APRENDE

JEFF-4.0 validation for Pu isotopes

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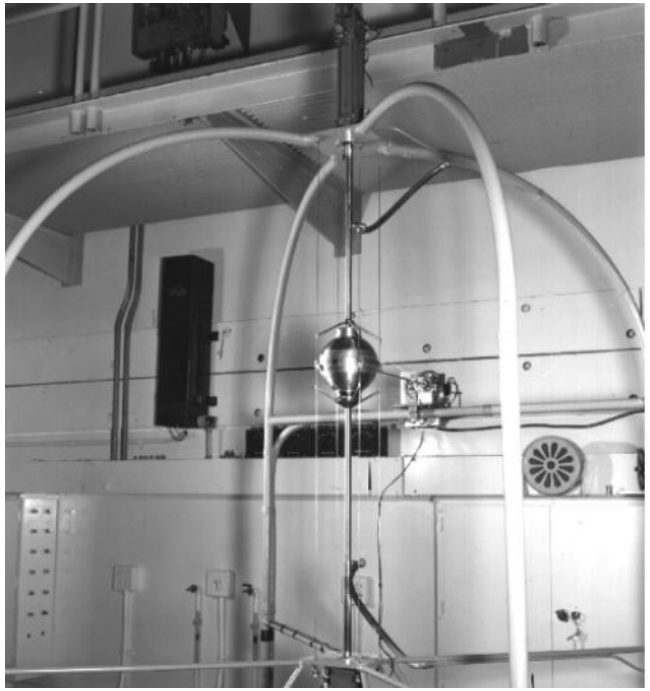
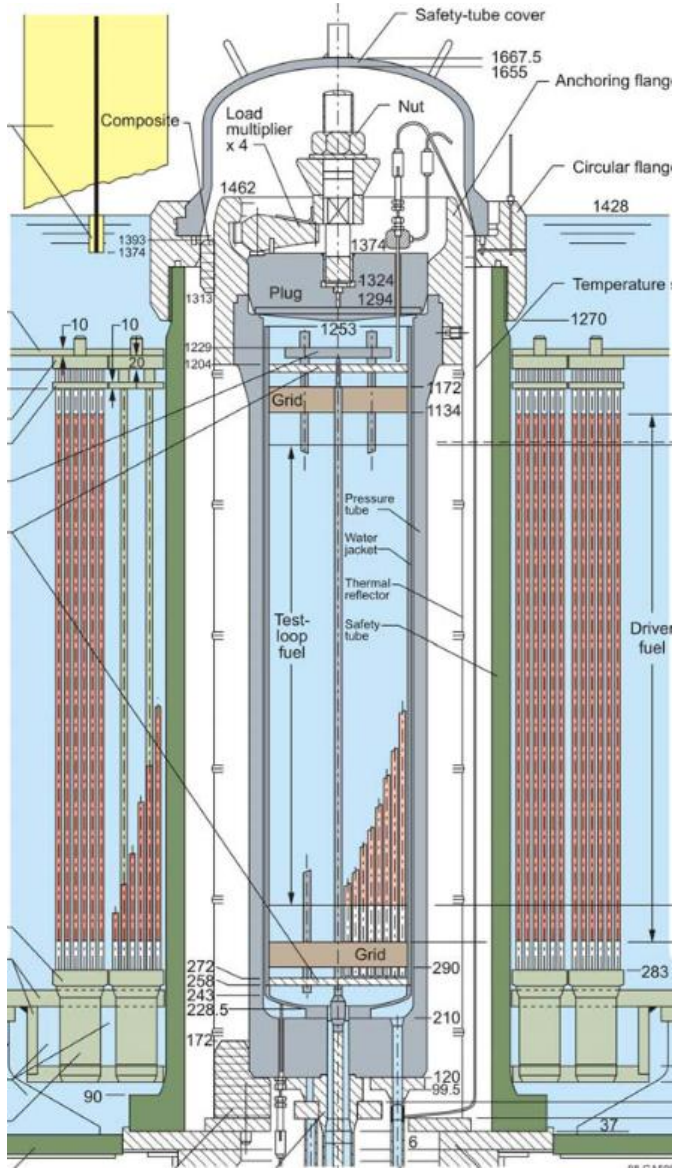
Integral benchmarks

- Macro-level experimental set-up
- Measure a ‘system-response’ such as
  - ✓ k_{eff}
  - ✓ Reaction rates
  - ✓ Power distribution
  - ✓ Spectral characteristics
  - ✓ Kinetics parameters (β_{eff}, Λ)
  - ✓ Feedback effect (T, void)
  - ✓ Isotopic
  - ✓ …
- These benchmarks were developed for validation of criticality safety calculations and reactor physics calculations.
  NOT for nuclear data feedback …



pu-met-fast-001
(Jezebel)



creole-pwr-exp-001

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Benchmarks with Pu isotopes

- ICSBEP
  - Thermal spectrum (and intermediate & mixed)
    - PST 515 cases ← Extensive discussion today
    - PCI 1, PCM 34, PMI 5, PMT5 3, PMM 16
  - Fast spectrum
    - PMF 100 cases ← Brief discussion today

k_{eff}

- IRPhE
  - Thermal spectrum
    - Creole (MoX), Kritz-1 (MoX) — temperature feedback, reaction rate distribution
    - Venus (MoX) — reaction rate distribution, power distribution, spectral indices, reactivity effects
    - Duke (UO_2) — reactivity as a function of depletion
  - Fast spectrum
    - MoX: BFS2, Joyo, Proteus, SNEAK, Zebra, ZPR, ZPPR

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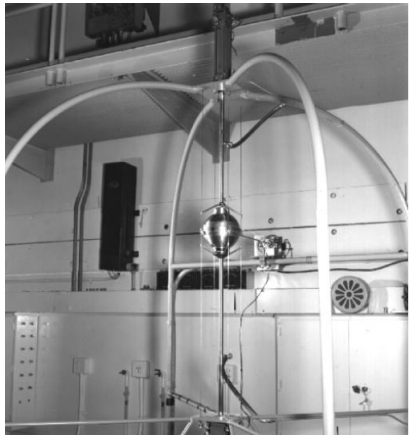
Pu-met-fast



Fuel geometry	Reflector	PMF benchmark
Sphere		1, 2, 22, 29
Metal button array		3, 4
Rods		12
Rods, 'flooded'		16, 17, 37
Molten Pu	Ni, Fe	45
'Jupiter'	Pb	47
Sphere	Water	11
Sphere	Polyethylene	24, 27, 31
Sphere	Cd + polyethylene	36
Sphere, Cylinder	Be, BeO	18, 19, 21, 38, 44
Sphere, Cylinder	Graphite	23, 30, 33, 44
Sphere	Al	9, 39, 44
Sphere, Rods	Fe	15, 44
Rods	Ni	14
Sphere	Steel	25, 26, 28, 32
Sphere, Rods	Cu	13, 40
Sphere	Mo	44
Sphere	W	5
Reactor	Hg (coolant)	46
Sphere	Pb	35
Sphere	Th	8
Sphere	U-nat or U-dep	6, 10, 20, 41

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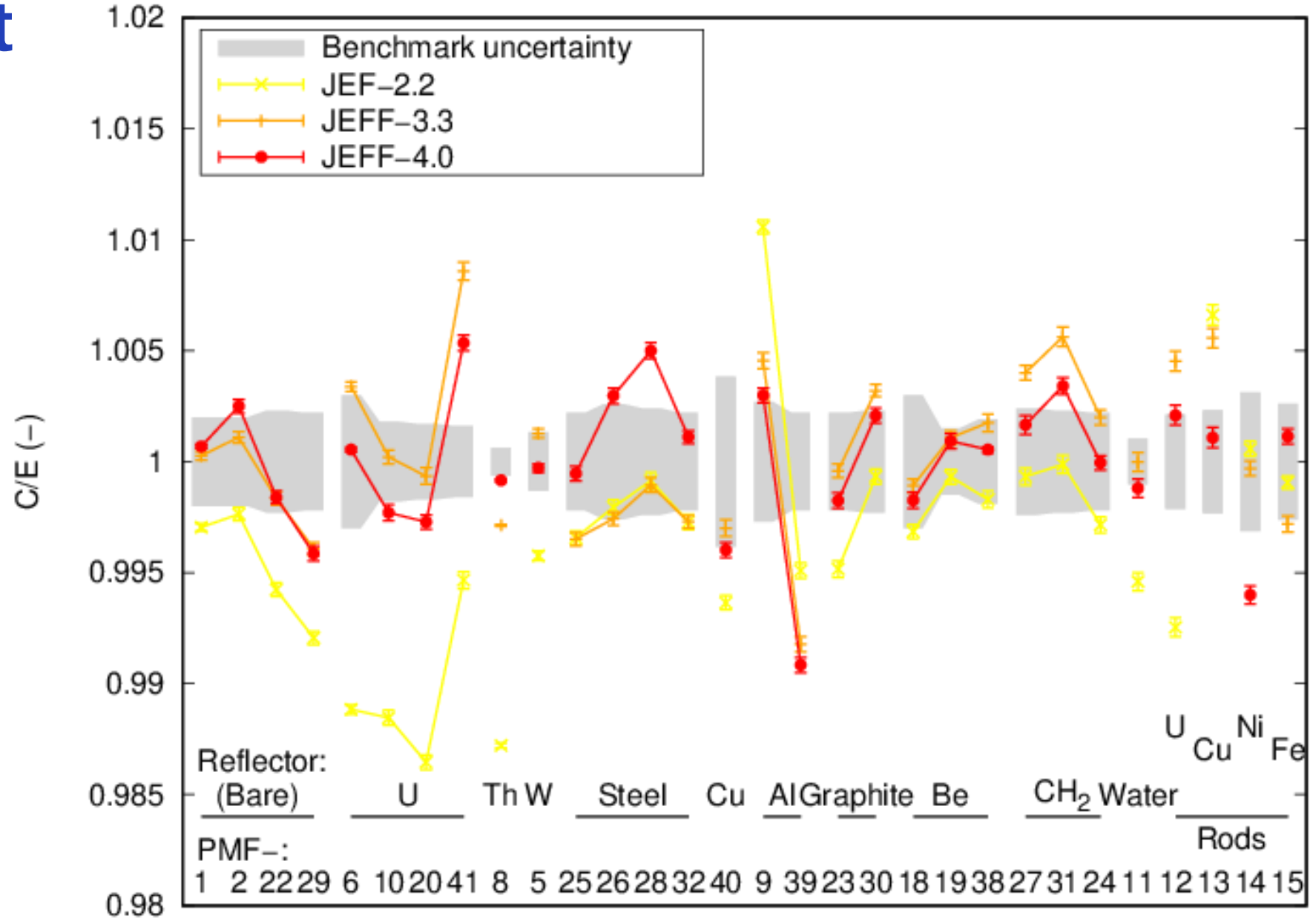
Pu-met-fast



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Pu-met-fast: χ^2

$$\chi^2/N = \frac{1}{N}\sum \frac{(calculated\ -measured)^2}{(combined\ uncertainty)^2}$$

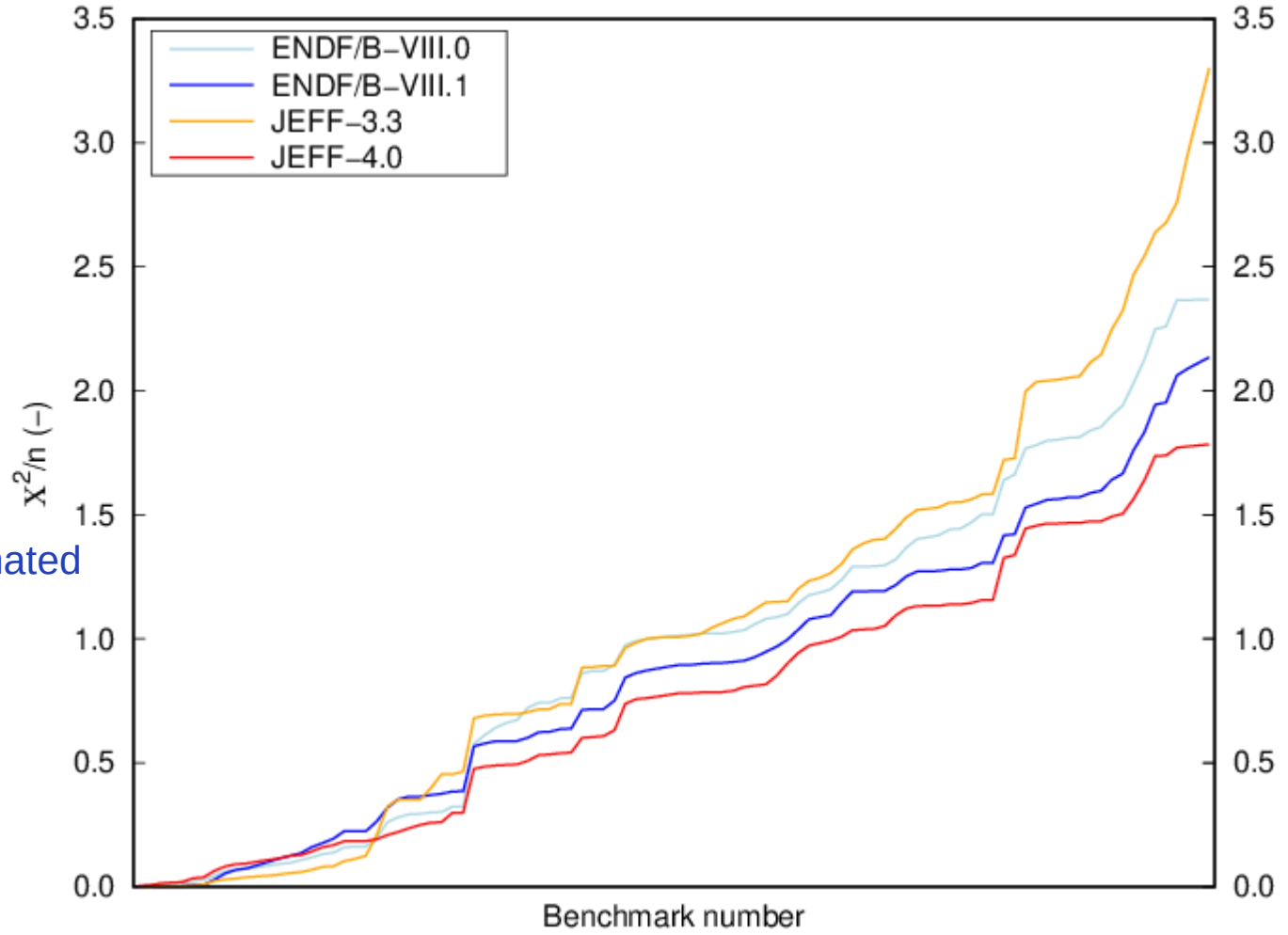
Reduced chi-squared statistic

$\approx$ 1 $\rightarrow$ good agreement

$\gg$ 1 $\rightarrow$ data mismatch or uncertainty underestimated

$\ll$ 1 $\rightarrow$ overfitting or uncertainty overestimated

JEFF-4.0	1.78	
'bare' only	1.42	(without PMF16-case1: 1.03)
The rest	2.13	



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Pu-sol-therm

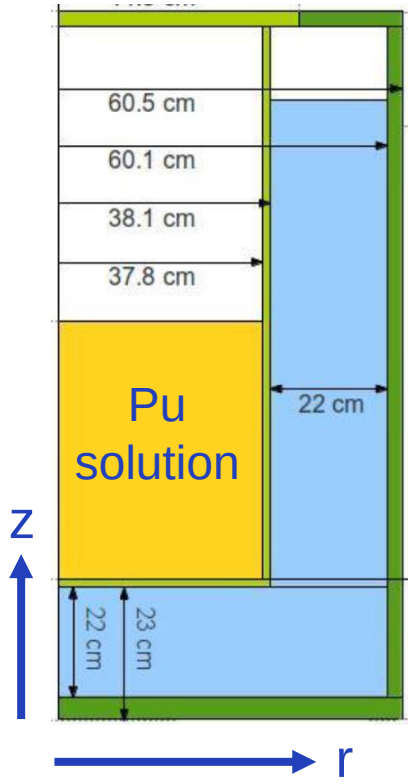
PNNL/Hanford

- Spheres: PST1 – 11, 18, 20, 21
  - Diameter range 29 – 61 cm
  - Pu-240 content 0.54% – 42.9%
- Cylinders: PST10, 34
  - Diameter range 20 – 30 cm
  - PST34: with Gd in solution
- Slabs: PST24, 25
  - Thickness range 11 – 22 cm
  - Pu-240 content 4.7% – 23.2%

Concentration range 10 – 400 g Pu / liter

Valduc

- Cylinder: PST38
  - Diameter 38 cm
  - Pu concentration 14 – 20 g Pu / liter
- Annular cylinders: PST22, 28, 30, 32, 41
  - Diameters 20/50 and 30/50 cm
  - Pu concentration 20 – 190 g Pu / liter
  - Pu-240 content 1.5% - 19%
- Interacting cylinders: PST13 – 17
  - Diameter range 25 – 30 cm
- Tank in tank: PST23
  - Pu-240 content 4.23% and 33.89%
  - Pu concentration 10^{-2} – 140 g Pu / liter
- Cubic tank: PST12
  - Pu concentration 13 – 105 g Pu / liter



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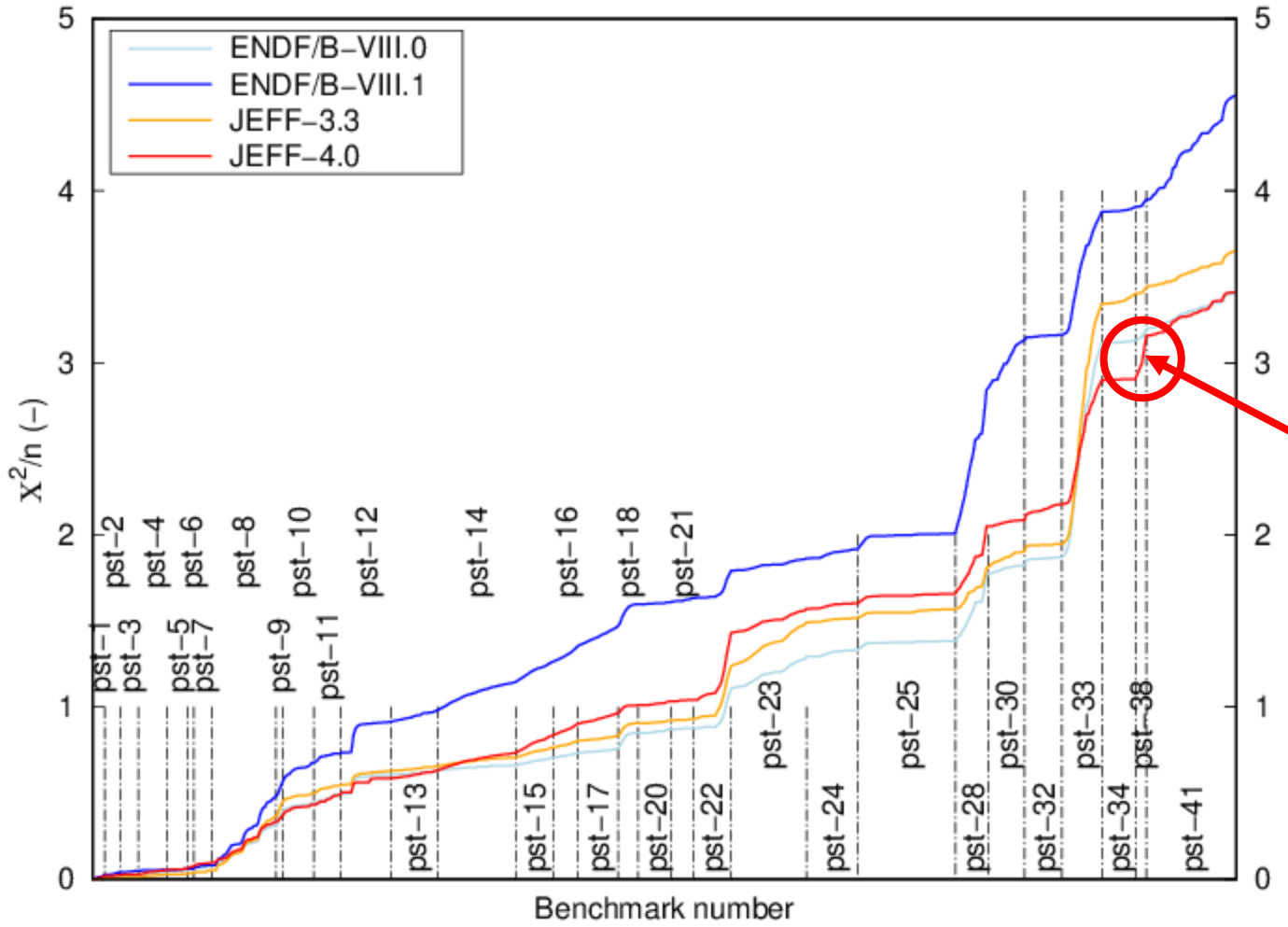
Pu-sol-therm: χ^2



pst38 has high χ^2 values for JEFF-4.0

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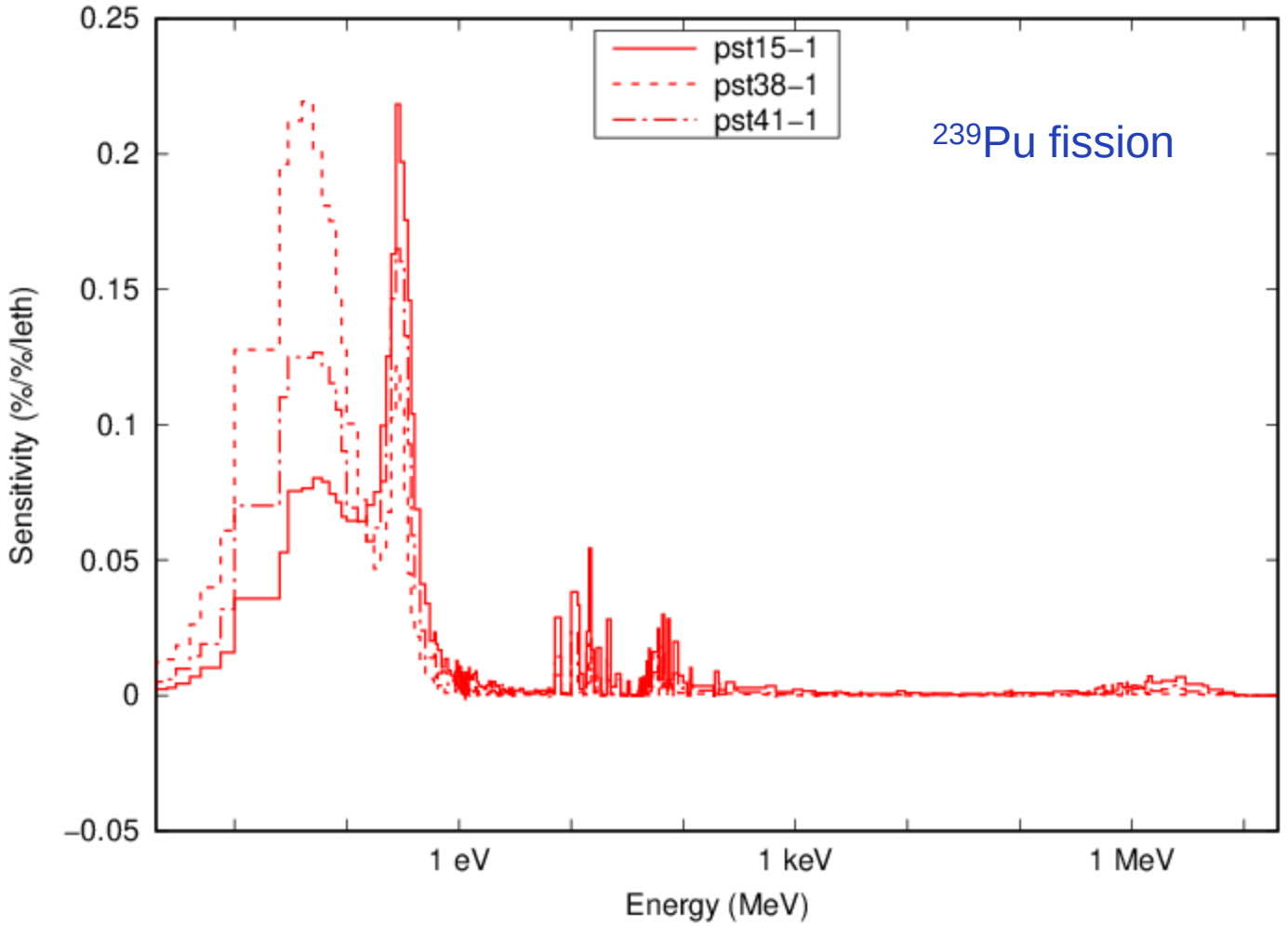
Pu-sol-therm: sensitivity profiles; examples



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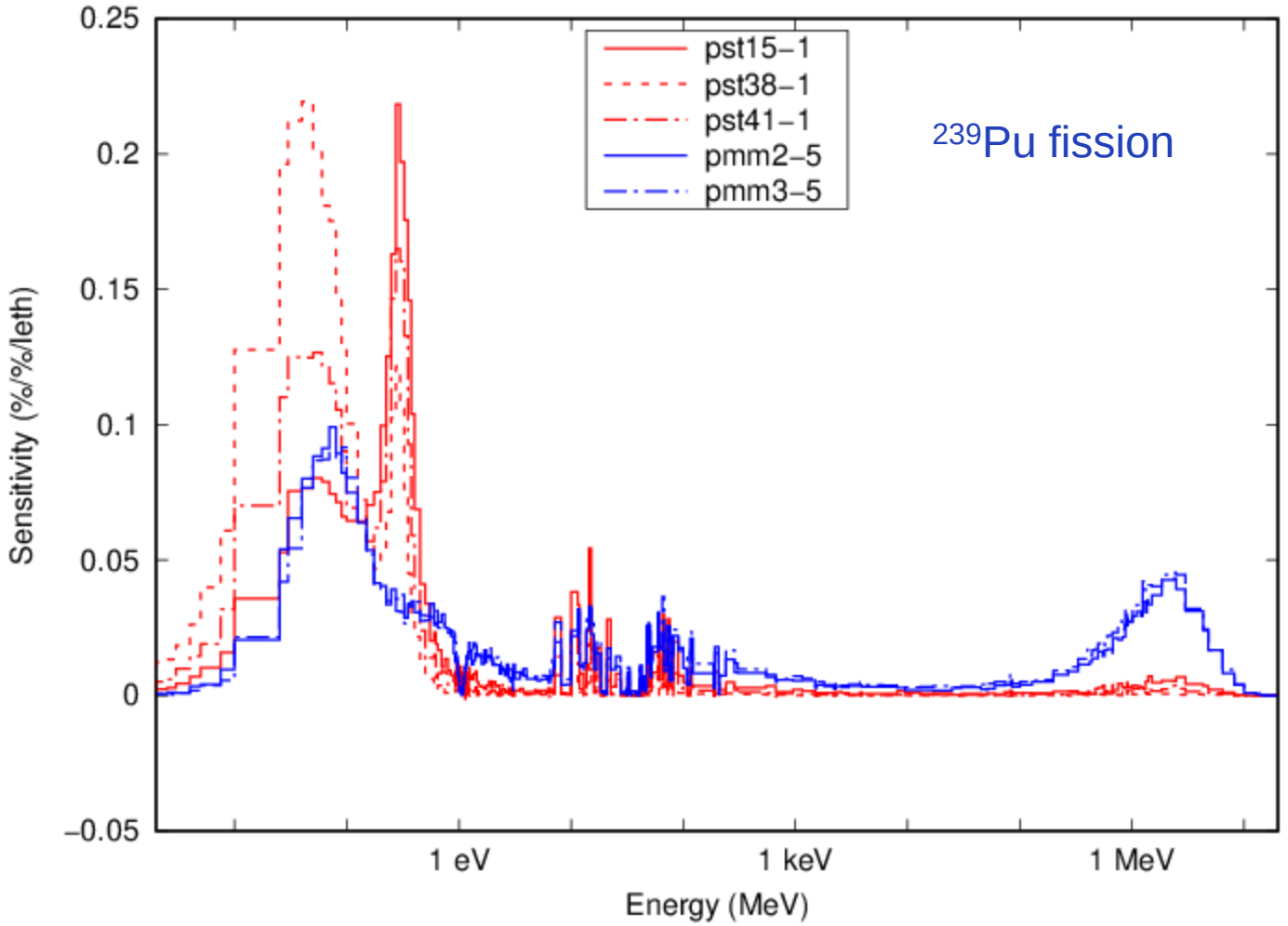
Pu-sol-therm: sensitivity profiles; examples



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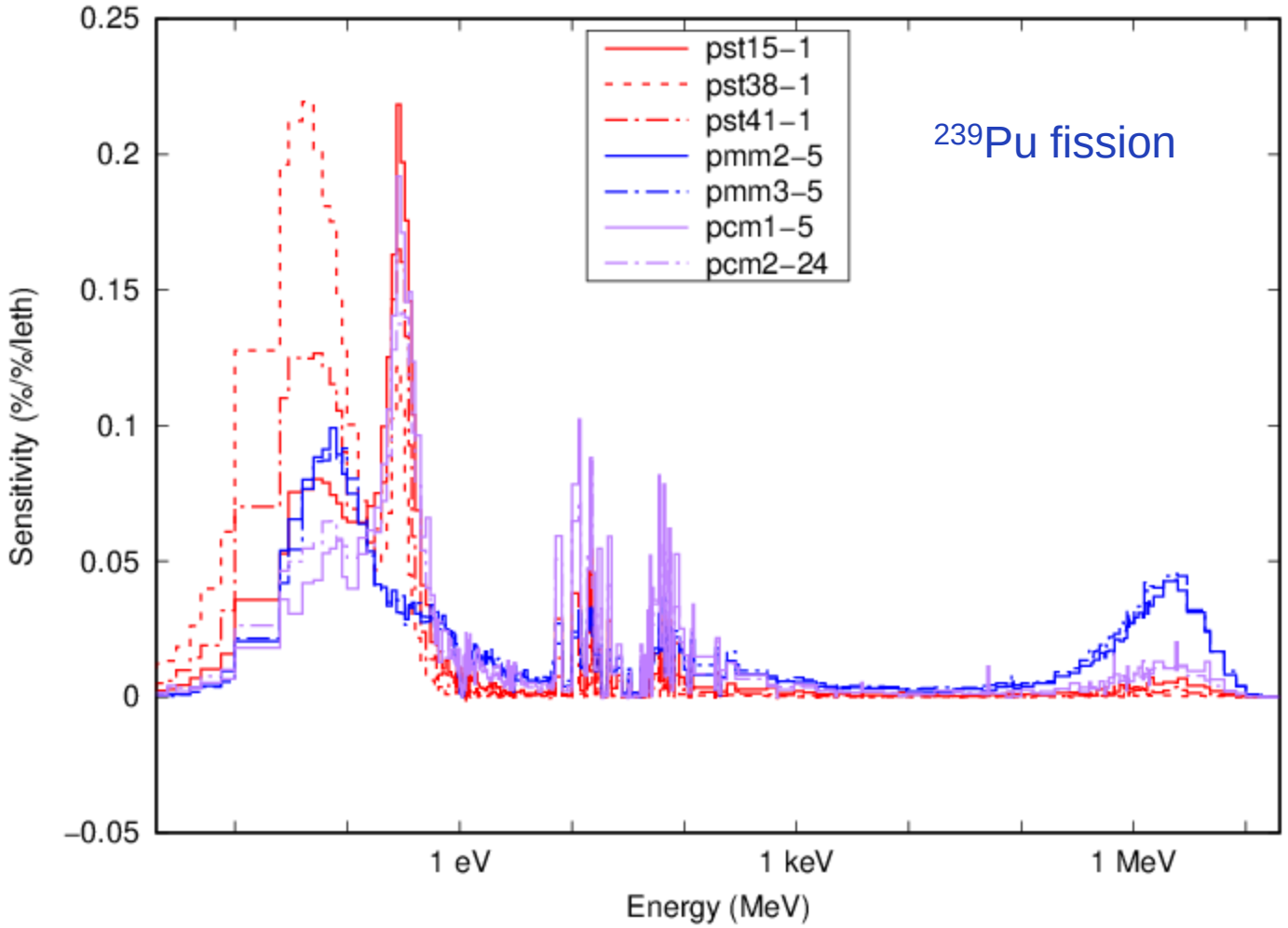
Pu-sol-therm: sensitivity profiles; examples



There are ‘pmm’ and ‘pcm’ benchmarks with sensitivity to the thermal range cross sections …

… but not as sensitive as some pst’s (such as pst38)

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Comparison pst38-4 and pst12-23: spectrum

pst38 case 4

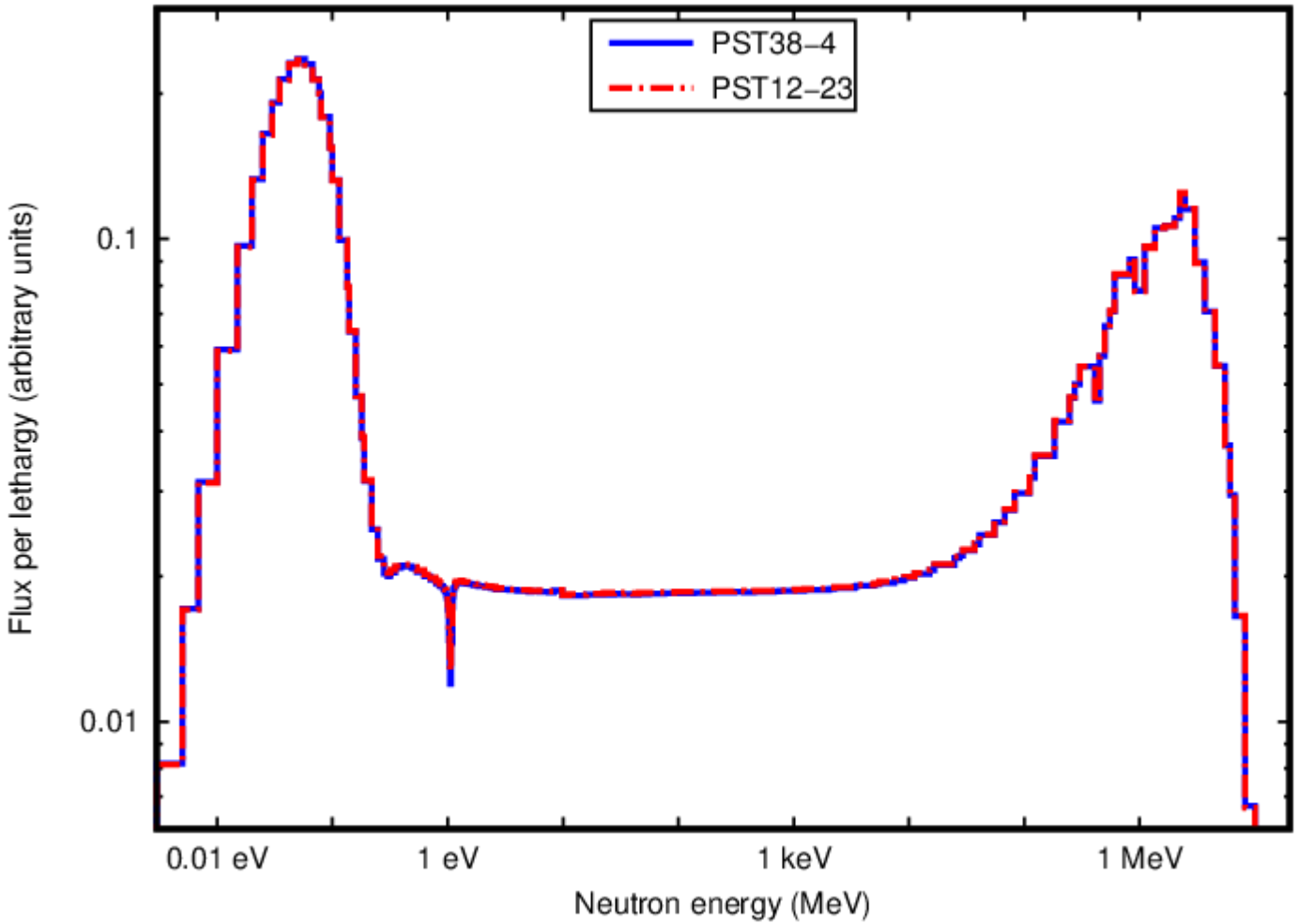
- ∅ 76 x 135 cm^3, reflected
- Pu concentration 14.2 g Pu / liter
- ^{240}Pu 20.8%
- 2006–2007

pst12 case 23

- 130 x 130 x 70 cm^3, unreflected
- Pu concentration 13.2 g Pu / liter
- ^{240}Pu 18.9%
- 1974

pst38 case 4: C/E = 0.99157 ± 0.00130

pst12 case 23: C/E = 1.00081 ± 0.00580



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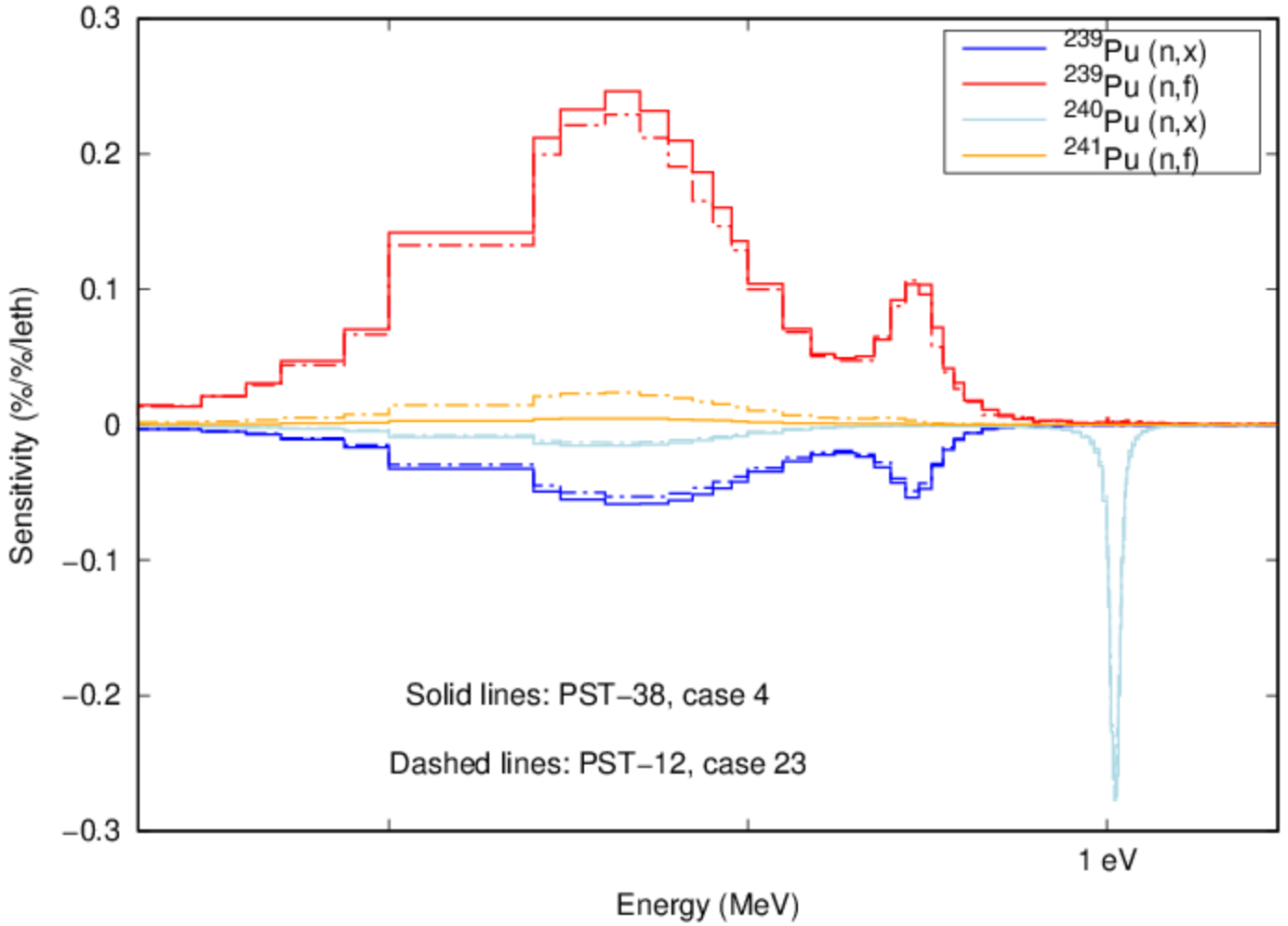
pst38-4 and pst12-23: sensitivity profiles



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Single parameter correlation?

Data set:

- 2 Labs, 31 benchmark series, 515 cases
- Parameters
    1. Pu-240 content (wt%)
    2. Pu concentration (g Pu / liter)
    3. EALF* (MeV)
    4. Laboratory
- Results
    1. C/E
    2. Calculation uncertainty (statistics only)
    3. Benchmark uncertainty

* EALF = Energy corresponding to the average lethargy causing fission

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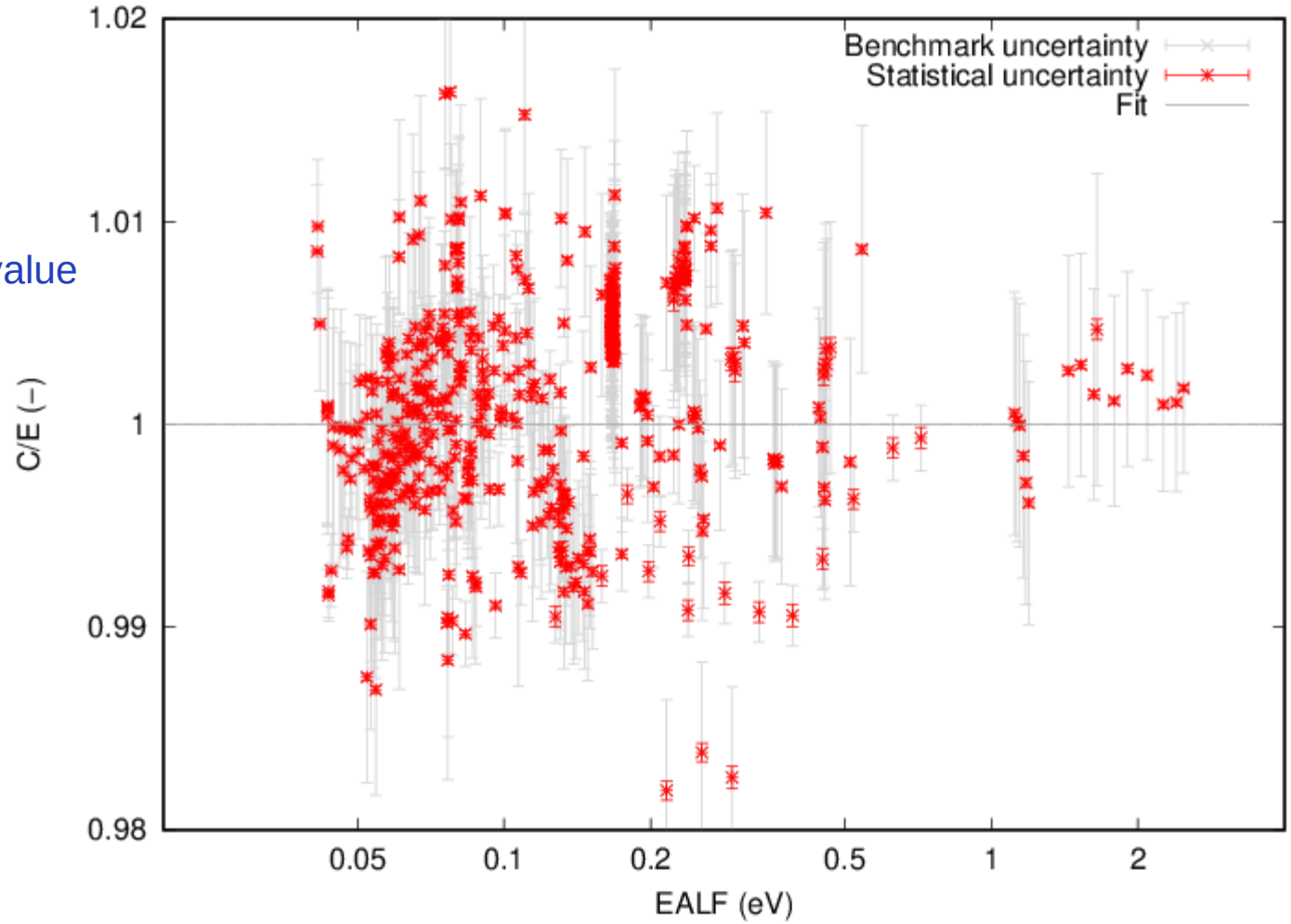
Single parameter correlation: EALF

No clear trend

Large variability for single parameter value



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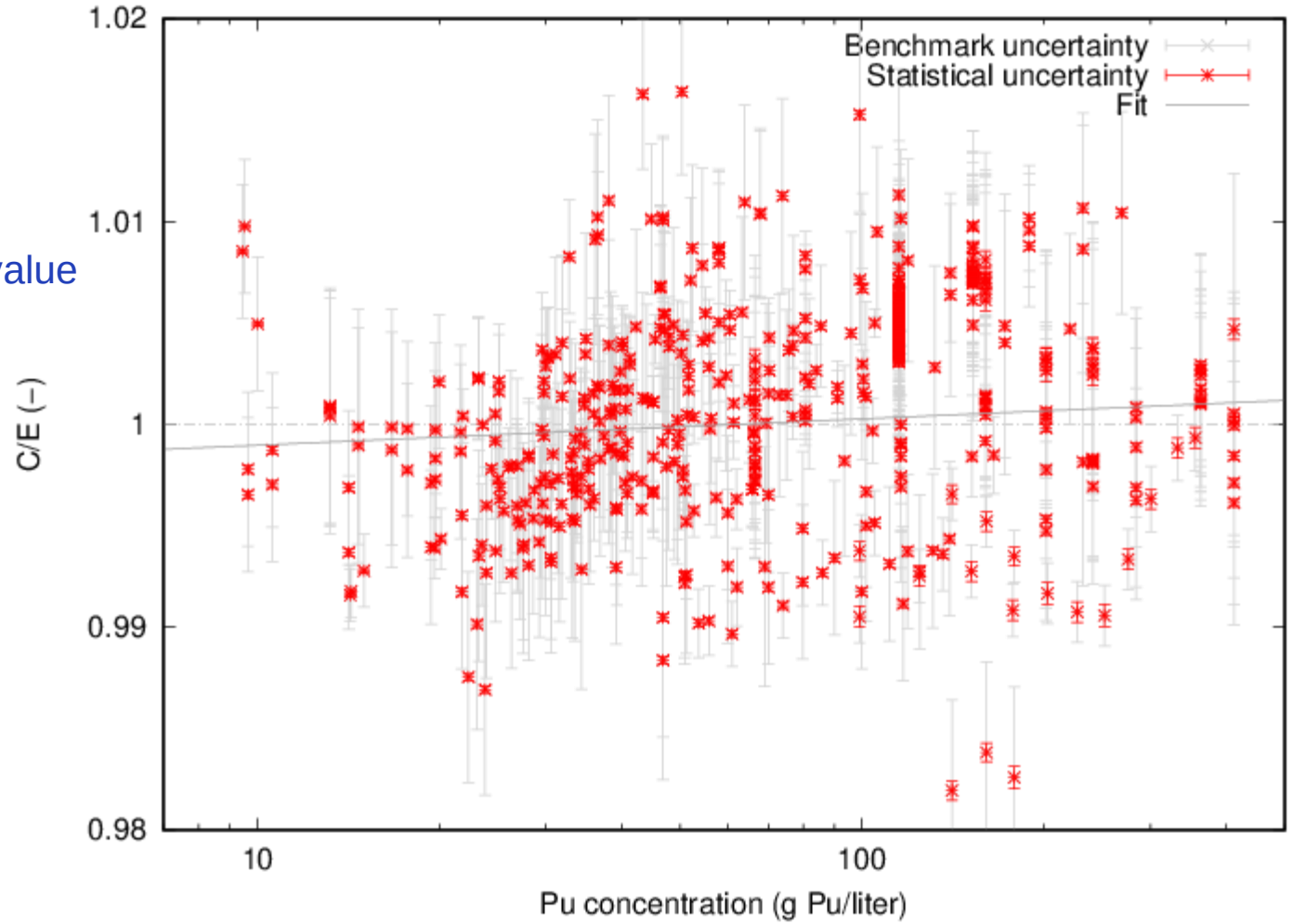
Single parameter correlation: Pu concentration

Weak trend

Large variability for single parameter value



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Single parameter, now per benchmark series

For each individual benchmark series, the trends with Pu concentration and EALF can be quantified (provided the benchmark series has several cases with a range of values for these parameters).

For most benchmark series: no statistically significant result.

Varying results; sometimes with a different sign

PST	Pu concentration		EALF	
1	**0.63**	**34%**	**0.59**	**36%**
2	**1.06**	**43%**	**1.34**	**44%**
3	**1.33**	**40%**	**1.57**	**63%**
4	0.37	138%	0.38	223%
5	**1.57**	**32%**	**2.30**	**33%**
6	1.54	121%	2.46	128%
7	**0.93**	**45%**	**0.88**	**46%**
8	0.13	204%	0.05	589%
9	**-7.42**	**40%**	0.10	40570%
10	**1.17**	**32%**	**2.10**	**33%**
11	**2.90**	**17%**	**5.40**	**23%**
12	**0.38**	**15%**	**0.68**	**13%**
16	**0.25**	**52%**	**0.23**	**53%**
18	**1.01**	**11%**	**1.13**	**14%**
20	0.02	1850%	-0.01	4406%
21	**0.38**	**30%**	**0.39**	**38%**
22	0.06	291%	0.16	133%
23	**-0.04**	**35%**	**-2.03**	**18%**
24	**0.18**	**47%**	**0.11**	**63%**
25	**-0.25**	**29%**	**-0.19**	**34%**
28	-0.04	639%	0.10	419%
30	0.03	530%	-0.05	700%
32	**-0.18**	**69%**	**-0.45**	**52%**
33	**0.30**	**62%**	**0.24**	**59%**
34	**0.30**	**15%**	**0.15**	**17%**
38	**0.71**	**13%**	**2.65**	**14%**
41	**0.15**	**64%**	**0.26**	**54%**

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Multi-parameter analysis using AI (1)

‘Anonymous data set’ used in CoPilot

First pass quantitative analysis:

1. Parameter 2 (Pu concentration) is a ‘very strong driver’
2. Parameter 3 (EALF) strongly correlated with parameter 2 (Pu concentration)
3. Parameter 1 (Pu-240 content): weak grouping effect. In a single benchmark series, it is constant; across series it shifts C/E slightly.
4. Possibly laboratory-dependent bias

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Multi-parameter analysis using AI (2)

Full regression analysis:

1. Parameter 2 (Pu concentration) is the primary driver; evidence:
   a. Strong Pearson/Spearman correlation (~0.8+)
   b. Significant in regression
   c. Stable trend across *all benchmark series*
2. Parameter 3 (EALF) is not a true independent driver; acts as a proxy driver and should be removed
3. Parameter 1 (Pu-240 content): Regression result not statistically significant, but there are shifts between benchmark series

The dataset is NOT a simple regression problem, but ‘a set of parametric sweeps (per benchmark series)’.

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Multi-parameter analysis using AI (3)

Normalised per benchmark series: removes series-specific bias

1. Parameter 1 (Pu-240 content) disappears as a driver
2. Parameter 2 (Pu concentration) remains dominant
3. Parameter 3 (EALF) still not independent

All cases collapse onto a '**near-universal curve**'

Laboratory effect:

- Valduc data: 'tight', centred around 1
- PNNL data: wider spread, more bias

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Multi-parameter analysis using AI (4)

Final ‘predictive model’

$$C/E = (1.0015 – 0.00015*p_1 + 0.0025*a_{PNNL})*(0.9966 + 4.3\cdot10^{-5}\ p_2)$$

- p_1 = Pu-240 content (%wt)
- p_2 = Pu concentration (g Pu / liter)
- a_{PNNL} = 1 for PNNL, 0 for Valduc
- With a normalisation per benchmark series

Optional refinement: slight non-linearity in p_1

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Multi-parameter analysis using AI (5)

Second analysis, this time including 3 more parameters: ^{241}Pu, ^{242}Pu, and ^{241}Am.

- Pu conc Dominant (strong monotonic trends across many benchmark series)
- ^{241}Pu Moderate (small but consistent shifts)
- ^{240}Pu Weak (only global/structural influence)
- ^{242}Pu Weak (limited variation effect)
- ^{241}Am Weak (limited variation effect)
- EALF Derived (not independent)

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Tentative conclusions for discussion

- Sensitivity profiles for 515 PST cases available for analysis
- Single parameter correlations are not very successful

- If the AI analysis can be trusted, then:
  - ✓ There is a ‘Laboratory-effect’
  - ✓ C/E results can be explained better if we assume a normalisation per benchmark series (in other words, each benchmark series may have its own bias)
  - ✓ The most important variable to correlate with is the Pu concentration; not EALF
  - ✓ The Pu-240 and Pu-241 contents have ‘secondary effects’

Many parameters were not included in the AI analysis (e.g. Geometry: what about angular distributions?)

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Get in touch for more information:

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Thank you!

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