



serco

Serco Assurance

Presentation by

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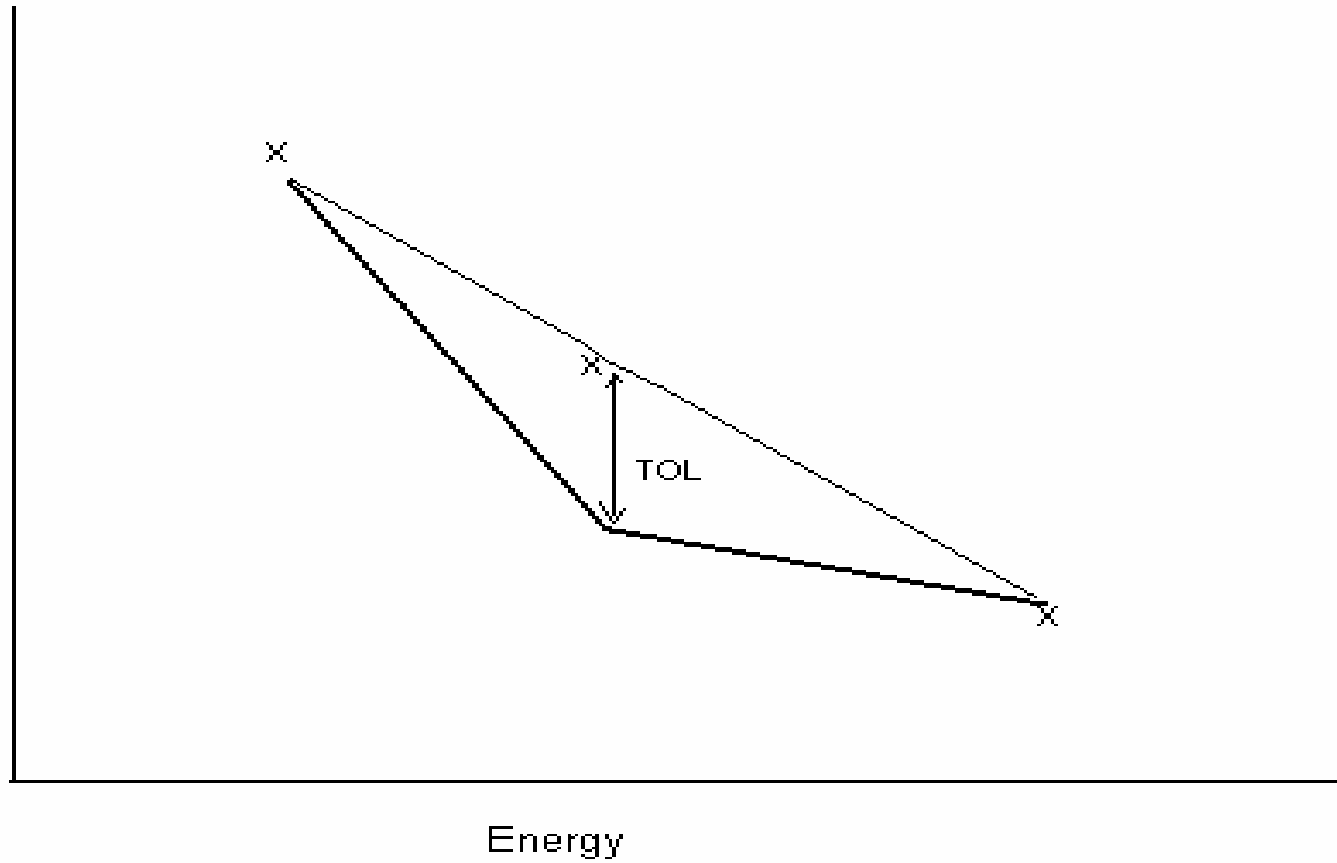
***Numerical Precision in
RECONR and BROADR
Following Improvements to
U-238 Nuclear Data***

2 May 2005

Reminder of Unified Grid and Interval Halving (1)

- Energy grid constructed in RECONR and BROADR
- Designed so that cross sections for all reactions are on the same grid
- Linear interpolation can be assumed between points
- Eases integration in later modules
- Several user parameters control the grid
- For our use $ERR = ERR_{THN} = ERR_{MAX} = 0.001$ and $ERR_{INT} = 1E-30$

Reminder of Unified Grid and Interval Halving (2)



Early NJOY application via SIGFIG

- Checking floating point values requires the use ABS function
IF(ABS(A-B).LT.TOL) THEN
- There are many of these checks in NJOY modules
- Routine SIGFIG rounds to a defined number of significant figures (NSF) – Then
IF(A.EQ.B)THEN
- User defined NSF in RECONR
- BROADR “worked out” user NSF input
- Many Hours worked by ENRICO+BOB+ Others
- SIGFIG very machine dependent @ 6-7 SF

Application at Winfrith

- Use Double Precision
- Use `-R8` compiler option
- Apply international updates without change
- Set number of significant figures to 9 (after study)
- Set reconstruction tolerance to 0.001 (0.1%)

STATUS in NJOY99

- Double precision
- SIGFIG sets values to 7SF
- UNLESS POINTS ARE EQUAL when 9SF are applied
- User tolerance of 0.001 appropriate

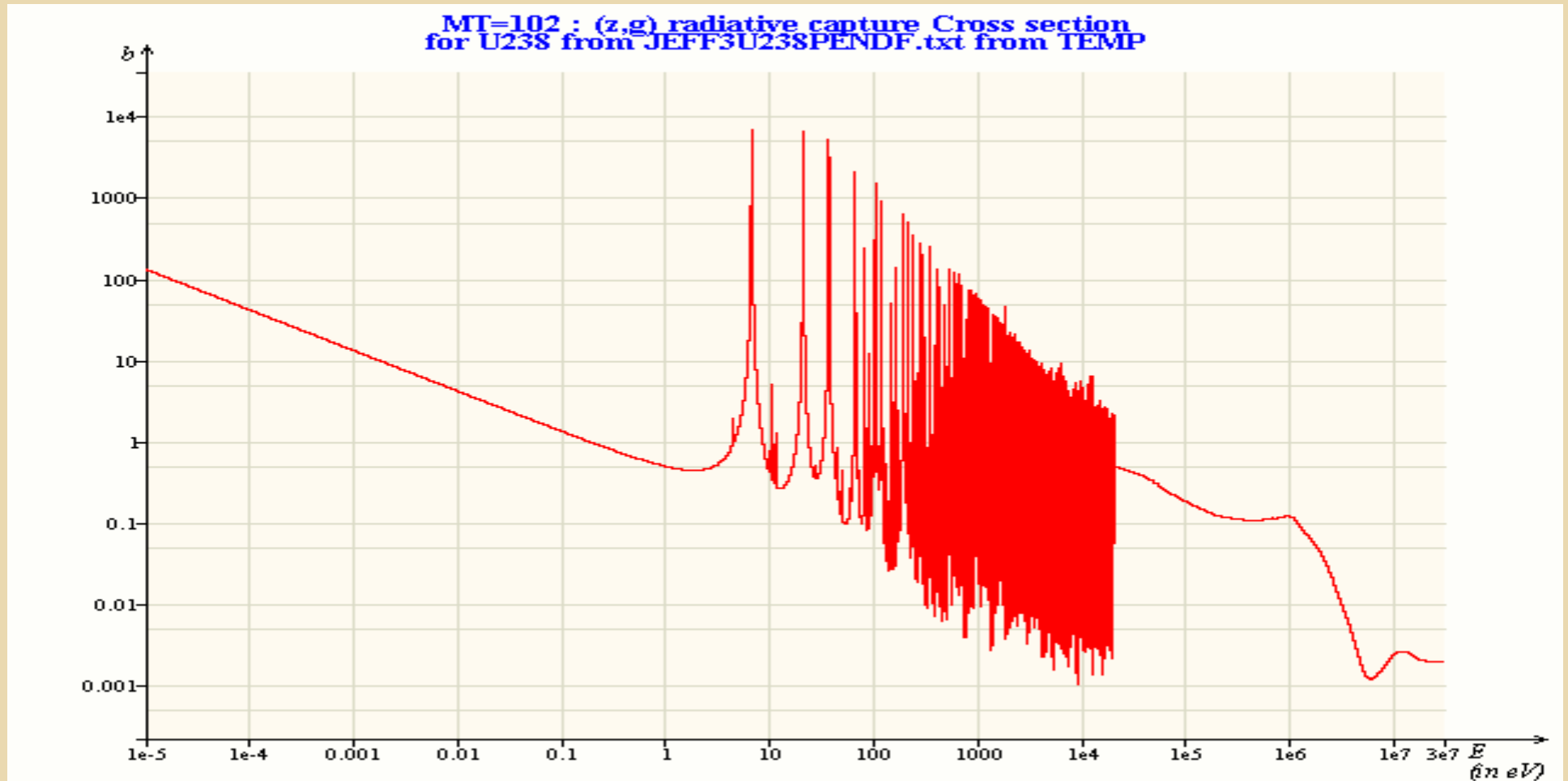
Conclusion for ENDF/B-VI_r8, JEFF3.0, JENDL3.3

- U238 is the most detailed file
- Resolved resonances to 10KeV
- 9SF needed for many points at 0K
- 9SF needed for few points at 300K
- NJOY99 solution for the grid is appropriate
- Possible problem –
Error on the grid increases as the points
APPROACH equality at 7SF

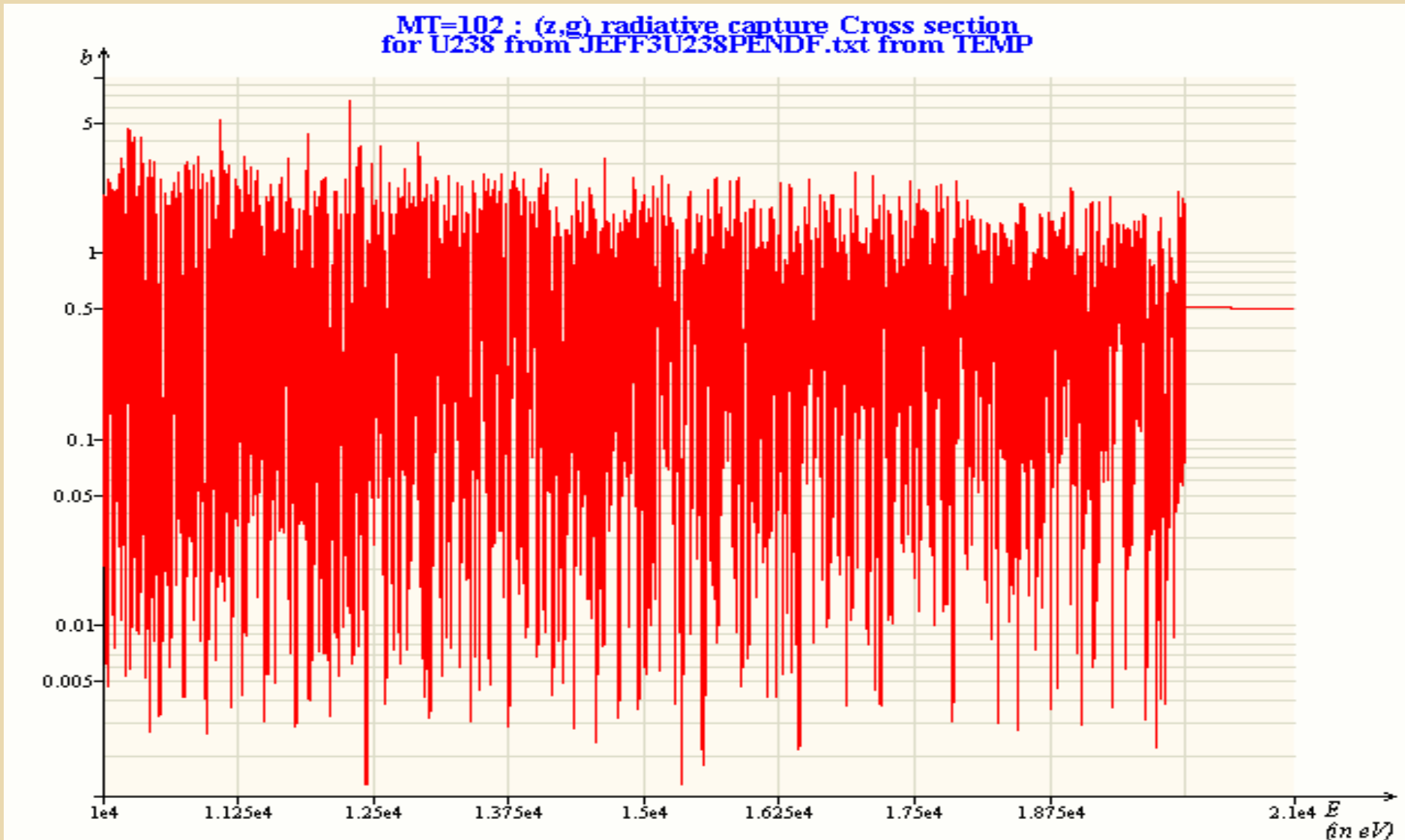
NEW U238 Evaluation (1)

- WPEC 22 study of low LWR K for :-
Leal/Larson... U235
WITH
Moxon/Sowerby .. U238
- At resonance energies freeze U235 consider improvements to U238
- New U238 Derrien /Courcelle/ Leal/Larson
- Resonance range extended to 20KeV from 10KeV
- As the resolved range increases in energy resonance spacing on a LOG scale tightens
- More close energy points.

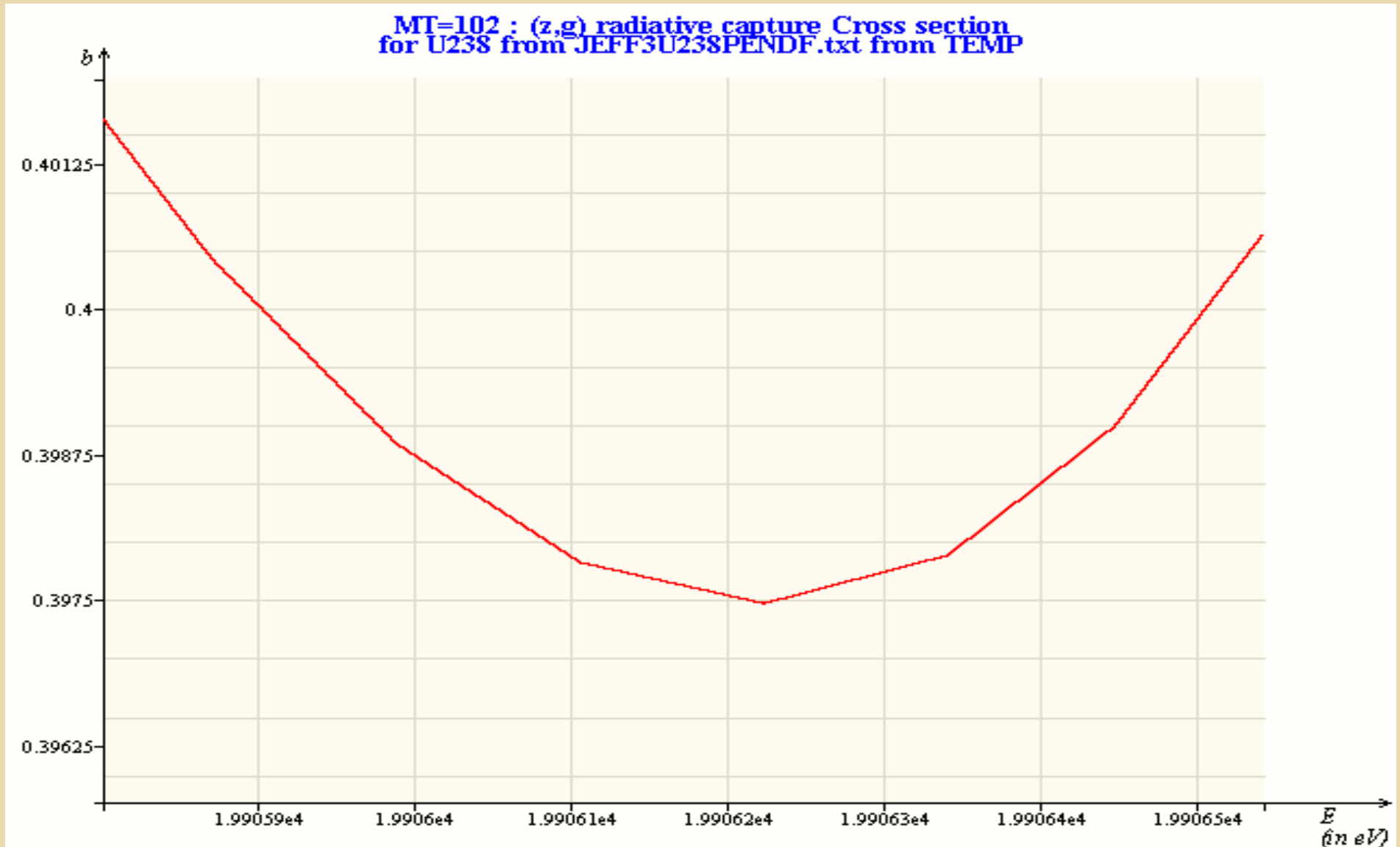
NEW U238 Evaluation (2) Capture Cross Section from JEFF3.1T4



NEW U238 Evaluation (3) Capture 10-20KeV



NEW U238 Evaluation (4) Capture - typical detail



Future developments and Unresolved data

- As accuracy increases the top of the Resolved range rises
- Above this, Unresolved resonance shielding is important for:-
fast reactors and
thermal reactors (resonance escape probability)
Reflected critical spheres
- PURR, CALENDF, GENEX – generate ladders
- All will require tight energy grids
- Revisit NJOY precision

NJOY Code Changes

- In RECONR + BROADR
- Changed NSF in SIGFIG calls from 7 to 9
- Did not cut out searches checking 7 figure accuracy
- Hence, other international changes can be applied
- NJOY99.90w22 created

Number of grid points from RECONR (0K)

Tolerance	NJOY99.90 w21	NJOY99.90 w22	Difference
0.001	1152817	1151742	-1075 (-0.09%)
0.002	820131	815407	-4724 (-0.57%)
0.005	520087	519221	-866 (-0.17%)
0.01	368984	367945	-1039 (-0.28%)

Number of grid points from BROADR (300K)

Tolerance	NJOY99.90 w21	NJOY99.90 w22	Difference
0.001	340207	335720	-4487 (-1.32%)
0.002	245939	242102	-3837 (-1.56%)
0.005	160808	157000	-3808 (-2.37%)
0.01	117371	116211	-1160 (-0.99%)

Grid Changes

- Using 9 SF gives less points
- Savings in BROADR are better than RECONR
- All are less than 3%
- Coarsening the tolerance has MUCH greater effect
- Detailed review indicated the new grid is noticeably different
- Possibly caused by removing the hidden error near points that are equal to 7SF
- What about practical links to single precision MONTE CARLO?

Number of Duplicated points at 7SF

Tolerance	NJOY99.90 w21	NJOY99.90 w22
0.001	431	7024
0.002	387	4068
0.005	32	1770
0.01	24	1284

MAXIMUM Effect on one of 13,193 Group Data (MONK8)

Tolerance	% Diff. due to Code Modification	% Diff. due to Tolerance Relaxation	
		NJOY99.90 w21	NJOY99.90 w22
0.001	0.09	-	-
0.002	0.10	0.25	0.25
0.005	0.19	0.48	0.48
0.01	0.41	1.25	1.25

Effect on a Sensitive Benchmark :- Zebra8A

Case	²³⁸ U Data Source	NJOY Version	K
1	JEF2.2	NJOY94.10 w23	0.9955 ±0.0002
2	JEFF3.1R2	NJOY99.90 w21	0.9899 ±0.0002
3	JEFF3.1R2	NJOY99.90 w22	0.9901 ±0.0002
Expt.			0.9920 ±0.0063

Conclusions

- Very little practical effect on K-eff
- Slightly more efficient energy grids
- Potential efficiency saving by not checking 7 SF
- “Cleaner” coding would result
- Disruptive – current method works
- Interface with Single Precision MONTE CARLO data is affected
- BUT as resonances are resolved more problems are likely with the current method
- Double precision MUST be used in unresolved ladders.