First results on assimilation of major actinides

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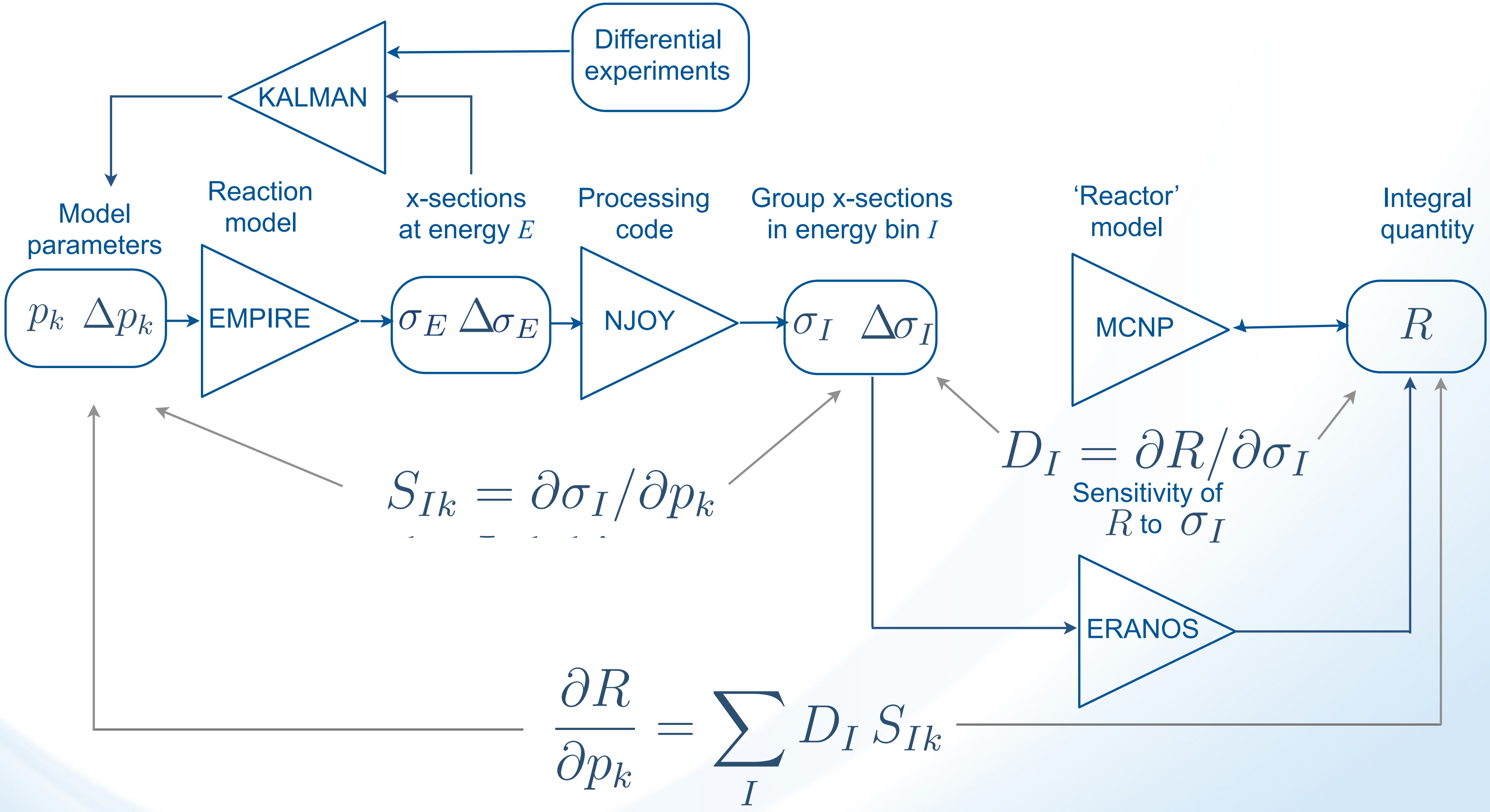
Assimilation
Linking integral experiments with reaction model parameters



Differential experiments

KALMAN

Model parameters

Reaction model

x-sections at energy E

Processing code

Group x-sections in energy bin I

'Reactor' model

Integral quantity

$p_k \ \Delta p_k$

EMPIRE

$\sigma_E \ \Delta\sigma_E$

NJOY

$\sigma_I \ \Delta\sigma_I$

MCNP

R

$$S_{Ik} = \partial\sigma_I/\partial p_k$$

$$D_I = \partial R/\partial\sigma_I$$

Sensitivity of R to σ_I

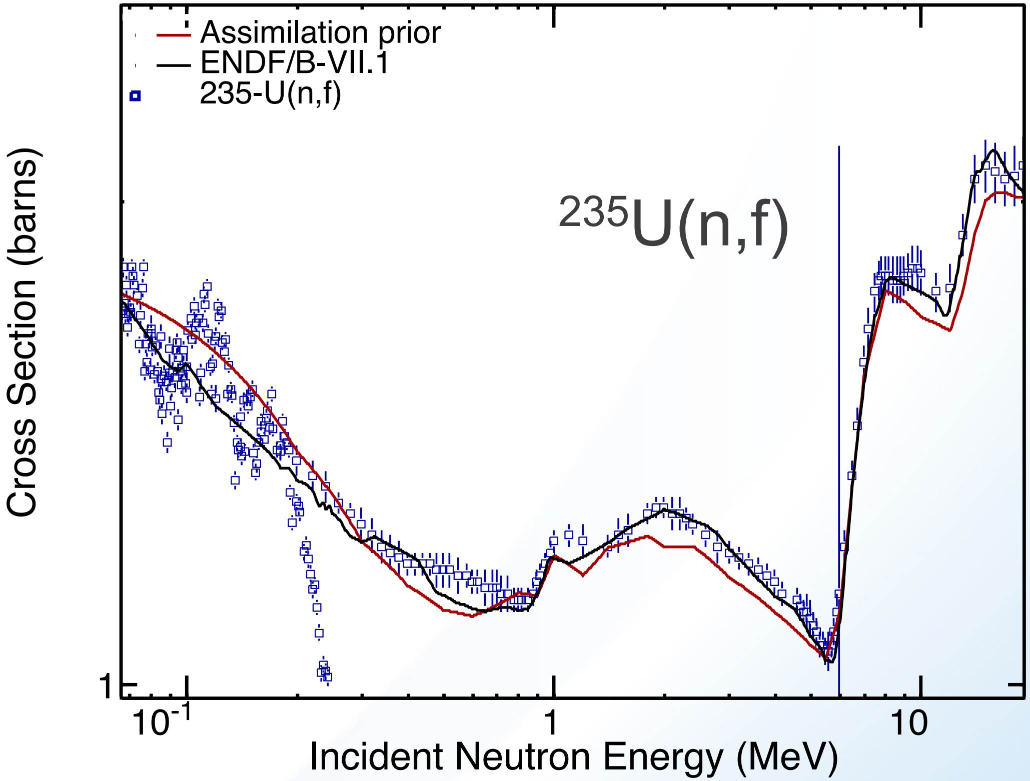
ERANOS

$$\frac{\partial R}{\partial p_k} = \sum_I D_I \, S_{Ik}$$

Using S_{Ik} differential exp. data, and Kalman filter ==> $\langle\Delta p_k \, \Delta p_\ell\rangle$ covariance matrix, which contains constraints imposed by microscopic exp. data.

^{235}U assimilation starting point (prior)

- EMPIRE calculations
  - EGSM lev. den.
  - CC with RIPL #2408
    4 coll. lev. & 76 in continuum
  - Exciton model
  - E1 strength MLO1
  - OM for fission
  - Fission barriers RIPL1
- Roughly adjusted parameters but **no** energy-dependent tuning!
- PFNS and nu-bars from VII.1



- Input to INL
  - central values in 33 energy groups
  - group-wise sensitivity matrices for 50 parameters (no PFNS & nu-bars!)
  - parameter covariance matrix

Performance of the prior file

k_{eff} results (experimental k_{eff} =1.0 (±100~300pcm))

Experiment	EMPIRE (±pcm)	ENDF/B–VII.0 (±pcm)
JEZEBEL–239	0.98567 (±8)	0.99986 (±9)
GODIVA	0.99072 (±9)	0.99983 (±9)
FLATTOP–Pu	0.98838 (±18)	1.00097 (±18)
FLATTOP–25	1.00182 (±17)	1.00217(±17)

C/E ratio of spectral indices at the center of JEZEBEL–239 and GODIVA

	JEZEBEL–239		GODIVA	
	EMPIRE	ENDF/B–VII.0	EMPIRE	ENDF/B–VII.0
$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	0.956±0.009	0.974±0.009	1.053±0.013	0.954±0.012
$\sigma_f(^{233}U)/\sigma_f(^{235}U)$	1.000±0.017	0.986±0.017	0.996±0.019	0.987±0.019
$\sigma_f(^{237}Np)/\sigma_f(^{235}U)$	0.999±0.017	1.009±0.017	1.070±0.017	0.990±0.016
$\sigma_f(^{239}Pu)/\sigma_f(^{235}U)$	0.971±0.020	0.984±0.020	0.992±0.018	0.986±0.018

Assimilation of the ^{235}U data

C/E for GODIVA

Experiment	old C/E ± σ	new C/E ± σ
K_{eff}	0.9907 ± 0.002	1.0010± 0.002
Fis.^{238}U/Fis.^{235}U	1.0527 ± 0.013	1.0357 ± 0.004
Fis.^{239}Pu/Fis.^{235}U	0.9917 ± 0.018	0.9771 ± 0.003
Fis.^{237}Np/Fis.^{235}U	1.0703 ± 0.017	1.0536 ± 0.003
Fis.^{233}U/Fis.^{235}U	0.9964 ± 0.019	0.9820± 0.004

Parameter variations and standard deviations obtained by data assimilation

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
FUSRED [a)]	1.402	1.257	0.878
TOTRED [b)]	0.461	0.966	0.917
ATILNO [c)]	-0.236	0.950	0.946
DELTAF [d)]	-0.025	0.649	0.621
VB0 [e)]	-0.006	0.133	0.118
UOMPVV101 [f)]	0.033	0.116	0.116
UOMPRS101 [g)]	0.072	0.834	0.834
UOMPWS101 [h)]	-0.110	2.023	2.022
TUNE000000 [i)]	-0.099	1.908	1.908

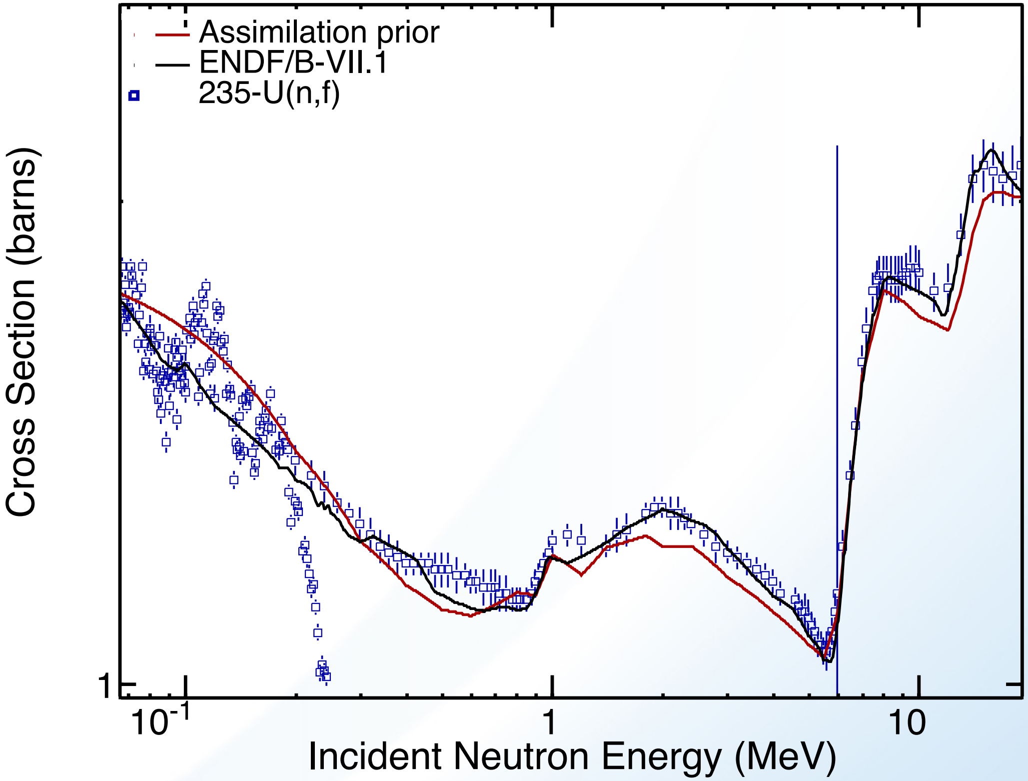
[a)] Factor multiplying the reaction (fusion, absorption, compound nucleus formation) cross section, [b)] Factor multiplying total cross section, [c)] Asymptotic level density parameter in Compound Nucleus, [d)] Pairing energy in the level densities at the saddle point in Compound Nucleus (first chance fission), [e)] Hight of the second hump in the fission barrier in Compound Nucleus, [f)] Real depth of the Optical Model potential for n + target, [g)] Surface imaginary Optical Model potential radius for n + target, [h)] Surface imaginary Optical Model potential depth for n + target, [i)] Factor on the gamma emission width in Compound Nucleus (scales capture).

Verification - EMPIRE/MCNP calculations using posterior parameters

k_{eff} C/E for GODIVA

	prior **C/E ± σ**	**posterior** **C/E ± σ**
INL	0.9907 ± 0.002	1.0010± 0.002
BNL	0.98418 ± 0.00008	0.99526 ± 0.00008

INL and BNL calculations show ~1000 pcm improvement in spite of the difference in the starting values.



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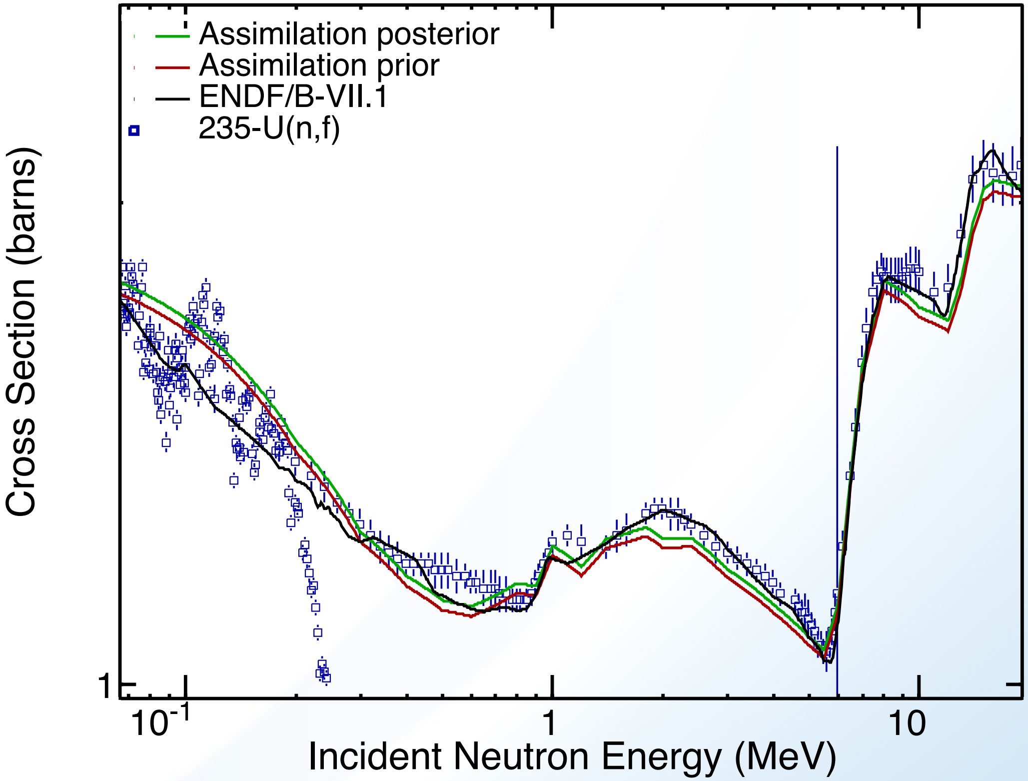

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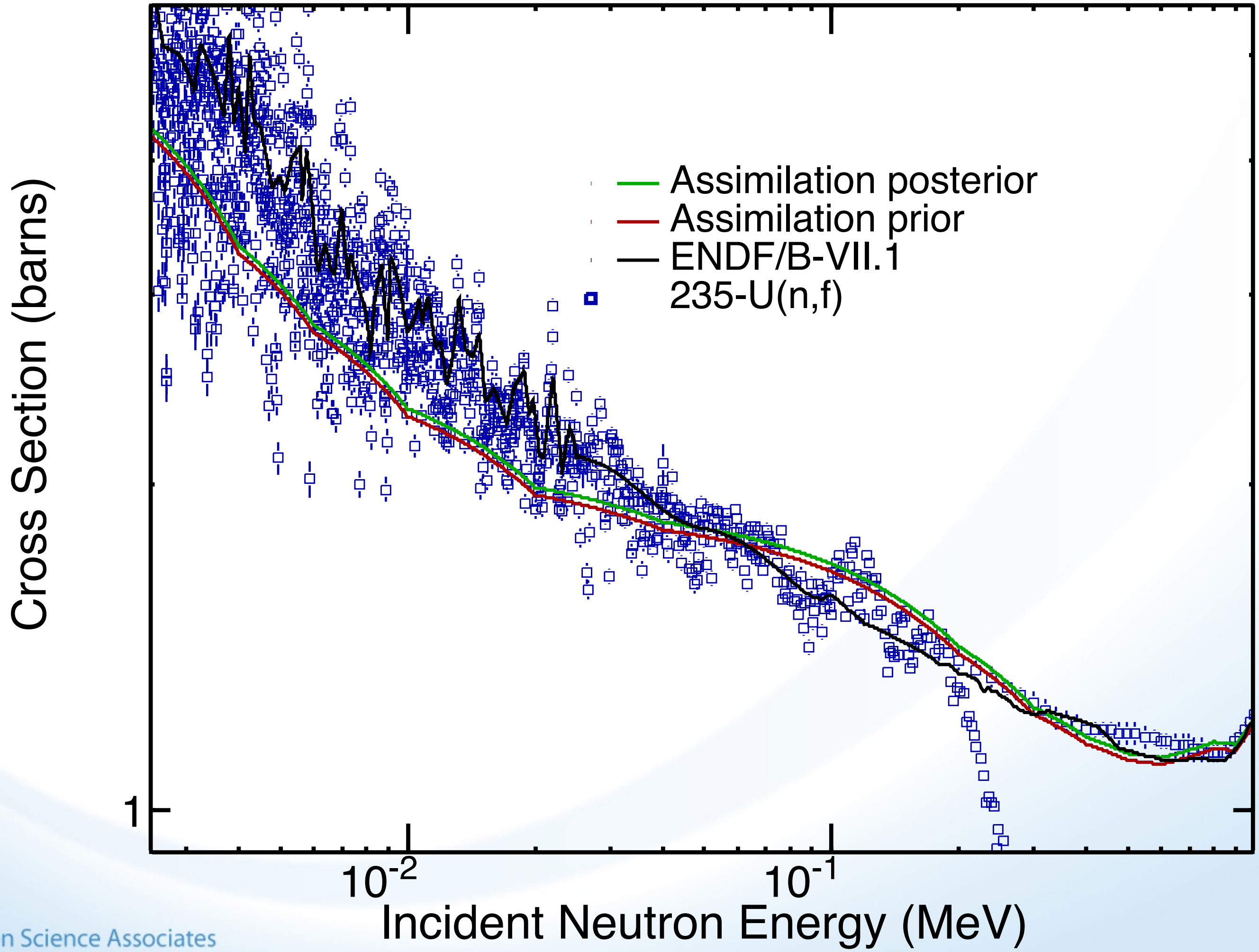

Further developments

- Better ‘a priori’ calculations
- Developing PFNS capabilities in EMPIRE
- Allowing variations of PFNS and nu-bars
- Allowing variations of resonance parameters
- Including more integral experiments

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 predominantly sensitive to a single material.

Conclusions

- Assimilation is feasible!
- Very small changes in cross sections can be enough to fix k_{eff}
- Pretty 'bad' cross sections can still produce reasonable k_{eff}, i.e., integral data should not overwrite differential data, lot of space for error compensation
- Non-linearity must be kept under control
- Advantages of consistent assimilation over Total MC
  - provides better insight into physics (sensitivities)
  - does not make 'unnecessary violence' to the parameters
  - calculation time - can be used for multi-material and multi-experiment adjustment
- Total MC advantages
  - not affected by non-linearity issues
  - can be used to find other local minima