From nuclear data to nuclear reactors

Looping over nuclear science

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NRG Petten

The Netherlands

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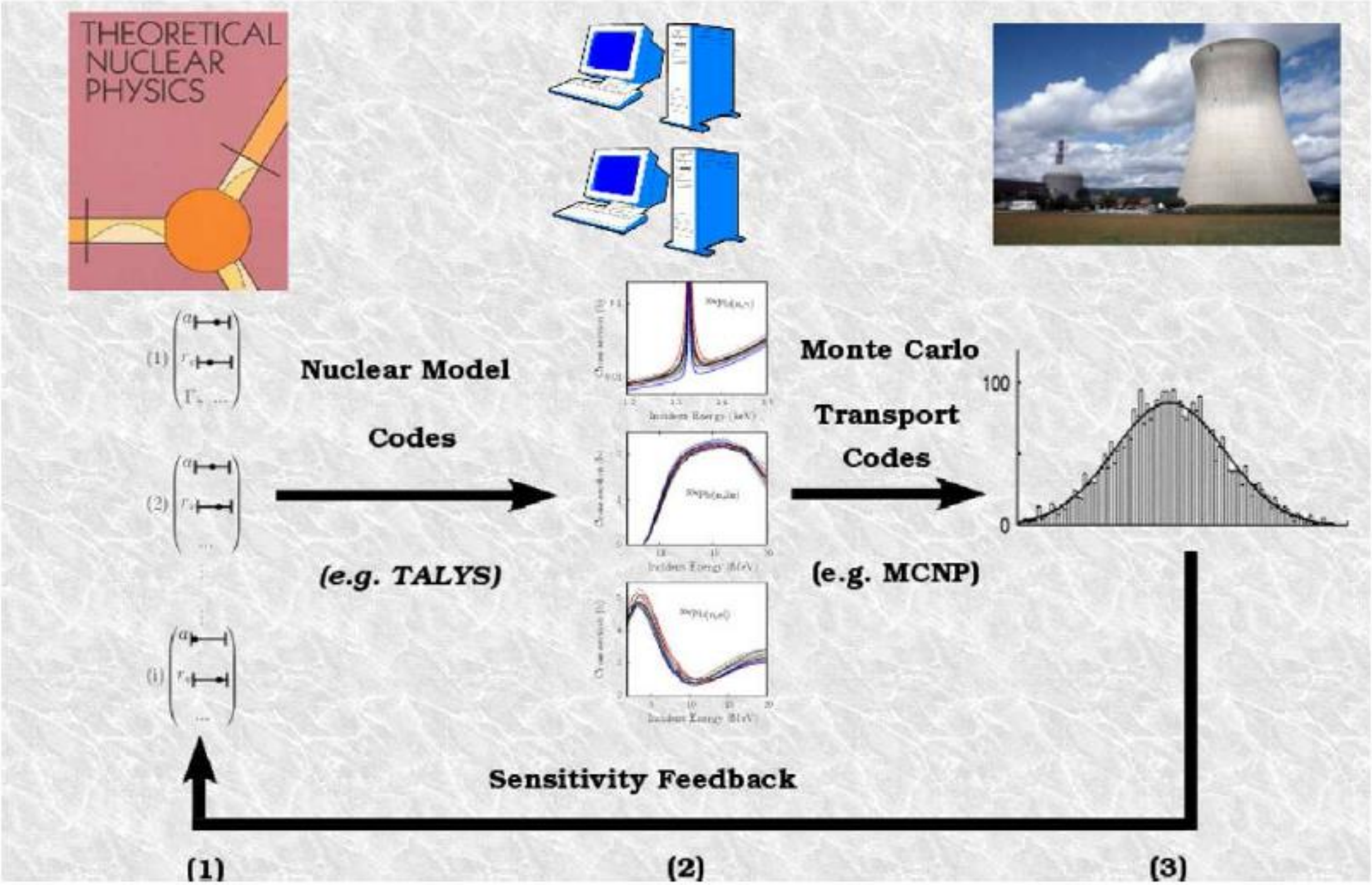
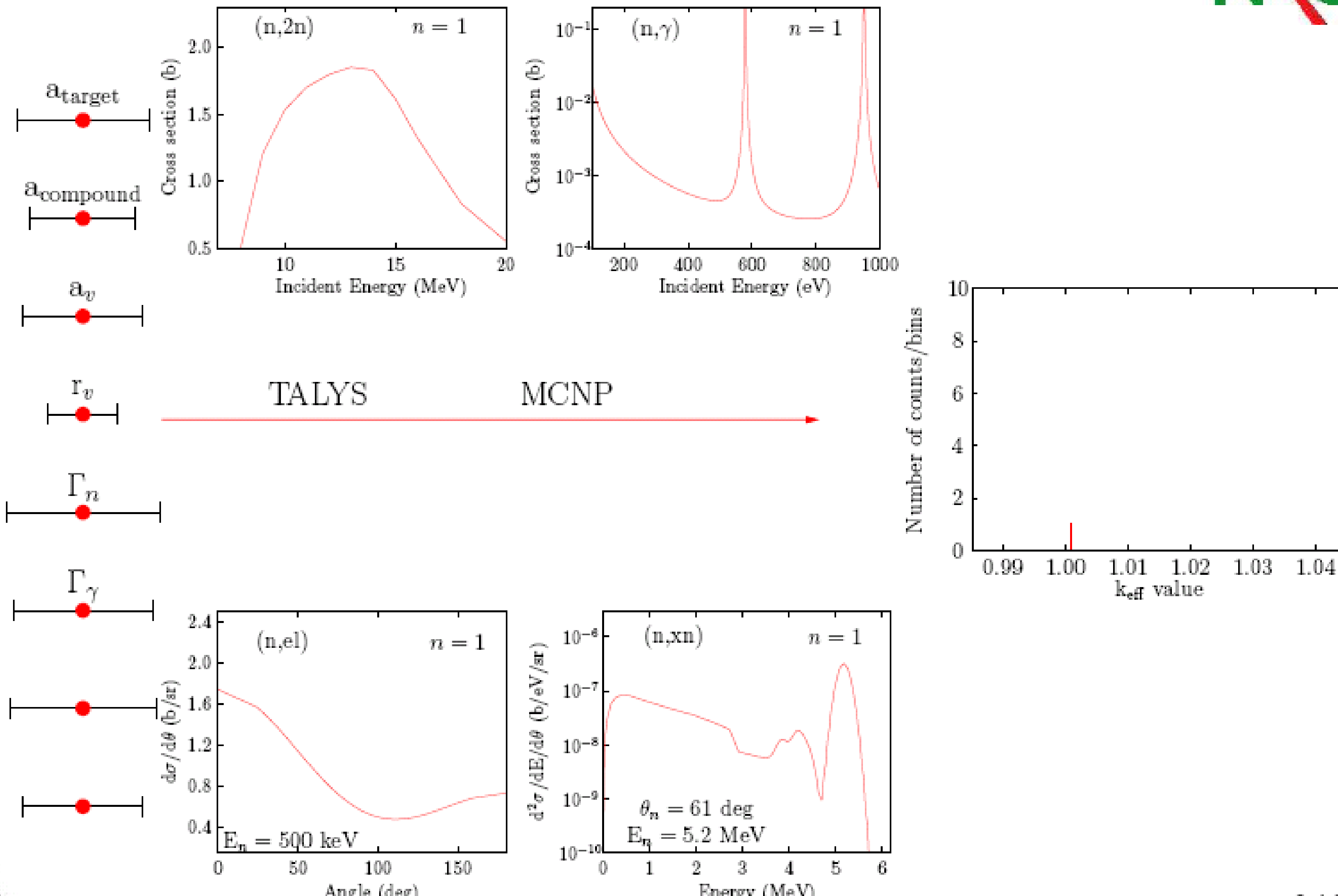
P(ND)^2-2, CEA-DAM, Bruyeres-le-Chatel

From nuclear data to reactors



A.J. Koning and D. Rochman, ``Towards sustainable nuclear energy: Putting nuclear physics to work'', Ann. Nuc. En. 35, p. 2024-2030 (2008).

“1000 ×(Talys + ENDF + NJOY + MCNP) calculations for Pb”



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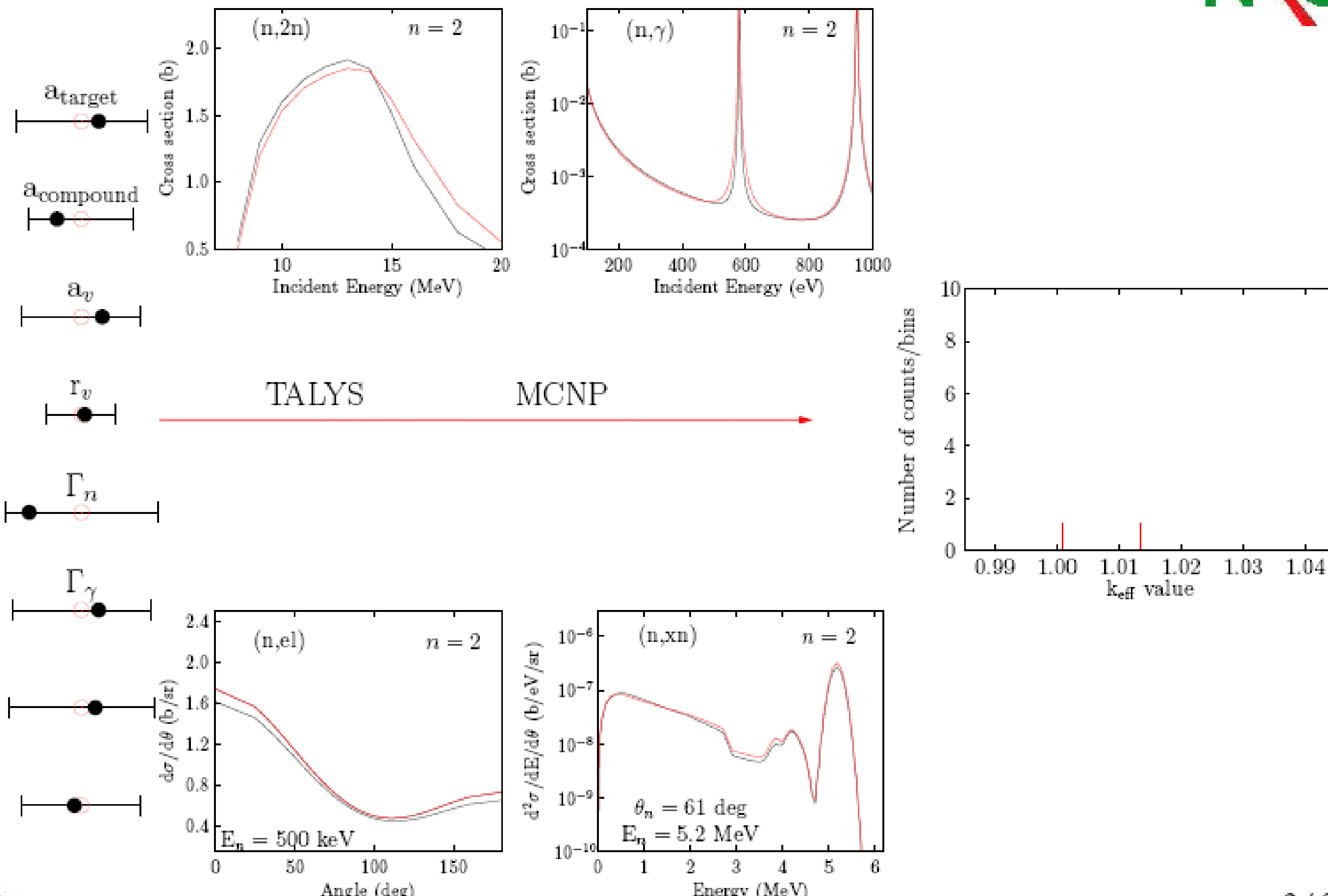

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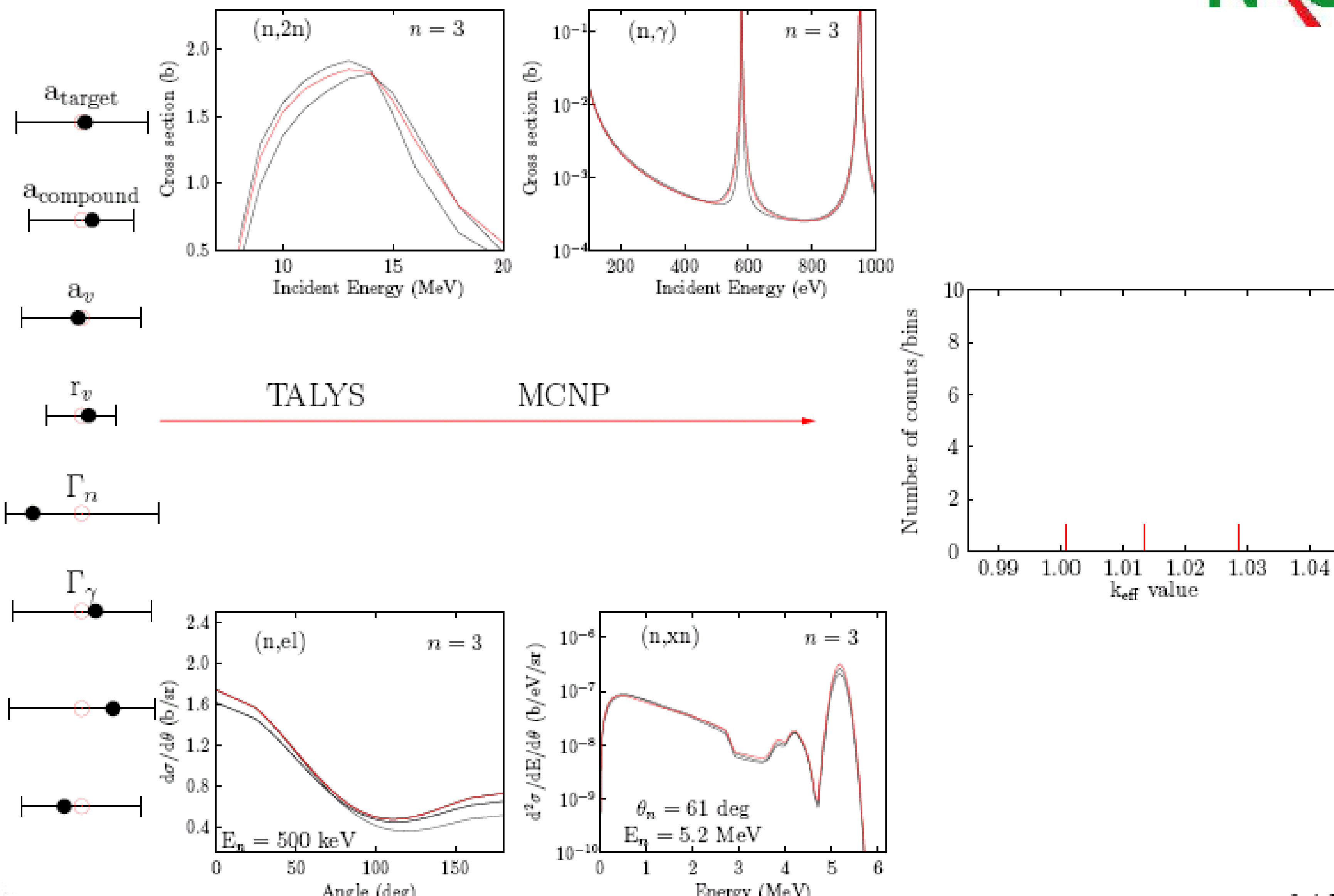

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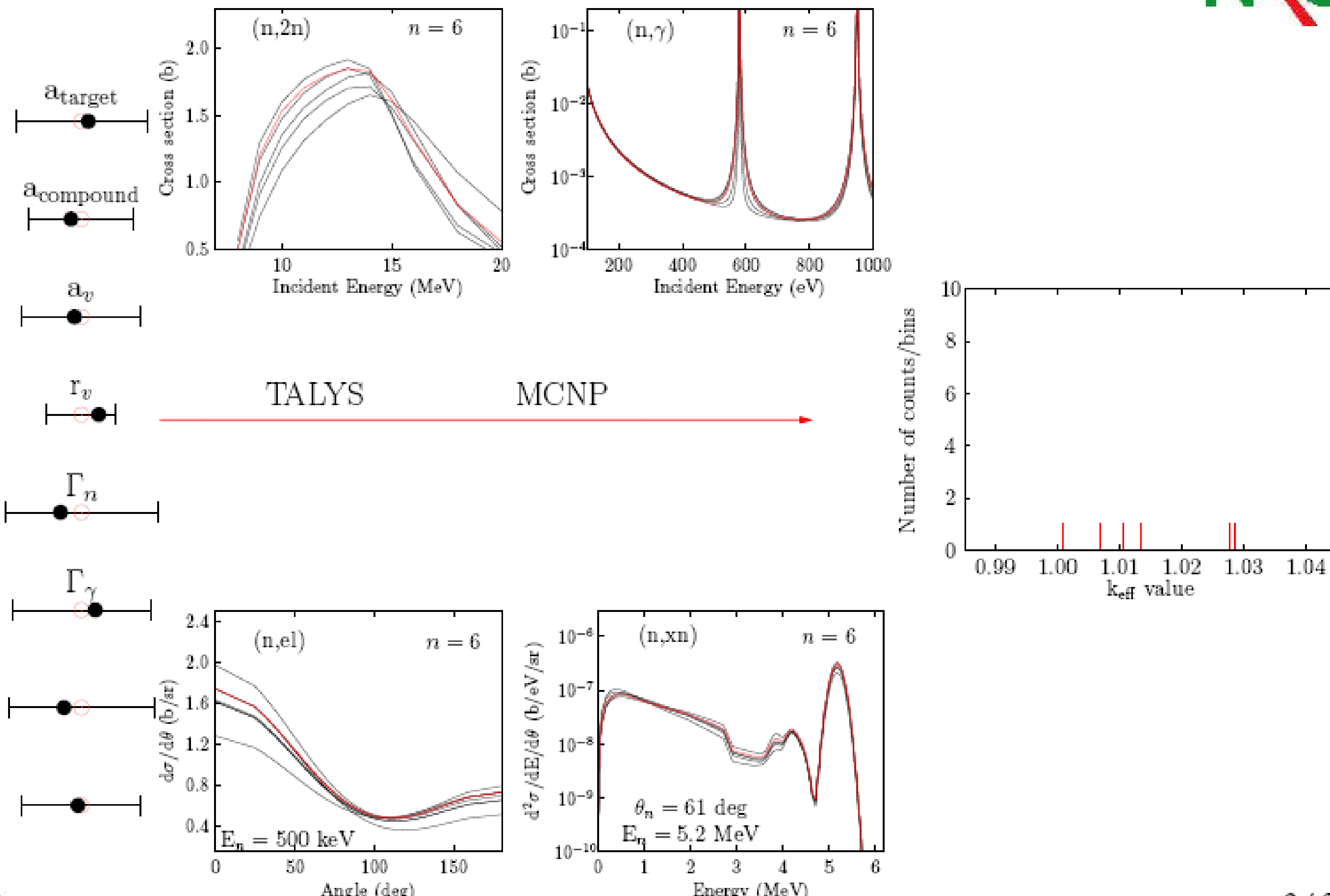

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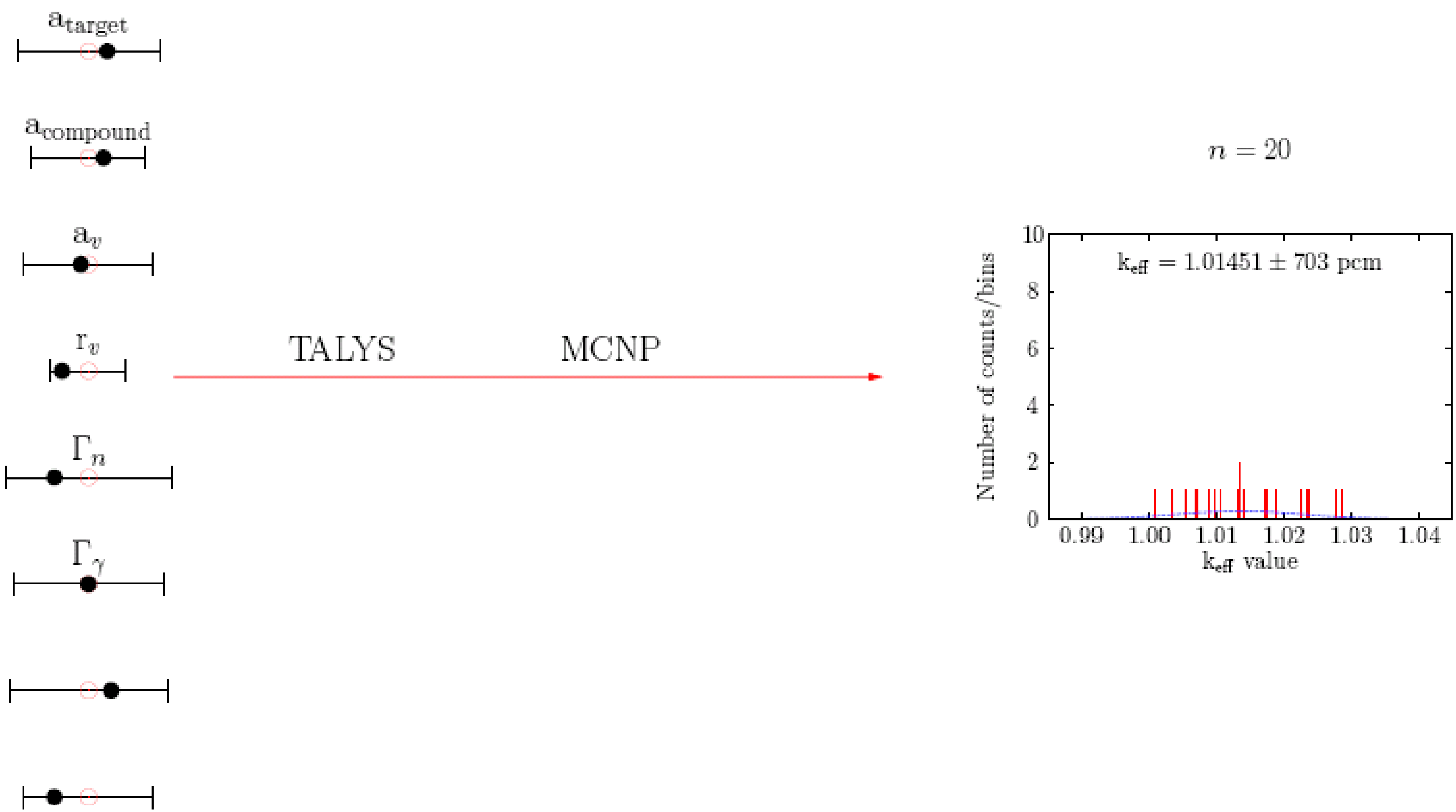

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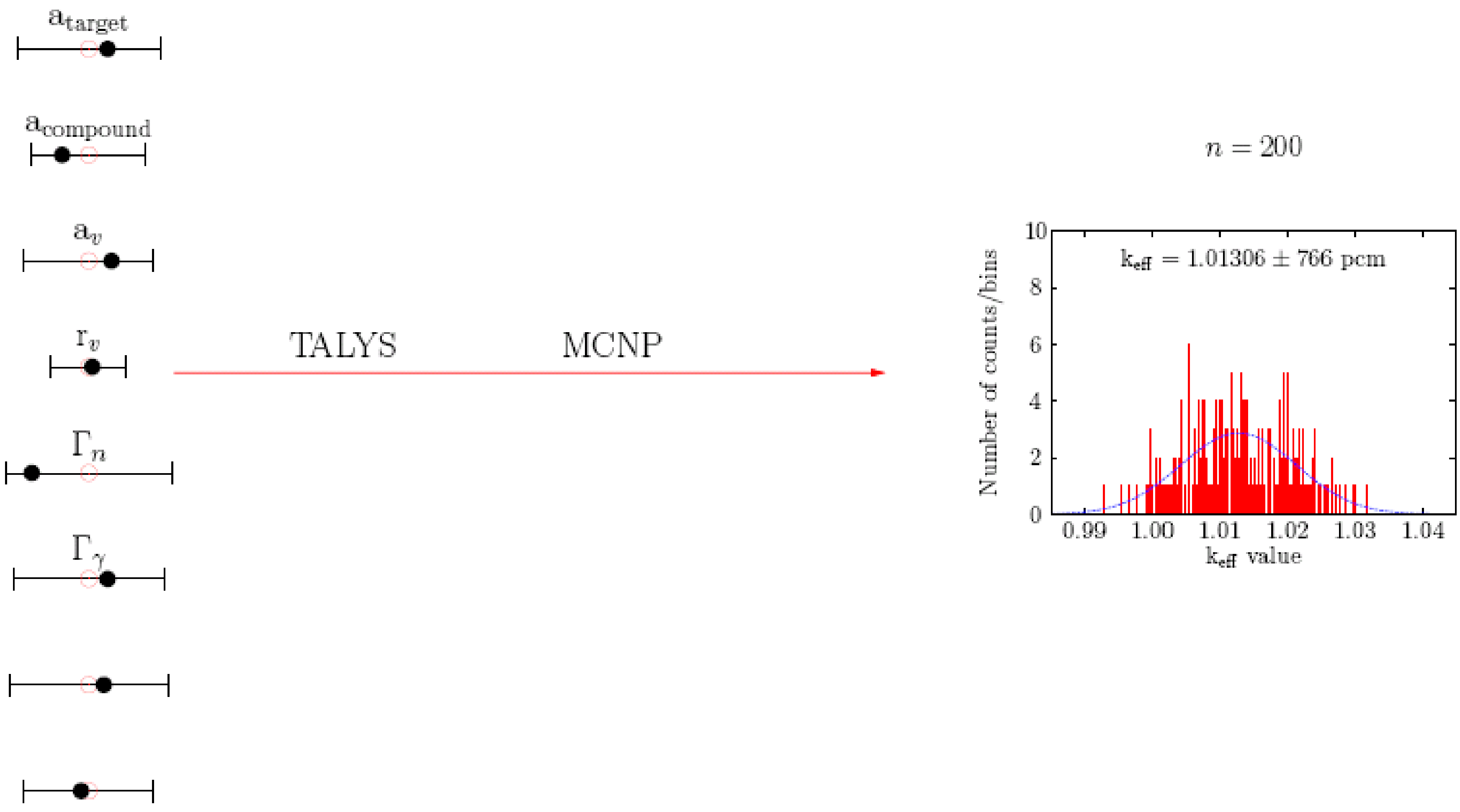
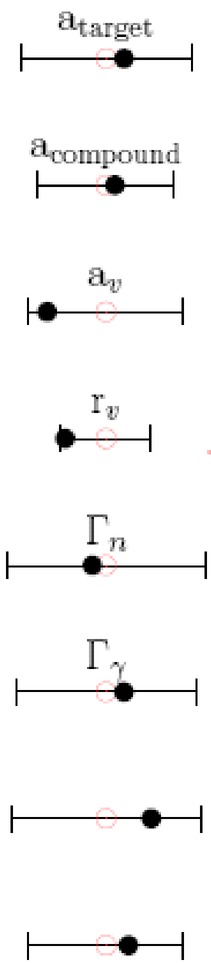
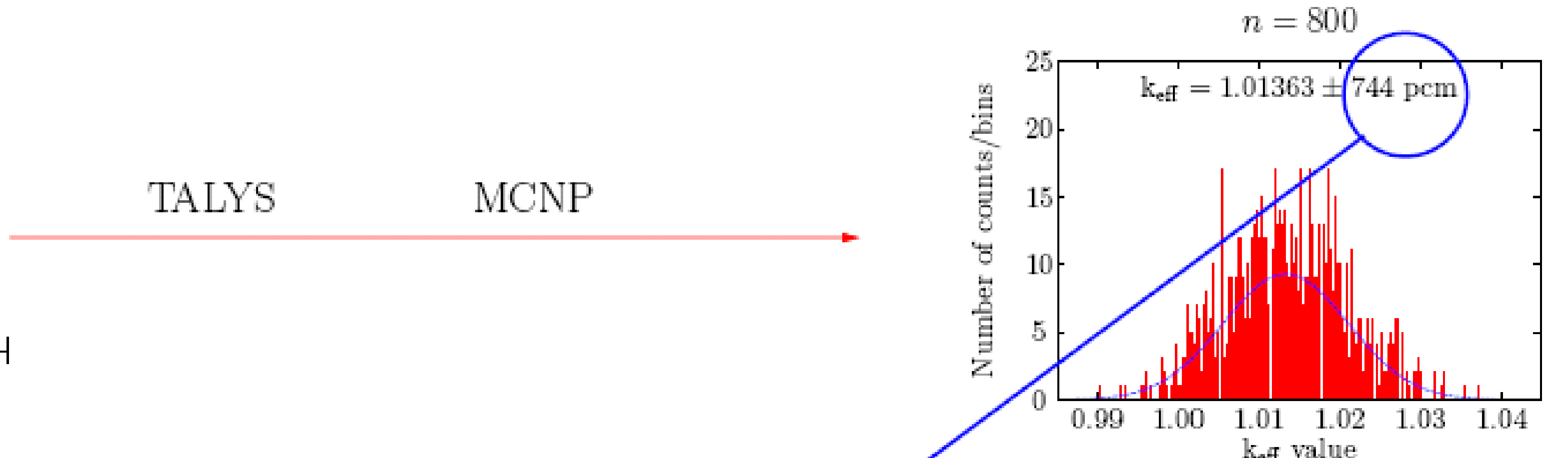


“1000 ×(Talys + ENDF + NJOY + MCNP) calculations for Pb”

Mike Herman (BNL) called this method:
“Total Monte Carlo” (TMC)

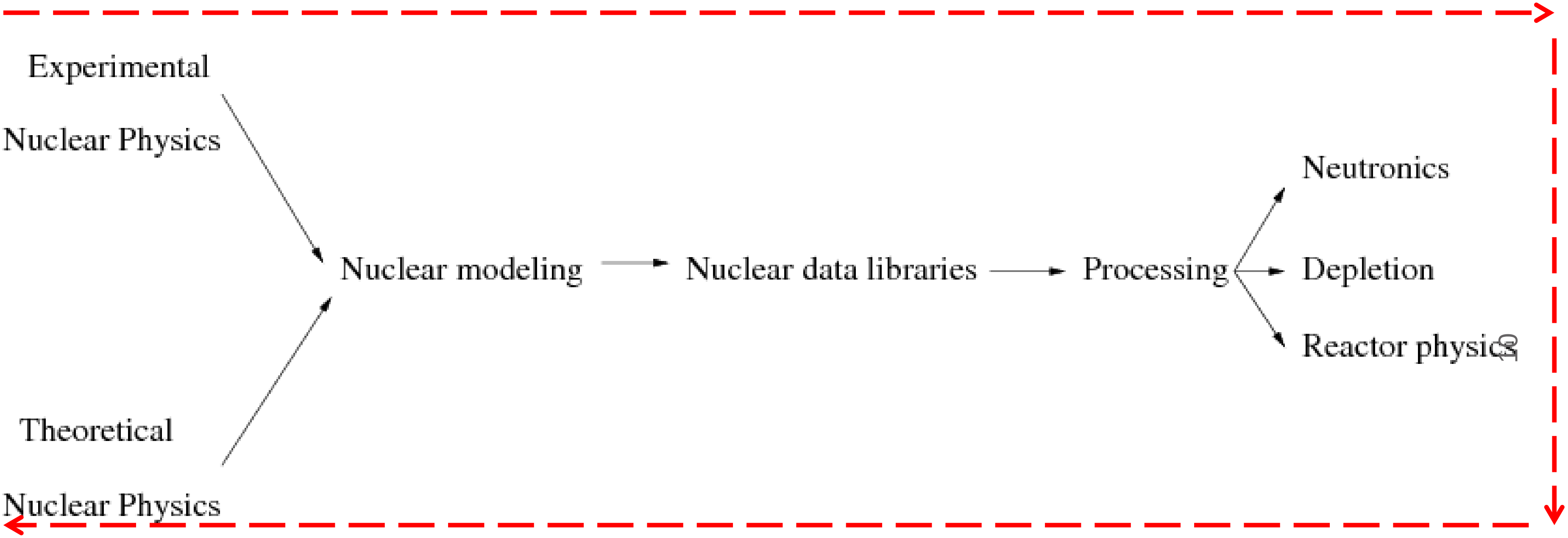




Statistical uncertainty $\simeq$ 68 pcm

$\Longrightarrow$ uncertainty due to nuclear data $\simeq$ 740 pcm

Looping over nuclear science

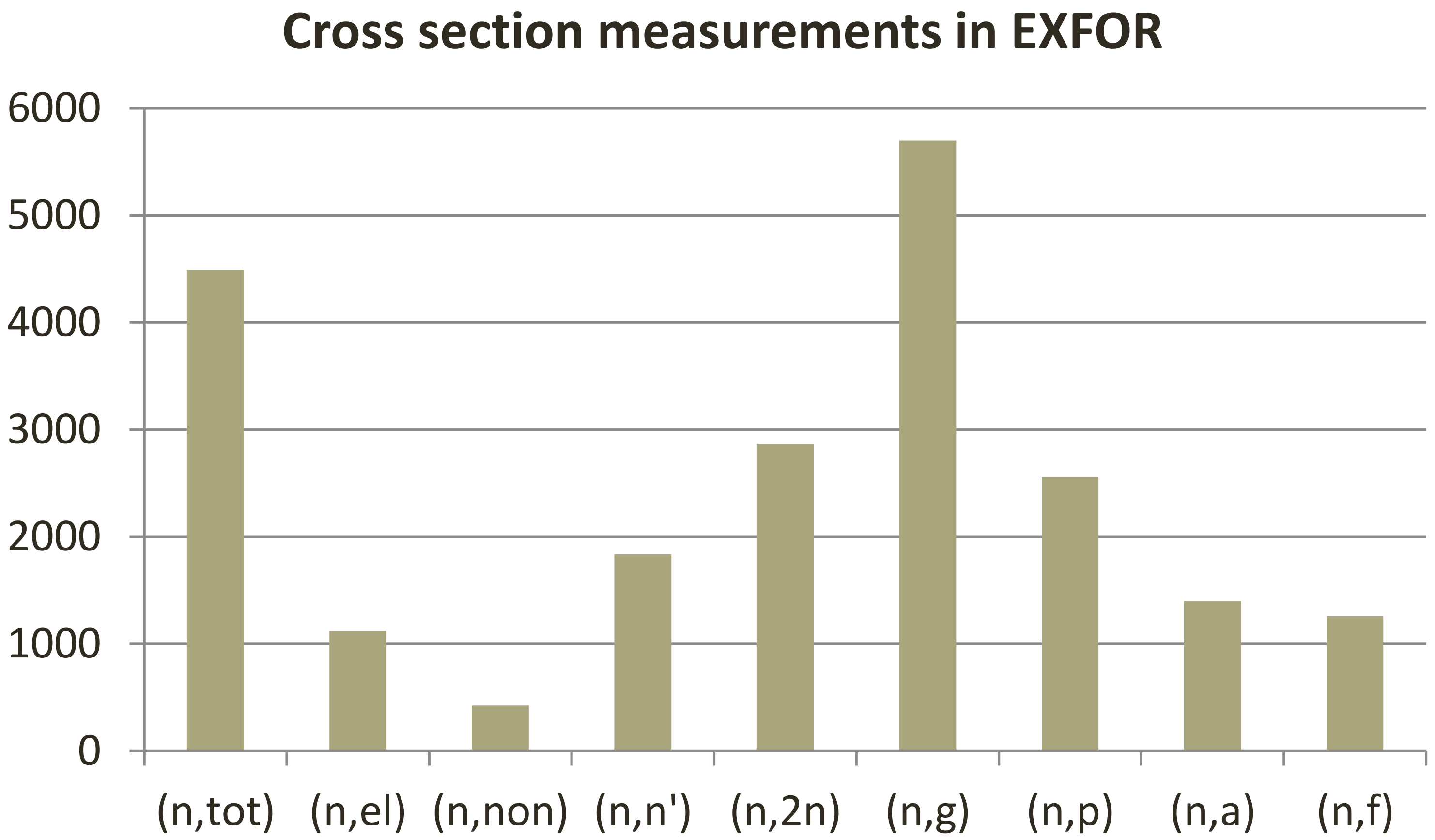


Feedback, sensitivity, uncertainty propagation, …..

Road to success:

- Use (extremely) robust software
- Store all human intelligence in input files and scripts
- Rely on reproducibility and quality assurance

EXFOR database
(Nuclear Reaction Data Center Network: IAEA, NEA, NNDC, JAEA, Obninsk, etc)



Total estimated cost of EXFOR (AK, private comm.): between 20 – 60 Billion Euro
Total estimated value of EXFOR : priceless

TALYS code

General use:

- TALYS can be used for
  - In-depth single nuclide/reaction analyses
  - Global multi-nuclide calculations

Complete output:

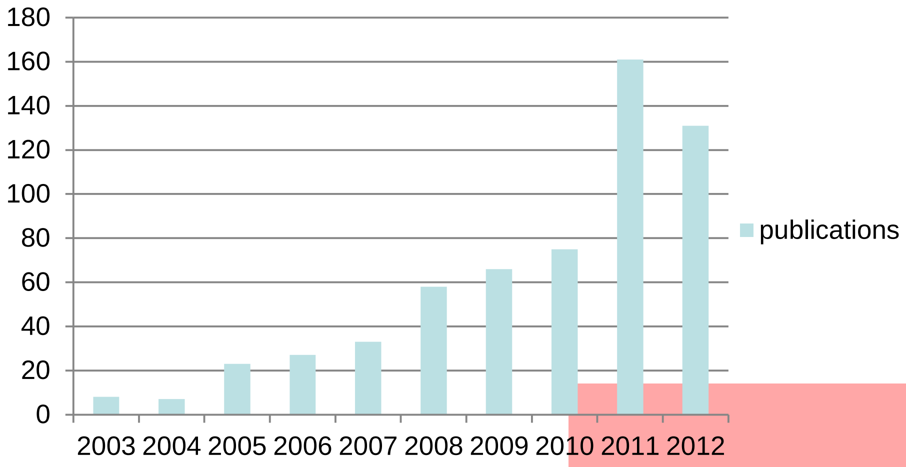
Total, partial and residual production cross sections, (Double)-differential spectra, Angular distributions per discrete level, Fission yields, Recoils, Isomeric production, Astrophysical reaction rates Gamma production, etc, (upcoming: integration of GEF: FY, nu, nubar, PFNS etc.)

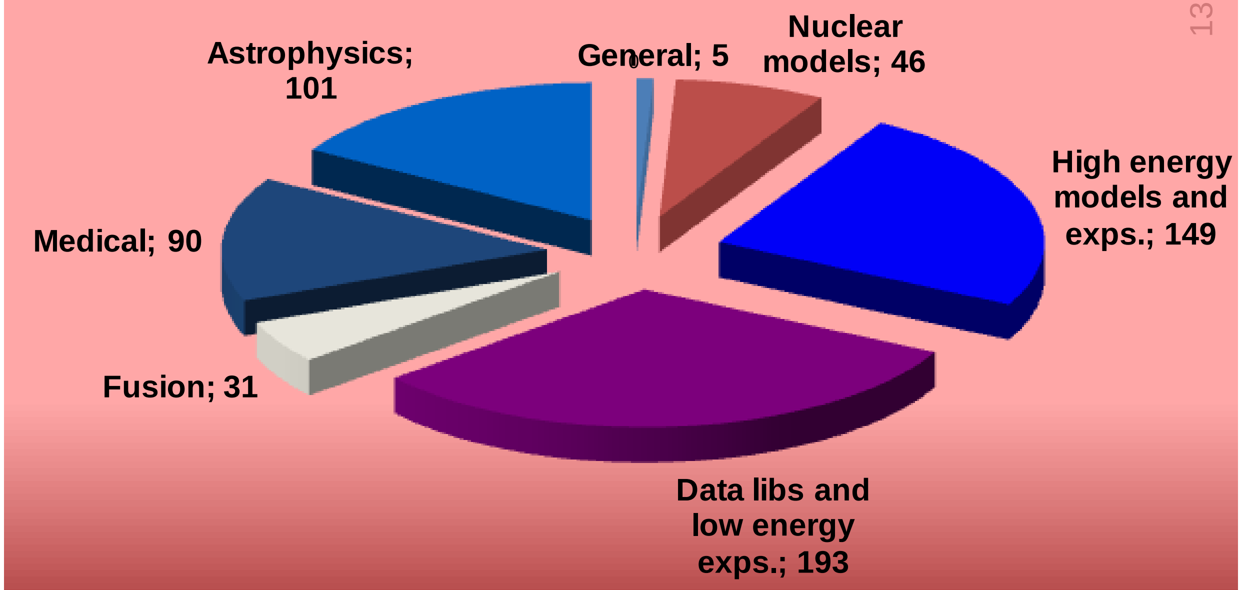
Recent accomplishment: option to use all optical, level density, fission and pre-equilibrium models phenomenological (Woods-Saxon, Fermi gas, Hill-Wheeler, exciton) or microscopical (Hartree-Fock-Bogolyubov-based, by Hilaire, Goriely, Bauge)

Total estimated cost of TALYS : between 2 – 4 Million Euro

Total estimated value of TALYS: no comment

TALYS publications





Initial probability distribution for TALYS parameters

For all nuclides for which experimental data exists:

- Sample parameters from a wide uniform distribution
- Obtain a wide scattering of random TALYS results and the standard deviation for every reaction channel of every nuclide
- Compare the results with all EXFOR data: 23490 experimental data sets = 2.7 million data points
- Count how many EXFOR points fall inside the 1-sigma uncertainty band.
- Assess the width of the (prior) uniform distribution for the model parameters.

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Starting point: "Expert" (Gaussian) parameter uncertainties

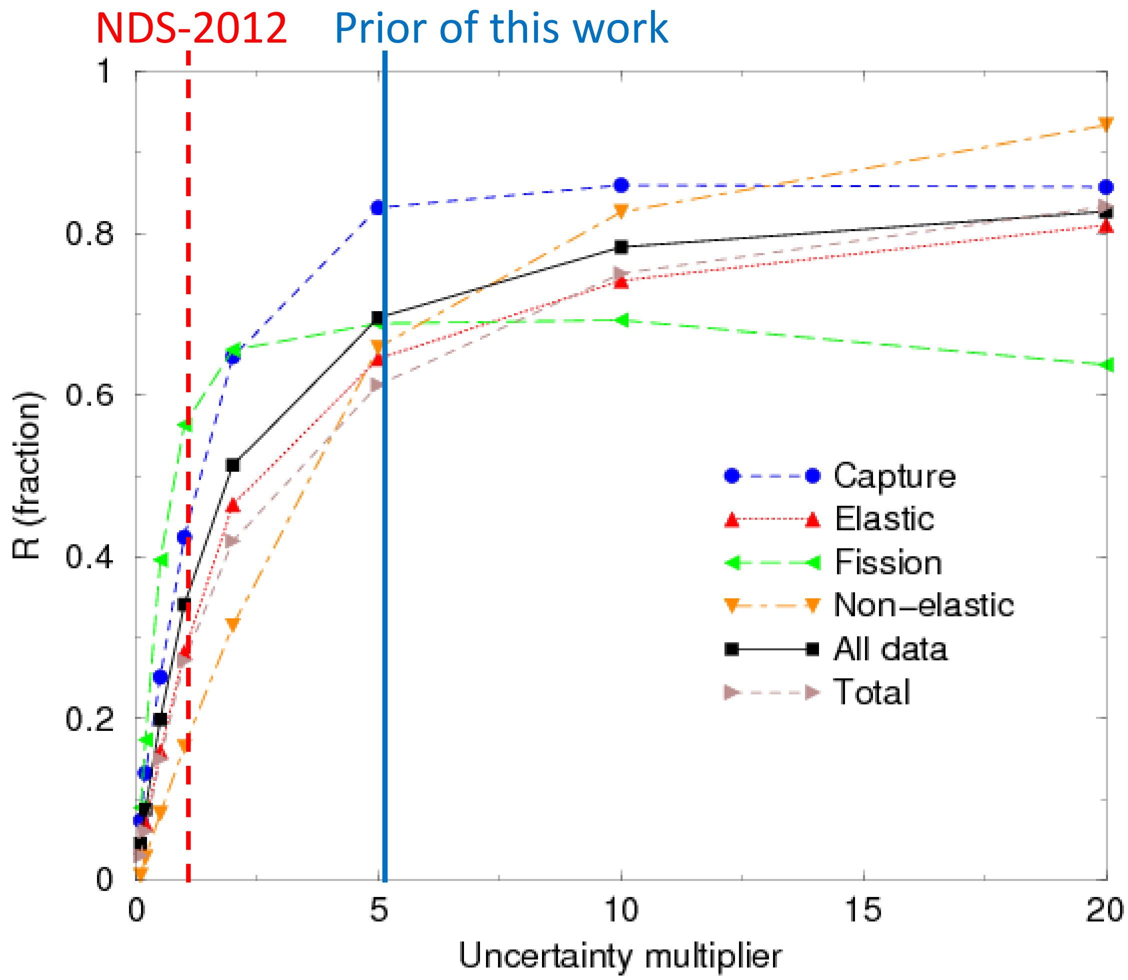
(A.J. Koning and D. Rochman, ``Modern nuclear data evaluation with the TALYS code system", Nucl. Data Sheets 113, 2841 (2012).) Origin: *Fingerspitzengefühl*

Parameter	uncertainty (%)	Parameter	uncertainty (%)
Optical model			
r_V^n	2	d_1^n	10
a_V^n	2	d_2^n	10
v_1^n	2	d_3^n	10
v_2^n	3	r_{SO}^n	10
v_3^n	3	a_{SO}^n	10
v_4^n	5	v_{so1}^n	5
w_1^n	10	v_{so2}^n	10
w_2^n	10	w_{so1}^n	20
r_D^n	3	w_{so2}^n	20
a_D^n	4		
r_V^p	4	d_1^p	20
a_V^p	4	d_2^p	20
v_1^p	4	d_3^p	20
v_2^p	6	r_{SO}^p	20
v_3^p	6	a_{SO}^p	20
v_4^p	10	v_{so1}^p	10
w_1^p	20	v_{so2}^p	20
w_2^p	20	w_{so1}^p	40
r_D^p	6	w_{so2}^p	40
a_D^p	8	r_C^p	10
λ_V	5	λ_{V1}	5
λ_W	5	λ_{W1}	5
λ_{Vso}	5	λ_{Wso}	5

Level density			
a	11.25-0.03125.A	σ^2	30
γ	30	δW	$\pm$ 1 MeV
α	30	β	30
R_σ	30	γ	30
E_0	20	E_M	20
T	10	δ	$\pm$ 2 MeV
K_{rot}	80		
C_{HFM}	30	δ_{HFM}	30
Gamma-ray strength			
Γ_γ	20	$\sigma_{E\ell}$	20
$\Gamma_{E\ell}$	20	$E_{E\ell}$	10
$E_{\rm nor}$	20	$E_{\rm shift}$	$\pm$ 0.8 MeV
Fission			
B_f	10	$\hbar\omega_f$	10
Pre-equilibrium			
M^2	30	$R_{\pi\pi}$	30
$R_{\nu\pi}$	30	$R_{\pi\nu}$	30
$R_{\nu\nu}$	30	R_γ	50
g_ν	11.25-0.03125.A	$E_{\rm surf}$	20
g_π	11.25-0.03125.A	$C_{\rm break}$	80
$C_{\rm knock}$	80	$C_{\rm strip}$	80

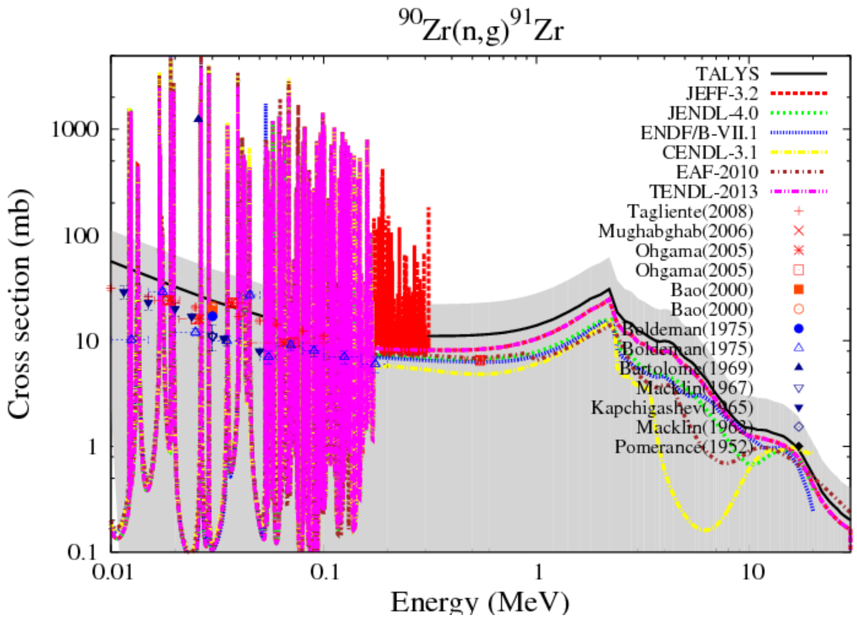
Multiply these uncertainties by 5 and sample ~200 parameters from uniform distribution

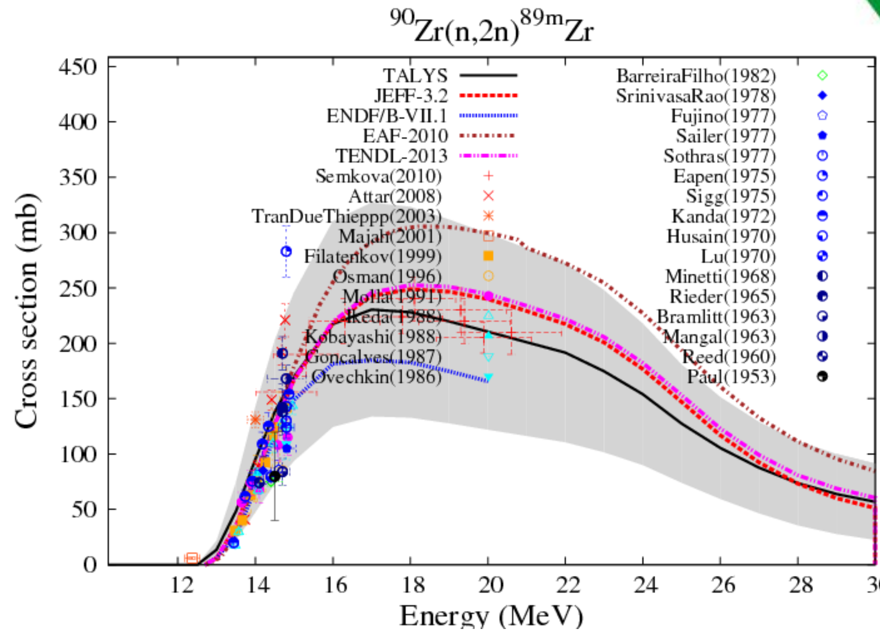
Fraction of EXFOR data inside 1-sigma uncertainty band

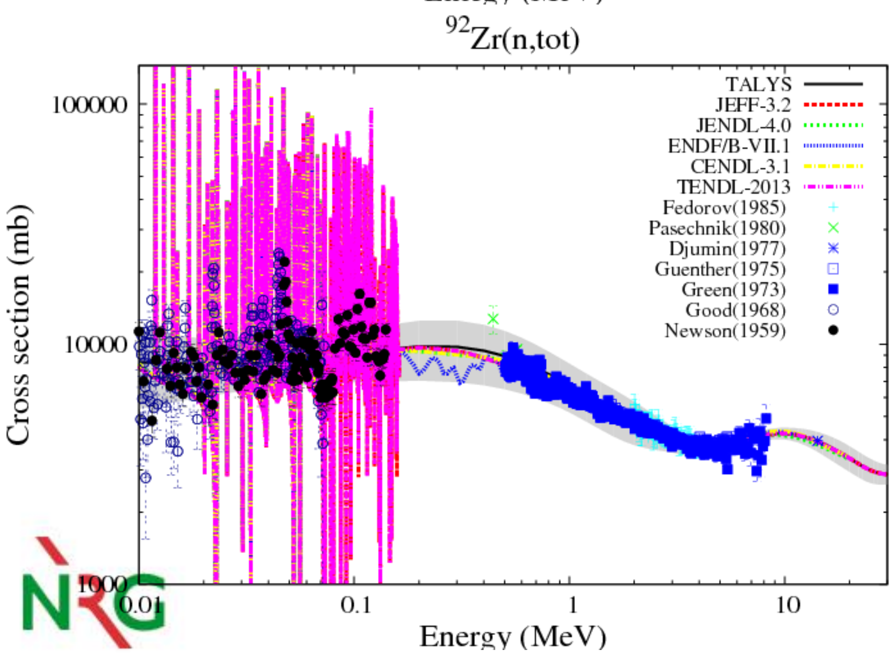


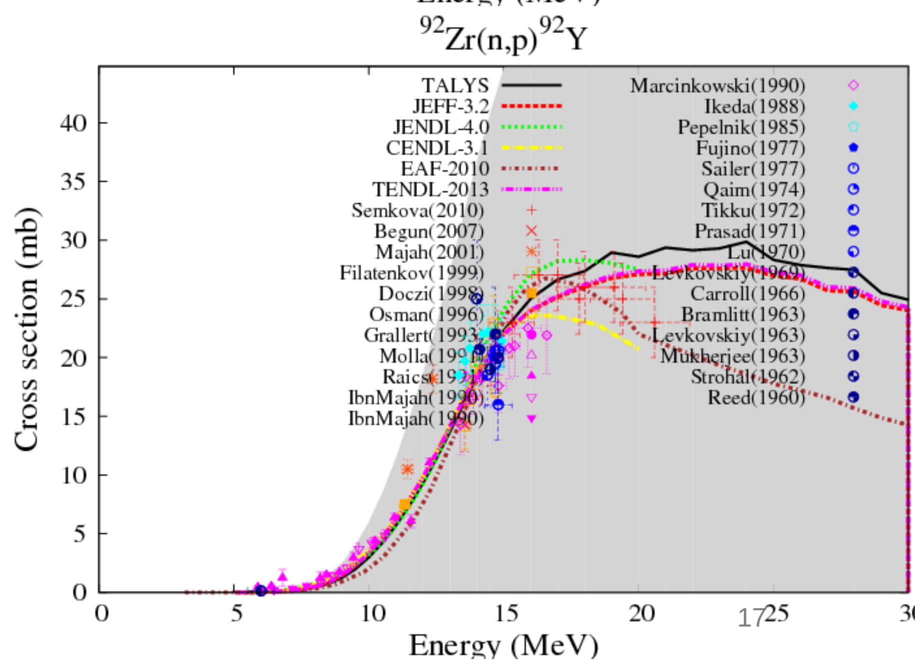
Random TALYS calculations for all nuclides compared with 23490 experimental data sets = 2.7 million data points

"Knowing nothing": Random TALYS parameters from initial parameter pdf: uniform distribution with uncertainty multiplier = 5









Initial probability distribution for cross sections

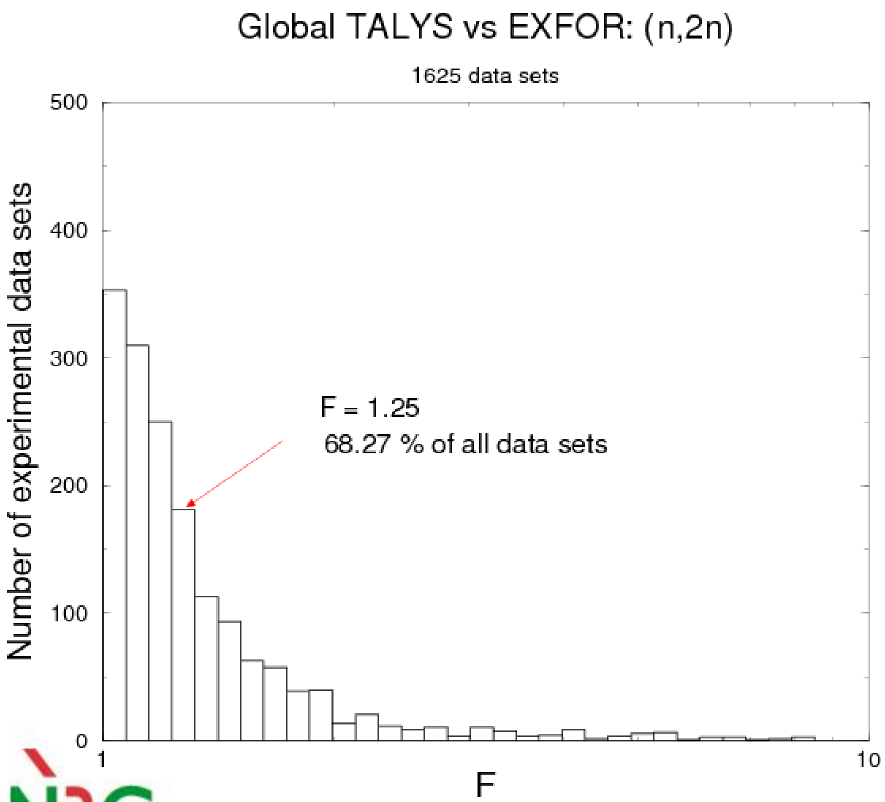
- **Perform 1 global, unadjusted TALYS calculation for the entire periodic table of elements**
- **Compare the results with all EXFOR data: 23490 experimental data sets = 2.7 million data points**
- **Determine the average deviation between TALYS and experiment.**
- **Use the results as knowledge (“pseudo-experimental data”) in a Bayesian Monte Carlo updating scheme.**

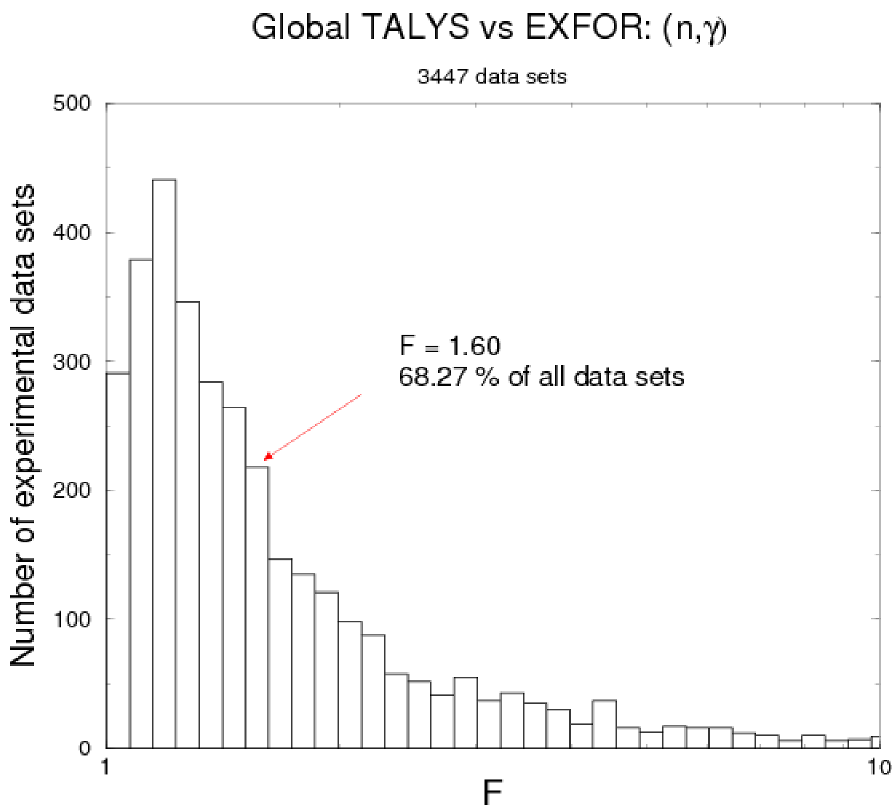
Initial probability distribution for cross sections

- **Use F-factor for each experimental data set:**

$$F = 10^{\sqrt{\frac{1}{N}\sum_{i}^{N}\left(\log\frac{\sigma_T^i}{\sigma_E^i}\right)^2}}$$

WPEC SG-30 on quality assessement of EXFOR

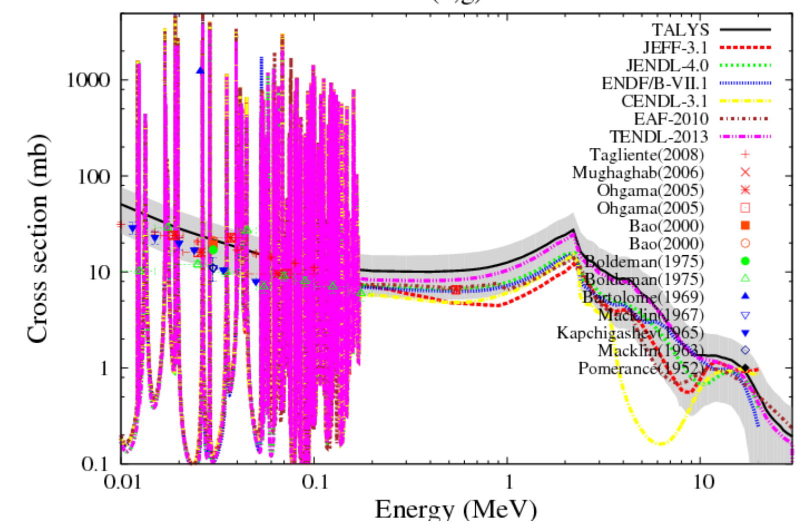




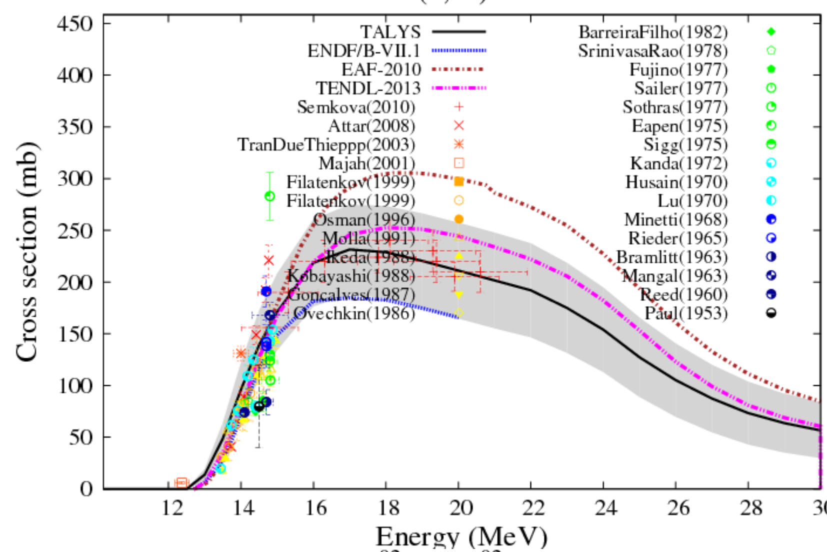
Initial probability distributions for cross sections

Starting point: global TALYS central values and uncertainties based on cross sections for all nuclides

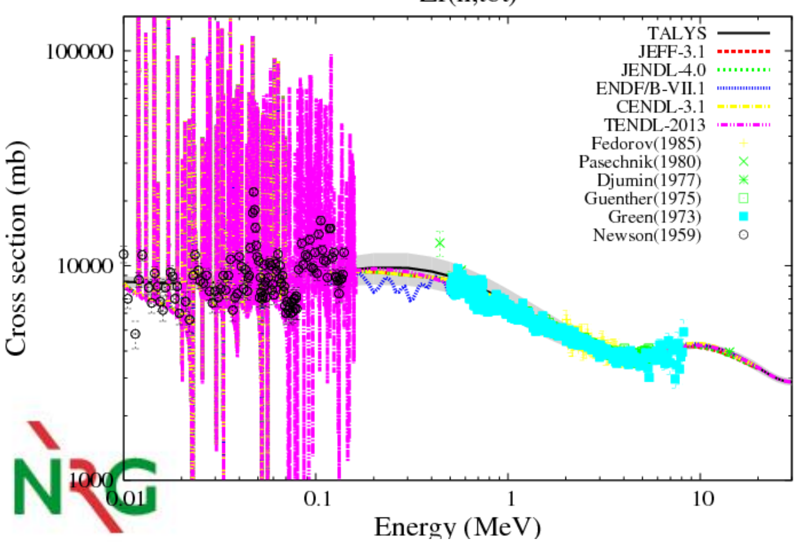
$^{90}Zr(n,g)^{91}Zr$



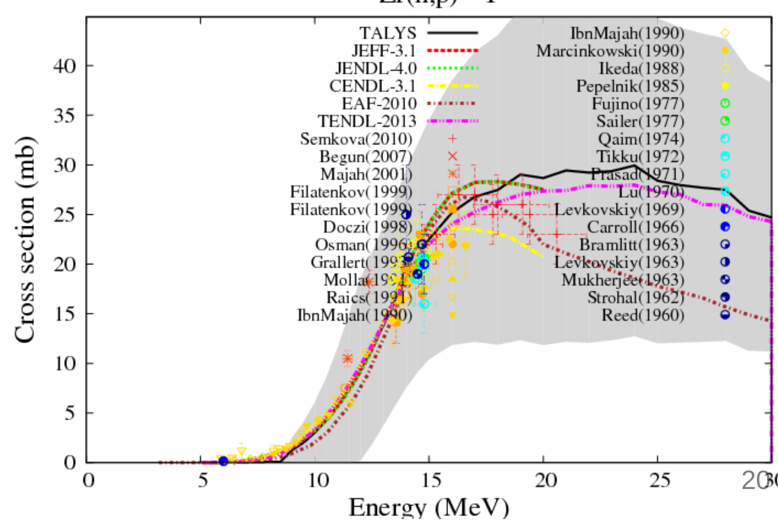
$^{90}Zr(n,2n)^{89m}Zr$



$^{92}Zr(n,tot)$



$^{92}Zr(n,p)^{92}Y$

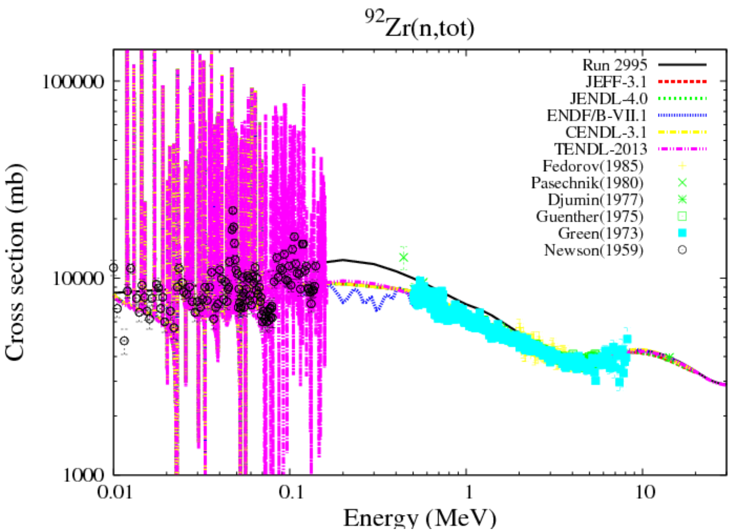


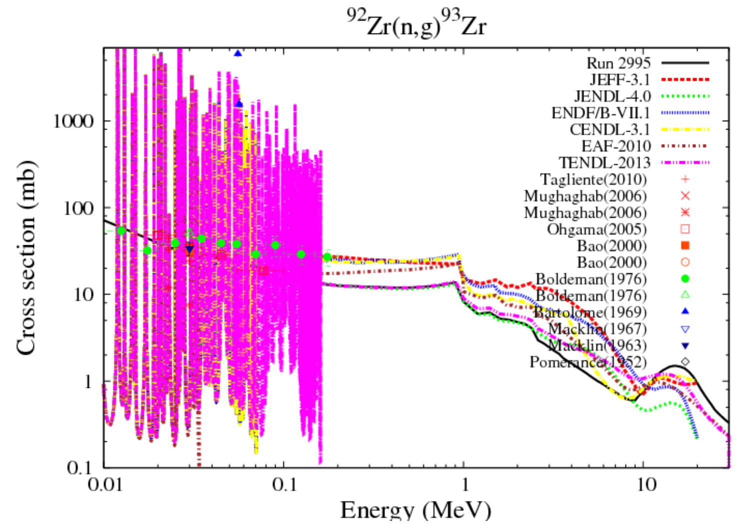
Create new parameter distributions using weights based on EXFOR

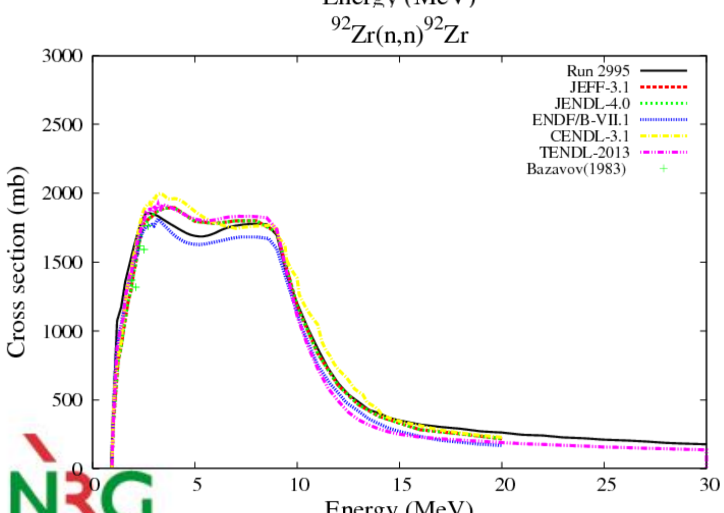
Each random data set k has a weight

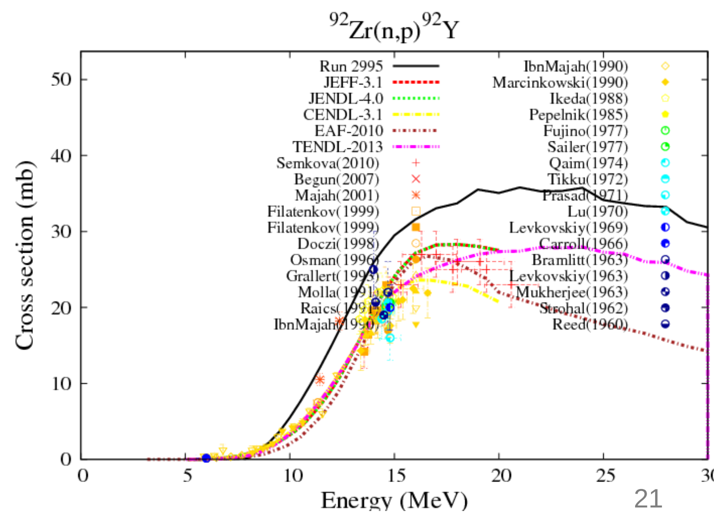
Bauge: BFMC, Capote-Trkov: UMC-B

$$w^{(k)} = \exp(-\chi^{2(k)}) / \exp(-\chi^{2(0)})$$





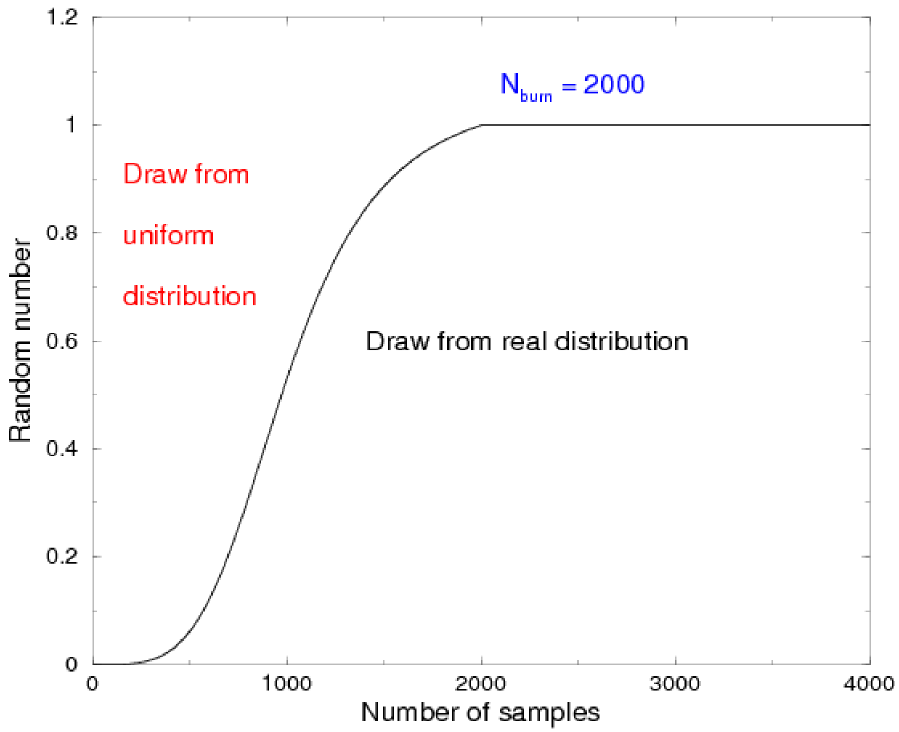




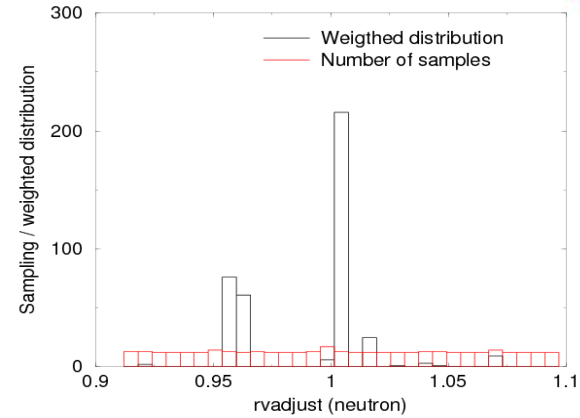
Create new parameter distributions using weights based on EXFOR

Assign the weight $w^{(k)}$ of random data set k to all TALYS parameters of that run

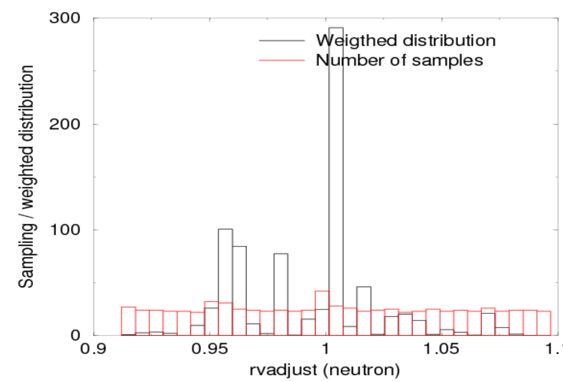
"Self–learning" sampling



400 random TALYS samples: n + ^{90}Zr



800 random TALYS samples: n + ^{90}Zr



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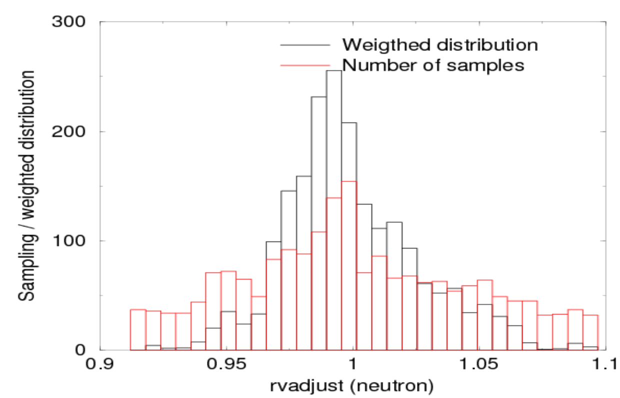

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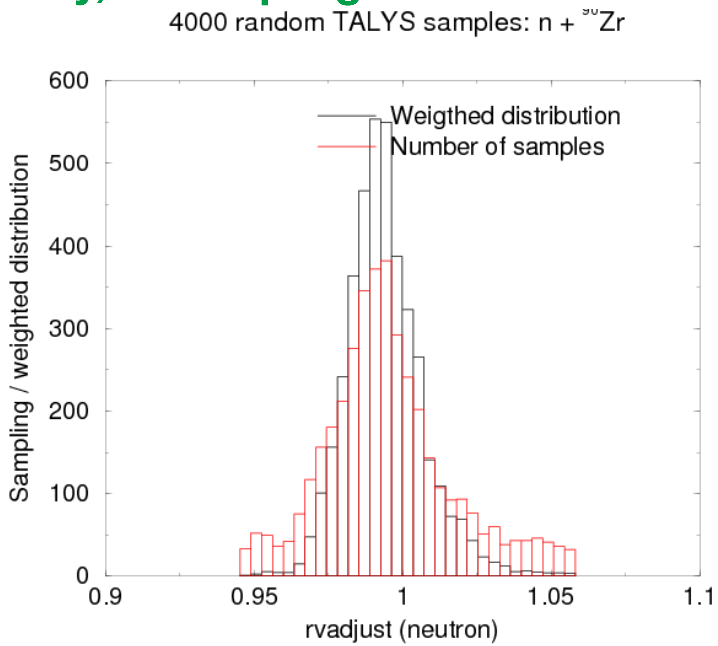
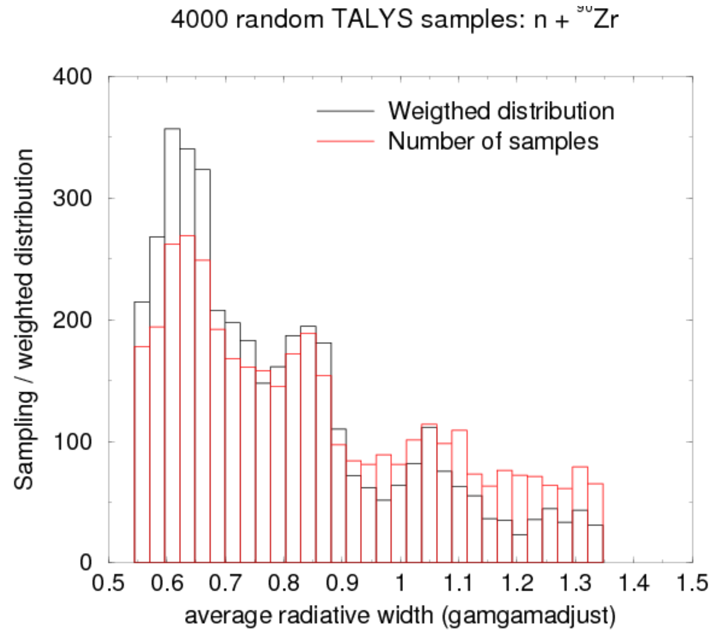
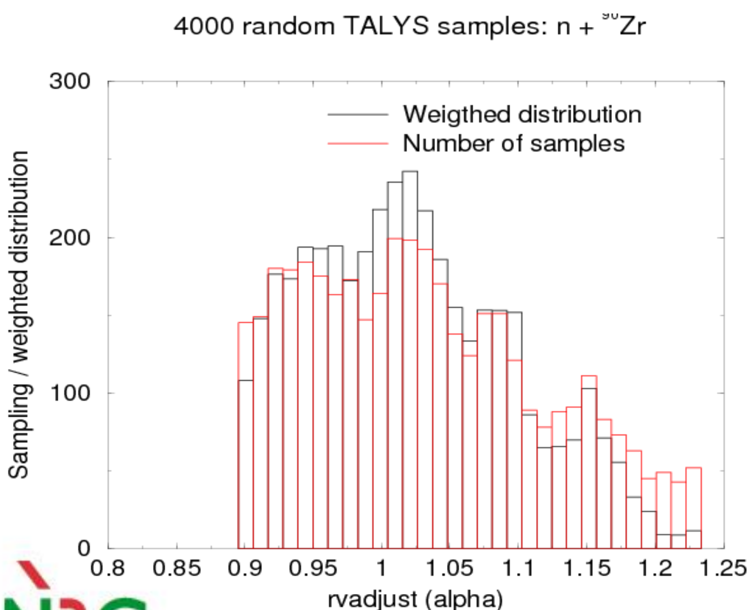
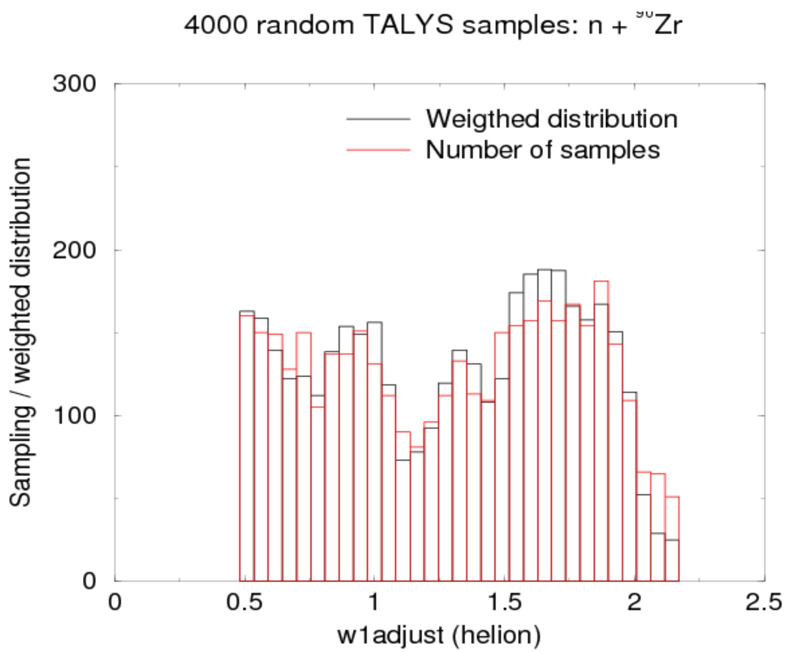
Finally, all sampling is done from the real weighted parameter distributions



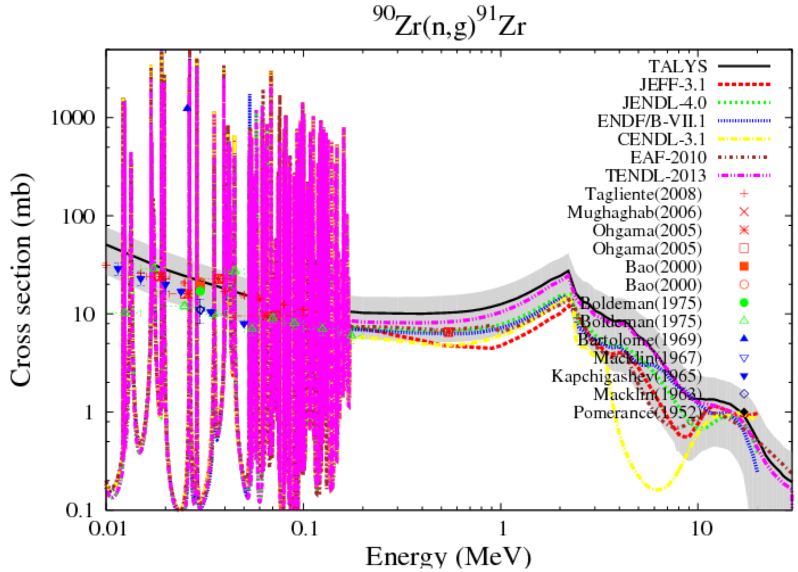


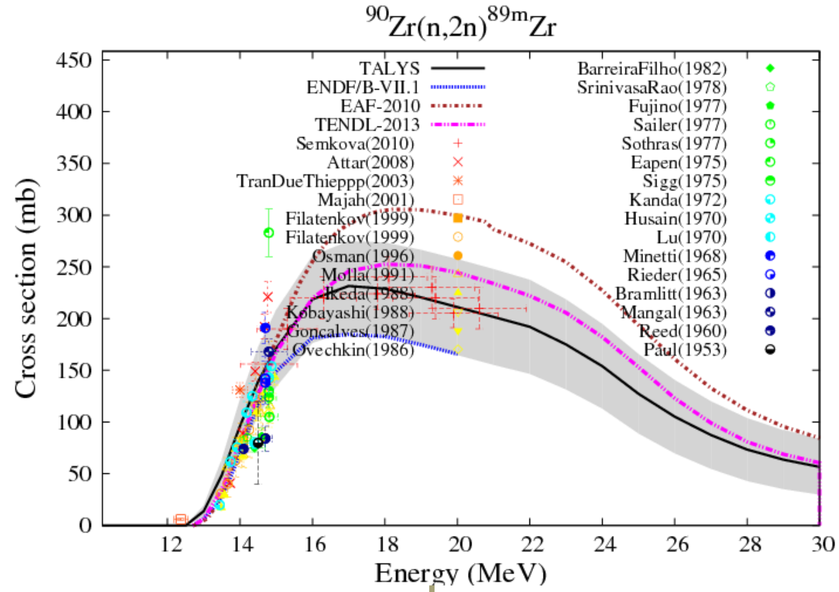




Zooming in

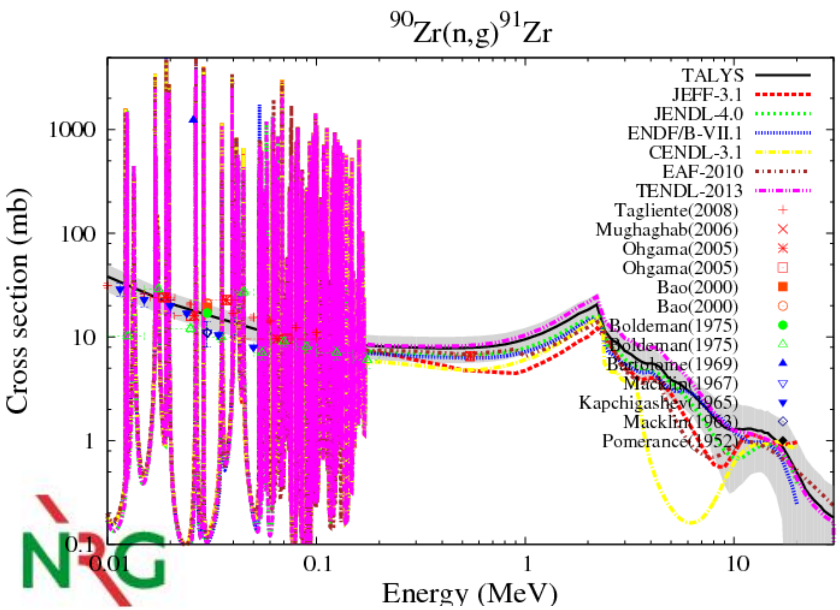
Prior: Global TALYS – uncertainties from all EXFOR data

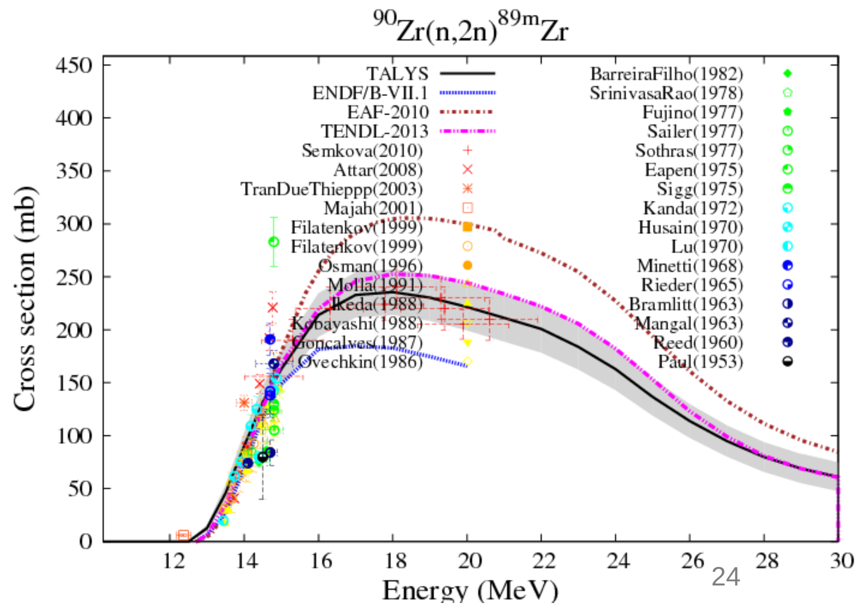




Use weights based on EXFOR for ^{90}Zr

Final





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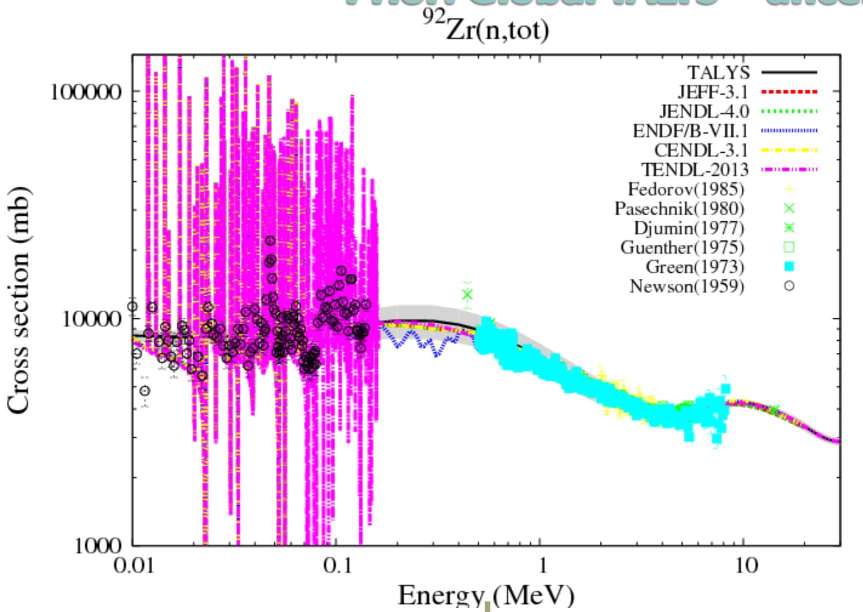
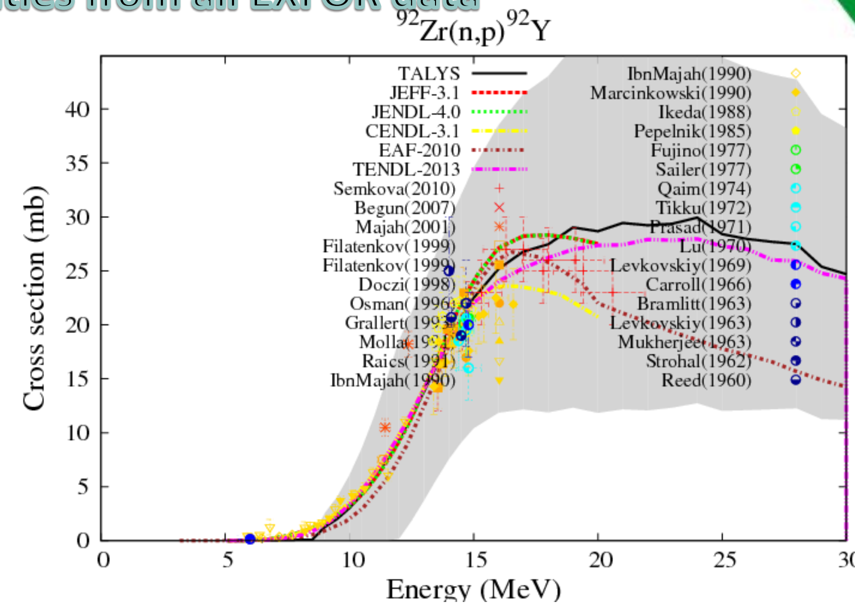
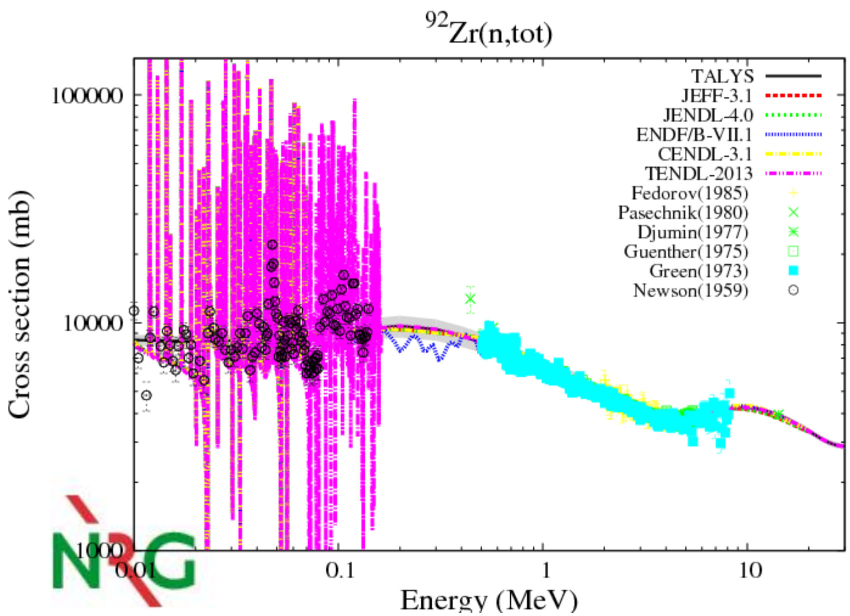
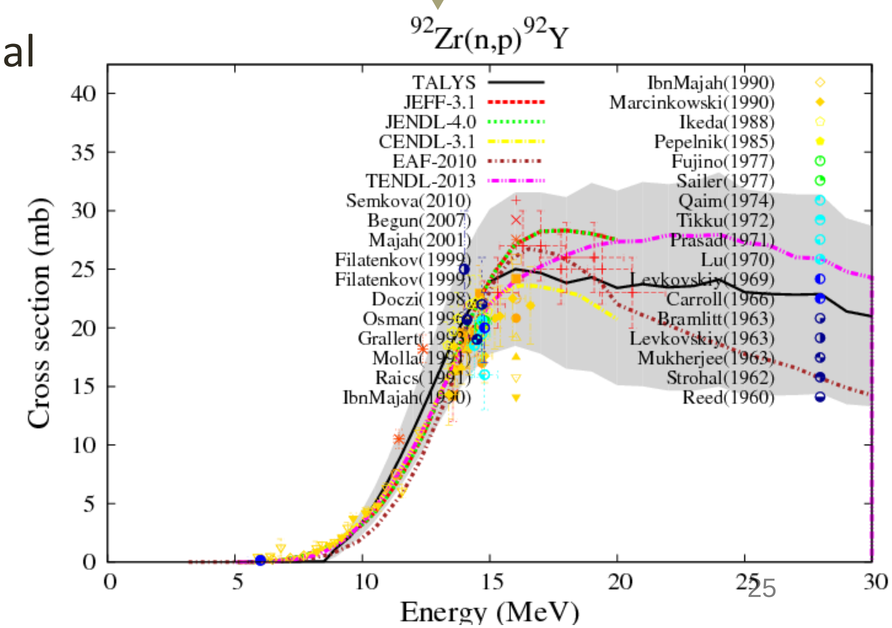




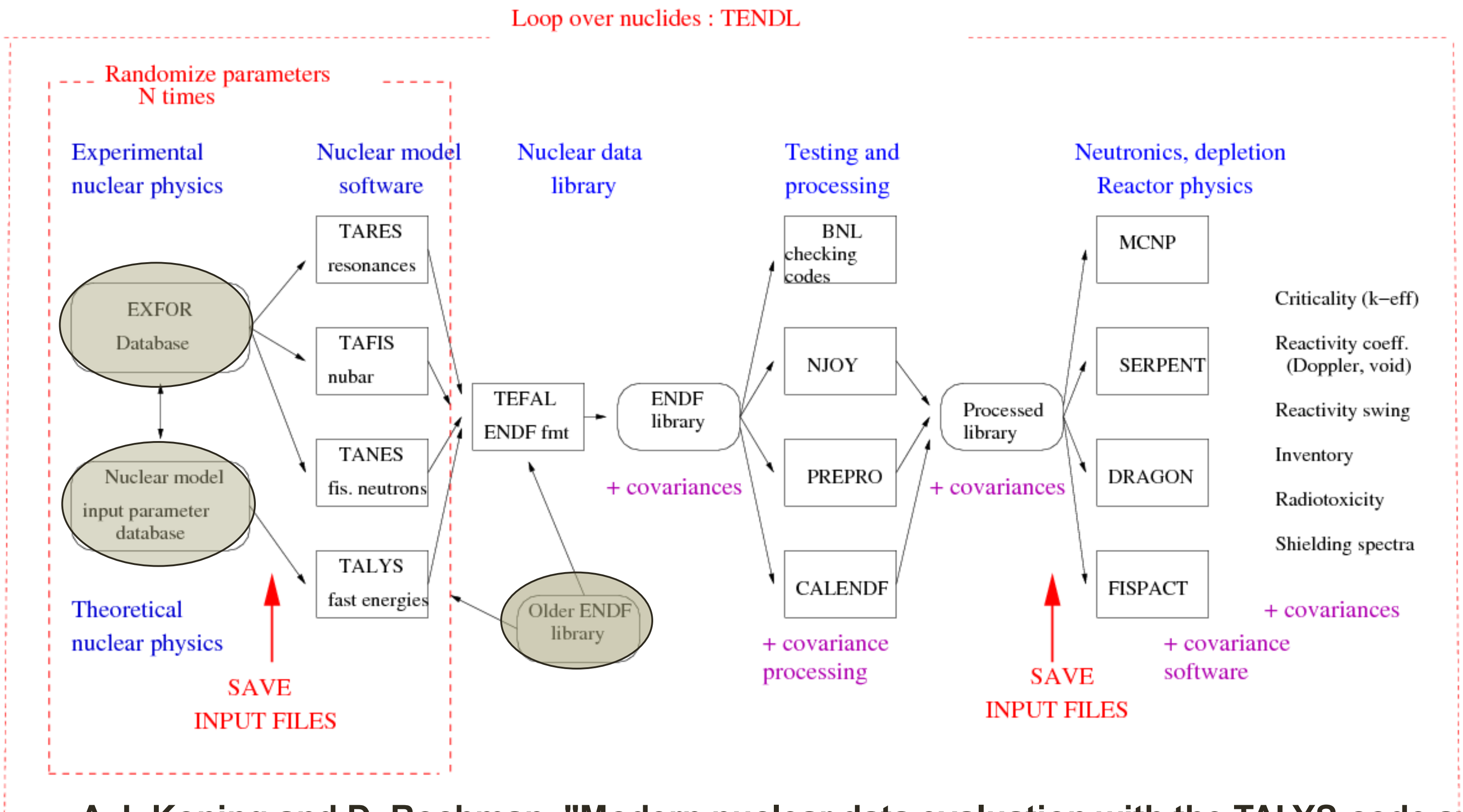
Use weights based on EXFOR for ^{90}Zr

Final



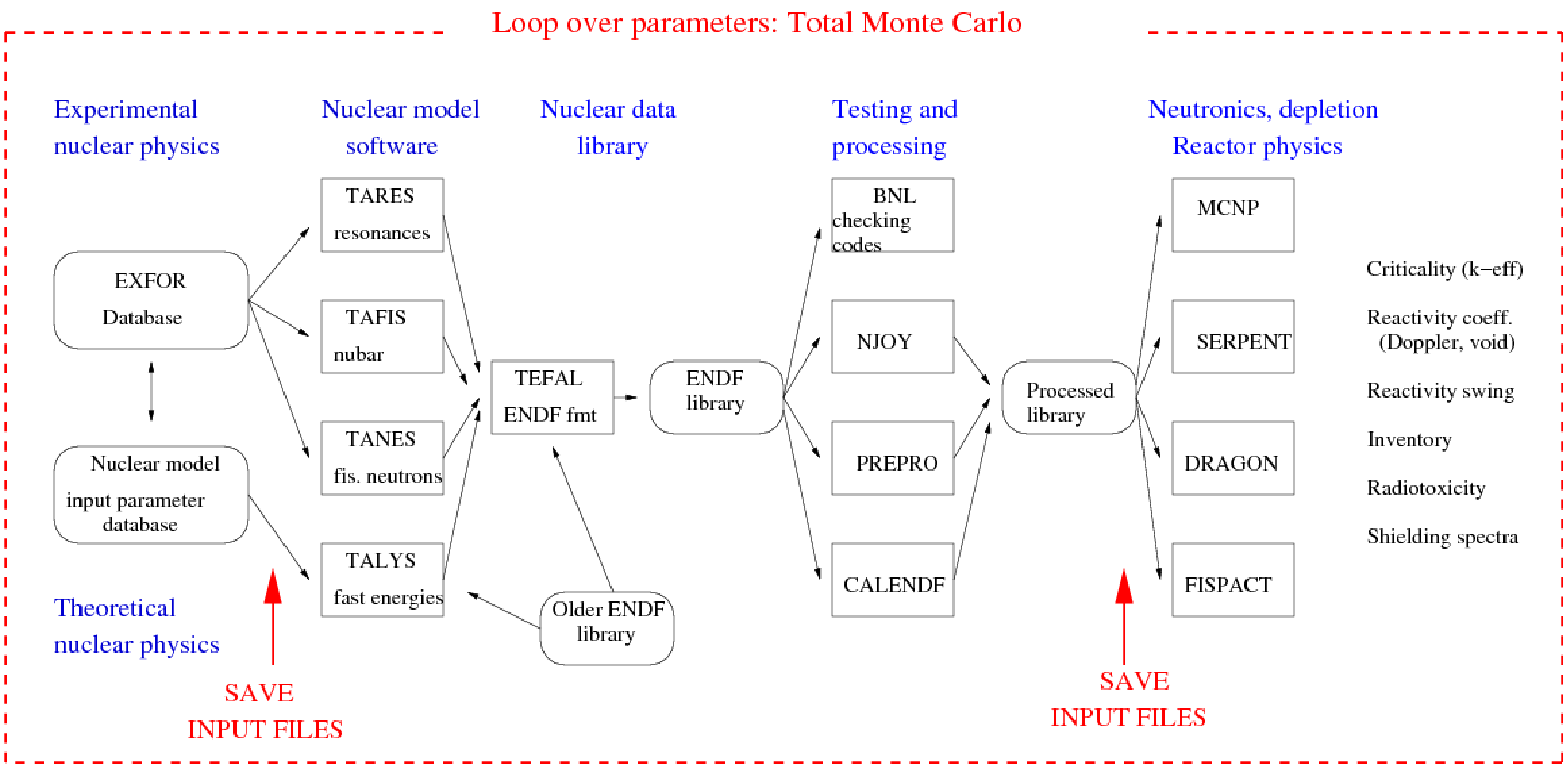


TENDL nuclear data library



A.J. Koning and D. Rochman ,"Modern nuclear data evaluation with the TALYS code system“, Nuclear Data Sheets 113, 2841 (2012).

Total Monte Carlo



NRG

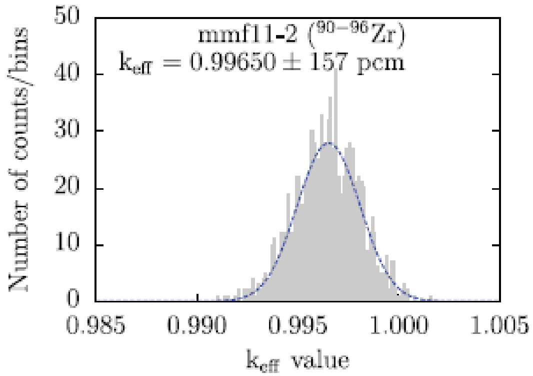
TMC example: criticality benchmarks

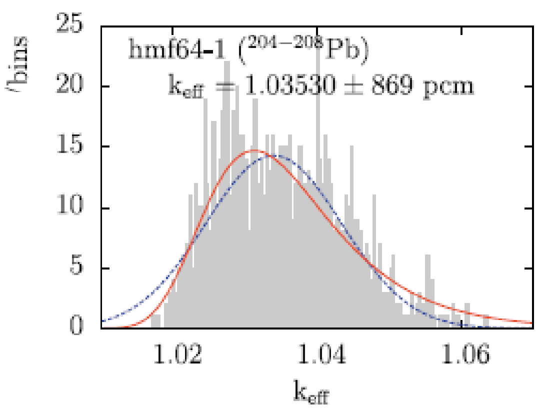
Total of 60000 random ENDF-6 files

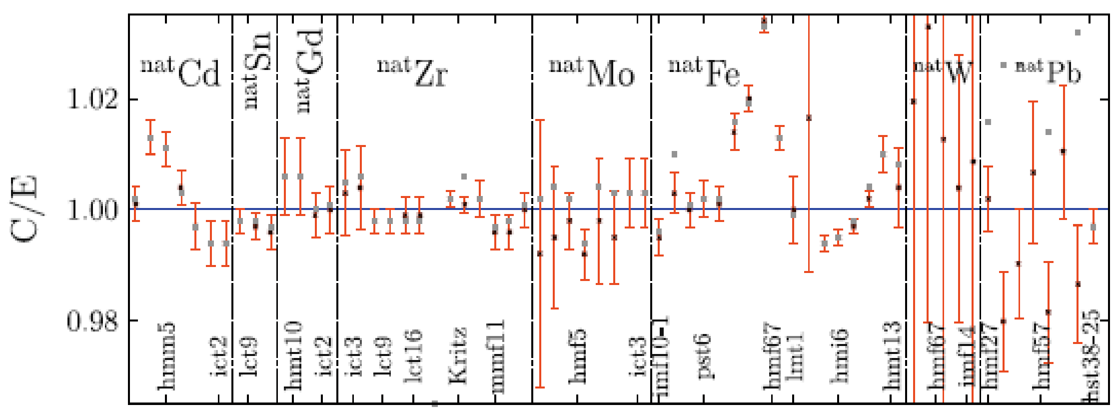
Sometimes deviation from Gaussian shape

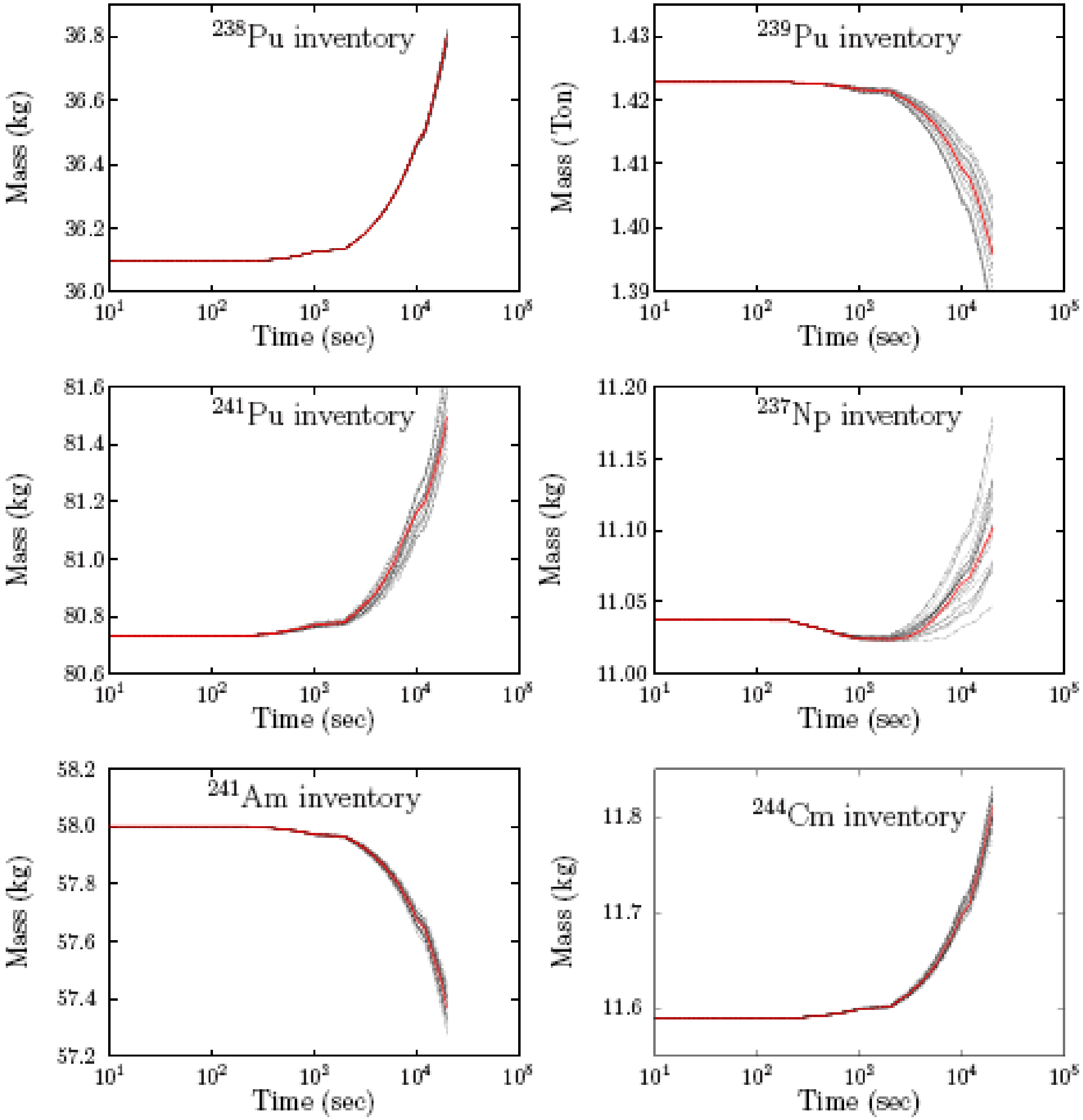
D. Rochman, A.J. Koning and S.C. van der Marck, *[``Uncertainties for criticality-safety benchmarks and keff distributions'']*, *Ann. Nuc. En. 36 810-831 (2009).*

Yields uncertainties on benchmarks !





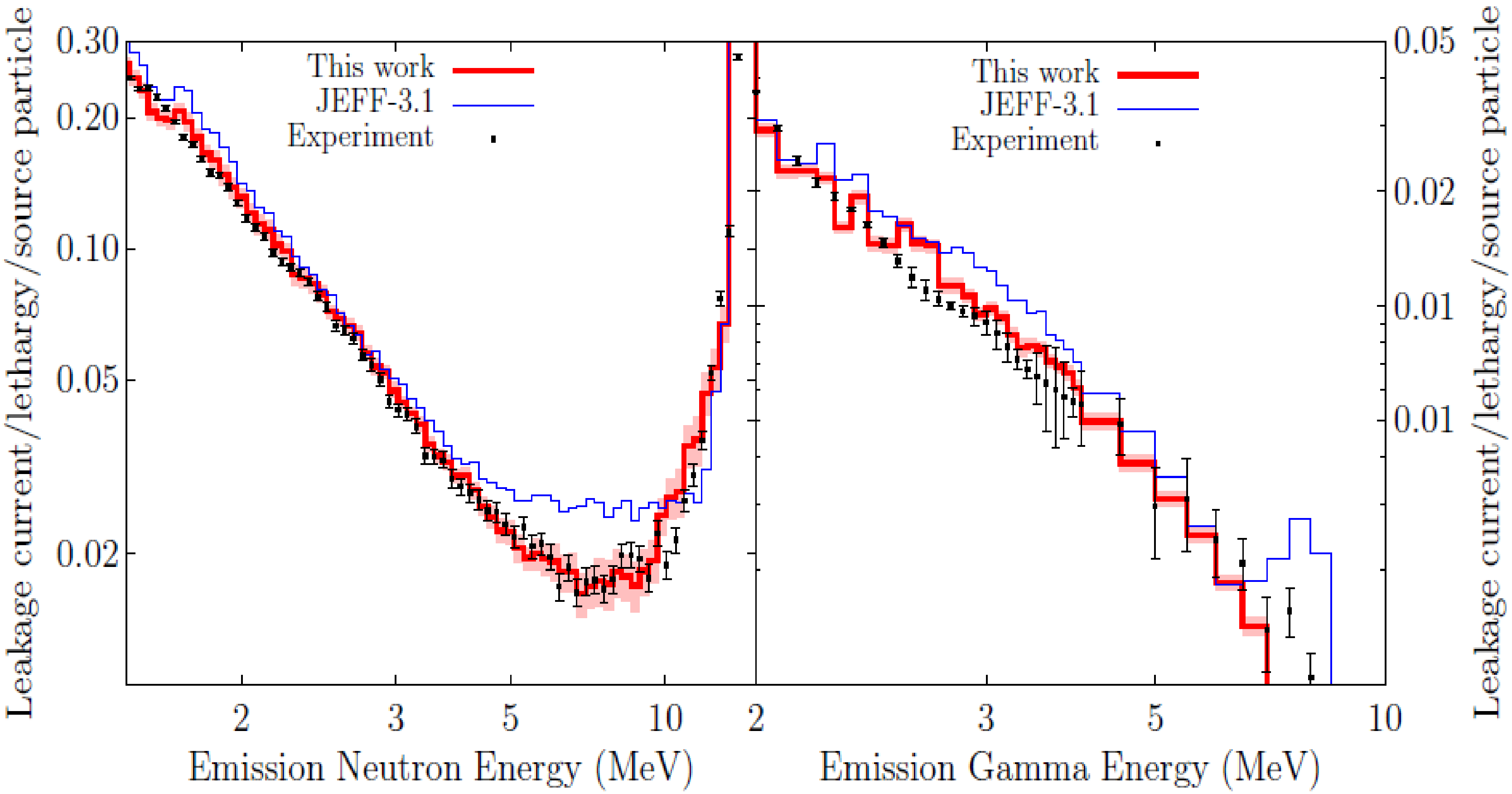




TMC example
PWR burn-up calculations

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'', Nuclear Technology 179, no. 3, 323-338 (2012).

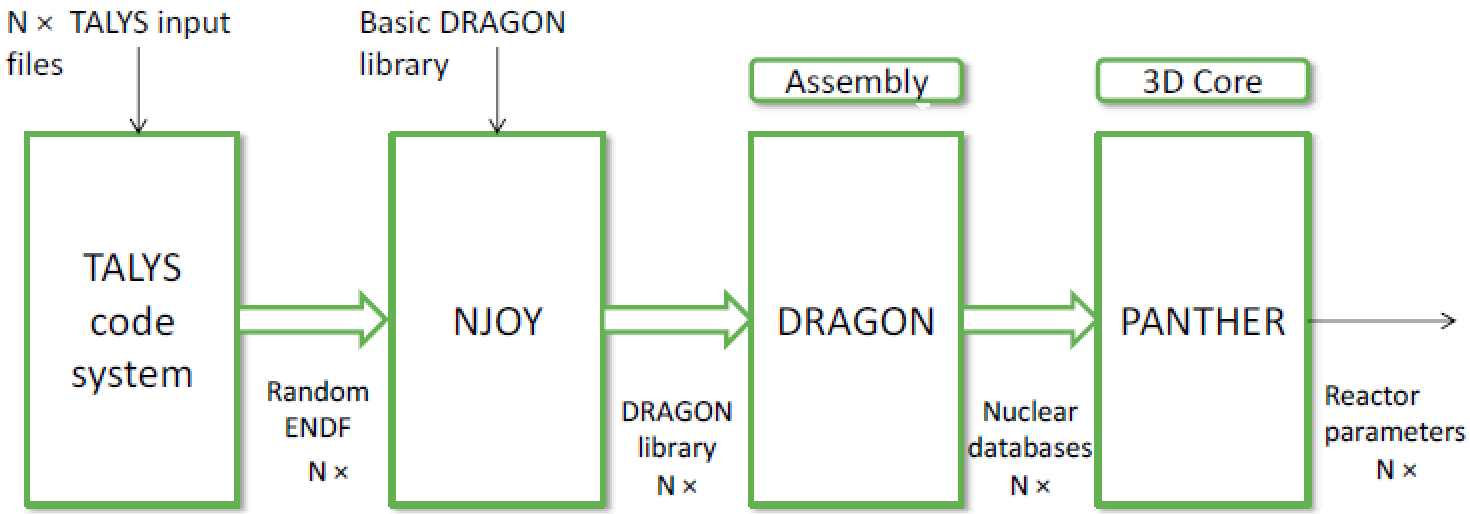
Fusion : Optimized Cu63,65 file vs Oktavian exp.



D. Rochman, A.J. Koning and S.C. van der Marck, [``Exact nuclear data uncertainty propagation for fusion design''], Fusion Engineering and Design 85, 669-682 (2010).

TMC beyond static systems: control rod ejection

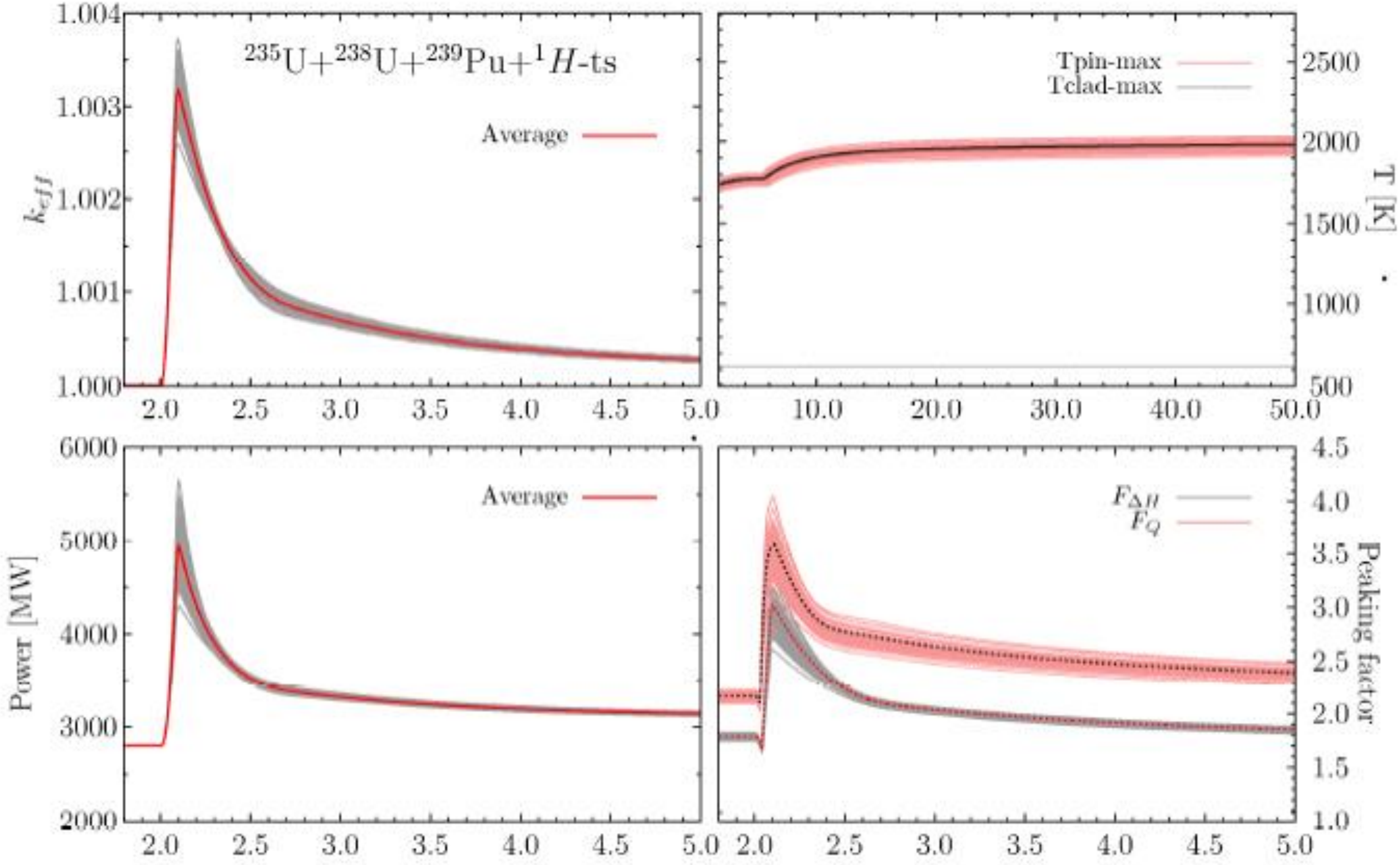
- Reminder: **Total Monte Carlo has nothing to do with the Monte Carlo or deterministic nature of the underlying software**
- **Produce nuclear databases for PANTHER containing macroscopic cross sections, kinetic parameters, isotope concentrations, in two energy groups, tabulated as function of burn-up, fuel and coolant temperature, boric acid concentration, control rod state, etc.**



Da Cruz, Rochman, Koning, Physor2014

Westinghouse 3-loop reactor: k-eff, power, temperature and peaking factor after control rod ejection

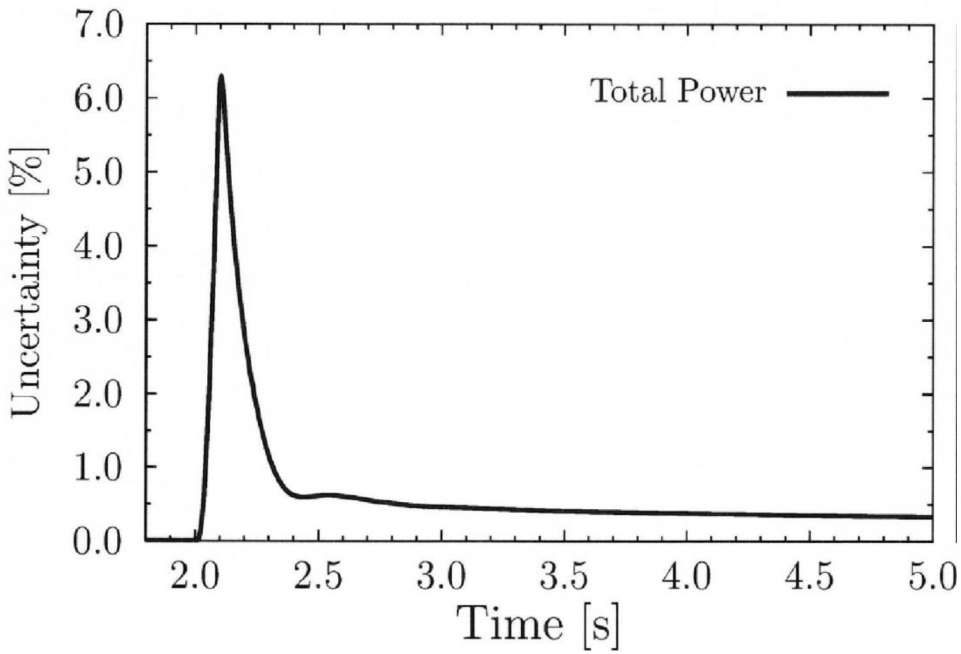
400 Random data libraries for U-235, U-238, Pu-239 and thermal scattering

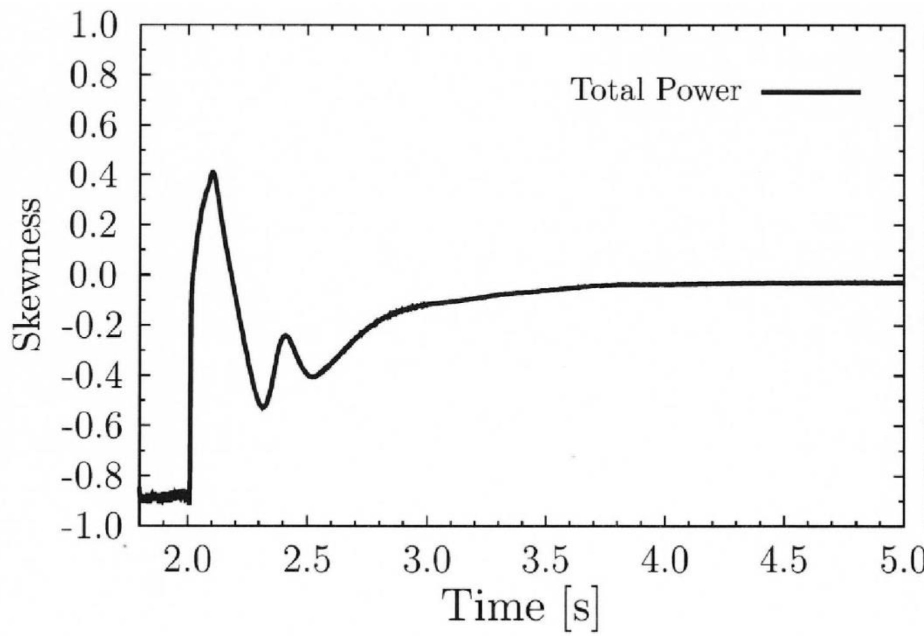


Time (s)

Time (s)

Uncertainty profile: Deviation from normal distribution





Final thought: Computers allow us to go back in time

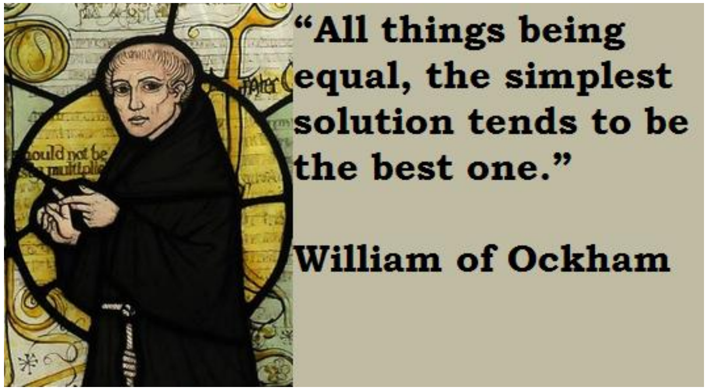
- **Monte Carlo: von Neumann**

- **Normal distribution: Gauss**

- **Inference: Bayes**

- **The methods are more and more reduced to sampling and counting.**

Among competing hypotheses, the one with the fewest assumptions should be selected.



Ockham's razor - William of Ockham (c. 1287 - 1347)