IAEA
60 Years
Atoms for Peace and Development

CIELO Data Validation and Benchmarking Activities at the IAEA

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Acknowledgement

- The work presented herein is the result of contributions from several IAEA consultants and voluntary contributions from external collaborators…

Overview

- Scope of data testing at the IAEA with examples
- Pitfalls in the use of figures of merit (FoM)
- Discrepancies in integral benchmarks
- Uncertainties due to data processing and self-shielding treatment

Scope of data testing

Strategy – taking ^{235}U as an example:

- Start with clean bare configurations
- Proceed with thermal solutions
- Include well-tested reflected systems
- More complex assemblies and broad scope testing

Bare ^{235}U configurations

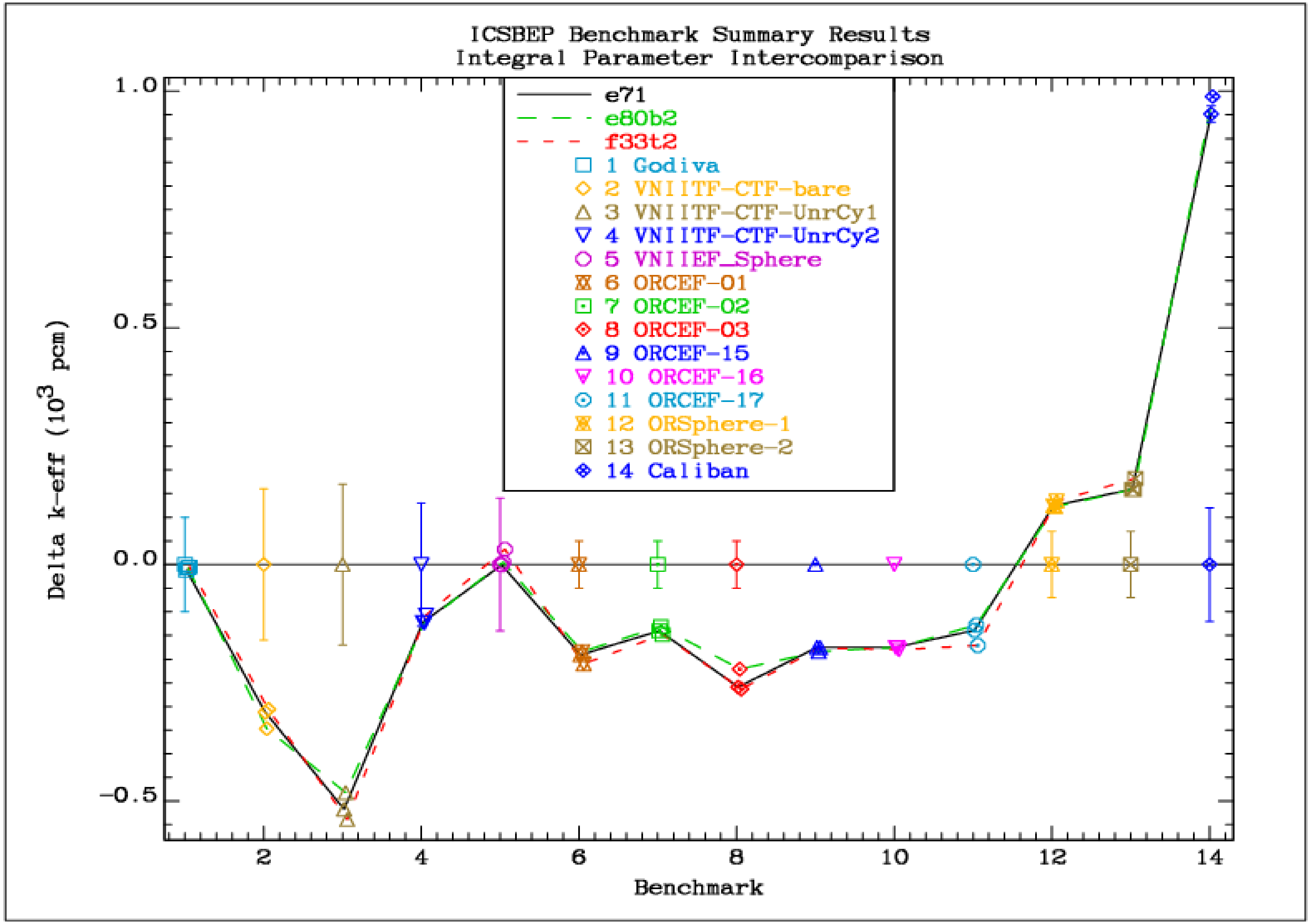
Observations:

Large discrepancies in predicted reactivity, which is unreasonable since sensitivities to nuclear data are similar. Examples:

- Caliban: 1% over-prediction (MCNP and TRIPOLI), 0.5% inconsistency in mass of fissile material, neglecting measured abundances of B, etc.)
- ORNL spheres predicted high compared to cylinders
- Discrepancies in the Russian benchmarks (0.5%)…

→ **There is a need to resolve the discrepancies**

Bare ^{235}U configurations

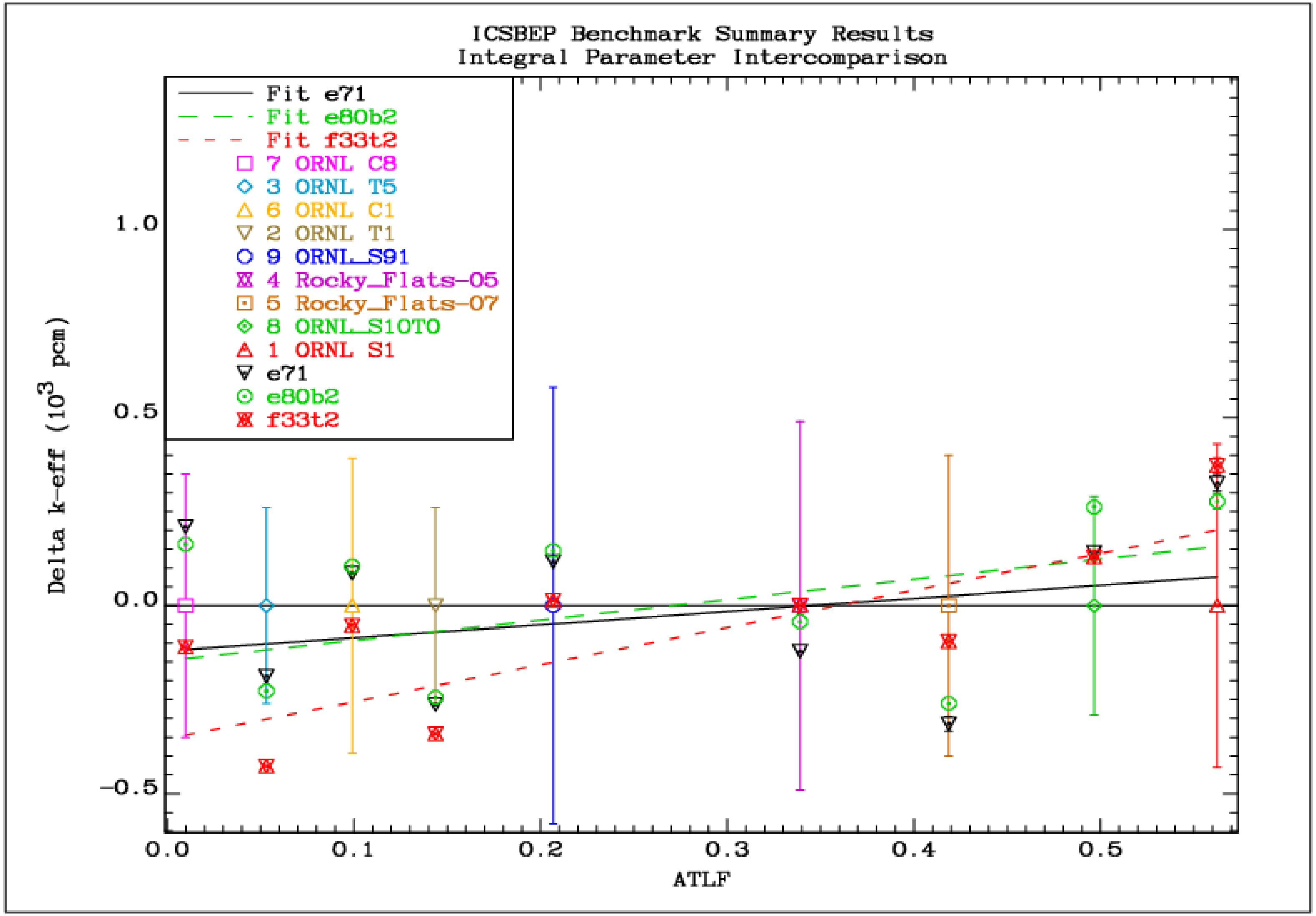


HEU Thermal Solutions

- Traditionally, the "above-thermal leakage fraction" (ATLF) is an established parameter for characterising solution assemblies
- To save time, representative cases were chosen that span the wide range of values
- With "beta-2" good performance is preserved

Again, there is large scatter in some groups of benchmarks

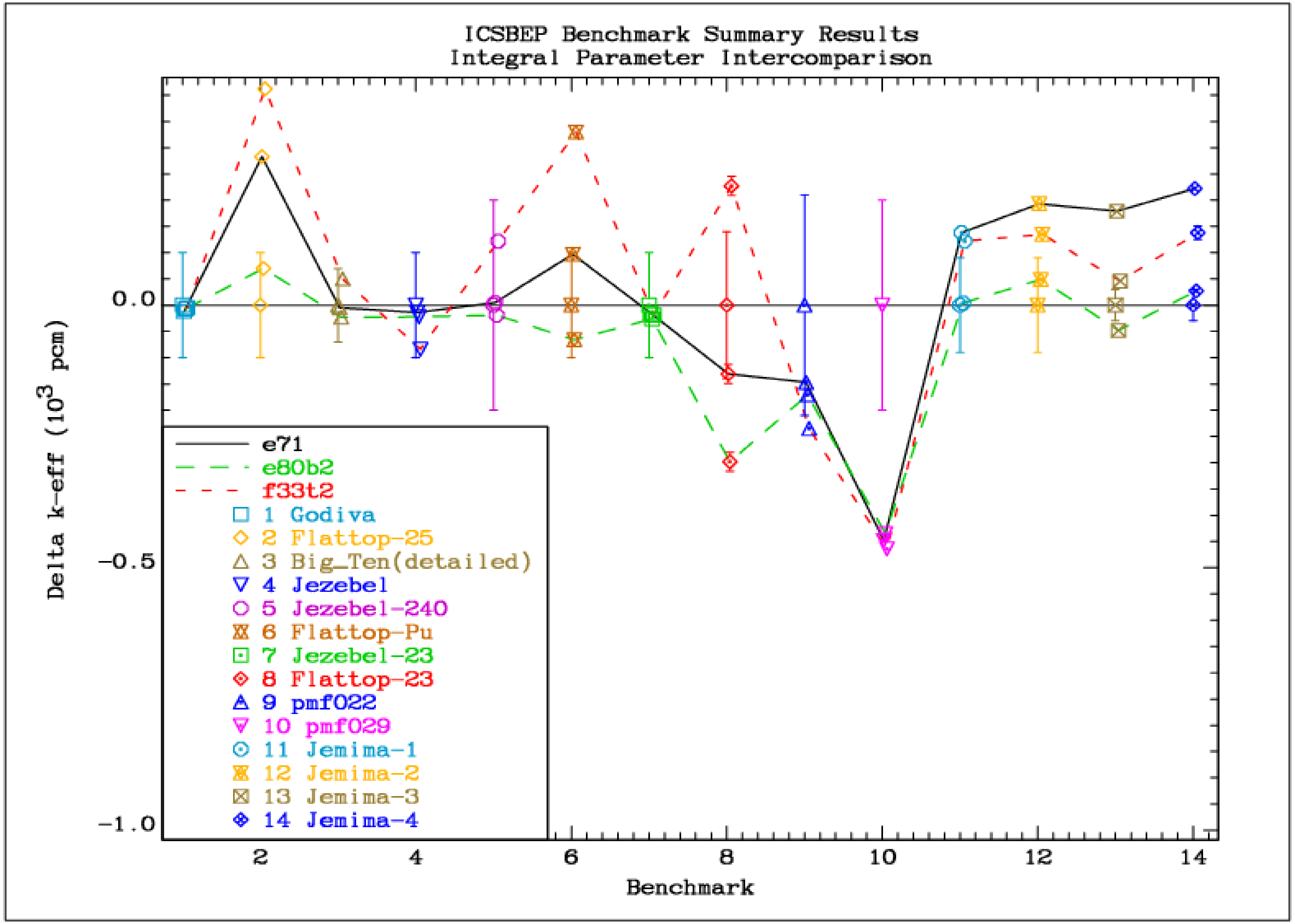
HEU Thermal Solutions



Reflected assemblies

- Preference for simple configurations with few materials that have well-known cross sections
- A selection of traditionally used assemblies was collected into the so-called “main” list

Reflected and other assemblies (main)



List of “main” benchmarks

1	HEU-MET-FAST-001	hmf001	Godiva
2	HEU-MET-FAST-028	hmf028	Flattop-25
3	IEU-MET-FAST-007	imf007d	Big_Ten(detailed)
4	PU-MET-FAST-001	pmf001	Jezebel
5	PU-MET-FAST-002	pmf002	Jezebel-240
6	PU-MET-FAST-006	pmf006	Flattop-Pu
7	U233-MET-FAST-001	umf001	Jezebel-U233
8	U233-MET-FAST-006	umf006	Flattop-23
9	PU-MET-FAST-022	pmf022	Bare(98
10	PU-MET-FAST-029	pmf029	Bare(88
11	IEU-MET-FAST-001	imf001-001	Jemima-1
12	IEU-MET-FAST-001	imf001-002	Jemima-2
13	IEU-MET-FAST-001	imf001-003	Jemima-3
14	IEU-MET-FAST-001	imf001-004	Jemima-4

Broad scope testing

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Benchmarking depends on:

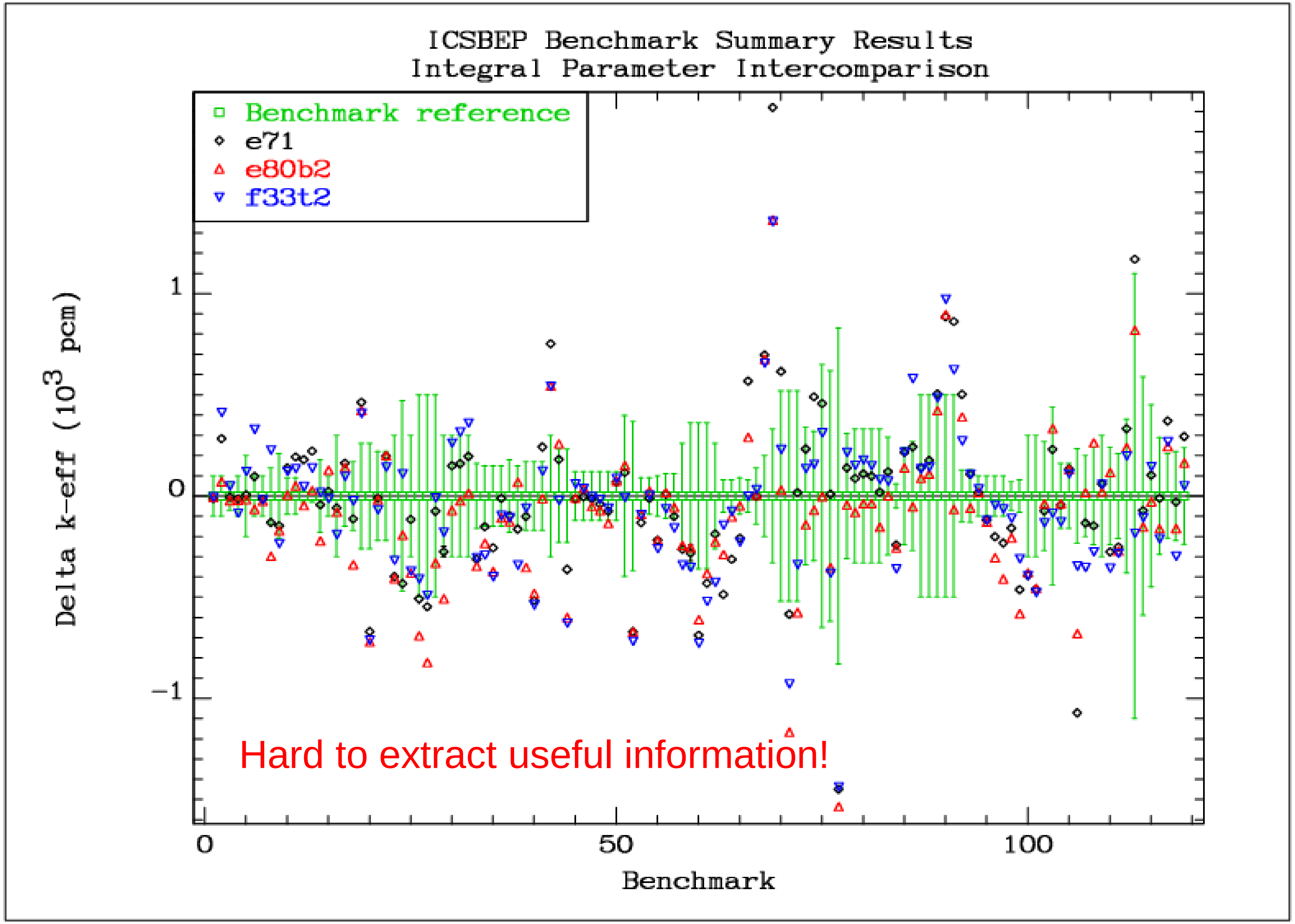
- Availability of input models
- Computer resources
- Capacity to analyse the results

Different sets are used at various places (NRG, LANL, CEA…)

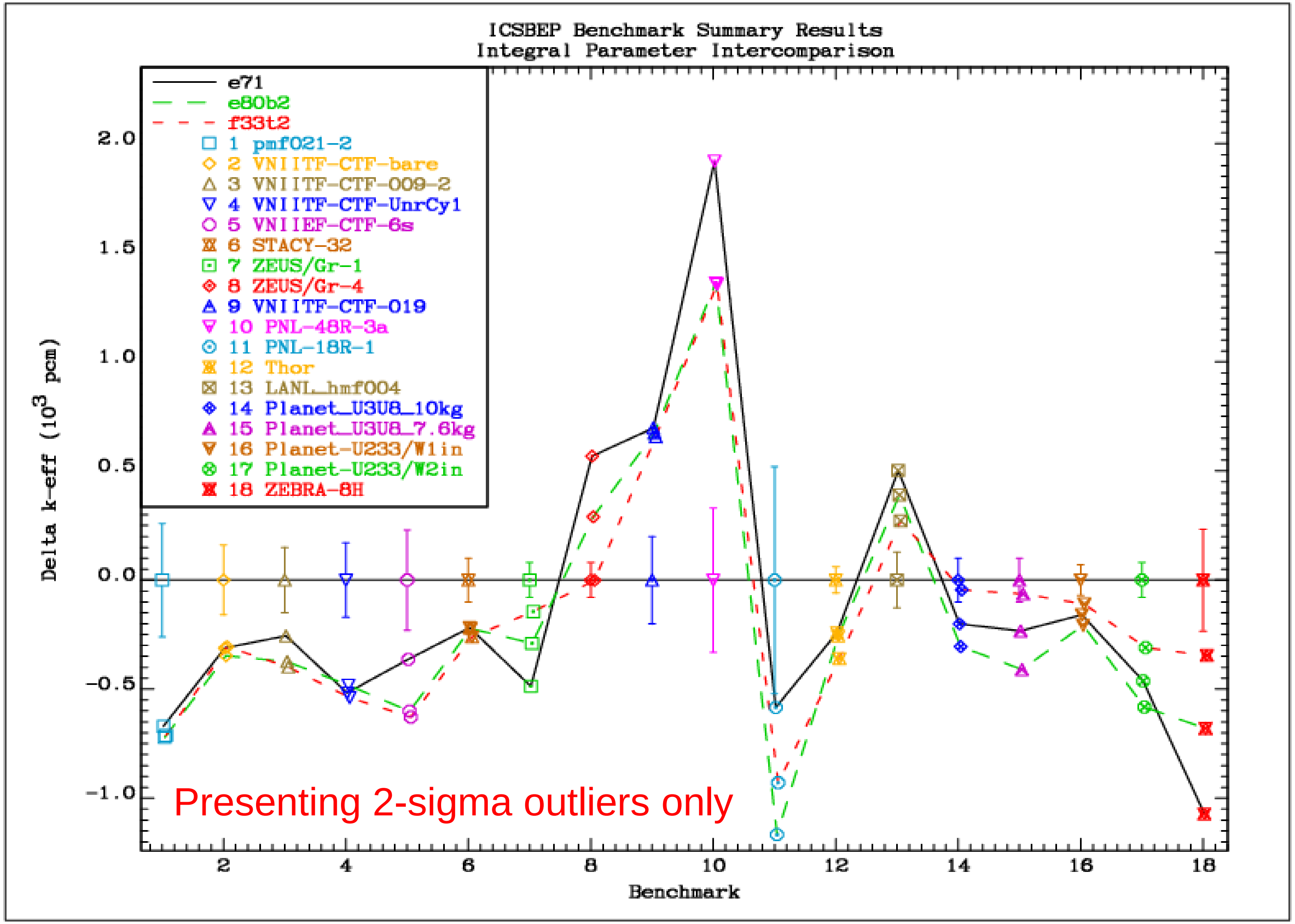
Example:

- Los Alamos suite of 119 ICSBEP benchmarks

Broad scope testing



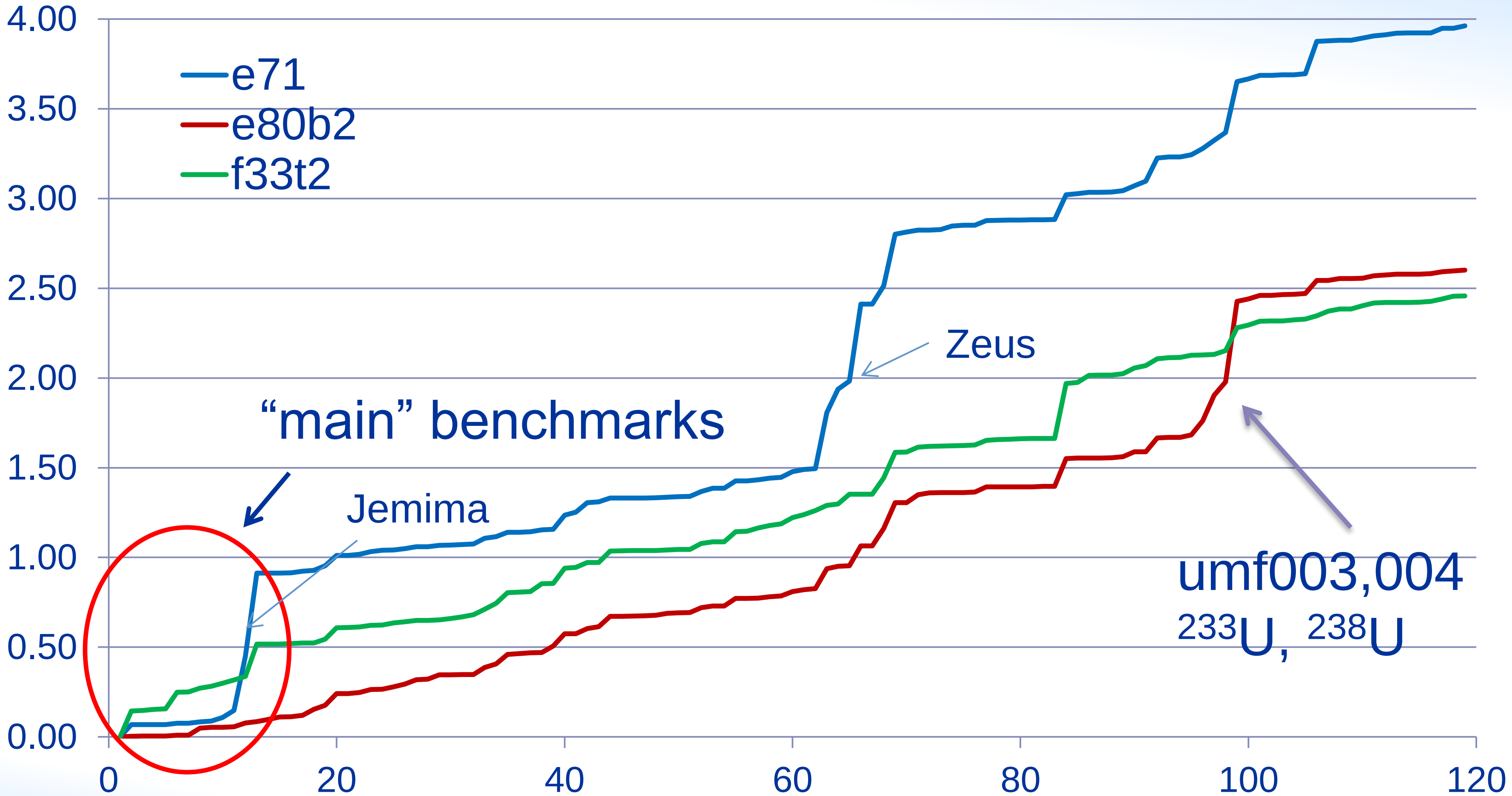
Broad scope testing (2σ outliers e80b2)



Pitfalls in the use of FoM

- Different possibilities for defining Figures of Merit (FoM) exist:
  - r.m.s. Delta-k – equal weight to all, including cases of low accuracy
  - X^2/DoF – sensitive to cases with unrealistically small uncertainties
  - … other

Cumulative contribution to X^2/DoF



Discrepancies in integral benchmarks

- As illustrated in the case of bare ^{235}U assemblies, discrepancies of several hundred pcm (parts per 100 000) for cases with similar spectra and sensitivity profiles are more likely caused by bad description or bad benchmark models
- A strong effort is needed to resolve such discrepancies

Data processing and methods

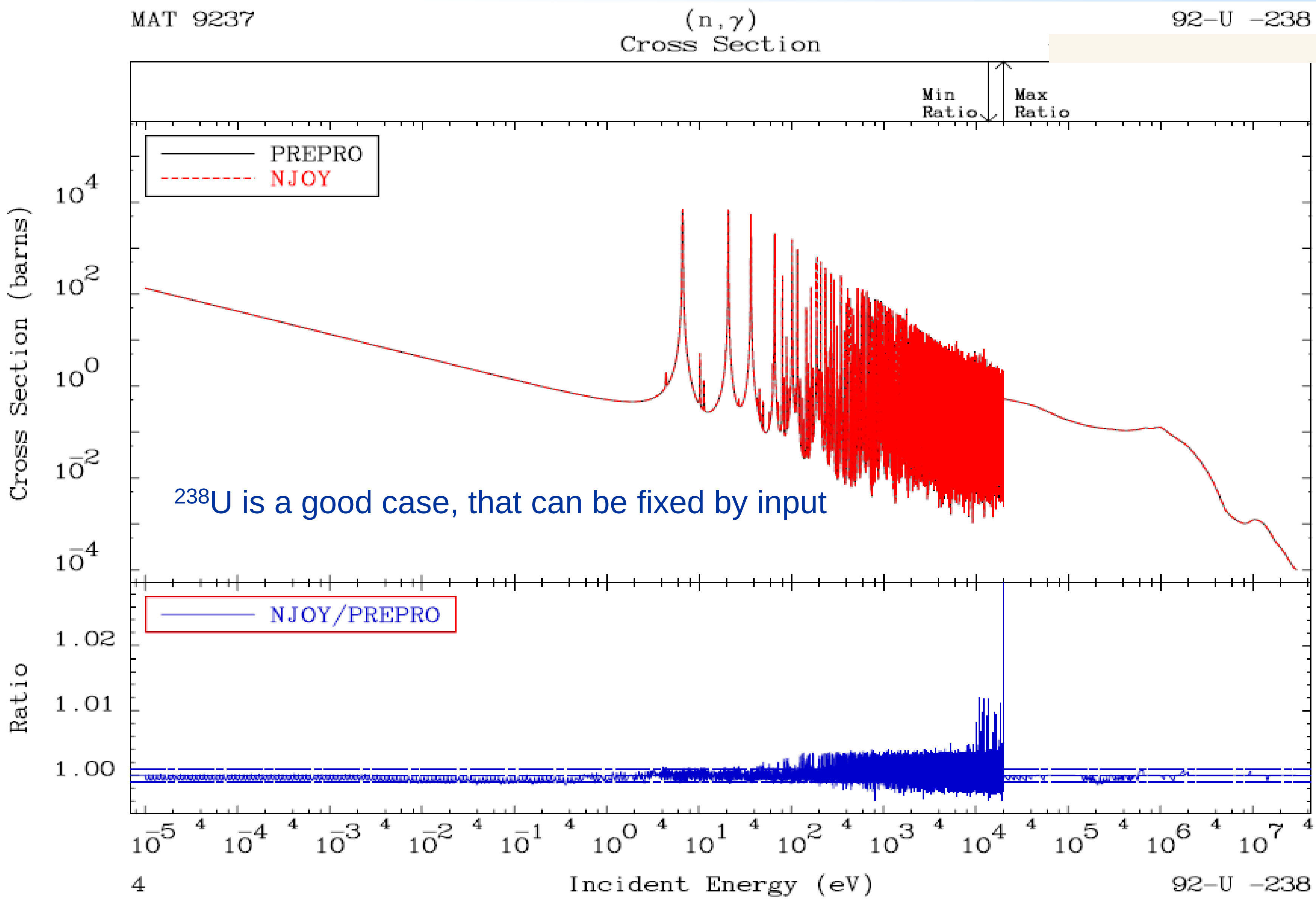
- Monte Carlo codes can treat geometry accurately
- Starting from the same data source they should give the same result
- Differences occur due to:
  - Data processing (e.g. resonance reconstruction)
  - Methods (e.g. self-shielding in the unresolved resonance range (URR))
  - Other …

Resonance reconstruction

Example:

- Make an ACE file with NJOY
- Convert back to ENDF
- Process the same library with PrePro with 0.1% reconstruction tolerance and same temperature
- Compare the two files
- Study the impact of differences on benchmarks
  - E.g. NJOY, PrePro, GRUCON (preliminary, ACE files provided by V. Sinitsa)

^{238}U Resonance reconstruction



^{238}U is a good case, that can be fixed by input

^{239}Pu Unresolved resonance range

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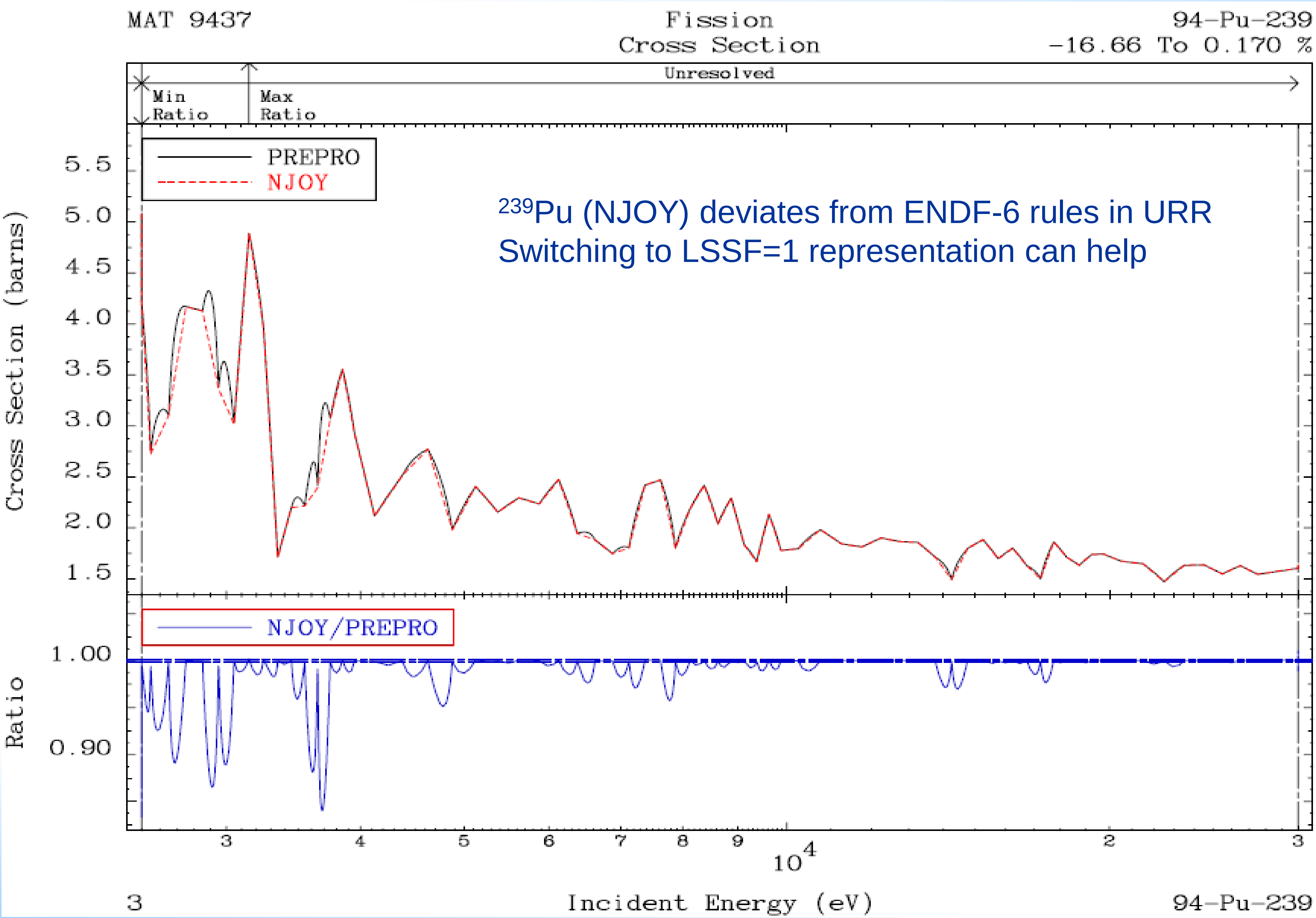
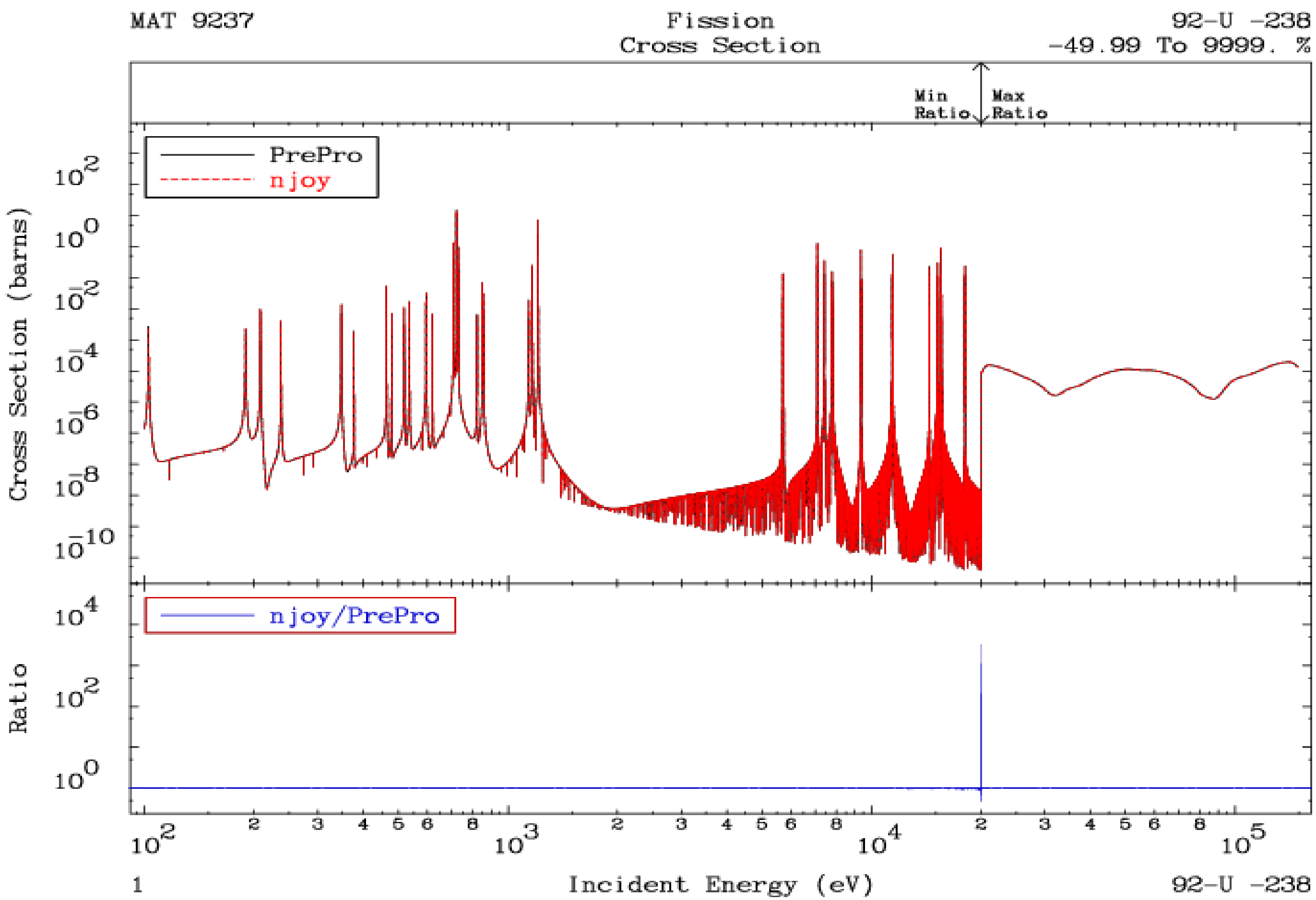


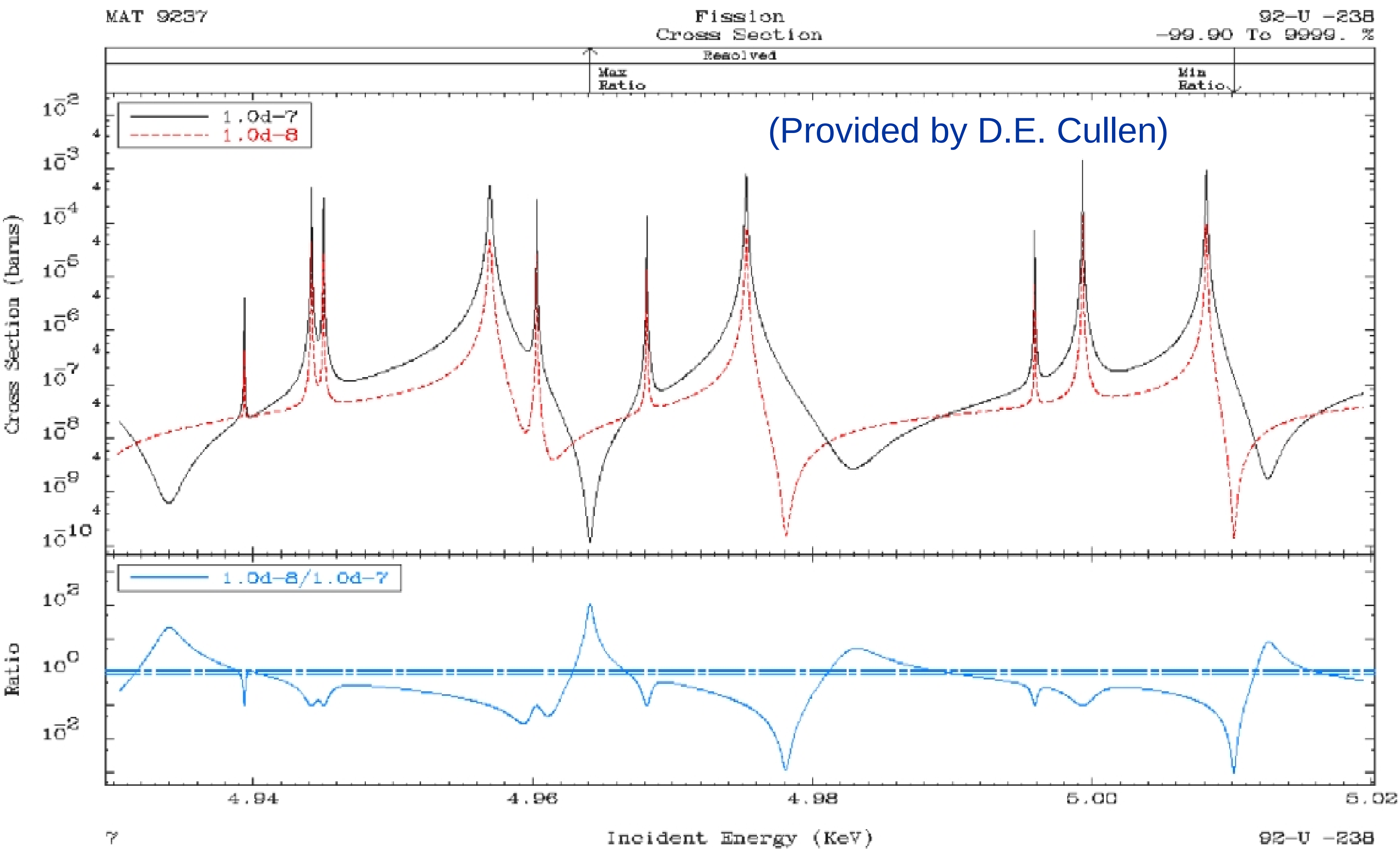
^{239}Pu (NJOY) deviates from ENDF-6 rules in URR

Switching to LSSF=1 representation can help

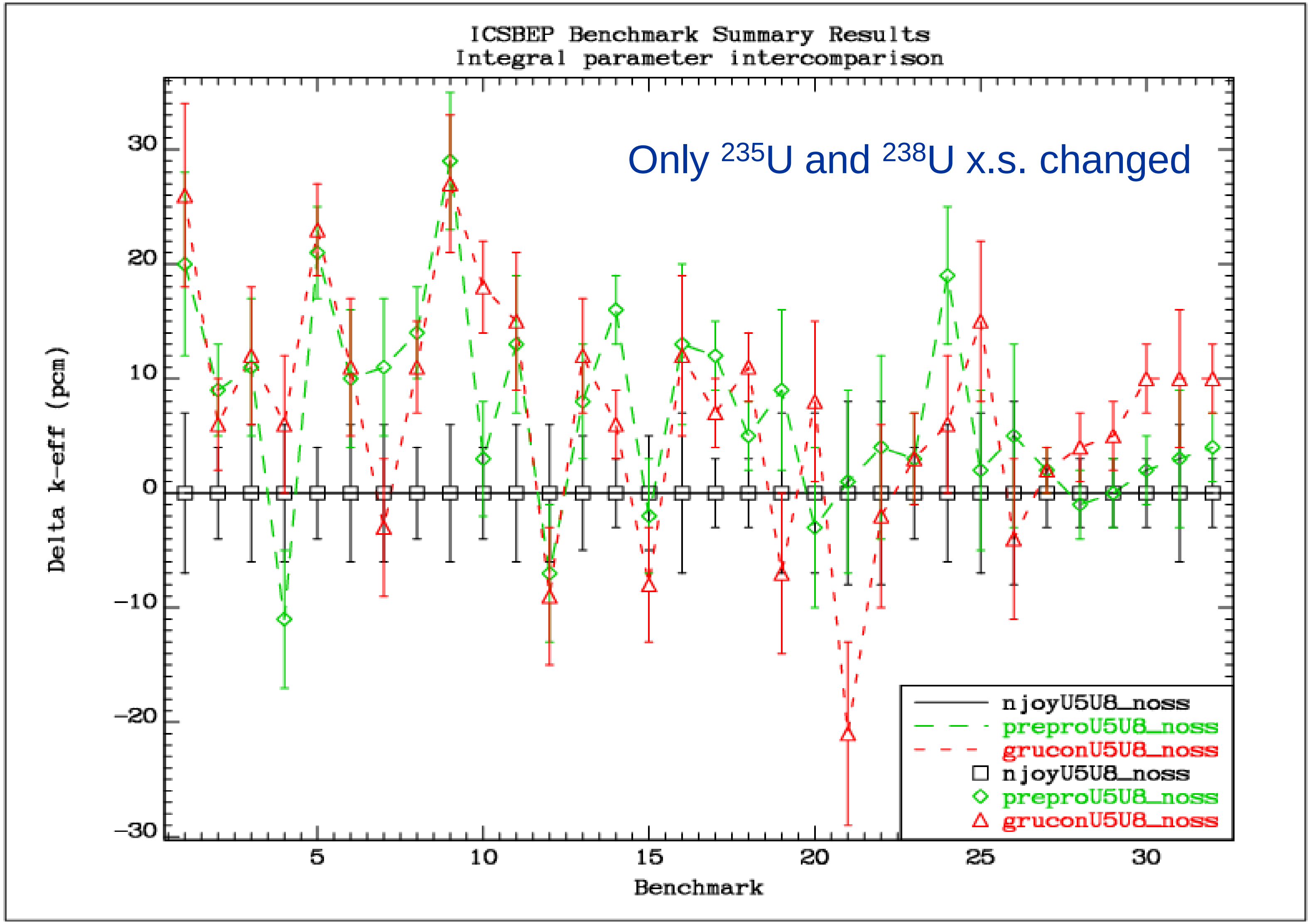
^{238}U Fission Cross Section



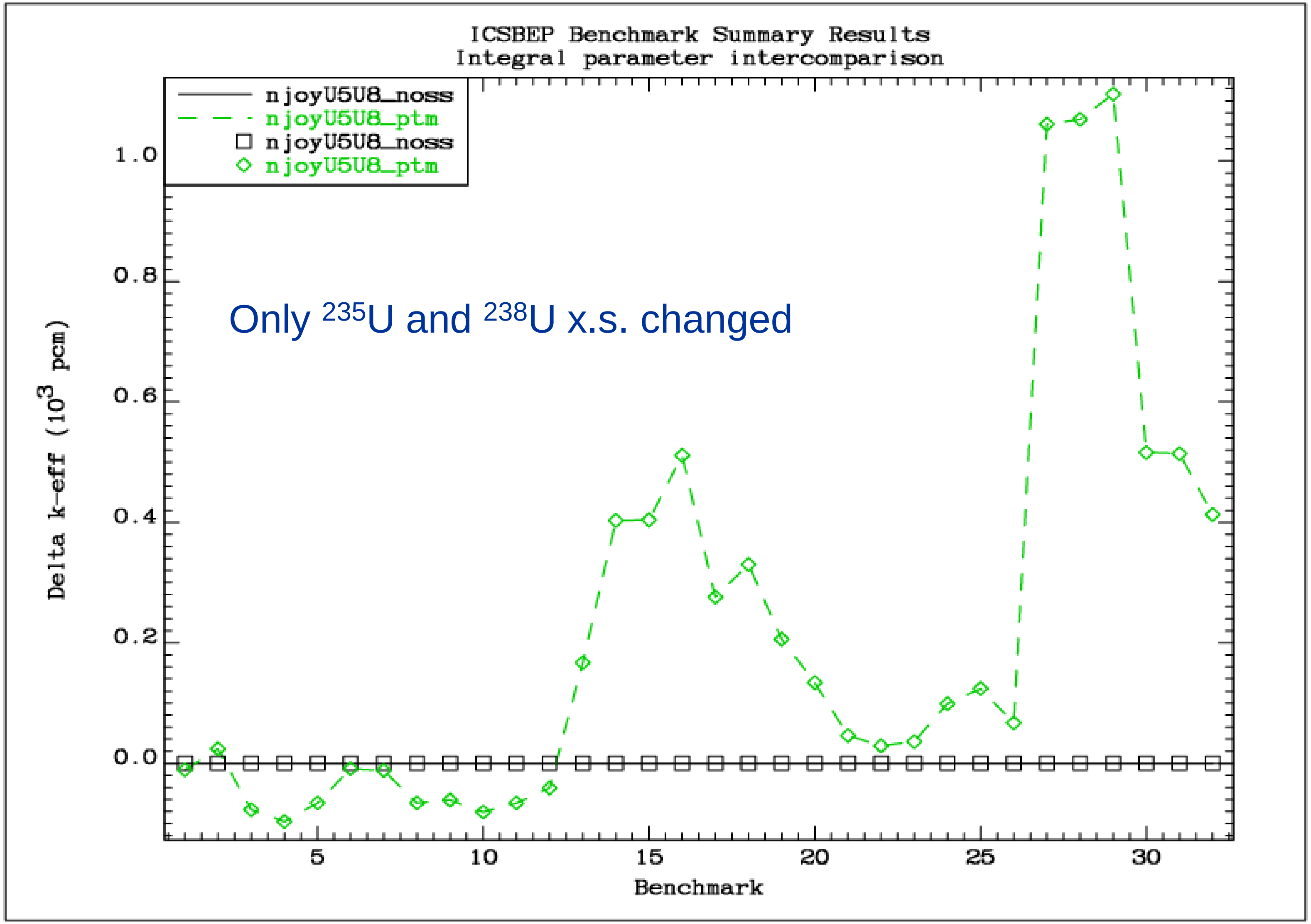
^{238}U Fission Cross Section



Impact on selected ICSBEP benchmarks



Self-shielding in the URR - importance

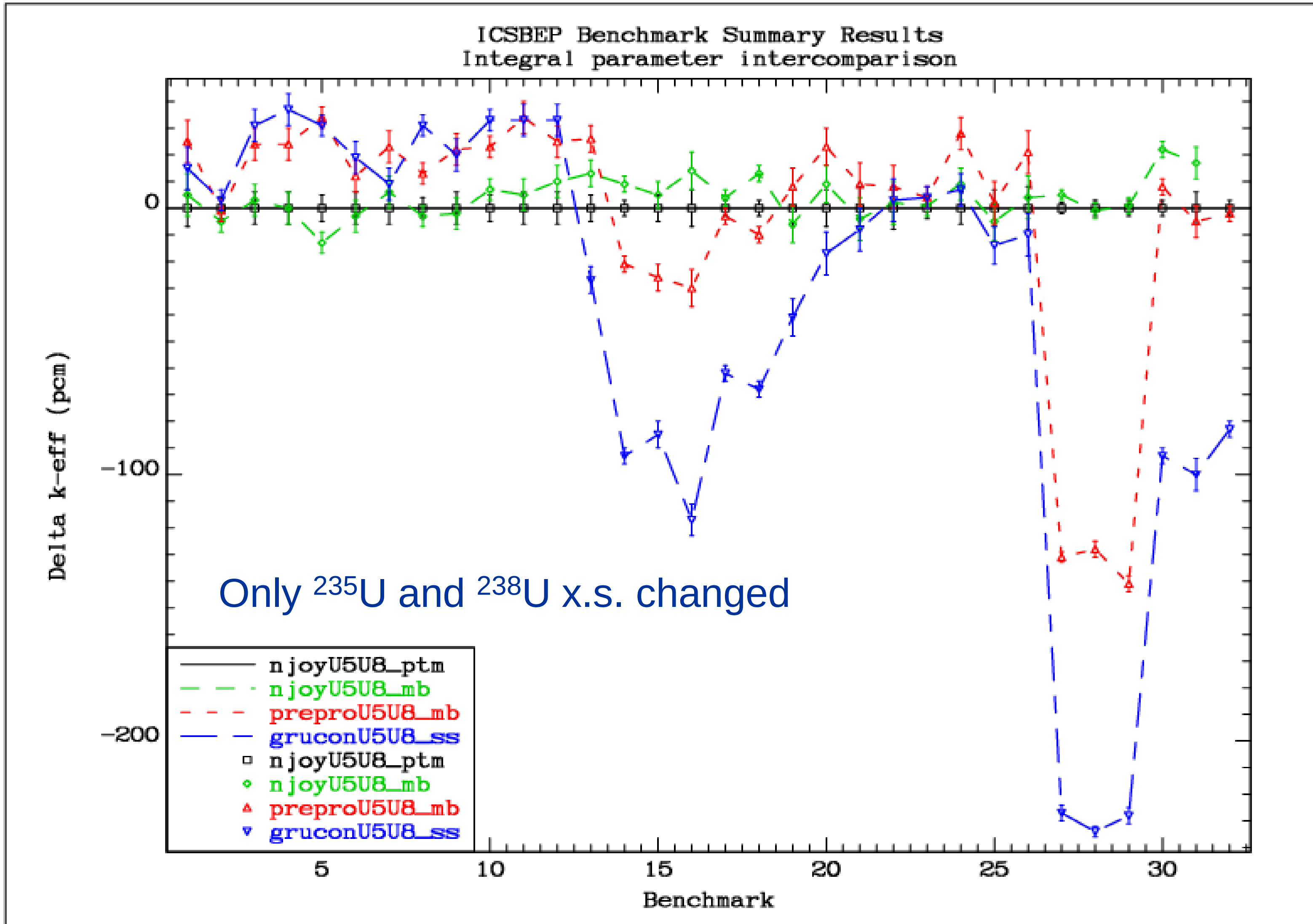


Self-shielding in the URR - methods

- NJOY probability table method (PTM)
- PrePro multi-band parameters
- GRUCON average parameters (preliminary , ACE files provided by V. Sinitsa)

Analysis is limited to ^{235}U and ^{238}U, the rest is taken from the generic MCNP library)

Self-shielding in the URR - methods



Conclusions

- Discrepancies in integral benchmarks with similar spectra and sensitivities should be resolved
- One should be careful in the interpretation of FoM
- MC calculations are NOT exact – be aware of uncertainties due to data processing and due to methods

Conclusions (cont.)

- With current data libraries we are converging for well-defined benchmarks; tight convergence criteria are needed
- Detailed benchmark models should be used whenever possible to avoid ambiguities

List of benchmarks in the study of methods

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1	HEU-MET-FAST-001	hmf001	Godiva
2	HEU-MET-FAST-002	hmf002-2	Topsy-2
3	HEU-MET-FAST-003	hmf003-01	Topsy-U_2.0in
4	HEU-MET-FAST-003	hmf003-02	Topsy-U_3.0in
5	HEU-MET-FAST-003	hmf003-03	Topsy-U_4.0in
6	HEU-MET-FAST-003	hmf003-10	Topsy-W_4.5in
7	HEU-MET-FAST-003	hmf003-11	Topsy-W_6.5in
8	HEU-MET-FAST-014	hmf014	VNIIEF-CTF-DU
9	HEU-MET-FAST-032	hmf032-1	COMET-TU1_3.93in
10	HEU-MET-FAST-032	hmf032-2	COMET-TU1_3.52in
11	HEU-MET-FAST-032	hmf032-3	COMET-TU1_1.742in
12	HEU-MET-FAST-032	hmf032-4	COMET-TU1-0.683in
13	IEU-COMP-FAST-004	icf004	ZPR-3/12
14	IEU-MET-FAST-007	imf007	Big_Ten
15	IEU-MET-FAST-007	imf007d	Big_Ten(detailed)
16	IEU-MET-FAST-010	imf010	ZPR-6/9(U9)
17	IEU-MET-FAST-012	imf012	ZPR-3/41
18	IEU-MET-FAST-013	imf013	ZPR-9/1
19	IEU-MET-FAST-014	imf014-2	ZPR-9/2
20	IEU-MET-FAST-022	imf022-01	FR0_3X-S
21	IEU-MET-FAST-022	imf022-02	FR0_5-S
22	IEU-MET-FAST-022	imf022-03	FR0_6A-S
23	IEU-MET-FAST-022	imf022-04	FR0_7-S
24	IEU-MET-FAST-022	imf022-05	FR0_8-S
25	IEU-MET-FAST-022	imf022-06	FR0_9-S
26	IEU-MET-FAST-022	imf022-07	FR0_10-S
27	MIX-MISC-FAST-001	mif001-01	BFS-35-1
28	MIX-MISC-FAST-001	mif001-02	BFS-35-2
29	MIX-MISC-FAST-001	mif001-03	BFS-35-3
30	MIX-MISC-FAST-001	mif001-09	BFS-31-4
31	MIX-MISC-FAST-001	mif001-10	BFS-31-5
32	MIX-MISC-FAST-001	mif001-11	BFS-42