Pu239 CIELO Nuclear Data Testing With Nuclear Data and Sensitivity Tool (NDaST)

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Overview

- **NDaST:** an NEA developed web tool that provides rapid feedback on the impact of changes to nuclear data on integral experiments, by accessing a database with sensitivity coefficients. http://www.oecd-nea.org/ndast/
- **WPEC SG34:** Working Party, motivated by a 500 pcm over prediction of PST benchmarks by ENDF/B-VII.0, that revised the cross section of Pu239 and identified a subset of ICSBEP Benchmarks that are representative of the set of PST benchmarks
- **CIELO:** An international collaboration currently revising major nuclear data cross sections, candidates for ENDF/B-VIII

Goal: Apply NDaST to a practical situation (helping CIELO) and gain an appreciation of the pros and cons of the tool when used for PREDICTION. Help improve default options and recommendations

Overview-Recent Pu239 backstory

ENDF/B-VII.0 +0.5% (500 pcm) over prediction of Plutonium Solution Thermal Benchmarks

(2010-2012)

WPEC SG34

Coordinated evaluation of ^{239}Pu up to and inc URR

New Pu239 Eval

RR Parameters +

σ_f=747±7 b

σ_γ=270±11b

Set of Representative ICSBEP Benchmarks

Table 9: Calculated k_{eff} C/E values

Benchmark Name	ENDF/B-VII.1 (i)	JEFF-3.1.2 (ii)	JENDL-4.0 (iii)	SG34 (iv)
PST1.4	1.00500(13)	1.00127(6)	1.00588(6)	1.00199(6)
PST4.1	1.00389(11)	0.99907(5)	1.00482(5)	1.00044(5)
PST9	1.01939(5)	1.01367(2)	1.02510(3)	1.01543(2)
PST12.10	1.00402(10)	0.99973(5)	1.00498(3)	1.00083(5)
PST12.13	1.00970(6)	1.00468(3)	1.01069(3)	1.00611(3)
PST18.6	1.00462(11)	1.00153(5)	1.00557(5)	1.00202(5)
PST34.4	1.00254(11)	0.99999(5)	1.00417(5)	0.99922(5)
PST34.15	0.99731(10)	0.99563(5)	0.99844(5)	0.99679(5)
8 assembly average	**1.00581**	**1.00195**	**1.00746**	**1.00285**

Major libraries agree Jezebel k_{eff} near 1.0000 but for different reasons!

(2012-2016)

WPEC SG40

CIELO- Collaborative International Evaluated Library Organization

H1

O16

Fe56

U235, U238

Pu239

Benchmarking

ICSBEP has Approximately 750 Pu and 500 Mixed Benchmarks

https://www.oecd-nea.org/science/wpec/volume34/volume34.pdf
https://www.oecd-nea.org/science/wpec/sg40-cielo/

Depending on What You Want Benchmarking Can Be Computer Intensive

To assess the impact on all PU-SOL-THERM

→ Run 600 Benchmarks, k_{eff} ~10 pcm

To assess the impact of each reaction on the benchmarks

→ 600 X #Reactions [Look what is driving the k_{eff} change]

To assess the impact of each reaction and each energy range on the benchmarks

→ 600 X #Reactions X #Energies [Look at energy region driving the change]

To decide between different options in each reaction and energy

→ 600 X #Reactions X #Energies X #Options

Example: 10 h per run, 5 reactions, 10 energy groups, 5 options
= 600 X 10 h X 5 X 10 X 5 = **1.5 Million Computer Hours** or **171 Computer Years! (per isotope ☺)**

Attempt to reduce this to minutes!

Nuclear Data Sensitivity Tool (NDaST) Flowchart

Benchmarks (Sensitivities) → Nuclear Data (% Change or Covariance) → Integral Results

Select / load benchmarks

Sensitivities (S) & C/E data

DICE

IDAT

Personal

Numerical Benchmarks

Database of over 4000 Sensitivity Data Files

User Input Perturbation (P)

isotope/reaction/energy cross section

AND /OR

JANIS 4

Covariance data via JANIS (C)

Built in processed data for major libraries

Load personal (coverx)

M energy groups (fixed)

S*P

Δk_{eff} for selected cases

C/E output plot grouped by criteria

S*C*S^T

$U_{C(XS)}$ for selected cases

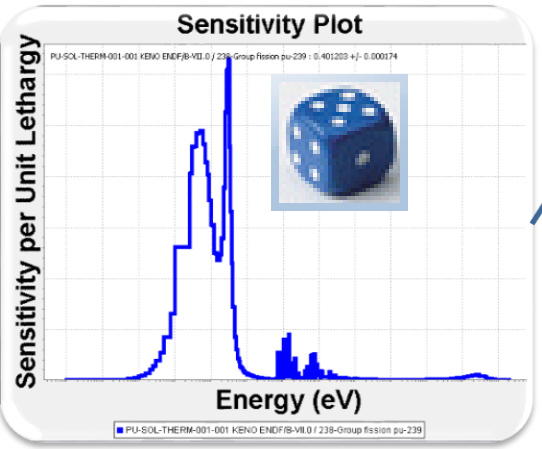
Additional uncertainty on output plot grouped by criteria

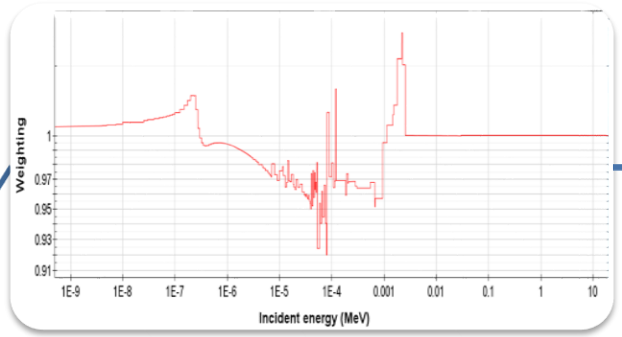
Matrix plot showing individual contribution to $U_{C(XS)}$ by isotope-reaction

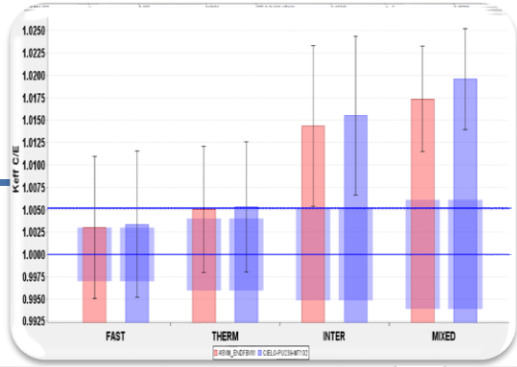
JANIS MF33: ENDF/B-VII.1 = 2138 files, JEFF-3.2 = 5688 files JENDL-4.0 = 2155 files TENDL-2013 = 77811 files

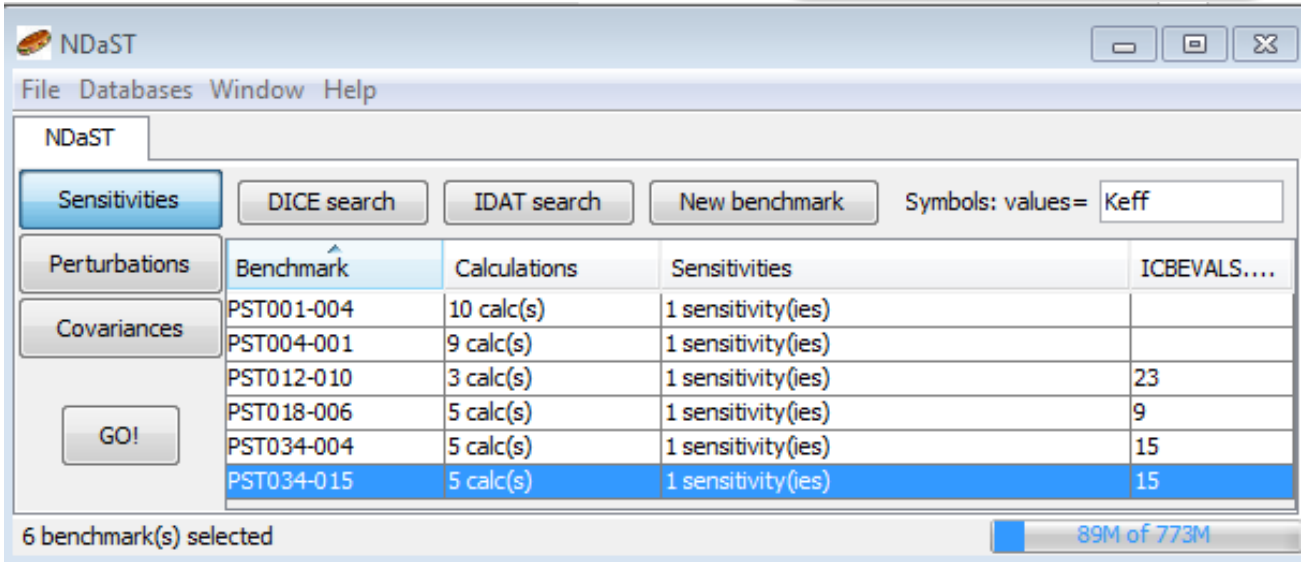
Nuclear Data Sensitivity Tool (NDaST) Flowchart

Benchmarks (Sensitivities) → Nuclear Data (% Change or Covariance) → Integral Results





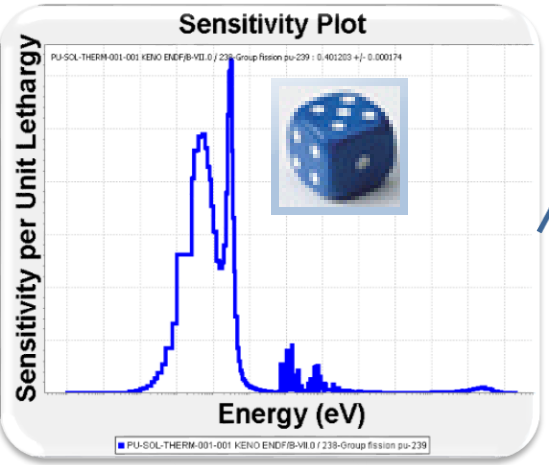




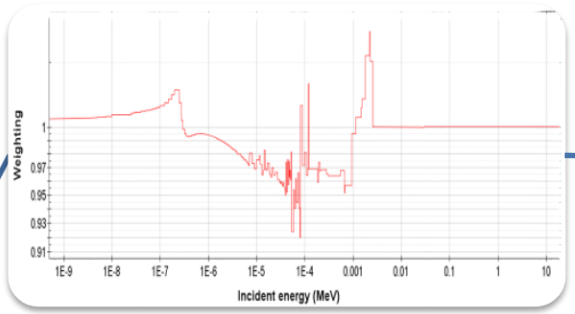
Database of over 4000 Sensitivity Data Files

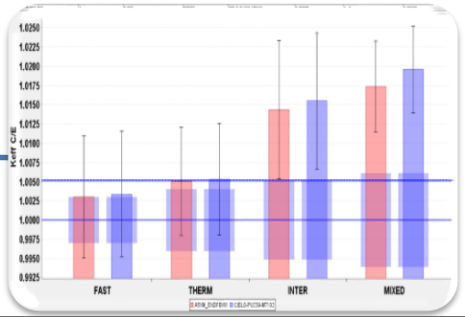
Nuclear Data Sensitivity Tool (NDaST) Flowchart

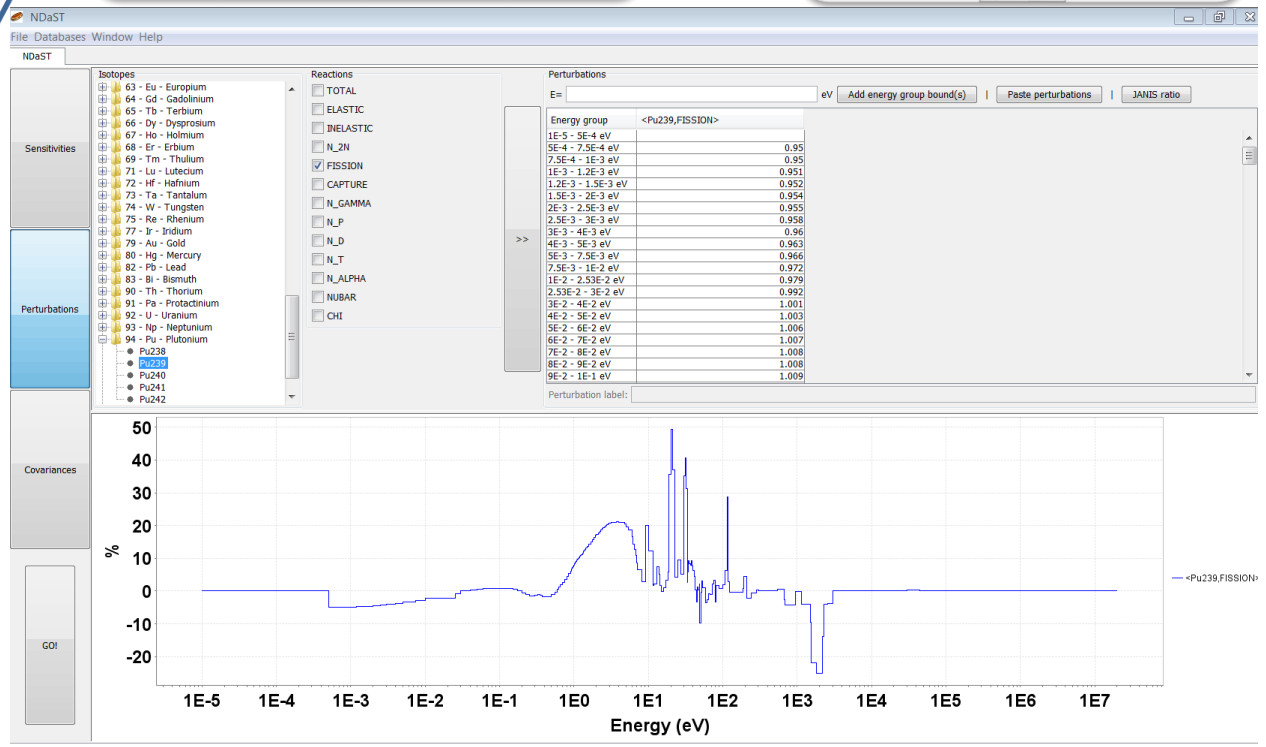
Benchmarks (Sensitivities) → Nuclear Data (% Change or Covariance) → Integral Results



Database of over 4000 Sensitivity Data Files







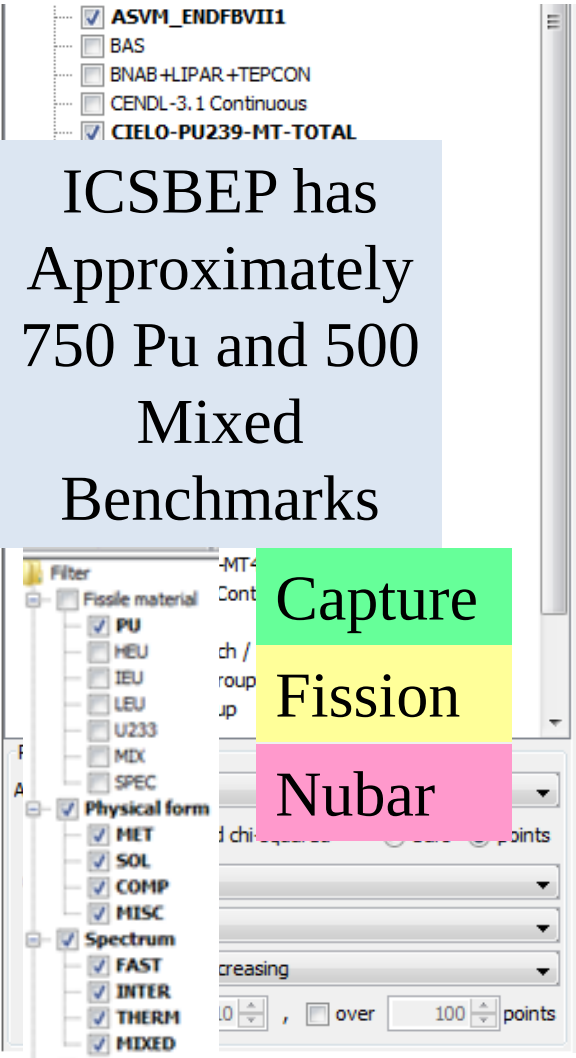
Pu239 CIELO, Sum of MF18,MT102,MF452

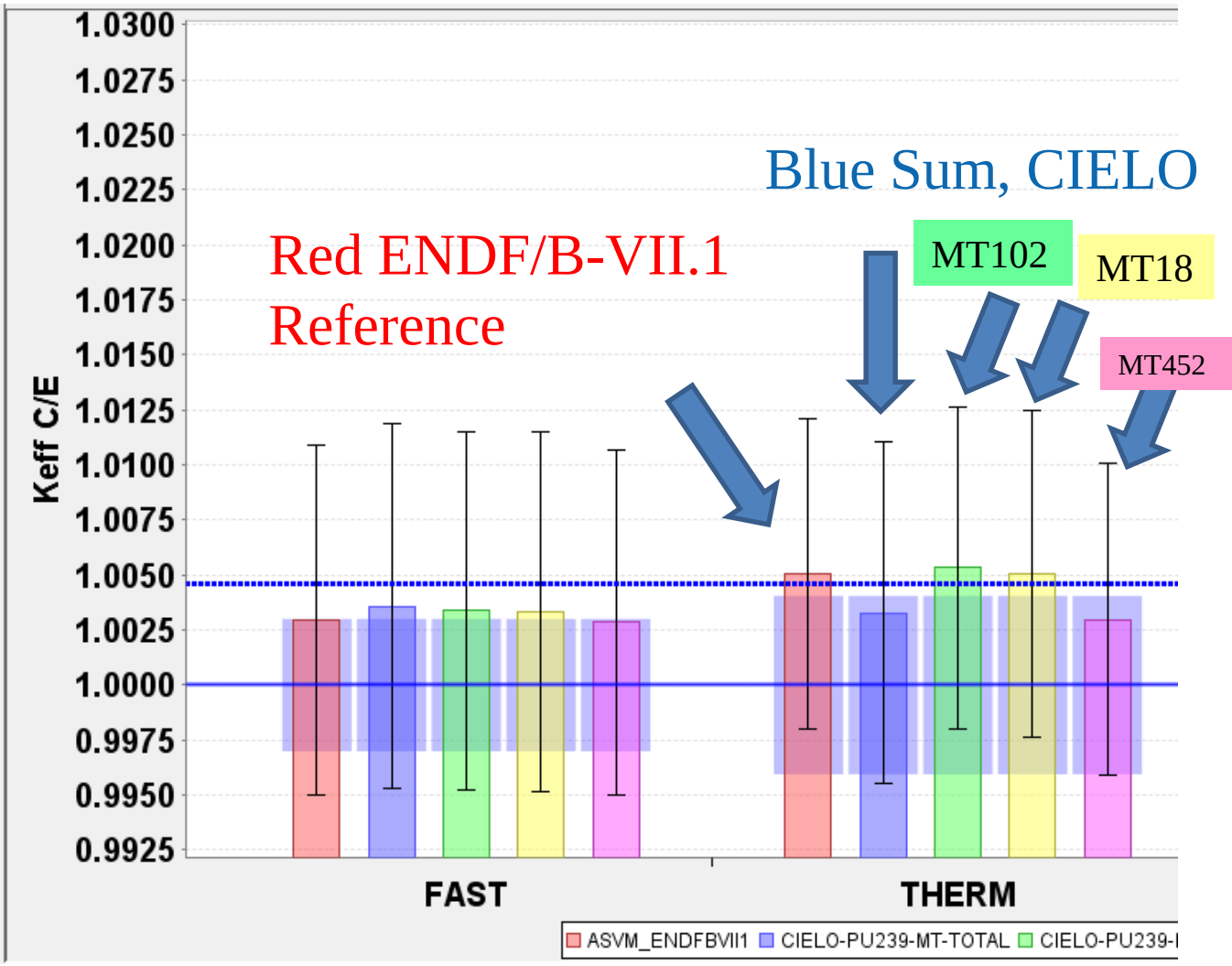
ICSBEP has Approximately 750 Pu and 500 Mixed Benchmarks

Capture

Fission

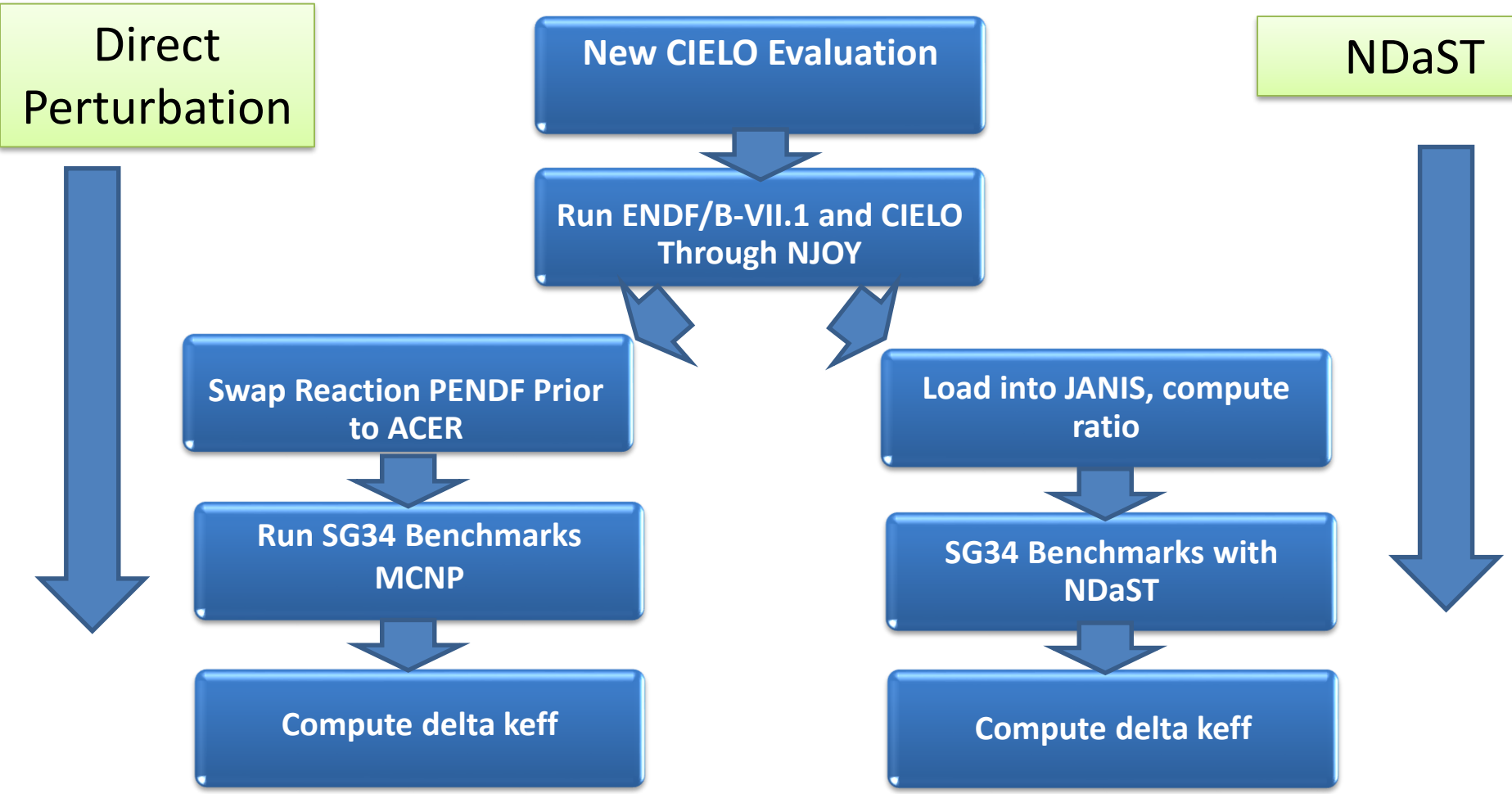
Nubar





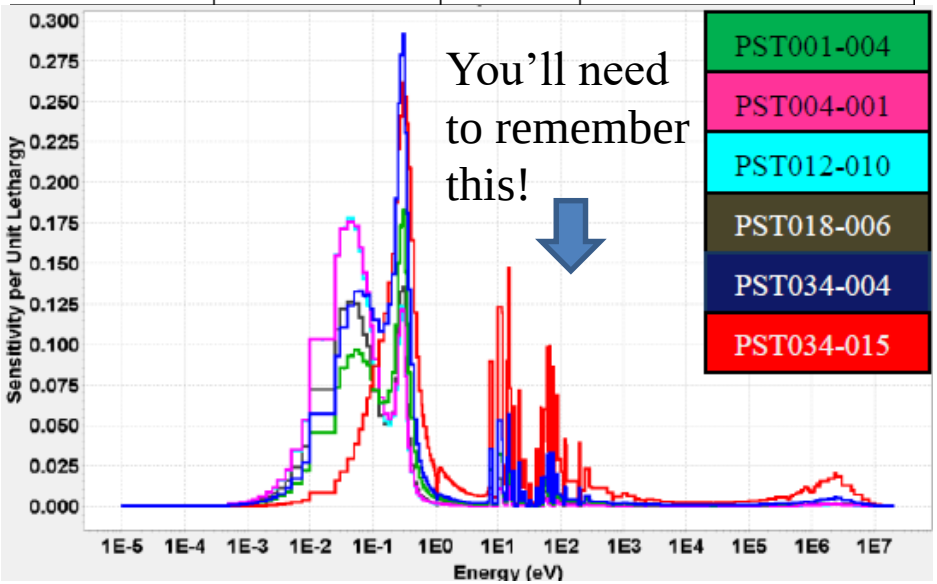
Check Reliability of NDaST Results for Individual Reaction Pertrubations

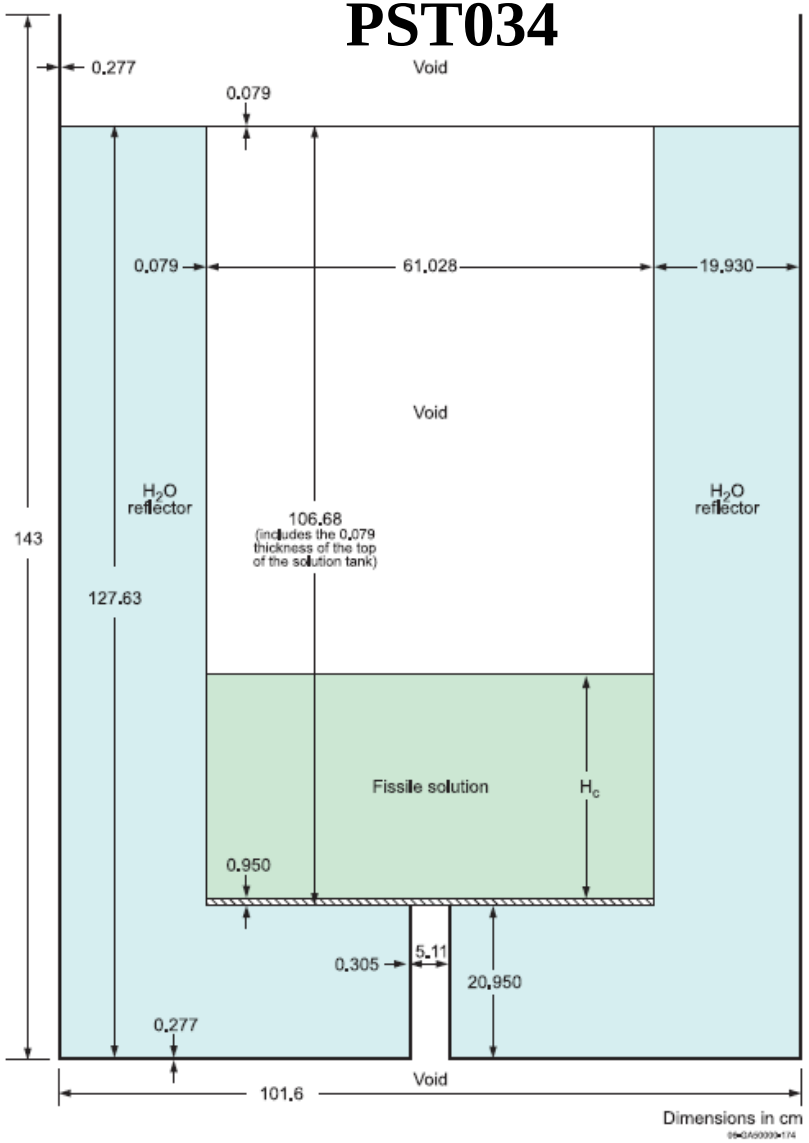
To what extent can we use first order sensitivity theory and NDaST to help?
Relevant to more than just NDaST as other codes/systems are based on similar principles



WPEC SG34 Benchmarks

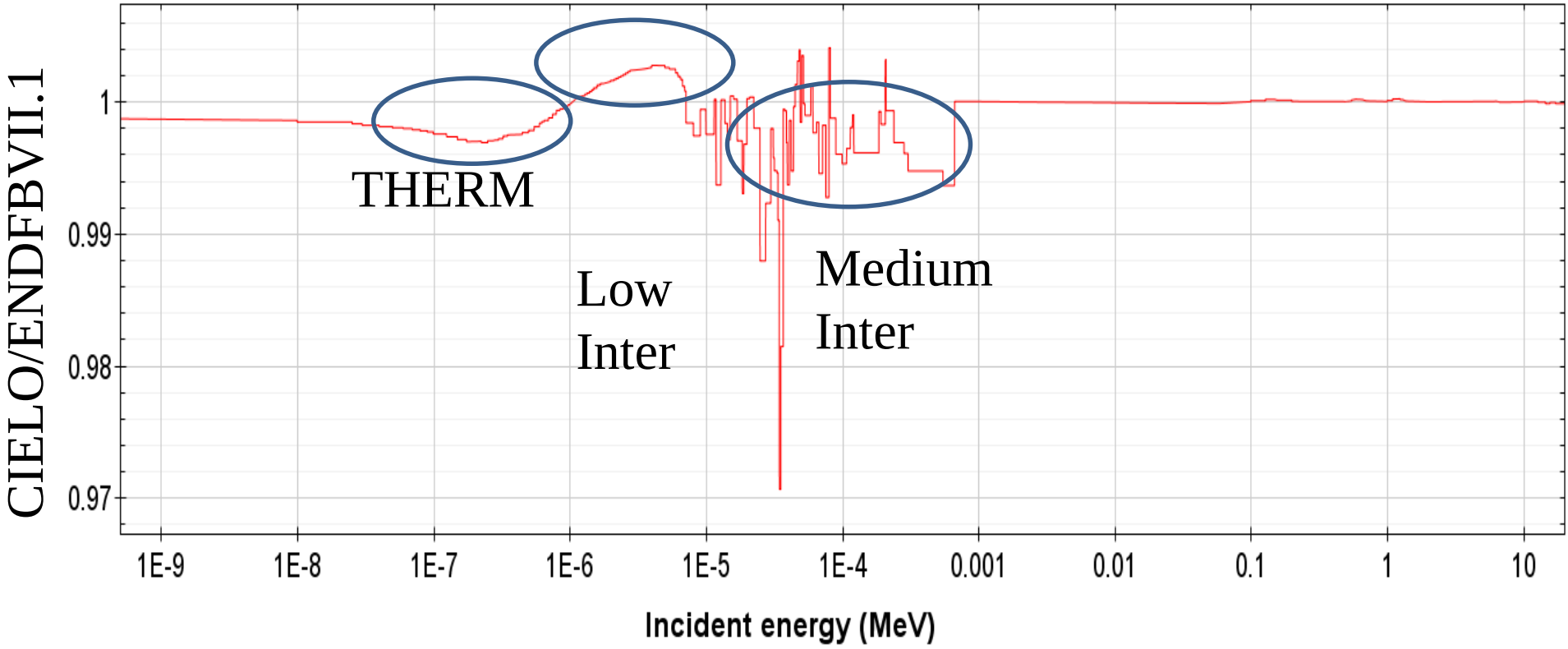
Evaluation-Case	Experimental keff	EALF (eV)	Source of SDF
PST001-004	1.0000 +/- 0.0050	0.0154	VALID-KENO MG [9]
PST004-001	1.0000 +/- 0.0047	0.0531	VALID- KENO MG
PST012-010	1.0000 +/- 0.0047	0.0535	NEA-CLUTCH
PST012-013	1.0000 +/- 0.0047	0.0428	N/A
PST018-006	1.0000 +/- 0.0047	0.0761	NEA-KENO MG
PST034-004	1.0000 +/- 0.0047	0.231	NEA-KENO MG
PST034-015	1.0000 +/- 0.0047	2.730	NEA-KENO MG





Nuclear Data Changes

Pu239-MT452 (Nubar) CIELO/ENDFBVII.1

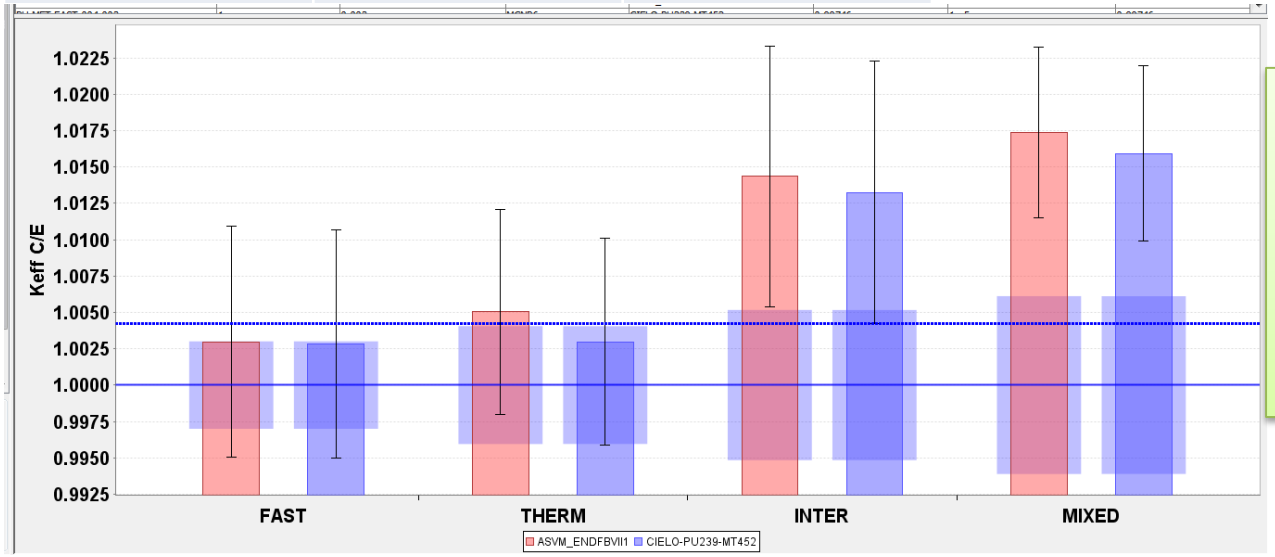


Effect of CIELO MT452 (nubar) changes

WPEC-SG34 BENCHMARK	Direct (pcm)	NDaST (pcm)
PST001-004	-231	-212
PST004-001	-199	-200
PST012-010	-197	-182
PST018-006	-183	-155
PST034-004	-215	-221
PST034-015	-220	-209

WPECSG34 Benchmarks

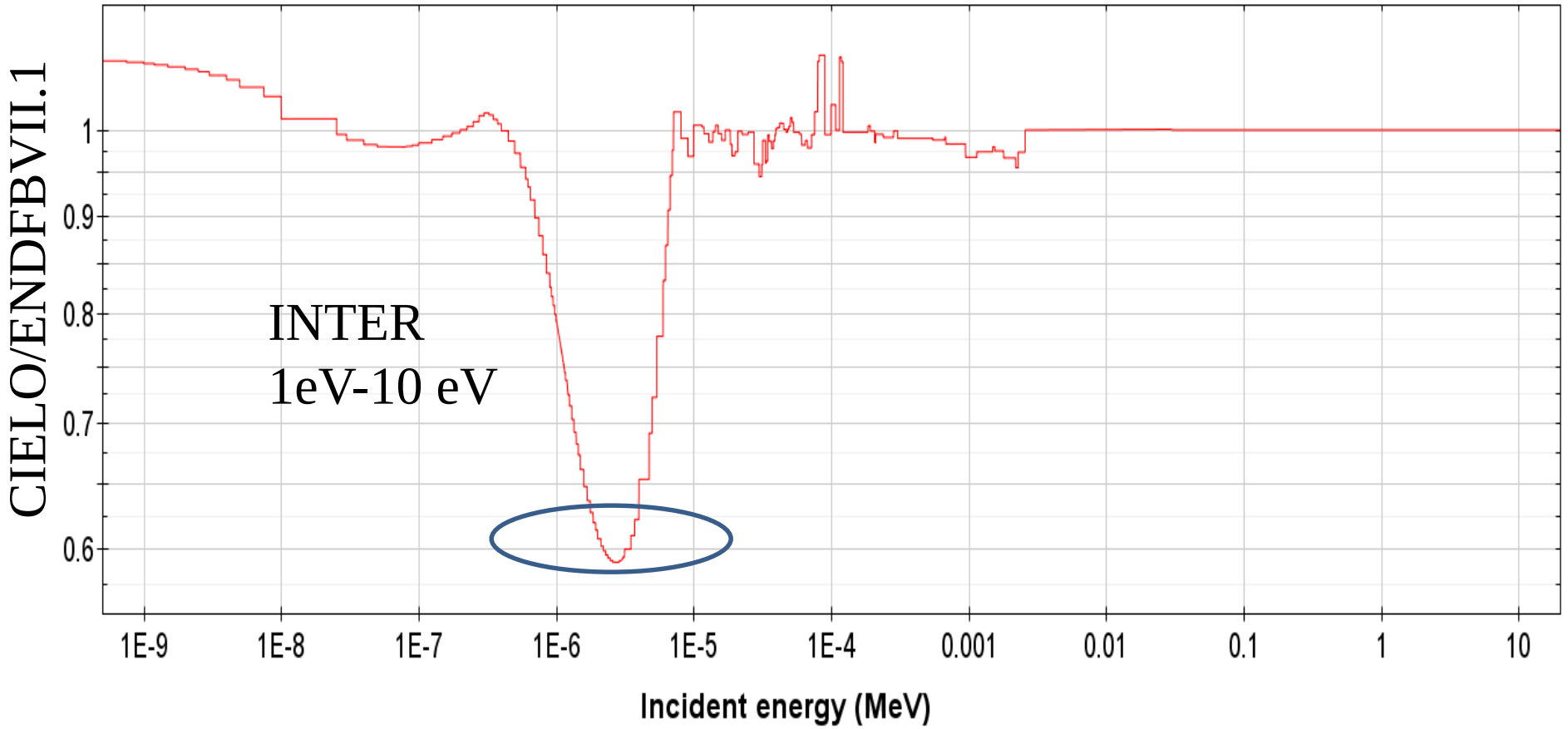
NDaST compares well with Direct perturbation (score one for 1st order perturbations!)



Larger Benchmark Suite

→Similar Conclusion

Pu239-MT102 CIELO/ENDFBVII.1



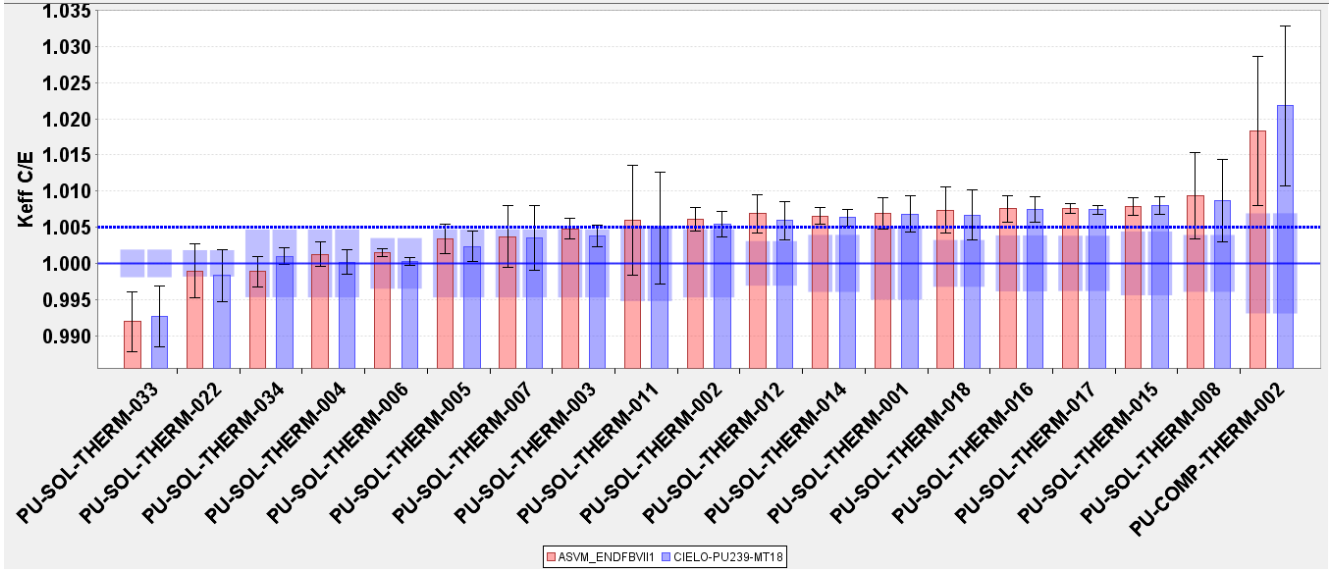
Effect of Capture Cross Section Changes

WPEC-SG34 BENCHMARK	Direct (pcm)	NDaST (pcm)
PST001-004	-1	+32
PST004-001	-8	0
PST012-010	-21	-2
PST018-006	-1	-8
PST034-004	-7	-7
PST034-015	-32	+26

WPECSG34 Benchmarks

Effect is small…NDaST predicts a small effect

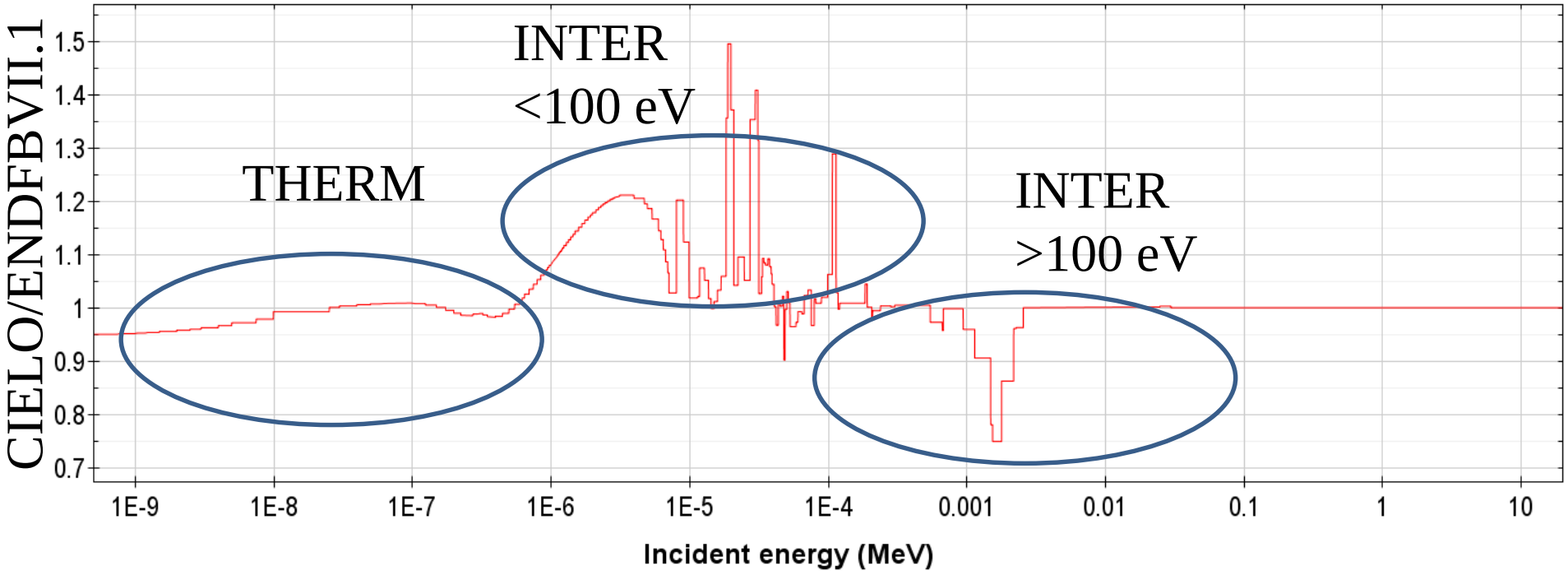
Not so good for PST034-015



Larger benchmark suite

Similar Conclusion

Pu239-MT18 CIELO/ENDFBVII.1



Effect of Fission Cross Section Changes

WPEC-SG34 BENCHMARK	Direct (pcm)	NDaST (pcm)
PST001-004	-52	-10
PST004-001	-150	-119
PST012-010	-156	-116
PST018-006	-116	-79
PST034-004	-73	-8
PST034-015	+234	+398

Most of the positive effect comes from 1eV to 10 eV

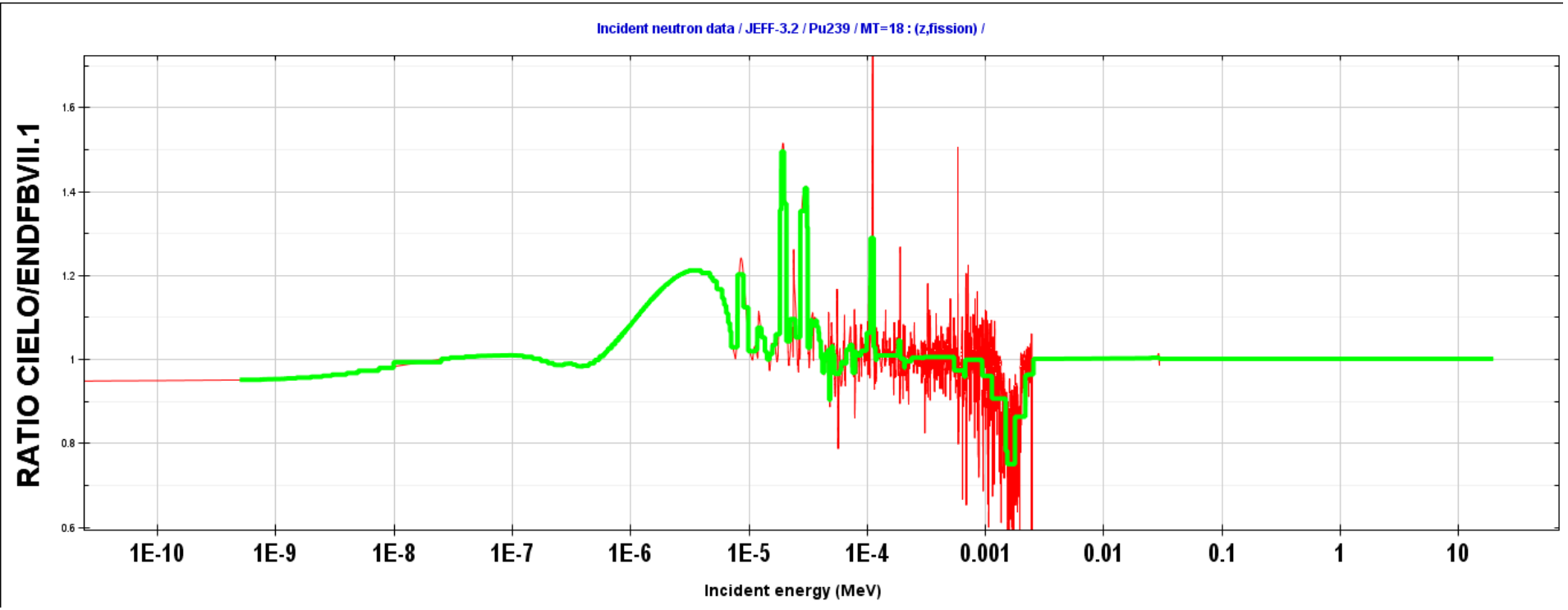
WPECSG34 Benchmarks

NDaST gives poor results for PST034

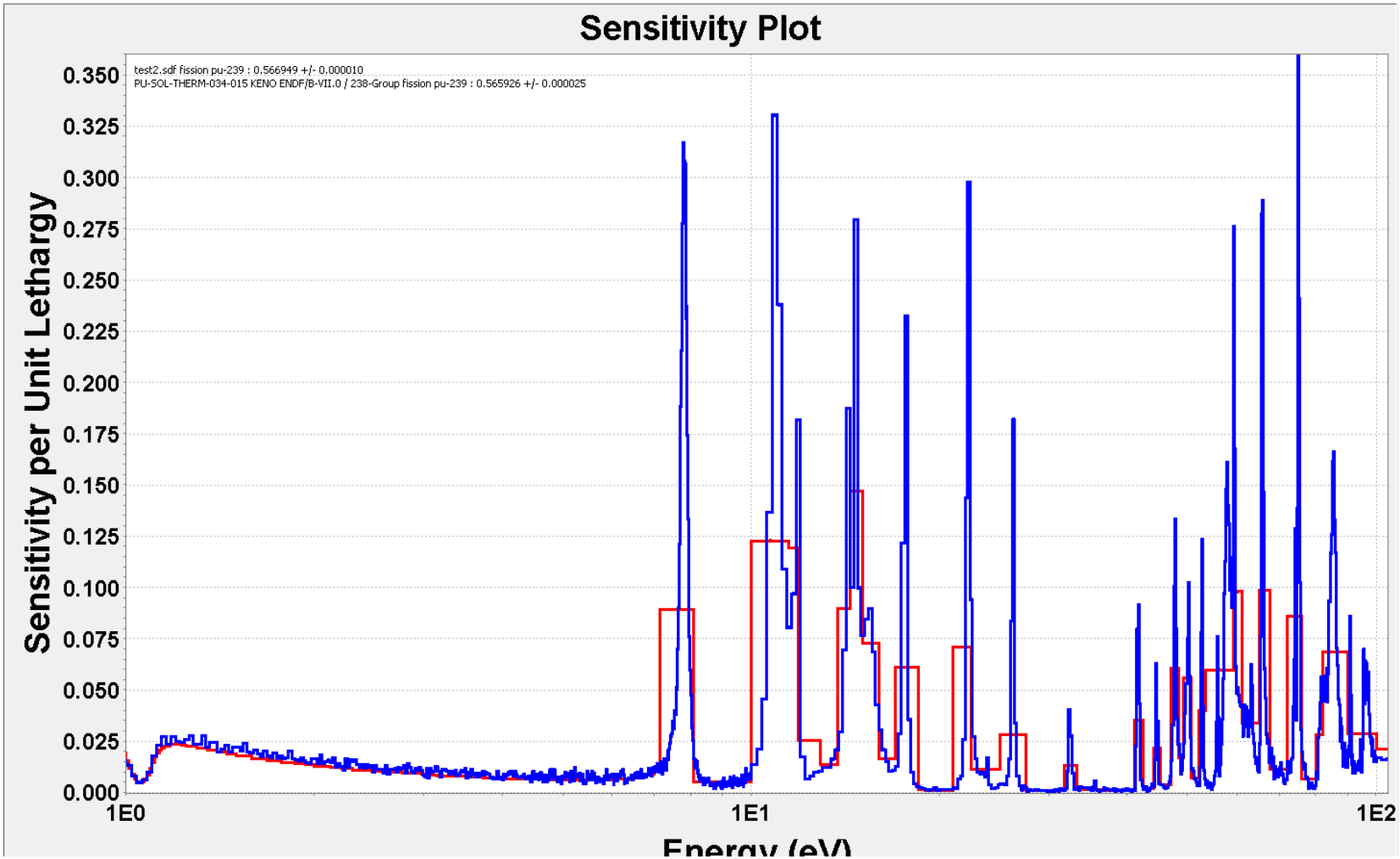
Why? Here are some options!

1) **Group structure of collapsed nuclear data**
2) **Group structure of sensitivity files**
3) **Higher order effects**

10000 Group vs. 238 Group Structure of Collapsed Cross Section Ratio



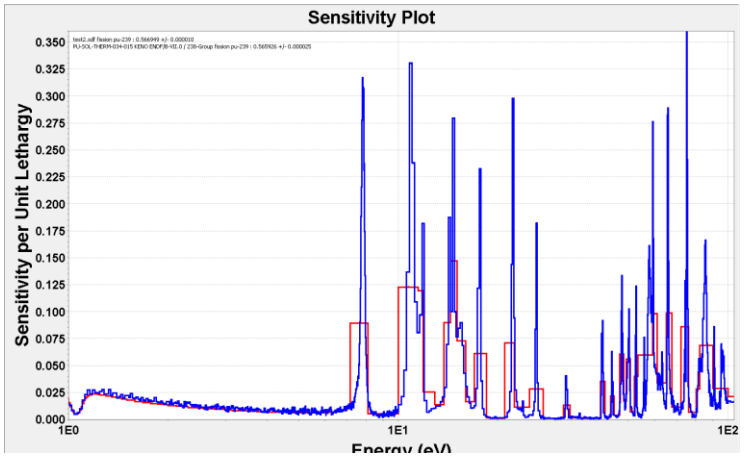
5450 Group vs. 238 Group Sensitivity File



PST034-015 NDaST Assumptions/Data

Effect of Cross Section Group Structure

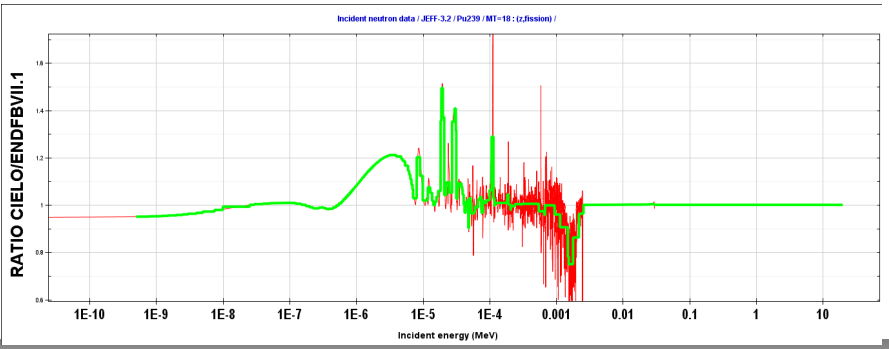
Nuclear Data	Sensitivity	NDaST
238G	**238G**	**+398 pcm**
640G	238G	+438 pcm
13072G	238G	+399 pcm



Effect of Sensitivity Group Structure

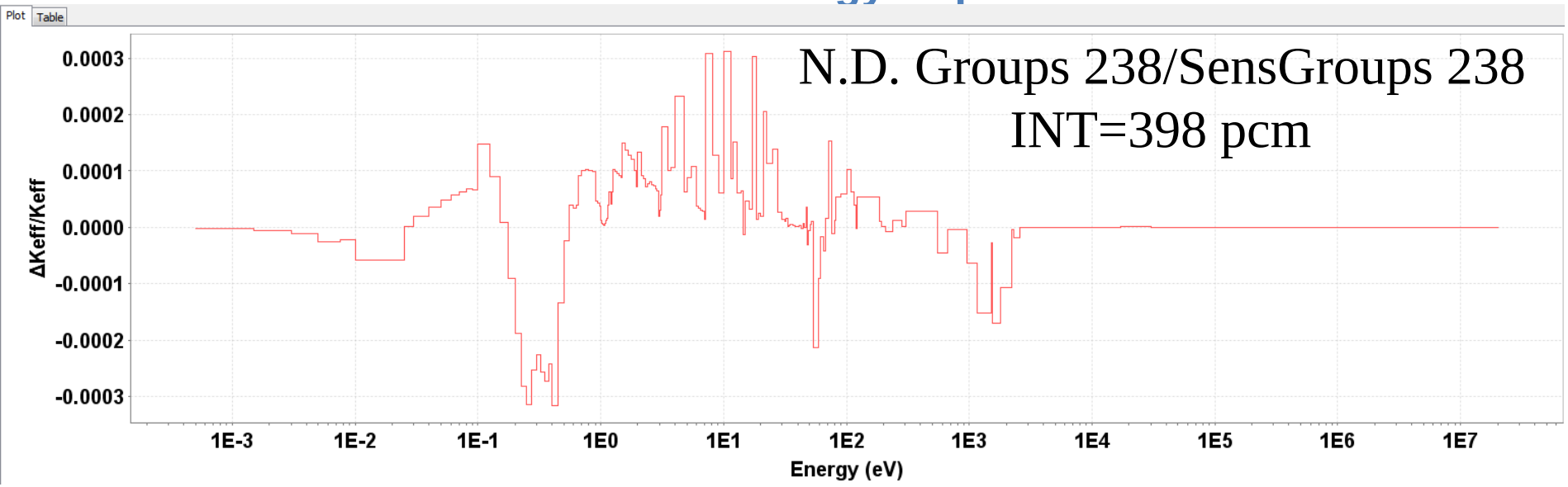
Nuclear Data	Sensitivity	NDaST
238G	238G	+398 pcm
238G	5450G	+477 pcm
13072G	**5450G**	**+317 pcm**

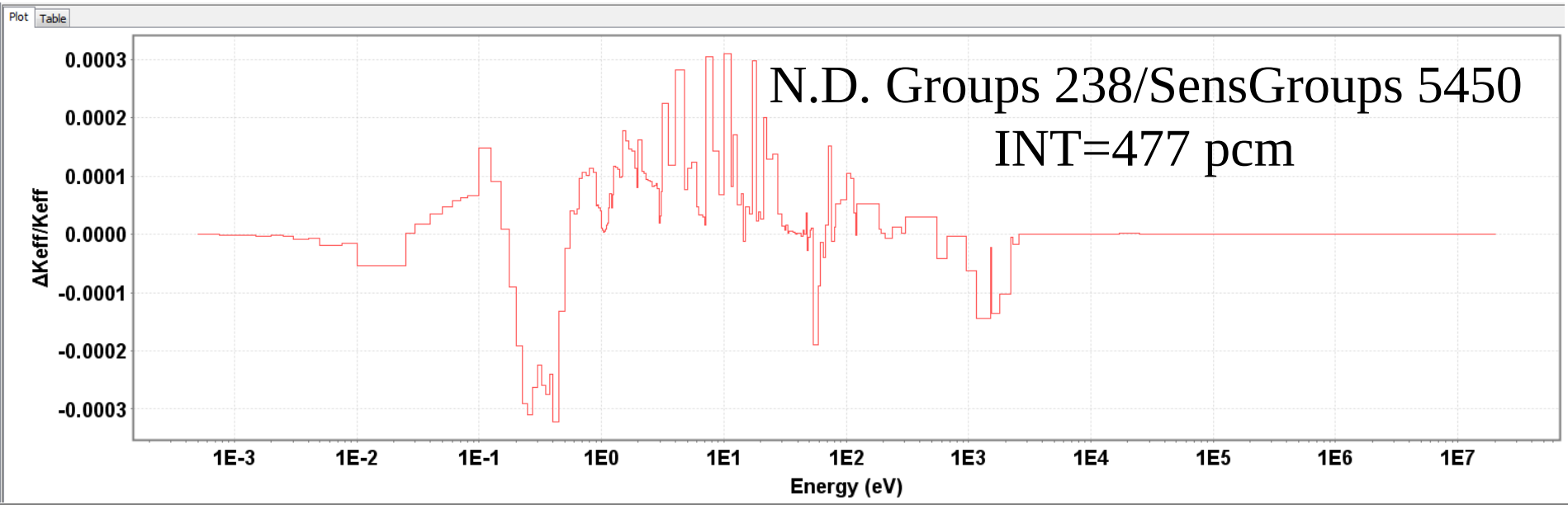
Energy (eV)	238/238	13072/5450
0.00-0.01	-9.0	-6.5
0.01-0.1	+30.5	+30.5
0.1-1.0	-156	-155
1.0-5.0	**+316**	**+369**
5.0-10.0	+84	+73
10-100	**+160**	**+28.4**
100-2.0e6	-28.1	-16.7



Direct +234 pcm

Plot of Detailed Energy Dependence





Full Results of Swapping Files, vs Summing the Separate Effect and NDaST

Eval-Case	MT18		MT102		MT452		PNFS		Total		
	Direct	NDaST	Direct	NDaST	Direct	NDaST	Direct	NDaST	Direct	Sep	NDaST[a]
PST001-004	-52	-10	-1	32	-231	-212	-143	N/A	-394	-427	-333
PST004-001	-150	-119	-8	0	-199	-200	-117	N/A	-466	-474	-436
PST012-010	-156	-116	-21	-2	-197	-182	-67	N/A	-415	-441	-367
PST018-006	-116	-79	-1	-8	-183	-155	-36	N/A	-311	-342	-278
PST034-004	-73	-8	-7	-7	-215	-221	-63	N/A	-384	-372	-299
PST034-015	234	398	-32	26	-220	-209	-53	N/A	-75	-71	162

a) NDaST Total is the sum of (MT18+MT102+MT452) from NDaST + PNFS from Direct

~13 pcm uncertainty

- Normally NDaST can do PNFS, but somewhat unusually CIELO has a dependence on incident neutron energy
- Existing NDaST and Underlying Sensitivity Data Currently Use an Energy Independent PNFS

Conclusion

- ✓ Applied NDaST to a practical problem
- ✓ NDaST compliments, DOES NOT REPLACE, direct perturbation testing
- ✓ Works reasonably well, depending on your accuracy requirements
- ✓ Limitations to assess changes to individual resonances
- ✓ Gives quick feedback when evaluating many options
- ✓ Can be used by people with no experience in Monte Carlo codes

http://www.oecd-nea.org/ndast/