Automated GENDF Data Validation @ AWE

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AWE Nuclear Data

- Maintain UK Nuclear Deterrent.
- Provide data for modelling needed to support physics based certification.
- Mainly groupwise data, processed initially using NJOY.
  - Currently building NJOY processing capability, processing was contracted out, now is coming in house.
- Most recent libraries ENDF/B-VII.0, JEFF3.1.0, JENDL3.3 +Actinoid file.

Automated GENDF Validation

- GENDF files are big, in depth checking of cross sections and secondary distributions is impractical for large libraries.
- Developed an automated tool, NDval.
- Scans GENDF files checking all cross sections and secondary energy distributions

NDval data checks

- Test 1: Ratio of Pythagorean Means
  - Test for Large data spikes.
  - Arithmetic Mean

$$\overline{\sigma_a} = \frac{1}{n}\sum_i^n \sigma_i$$

  - Harmonic Mean

$$\overline{\sigma_h} = \left(\frac{1}{n}\sum_i^n \frac{1}{\sigma_i}\right)$$

  - Geometric Mean

$$\overline{\sigma_g} = \sqrt[n]{\prod_i^n \sigma_i}$$

- Calculate ratio of these three means.

$$r = \frac{\overline{\sigma_a \sigma_h}}{\left(\overline{\sigma_g}\right)^2}$$

- If r>> 1 data are dominated by few high values.
- Due to diagonal terms in elastic scattering matrices. Only off diagonal data are considered.

- Test 2: The Gradient Test
- Test for extreme changes in data, discontinuities etc.
- Checks the gradient $$\frac{d\sigma}{d\ln E}$$
- Extreme gradients can be physical features, diagonal in matrix data, resonances.

- Test 3: Gradient sign change test.
- Tests for rapidly changing data eg many small spikes.
- Calculates the number of times the sign of the gradient changes over a predefined bin.

- Can be physical features eg RRR

- Test 4: Comparison with a second library.
- Test for differences between two files.
- Reports significant data differences.

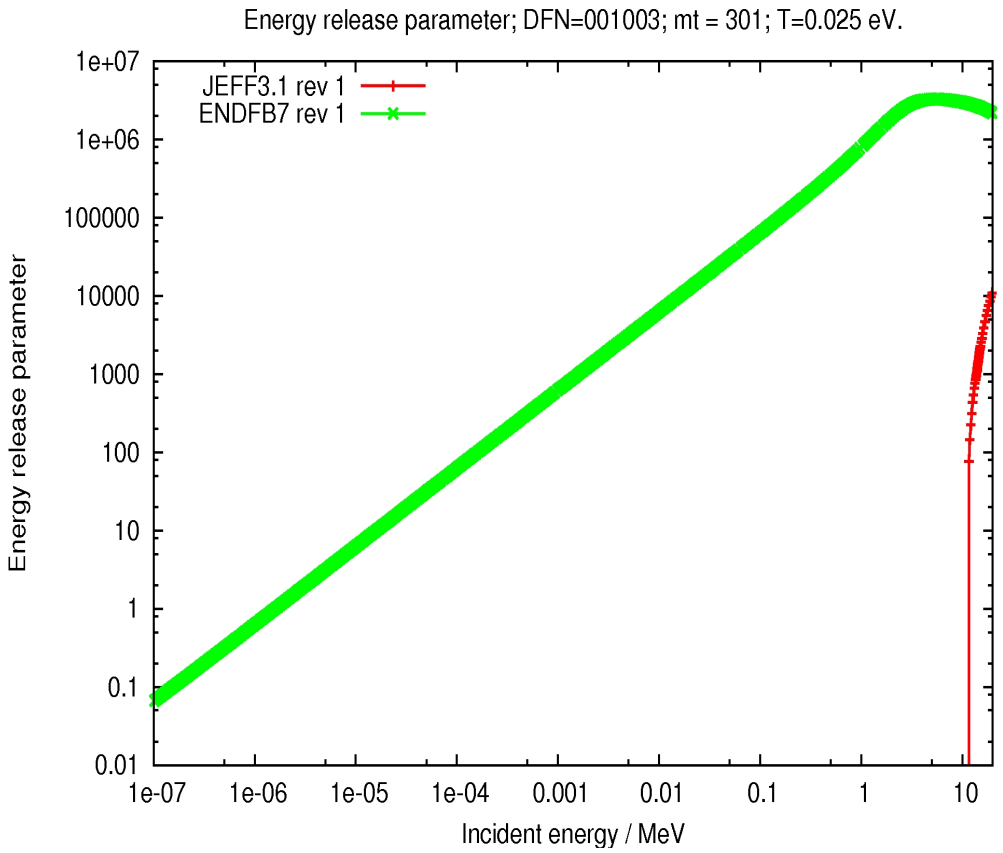
- What do you compare against, old data? Another evaluation eg JEFF, JENDL.

Interesting features in data.

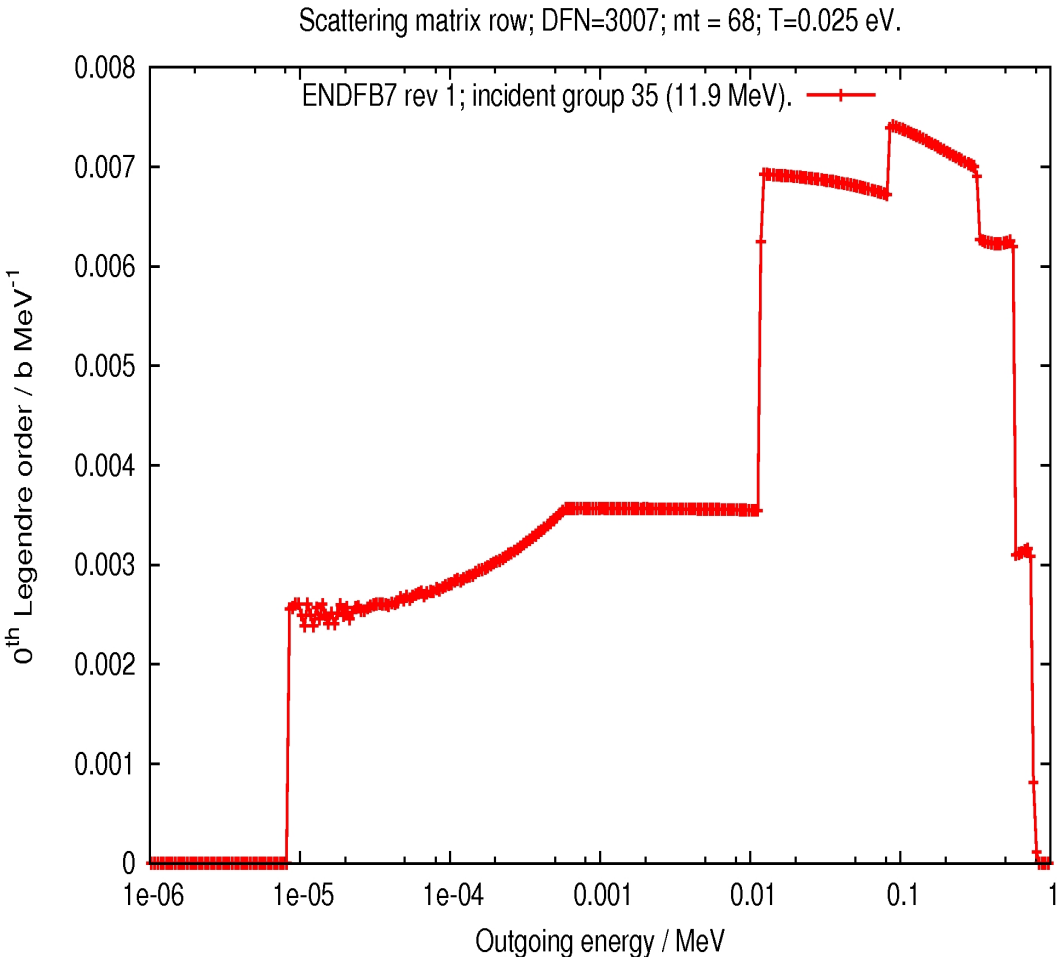
- Used NDval on ENDF/B-VII.0 and JEFF3.1 GENDF files.
- Found a number of interesting features.
  - Missing data in total KERMA (MT301).
  - Discontinuities in data matrices and cross sections.
  - Spikes near threshold in secondary distributions.
  - Thermal tails in fission spectra.
  - Differences in cross sections.

The energy release bug.

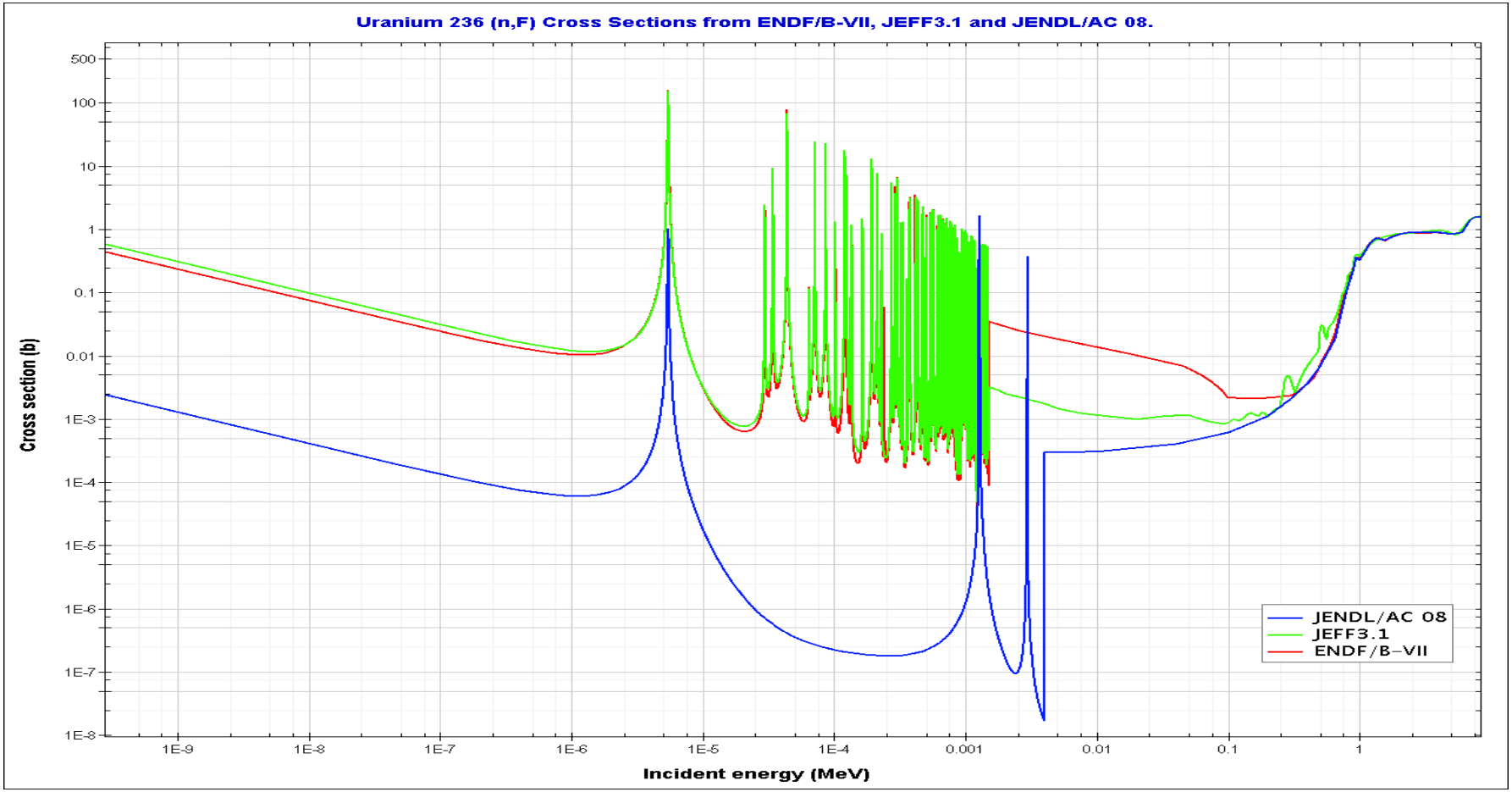
- JEFF3.1 and ENDF/B-VII vastly different.
  - 3 orders of magnitude.
- ENDF/B-VII agrees with older data.
- All reactions were not included in the calculation of the total.



Data Discontinuities

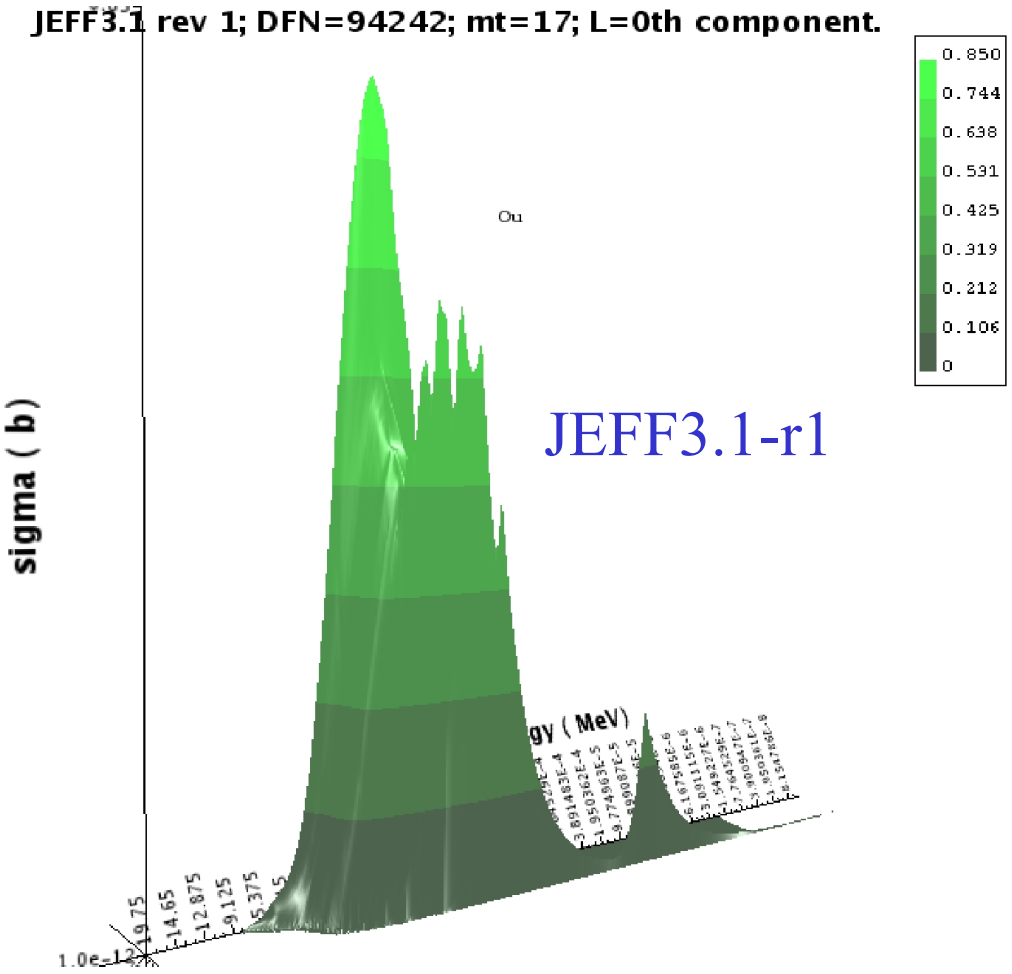


- ^{7}Li inelastic scattering.
- Occur in other secondary distributions.
- Discontinuities in the data.
- Caused by low resolution underlying data

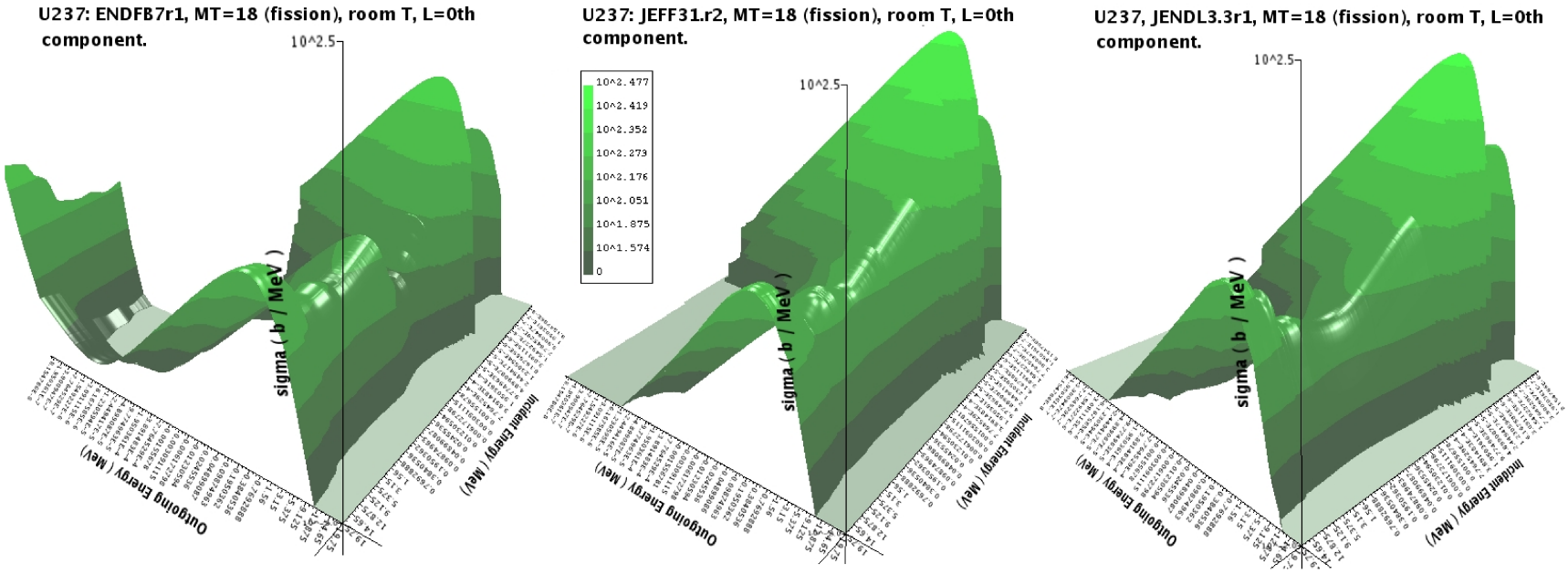

Uranium 236 (n,F) Cross Sections from ENDF/B-VII, JEFF3.1 and JENDL/AC 08.
Cross section (b)
500
100
10
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
1E-8
1E-9
1E-8
1E-7
1E-6
1E-5
1E-4
0.001
0.01
0.1
1
Incident energy (MeV)
JENDL/AC 08
JEFF3.1
ENDF/B-VII

Threshold Spikes

- Occur in reactions with a threshold energy.
- Spikes in secondary distributions near threshold energy.

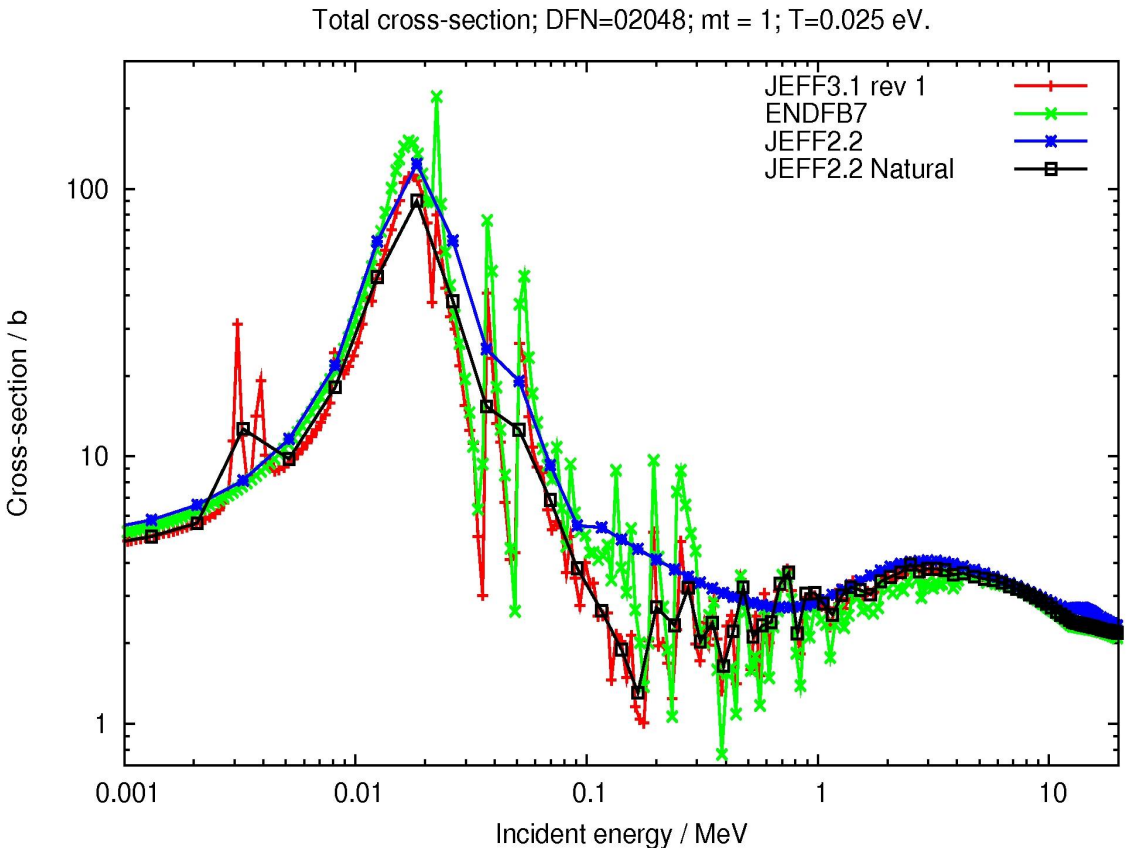


Thermal Tails in Fission Spectra.

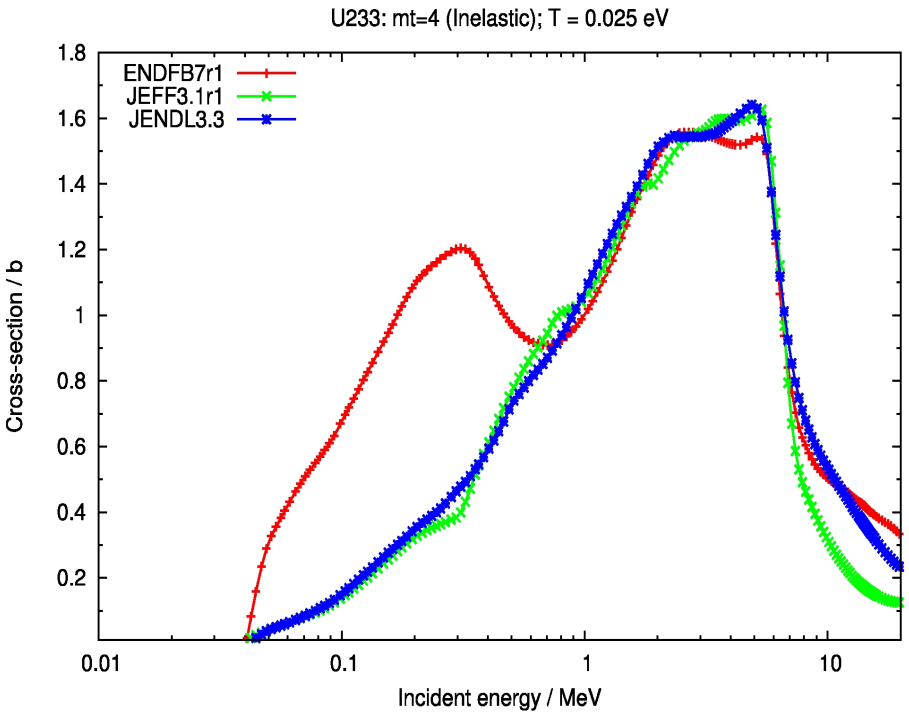


- U237 ENDF/B-VII has an unexpected thermal tail.
  - JENDL3.3 and JEFF3.1 don't have this.

Cross Section Differences

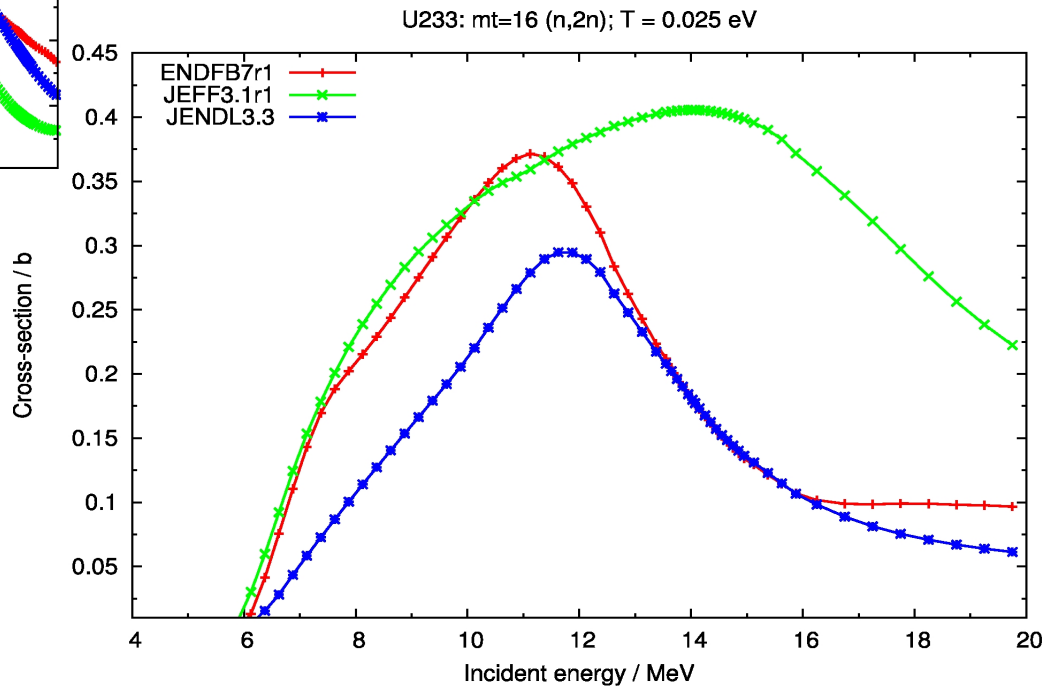


- Factor of 2 disagreement.
- JEFF3.1 matches JEF2.2 Ti Nat data
- ENDF/B-VII shows better match to JEF2.2 Ti 48 data



Inelastic scatter

(n,2n)



- Creation and Development of NDval forms part of a greater programme of validation and data assessment.

- A project aiming to provide the best, validated cross sections to our users.
  - The LINDA project.
- NDval to be applied to ENDF/B-VII.1 when finalised.