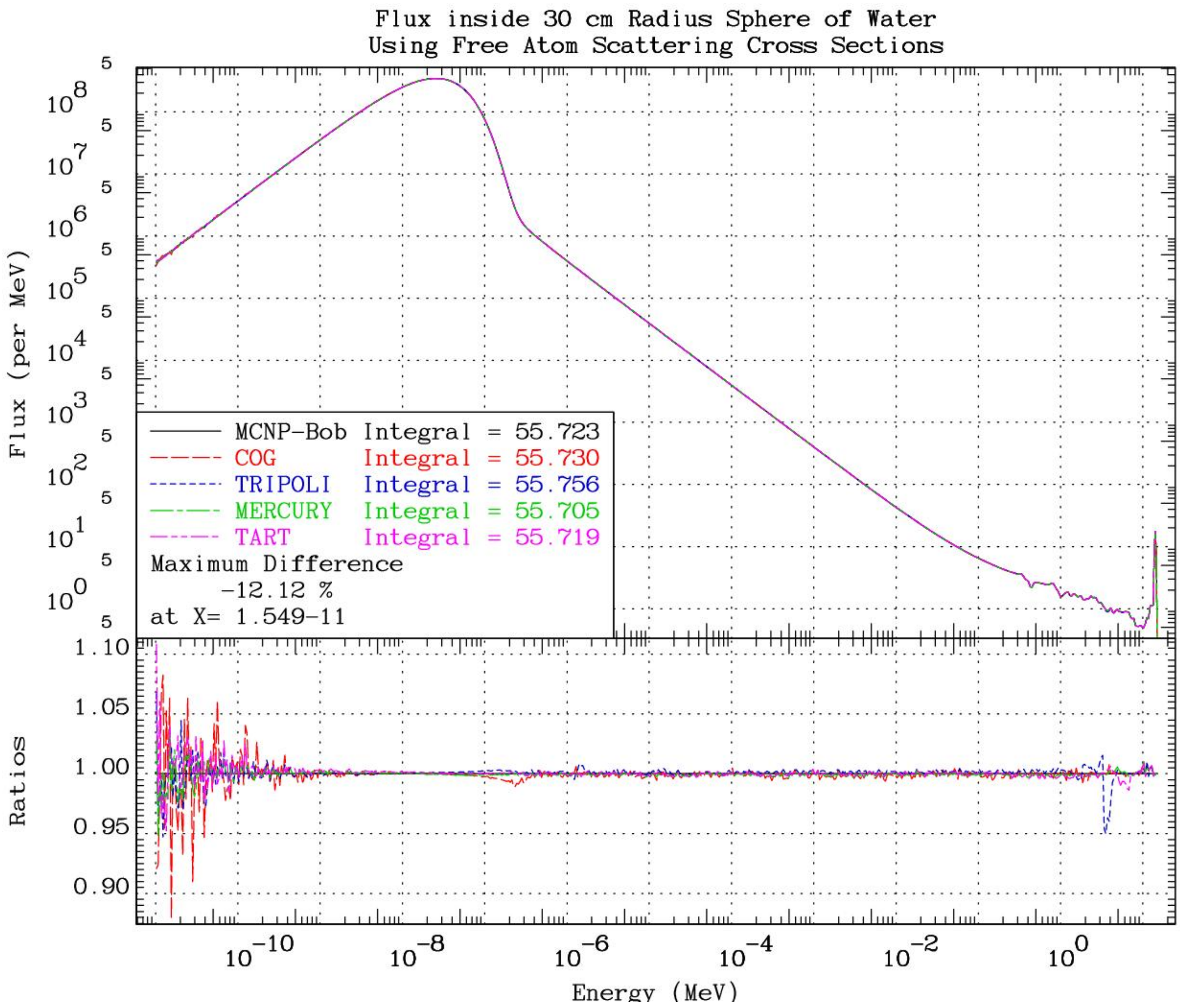
39.75% leaks

60.25% are absorbed in the sphere

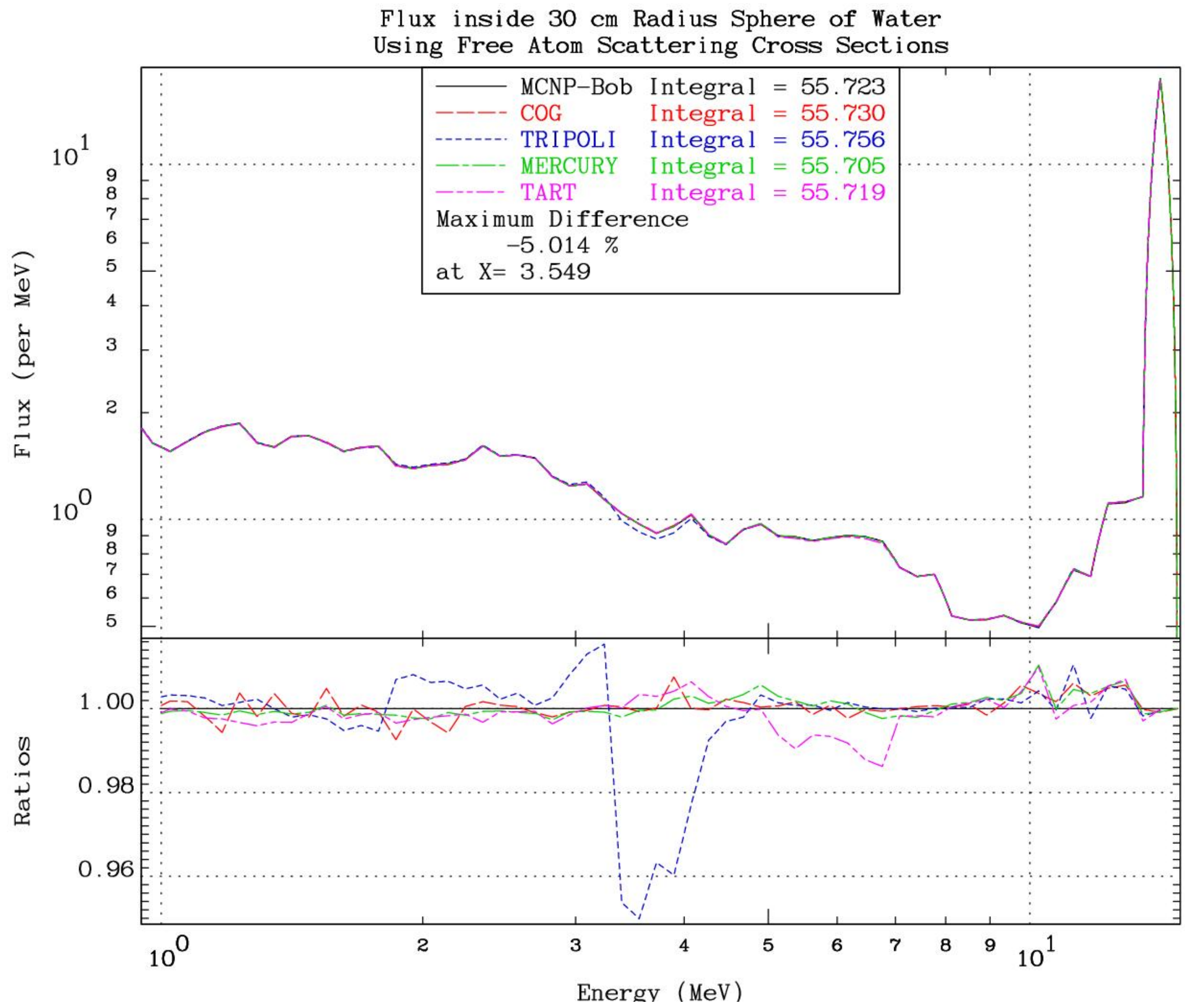


Free Atom Scattering Results

Integral flux
0.041 or 0.07%



5%TRIPOLI (3-4 MeV) and 1% TART05 (5-7 MeV)



Identical as when using bound data

up to 5%

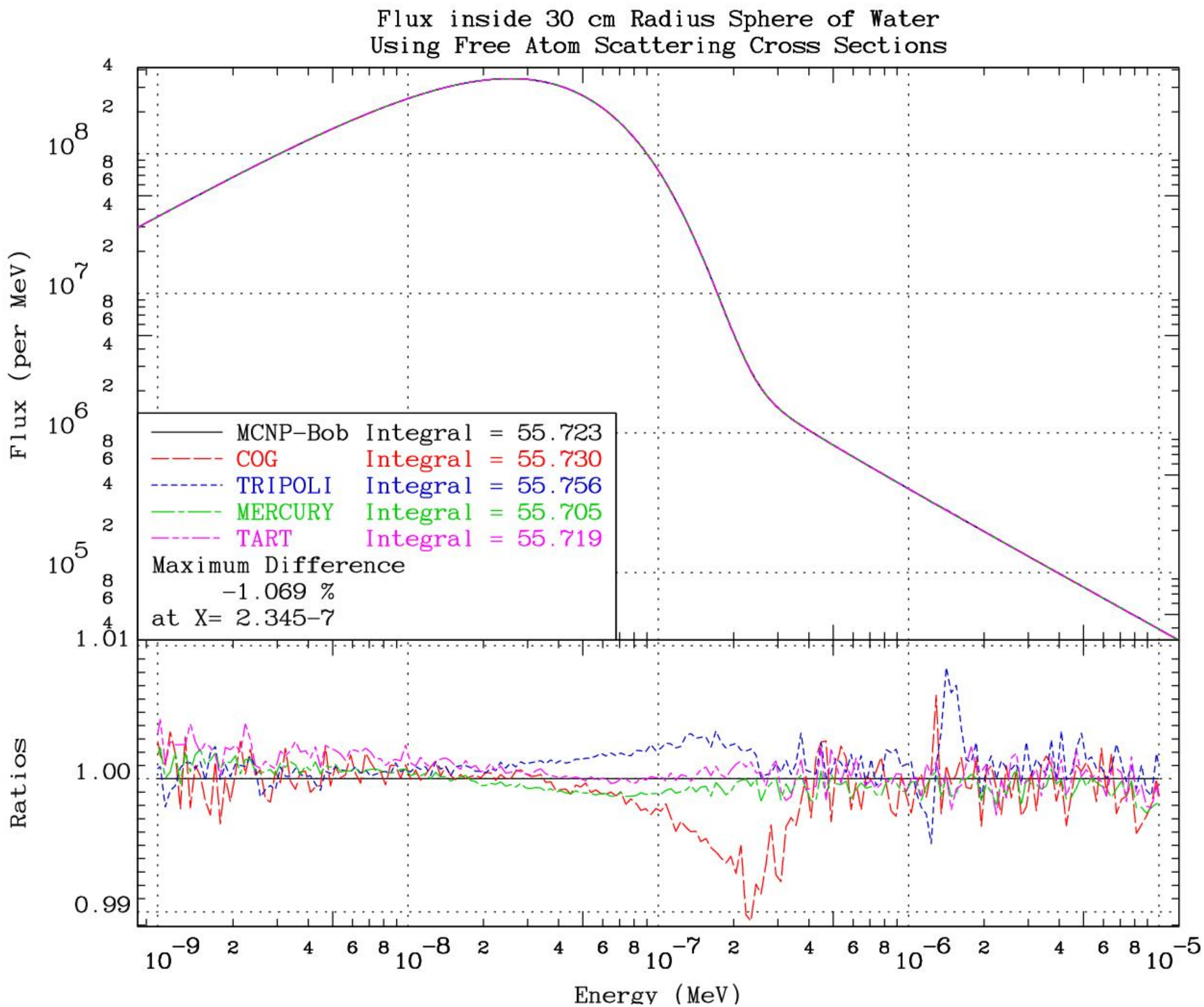
(initially 80%)

The most important energy range for PWR, BWR

s.d. = 0.1-0.2%

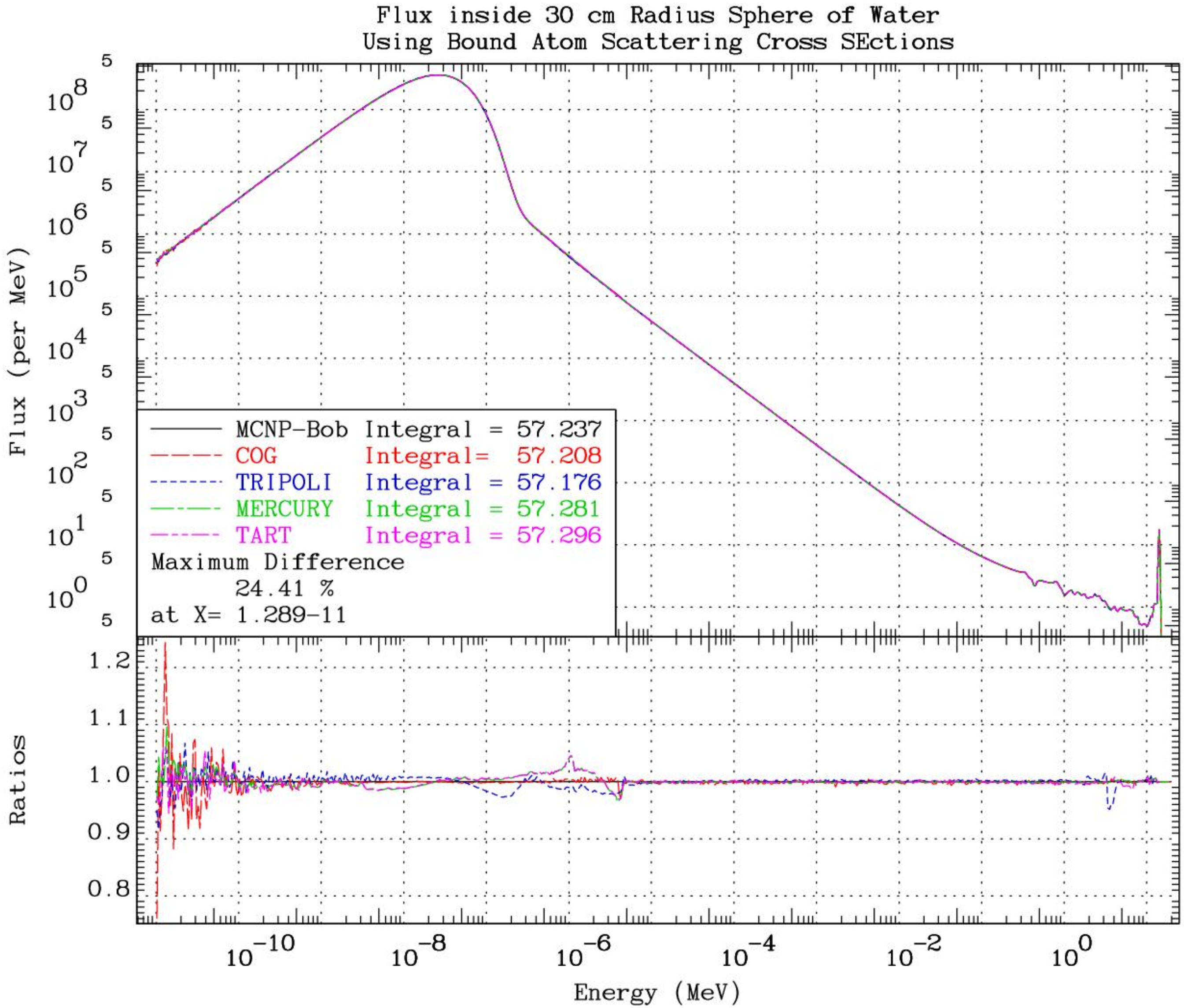
up to 1%

(initially 10%)



Bound Atom Scattering Results

Integral flux
0.120 or 0.21%



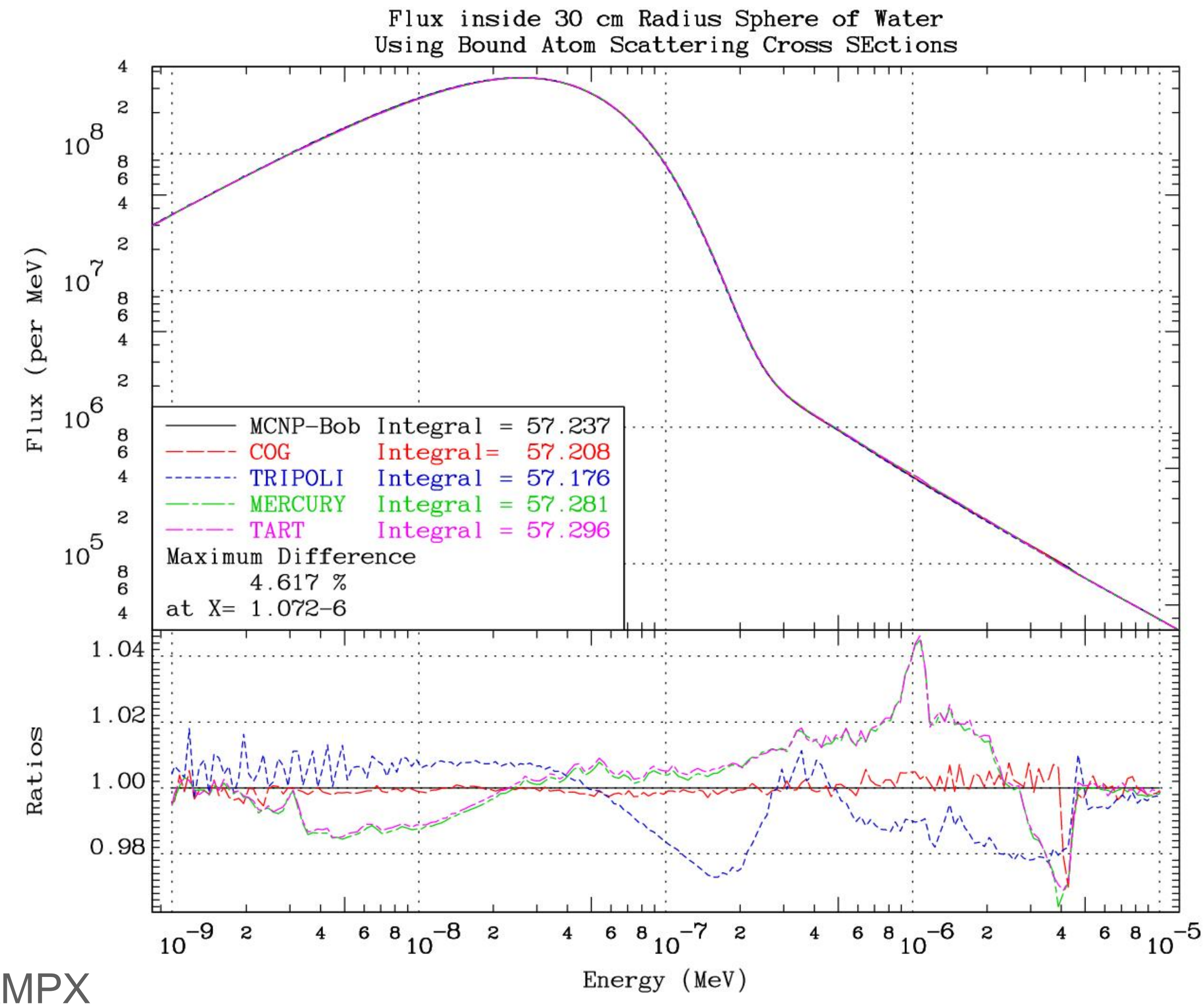
The most important energy range for PWR, BWR

- 0.2 to 24 eV -
the pcm "roller" range

up to 4%

Achieved after several iterations

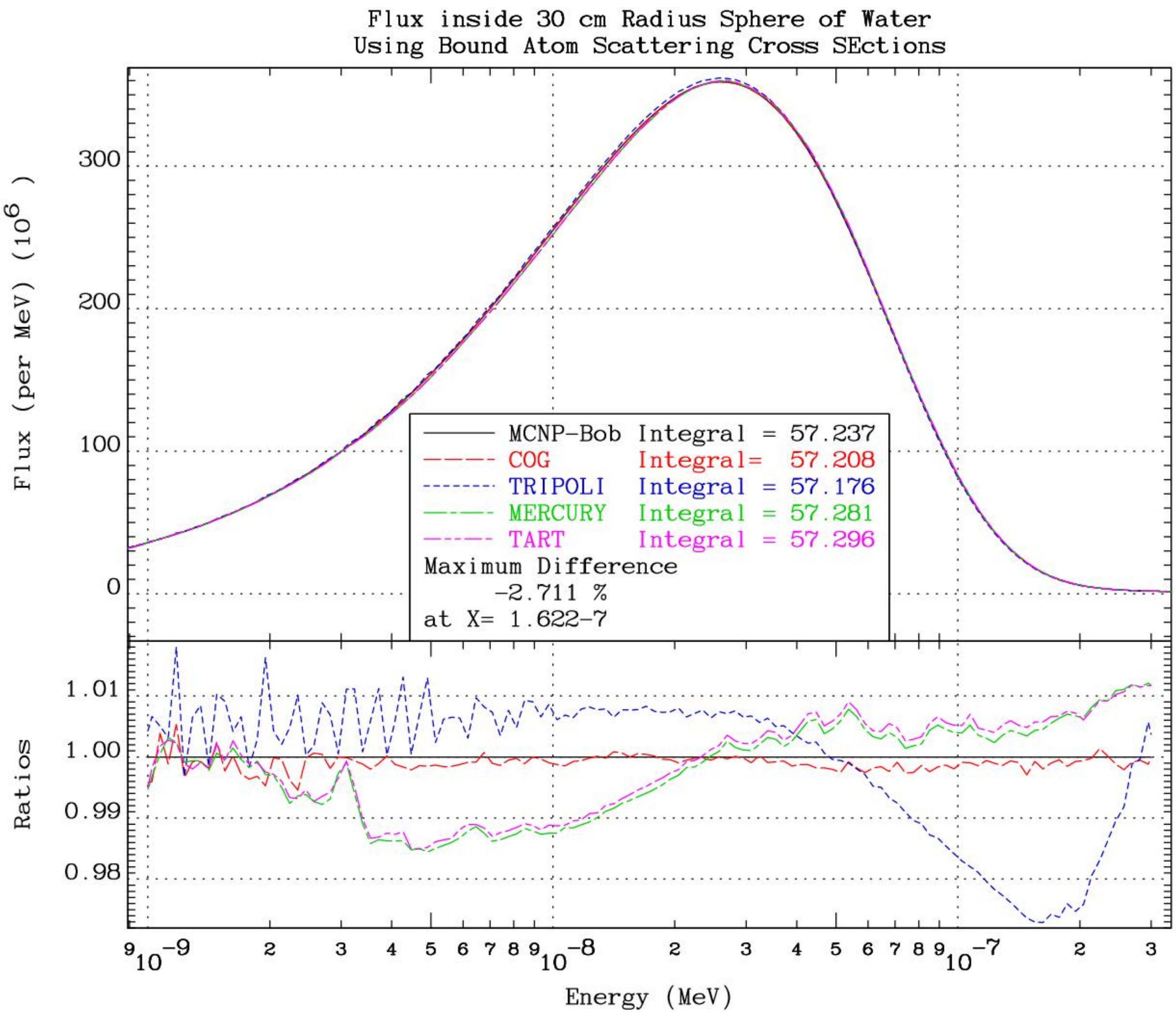
Join energy ??
1.6 eV VIM
4 eV TART, COG
4.5 eV MCNP's
4.95 eV TRIPOLI, AMPX



Near the peak of the Maxwellian

up to 1%

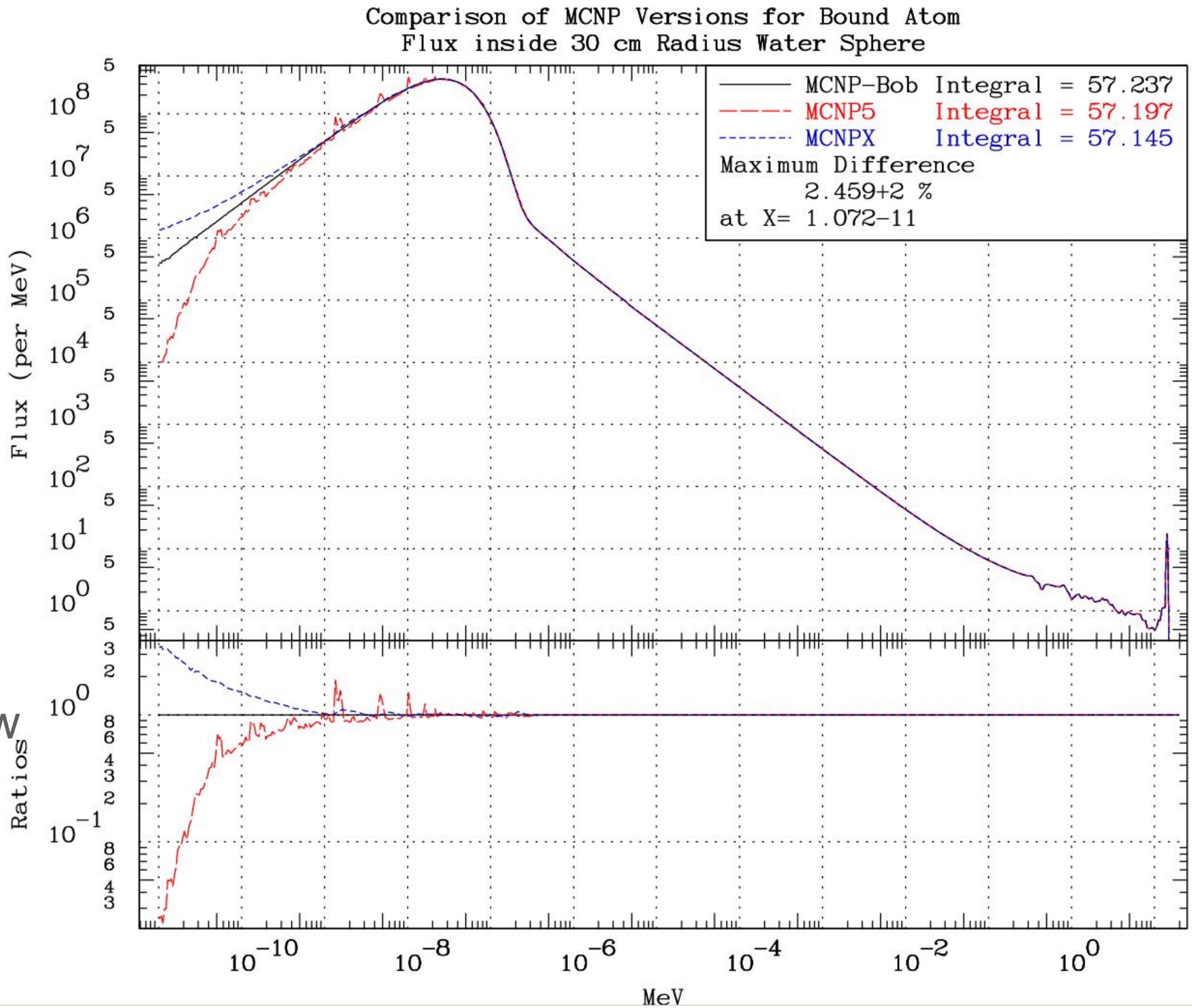
Not great
with s.d.
~ 0.1%



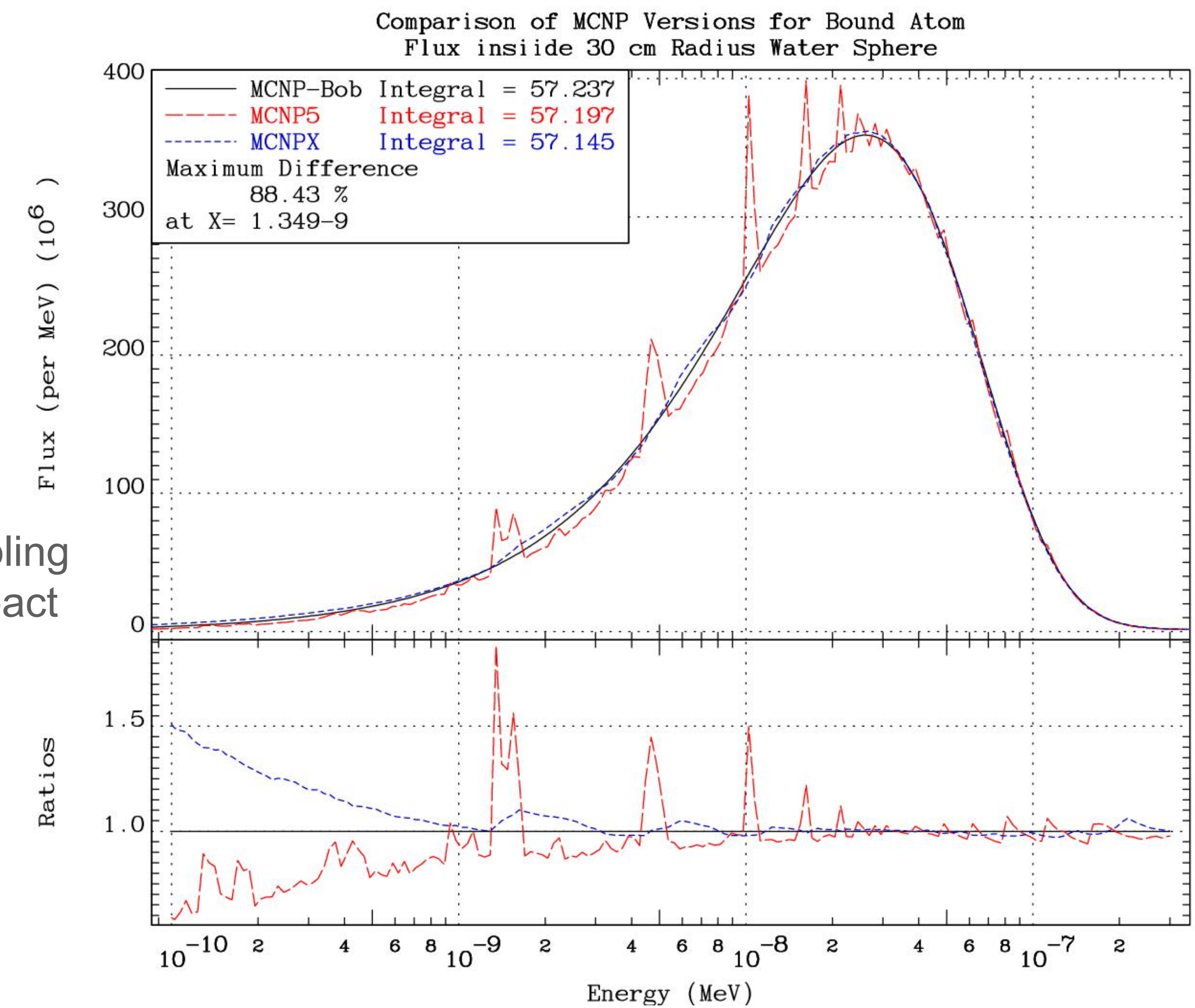
MCNP Family of Codes

MCNP4c3 & MCNP5 use discrete values (energy and cosine)

MCNP5-Bob and NJOY-99.161 new thermal handling give the better answer



Smoothing of MCNPX, spike of MCNP5 & MCNP4c3



Discrete thermal sampling versus continuous impact on Keff

LCT6-2,-4,-6,-8,-10
4 to 27 pcm
with s.d. of 10 pcm

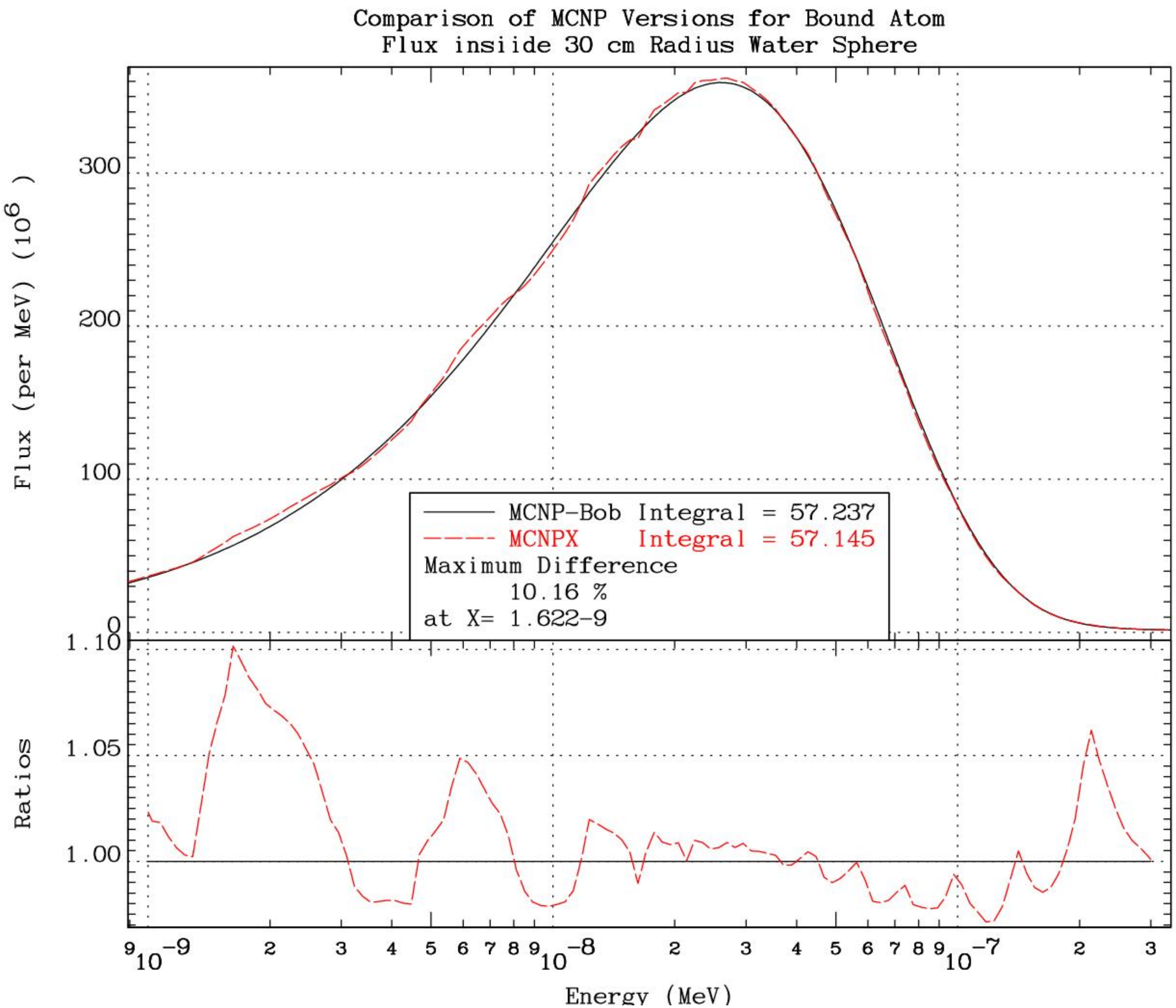
Use discrete thermal sampling instead of continuous

ICSBEP	MCNP5-Bob Keff results with ENDF/B-VII
HST42-1	1.00100(07)-1.00100(06) = .00000(07)
-2	0.99995(07)-1.00006(06) = -.00011(07)
-3	1.00155(05)-1.00153(05) = .00002(05)
-4	1.00230(05)-1.00222(05) = .00008(05)
HST32	0.99789(13)-0.99800(13) = -.00011(13)
LST20-1	1.00024(09)-1.00023(08) = .00001(09)
-2	1.00003(08)-0.99983(08) = .00020(08)
HST1-1	0.99843(14)-0.99838(15) = .00005(15)
-5	0.99864(13)-0.99885(13) = -.00019(13)
LCT6-2	1.00074(10)-1.00058(10) = .00016(10)
-4	1.00031(10)-1.00004(10) = .00027(10)
-6	1.00054(10)-1.00050(10) = .00004(10)
-8	1.00015(10)-1.00019(10) = -.00004(10)
-10	1.00013(10)-1.00001(10) = .00012(10)

discrete tables Keff - new continuous tables Keff

MCNPX26c?? still differ from MCNP5-Bob

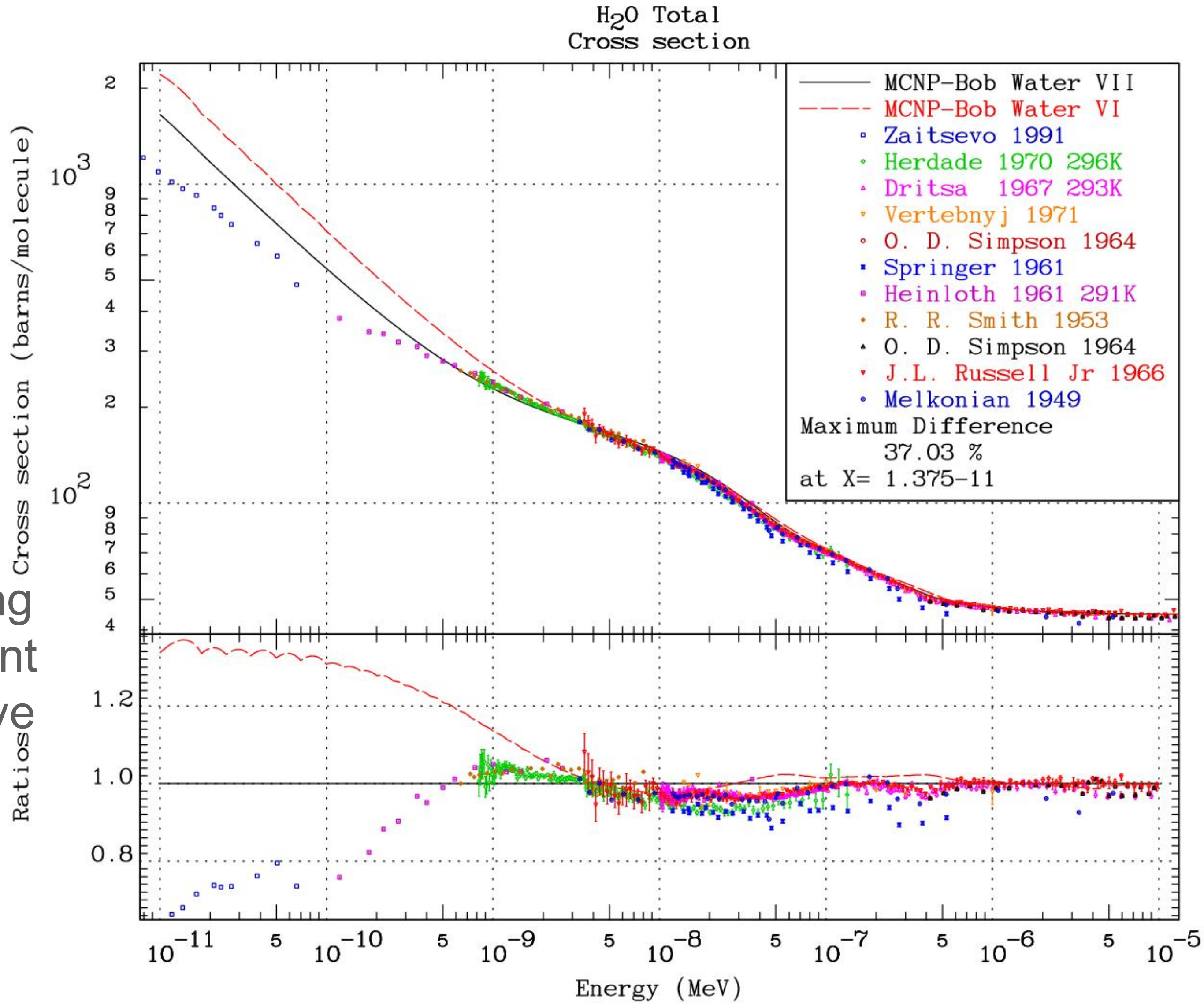
Thermal smoothing impact



Prospects for cross section

Why such differences below 1 milli-ev ?

Diffusive clustering becomes important but we do not have a good model….



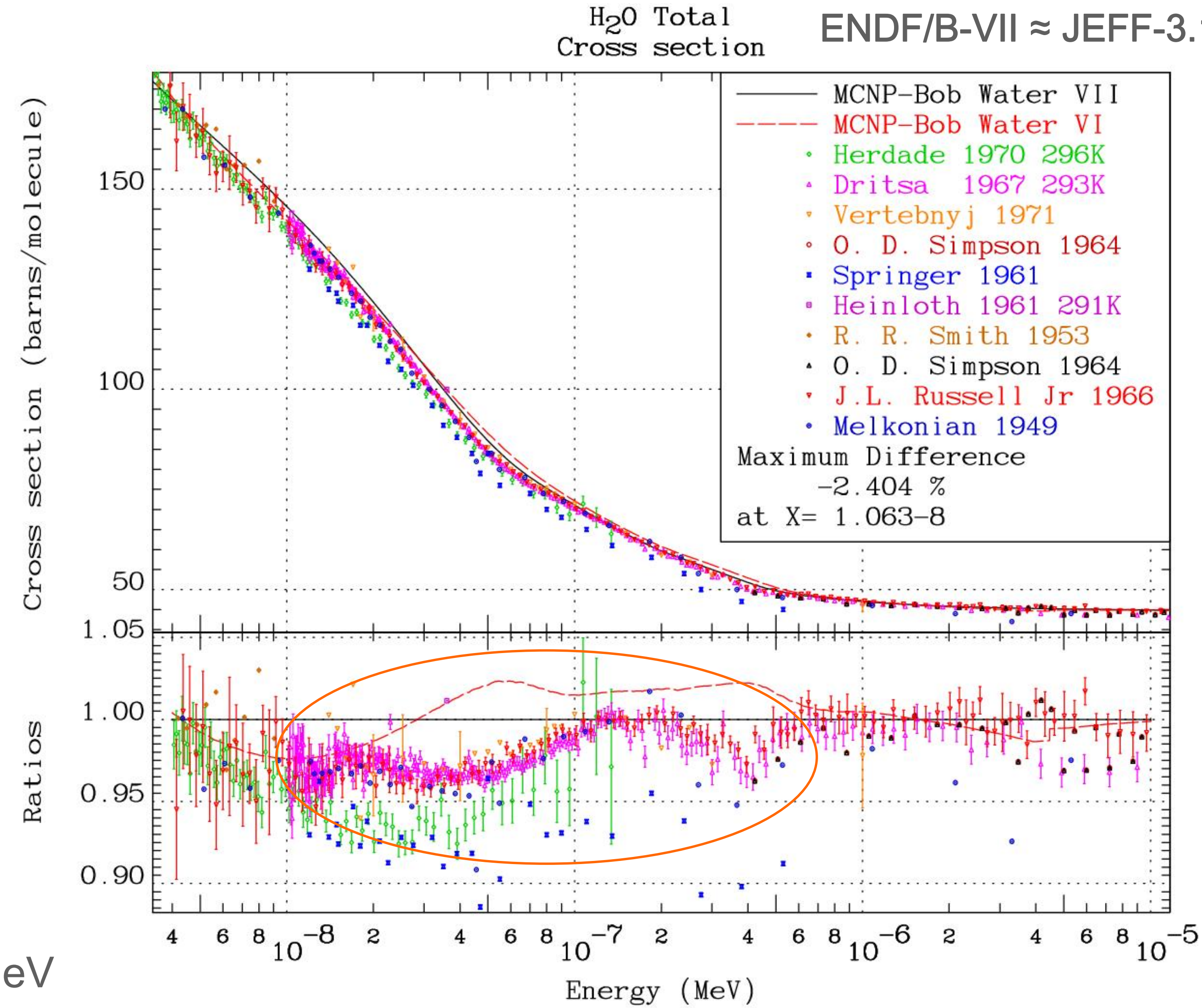
Back up to ENDF/B-VII beta1 H(H2O)

ICSBEP	MCNP5 Keff results	
HST42-1	1.00017(04)-1.00022(04)	= -.00005(04)
HST9-2	1.00084(14)-1.00275(14)	= -.00191(14)
LCT6-06	0.99929(10)-1.00050(10)	= -.00121(10)
LCT39-01	0.99675(11)-0.99805(11)	= -.00130(11)
PST1-1	1.00414(13)-1.00612(13)	= -.00198(13)
PST11-1.18	0.99514(16)-0.99398(16)	= .00116(16)

Cross sections variations impact still dominate the Keff variations and reactions rates

Prospects for cross section

ENDF/B-VII ≈ JEFF-3.1



Still 3 to 4% higher just above 2.53×10^{-8} MeV

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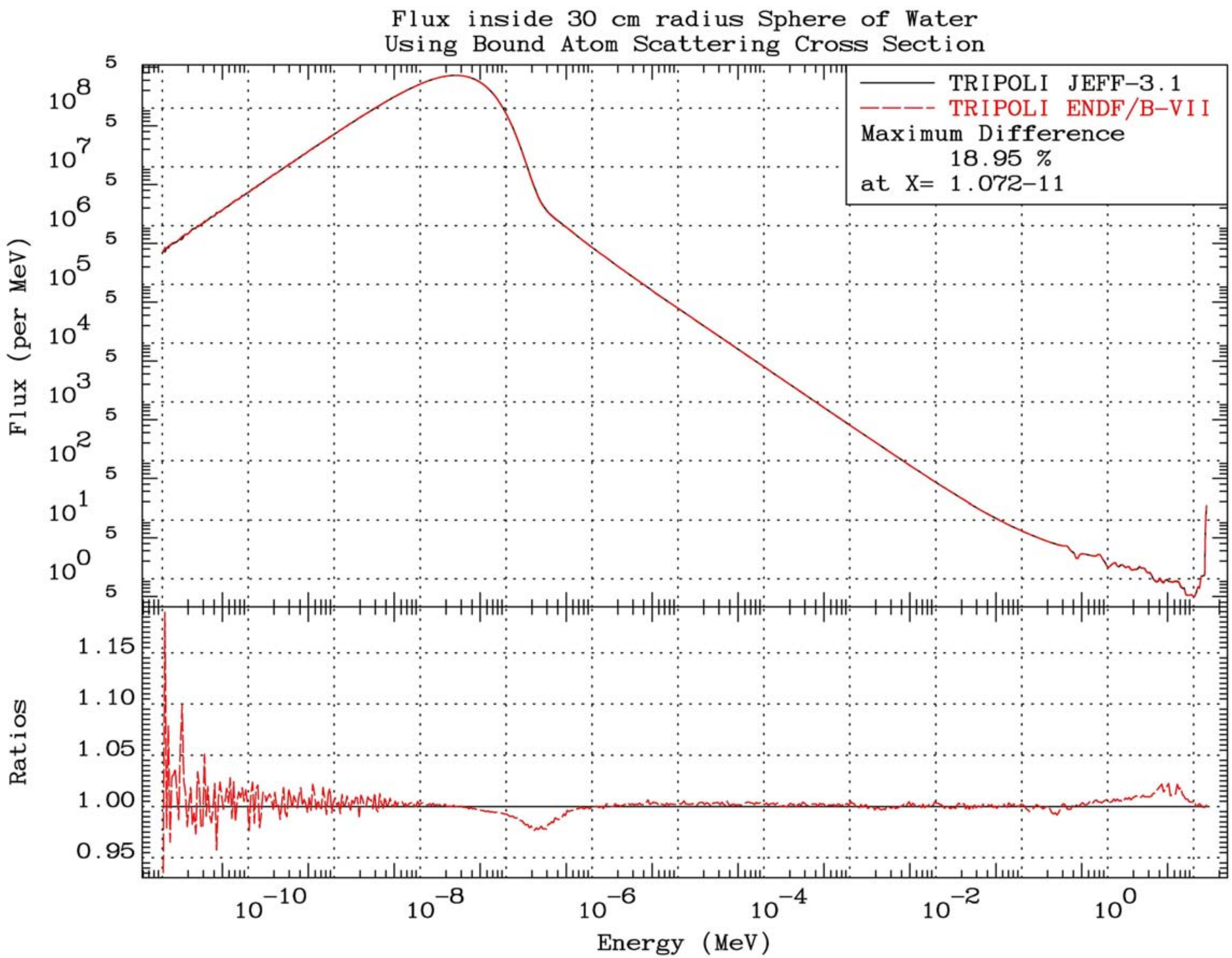
TRIPOLI-4.4 results: thermal data files influence



JEFF-3.1 and ENDF/B-VII thermal data converge ..

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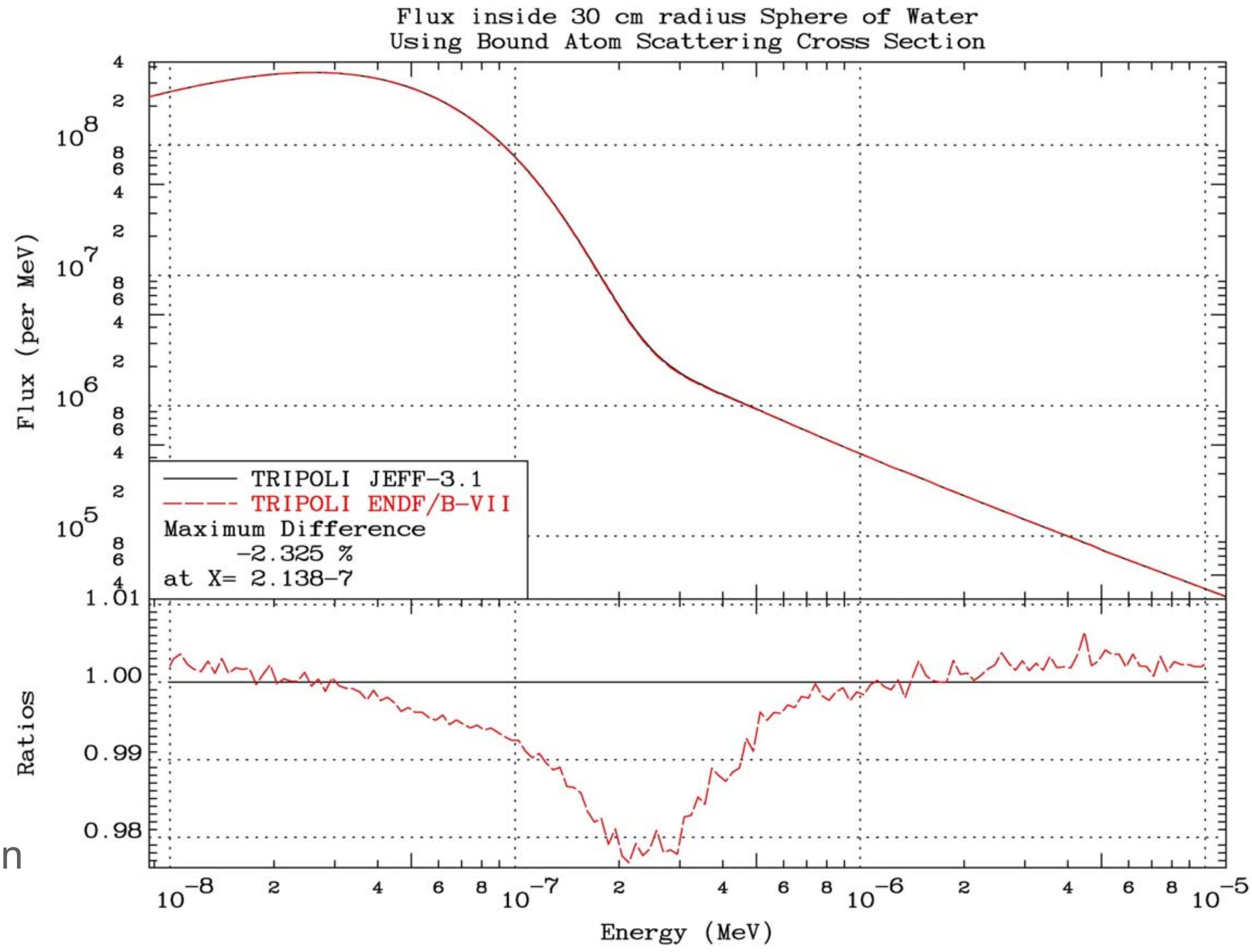
TRIPOLI-4.4 results: thermal data files influence

ENDF/B-VII slightly different than JEFF-3.1

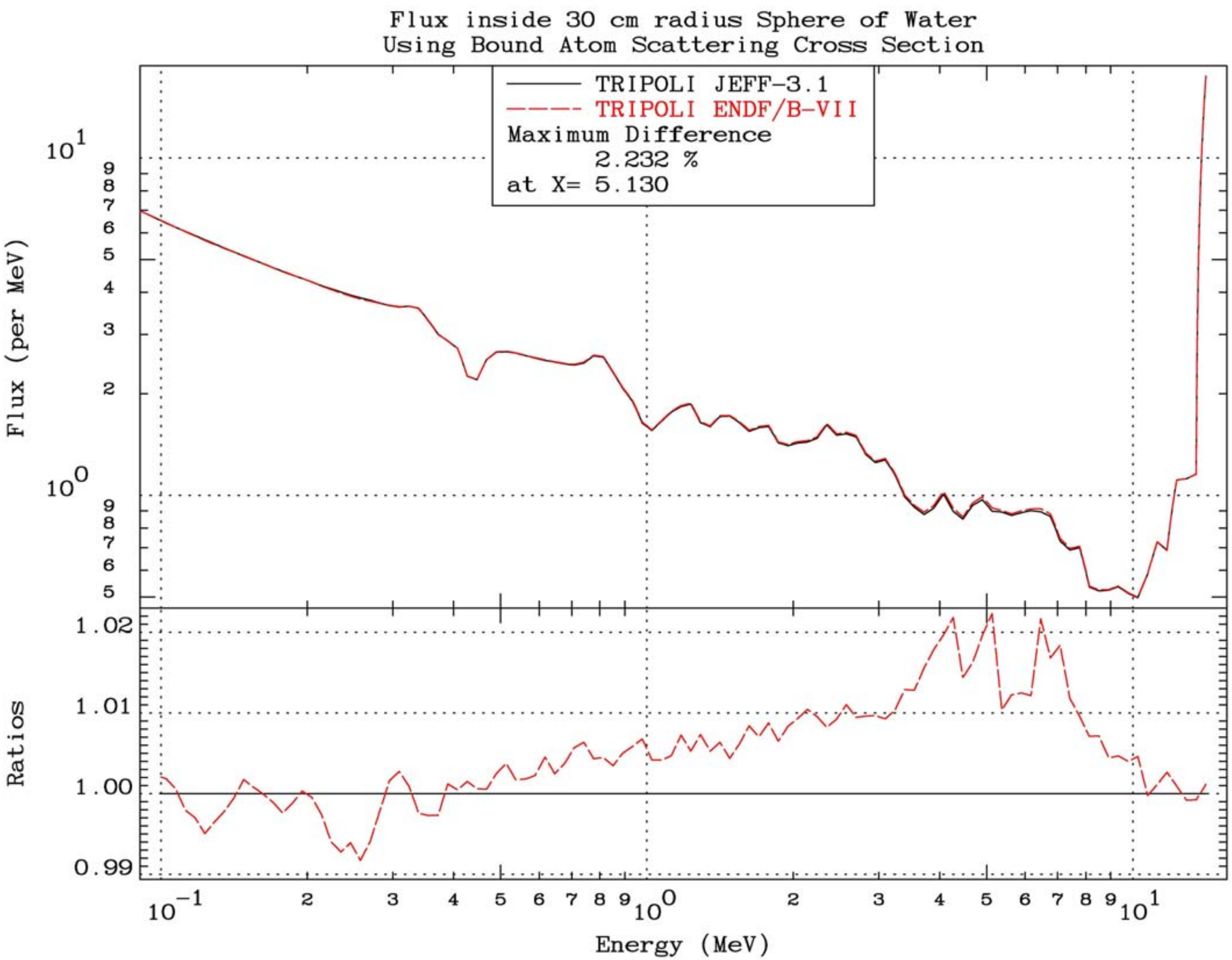
Temperature grid
α, β points
.01 to .1 eV
phonon distribution
(dip at 0.025 eV)



TRIPOLI-4.4 results: thermal data files influence

New O16 of ENDF/B-VII

(n,α0) <32%
2.4 - 8.9 MeV impact



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Same (latest) thermal data but different Monte Carlo

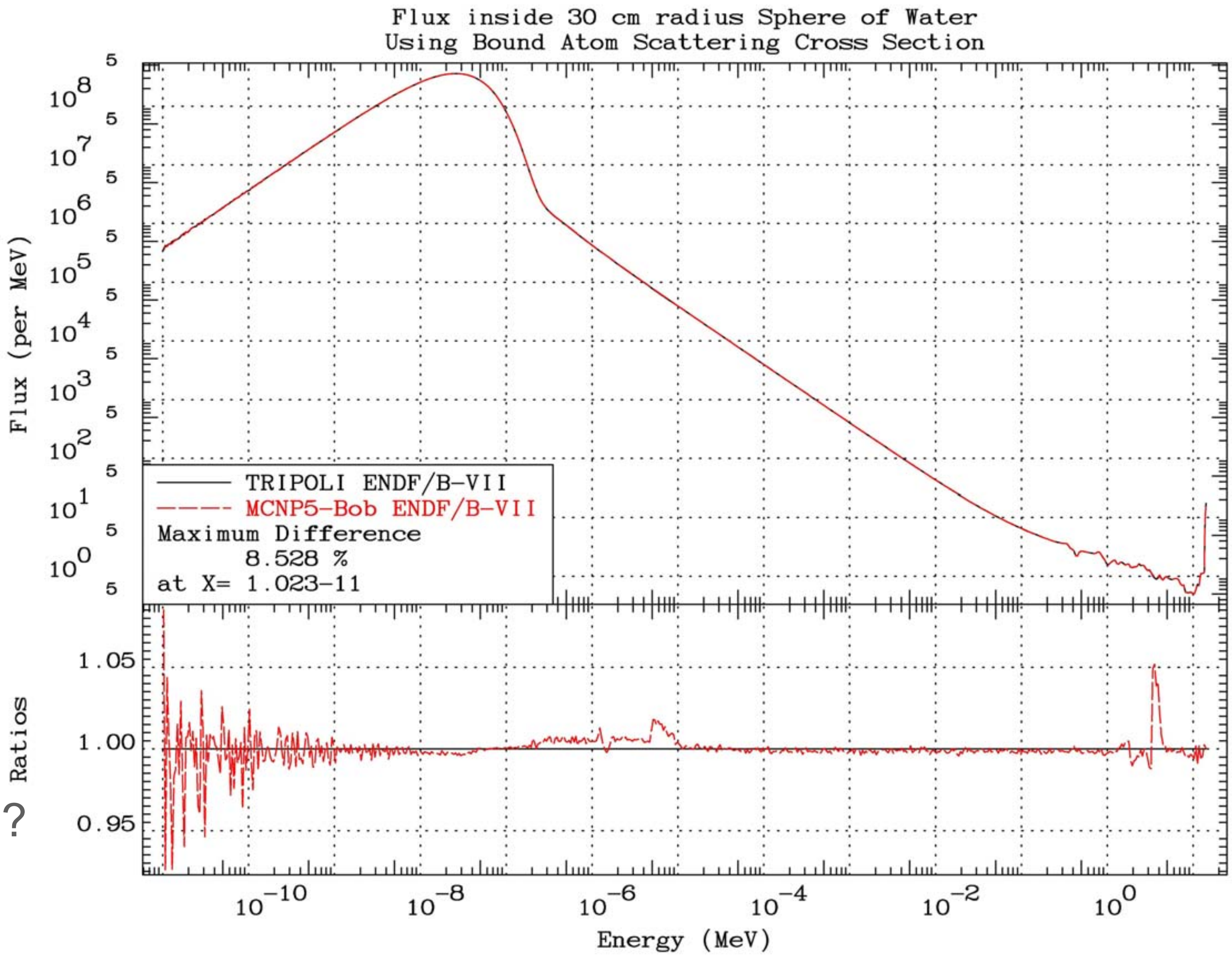
NJOY-99.161

MCNP5-Bob
20 bins, 10 eV
equipro. bin

TRIPOLI
32 bins, 4.95 eV
equipro. cos.

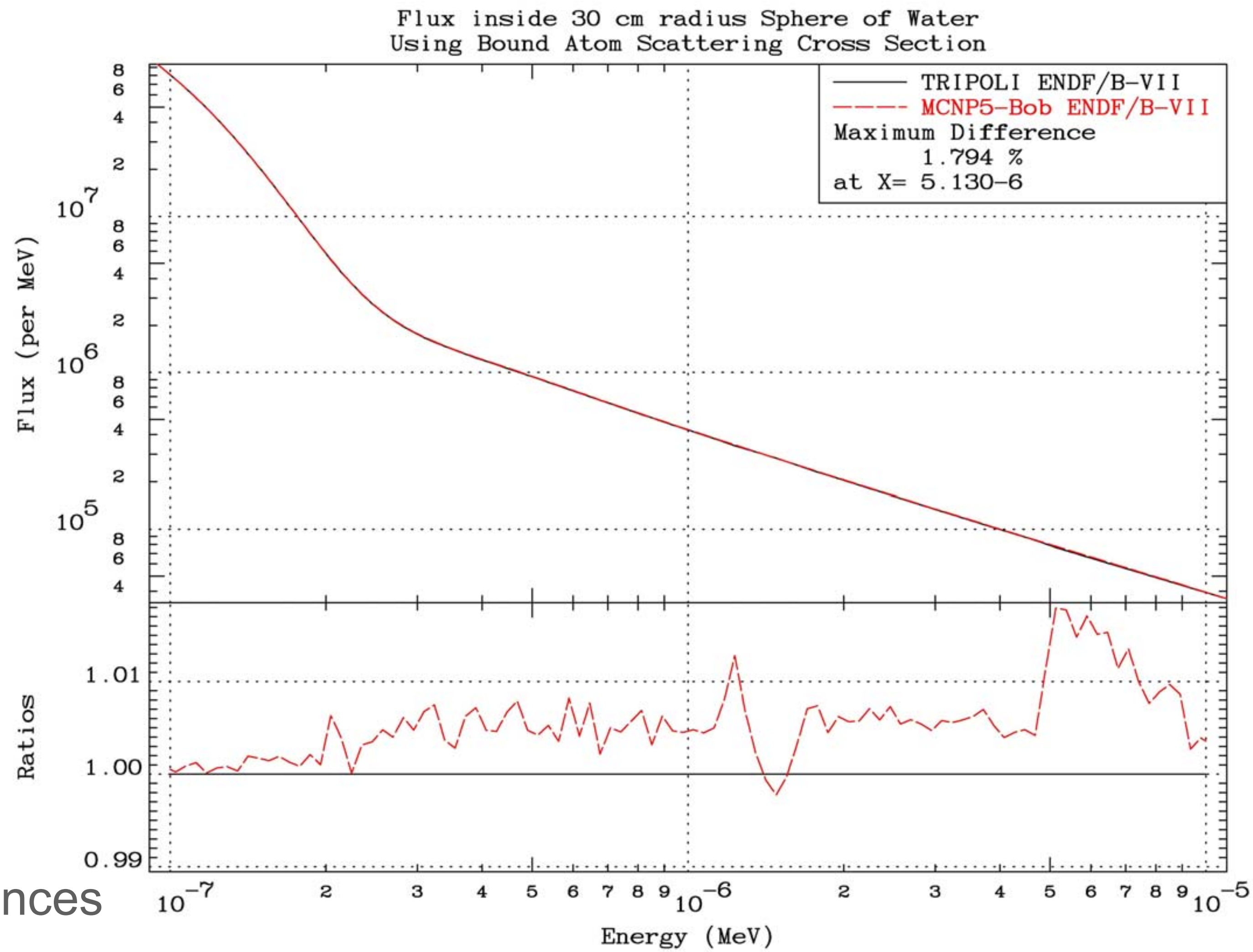
Processing dials?

Else excellent
agreement



s.d. = 4 to 1% then well below ~0.1%

Same (latest) thermal data but different CODE

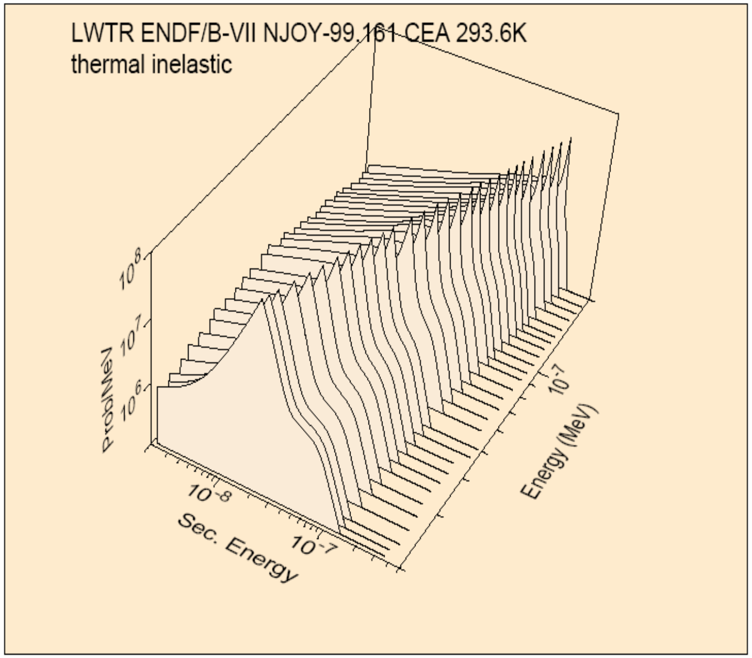


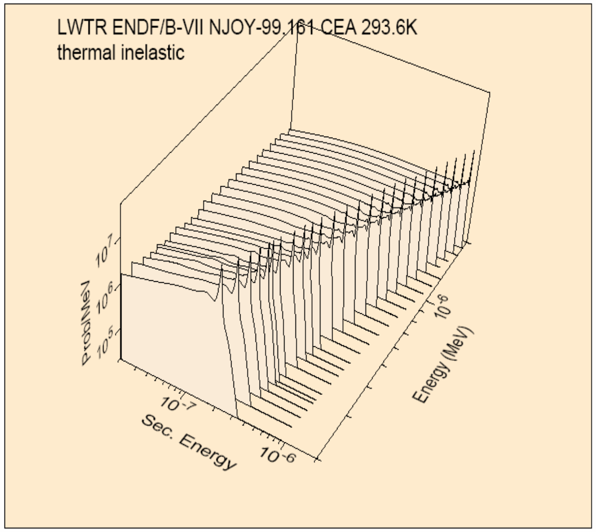
Upper threshold influence

4.95 or 10 eV ?

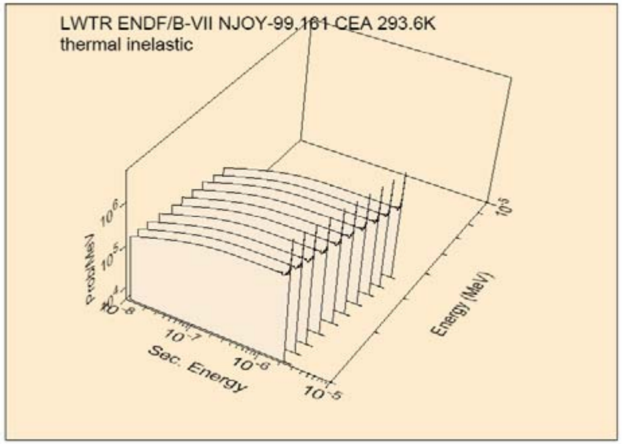
Direct influence in the eV regions where the resonances are at their best..

Inelastic thermal energy distribution

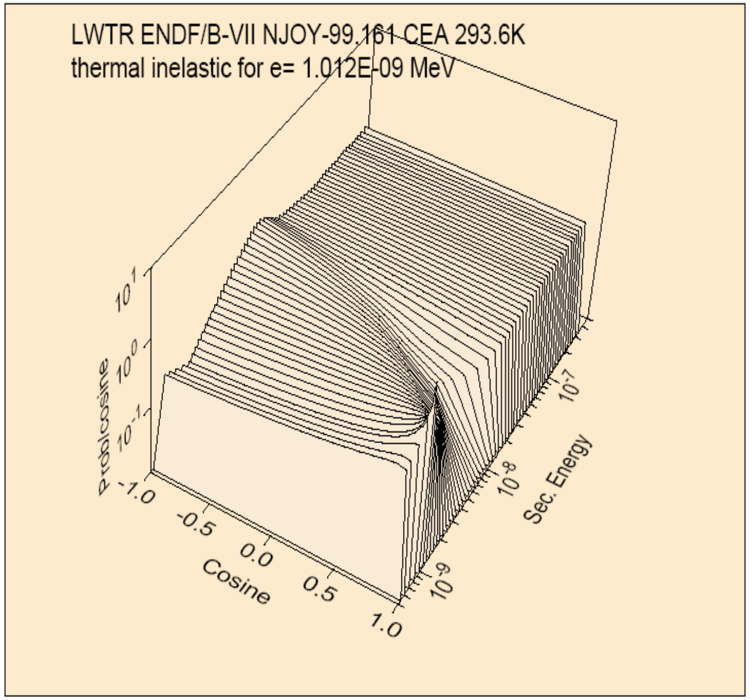


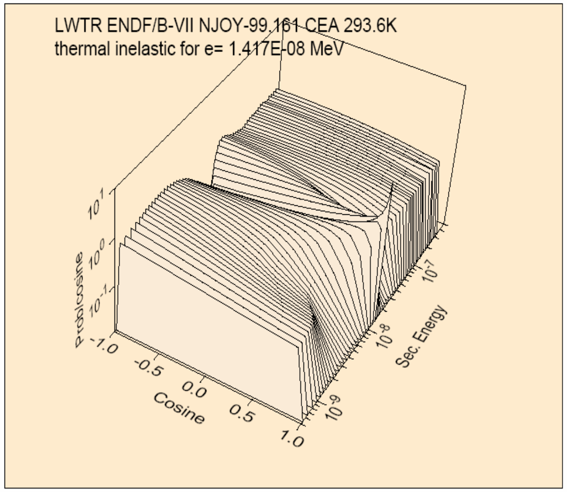


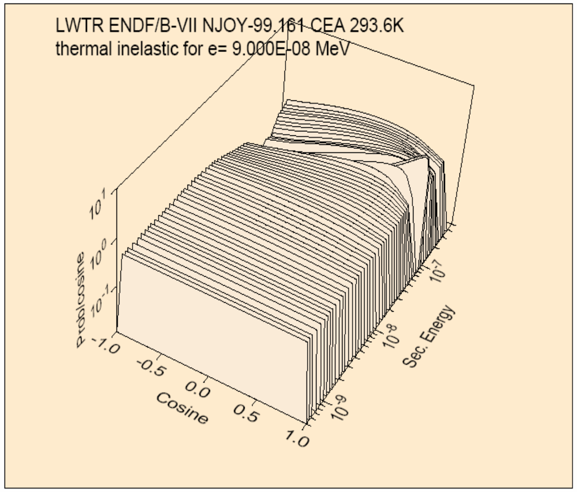
Peaked and evolving…



Inelastic thermal angular distribution







Structured …with valley

Conclusions

ALL of the participating codes or data were improved based on this code comparisons

There is one positive conclusion that we can reach from this study: regardless of how much time and effort we put into improving our Monte Carlo codes, we are never going to eliminate differences unless we improve our nuclear data and processing codes

We hope that the results presented here serve as a wake up call to those who think our Monte Carlo codes or other systems and the nuclear data they use are "now perfect". This should serve as a WARNING for current code system

Be aware that there is more uncertainty in Monte Carlo answers than the estimates of statistical uncertainty printed out by the codes