

US Nuclear Data Program

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NATIONAL LABORATORY

a passion for discovery



U.S. DEPARTMENT OF
ENERGY

Office of
Science

ARRA project (2009-2012)

Use of Covariances in a Consistent Data Assimilation for Improvement of Basic Nuclear Parameters in Nuclear Reactor Applications: From Meters to Femtometers

BNL - EMPIRE prior calculations, covariances for model parameters, group-wise sensitivity matrices

INL - integral experiment sensitivities to group-wise cross sections, assimilation

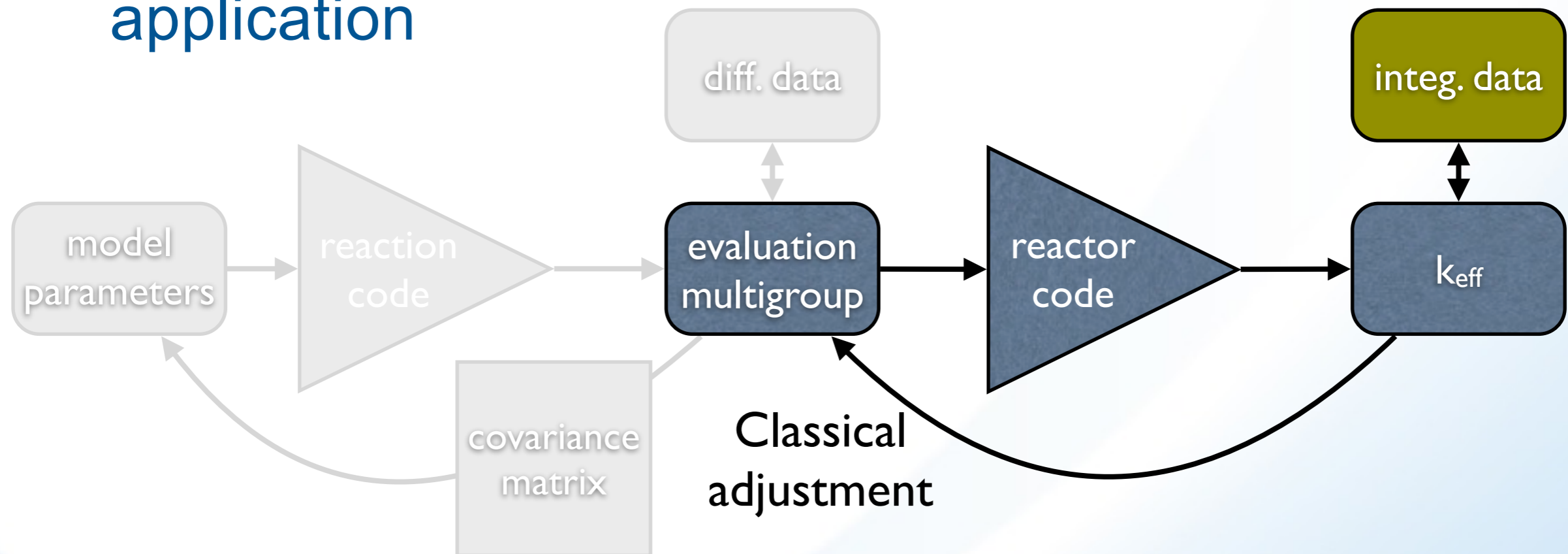
"It has been a bit forgotten that in all really creative thinking in reactor design, a working knowledge of nuclear reaction theory is required."

E. Wigner

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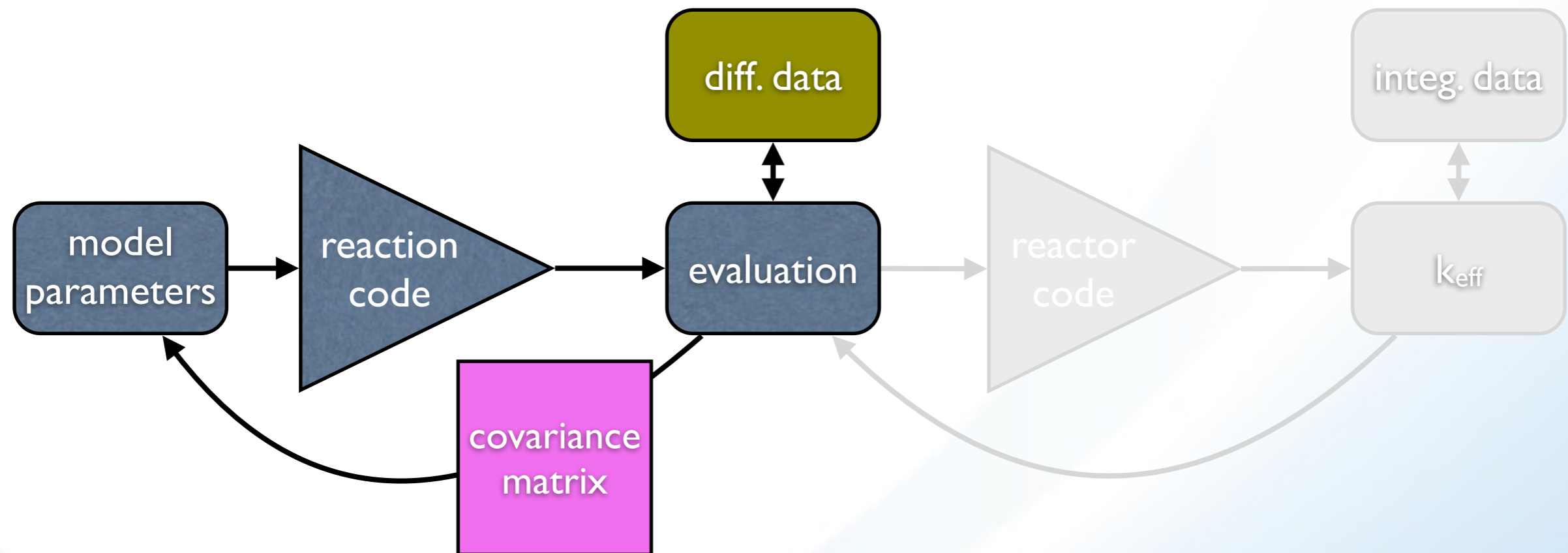
Consistent adjustment (assimilation) linking reaction theory and integral experiments

- Users often tune multi-group evaluated files to a certain type of integral experiments
- Such adjusted file is only valid for a specific application



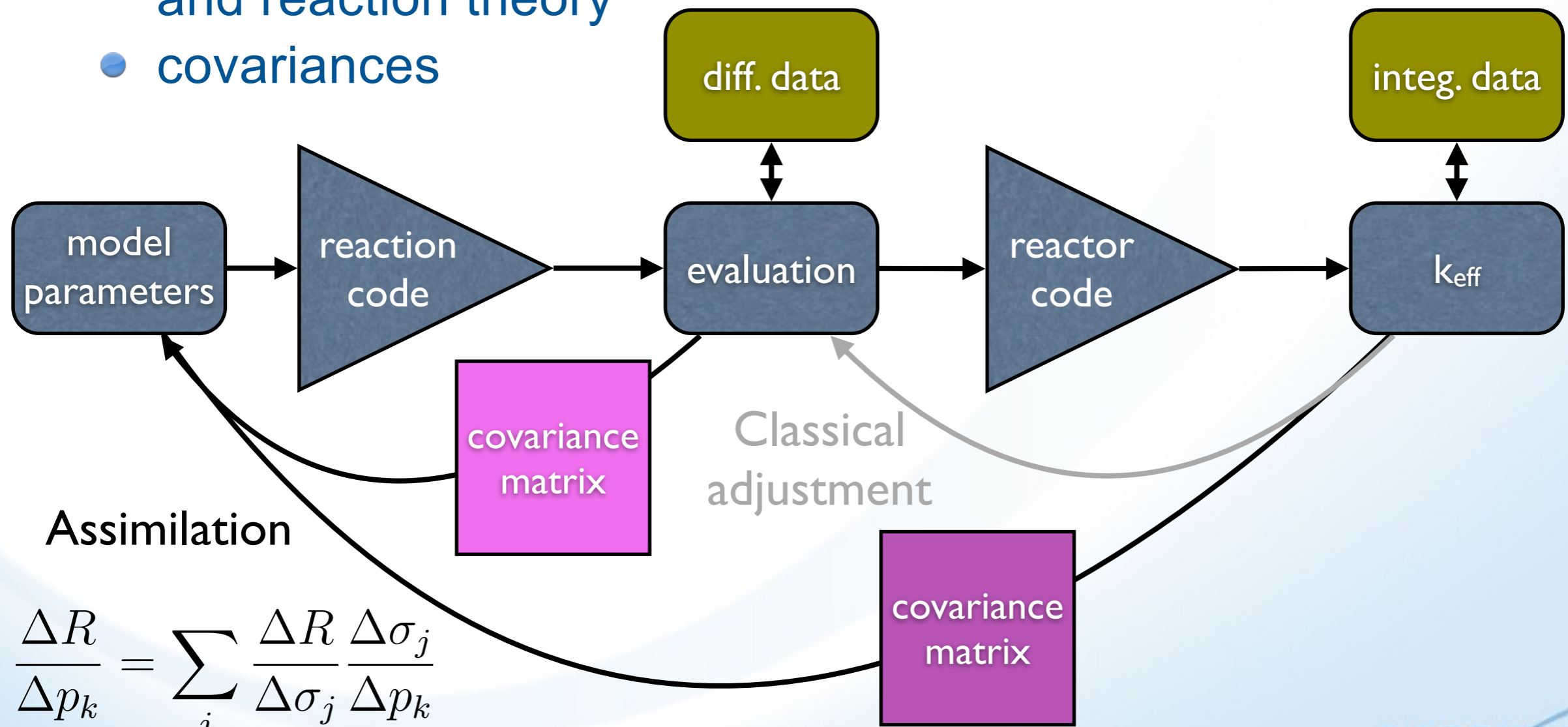
Consistent adjustment (assimilation) linking reaction theory and integral experiments

- Modern practice is to use nuclear reaction code constrained by experimental data to produce evaluation and covariances



Consistent adjustment (assimilation) linking reaction theory and integral experiments

- Tuning is moved from multi-group file to reaction model parameters providing
 - evaluation constrained by differential and integral data and reaction theory
 - covariances



$$\frac{\Delta R}{\Delta p_k} = \sum_j \frac{\Delta R}{\Delta \sigma_j} \frac{\Delta \sigma_j}{\Delta p_k}$$

Scope of the project

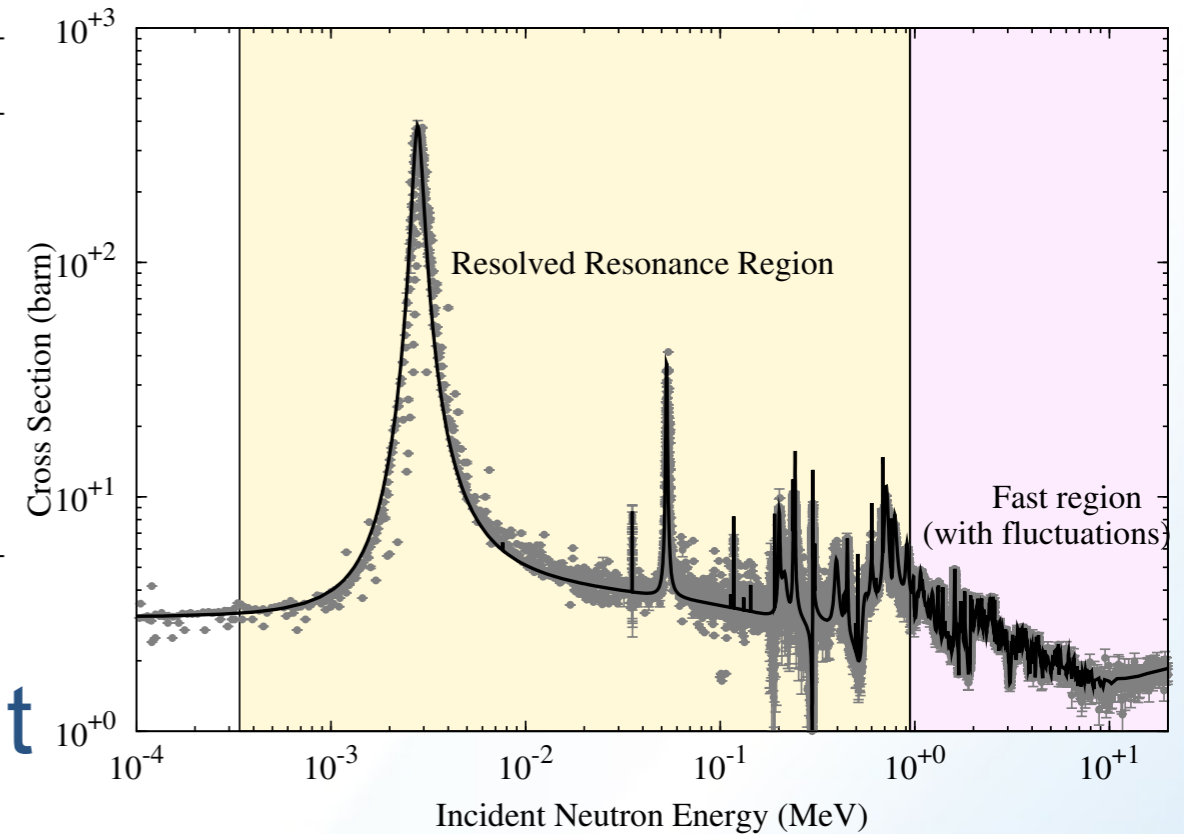
Investigate feasibility of the assimilation concept for priority materials

- ^{23}Na - coolant
- ^{56}Fe - structure material
- ^{105}Pd - fission product
- $^{235,238}\text{U}$, ^{239}Pu - major actinides
- ^{242}Pu - minor actinide

Clean integral experiments available

Assimilation of ^{23}Na

Detector	prior C/E	posterior C/E
EURACOS ^{32}S	0.770 ± 0.085	0.997 ± 0.057
EURACOS ^{197}Au	0.954 ± 0.102	0.946 ± 0.010
JANUS-8 ^{32}S	0.538 ± 0.022	1.000 ± 0.022
JANUS-8 ^{197}Au	1.010 ± 0.033	0.959 ± 0.028
JANUS-8 ^{55}Mn	1.158 ± 0.025	1.028 ± 0.023
JANUS-8 ^{103}Rh	0.960 ± 0.106	0.976 ± 0.047

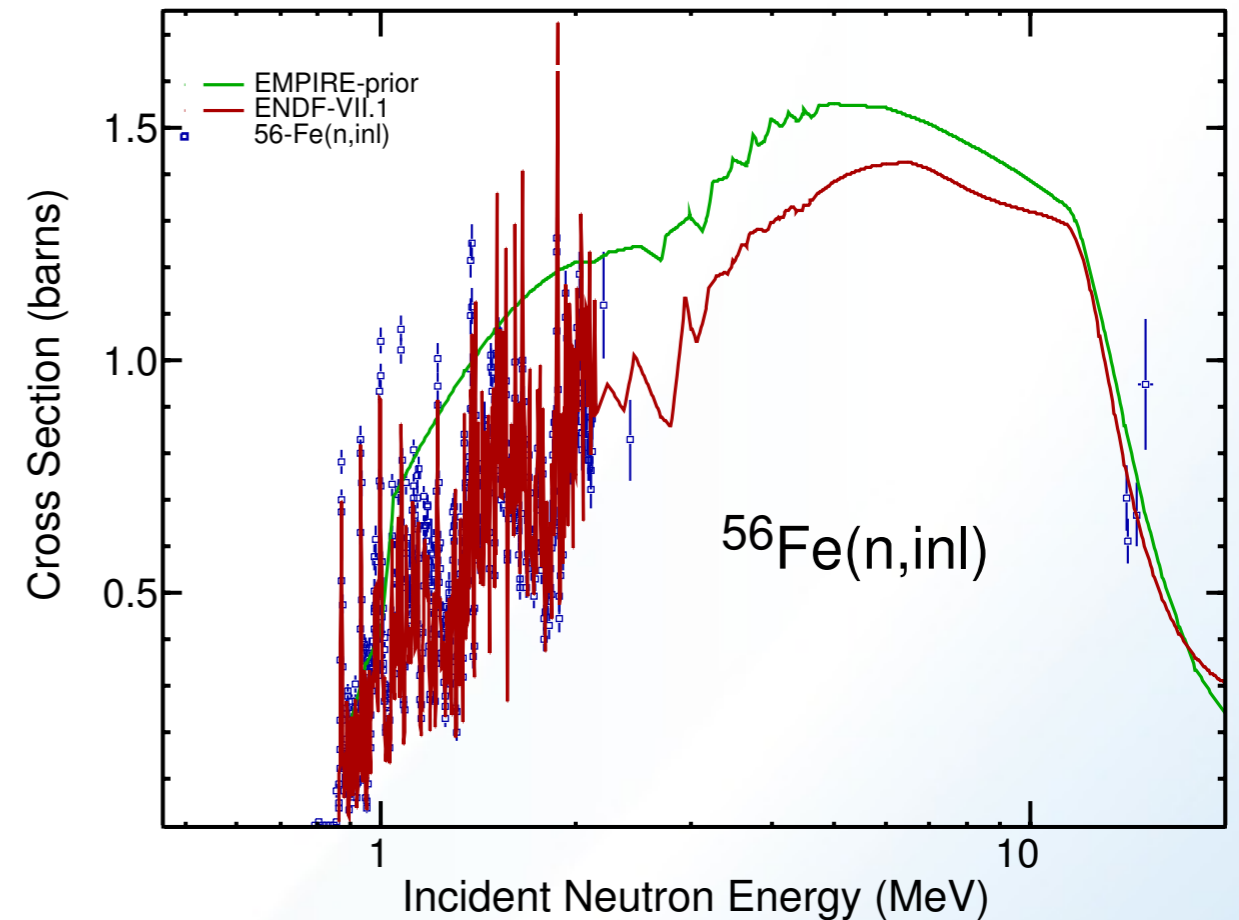
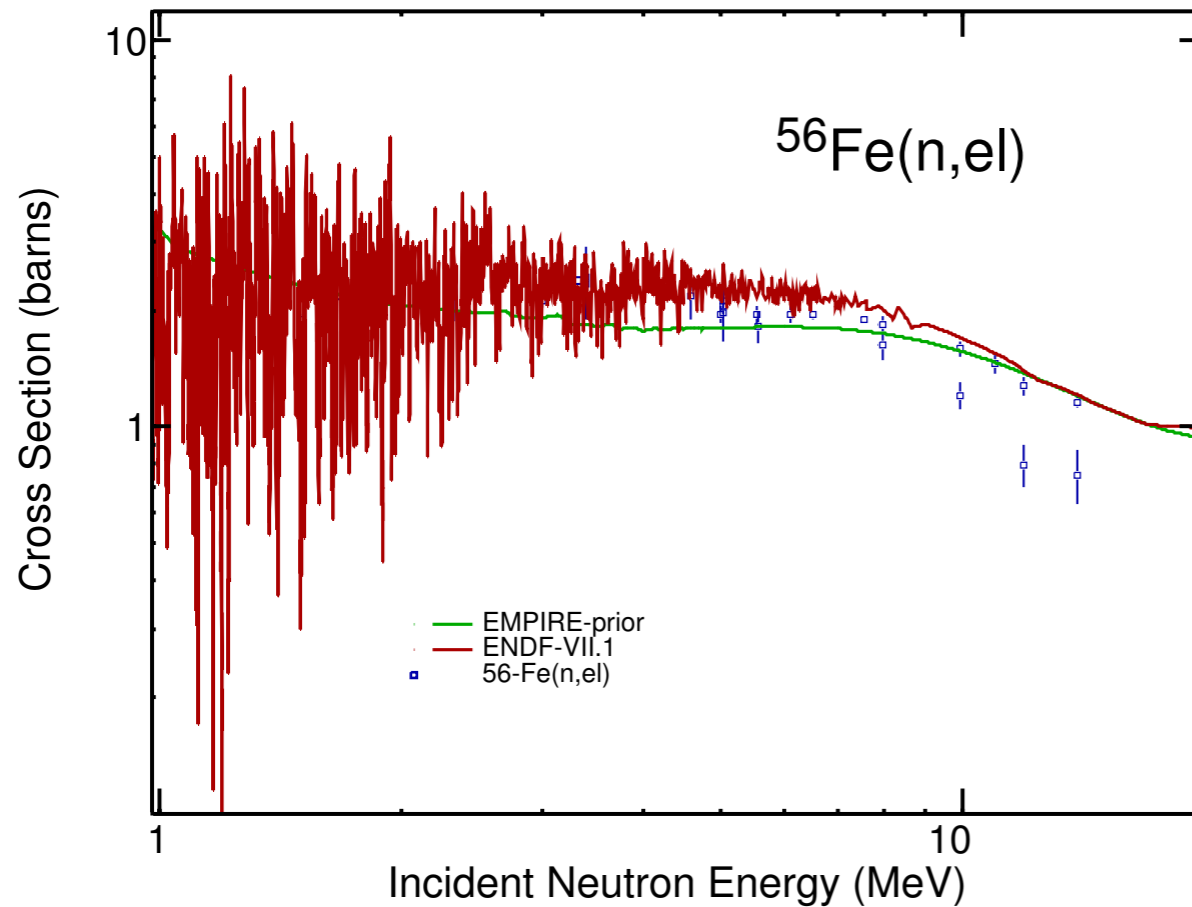


- Apparently excellent result but **failed 'retrofitting test'**

- Lesson learned

- non-linearity effects may distort the assimilation procedure and must be kept under control.
- cross section fluctuations represent a challenge (in ^{23}Na treated via energy dependent scaling factor)

Assimilation of ^{56}Fe



- Hopeless resonance-like structure up to 8 MeV
- Poor prior - better CC omp needed

C/E after assimilation of ^{56}Fe

Experiment		C/E \pm	(before)	C/E \pm	(after)
$^{10}\text{B}(n, \gamma)$ slope	ZPR3-54	0.853	± 0.030	1.012	± 0.022
$^{235}\text{U}(n,f)$ slope	ZPR3-54	0.907	± 0.030	1.015	± 0.013
$^{239}\text{Pu}(n,f)$ slope	ZPR3-54	0.889	± 0.030	0.996	± 0.013
$^{238}\text{U}(n,f)$ slope	ZPR3-54	1.455	± 0.030	1.284	± 0.014
$^{32}\text{S}(n,p)$ slope	EURACOS	0.879	± 0.093	1.197	± 0.055
$^{197}\text{Au}(n, \gamma)$ slope	EURACOS	1.288	± 0.098	1.054	± 0.032
$^{115}\text{In}(n,n')$ slope	EURACOS	0.327	± 0.156	0.455	± 0.042
$^{103}\text{Rh}(n,n')$ slope	EURACOS	0.478	± 0.071	0.511	± 0.010

- Certain improvement achieved but VII.0 performs better
- Poor prior - better CC omp needed

^{56}Fe - posterior parameters

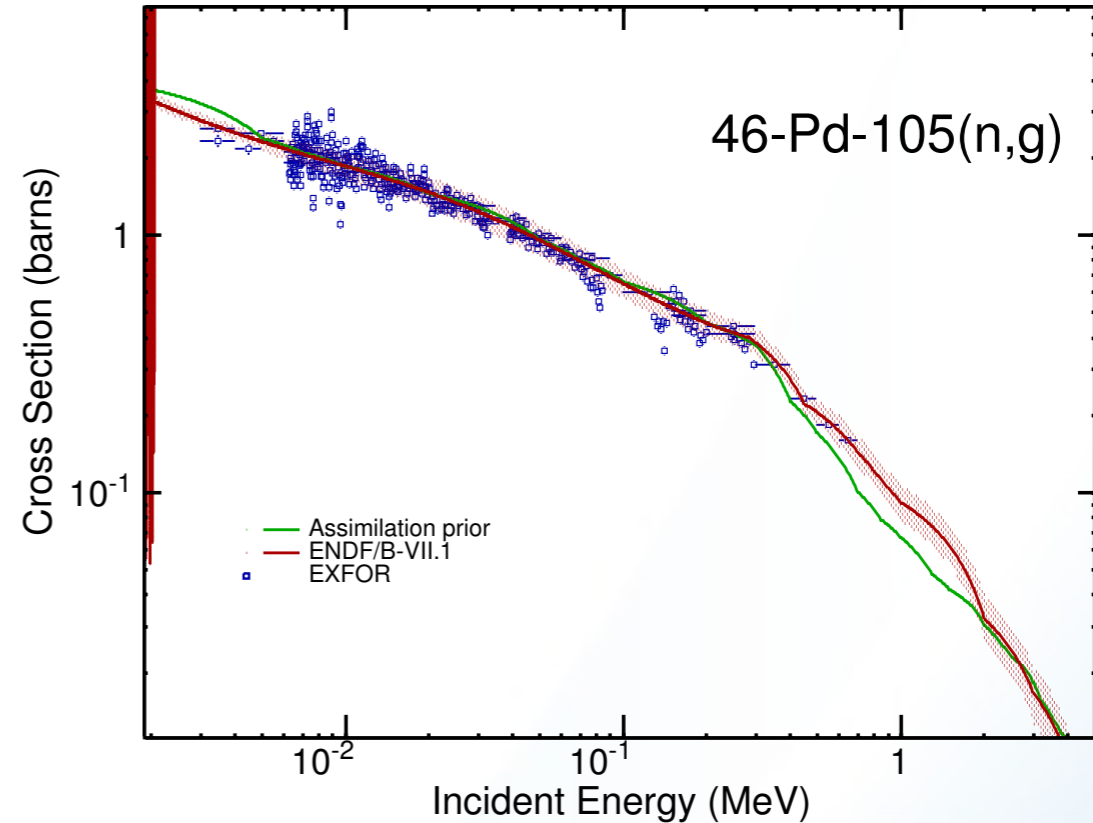
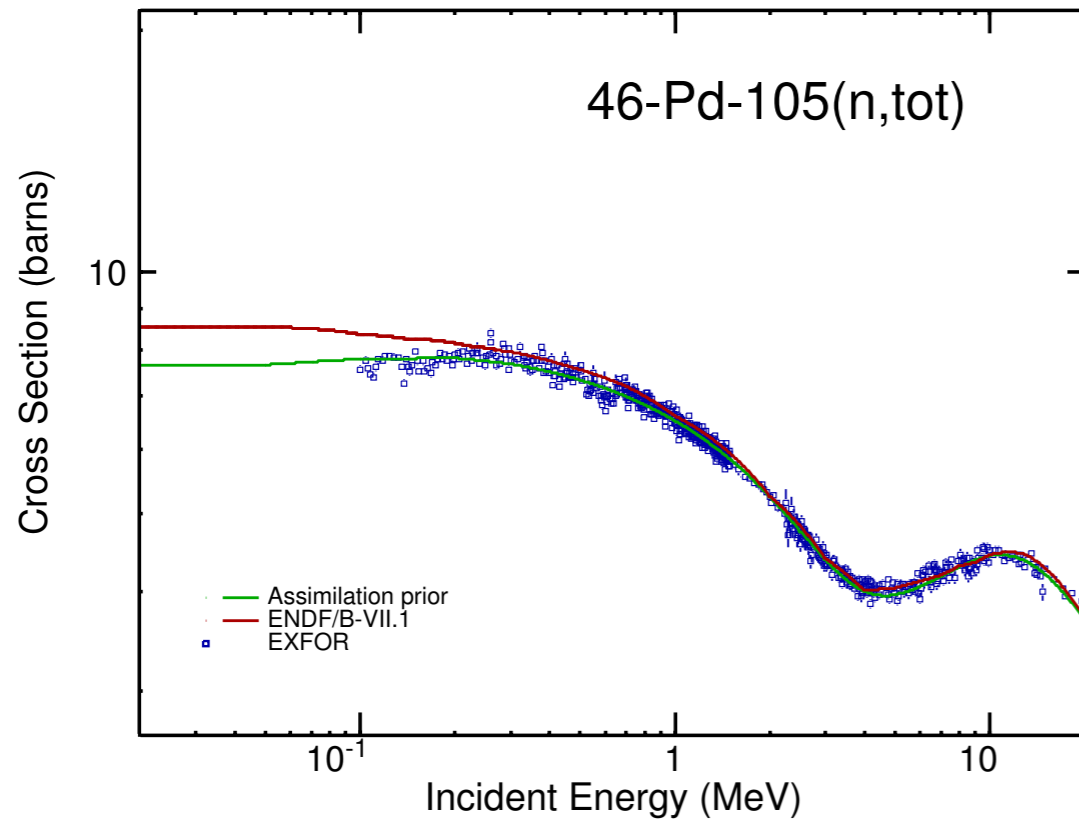
Parameter	Variation (%)	Init. Std. Dev. (%)	Final Std. Dev. (%)
Scat. Rad. ^a	-13.25	5.1	2.1
Γ_n Bound Level ^b	1.9	4.0	3.7
Γ_g Bound Level ^b	-2.1	5.0	4.8
Γ_n 277 keV ^c	-1.1	8.0	8.0
Γ_n 317 keV ^c	-2.2	8.0	8.0
Γ_n 361 keV ^c	-2.9	8.0	8.0
Γ_n 381 keV ^c	-3.0	8.0	8.0
Γ_n 665.6 keV ^c	1.3	8.0	8.0
Real well volume ^d	15.1	3.0	2.2
Nuclear radius Real Surf. ^e	10.5	3.0	2.9
Imag. & Real Surf. ^f	10.8	5.0	4.9
TOTRED ^g	-0.9	1.0	1.0
FUSRED ^h	-2.0	1.3	1.2

Unphysical changes
in the parameters

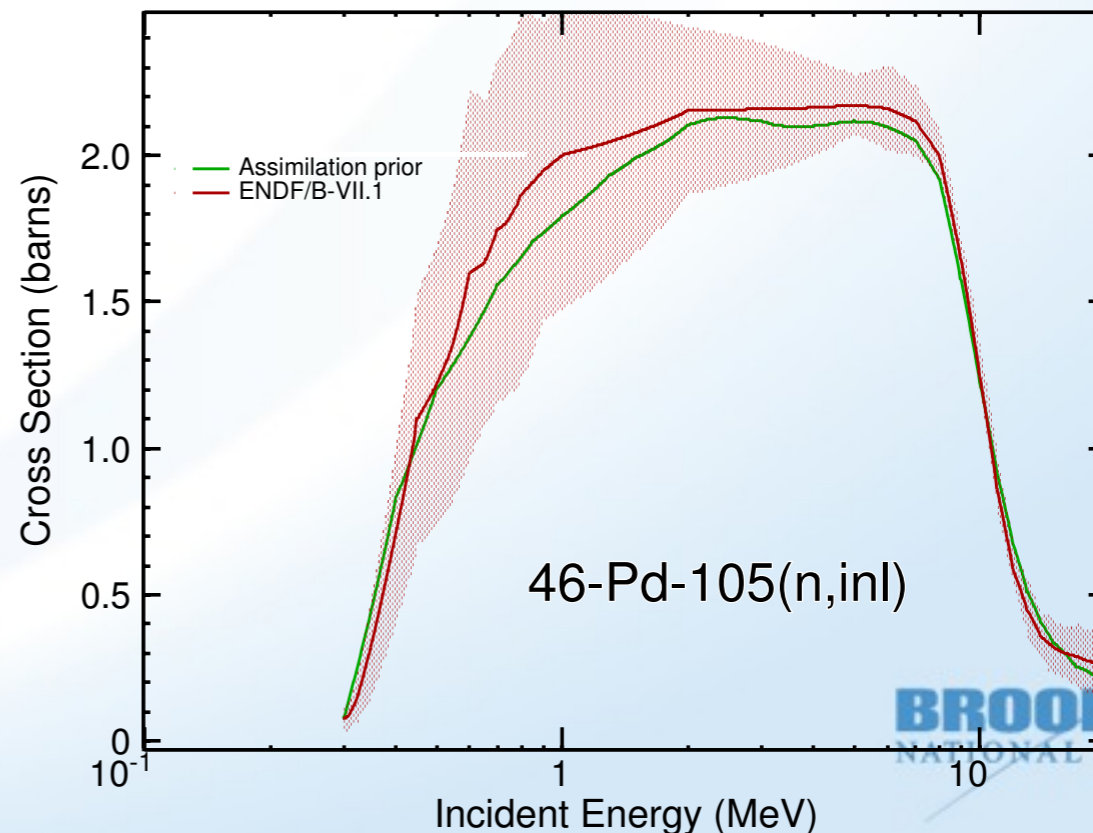
^{56}Fe lesson learned

- Integral experiments alone do not ensure restoring agreement with differential data if the prior is of poor quality.
- A practical, necessarily approximative, method should be developed for treating fine energy fluctuations that can't be treated in terms of the reaction theory
- Possible discrepancies among differential and integral experiments might make consistent assimilation difficult or impossible.

Assimilation of ^{105}Pd



- Pretty good prior
- Integral experiment PROFIL-1 sensitive to capture \Leftrightarrow should be easy!



¹⁰⁵Pd - prior parameter correlations

Parameter	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1 UOMPRV-011 ^a	100																							
2 UOMPVV-011 ^a	-99	100																						
3 UOMPRS-011 ^a	-72	67	100																					
4 UOMPWS-011 ^a	89	-89	-78	100																				
5 UOMPRW-011 ^a	0	0	0	0	100																			
6 UOMPWV-011 ^a	0	0	0	0	0	100																		
7 TOTRED-000 ^b	0	0	0	0	0	0	100																	
8 FUSRED-000 ^b	0	0	0	0	0	0	0	100																
9 ATILNO-000 ^c	-4	4	2	-5	0	0	0	0	100															
10 ATILNO-010 ^c	-40	40	26	-35	0	0	0	0	1	100														
11 ATILNO-020 ^c	0	0	0	0	0	0	0	0	0	0	100													
12 ATILNO-030 ^c	0	0	0	0	0	0	0	0	0	0	0	100												
13 GTILNO-000 ^d	30	-30	-20	26	0	0	0	0	-1	-38	0	0	100											
14 GTILNO-010 ^d	2	-2	-1	2	0	0	0	0	0	1	0	0	-5	100										
15 GTILNO-020 ^d	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100									
16 GTILNO-030 ^d	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100								
17 TUNEPE-100 ^e	4	-4	-3	4	0	0	0	0	0	1	0	0	-10	-1	0	0	100							
18 TUNE-000 ^f	6	-6	-4	7	0	0	0	0	-99	-2	0	0	2	0	0	0	0	100						
19 TUNE-011 ^f	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100					
20 TUNE-010 ^f	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100				
21 PCROSS-000 ^g	-25	25	17	-23	0	0	0	0	1	68	0	0	36	2	0	0	5	-1	0	0	100			
22 RESNOR-100 ^h	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100		
23 RESNOR-200 ^h	-1	1	1	-1	0	0	0	0	0	-24	0	0	5	0	0	0	1	0	0	0	0	0	100	
24 RESNOR-300 ^h	0	0	0	0	0	0	0	0	0	-5	0	0	0	0	0	0	0	0	0	0	0	0	0	100

Strong anti-correlation between CN level density and gamma strength function

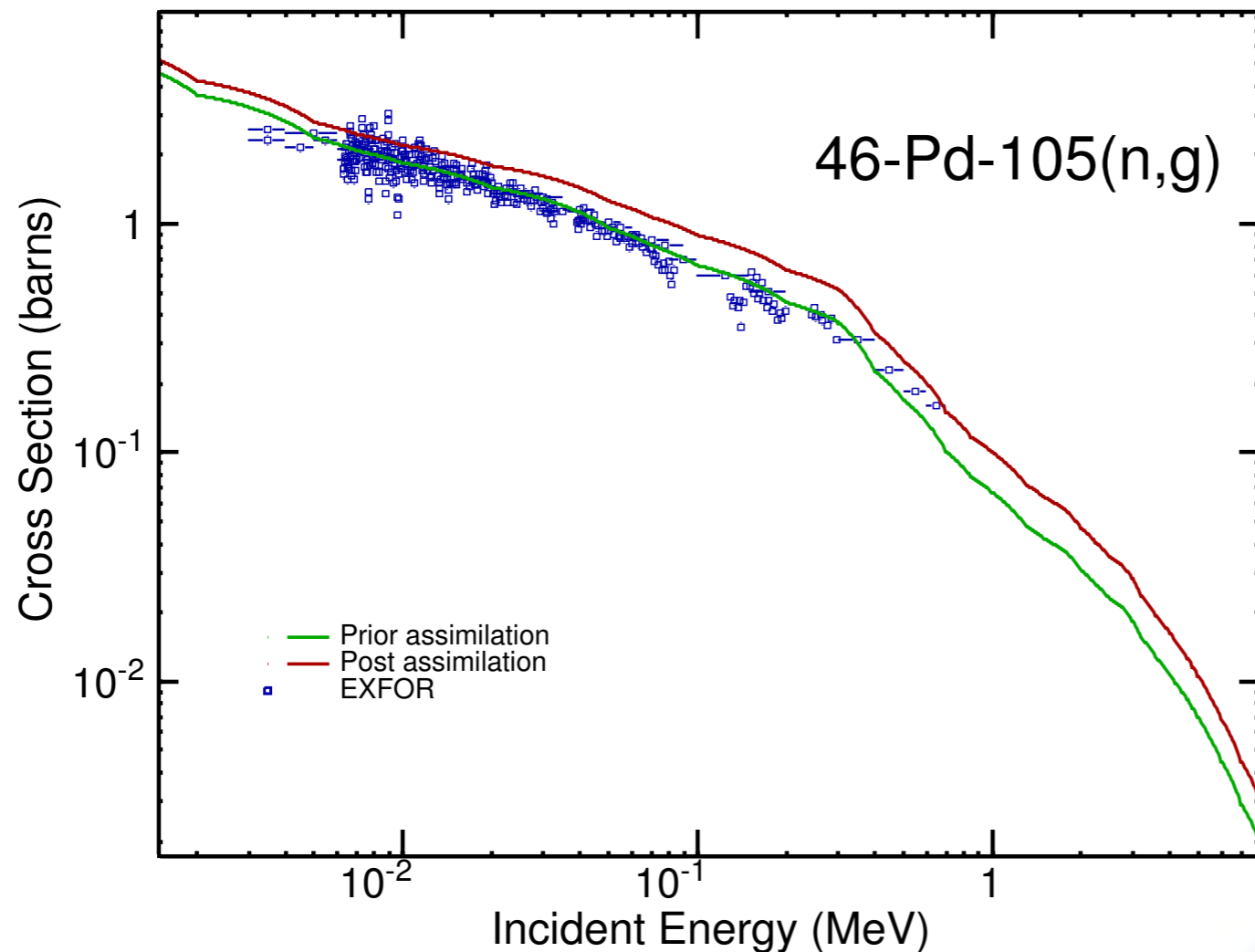
^{105}Pd - assimilation results

Experiment	old C/E $\pm \sigma$	new C/E $\pm \sigma$
PROFIL-1	0.835 \pm 0.028	0.990 \pm 0.027

Parameter	Variation (%)	Init. % Std. Dev.	Final % Std. Dev.
TUNE000 ^a	69.253	40.00	10.77
ATILNO000 ^b	-2.573	1.49	0.43
FUSRED000 ^c	0.353	2.00	1.99

- TUNE-ATILNO anti-correlation keeps capture cross section constant!
- Assimilation required modification of the covariance matrix (increasing gamma-strength uncertainty keeping CN level density constrained)

^{105}Pd - assimilation results (cont.)



- posterior disagrees with differential data
- differential and integral experiments discrepant

Assimilation concept worked! Violence had to be done to the differential covariance matrix to fit integral data.

^{105}Pd - lesson learned

- If two parameters happen to be strongly anti-correlated assimilation may exploit this feature to drive both parameters out of the physical range.
- If assimilation is not possible without increasing properly defined prior uncertainties it either means that the model is not adequate or flexible enough, or that differential and integral experiments are inconsistent.

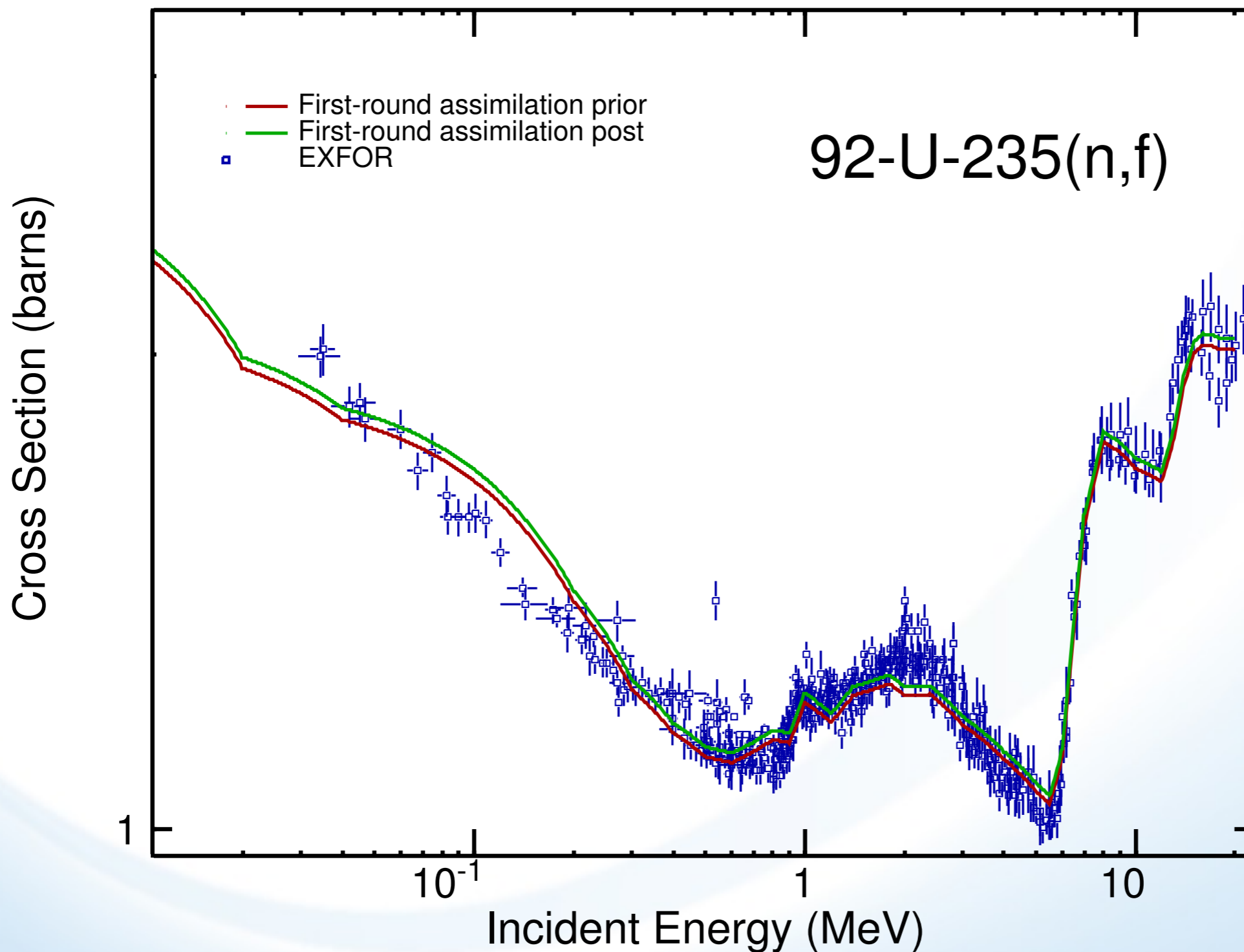
Assimilation of ^{235}U (1st round)

GODIVA

Experiment	C/E $\pm \sigma$ (before)	C/E $\pm \sigma$ (after)
k_{eff}	0.9907 \pm 0.002	1.0010 \pm 0.002
$^{238}\text{U}(\text{n,f})/^{235}\text{U}(\text{n,f})$	1.0527 \pm 0.013	1.0357 \pm 0.004
$^{239}\text{Pu}(\text{n,f})/^{235}\text{U}(\text{n,f})$	0.9917 \pm 0.018	0.9771 \pm 0.003
$^{237}\text{Np}(\text{n,f})/^{235}\text{U}(\text{n,f})$	1.0703 \pm 0.017	1.0536 \pm 0.003
$^{233}\text{U}(\text{n,f})/^{235}\text{U}(\text{n,f})$	0.9964 \pm 0.019	0.9820 \pm 0.004

Parameter	Variation (%)	Init. Std. Dev. (%)	Final Std. Dev. (%)
FUSRED000 ^a	1.402	1.257	0.878
TOTRED000 ^b	0.461	0.966	0.917
ATILNO000 ^c	-0.236	0.950	0.946
DELTA000 ^d	-0.025	0.649	0.621
VB000 ^e	-0.006	0.133	0.118
UOMPVV011 ^f	0.033	0.116	0.116
UOMPVS011 ^g	0.072	0.834	0.834
UOMPWS011 ^h	-0.110	2.023	2.022
TUNE000 ⁱ	-0.099	1.908	1.908

^{235}U (1st round) - assimilated fission



^{235}U (1st round) - lesson learned

- A single integral experiment can be successfully assimilated even with a poor prior. Here, $k_{\text{eff}}=1$ was obtained by scaling fission (fusion) cross sections regardless of differential data.
- More integral experiments with diverse characteristics should help.

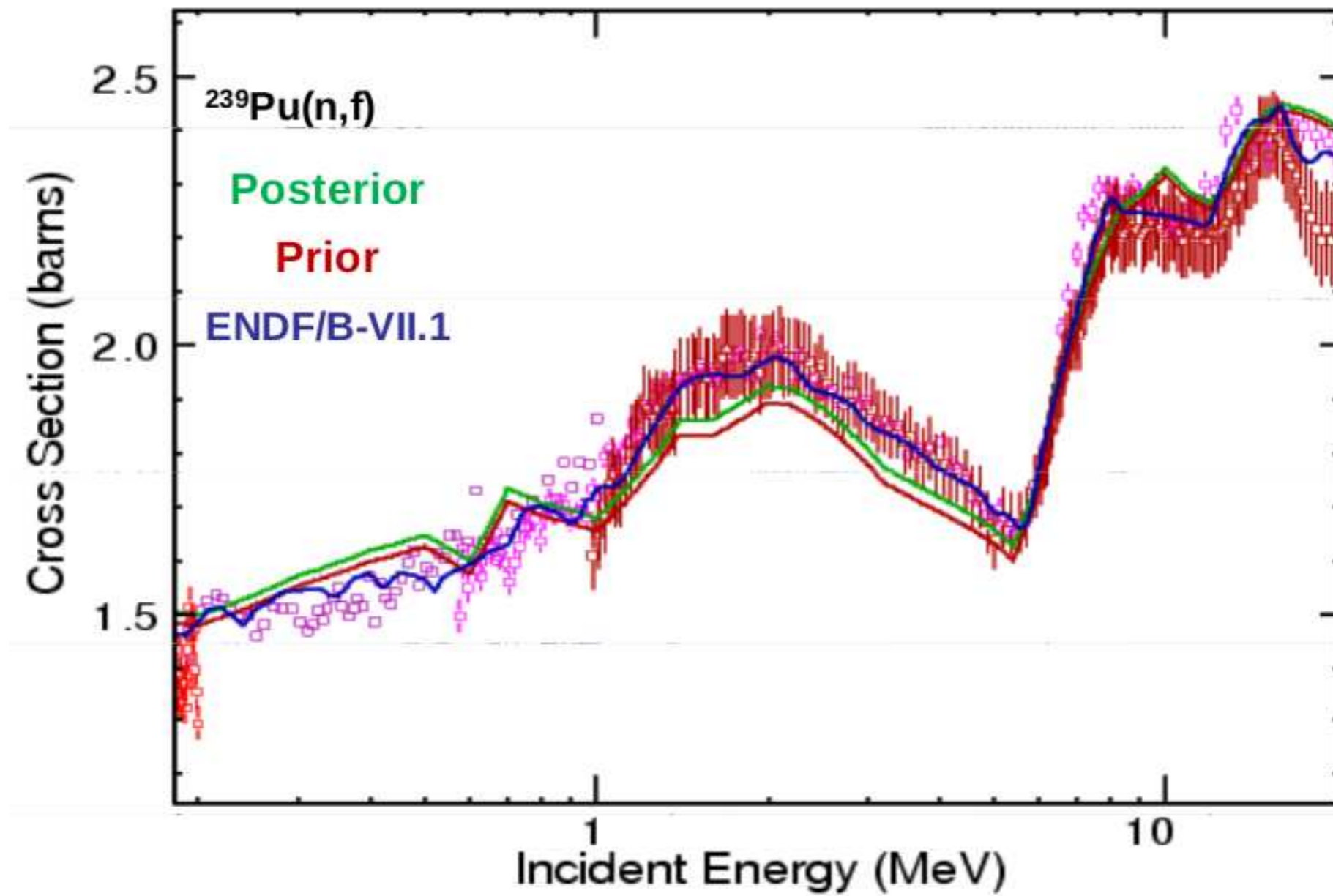
Assimilation of ^{239}Pu (1st round)

JEZEBEL

Experiment	prior C/E \pm	post C/E \pm
k_{eff}	0.9857 ± 0.002	0.9998 ± 0.002
Fis.238U/Fis.235U	0.9561 ± 0.009	0.9598 ± 0.002
Fis.239Pu/Fis.235U	0.9708 ± 0.020	0.9917 ± 0.003
Fis.237Np/Fis.235U	0.9988 ± 0.017	1.0010 ± 0.001
Fis.233U/Fis.235U	1.0003 ± 0.017	1.0002 ± 0.001

- Consistent improvement (except $^{238}\text{U}/^{235}\text{U}$)
- VII.1 and assimilated file equivalent on k_{eff} but...

^{239}Pu (1st round) - assimilated fission



... NOT for differential experiments

^{239}Pu (1st round) - assimilated parameters

Parameter	Variation (%)	Prior Std. Dev. (%)	Posterior Std. Dev. (%)
VA000 ^a	-0.141	0.134	0.121
FUSRED000 ^b	0.432	0.951	0.612
LDSHIF010 ^c	0.299	0.705	0.692
DELTA000 ^d	-0.120	0.671	0.668
ATILNO010 ^e	-0.076	0.965	0.958
VB000 ^f	-0.079	0.480	0.479
ATLATF000 ^g	0.128	1.240	1.239
TOTRED000 ^h	-0.0831	0.918	0.815
HA000 ⁱ	-0.155	0.474	0.471

Assimilation distributed over several parameters

^{239}Pu (1st round) - lesson learned

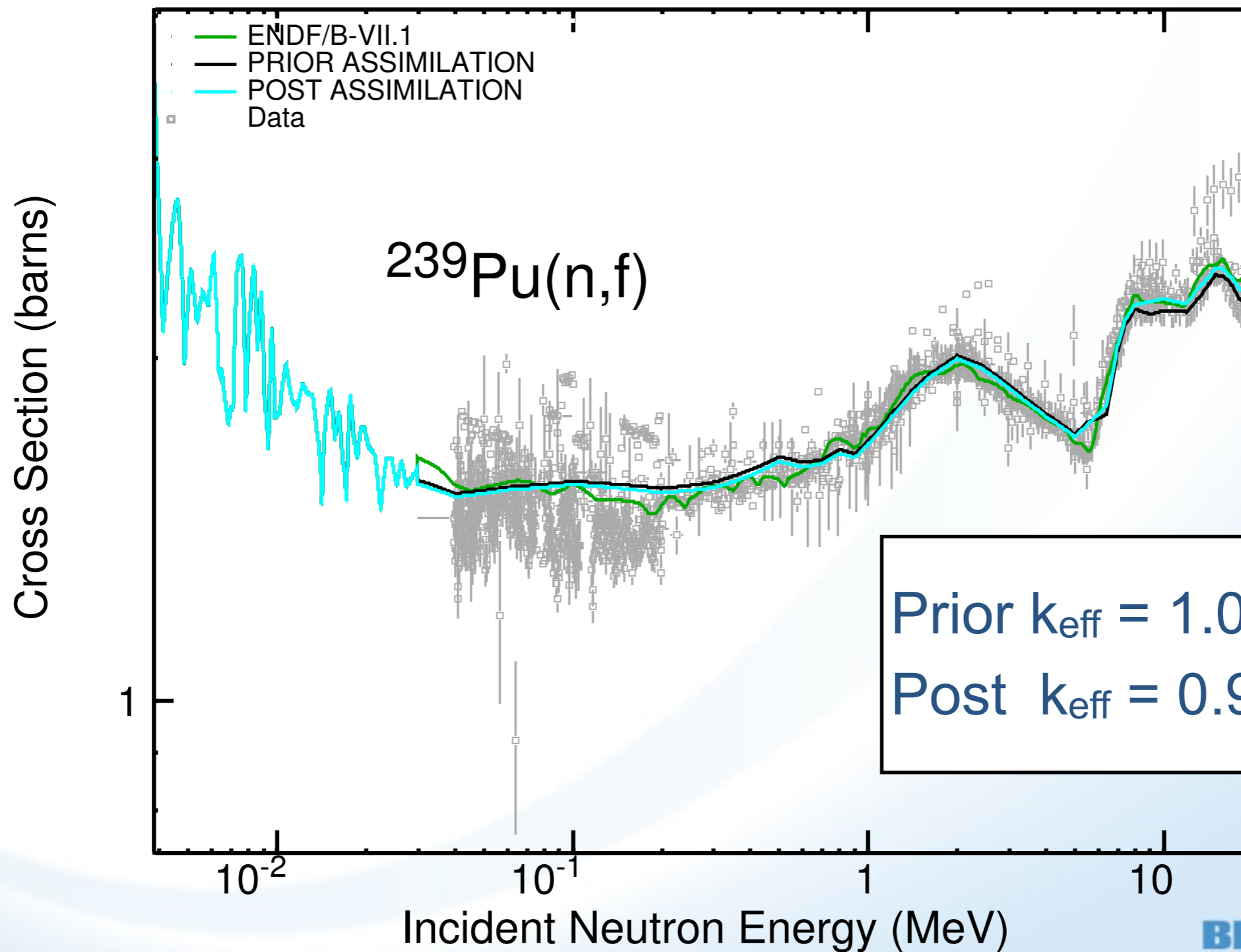
- Perfect agreement with integral parameter can be obtained without satisfactorily reproducing differential data.

There is no substitute for a good prior!

Assimilation of ^{239}Pu (2nd round)

- New version of EMPIRE with improved fission parametrization (M. Sin)
- Overall very good prior
- EMPIRE calculated PFNS included in assimilation
- Direct assimilation on JEZEBEL's k_{eff} using MCNP performed at BNL.

^{239}Pu (2nd round) assimilated fission



^{239}Pu (2nd round) - assimilated parameters

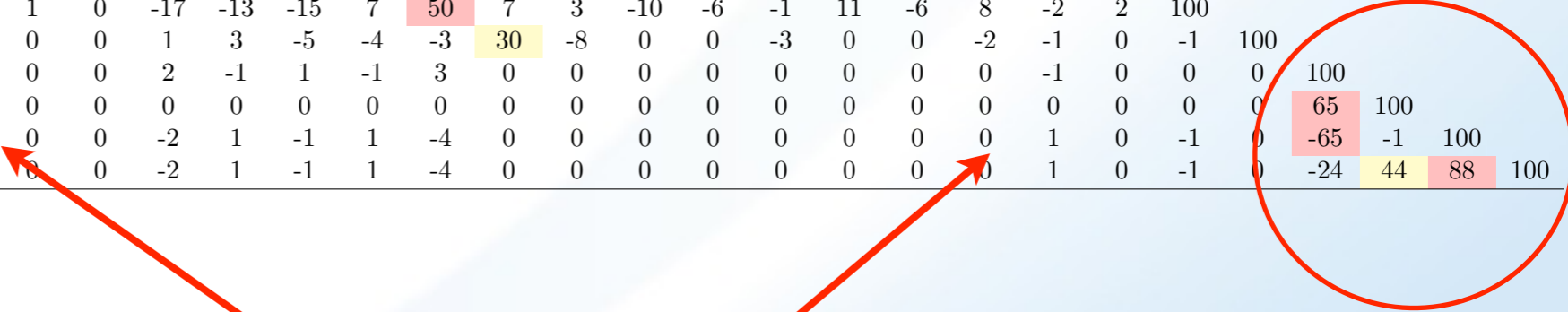
Parameter Name	pre-assimilation	post-assimilation
ATILNO-000	1.083	1.0851
ATILNO-001	0.907	0.9034
ATILNO-020	0.938	0.9380
ATILNO-030	0.988	0.9880
TUNEFI-010	0.833	0.8327
TUNE-000	2.228	2.2230
FUSRED-000	0.970	0.9700
RESNOR-000	1.320	1.3200
FISVF1-000	1.000	0.9995
FISVF1-010	1.000	1.0005
FISVF2-000	1.000	1.0042
FISVE1-000	1.000	0.9985
FISVE2-000	1.000	0.9995
FISHO1-000	1.000	0.9992
FISHO2-000	1.000	0.9992
FISAT1-000	0.917	0.9157
FISAT2-000	0.971	0.9717
FISAT2-010	0.981	0.9810
FISDL1-000	1.000	0.9999
FISDL2-000	1.000	0.9999
LDSHIF-000	1.100	1.0990
LDSHIF-010	1.063	1.0647
LDSHIF-020	0.917	0.9170
PFNALP-000	0.963	0.9613
PFNRAT-000	0.928	0.9279
PFNERE-000	0.999	1.0002
PFNTKE-000	0.984	0.9853

- The change required for assimilation is very small in comparison to the uncertainties of the experimental data sets.
- Tiny changes in the parameters are well within the prior uncertainties of the parameters

^{239}Pu (2nd round) - post-assimilation covariance matrix

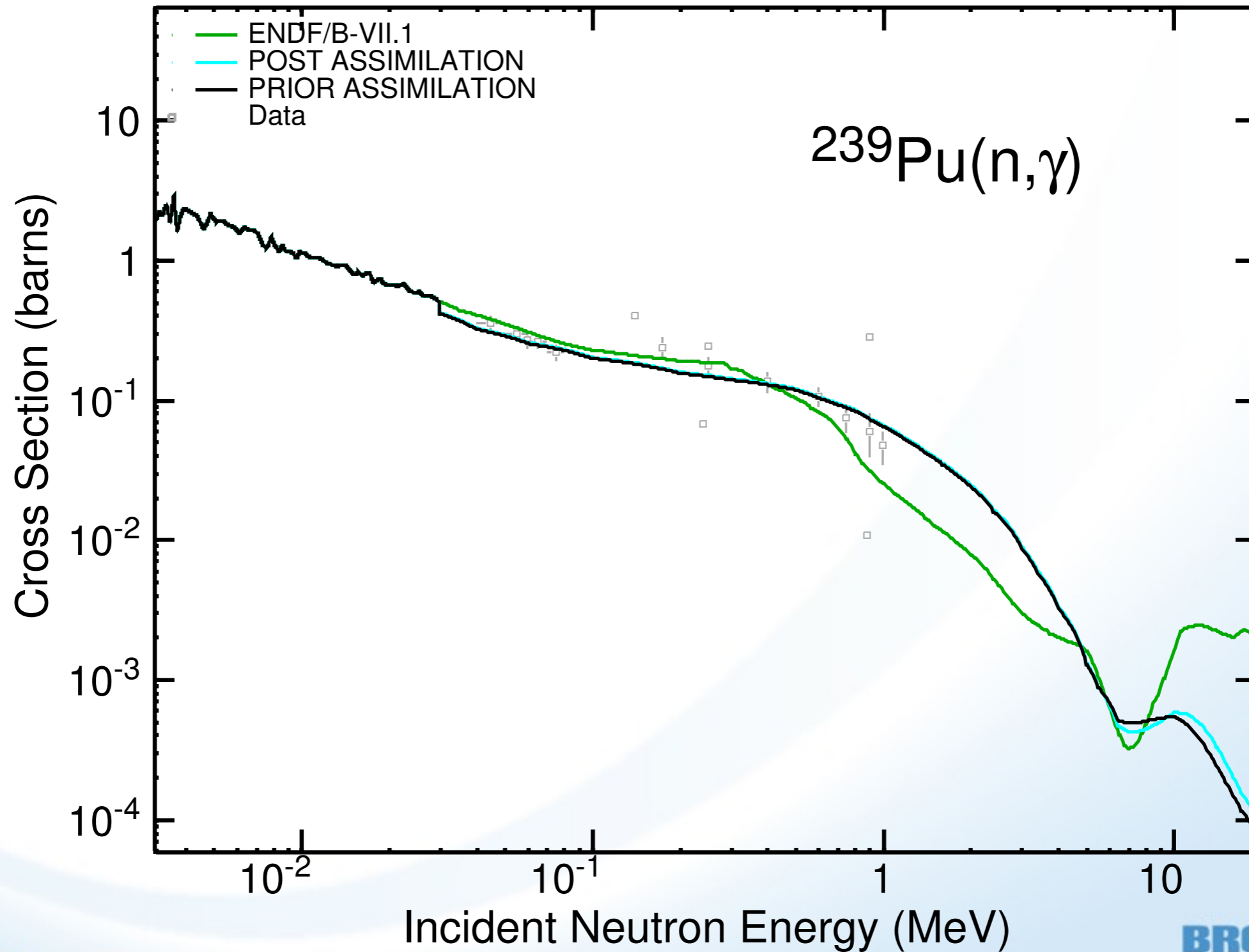
Parameter	1	2	3	5	6	7	9	10	11	12	13	14	16	17	18	20	23	24	26	34	37	38	46	47	48	50	51	52	53	
1 ATILNO-000 ^a	100																													
2 ATILNO-010 ^a	4	100																												
3 ATILNO-020 ^a	-2	0	100																											
5 TUNEFI-010 ^b	0	1	4	100																										
6 TUNEFI-000 ^b	-1	2	-1	0	100																									
7 TUNE-000 ^c	-19	-2	1	0	-1	100																								
9 TOTRED-000 ^d	0	0	0	0	0	0	100																							
10 FUSRED-000 ^d	0	0	0	0	0	0	-98	100																						
11 RESNOR-000 ^e	-5	15	-7	1	0	2	1	0	100																					
12 FISVF1-000 ^f	-3	47	-12	2	8	-3	0	0	17	100																				
13 FISVF1-010 ^f	-2	-13	22	-2	0	1	0	0	-47	-7	100																			
14 FISVF1-020 ^f	2	6	-21	-1	0	-1	0	0	0	0	-5	100																		
16 FISVF2-000 ^f	-13	-38	17	-3	12	4	0	0	-19	-67	6	3	100																	
17 FISVF2-010 ^f	-2	-5	-21	19	-1	0	0	0	-2	-16	-26	2	22	100																
18 FISVF2-020 ^f	0	3	-24	-1	0	0	0	0	0	-2	1	-29	4	6	100															
20 FISVE1-000 ^g	-1	-2	0	0	-1	-1	0	0	0	17	0	0	9	0	0	100														
23 FISVE2-000 ^g	-2	7	-2	0	-1	-1	0	0	0	0	0	0	18	-2	0	-1	100													
24 FISVE2-010 ^g	0	0	5	-2	0	0	0	0	0	2	-1	0	-3	12	0	0	0	100												
26 FISHO1-000 ^h	4	3	1	0	2	1	-1	0	6	34	0	-2	3	0	0	1	2	0	100											
34 FISAT1-000 ⁱ	-1	10	-3	1	-1	-1	0	0	1	3	-3	1	20	-4	0	-1	-2	0	-1	100										
37 FISAT2-000 ⁱ	-2	67	21	-3	-2	0	0	0	-4	-2	10	7	20	20	8	0	-4	-3	3	-3	100									
38 FISAT2-010 ⁱ	2	-1	37	-3	0	-1	0	0	4	7	-12	12	-10	17	17	0	1	-3	-1	2	-14	100								
46 LDSHIF-000 ^j	21	0	0	0	0	4	0	0	2	3	0	-1	2	0	0	0	1	0	-4	0	1	0	100							
47 LDSHIF-010 ^j	-9	-18	5	-1	-7	-1	1	0	-17	-13	-15	7	50	7	3	-10	-6	-1	11	-6	8	-2	2	100						
48 LDSHIF-020 ^j	0	1	1	-6	0	0	0	0	1	3	-5	-4	-3	30	-8	0	0	-3	0	0	-2	-1	0	-1	100					
50 PFNALP-000 ^k	0	-1	0	0	0	0	0	0	2	-1	1	-1	3	0	0	0	0	0	0	0	0	0	-1	0	0	0	100			
51 PFNRAT-000 ^k	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52 PFNERE-000 ^k	-1	2	-1	0	0	1	0	0	-2	1	-1	1	-4	0	0	0	0	0	0	0	0	0	1	0	-1	0	0	0	0	0
53 PFNTKE-000 ^k	-1	1	0	0	0	0	0	0	-2	1	-1	1	-4	0	0	0	0	0	0	0	0	0	1	0	-1	0	-24	44	88	100

PFNS

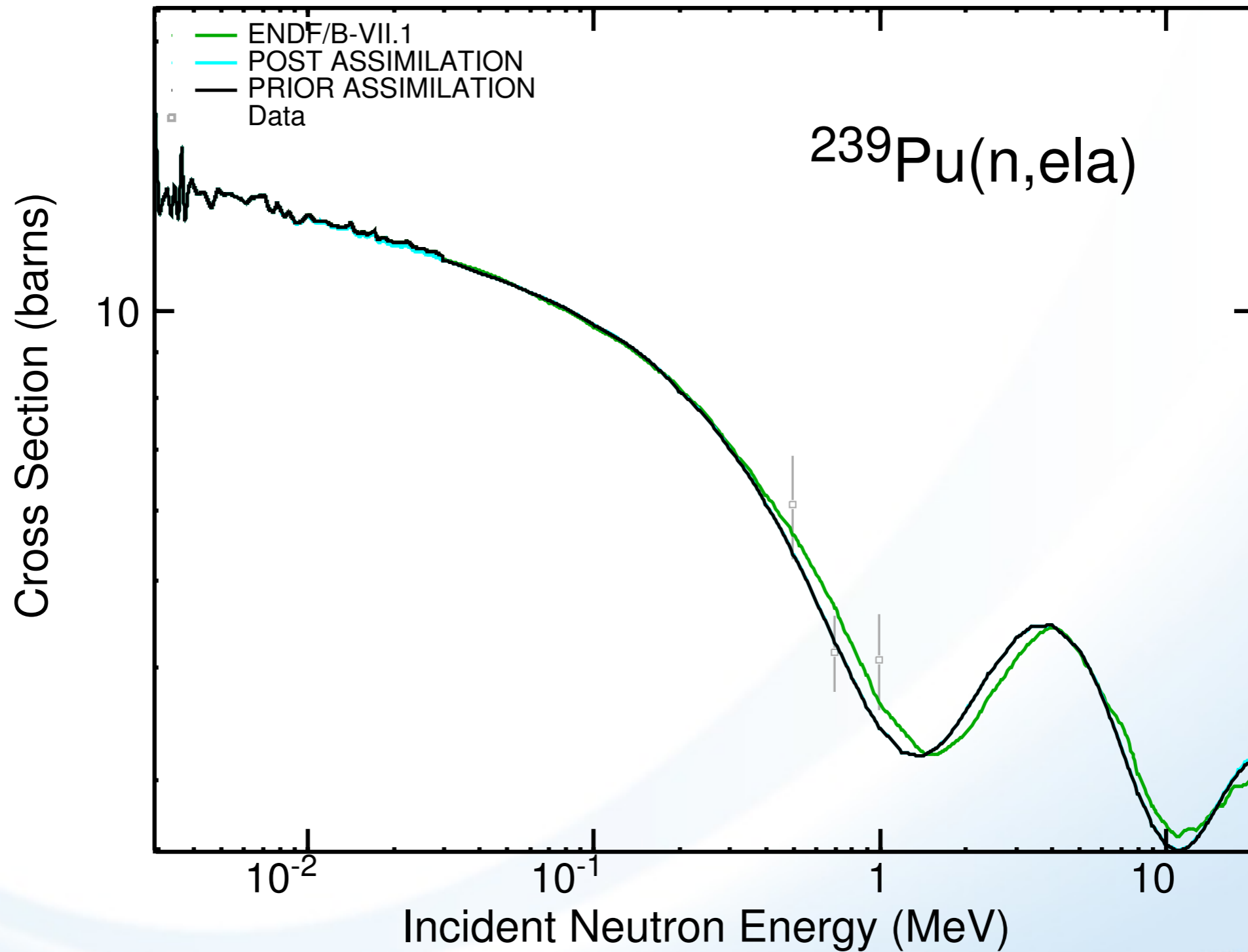


Little correlations between PFNS and x-sec parameters

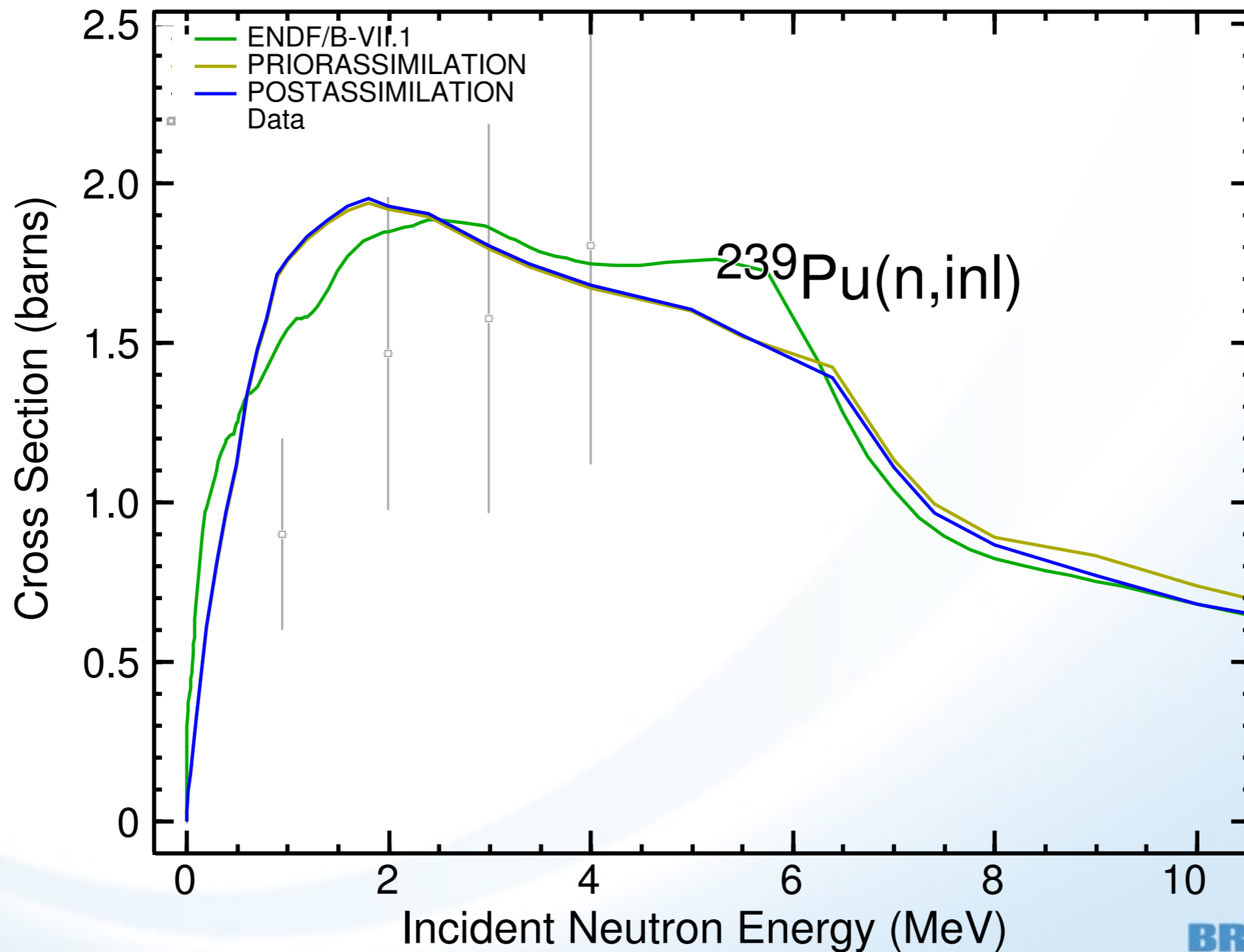
^{239}Pu (2nd round) - assimilated capture



^{239}Pu (2nd round) - assimilated elastic



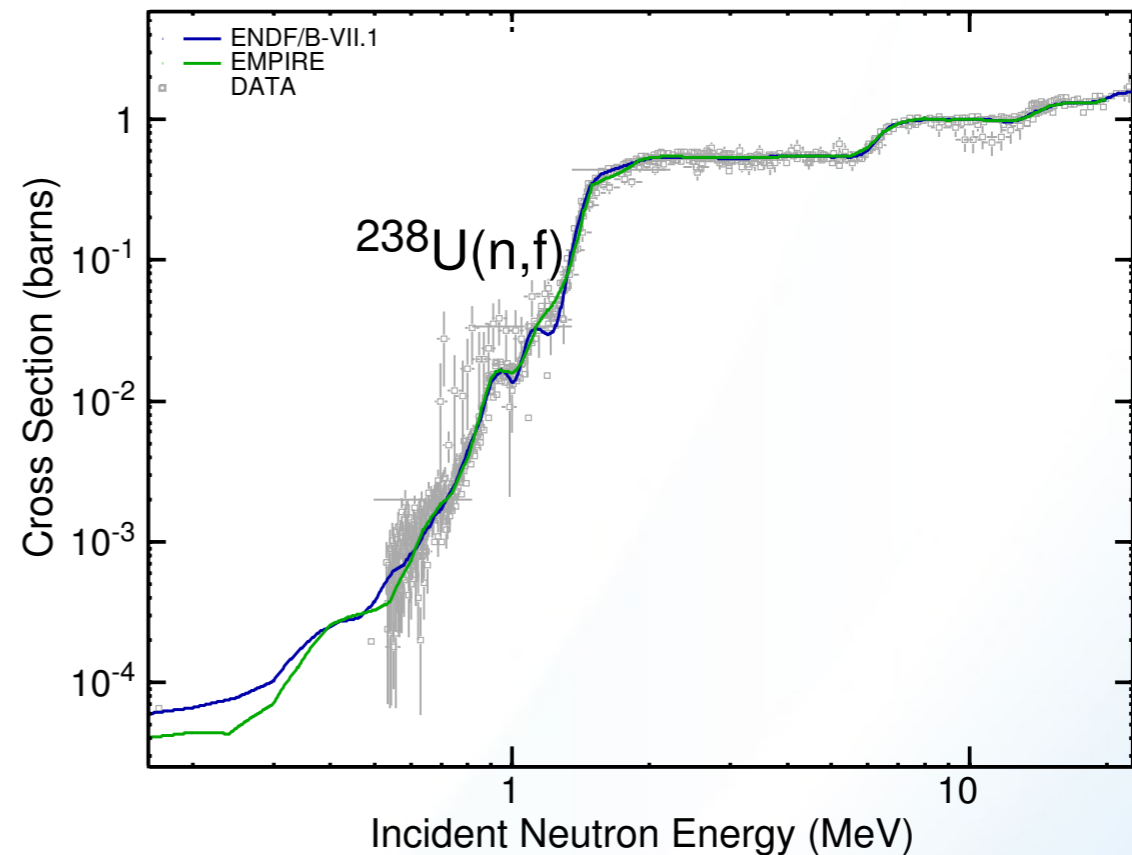
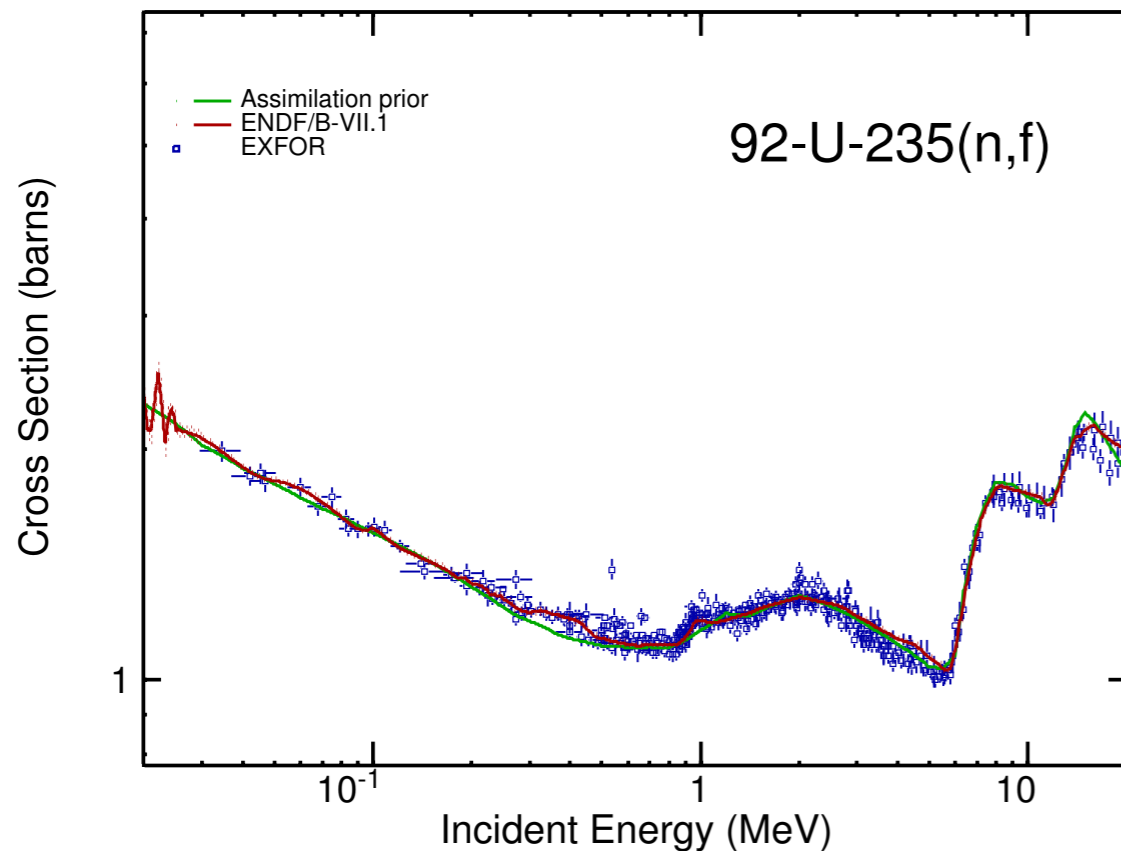
^{239}Pu (2nd round) - assimilated inelastic



^{239}Pu (2nd round) - lesson learned

- Successful assimilations when starting with good prior
- Reduction of uncertainties in the model parameters and consequently also in the calculated integral result
- Little correlations among x-sec and PFNS parameters

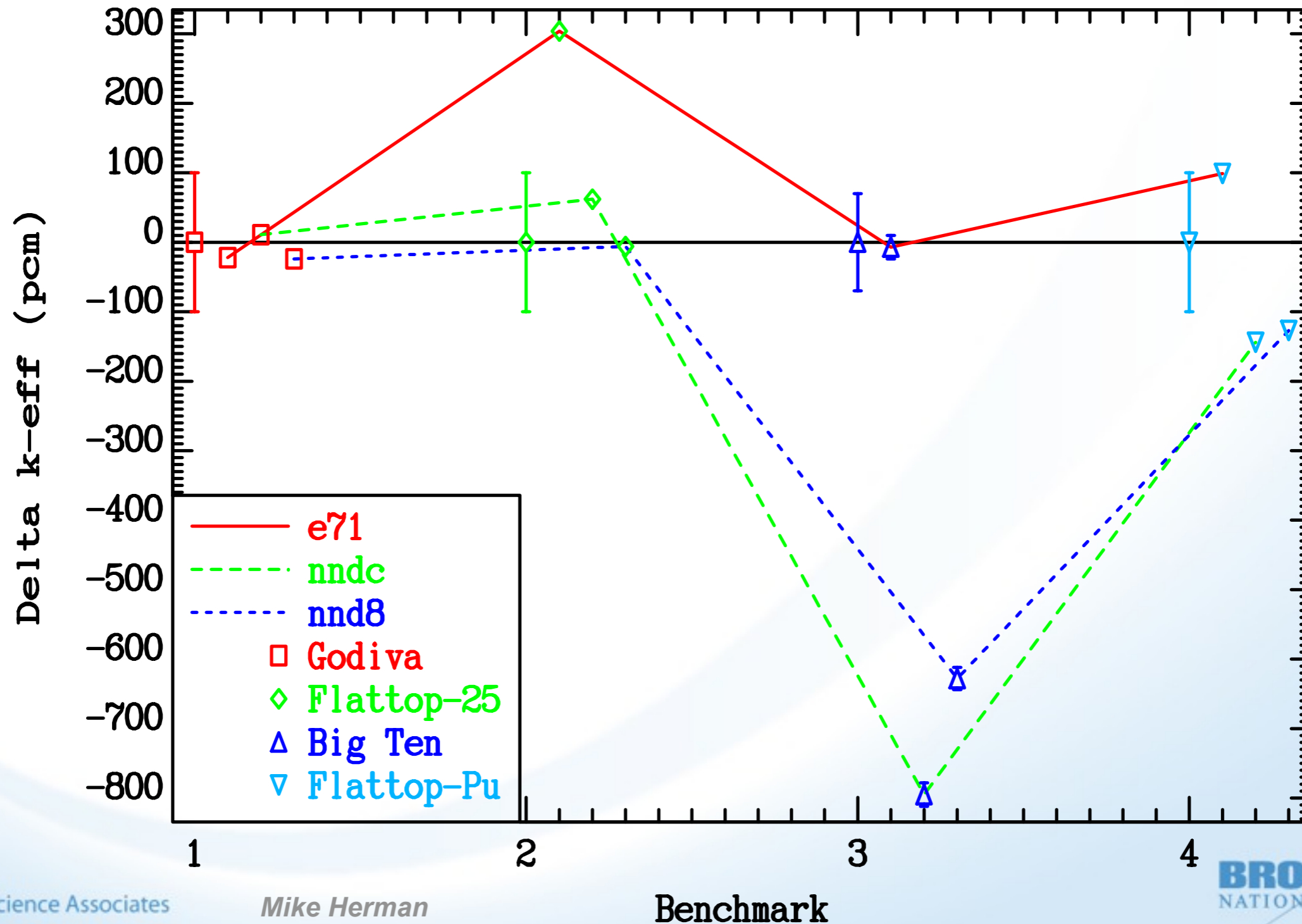
Assimilation priors for ^{235}U and ^{238}U (2nd round)



- Both standards and reproduced within about 2% (standards uncertainties)
- 14 levels coupled in ^{238}U calculations

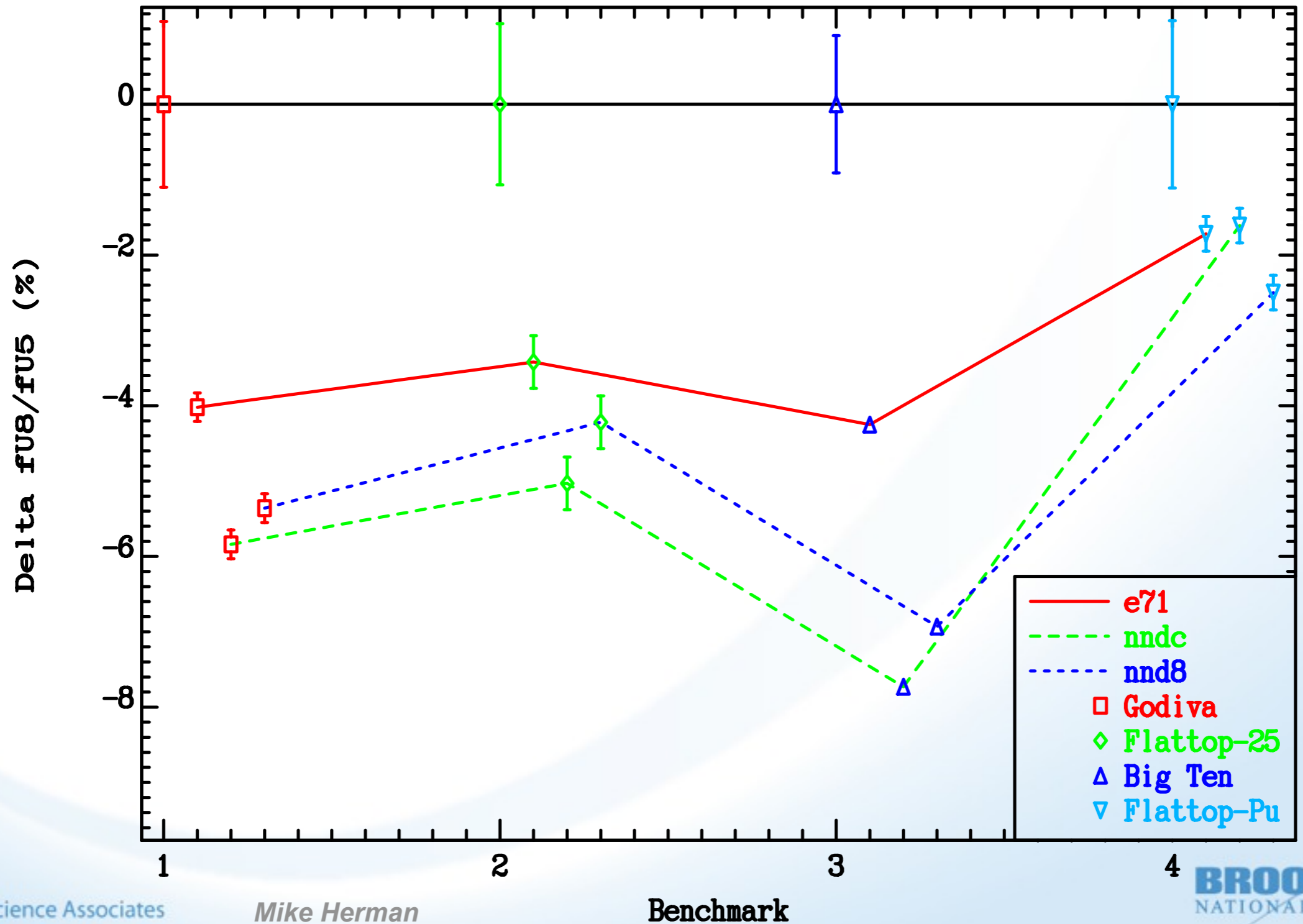
Benchmarking new priors for ^{235}U and ^{238}U

ICSBEP Benchmark Summary Results
Integral parameter intercomparison



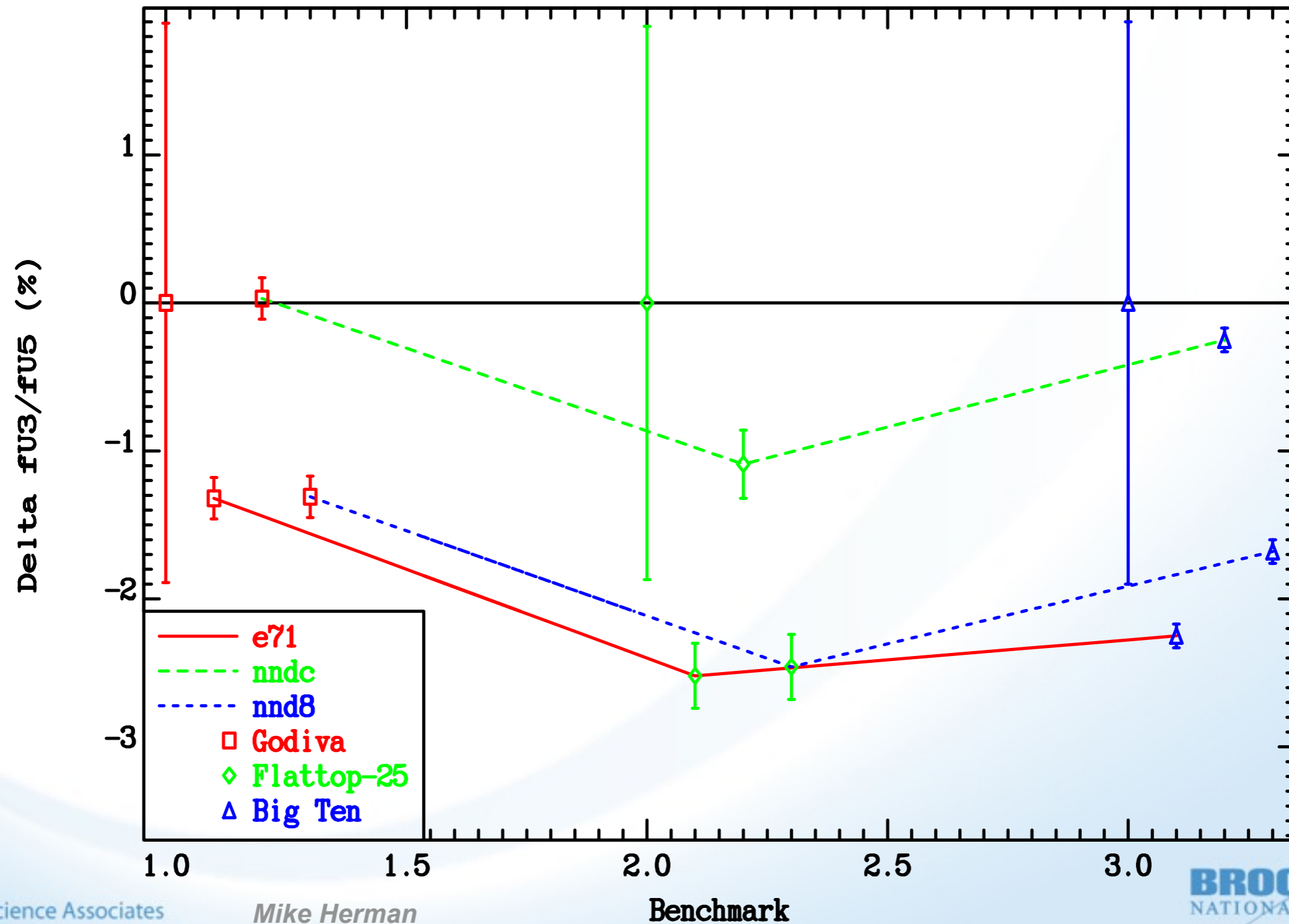
Benchmarking new priors for ^{235}U and ^{238}U

ICSBEP Benchmark Summary Results
Integral parameter intercomparison



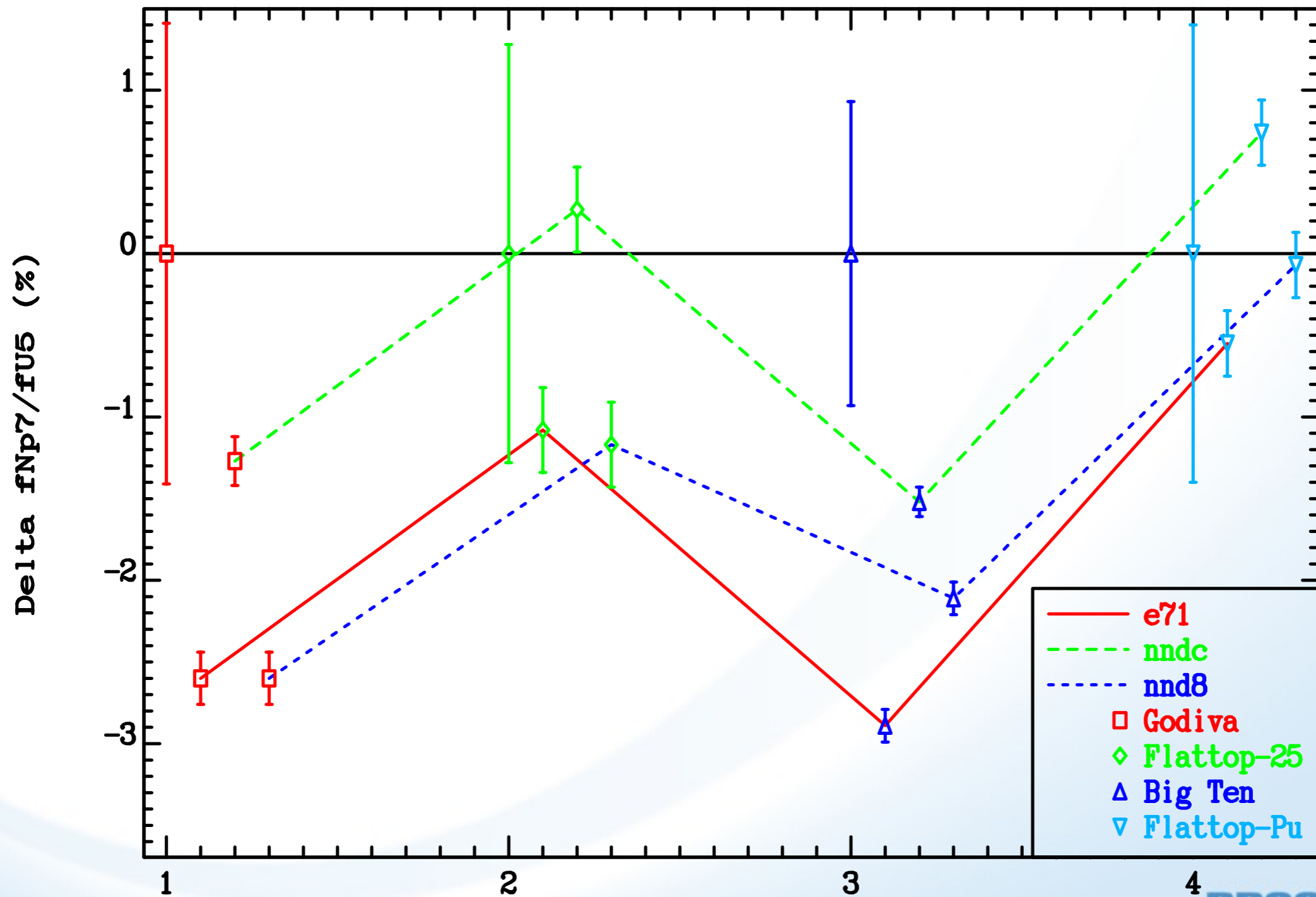
Benchmarking new priors for ^{235}U and ^{238}U

ICSBEF Benchmark Summary Results
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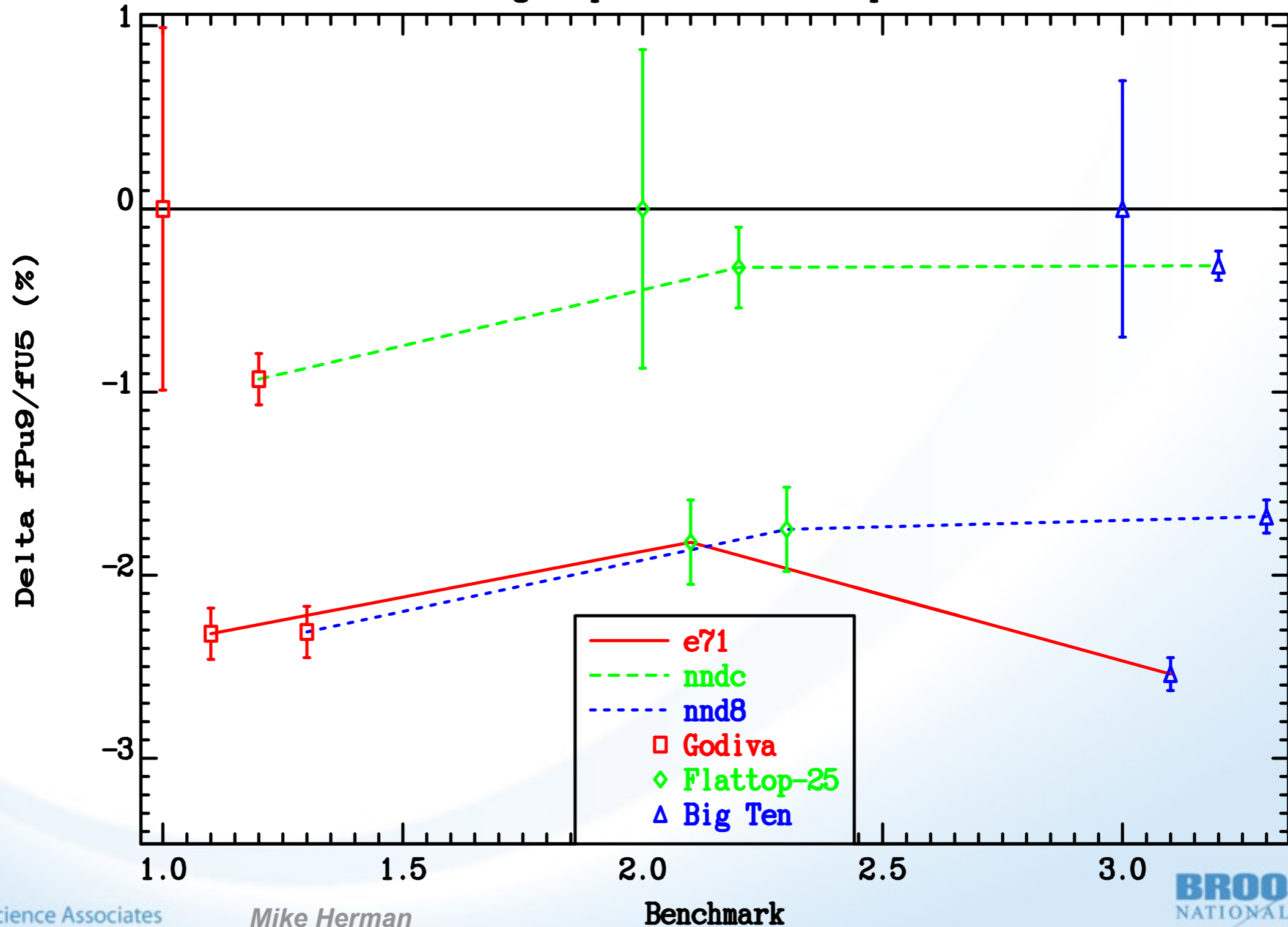
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Assimilation priors for ^{235}U and ^{238}U

- lesson learned

- Fully model based priors of a quality comparable to modern evaluations are possible!

Conclusions

- **Assimilation pitfalls**

- non-linearity
- fluctuations in cross sections
- selection of experimental data
- PPP
- anti-correlations driving parameters out of physical range

- **Assimilation prerequisites**

- realistic covariances and correlations among measurements
- good physics/modeling resulting in **good** prior
- realistic weighting of differential and integral experiments
- verity of experiments probing different aspects

- **Assimilation is feasible**

Conclusions

Changes much smaller than experimental cross section or model uncertainties are sufficient for a good prior to reproduce integral measurements. Thus:

- differential data based evaluation is unlikely to predict integral experiment within its precision
- integral data are not sufficient to turn a bad prior into a good one
- only all experimental information combined with the state of the art modeling may provide a right answer