Progress on TALYS data evaluation system (WP2)

Arjan Koning
NRG

ANDES annual meeting
April 23-24, 2012
NEA Data Bank, Issy-les-Moulineaux

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- State of the TALYS empire
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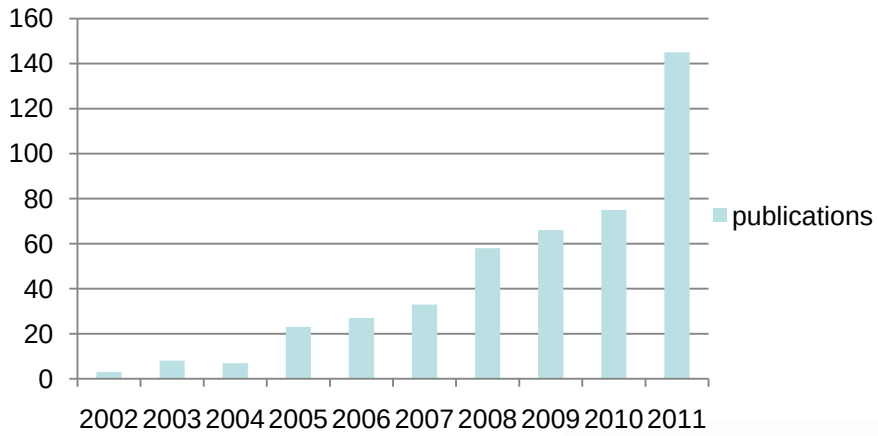
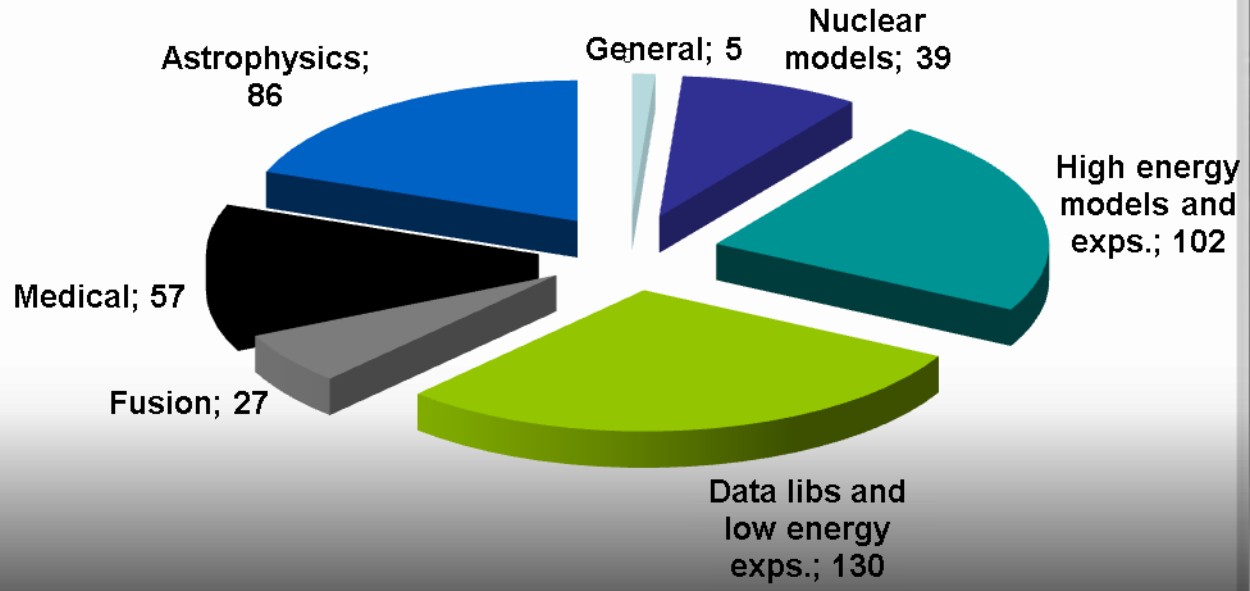
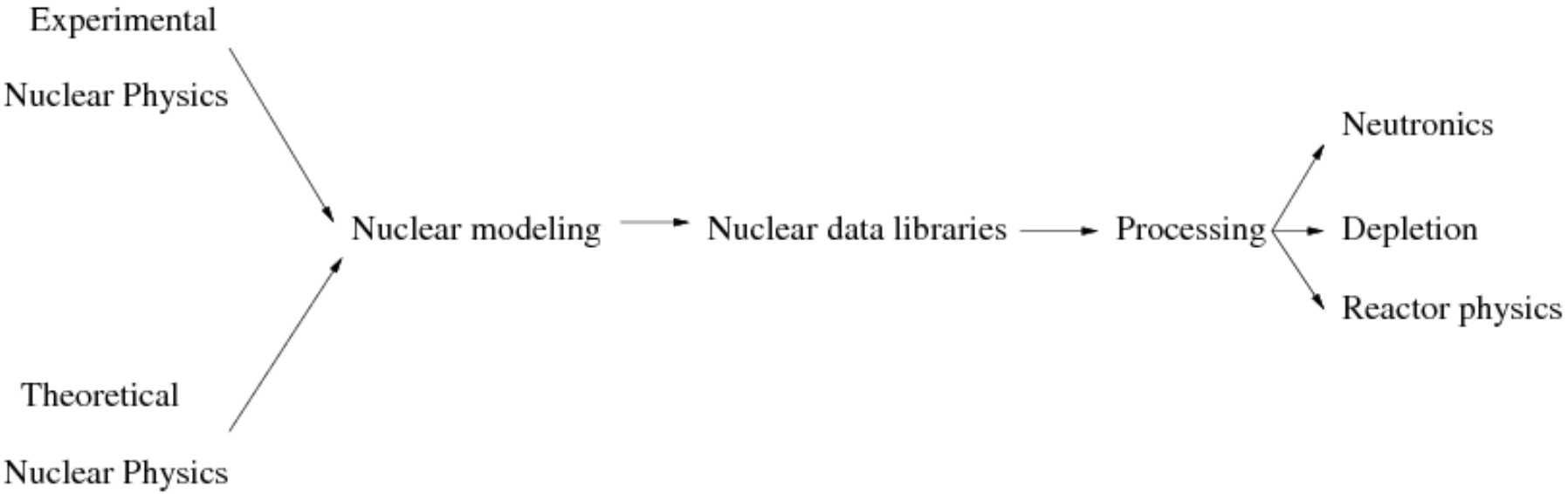
TALYS publications





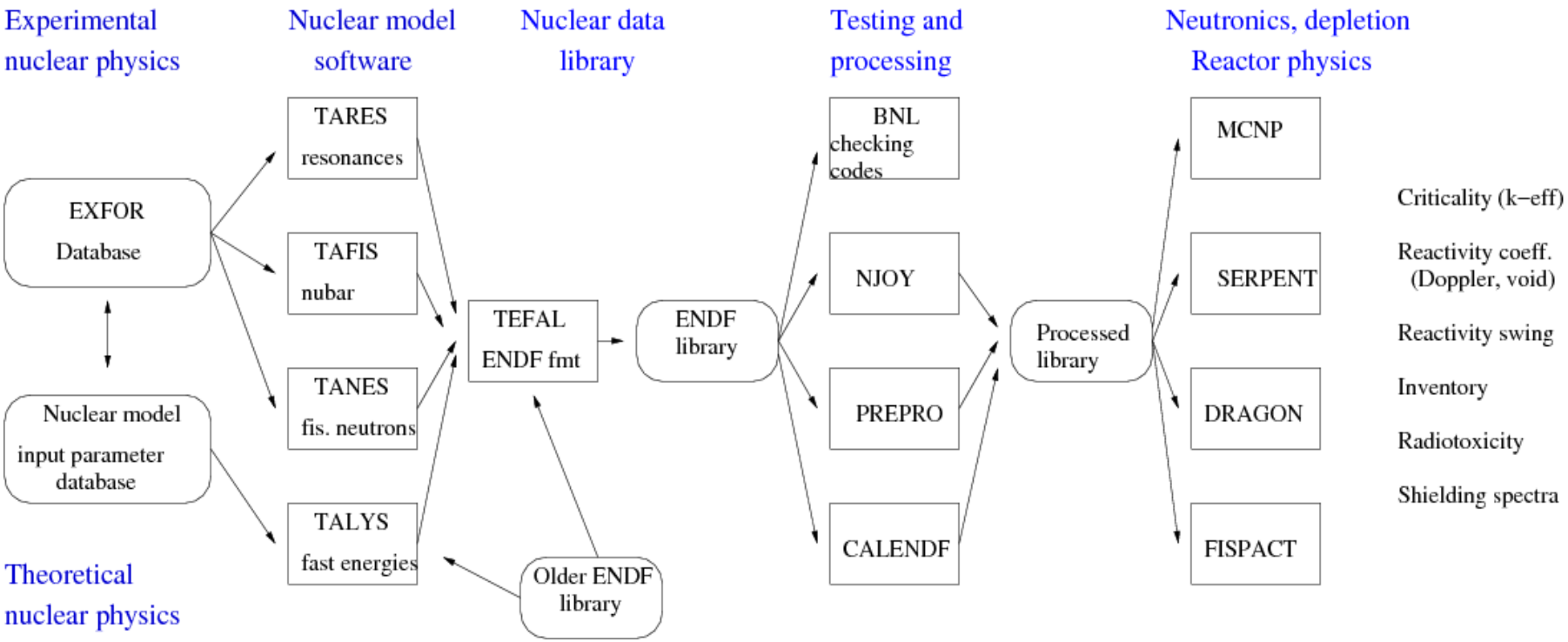
Automating nuclear science



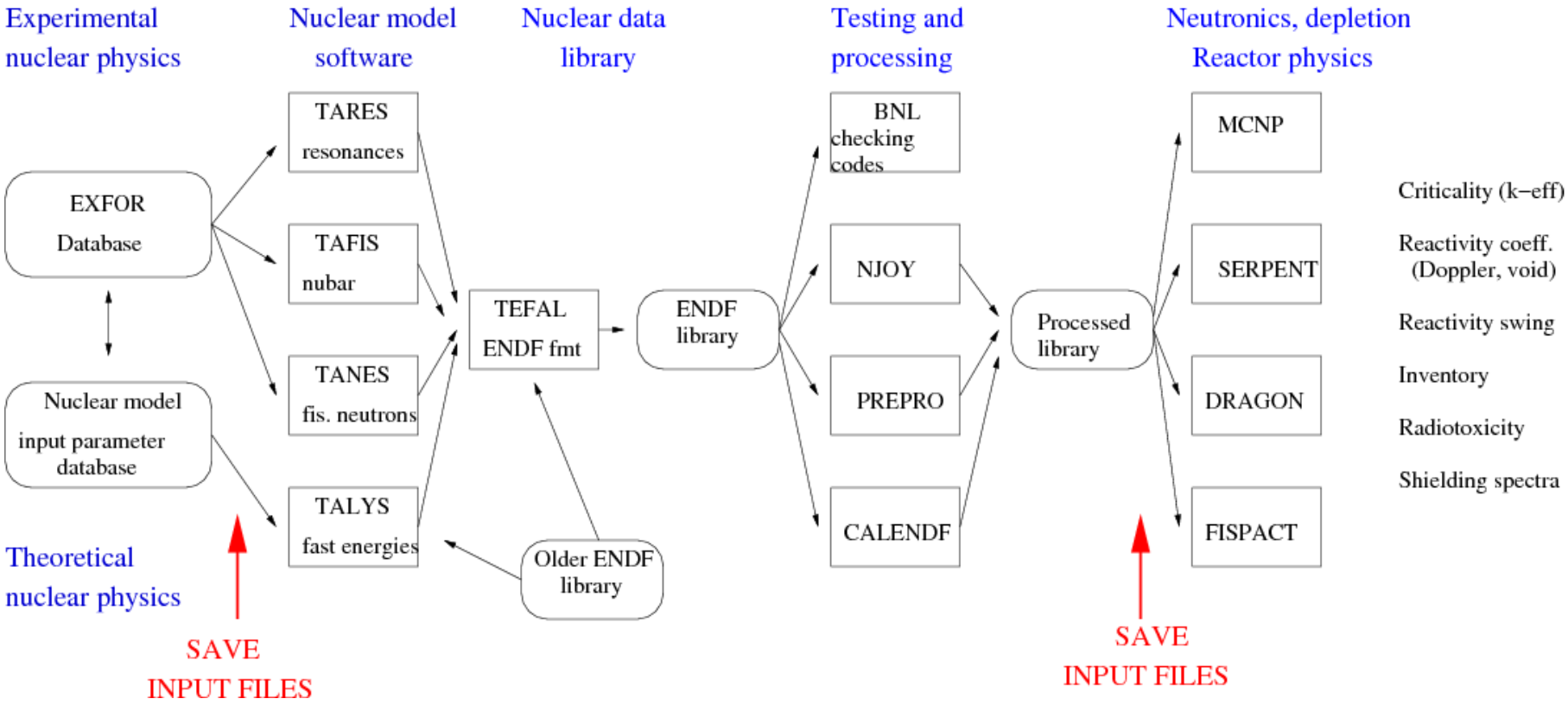
Road to success:

- Use (extremely) robust software
- Store all human intelligence per isotope in input files and scripts

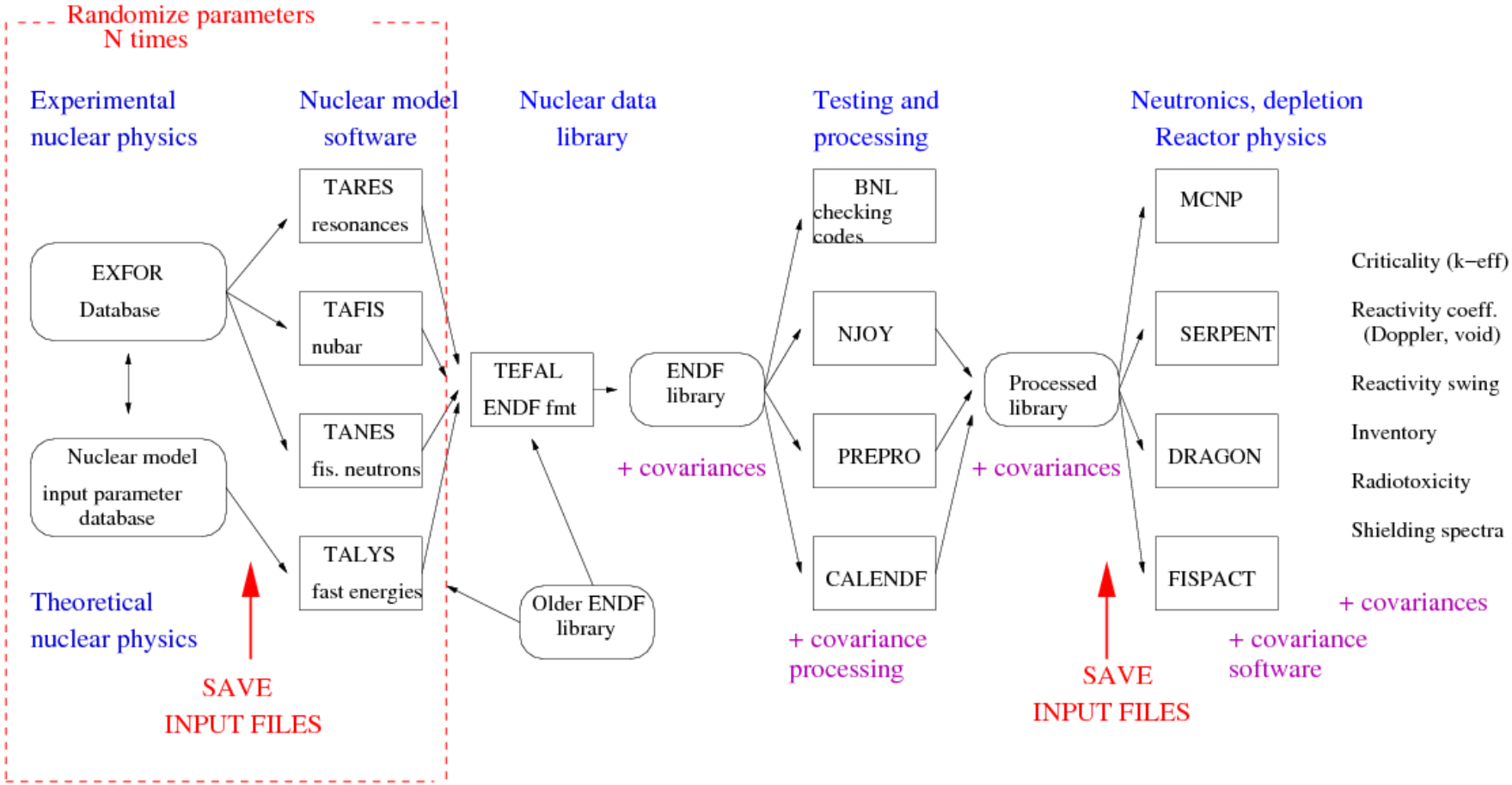
Automating nuclear science: Software



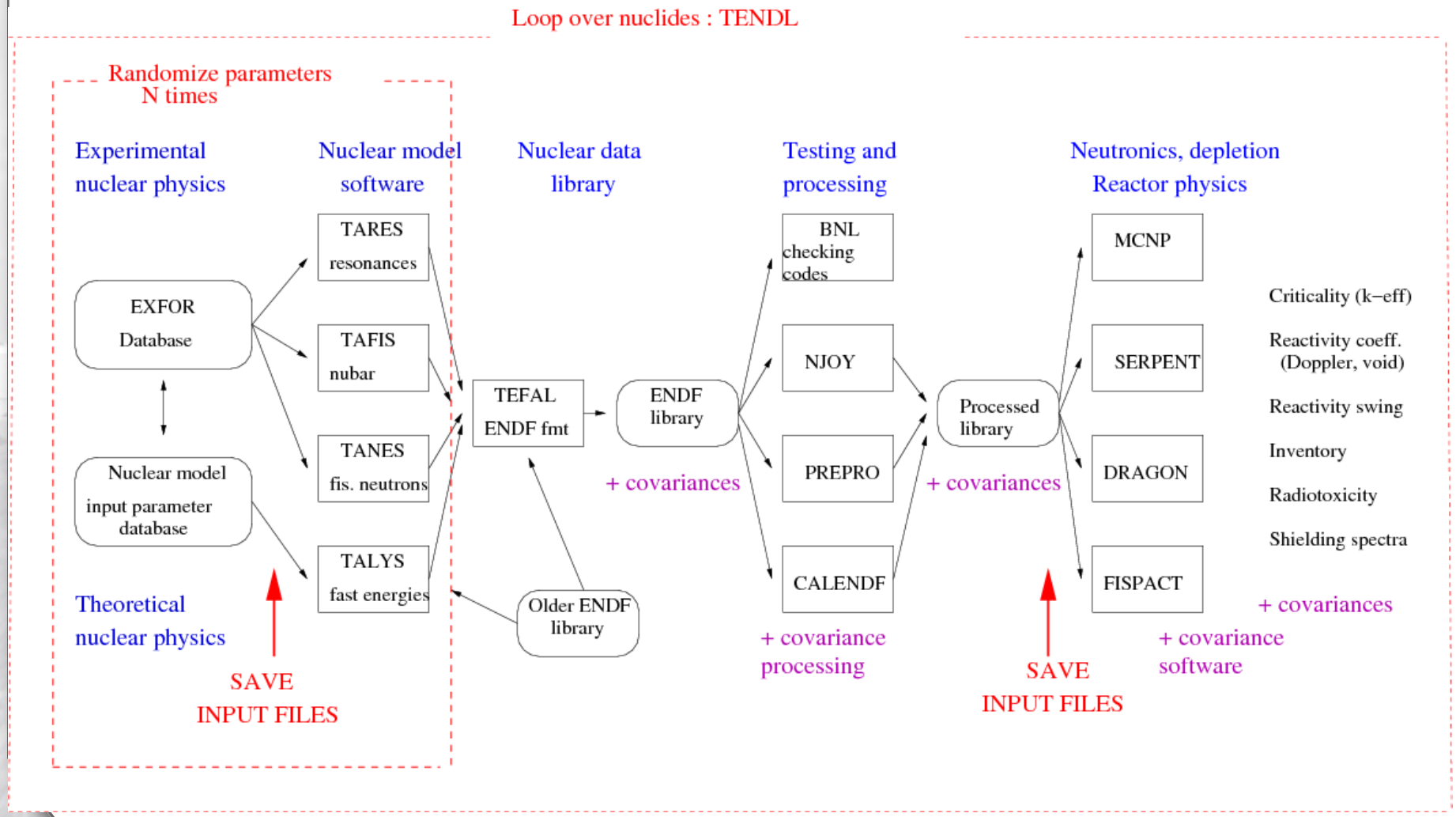
Automating nuclear science: Reproducibility



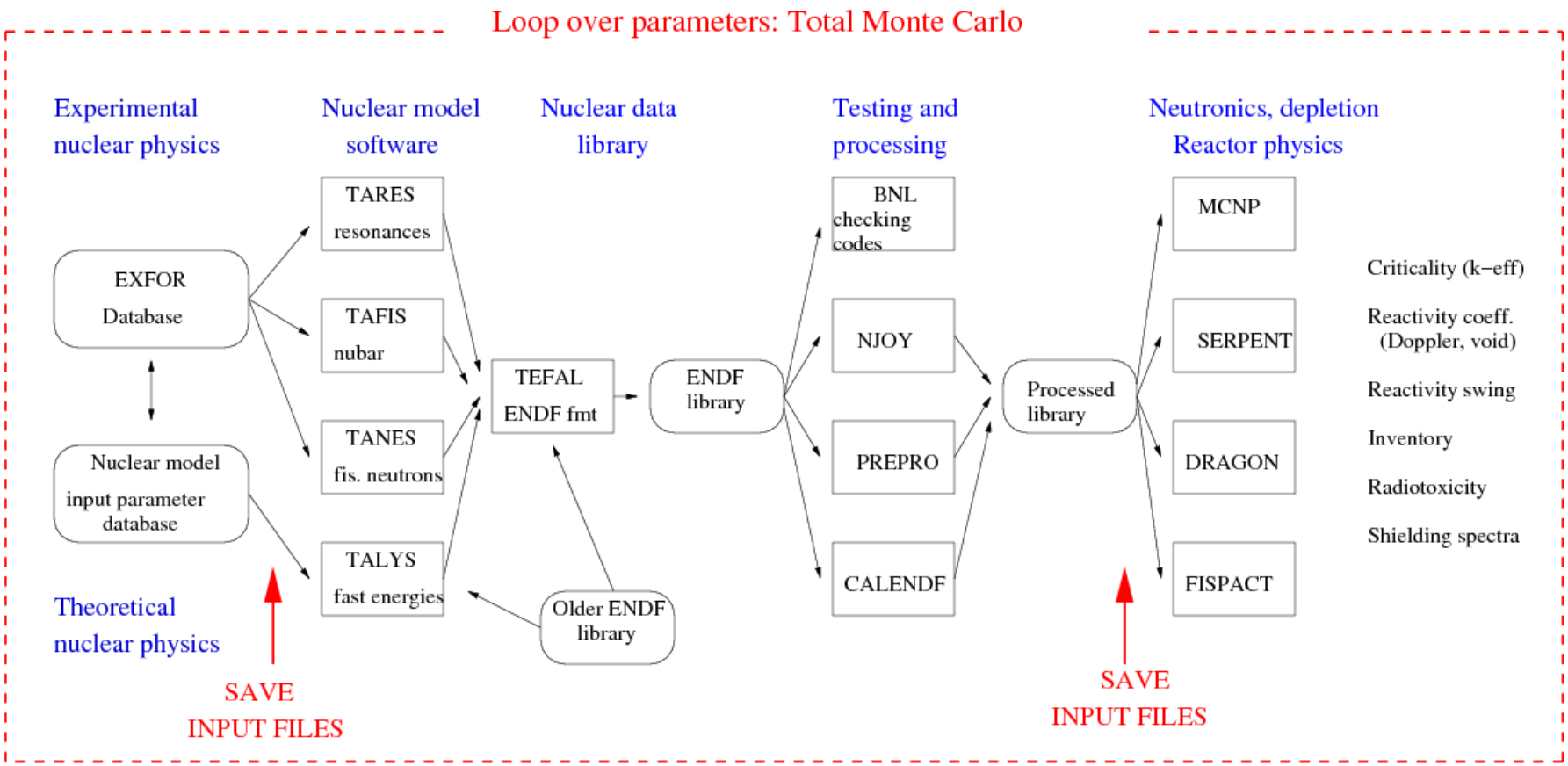
Automating nuclear science: Covariances



Automating nuclear science: Complete nuclear data library



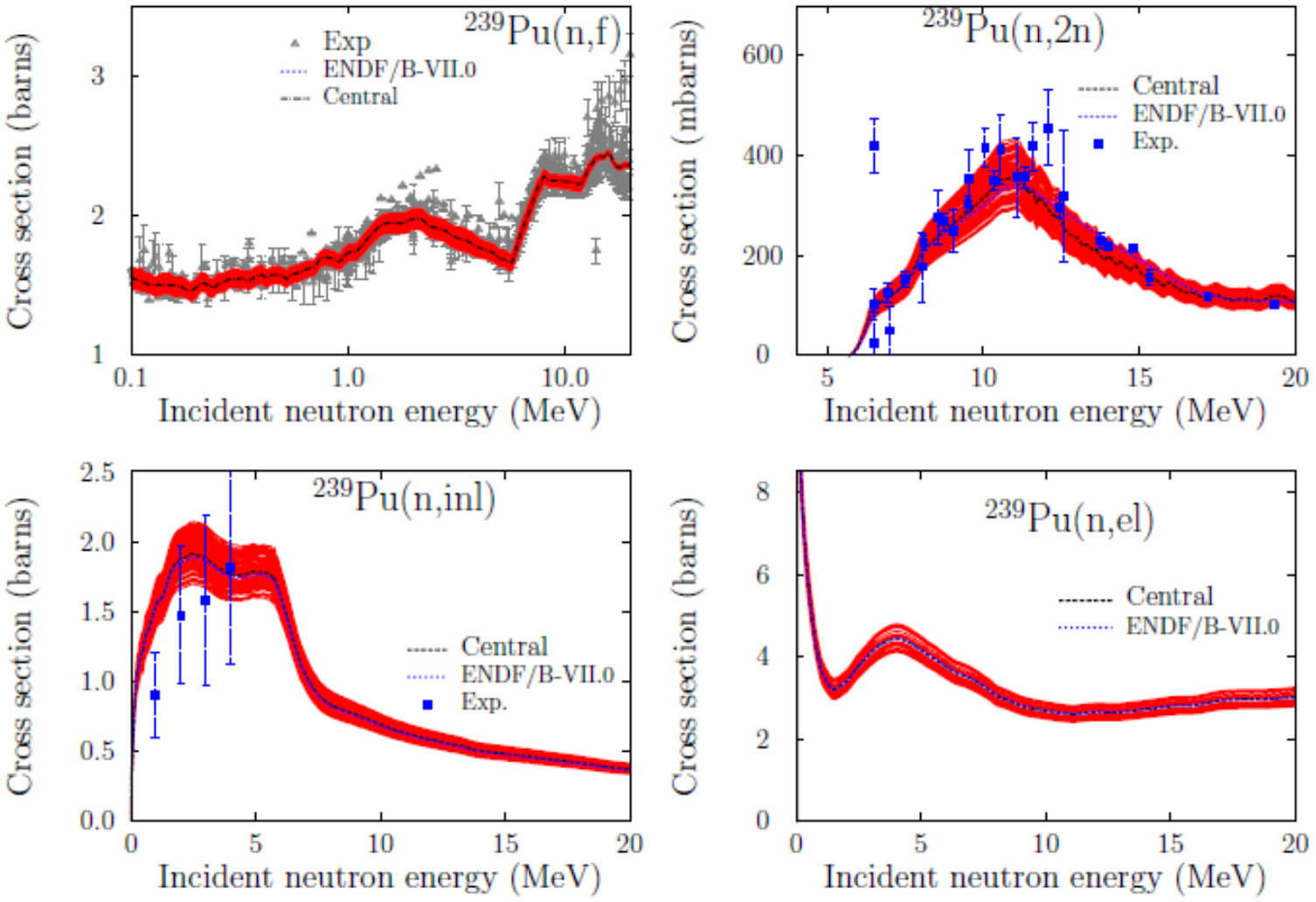
Automating nuclear science: Total Monte Carlo



Nuclear modeling for Pu-239

- Optical model: adjusted version of Soukhovitskii potential
- Level densities adjusted for each fission barrier
- Fission barrier parameters adjusted
- Pre-equilibrium strength adjusted
- A total of 25 adjusted parameters, rest default
- Final (small) empirical renormalization to experimental data
- Randomizing data takes place around that optimum
- Unphysically small uncertainties of theoretical parameters are needed to simulate (very) small experimental uncertainties.
- ….but it works great!

Pu239 cross sections + uncertainties

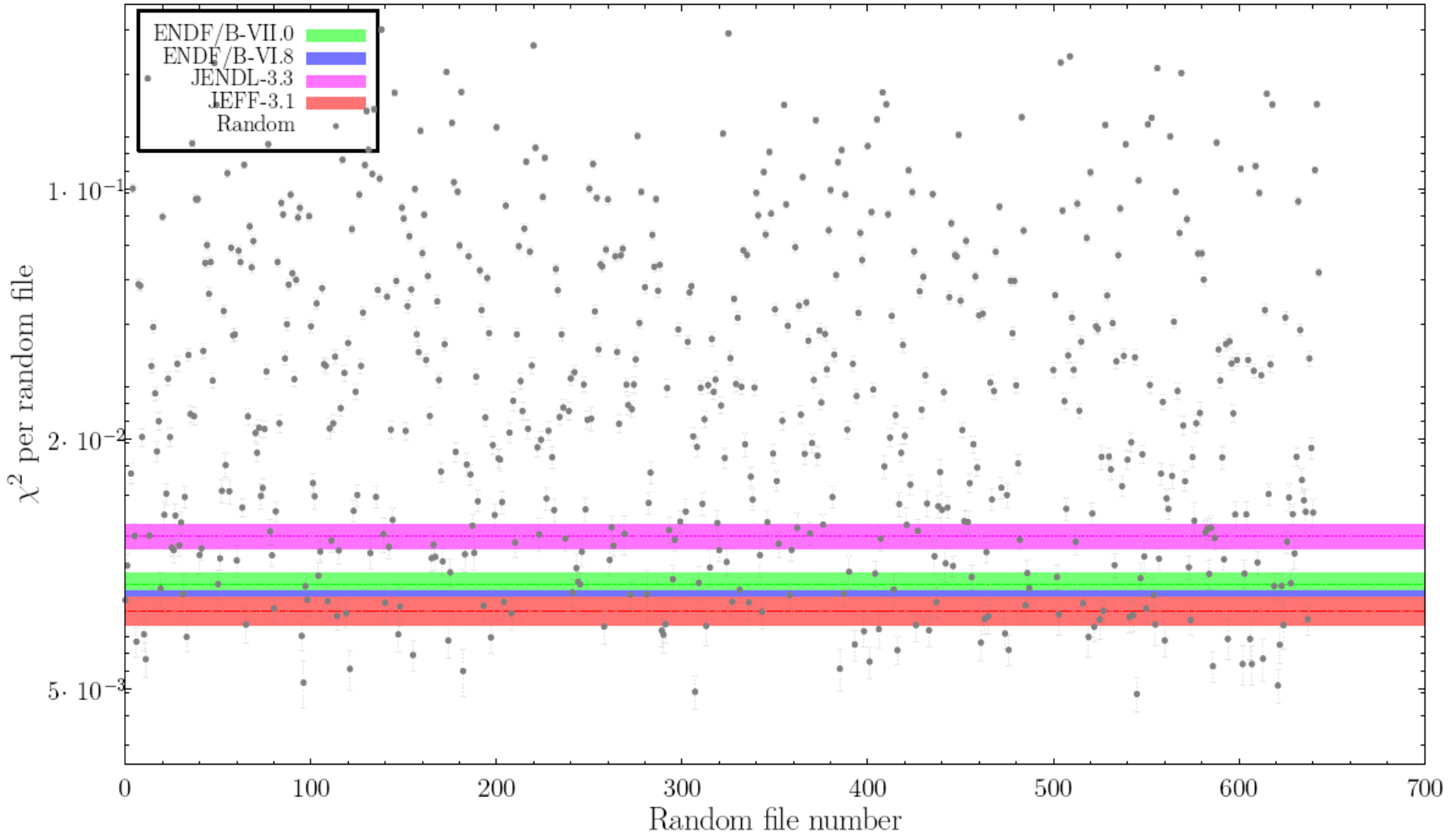


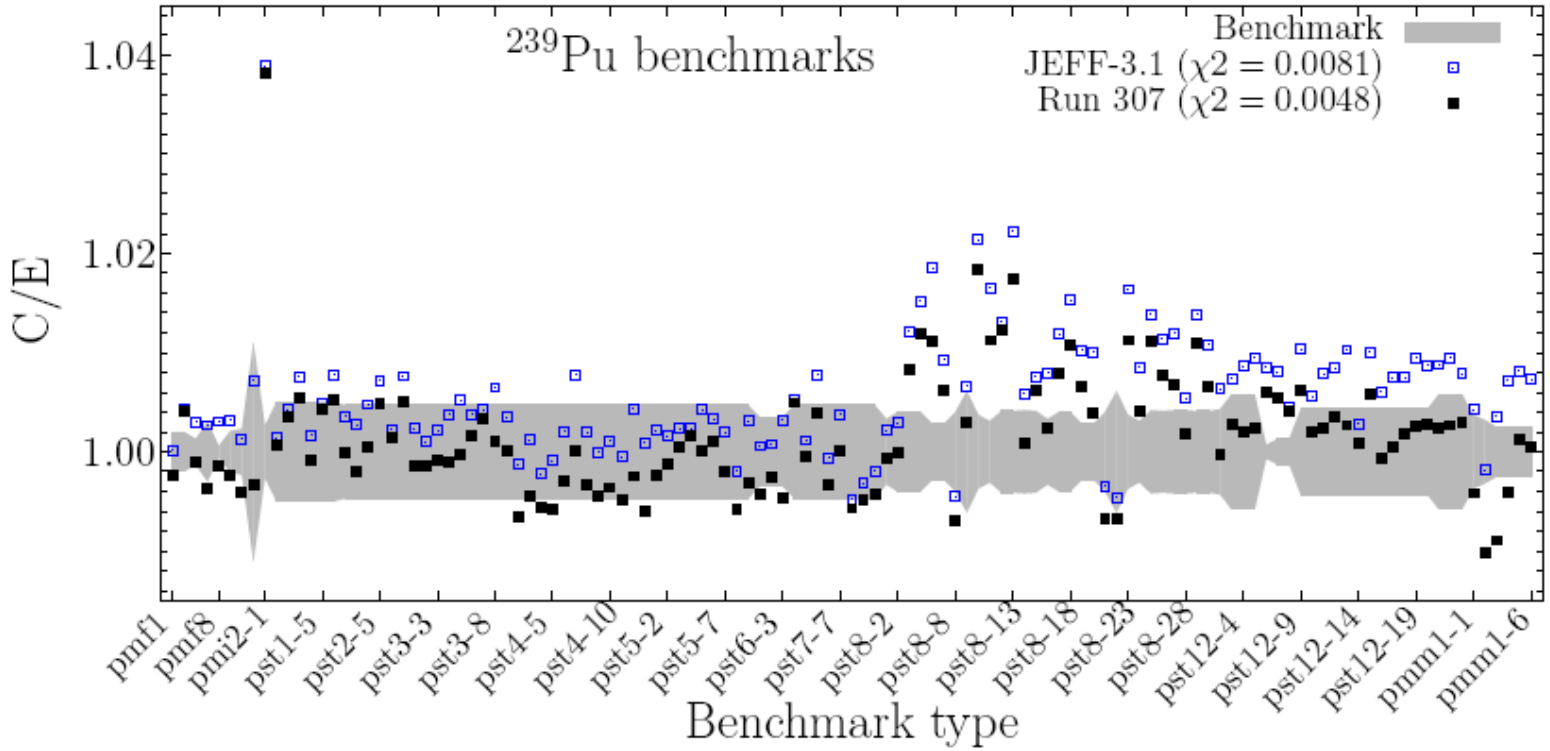
Optimization of Pu-239

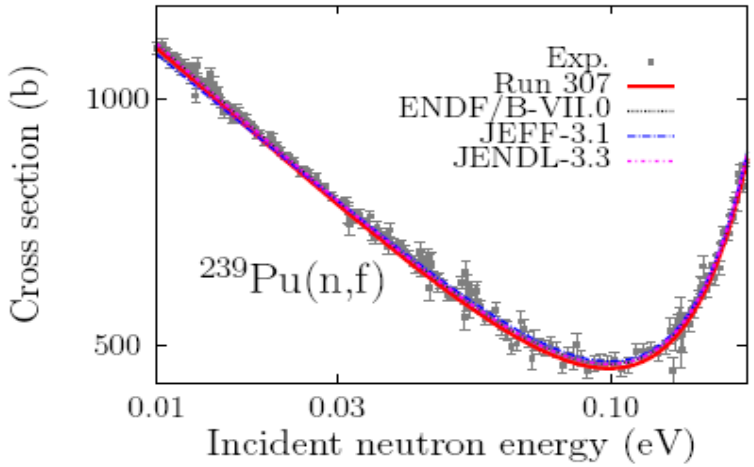
- Select 120 ICSBEP benchmarks
- Create 630 random Pu-239 libraries, all within, or closely around, the uncertainty bands
- Do a total of 120 x 630 =75600 MCNP criticality calculations
- Do another 120 x 4 calculations:

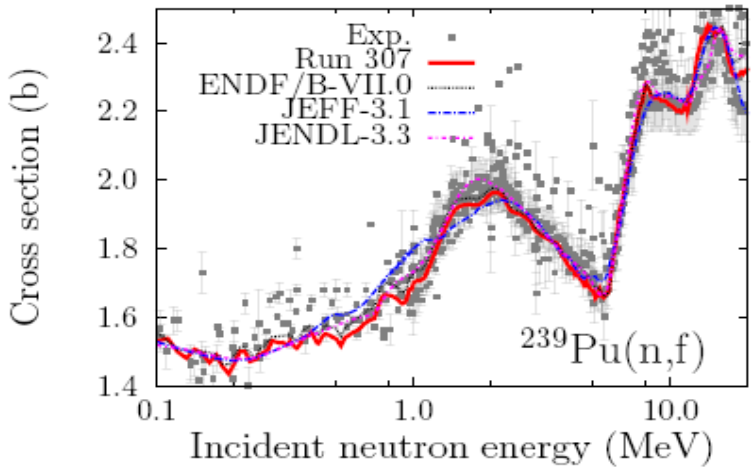
  - for JEFF-3.1, $\chi^2 = 8.08e^{-3} +/- 7.2e^{-4}$
  - for ENDF/B-VII.0, $\chi^2 = 9.55e^{-3} +/- 7.9e^{-4}$
  - for ENDF/B-VI.8, $\chi^2 = 8.45e^{-3} +/- 7.2e^{-4}$
  - for JENDL-3.3, $\chi^2 = 1.31e^{-2} +/- 1.0e^{-3}$

Optimization of Pu-239




^{239}Pu benchmarks
Benchmark
JEFF-3.1 ($\chi 2 = 0.0081$)
Run 307 ($\chi 2 = 0.0048$)
C/E
1.04
1.02
1.00
pmf1
pmf8
pmi2-1
pst1-5
pst2-5
pst3-3
pst3-8
pst4-5
pst4-10
pst5-2
pst5-7
pst6-3
pst7-7
pst8-2
pst8-8
pst8-13
pst8-18
pst8-23
pst8-28
pst12-4
pst12-9
pst12-14
pst12-19
pmm1-1
pmm1-6
Benchmark type


Exp.
Run 307
ENDF/B-VII.0
JEFF-3.1
JENDL-3.3
^{239}Pu(n,f)
Cross section (b)
1000
500
0.01
0.03
0.10
Incident neutron energy (eV)


Exp.
Run 307
ENDF/B-VII.0
JEFF-3.1
JENDL-3.3
^{239}Pu(n,f)
Cross section (b)
2.4
2.2
2.0
1.8
1.6
1.4
0.1
1.0
10.0
Incident neutron energy (MeV)

Some publications

D. Rochman and A.J. Koning, ``How to randomly evaluate nuclear data: a new method applied to Pu-239'', Nucl. Sci. Eng. 169(1), 68 (2011).

D. Rochman, A.J. Koning, S.C. van der Marck, A. Hogenbirk and C.M. Sciolla, ``Nuclear data uncertainty propagation: Perturbation vs. Monte Carlo'', Ann. Nuc. En. 38, 942 (2011).

D. Rochman, A.J. Koning, D.F. da Cruz, ``Uncertainties for the Kalimer Sodium Fast Reactor: void coefficient, keff, Beff, burn-up and radiotoxicity'' , Jap. Journ. Sci. Techn. 48 (8) 1193 (2011).

S. Goriely, S. Hilaire, A.J. Koning and R. Capote, ``Towards improved evaluation of neutron-induced cross section on actinides'', Phys. Rev. C83, 034601 (2011).

D. Rochman and A.J. Koning, ``Evaluation and adjustment of the neutron-induced reactions of 63,65Cu'', Nucl. Sci. Eng. 170 (3), 265 (2012).

D. Rochman, A.J. Koning and D. da Cruz, ``Propagation of 235,236,238U and 239Pu nuclear data uncertainties for a typical PWR fuel element'', to be published (2012).

Conclusions

- For uncertainty propagation, TMC is an easier tool than covariances + perturbation + sensitivity. It is also more exact: all correlations are taken into account.
- However, the world wants covariances, and they get covariances (TENDL)
- With a reproducible automated system, almost anything is possible. After some years of serious software development we can now fork into various branches:
  - TALYS Evaluated Nuclear Data Library (TENDL) including complete covariance data (MF31-35)
    - 2012: Zooming in on high-quality data per nuclide for the “Manhattan project” (ND2013 in New York)
  - Total Monte Carlo uncertainty propagation
  - Nuclear data library optimization
  - Other applications (not discussed here)

ANDES is the most important contributor to this.