Nuclear Data Parameter Adjustment BNL-INL

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November 29, 2013

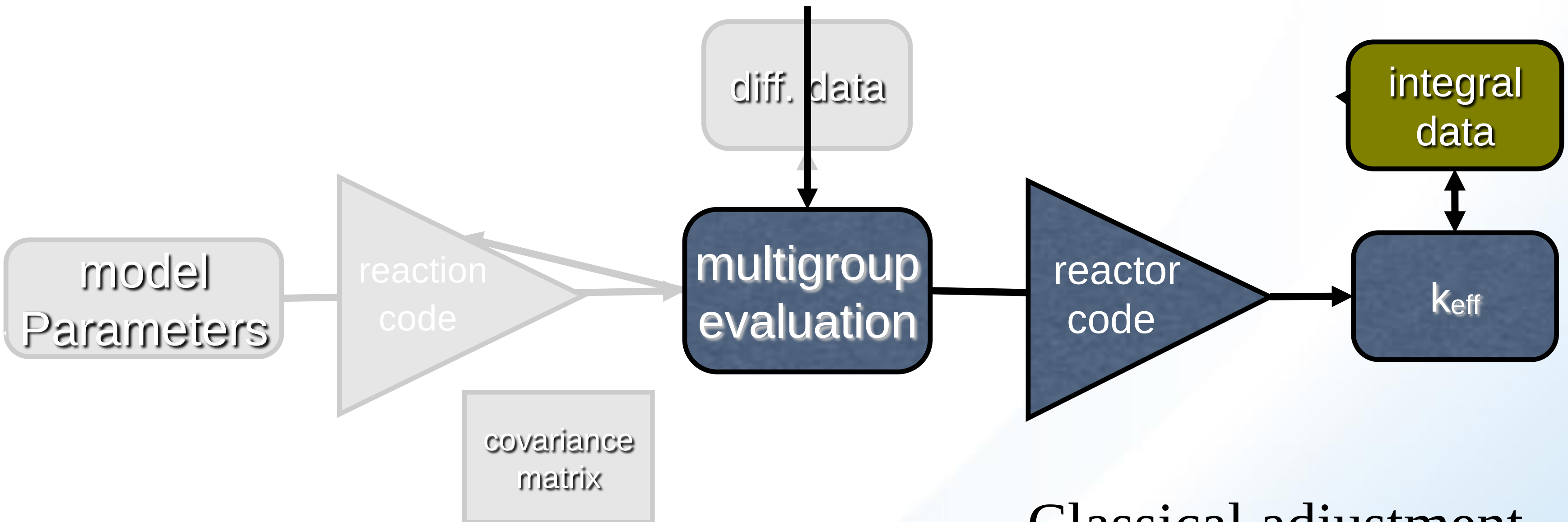
Introduction

- The major drawbacks of the classical adjustment method are related to the multigroup cross section approach. This implies several constraints:
  - potential limitation of the domain of application of the adjusted data
  - fixed energy multigroup structure
  - dependence on the neutron spectrum used as weighting function and the code used to process the basic data file
- The classical statistical adjustment method can be improved by “adjusting” reaction model parameters rather than multigroup nuclear data.
- The objective is now to correlate the uncertainties of some basic parameters that characterize the neutron cross section description, to the discrepancy between calculation and experimental value for a large number of clean, high accuracy integral experiments.

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

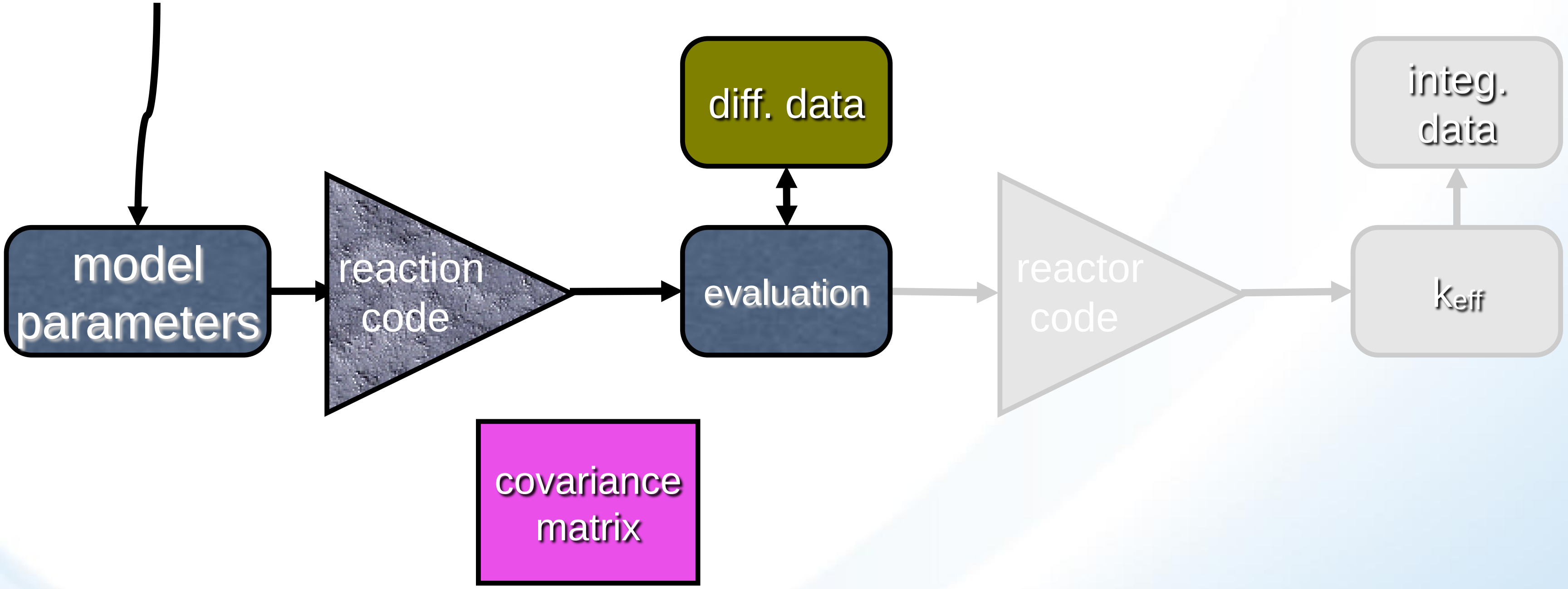


Classical adjustment

Consistent adjustment (assimilation)

linking reaction theory and integral experiments

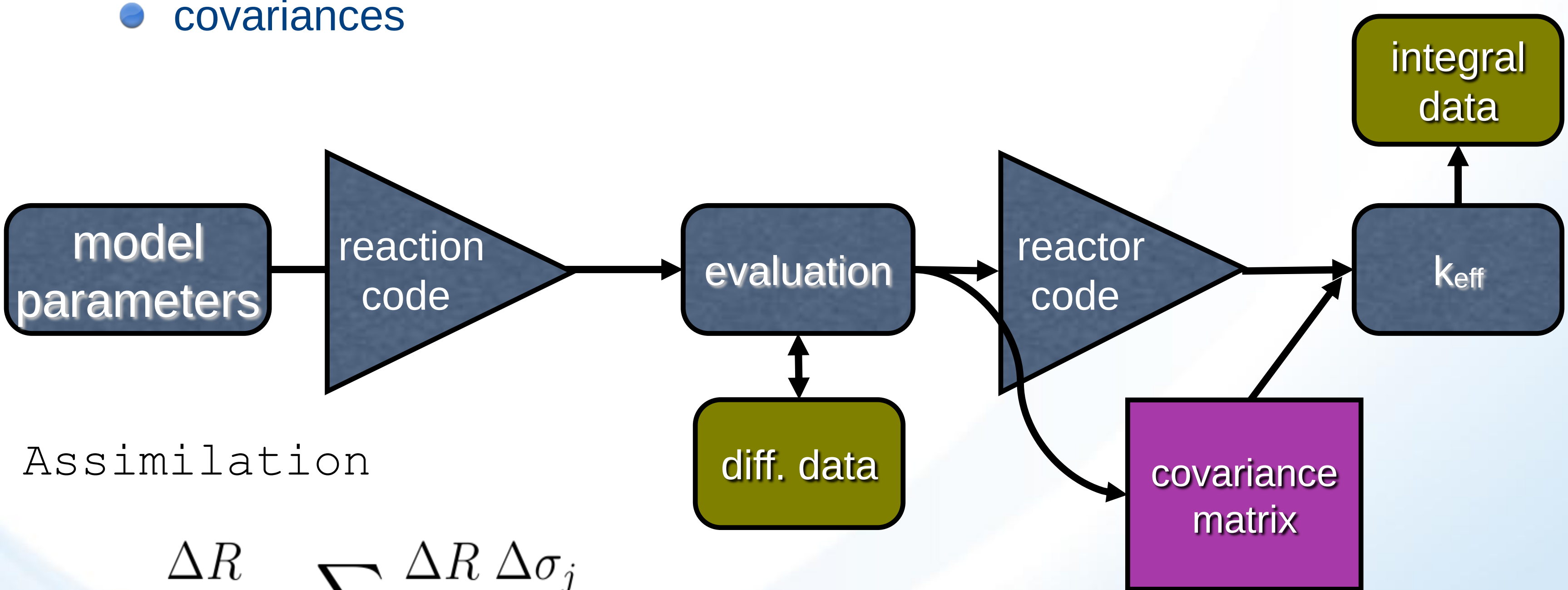
- Modern practice is to use nuclear reaction code constrained by experimental differential data to produce evaluations and covariances



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

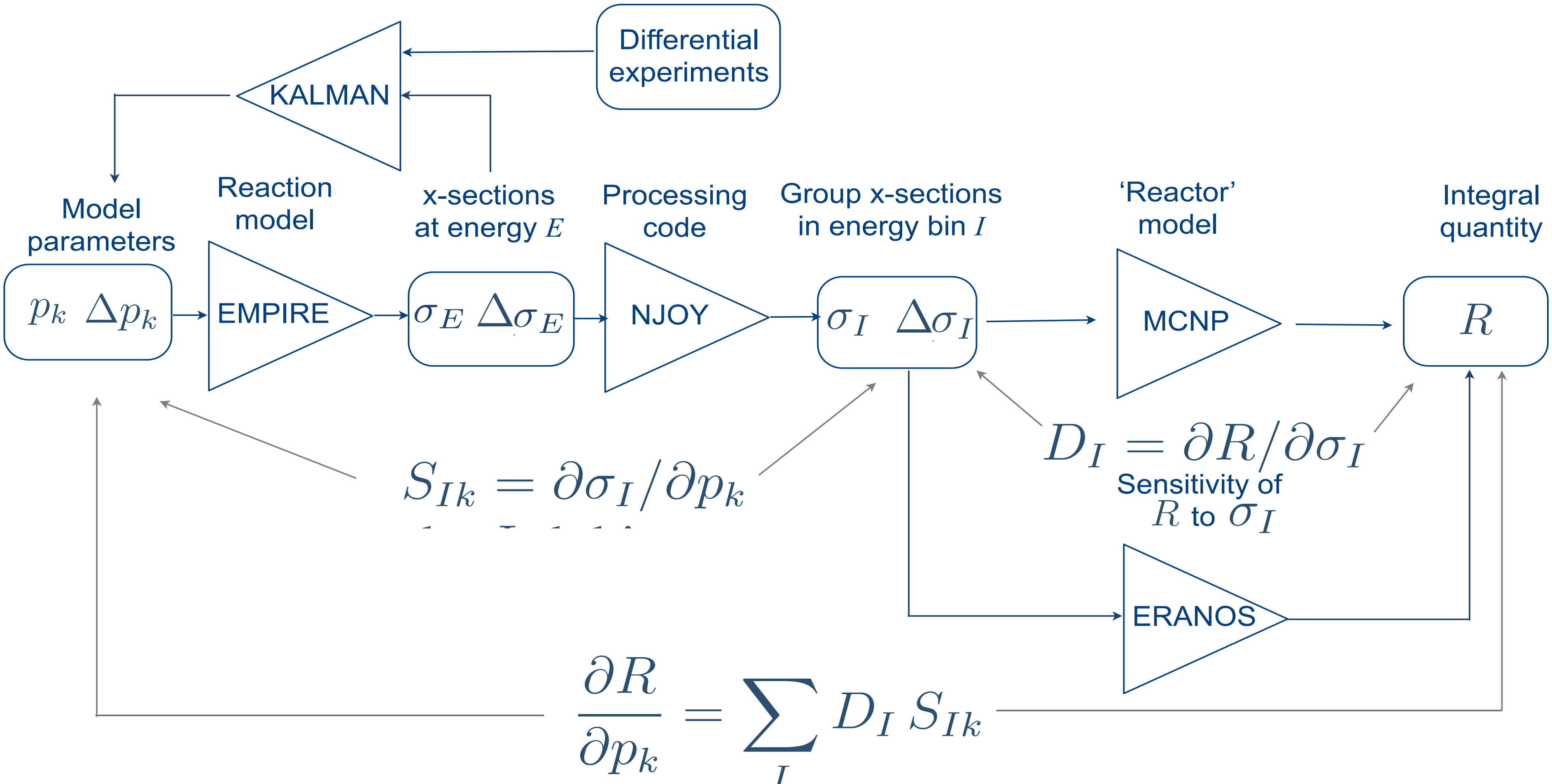


Assimilation

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

Consistent Data Assimilation

Linking integral experiments with reaction model parameters



S_{Ik} contains all restrictions imposed by differential data

Assimilation - consistent adjustment

- Benefits
  - Application independent (or less dependent) adjustment (no multi-group structure)
  - Correlations (x-experiment, x-materials, x-reactions)
  - Cohesion of integral and differential experiments and nuclear reaction theory
    - Better model parameters
    - More reliable (physics constrained) data

Requisites for assimilation

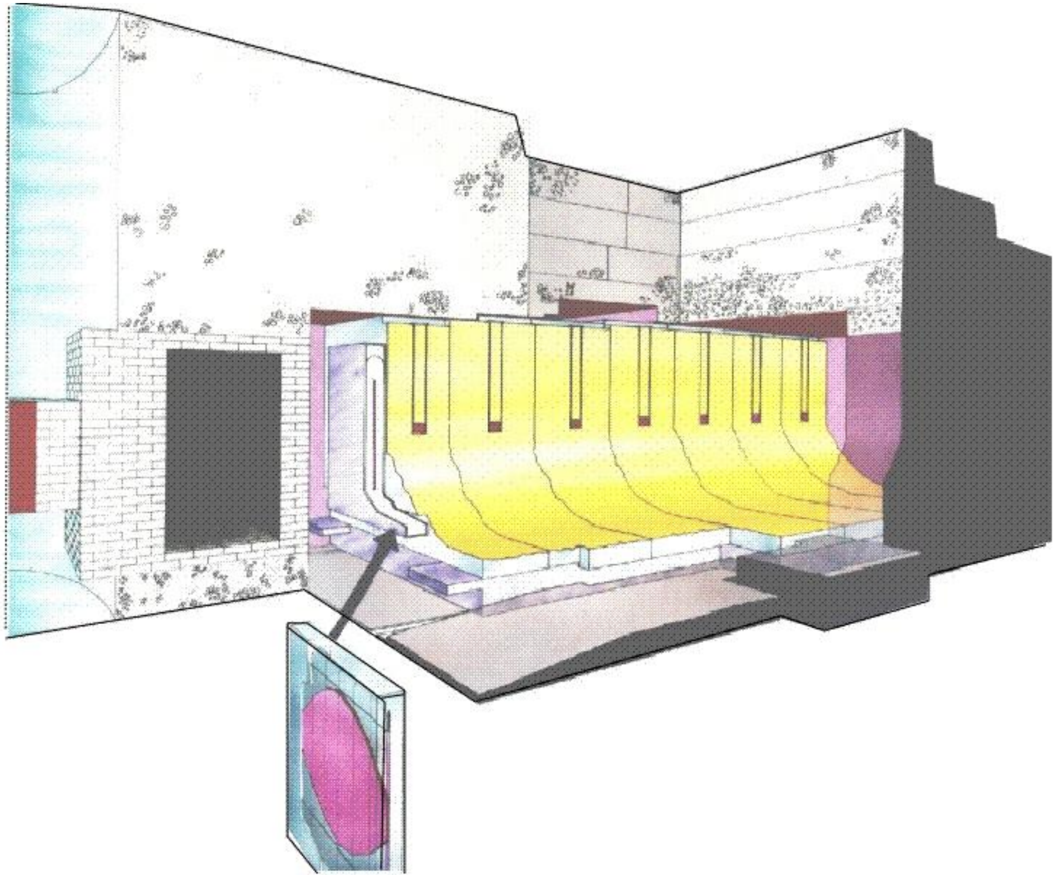
- Adequate set of reaction models
- Entire evaluation expressed in terms of model parameters
- Reaction model and its parameterization flexible enough to reproduce differential and integral data
- Clean, well defined, integral experiments possibly predominantly sensitive to a single material.

A few examples done up to now

- Investigate feasibility of the assimilation concept for priority materials
  - ^{23}Na - coolant
  - ^{56}Fe - structure material
  - ^{105}Pd - fission product
  - ^{235,238}U, ^{239}Pu - major actinides
  - ^{242}Pu - minor actinide
- Clean integral experiments available

Assimilation of ^{23}Na EURACOS

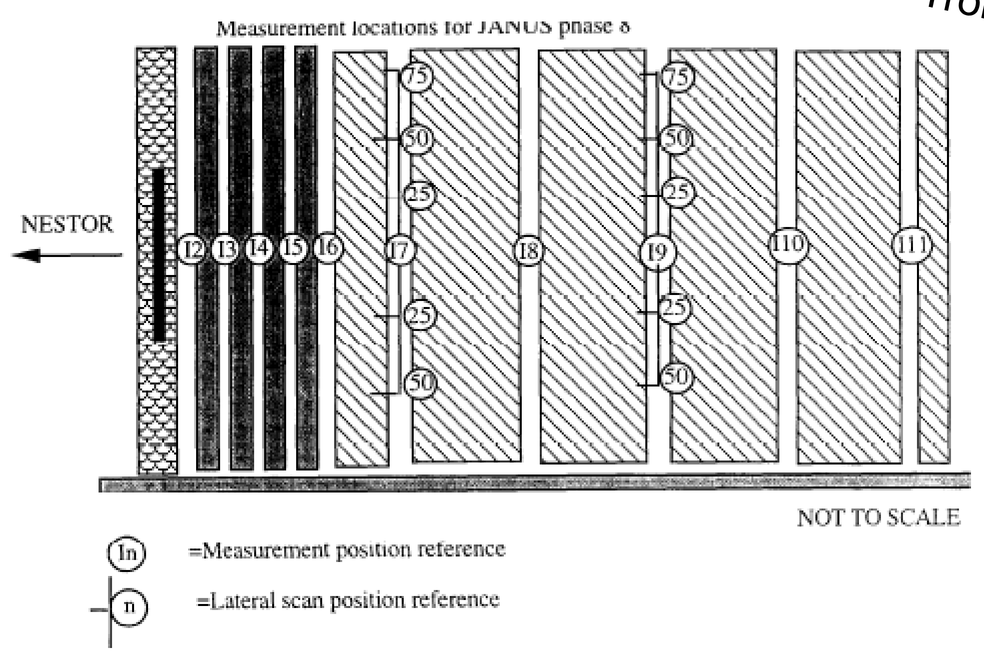
- The Ispra sodium benchmark project was performed under the EURACOS (Enriched URAnium COnverter Source) irradiation facility.
- Measurements with activation detectors were carried out at distances from the source for ^{32}S(n,p) and ^{197}Au (n,γ) in order to analyze fast and epithermal neutron attenuations.

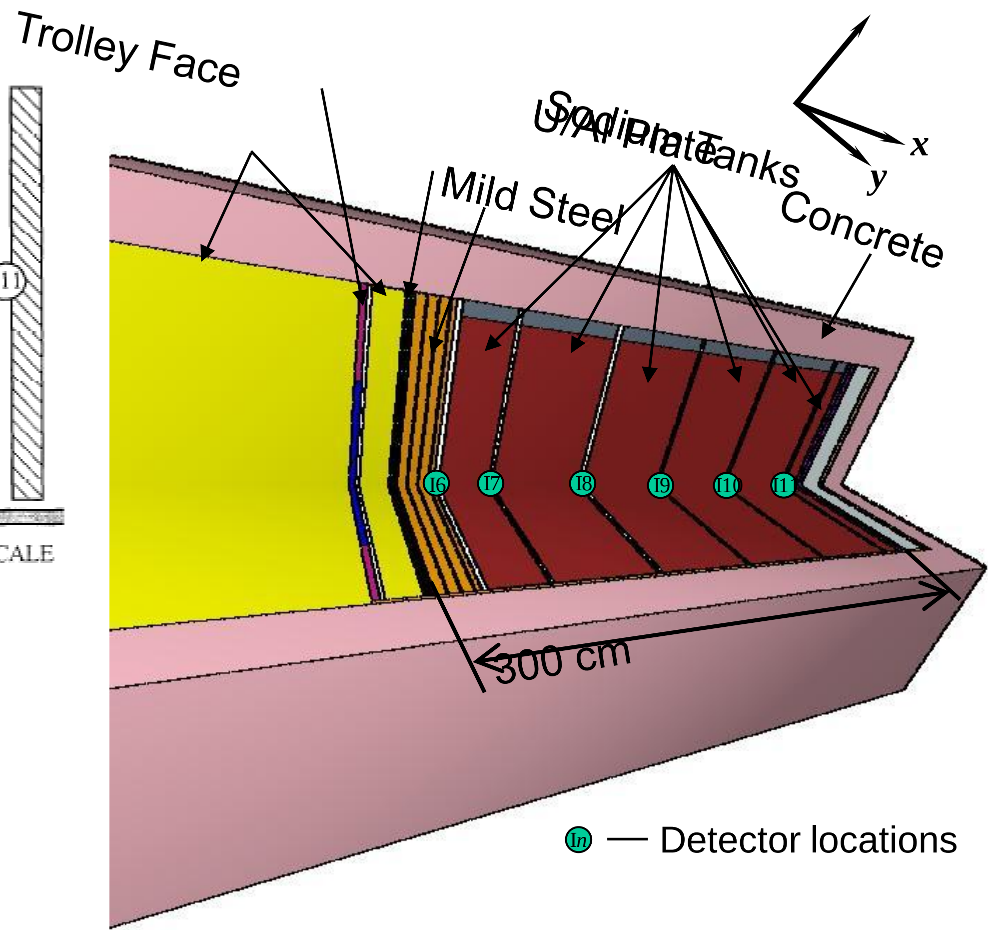


Assimilation of ^{23}Na

JANUS-8 Sodium Propagation Experiment

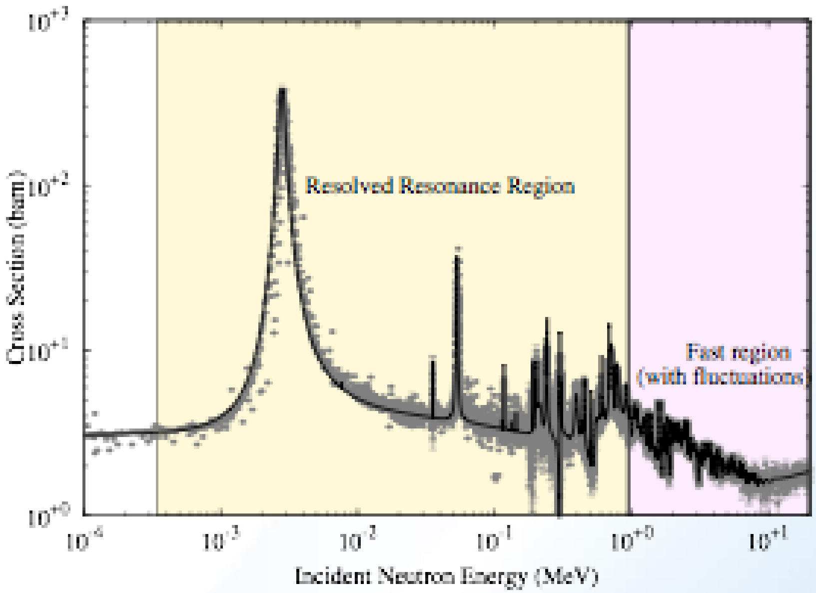
- The JANUS Phase 8 experiments were performed at the ASPIS facility.
- The neutron attenuations of several different detectors were analyzed and in particular for the following reaction rates: $^{32}S(n,p)^{32}P$, $^{103}Rh(n,n')^{103m}Rh$, $^{197}Au(n,\gamma)^{198}Au$, and $^{55}Mn(n,\gamma)^{56}Mn$.





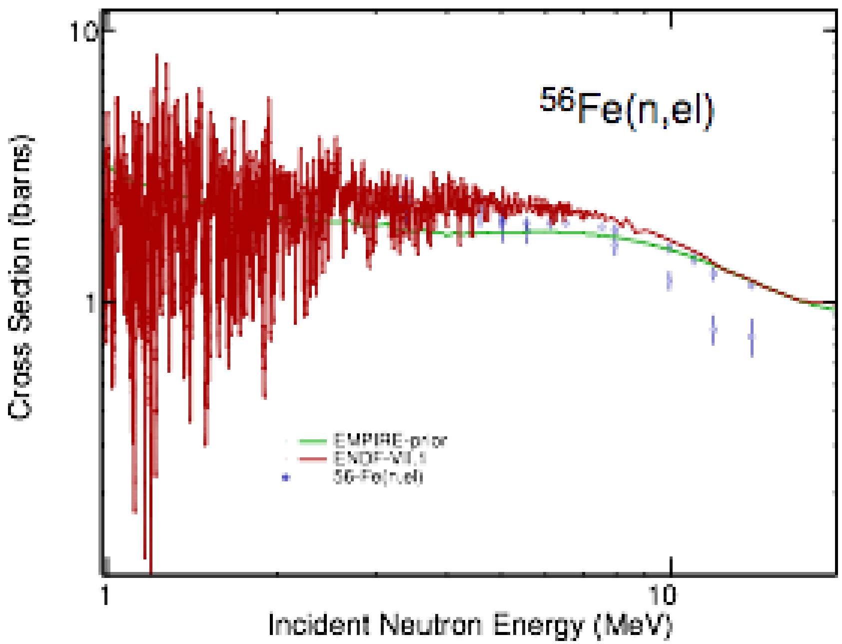
Assimilation of ^{23}Na

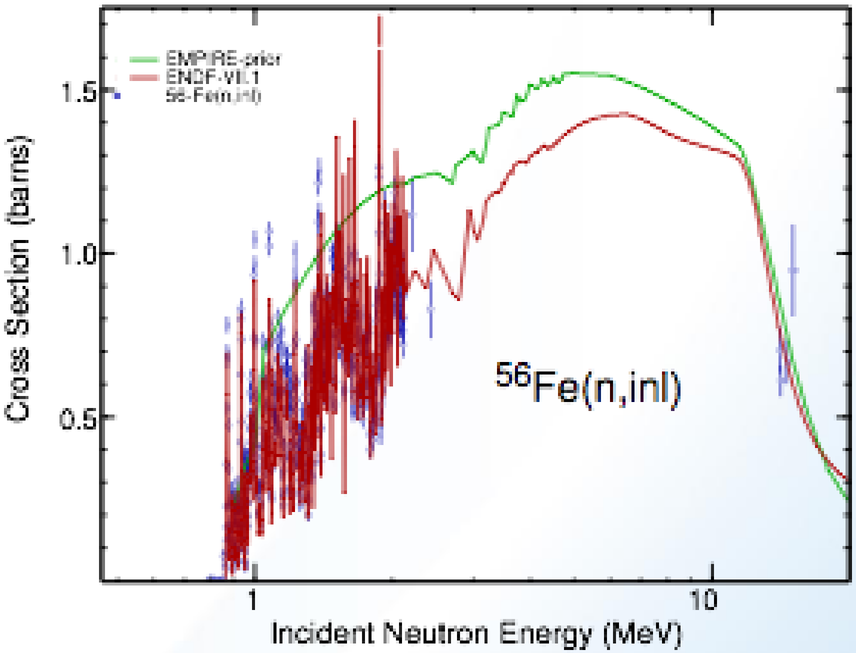
Detector	prior C/E	posterior C/E
EURACOS ^{32}S	0.770 ± 0.085	0.997 ± 0.057
EURACOS ^{197}Au	0.954 ± 0.102	0.946 ± 0.010
JANUS-8 ^{32}S	0.538 ± 0.022	1.000 ± 0.022
JANUS-8 ^{197}Au	1.010 ± 0.033	0.959 ± 0.028
JANUS-8 ^{55}Mn	1.158 ± 0.025	1.028 ± 0.023
JANUS-8 ^{103}Rh	0.960 ± 0.106	0.976 ± 0.047



- 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

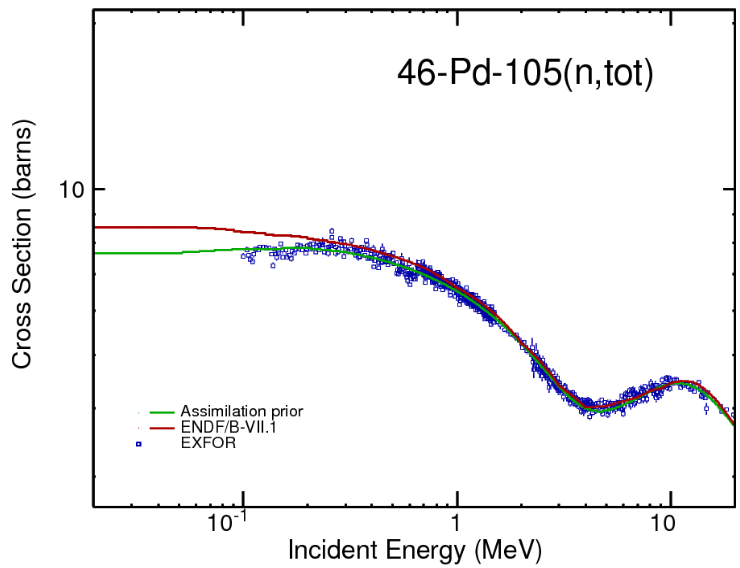
Experiment		C/E ± σ (before)	C/E ± σ (after)
^{10}B(n,α) slope	ZPR3-54	0.853 ± 0.030	1.012 ± 0.022
^{235}U(n,f) slope	ZPR3-54	0.907 ± 0.030	1.015 ± 0.013
^{239}Pu(n,f) slope	ZPR3-54	0.889 ± 0.030	0.996 ± 0.013
^{238}U(n,f) slope	ZPR3-54	1.455 ± 0.030	1.284 ± 0.014
^{32}S(n,p) slope	EURACOS	0.879 ± 0.093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

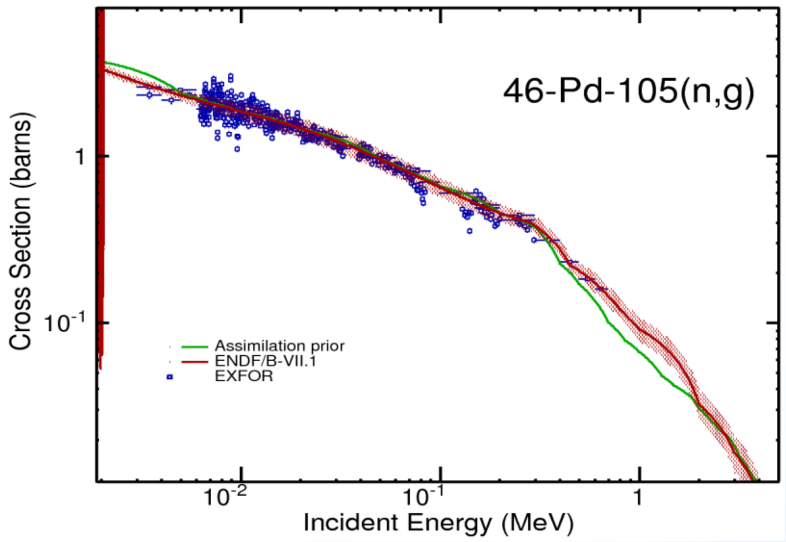
- Certain improvement achieved but VII.0 performs better
- Poor prior - better CC omp needed

^{56}Fe lesson learned

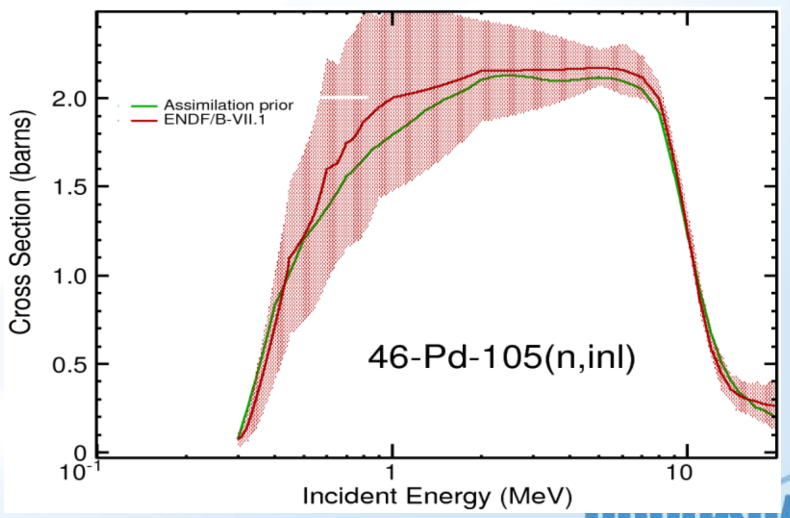
- Integral experiments alone do not ensure restoring agreement with differential data if the prior is of poor quality.
- A practical, necessarily approximative, method should be developed for treating fine energy fluctuations that can't be treated in terms of the reaction theory
- Possible discrepancies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

Assimilation of ^{105}Pd

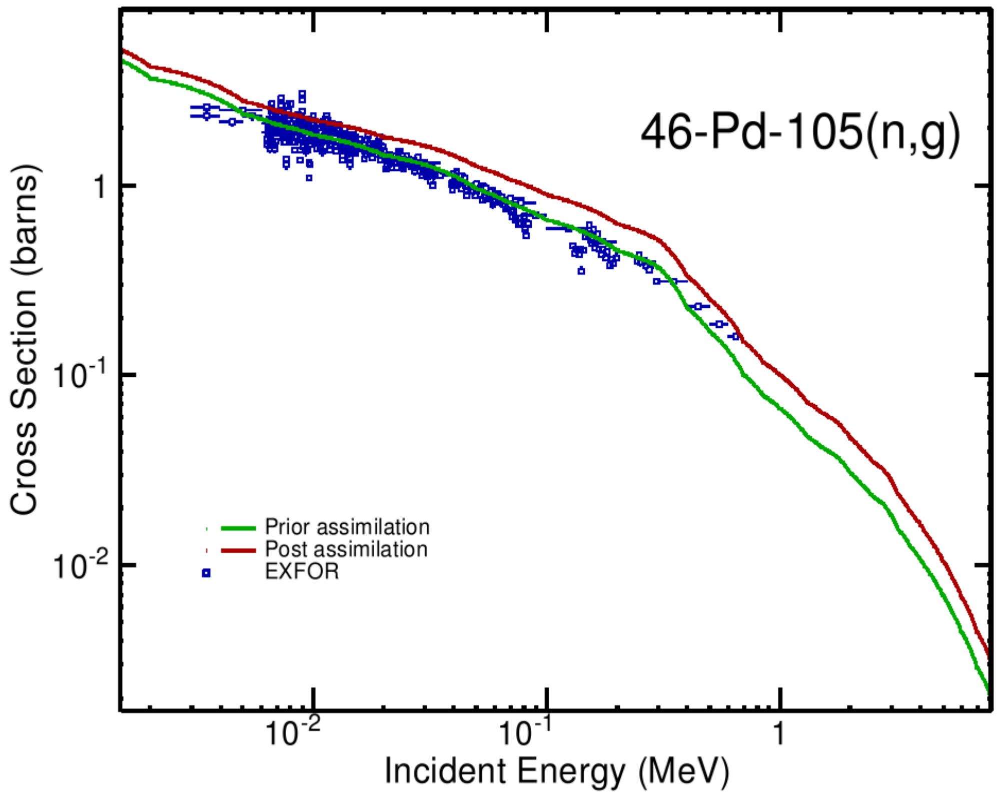




- Pretty good prior
- Integral experiment PROFIL-1 sensitive to capture -> should be easy!



^{105}Pd - assimilation results



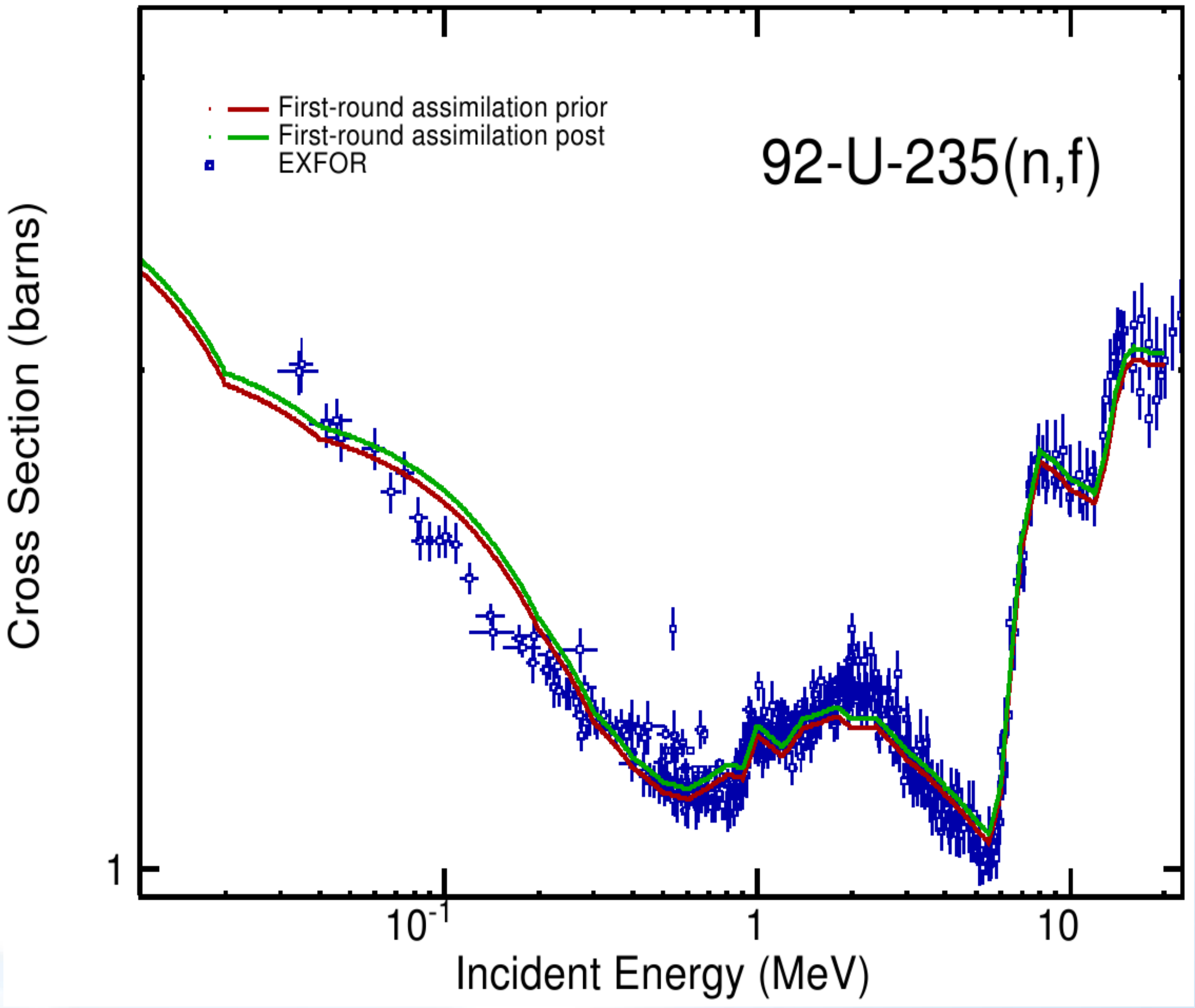
- posterior disagrees with differential data
- differential and integral experiments discrepant

Assimilation concept worked! However, 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 beyond 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.

^{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_{eff}=1 was obtained by scaling fission cross sections regardless of differential data.

- More integral experiments with diverse characteristics should help.

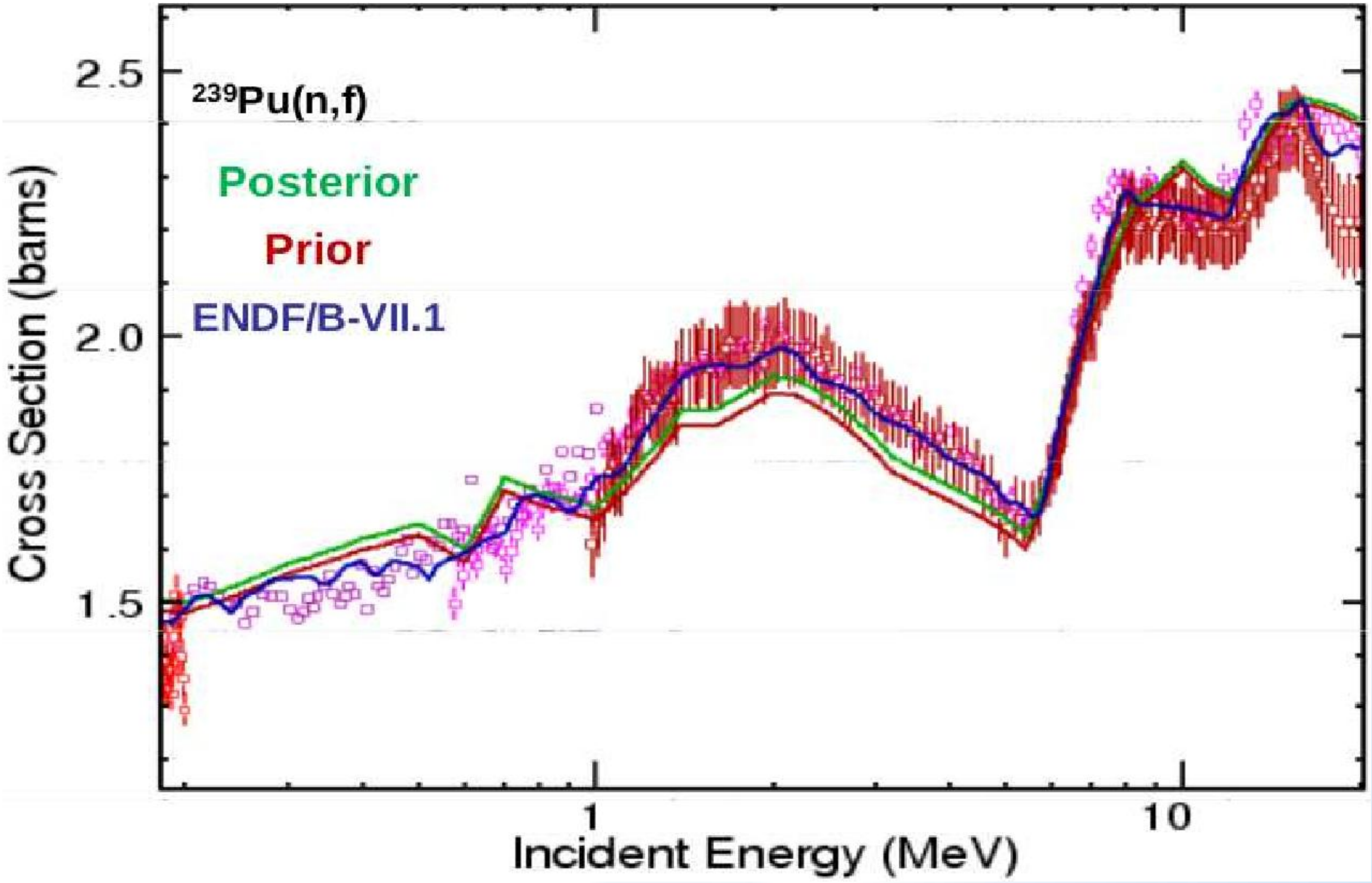
Assimilation of ^{239}Pu (1st round)

JEZEBEL

Experiment	prior C/E $\pm\ \sigma$	post C/E $\pm\ \sigma$
k_{eff}	0.9857 ± 0.002	$0..9998 \pm 0.002$
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}U/^{235}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
DELTAF000[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

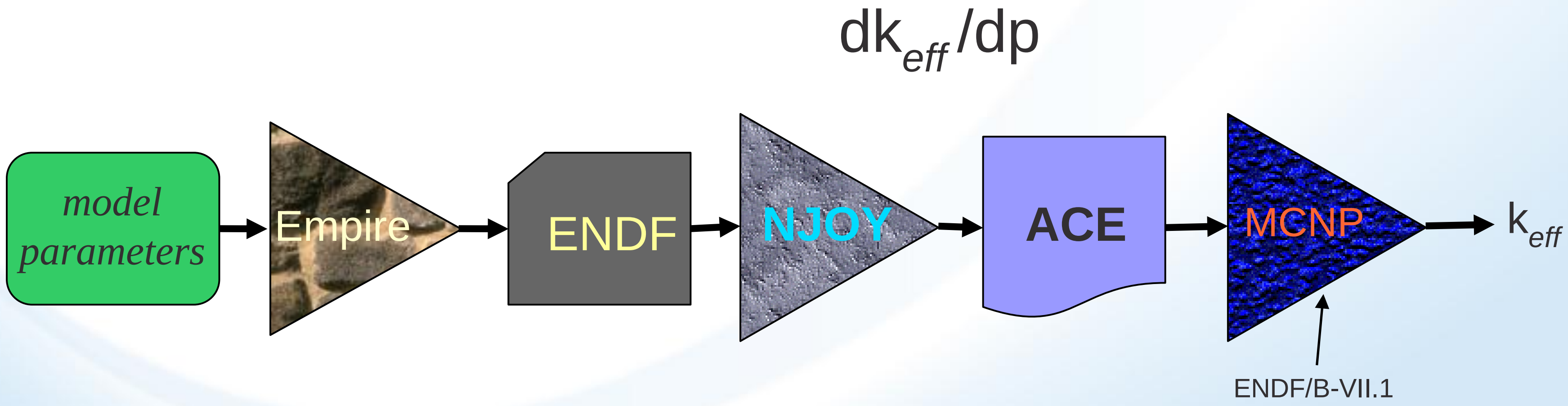
Assimilation distributed over several parameters

^{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 k_{eff} using MCNP performed at BNL.



^{239}Pu direct 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

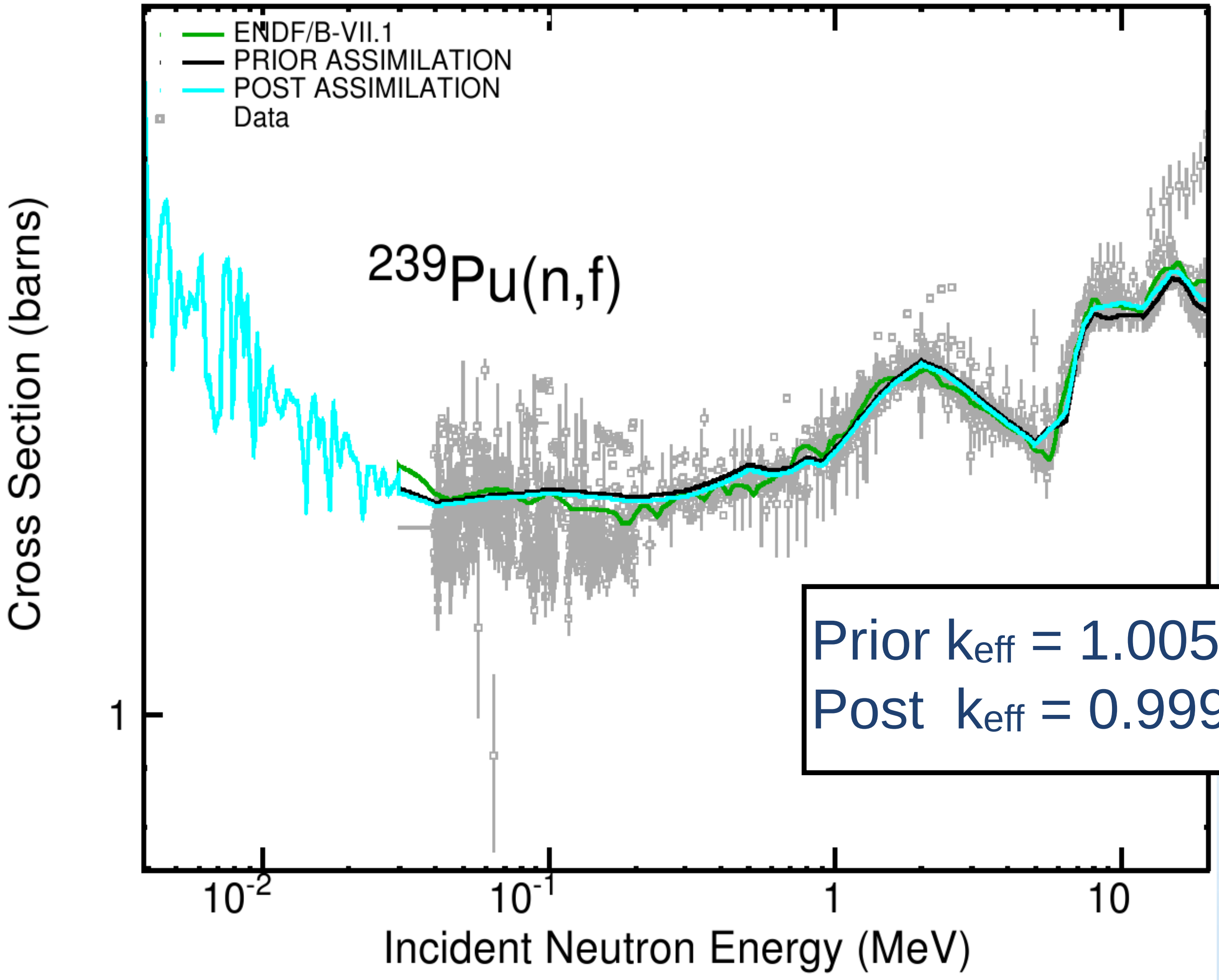
^{239}Pu direct assimilation covariance matrix

	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	-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	65	100		
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	1	0	-1	0	-65	-1	100	
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	1	0	-1	0	-24	44	88	100

PFNS

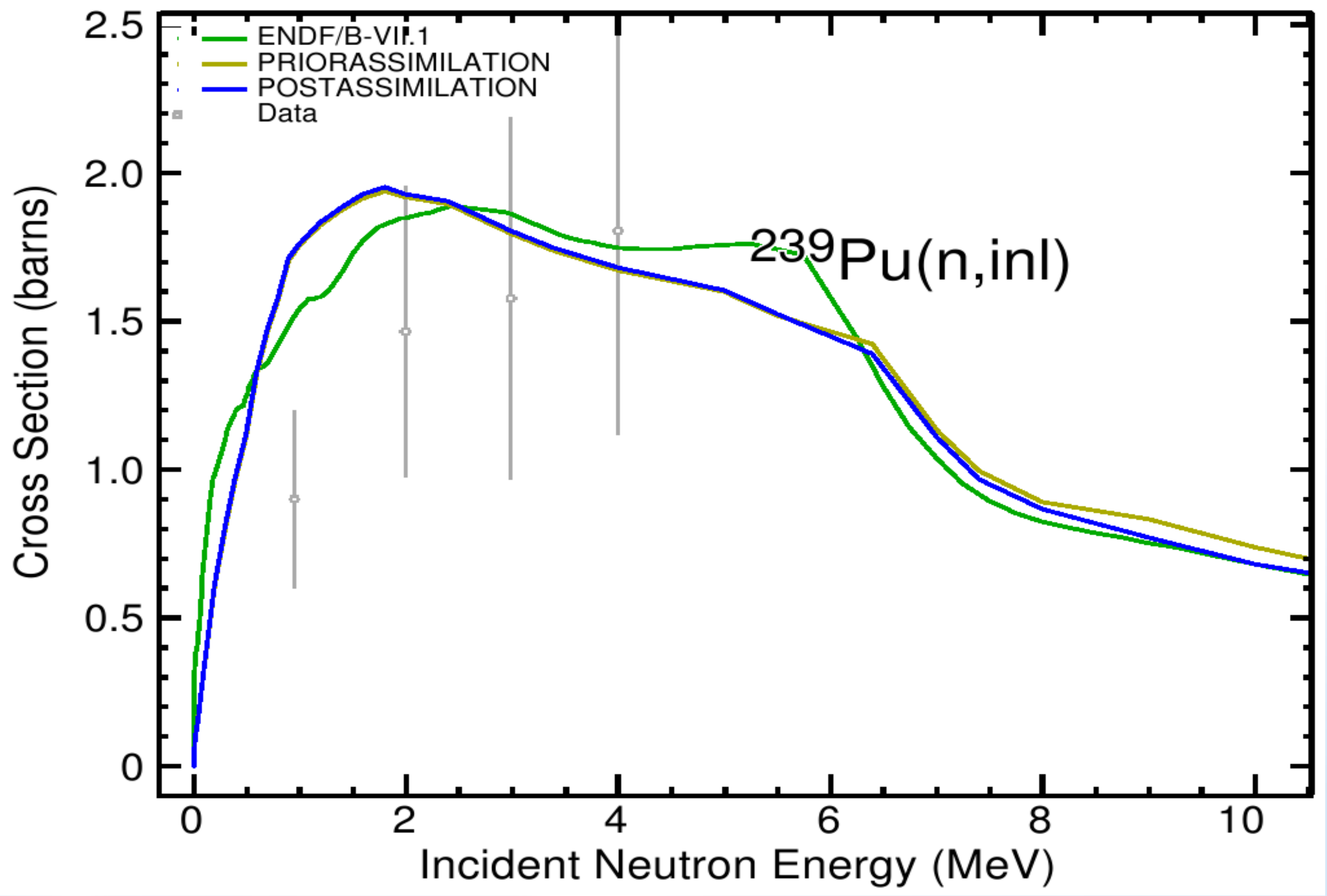
Little correlations between PFNS and x-sec parameters

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



Prior k_{eff} = 1.00516 (8)
Post k_{eff} = 0.99959 (8)

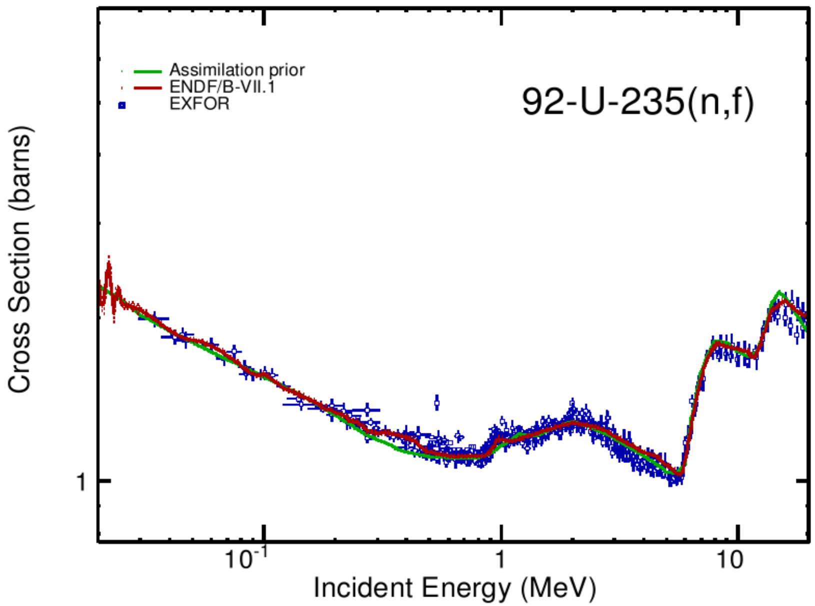
^{239}Pu (2nd round) - assimilated inelastic

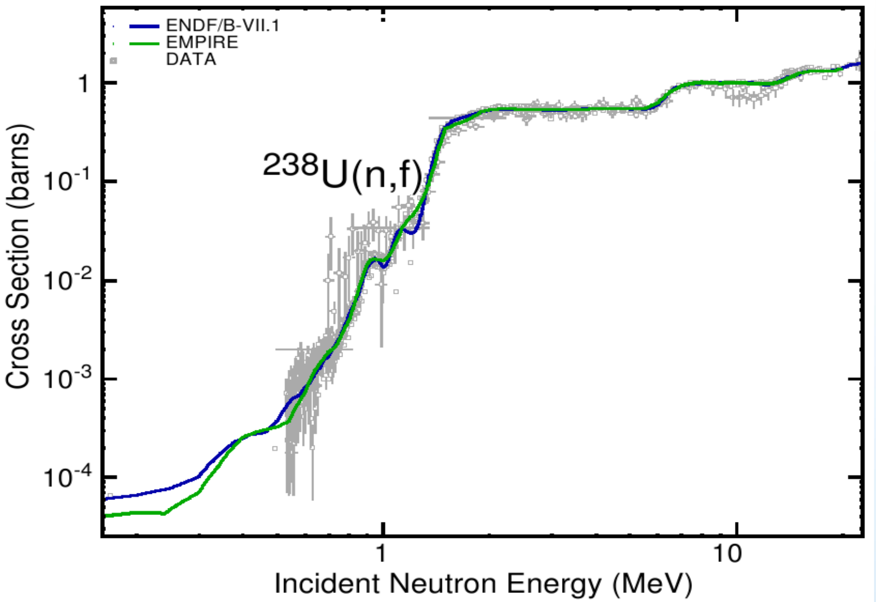


^{239}Pu (2nd round) - lesson learned

- Successful assimilations when starting with good prior
- Reduction of uncertainties in the model parameters and consequently also in the calculated integral result
- Little correlation between cross section & PFNS parameters

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





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

Multi-isotope assimilation

- Combine multiple integral experiments with sensitivities to multiple materials. The resulting assimilation should satisfy both differential and integral experiments and provide important cross-material covariances.

Integral Exp	^{235}U	^{238}U	^{239}Pu
FLATTOP-239		X	X
FLATTOP-HEU	X	X	
JEZEBEL-239			X
GODIVA	X		

- Preliminary results look promising – more work needed.

Conclusions

- Assimilation pitfalls
  - non-linearity
  - fluctuations in cross sections
  - selection of experimental data
  - 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
  - variety 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 ---

- purely differential data based evaluation is unlikely to reproduce 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