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Data Assimilation for ^{23}Na

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Data Assimilation Strategies

Strategy 1: Deterministic method

- Key issue is to have input parameter covariances
- Cross sections collapsed into 30-groups by NJOY
- Sensitivities can be produced using the method developed for low-fidelity project for 18 parameters (now ~50 parameters)
- Computational requirements: $2n+1$ runs needed, each EMPIRE run ~15' for a set of ~50 incident neutron energies
- New NNDC Dell Linux cluster with 75 nodes can be used

Strategy 2: Monte Carlo method

- Again, key issue is to have input parameter covariances
- Monte Carlo sampling for all parameters, then always EMPIRE and creation of ENDF-6 formatted file
- Next, NJOY to create continuous energy library (ACER format)
- Finally, MCNP

1st strategy adopted for ²³Na

Data Assimilation: Assumptions

Assumptions

- EMPIRE can reproduce ENDF/B-VII.0 evaluation with a proper set of nuclear physics parameters p_k , including both RR and fast neutron region.
- Covariance matrix of parameters p_k can be established, at least as diagonal matrix containing parameter uncertainties Δp_k .
- There is clean integral experiment of reactor quantity R which can provide sufficient feedback to update initial evaluation.

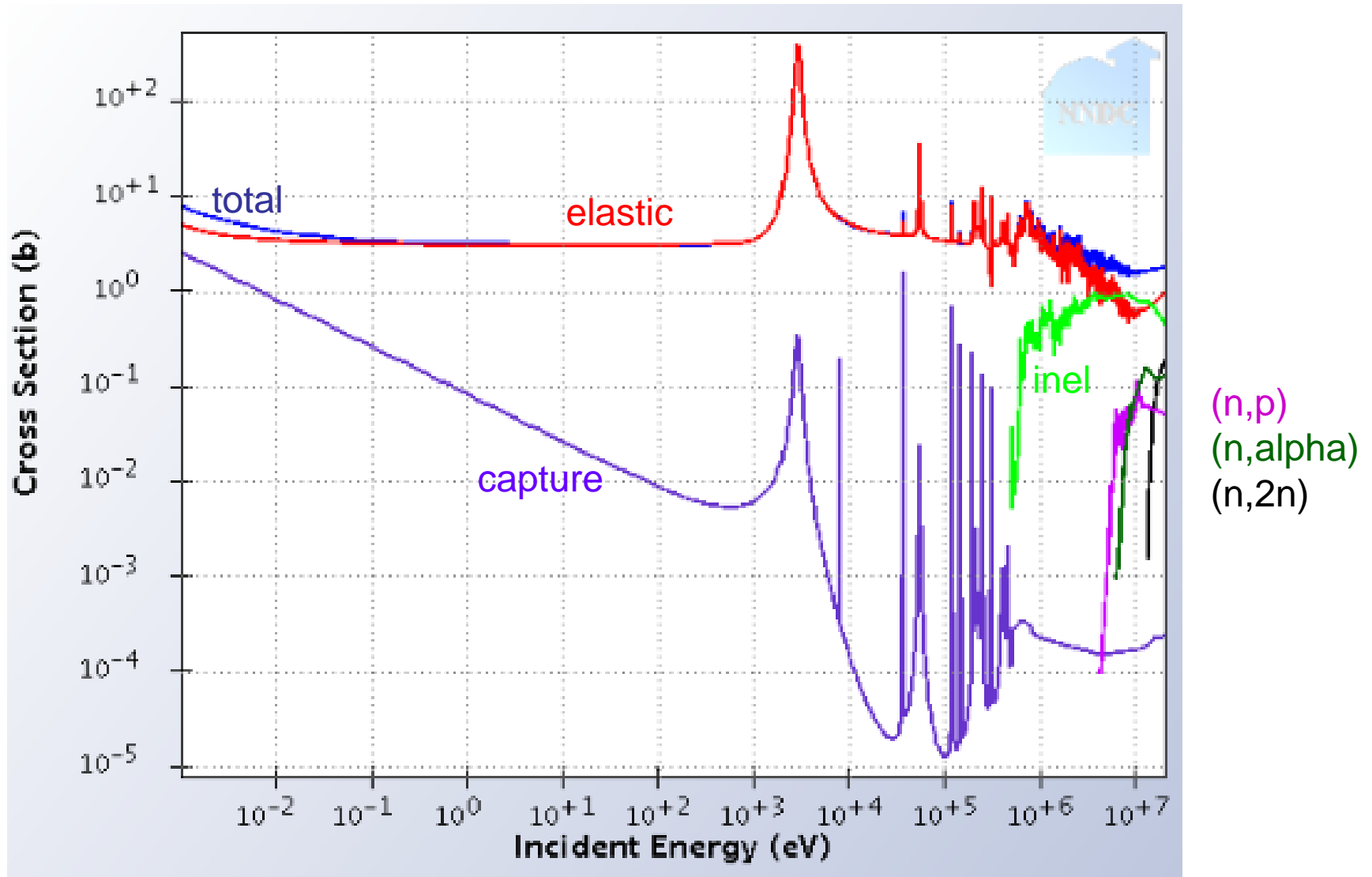
Data Assimilation: Procedures

Procedures

1. Calculate parameter sensitivities: $\Delta\sigma_j/\Delta p_k$ where σ_j is multi-group cross section
2. Calculate integral sensitivities: $\Delta R/\Delta\sigma_j$ and then
$$\frac{\Delta R}{\Delta p_k} = \sum_j \frac{\Delta R}{\Delta\sigma_j} \times \frac{\Delta\sigma_j}{\Delta p_k}$$
3. Update initial parameters using the above sensitivities and parameter uncertainties (covariances), produce $^{mod}p_k$
4. Produce updated evaluation using $^{mod}p_k$

23-Na cross sections

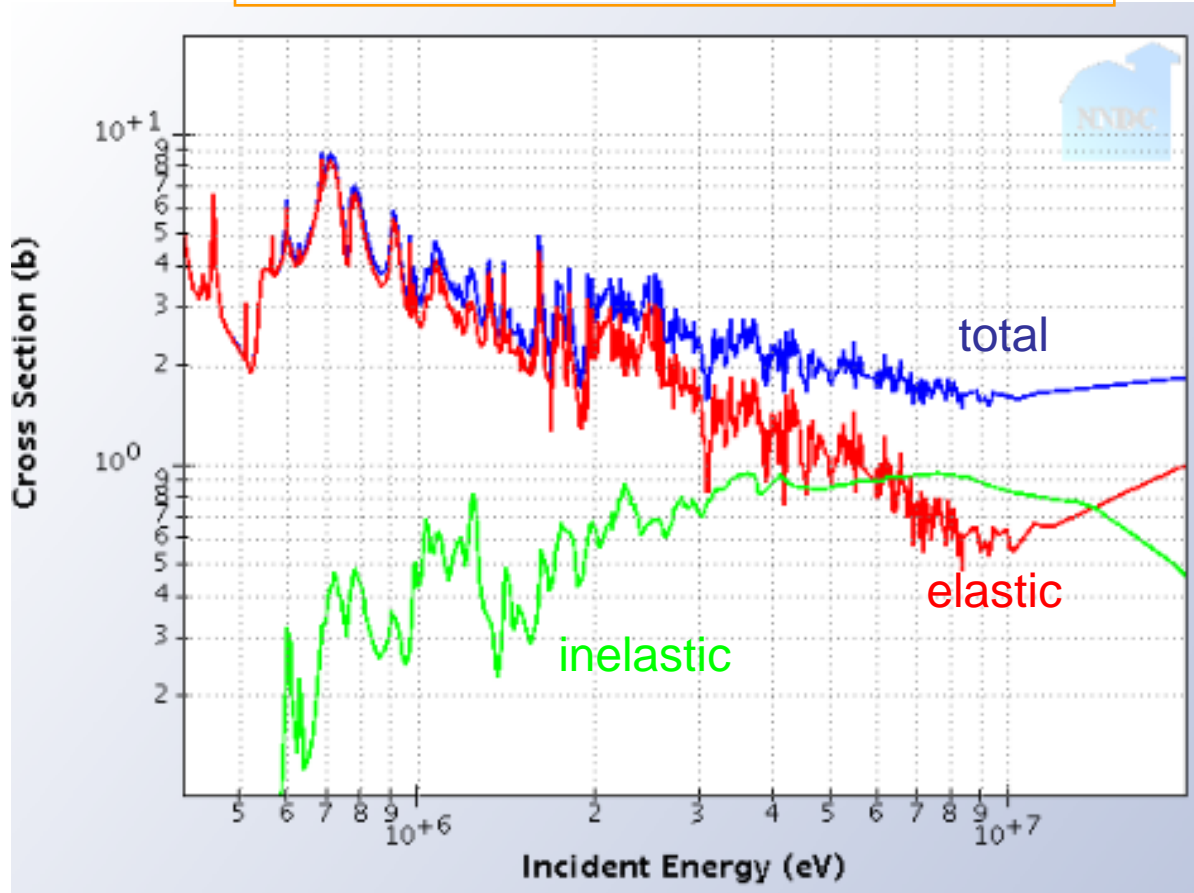
Most important channels: elastic, inelastic



23-Na challenges for EMPIRE

Challenge No.1:

Fluctuations above RR, up to ~10 MeV!



Challenge No.2:

Background in MF3 to fix RR region (evaluation by D. Larson, 1977)

Challenge No.3:

27 discrete levels in (n,n'), starting at 0.44, 2.08, 2.39 MeV,...

How good is ENDF/B-VII file for ^{23}Na ?

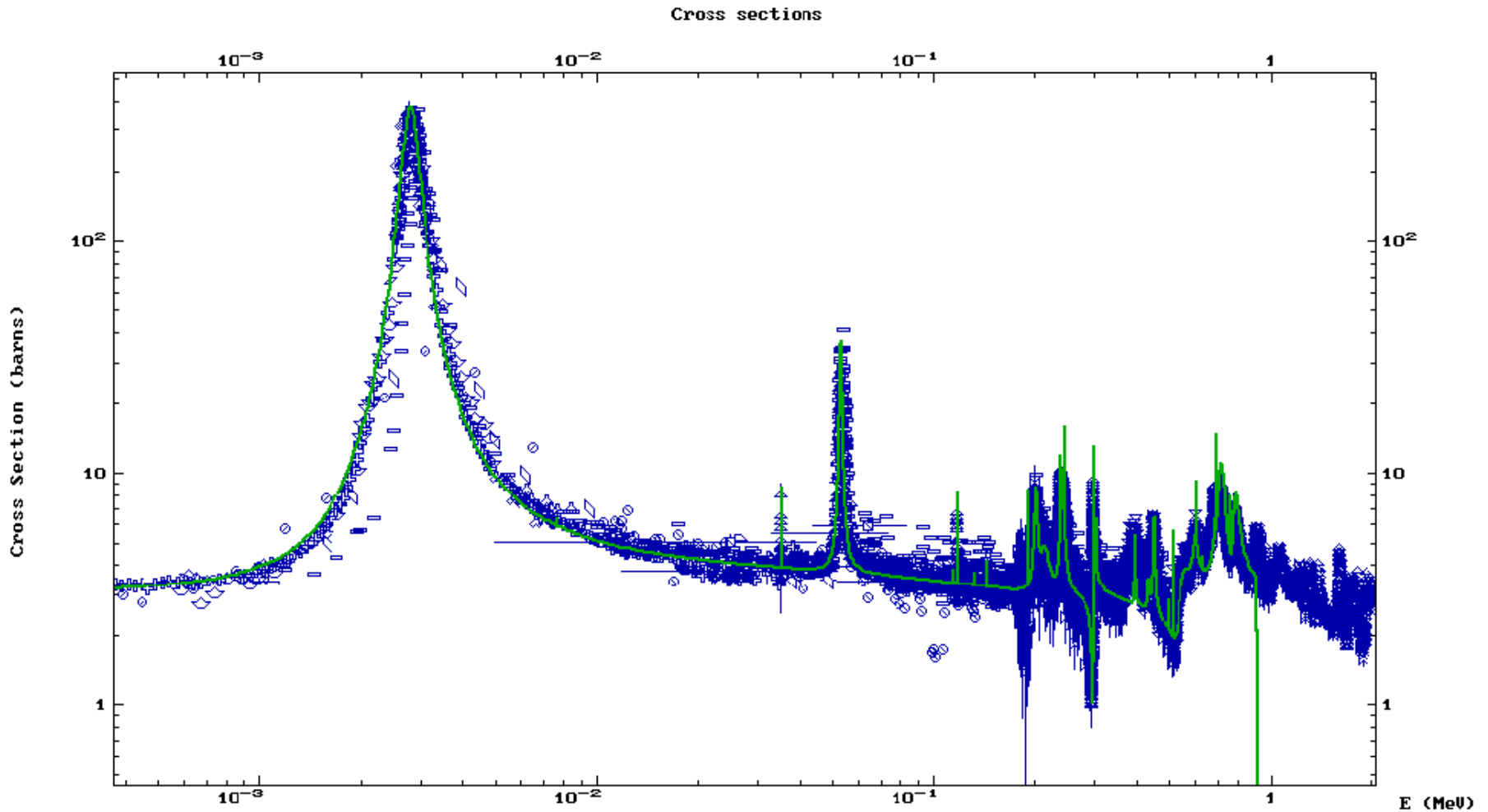
Evaluation adopted by ENDF/B-VII.0 was done by **D. Larson et al** in **1977!**

Recent review of all available evaluations by Nikolaev, Ignatyuk et al, Russia, to select best evaluations for **RUSFOND** library, completed in 2007. Their review of ^{23}Na is summarized in the report (32pp.):

- RR region → adopt Larson, though there is need for new evaluation
- Fast region → adopt Larson for total, elastic and inelastic
adopt Larson for (n,p), (n,a) up to 9 MeV
modify (n,2n), (n,na), (n,np), (n,t), ...
- Discussion of mu-bars
- Discussion of covariances

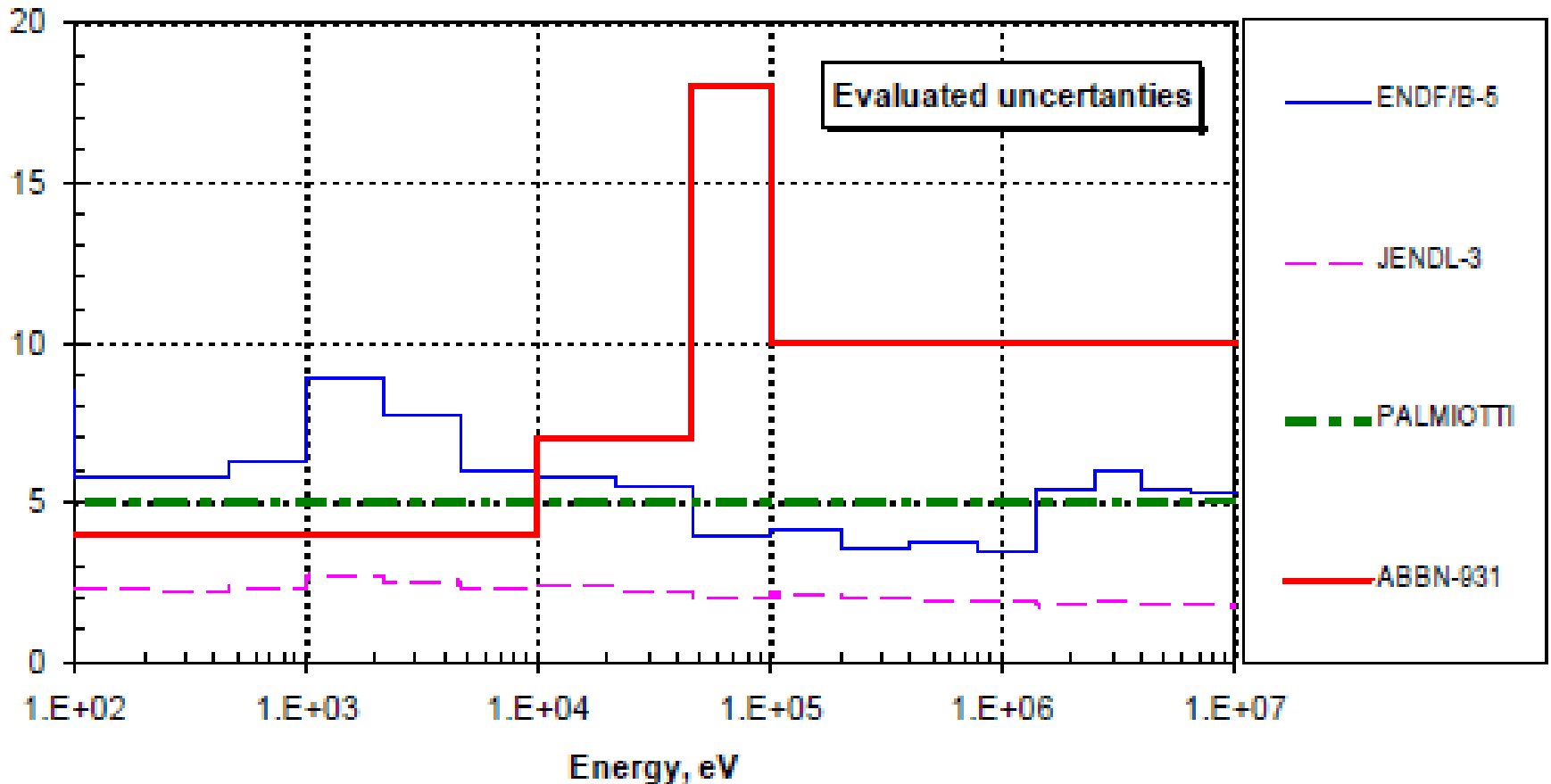
23-Na possible improvements

Capture in RR can be extended up to ~ 1 MeV (Pigni/Mughabghab)

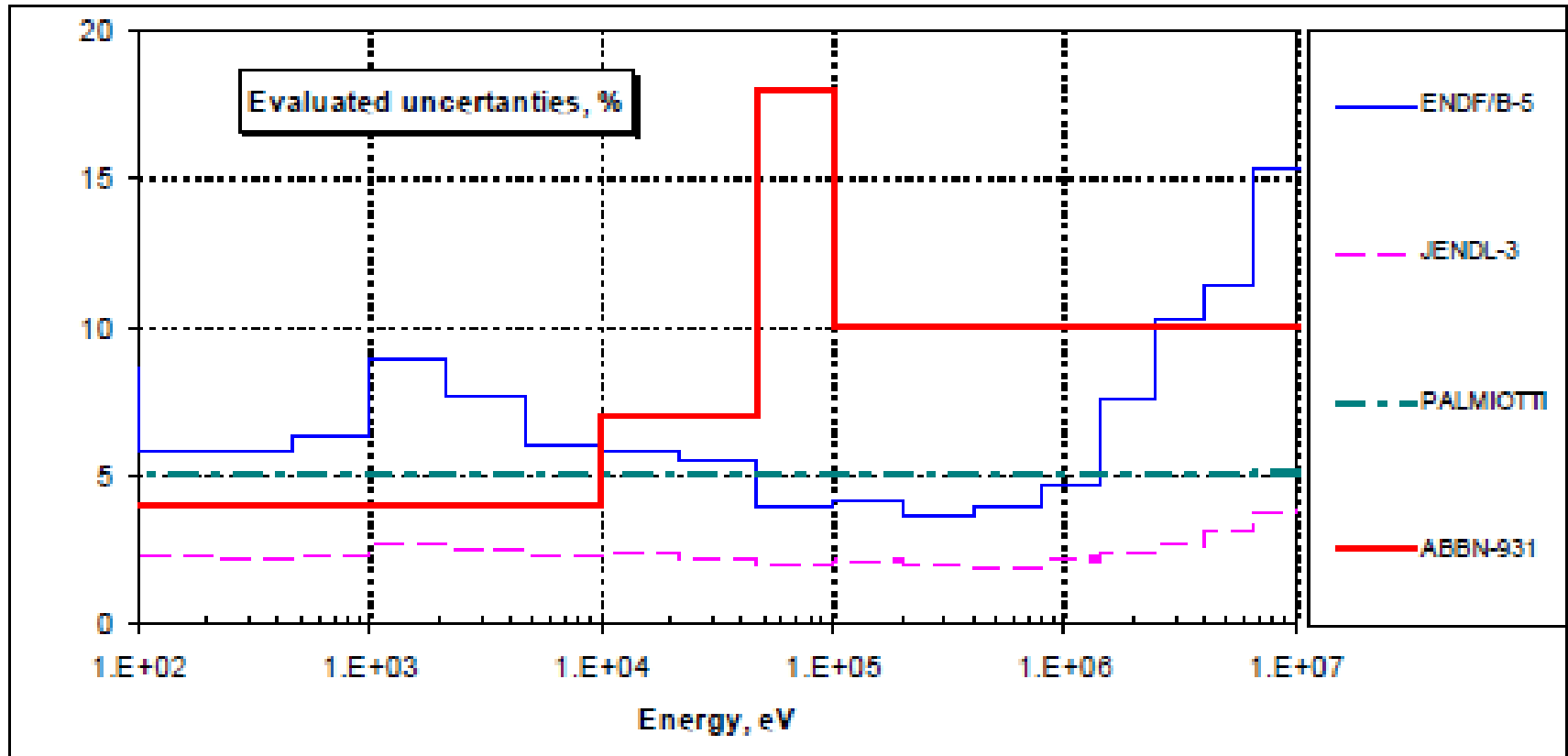


23-Na total, uncertainties

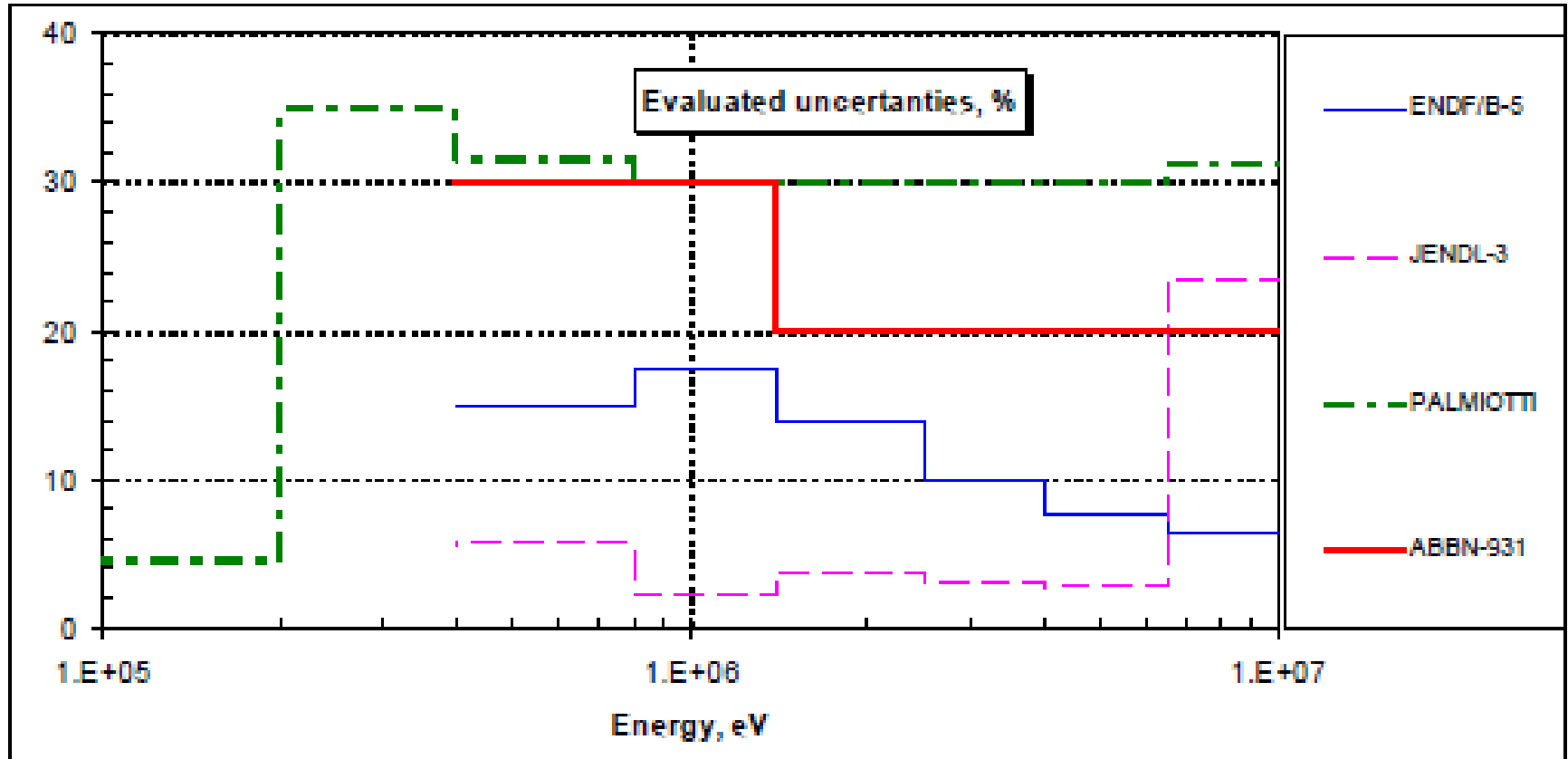
Analysis taken from RUSFOND report



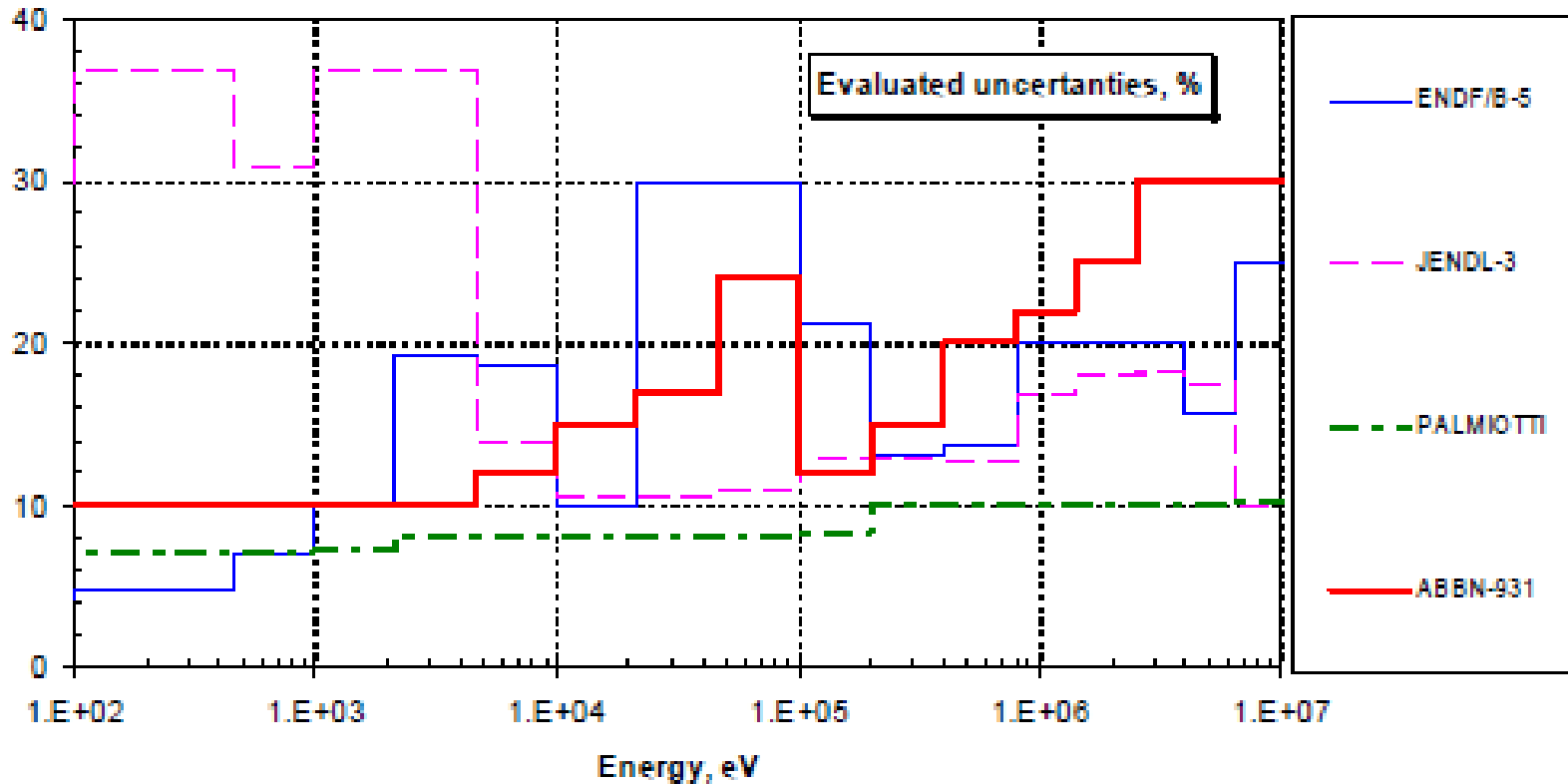
23-Na elastic, uncertainties



23-Na inelastic, uncertainties



23-Na capture, uncertainties



Our approach adopted for 23-Na

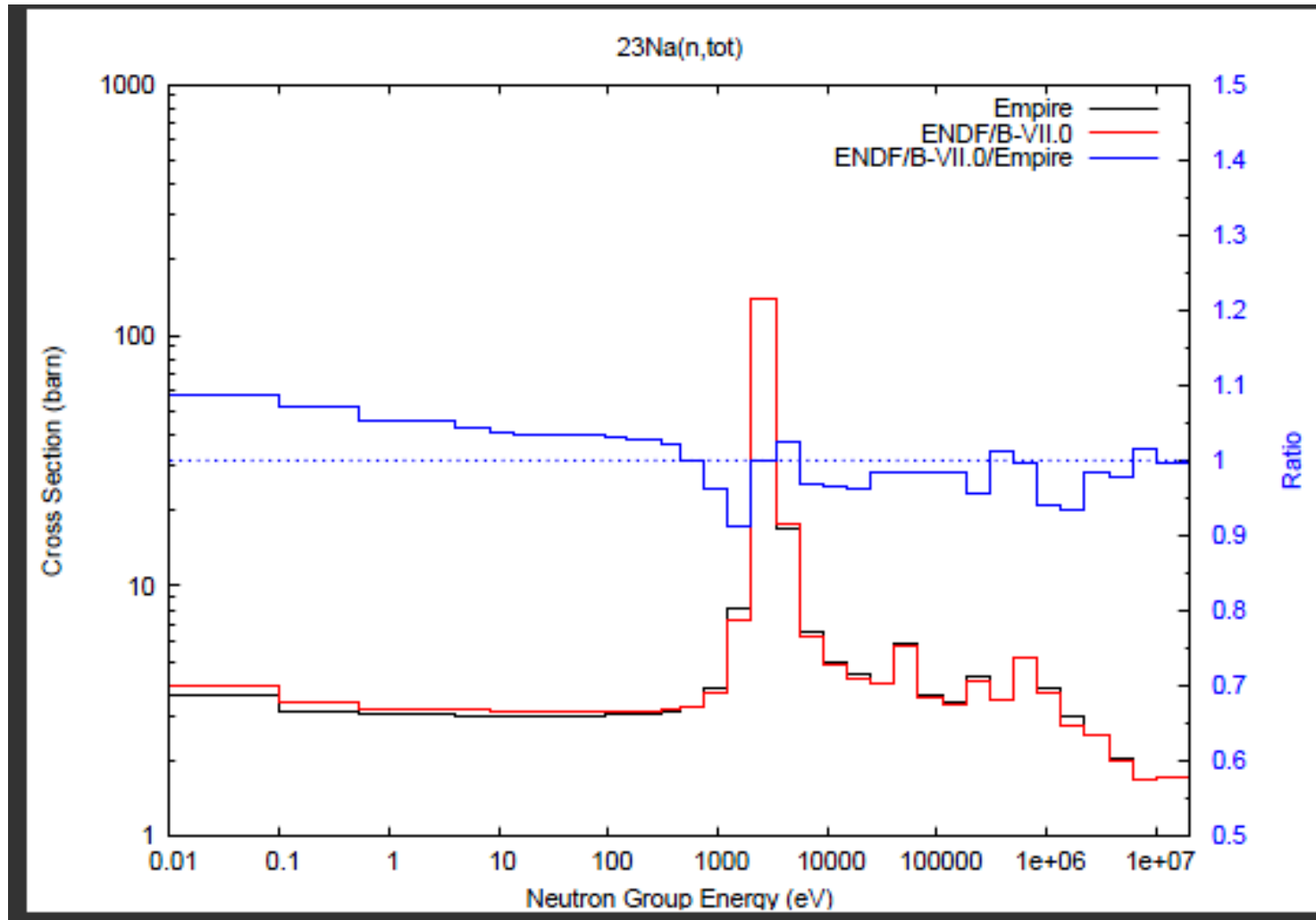
- Give up attempt to reproduce fluctuations via EMPIRE parameterization, it is too complicated and time consuming. (We did so later!)
- Select parameters p_k and their **covariances** so that EMPIRE can reasonably reproduce ENDF/B-VII.0 on the multigroup level, not trivial!
 - ❑ multigroup cross sections
 - ❑ multigroup cross section uncertainties
- Produce **diff file**, obtained as difference between EMPIRE and VII.0 for each reaction channel in the entire energy range:
 - ❑ **diff** = additive constants, precisely known, with strong energy dependence
 - ❑ these additive constants do not contribute to sensitivities
 - ❑ diff file should be stored and used when VII.0 update is constructed
- Calculate **sensitivities** for the above set of parameters.

Our approach adopted for 23-Na

- *Action on INL → produce modified set of parameters.*
- Produce **updated file** by using modified set of parameters and by adding back diff file to reproduce fluctuations.

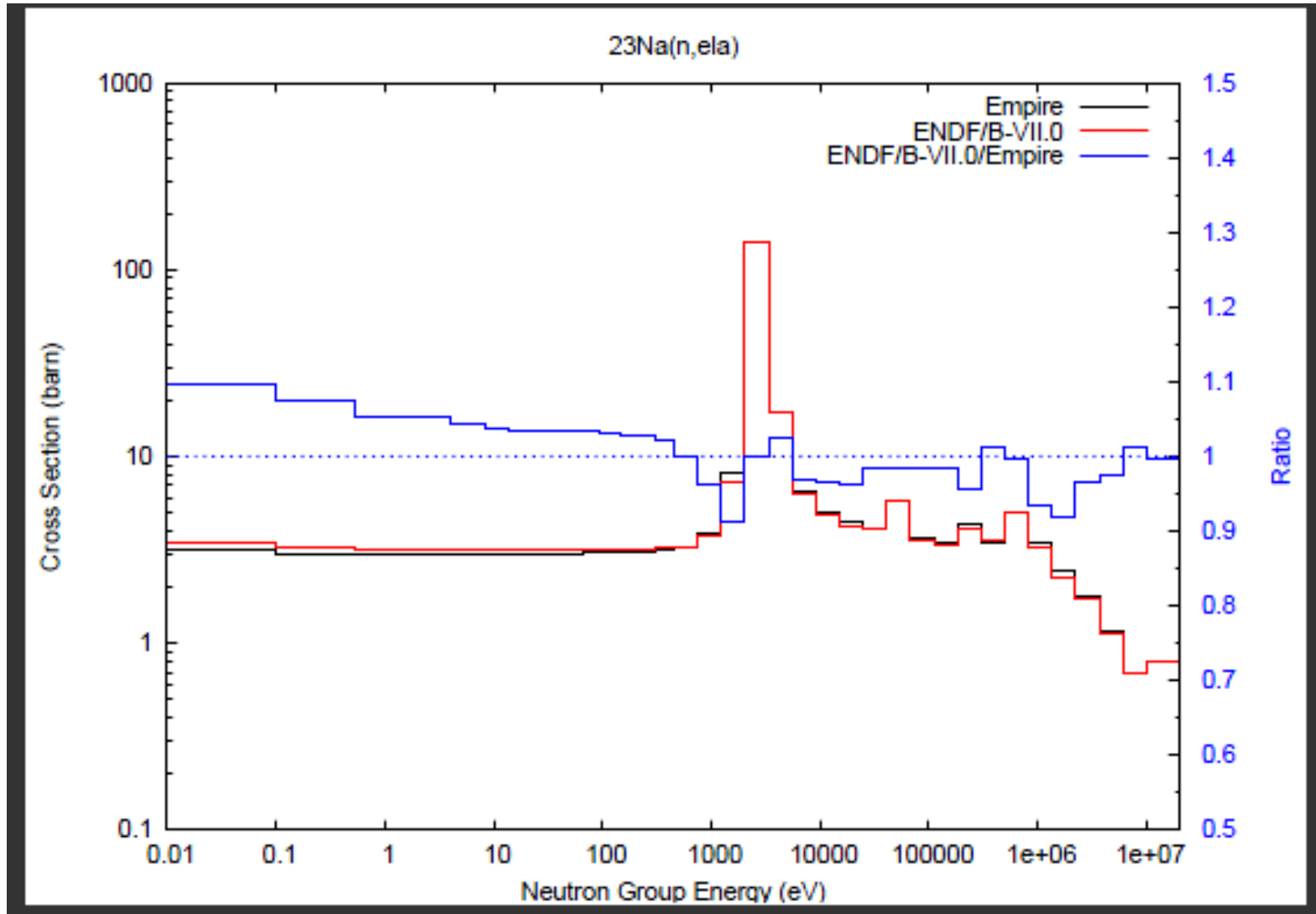
23-Na multigroup cross sections, total

33-groups, ENDF/B-VII.0 versus EMPIRE



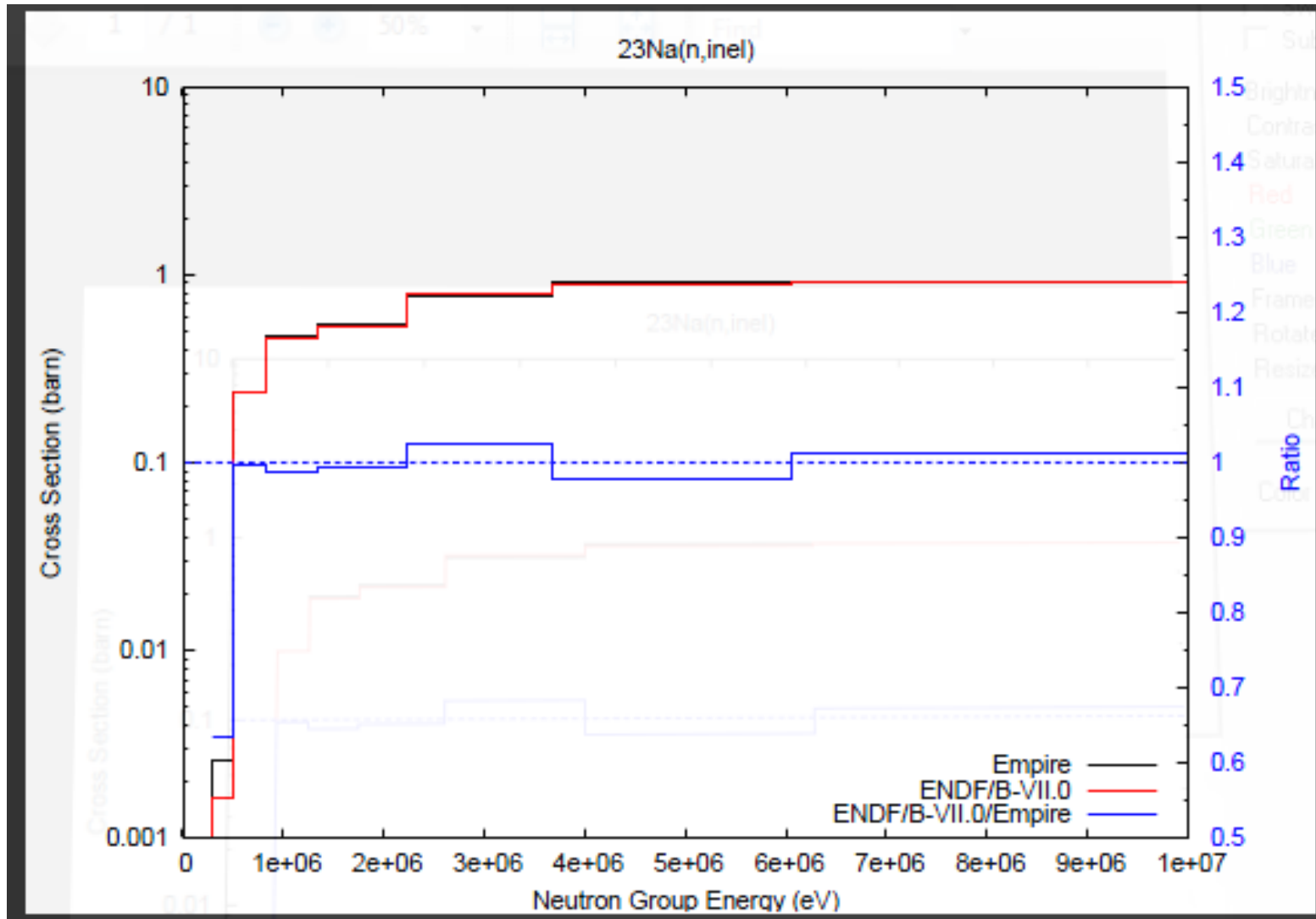
23-Na multigroup cross sections, elastic

33-groups, ENDF/B-VII.0 versus EMPIRE



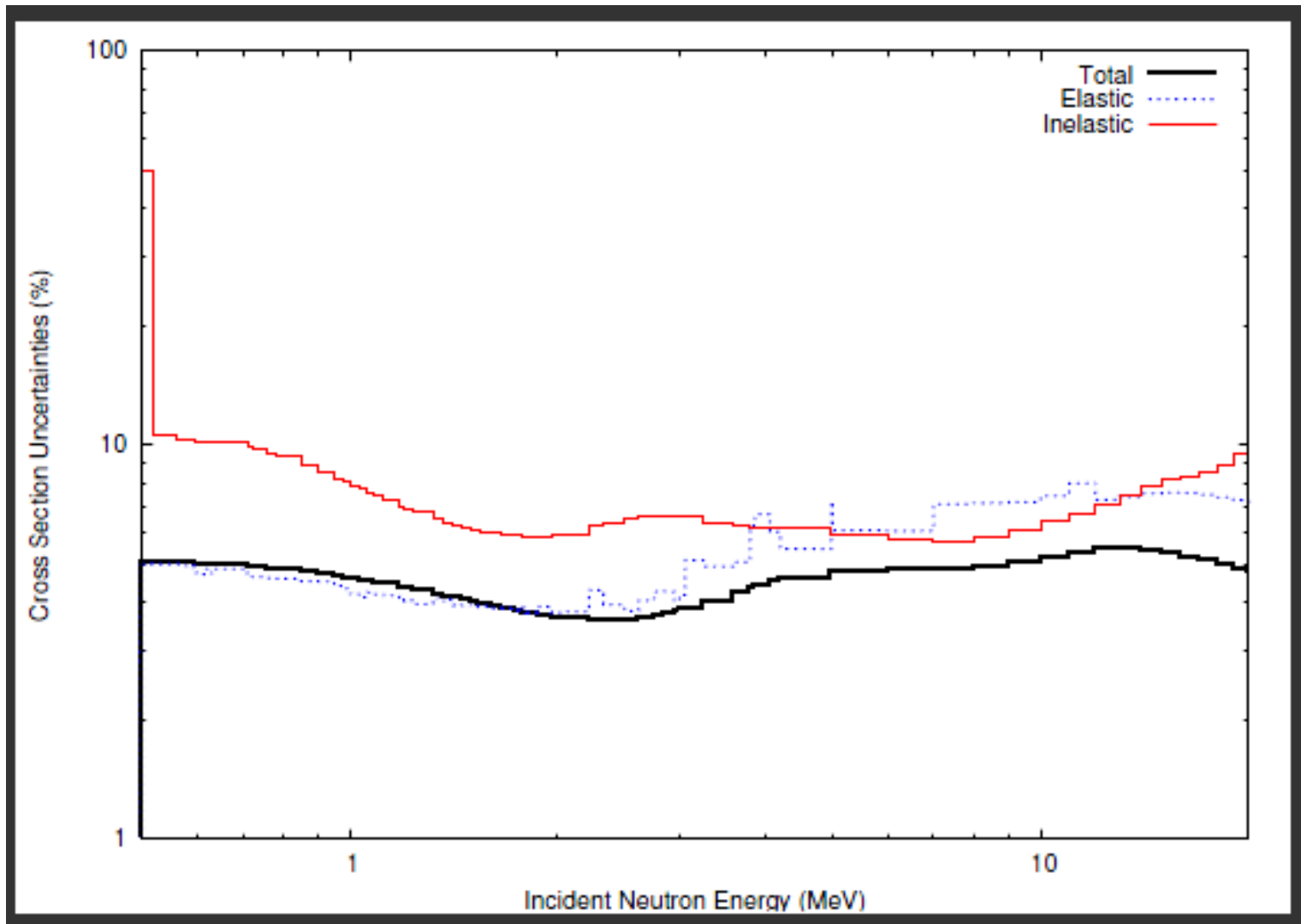
23-Na multigroup cross sections, inelastic

33-groups, ENDF/B-VII.0 versus EMPIRE



23-Na multigroup cs uncertainties

EMPIRE, pointwise values, fast region



Conclusions

We produced initial estimate of parameters for 23-Na (15 in RR region, 16 in fast region) and their covariances and produced sensitivities in 33-groups.

Lessons learned and issues:

1. We focused on elastic and inelastic, up to 10 MeV, **is this sufficient?**
2. To reproduce ENDF/B-VII.0 evaluation with EMPIRE cannot be done exactly (fluctuations, MF33 background, ...), further effort is needed to reach **~1%** (**is this reasonable requirement?**) agreement on the 33-group level in terms of cross sections.
3. Our parameter covariances propagate to **cross sections uncertainties**. Are our values reasonable?
4. ENDF/B-VII.0 dates back to **1977** and it would be desirable to **reevaluate** it first. This would require 3-6 months of effort. Can we afford it?
5. **Diff** file of additive constants is needed to reproduce fluctuations in ENDF/B-VII.0. The idea has **not been tested** yet.

Actions from the March meeting

1. New group structure will be supplied by INL, will add ~10 groups to current 33.
2. INL will supply list of ~10 resonances for which sensitivities should be calculated.
3. Our approach to go only up to ~10 MeV is ok.
4. When reproducing ENDF/B-VII.0 with EMPIRE we should reach ~5% agreement on the multigroup level, ~1% might be desirable but it is not necessary.
5. Uncertainties in inelastic should be ~20%, our current values (~10%) are too optimistic.
6. One can also use Empire file for assimilation directly, without the need to use diff file. We should do both: Empire file and ENDF/B-VII.0 file.
7. Full re-evaluation of 23-Na should not be done.
8. Hany Abdel-Khalik wants explicit values (+ Δ , - Δ) from Marco to check nonlinearities.

Progress since March 2009

Group structure

- New 41-energy group structure established, tailored to ^{23}Na .

Evaluation in parameter space

- RRR evaluations extended to 1 MeV
- Two tuning energy-dependent parameters introduced in fast region (total cs, absorption cs) to reproduce fluctuations
- Set of 40 parameters produced
 - RRR (ML Breit-Wigner) = 18 parameters
 - Fast region (OM, HF, preeq exciton) = 20 parameters
 - Fast region (tuning) = 2 parameters
- Improved analysis of covariances performed \rightarrow covariances in parameter space produced

Sensitivities

- Sensitivities to 40 parameters were calculated, $\Delta\sigma_j/\Delta p_k$
- Results supplied to INL