Establishment of best practices in reducing uncertainty of neutron cross-sections with Bayesian methods

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Presentation plan

- Accuracy limits of direct experimental measurements of neutron cross-sections
- What is the point of knowing neutron cross-sections accurately?
- Data assimilation
- Bayesian statistics algorithms
- Good practices in Bayesian statistics
- Summary

What is a neutron cross section?

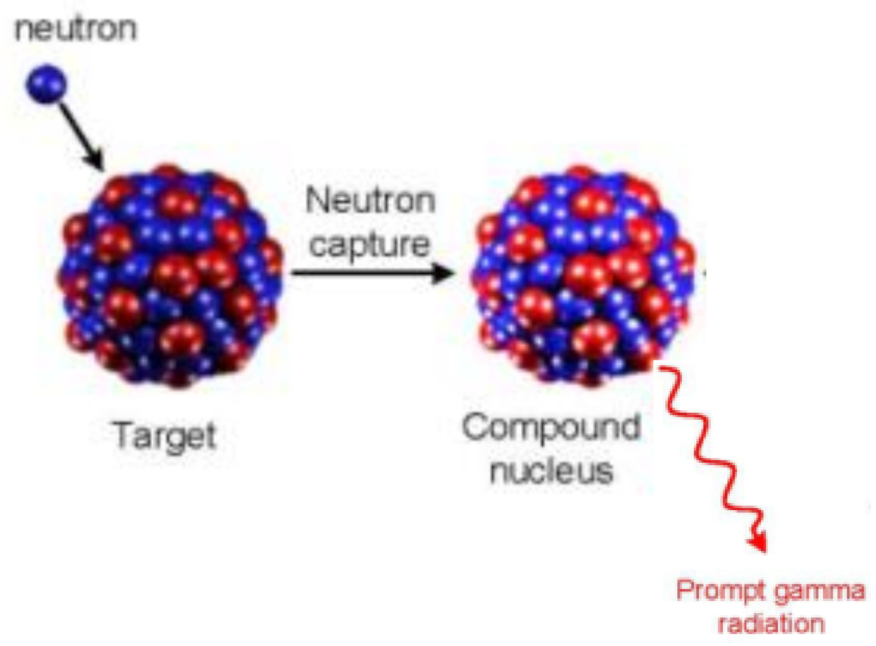
It is a measure of probability for a reaction between neutron and nucleus. Unit: 1 barn = 10^(-24)cm^2

Some of other reaction types:

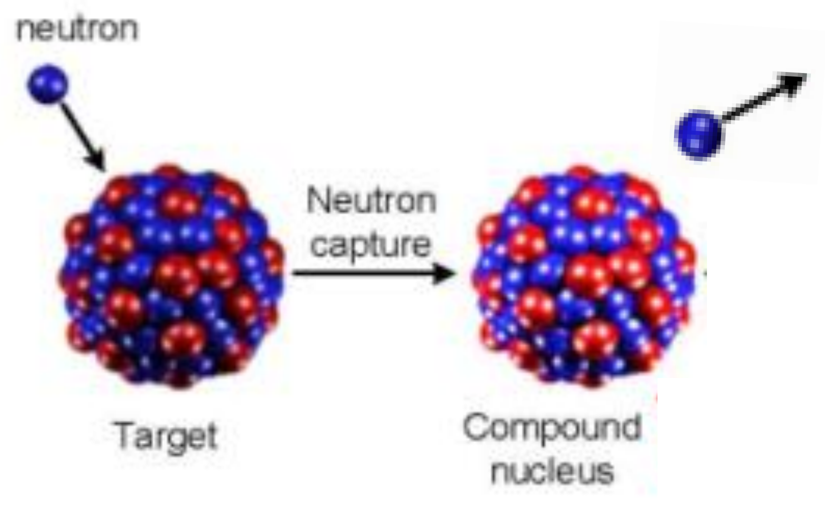
- n, 2n
- n, alfa

Some of reaction types:

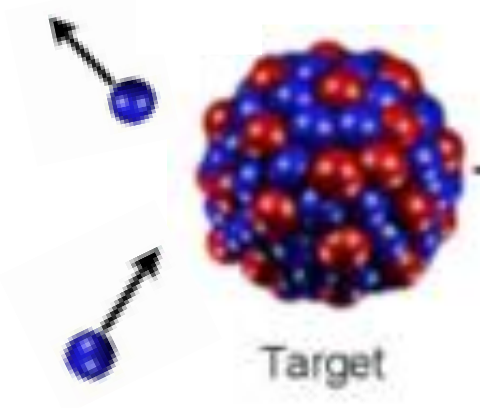
n, gamma



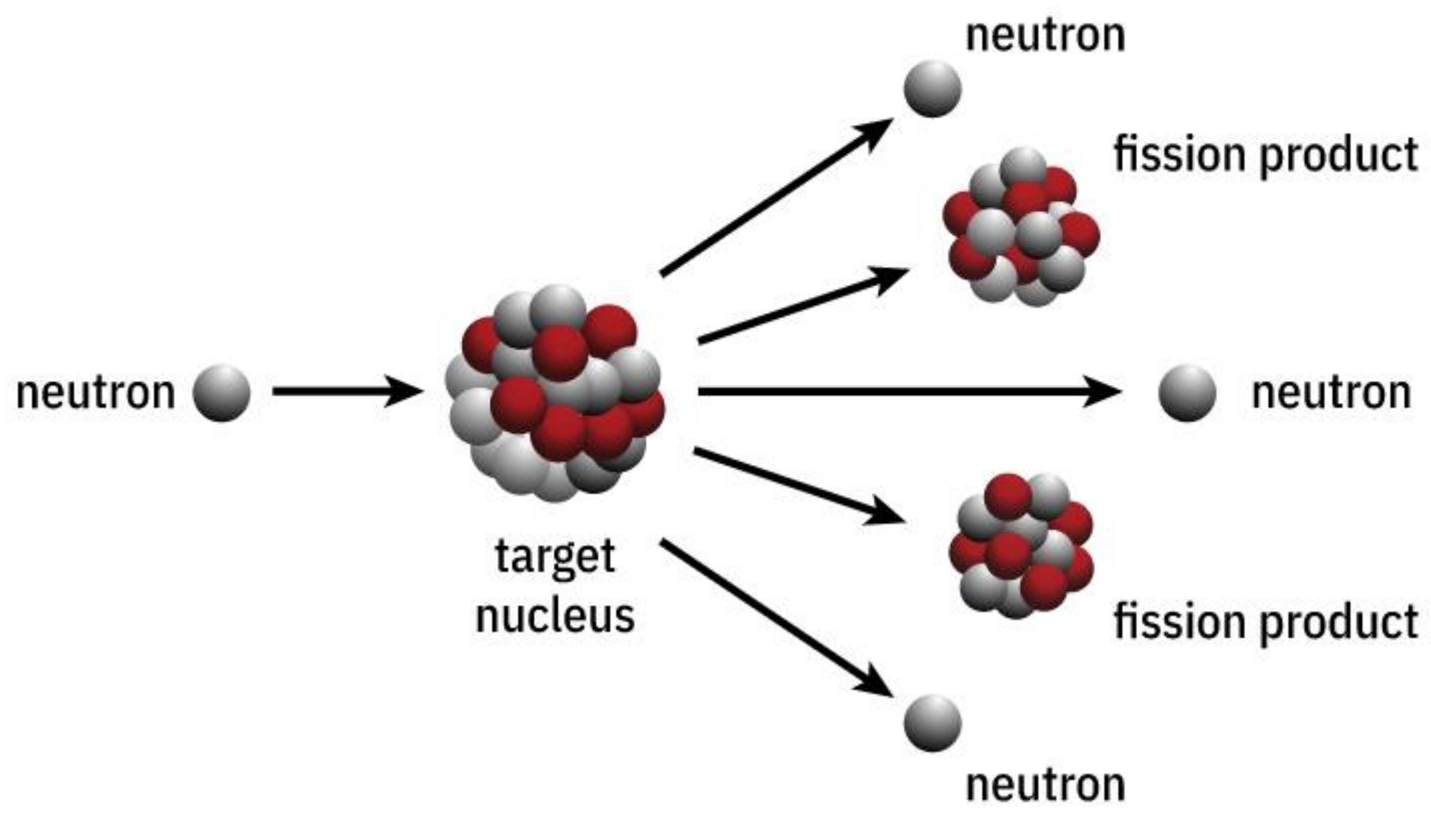
n, n’



n, elastic



n, fission



Graphics based on L. Hamidatou, H. Slamene et al. Concepts, Instrumentation and Techniques of Neutron Activation Analysis, DOI: 10.5772/53686

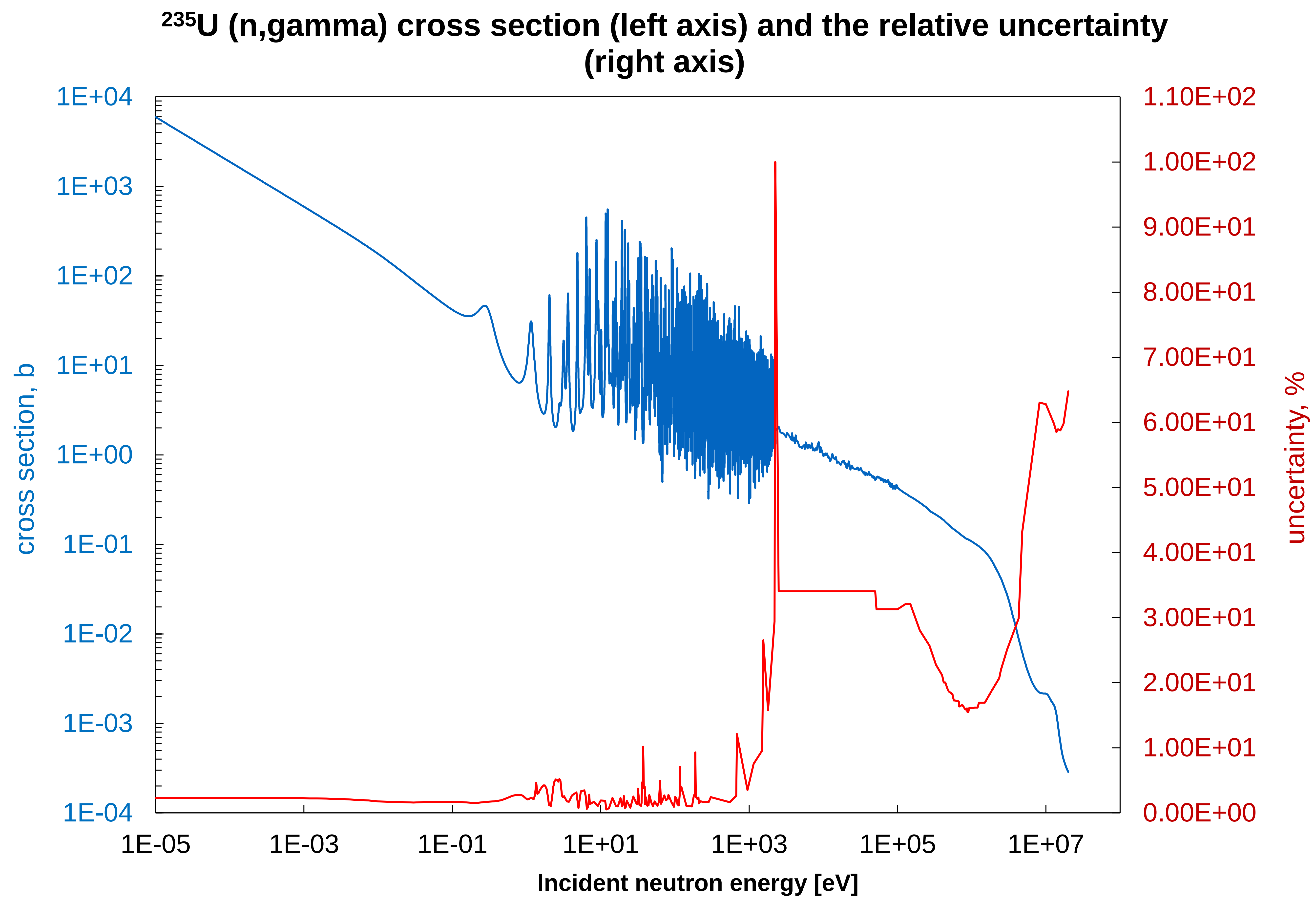
Graphics from https://www.atomicarchive.com/science/fission/index.html, access: 06.12.2021

Continuous neutron cross section library

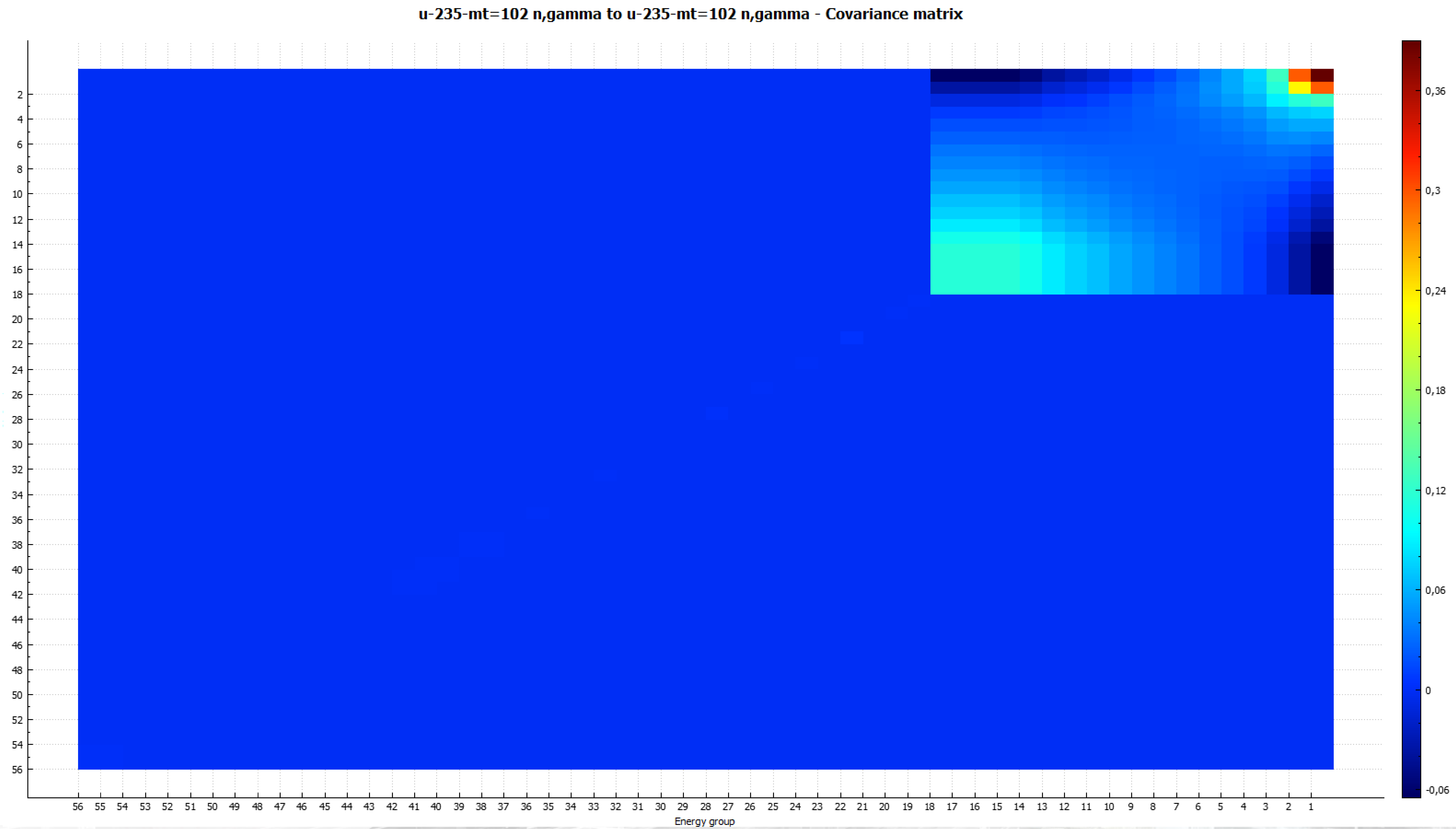
Fission measurement accuracy: ~0.8 %

Neutron capture measurement accuracy: measured by capture/fission ratio, so >0.8 %

Elastic scattering measurement accuracy limited by energy resolution limits



Covariance matrix example



Multiplication factor – a chain reaction parameter dependent on cross section values

$$k_{eff} = \frac{number\ of\ neutrons\ in\ one\ generation}{number\ of\ neutrons\ in\ preceding\ generation}$$

- For $k_{eff} = 1$ a reactor is critical (constant power).
- For $k_{eff} > 1$ the reactor's power increases.

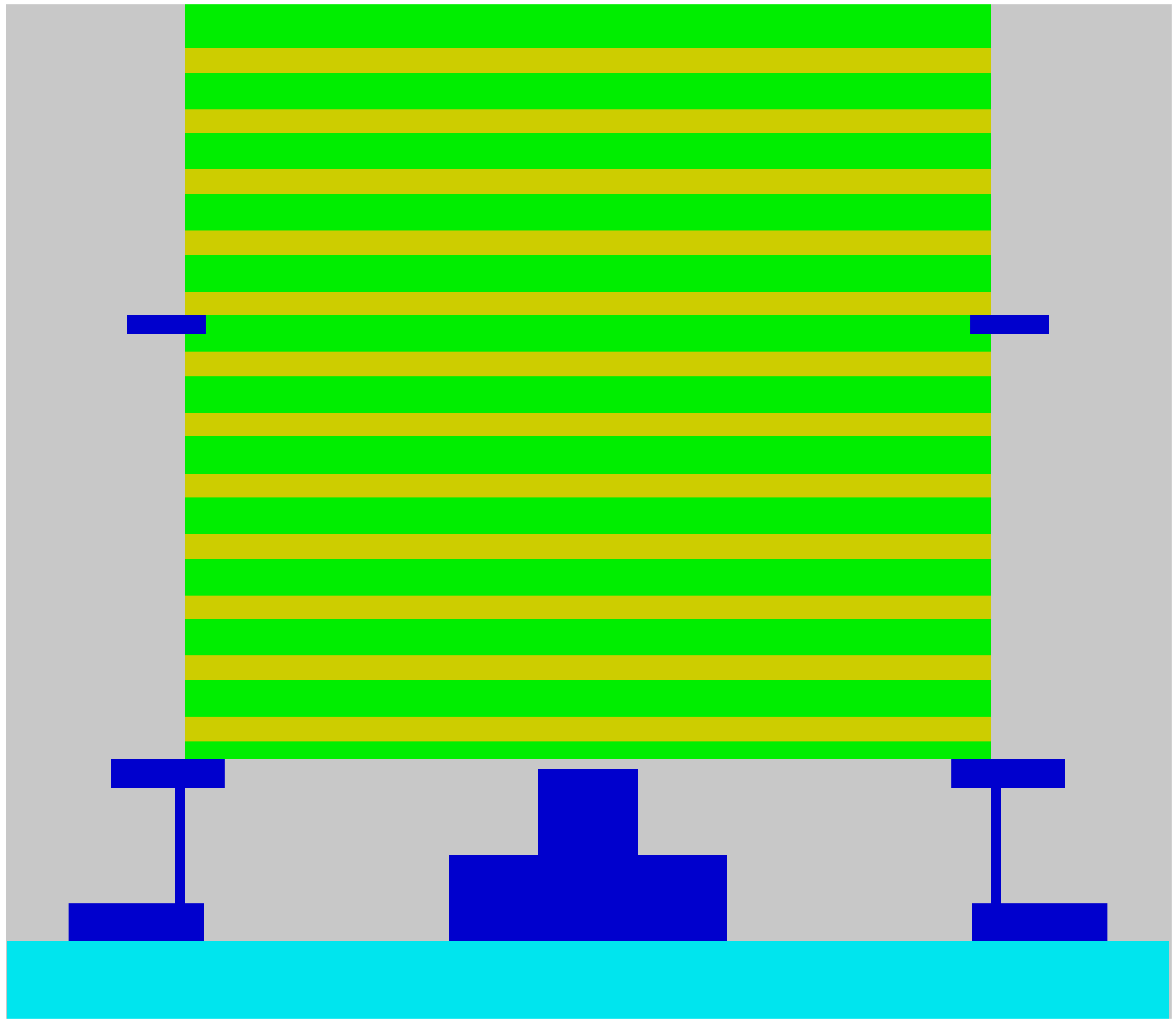
- When $k_{eff} > 1.0065$ in a typical thermal reactor, the power increases exponentially.
- Safety margin for thermal reactor: $k_{eff} < 1.0032$

Reactor geometry optimisation and safety requirements based on k_{eff}.

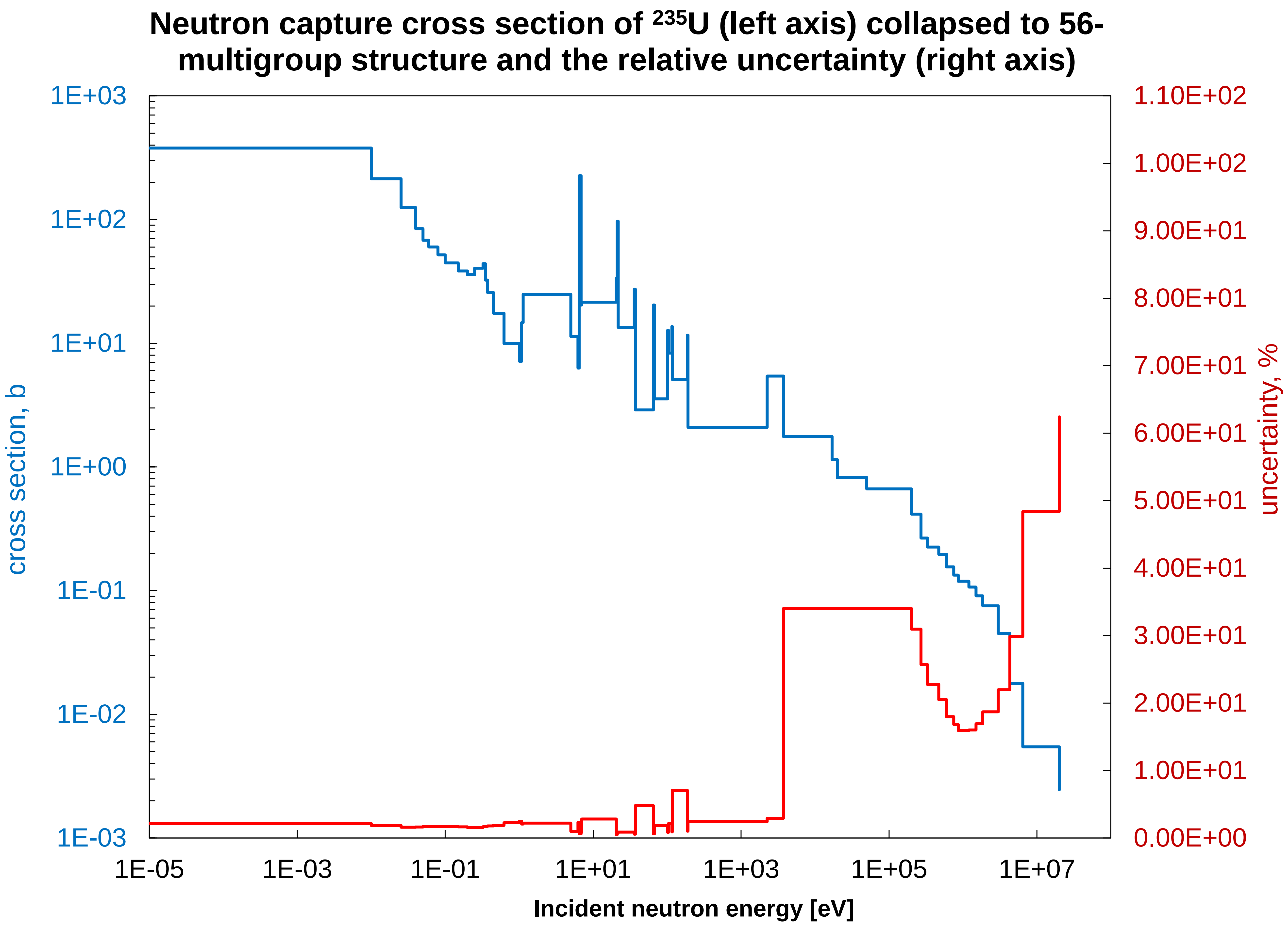
How is keff calculated?

- Geometry and material composition is defined in dedicated software
- Neutron behaviour is simulated with **Monte Carlo simulator**
- keff is calculated from formula presented earlier
- Enough generations are run for the **statistical uncertainty** of keff to be very small (typically ~0,0001**≈0,01%**)

A geometry example in SCALE simulator, a cylinder of uranium slabs, X-Z plane view:



Inaccuracies in k_{eff} calculations



Cross section uncertainties are the main contributor to the keff uncertainty.

Keff uncertainty can be calculated with an error propagation method:

$$\boldsymbol{E^2 = SMS^T}$$

E = uncertainty in 1 sd
S = sensitivity vector
M = covariance matrix of xs uncertainties

Another way: Monte Carlo sampling

Usually **keff uncertainty ≈ 1-2%**

Problem definition

- $k_{eff}\ unc = f(cross\ sections\ unc, geometrical\ unc, MC\ unc)$.
- Reducing neutron cross-section uncertainty with direct measurements is beyond the possibilities of current technology
- k_{eff} can be easily measured experimentally

Inverse procedure:

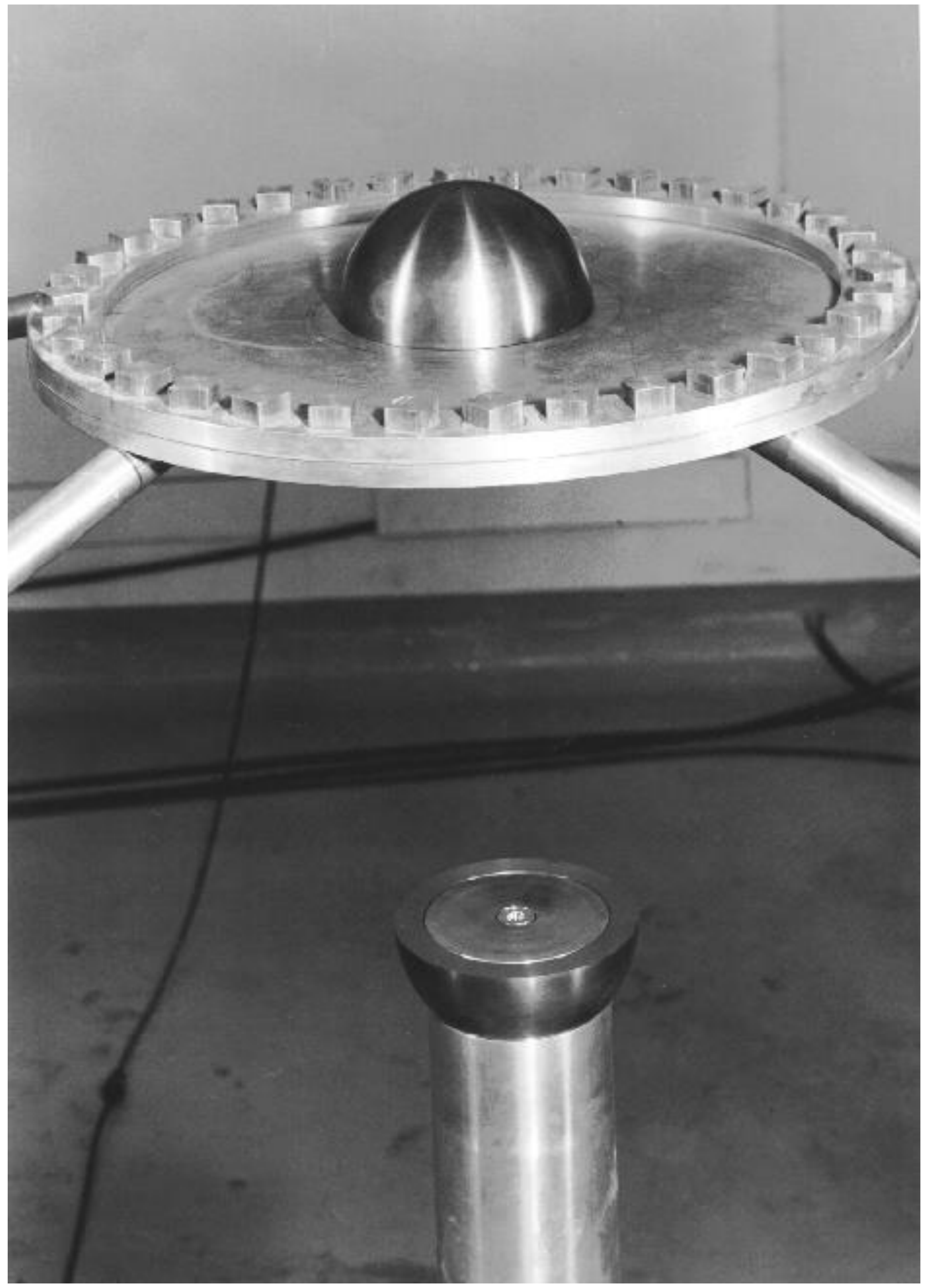
Can we reduce the neutron cross-section uncertainties using k_{eff} measurements?

Pool of historically measured k_{eff} - for existing experiments → Data assimilation algorithm

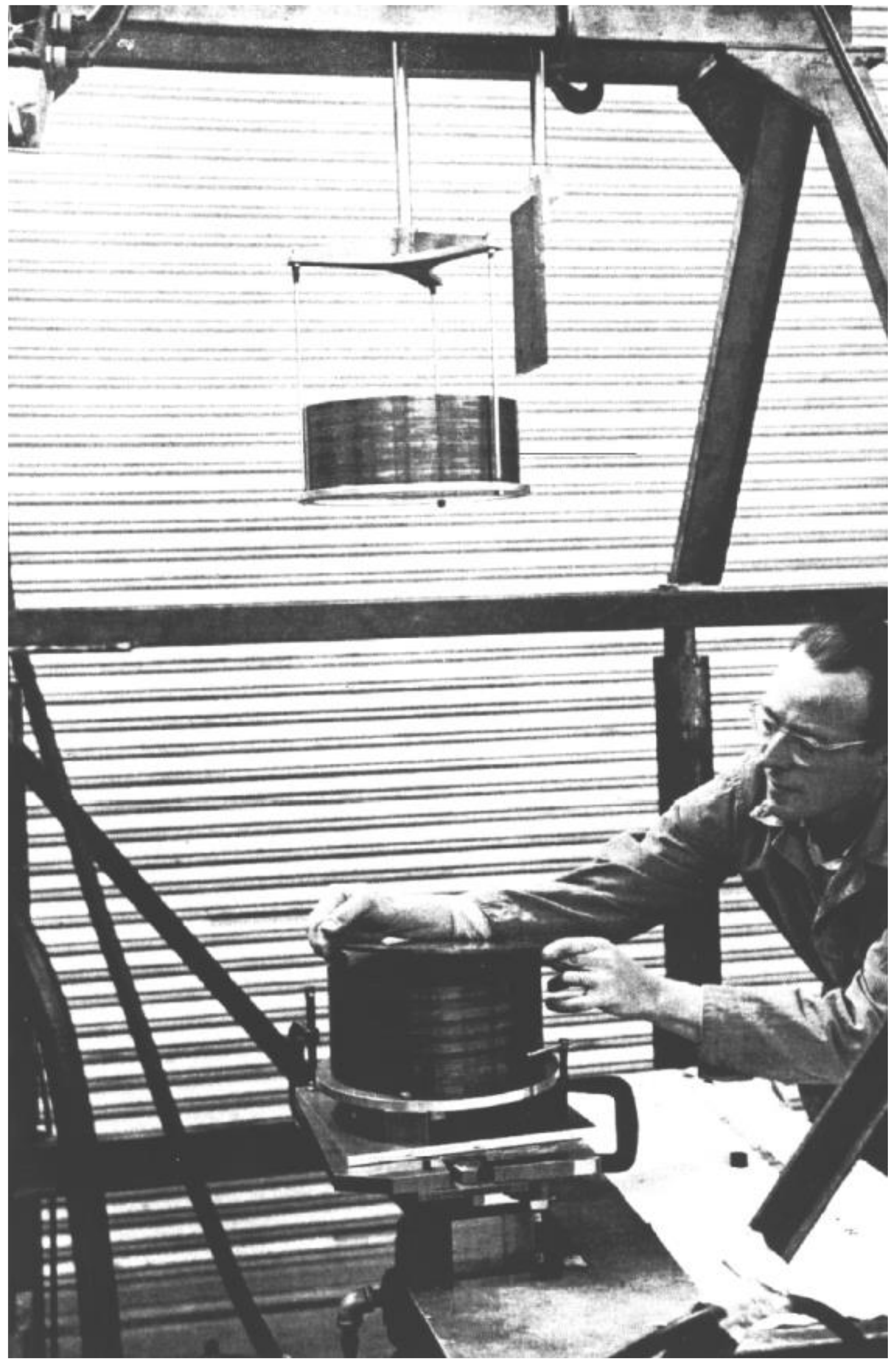
Prior neutron cross-sections → Data assimilation algorithm

Data assimilation algorithm → Posterior neutron cross-sections → Posterior k_{eff} for a system of interest

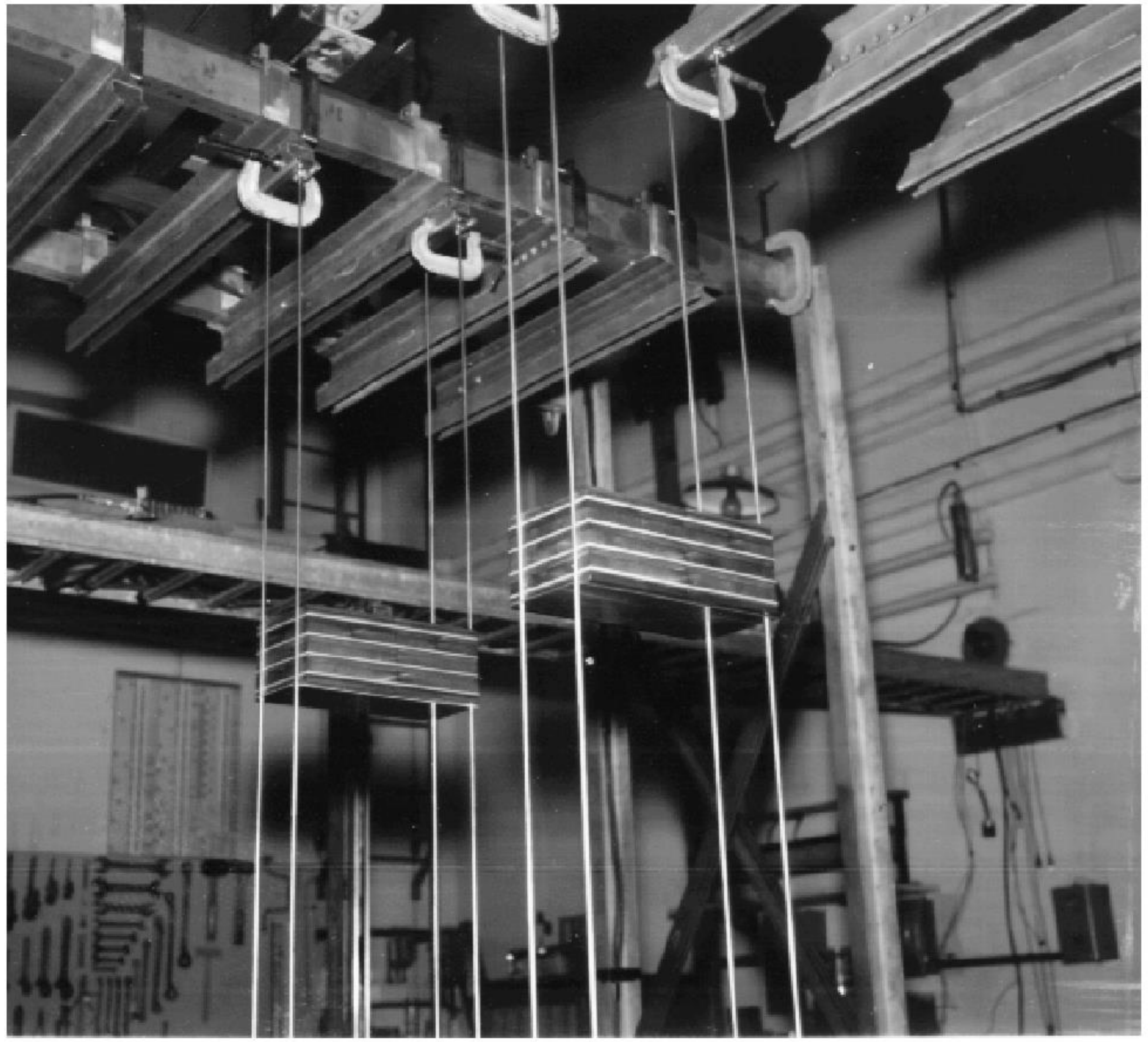
Experiment examples



Highly enriched uranium sphere



A stack of intermediately enriched uranium disks



Polyethylene reflected assemblies of uranium plates

Bayesian statistics

$$\text{Bayes}'\text{theorem: } P(\theta|y_0) \propto P(y_0|\theta)P(\theta)$$

$P(\theta)$ - prior (initial distribution of θ)

$P(\theta|y_0)$ - posterior (distribution of θ given data y_0)

$P(y_0|\theta)$ - likelihood (distribution of y_0 as a function of θ)

Successful procedure indications:

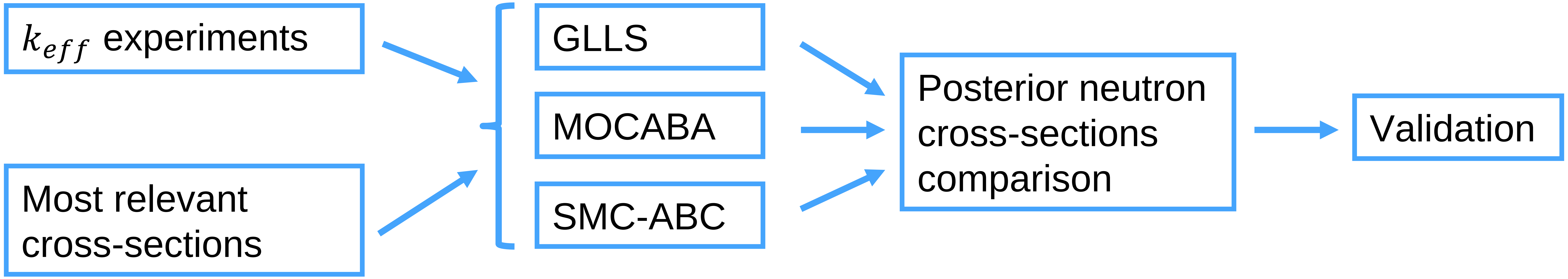
1. Uncertainty got reduced
2. Mean posterior got closer to its true value

Bayesian calibration algorithms

Method	GLLS	MOCABA	SMC-ABC
Model type	Linear approximation	Any model	Any model
Prior distribution of input parameter	Multivariate normal	Any distribution that can be transformed to a multivariate normal distribution	Any distribution
Posterior	Multivariate normal	Multivariate normal	Any distribution
Sampling	No sampling	Monte Carlo sampling	Complex algorithm with Markov Chain Monte Carlo within
Computational burden	Seconds once sensitivity analysis is complete	1-2 days	Months

Algorithm performance comparison based on example

Goal: reduction of uncertainty of neutron cross-sections relevant to fast U-235 rich systems



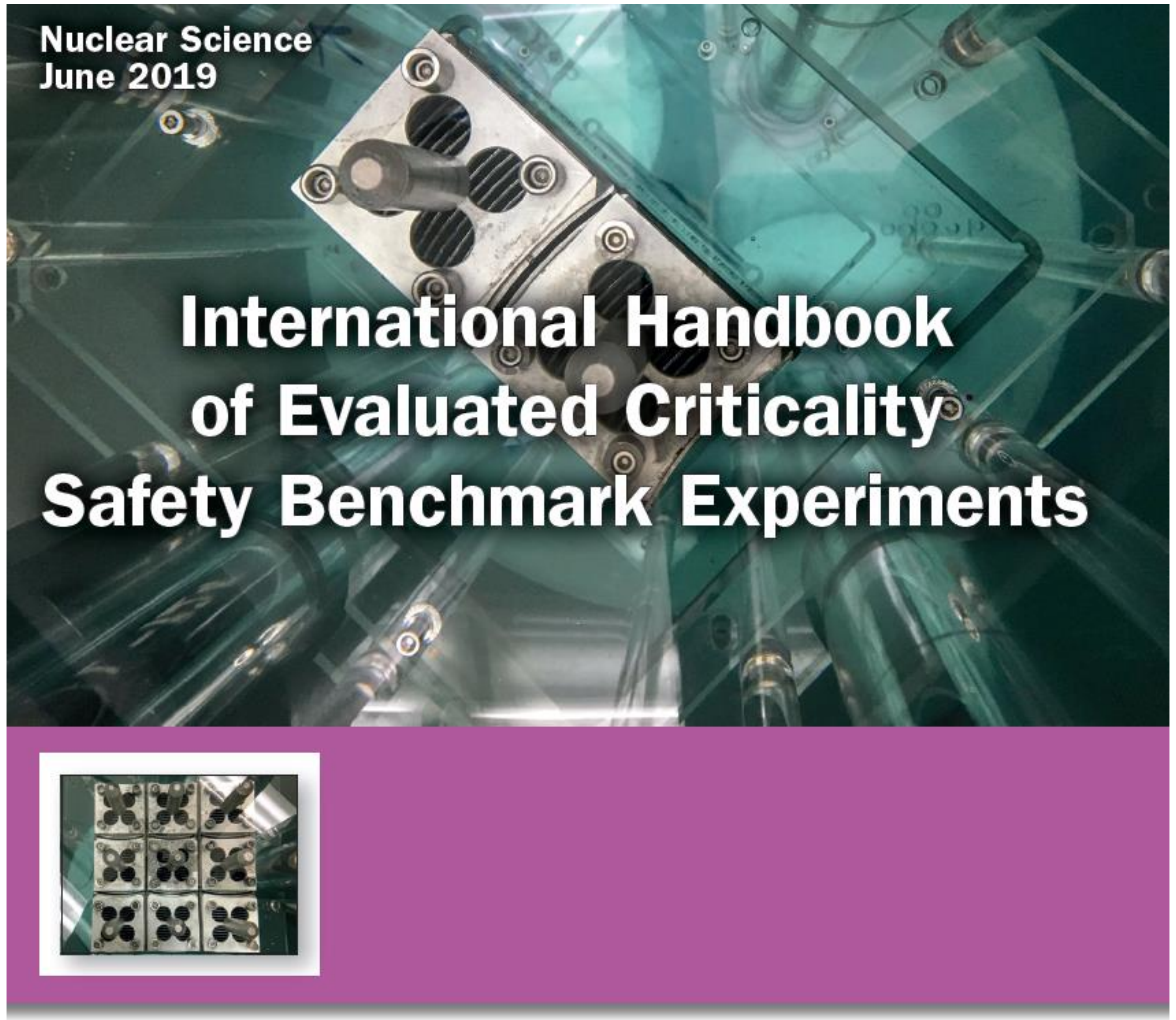
- **Top 23** cross-sections influence on a 93 % U-235 system: **80 % k_{eff} uncertainty**
- 24 experiments designated for assimilation

Cross-section list

Table 1: Calibrated perturbation factor list

Reaction type or quantity and energy group	Energy range [eV]
(n, gamma)4	(3.00E+06 - 1.85E+06)
(n, gamma)6	(1.50E+06 - 1.20E+06)
(n, gamma)7	(1.20E+06 - 8.61E+05)
(n, gamma)9	(7.50E+05 - 6.00E+05)
(n, gamma)10	(6.00E+05 - 4.70E+05)
(n, gamma)11	(4.70E+05 - 3.30E+05)
(n, gamma)12	(3.30E+05 - 2.70E+05)
(n, gamma)13	(2.70E+05 - 2.00E+05)
(n, gamma)14	(2.00E+05 - 5.00E+04)
(n, gamma)15	(5.00E+04 - 2.00E+04)
(n, gamma)17	(1.70E+04 - 3.74E+03)
(n, n')4	(1.85E+06 - 1.50E+06)
(n, n')7	(1.20E+06 - 8.61E+05)
(n, n')9	(7.50E+05 - 6.00E+05)
(n, n')10	(6.00E+05 - 4.70E+05)
(n, n')11	(4.70E+05 - 3.30E+05)
(n, elastic)14	(2.00E+05 - 5.00E+04)
(n, fission)2	(6.43E+06 - 4.30E+06)
(n, fission)4	(3.00E+06 - 1.85E+06)
(n, fission)7	(1.20E+06 - 8.61E+05)
(n, fission)11	(4.70E+05 - 3.30E+05)
(n, fission)14	(2.00E+05 - 5.00E+04)
(chi)1	(2.00E+07 - 6.43E+06)

Experimental database



NEA
NUCLEAR ENERGY AGENCY

EVALUATED EXPERIMENTS

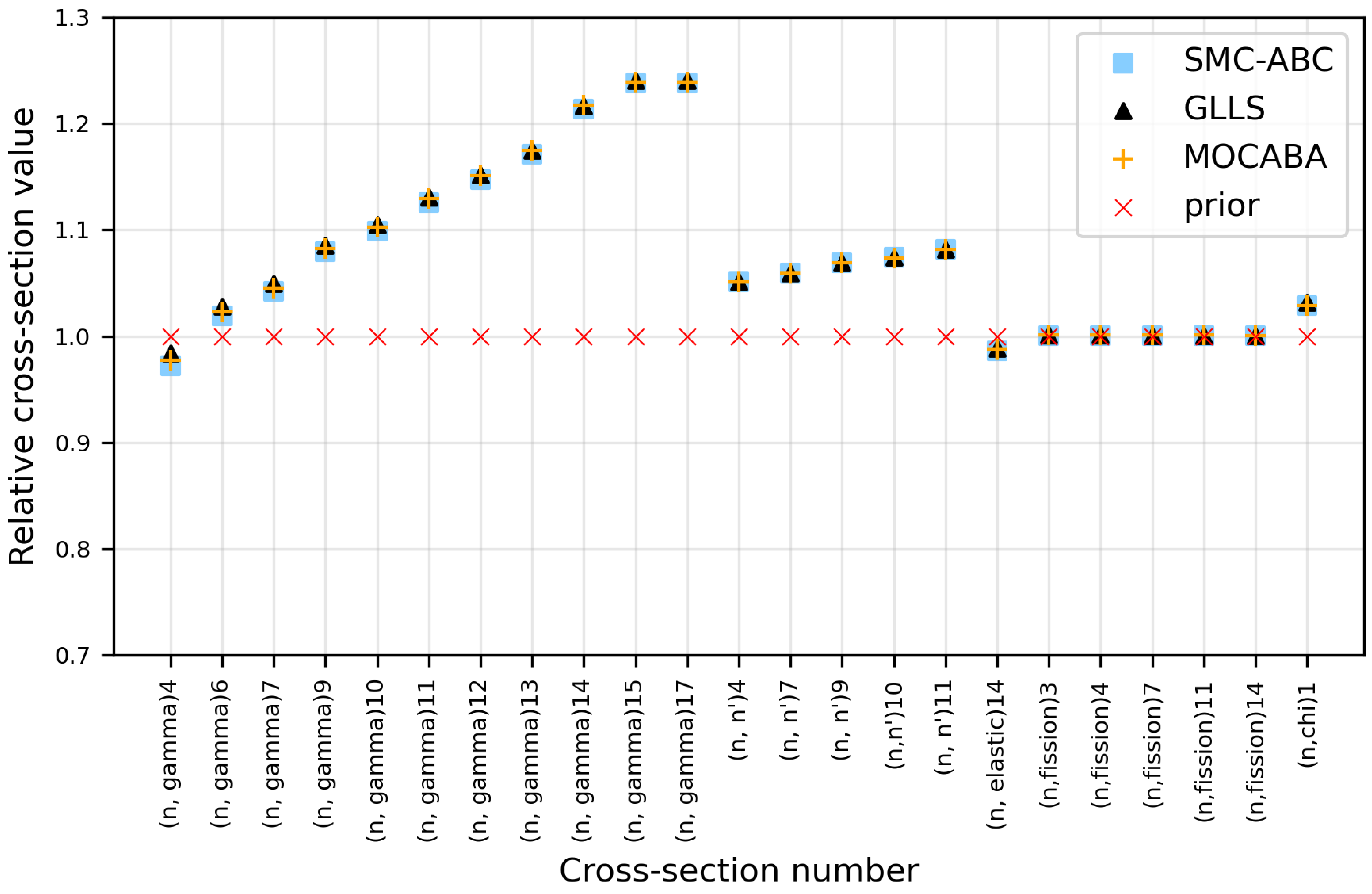
Highly Enriched Uranium Systems

METAL SYSTEMS

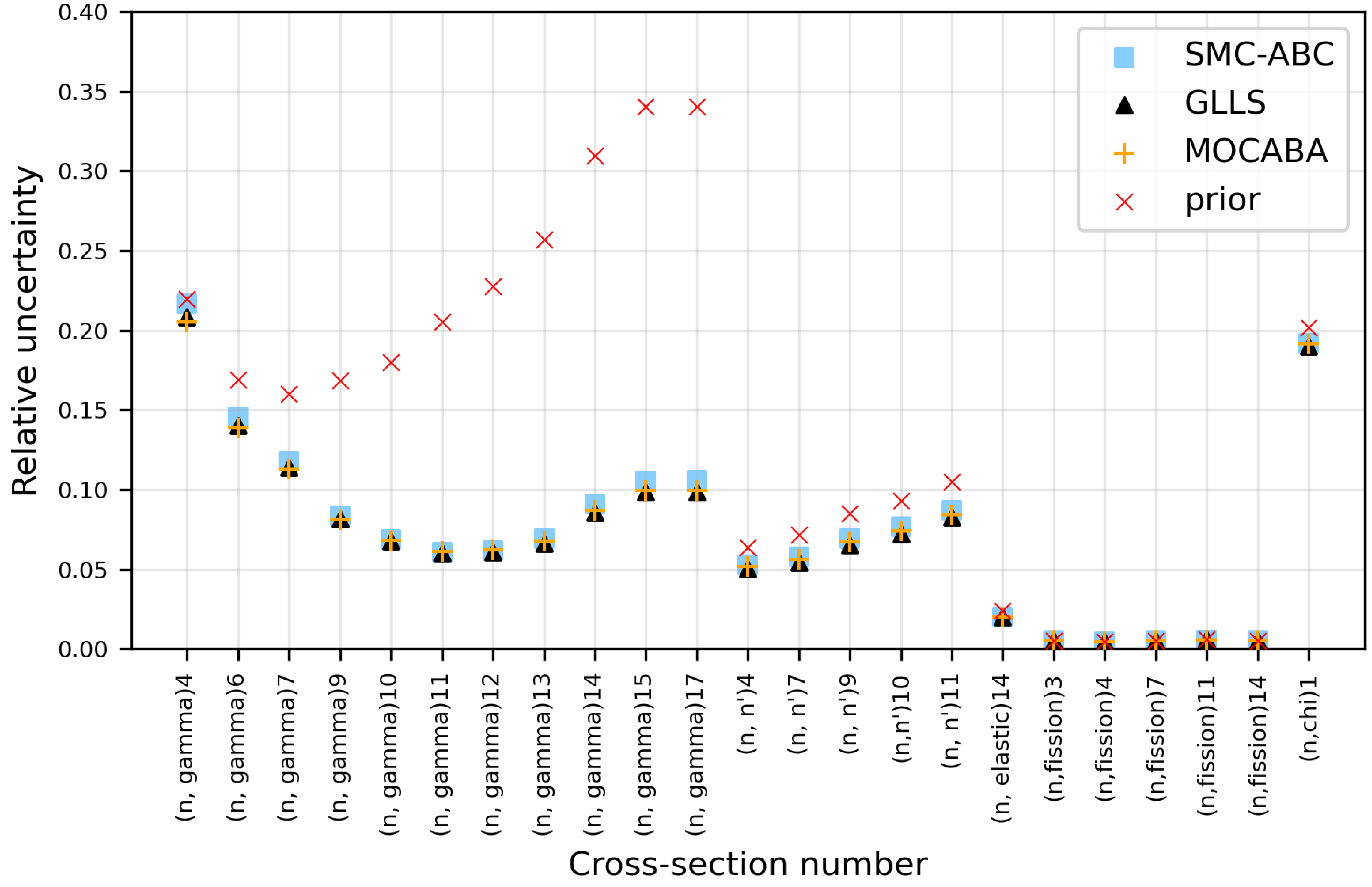
FAST METAL SYSTEMS

HEU-MET-FAST-001	Bare, Highly Enriched Uranium Sphere (Godiva)
HEU-MET-FAST-002	Topsy 8-Inch-Tuballoy-Reflected Oralloy Assemblies
HEU-MET-FAST-003	Reflected Oralloy Spherical Assemblies
HEU-MET-FAST-004	Water-Reflected, Highly Enriched Uranium Sphere
HEU-MET-FAST-005	Beryllium- and Molybdenum-Reflected Cylinders of Highly Enriched Uranium
HEU-MET-FAST-006	Lattices of Oralloy Cubes in Water
HEU-MET-FAST-007	Uranium Metal Slabs Moderated with Polyethylene, Plexiglas, and Teflon
HEU-MET-FAST-008	Bare Sphere of Highly Enriched Uranium
HEU-MET-FAST-009	Spheres of Highly Enriched Uranium Reflected by Beryllium or Beryllium Oxide
HEU-MET-FAST-010	Spheres of Highly Enriched Uranium Reflected by Boron+Beryllium or Boron+Beryllium Oxide
HEU-MET-FAST-011	Sphere of Highly Enriched Uranium Reflected by Polyethylene

Data assimilation results – posterior means



Data assimilation results – posterior uncertainties



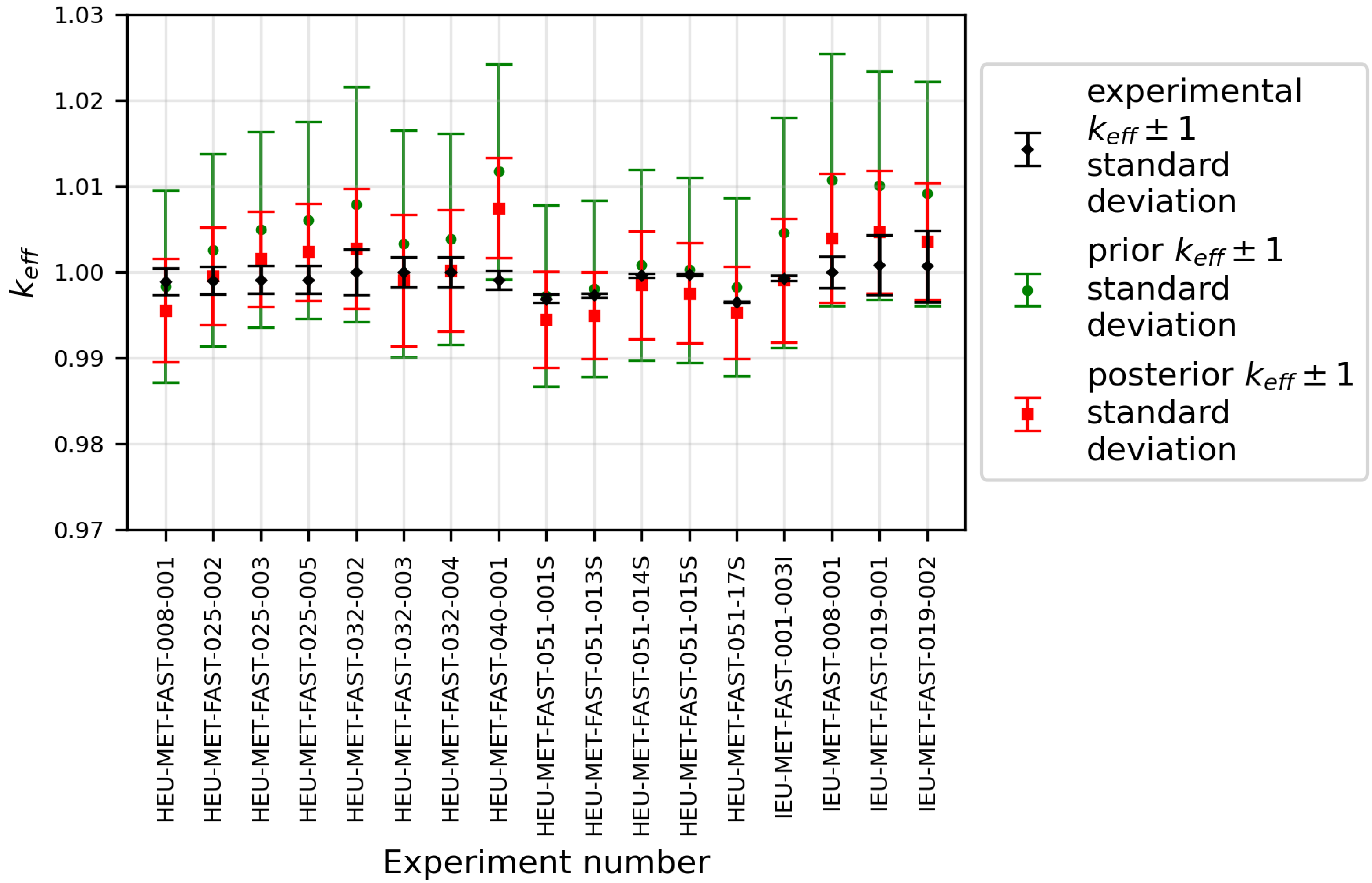
Most appropriate algorithm - MOCABA

Validation techniques

Two techniques are available to determine whether the data assimilation was successful

1. Validation using unassimilated experiments – checking if experimental data is close to simulated data
2. The use of so-called synthetic experiments

Validation 1 & Uncertainty reduction in calculated k_{eff}

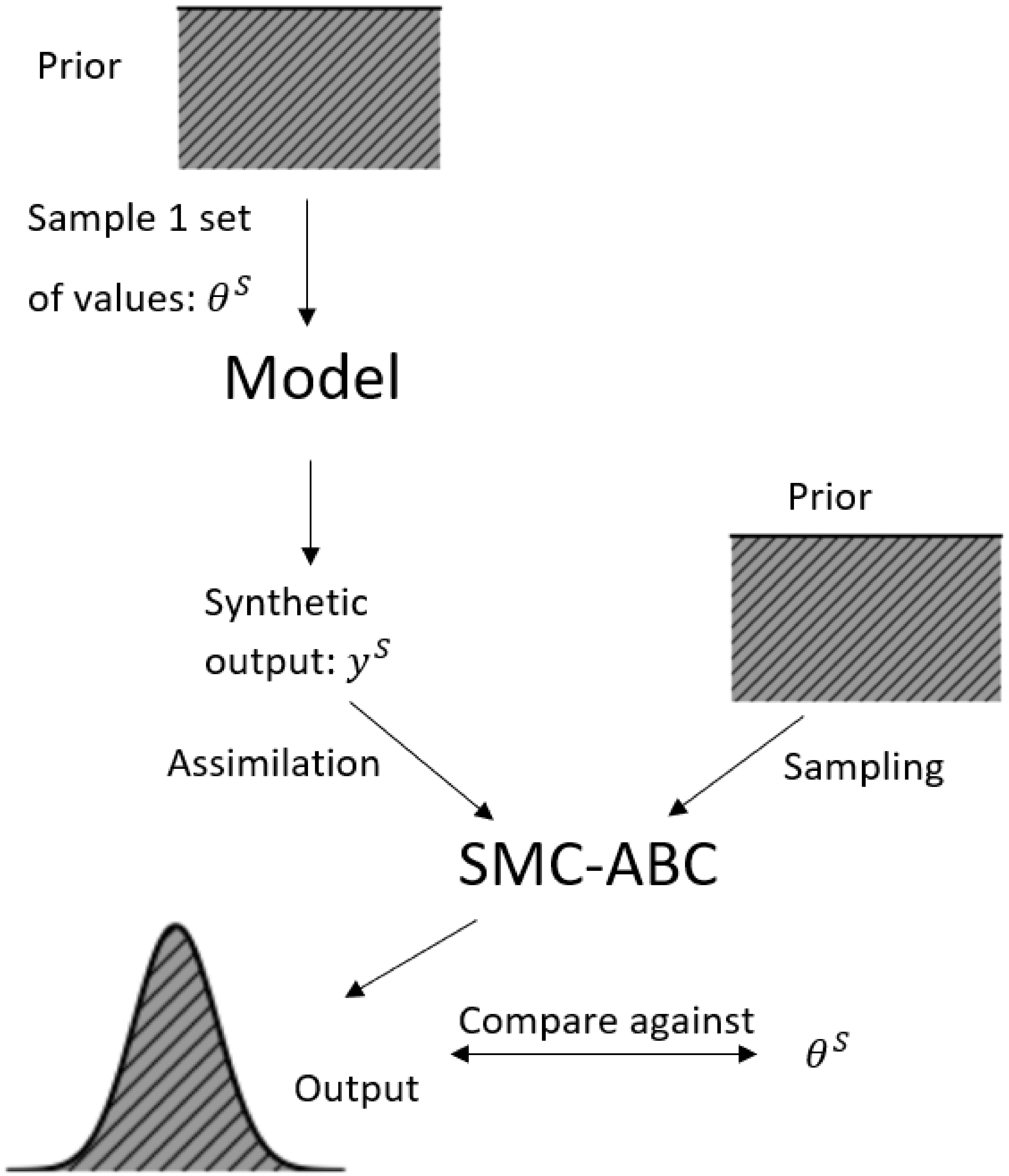


Distance between the mean calculated and experimental results reduced by 49 %

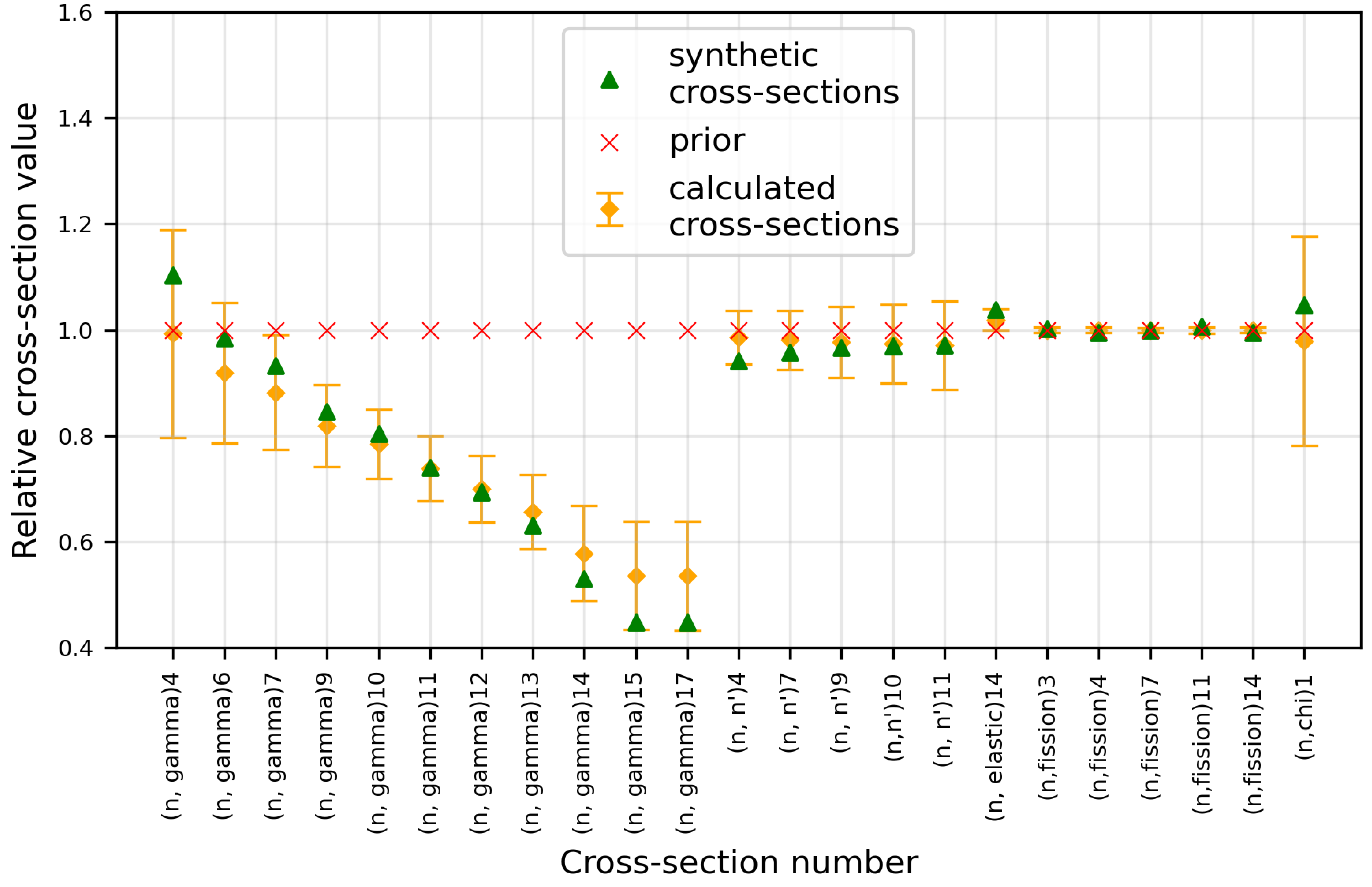
Posterior k_{eff} uncertainty reduced by 48 %

Validation 2: synthetic experiments

Synthetic experiments are simulation outputs generated computationally, based on inputs sampled from the prior. We assimilate the outputs and check how close posterior values are to the sample from the prior.



Synthetic experiment validation results



15 neutron cross-sections were calibrated successfully, 8 either stayed unchanged or were slightly overfitted.

Identifiability assessment

Identifiability problem answers the question on whether available measurement data is enough to find the true value of uncertain input parameters.

When is identifiability weak?

- In cases where output parameters are not sensitive to some input parameters or one input parameter is dominant sensitivity-wise
- When measurements are not diverse enough
- When there are too few measurements

Influence of unupdated cross-sections on results

Current treatment of uncalibrated parameters in nuclear engineering data assimilation

- Uncalibrated parameters' uncertainties are often ignored
- The correlations between experimental errors from uncalibrated parameters are ignored

Experimental vs unupdated cross-section correlated uncertainties

Experimental uncertainty covariance matrix:

- Experimental sources: geometry or material of some part of the experimental setup is the same across multiple experiments. Example: container dimensions
- Other source: uncertainty from unupdated cross-sections, which are present across multiple experiments. Example: cross-sections O and H if only U is considered

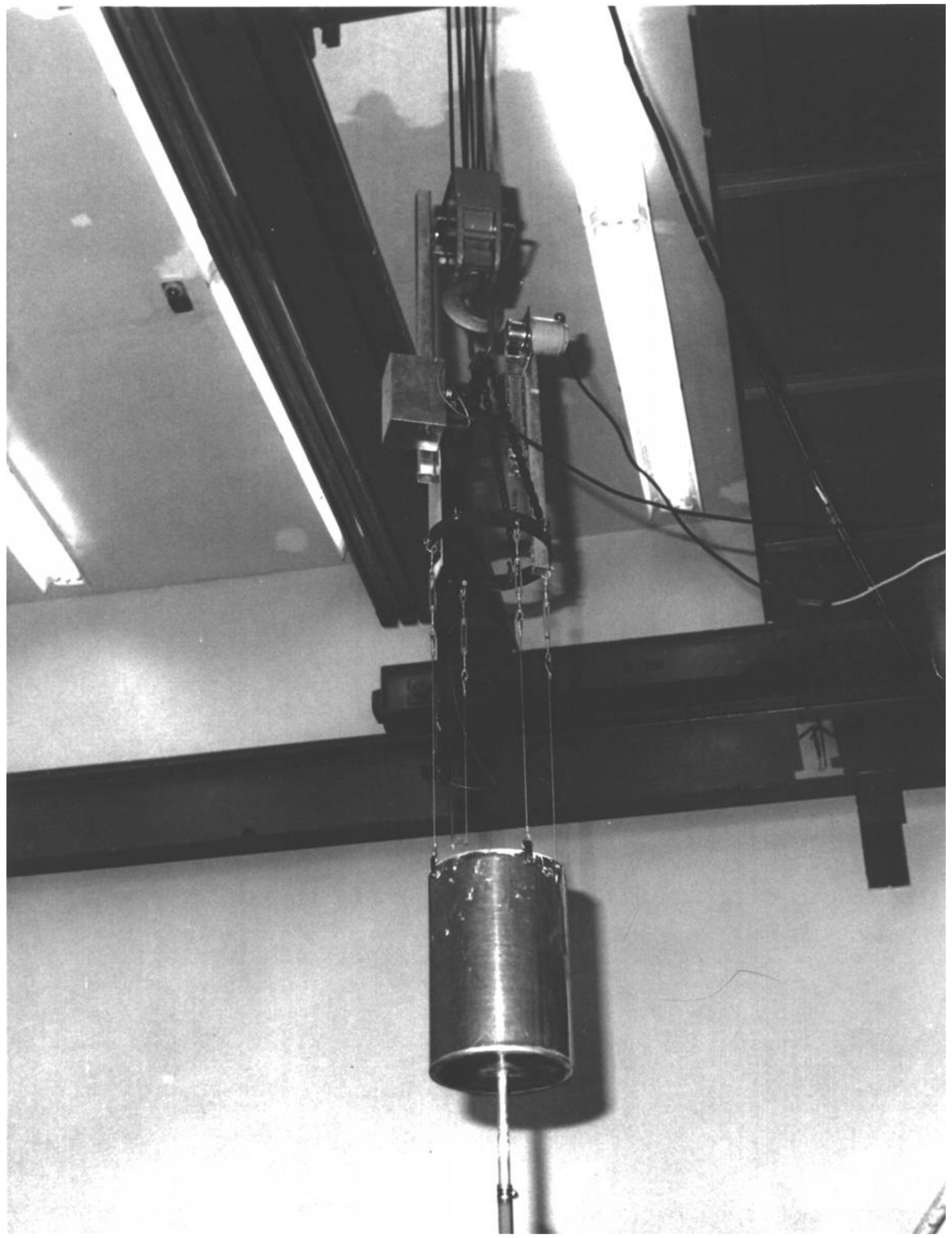


Photo of the vessel in which 10 critical solutions were researched

Example problem for unupdated cross-section treatment

Goal: reduction of uncertainty of neutron cross-sections relevant for thermal systems

k_{eff} experiments, 3 highly correlated sets

1904 cross-sections (U, B)

MOCABA, rigorous uncertainty treatment

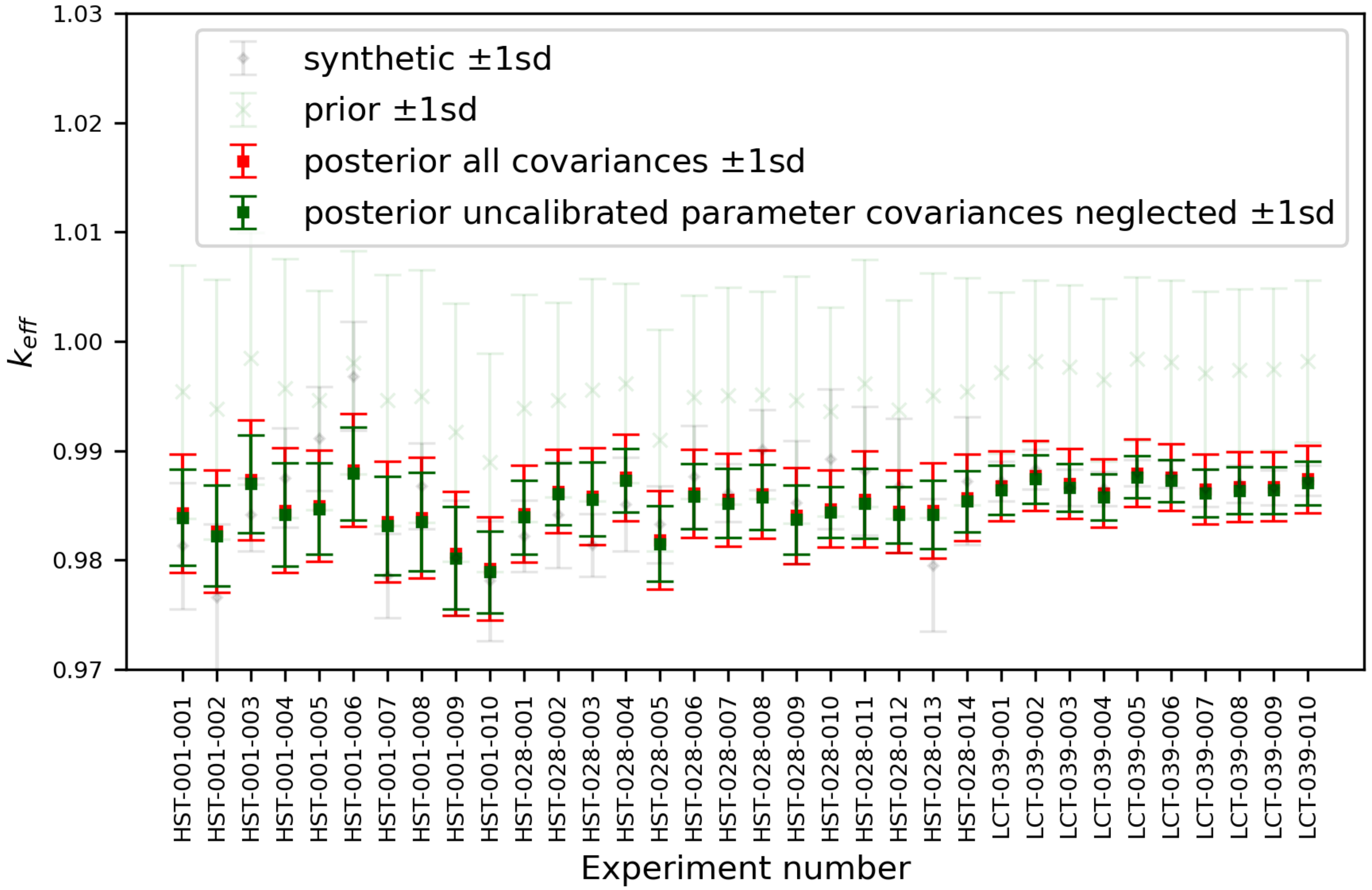
MOCABA, correlations from uncalibrated parameters ignored

Comparison of posterior k_{eff}

Consequences of neglecting covariances from unupdated cross-sections

The uncertainty **underestimated by 25 %** compared to what it should be.

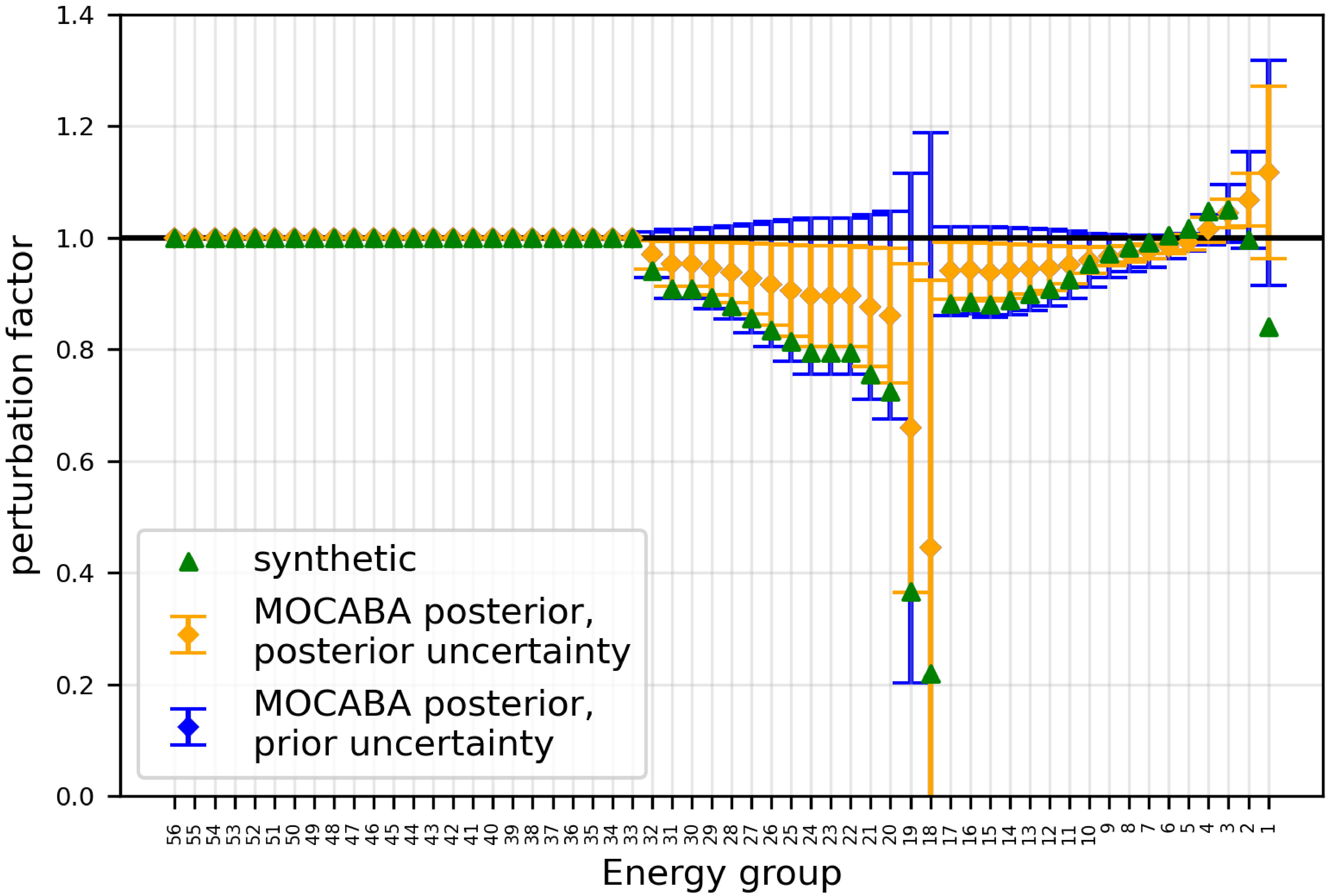
Posterior keff results after executing the algorithm from previous slide



Another finding: difficult to correctly update fastest neutron cross-sections

Synthetic validation result: the fastest groups overfitted. Additional experiments, other than k_{eff} measurements required.

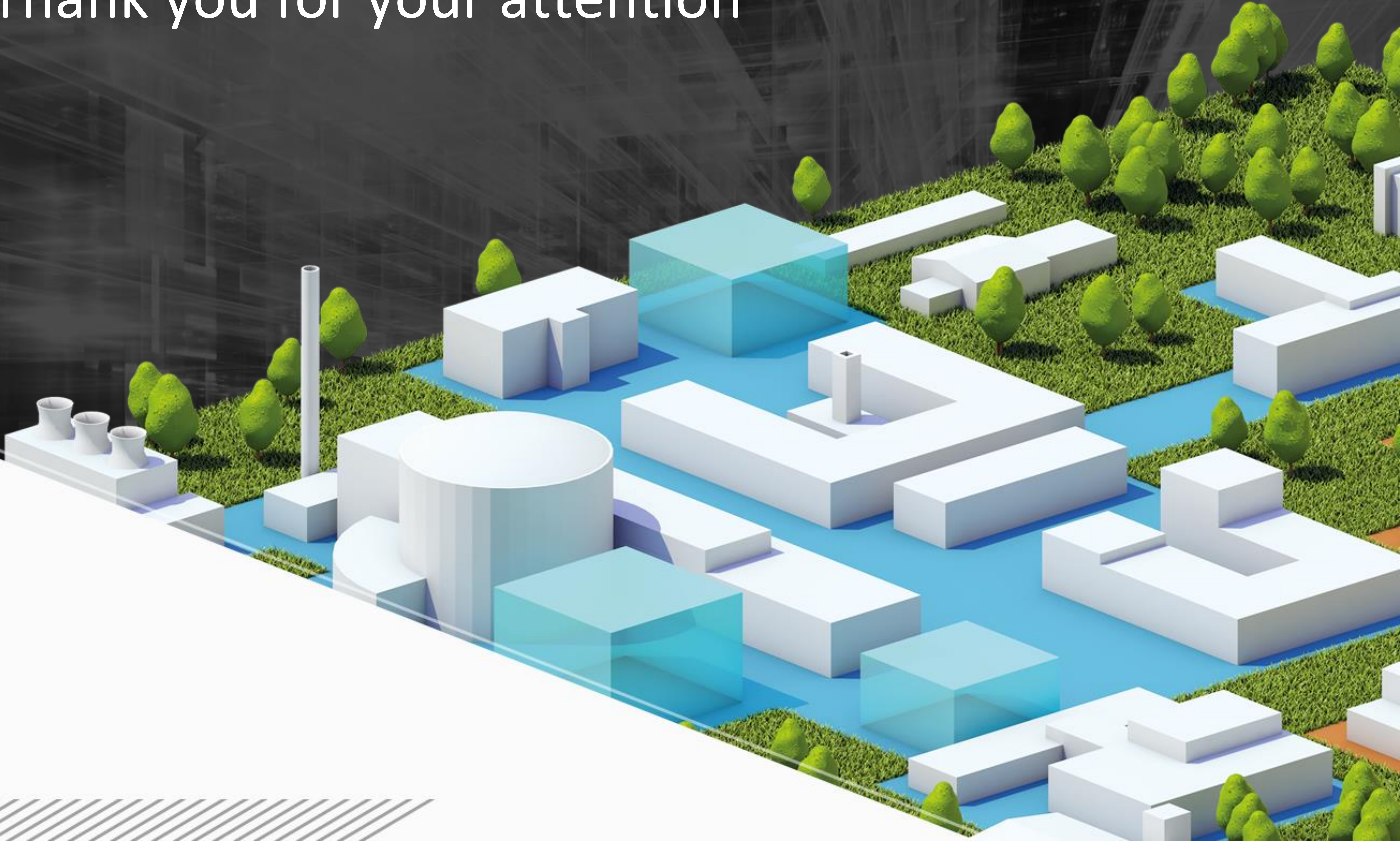
Comparison of U-235(chi) parameter posterior with synthetic values.



Summary

- The most appropriate algorithm for neutron cross-section Bayesian updating was found - MOCABA
- A novel in the context of nuclear engineering validation procedure was presented – the synthetic experiments
- The correct treatment of uncalibrated uncertain cross-sections was proposed
- It is found that for all cross-section to be successfully calibrated additional experiments, other than k_{eff} measurements are required

Thank you for your attention



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