Nuclear data, uncertainties and their applications

Part 1: Introduction and TMC

D. Rochman

Nuclear Research and Consultancy Group,

NRG, Petten, The Netherlands

EXTEND school Budapest, September 2012

Contents

① What are nuclear data ? (*Part 1*)
② Are they important ? (*Part 1*)
③ What are they ? (*Part 1*)
③ How can they be produced ? (*Part 1*)
④ Where are they used ? (*Part 1*)
⑤ Total Monte Carlo (TMCs) (*Part 1*)
⑥ Applications: adjustment of nuclear data (*Part 2*)
⑦ Applications: nuclear data and uncertainties for reactors and fuels (*Part 3*)
⑧ Discussions


You are here: Home / Top News / U.S. News / U.S., Russia exchange nuclear data

U.S. News

U.S., Russia exchange nuclear data

Recommend 0 Tweet 0 +1 0 (0)

President Dimitri Medvedev (L) of Russia and U.S. President Barack Obama hold a bilateral meeting at the United Nations in New York on September 23, 2009. UPI/Olivier Douliery/Pool

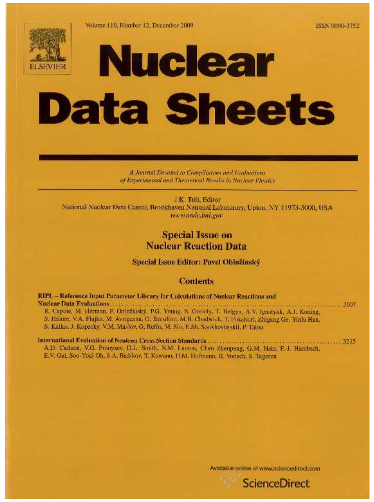
License photo

All slides can be found at:
ftp://ftp.nrg.eu/pub/www/talys/bib_rochman/presentation.html).

What are nuclear data ?

The term ”nuclear data” can have different meaning,

- dusty books, constants, mature field, code inputs,
- list, Schrodinger equation, unexciting...
- but this is not ! (I’m going to prove that)



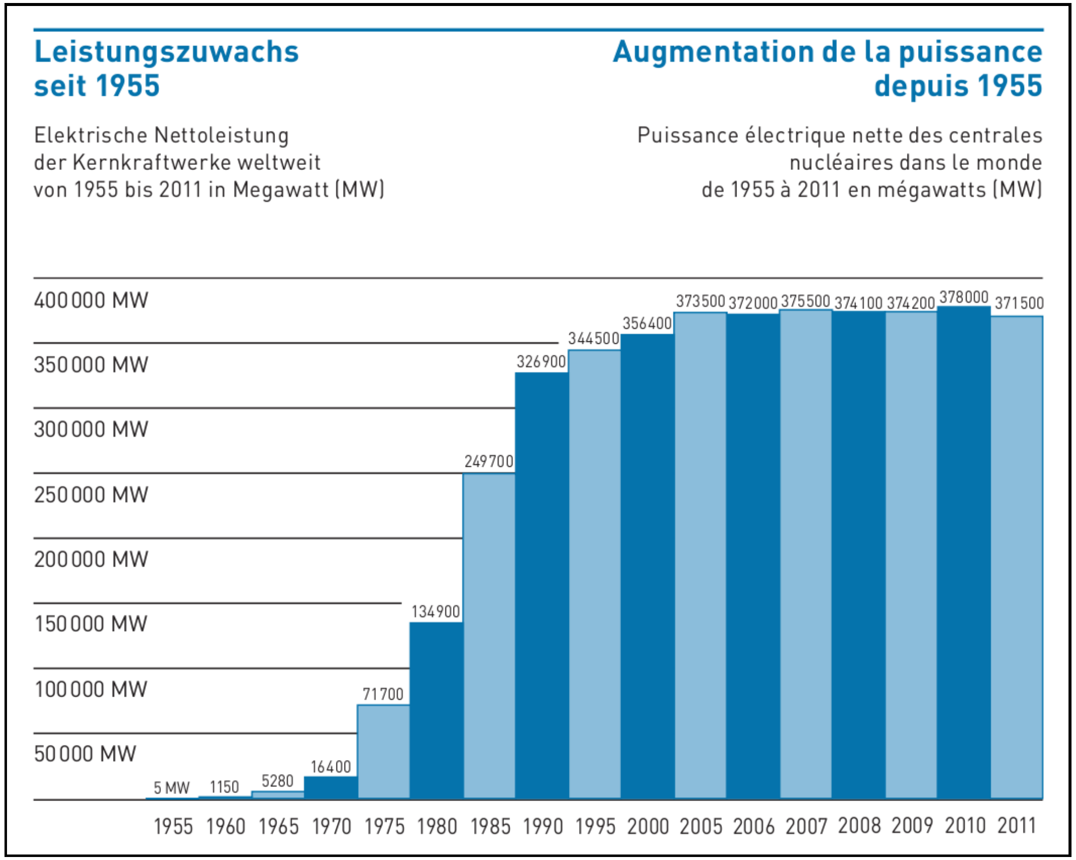
Are nuclear data important ?

Better nuclear data can help for:

- ▶ safety margins, fuel storage,
- ▶ life-time extension,
- ▶ cost reduction in design of new systems,
- ▶ isotope production,
- ▶ safety of people (shielding),
- ▶ waste transmutation,
- ▶ development of future systems.

Better nuclear data have a limited effect on:

- ◀ current reactor operation,
- ◀ current reactor safety,...
- ◀ accident simulation,
- ◀ proliferation,
- ◀ Chernobyl, TMI, Fukushima.

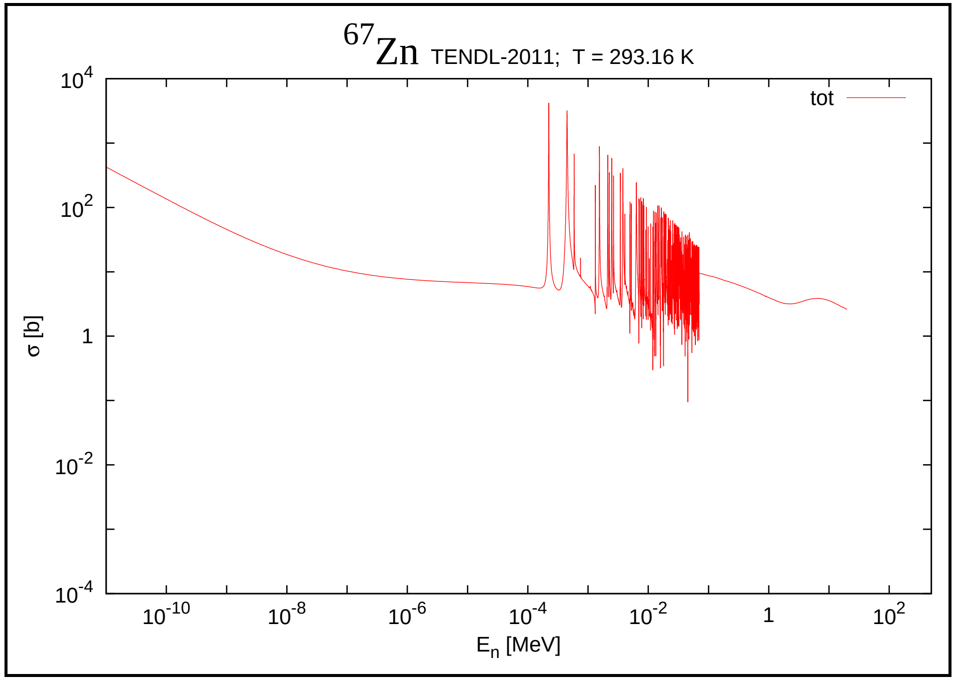


What are nuclear data in this presentation ?

- from ^{1}H to ^{280}Ds,
- from 0 to 20(0) MeV neutron induced,
- cross sections, particle emission,
- angular and energy distributions,
- decay data (half-lifes, γ-ray...), fission yields, neutron yields,

↪ and uncertainties.

All these data are nicely condensed in files in ENDF-6 format (the manual can be found here).



How to produce nuclear data ?

Independently of the quality of the data, there are 2 ways to produce them:

First solution: manual production

① widely used for decades and up to 2100,
② concerns all major libraries,
③ questionable QA practices ($\neq$ than the nuclear industry standards)
④ has produced very good data in the past and present,
⑤ we know less and less why.

Second solution: ”computer-assisted” production

❶ one word: ”reproducibility”,
❷ concerns only one library: TENDL,
❸ much better QA,
❹ spend your time on evaluation, and not on formatting, assembling...

The world perception is changing and the second solution might spread around. But this is not the case yet.

How to use nuclear data ?

In general, nuclear data are used by simulation codes:

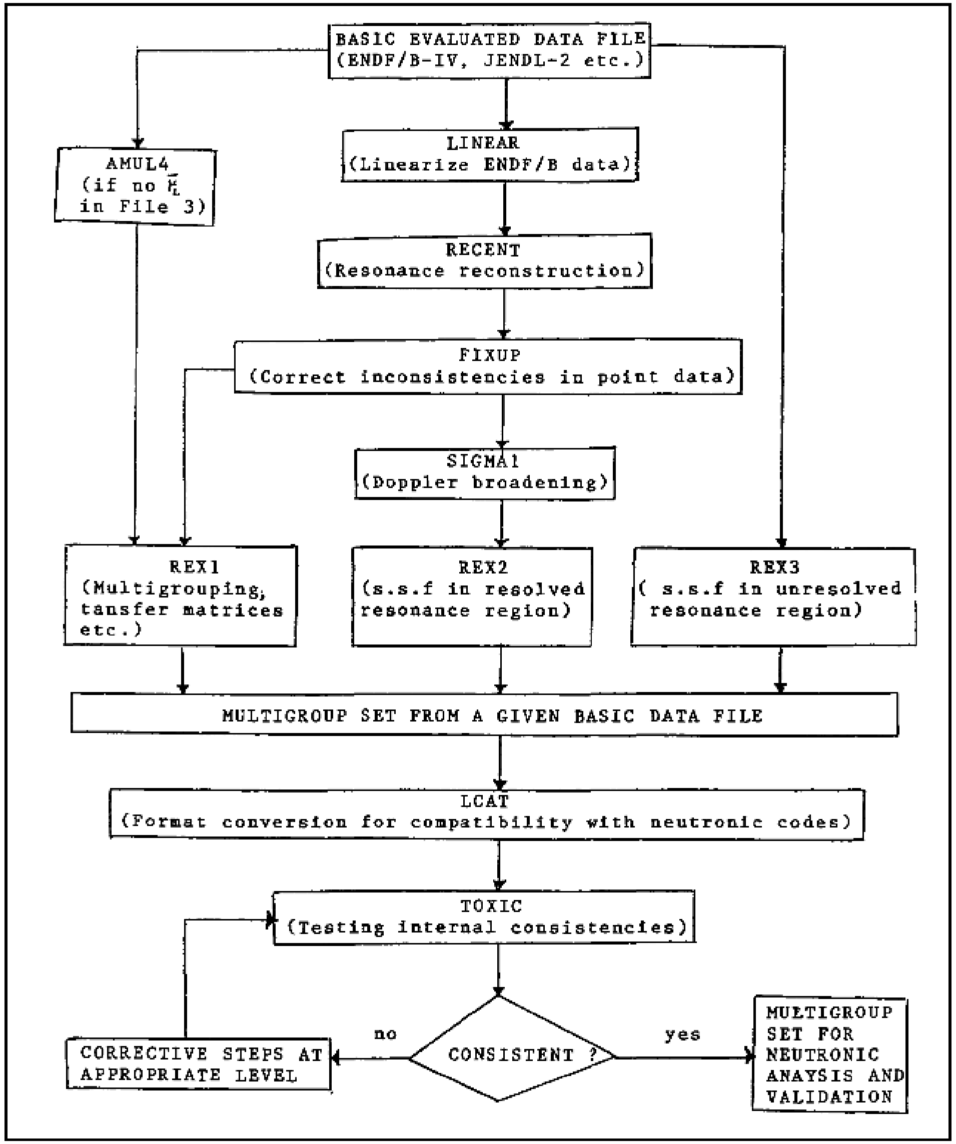
- Transport Monte Carlo: MCNP, SERPENT, TRIPOLI ... (see here for details),
- Transport deterministic: PARTSN, DRAGON, ATTILA ... (see here for details),
- High energy transport: GEANT4, FLUKA, MCNPX ...
- Depletion: FISPACT, ORIGEN, DARWIN ...
- Full core: PANTHER, SIMULATE...
- Transient: SIMULATE, RELAP (see here for details),
- and other...

using some processing codes:

- NJOY (USA LANL),
- CALENDF (France CEA),
- PREPRO (USA LLNL),
- AMPX, PUFF (USA ORNL),
- WIMS (UK), and many other.

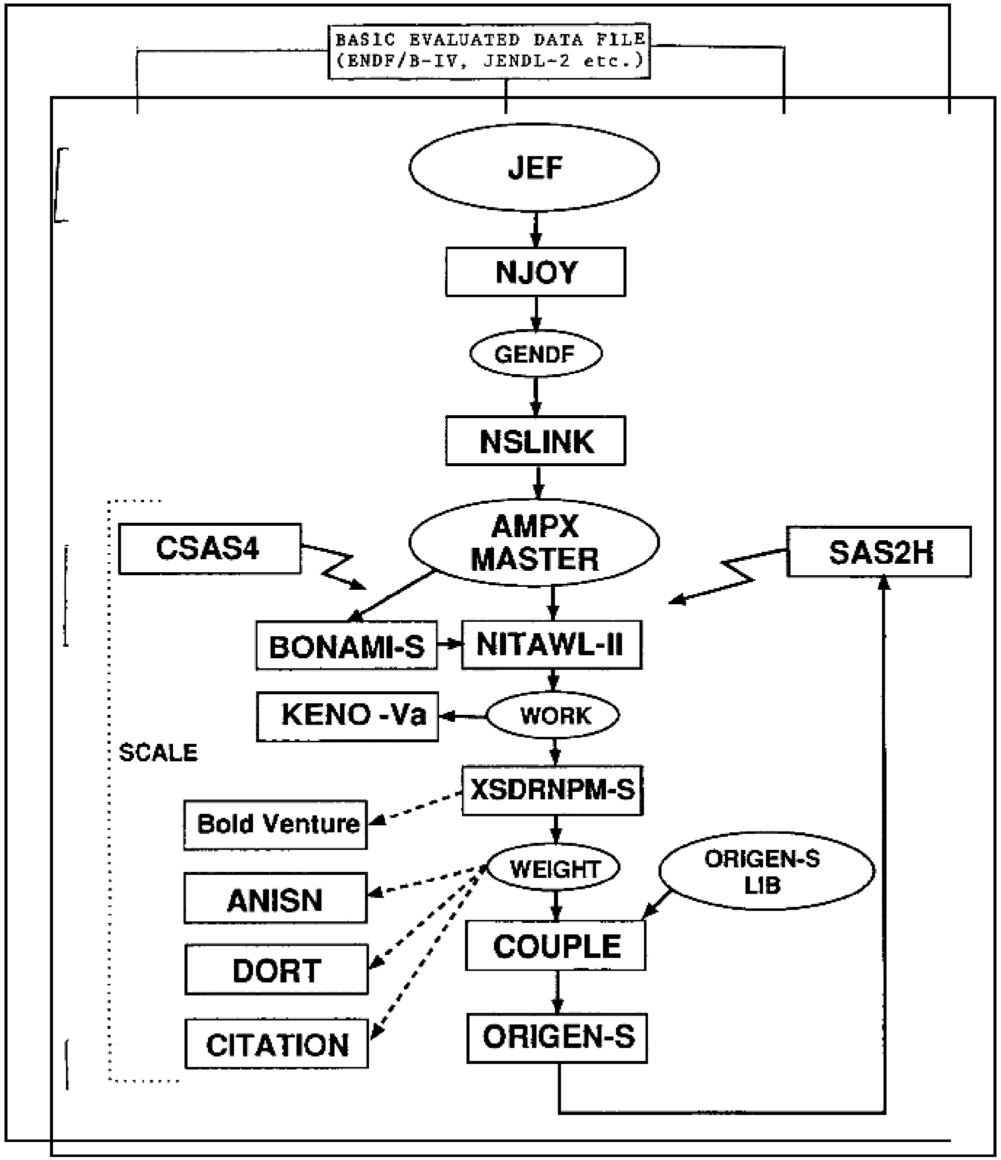
How to process nuclear data ?

One of the most complicated job in nuclear data:



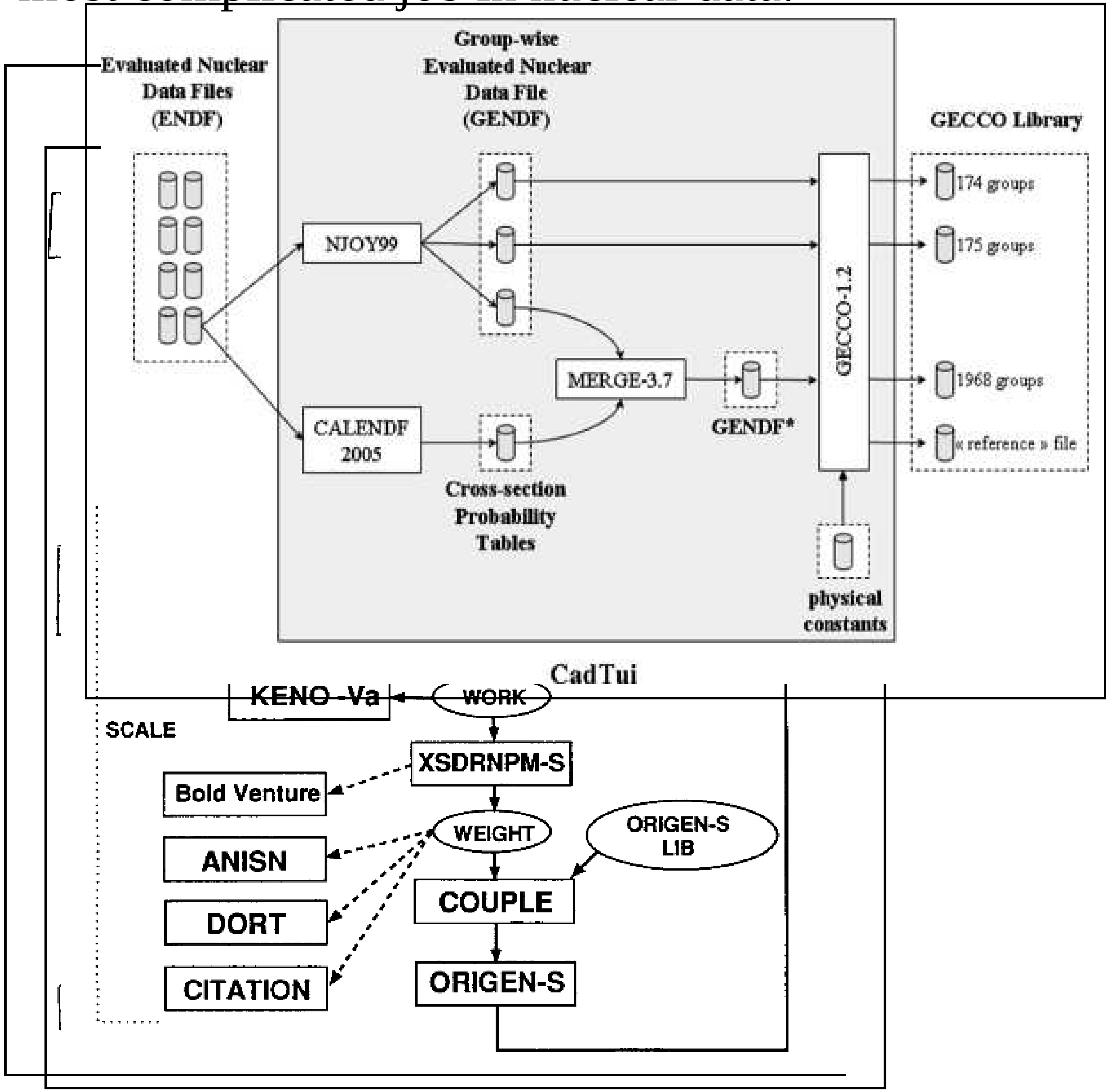
How to process nuclear data ?

One of the most complicated job in nuclear data:



How to process nuclear data ?

One of the most complicated job in nuclear data:



How to process nuclear data ?

One of the most complicated job in nuclear data:

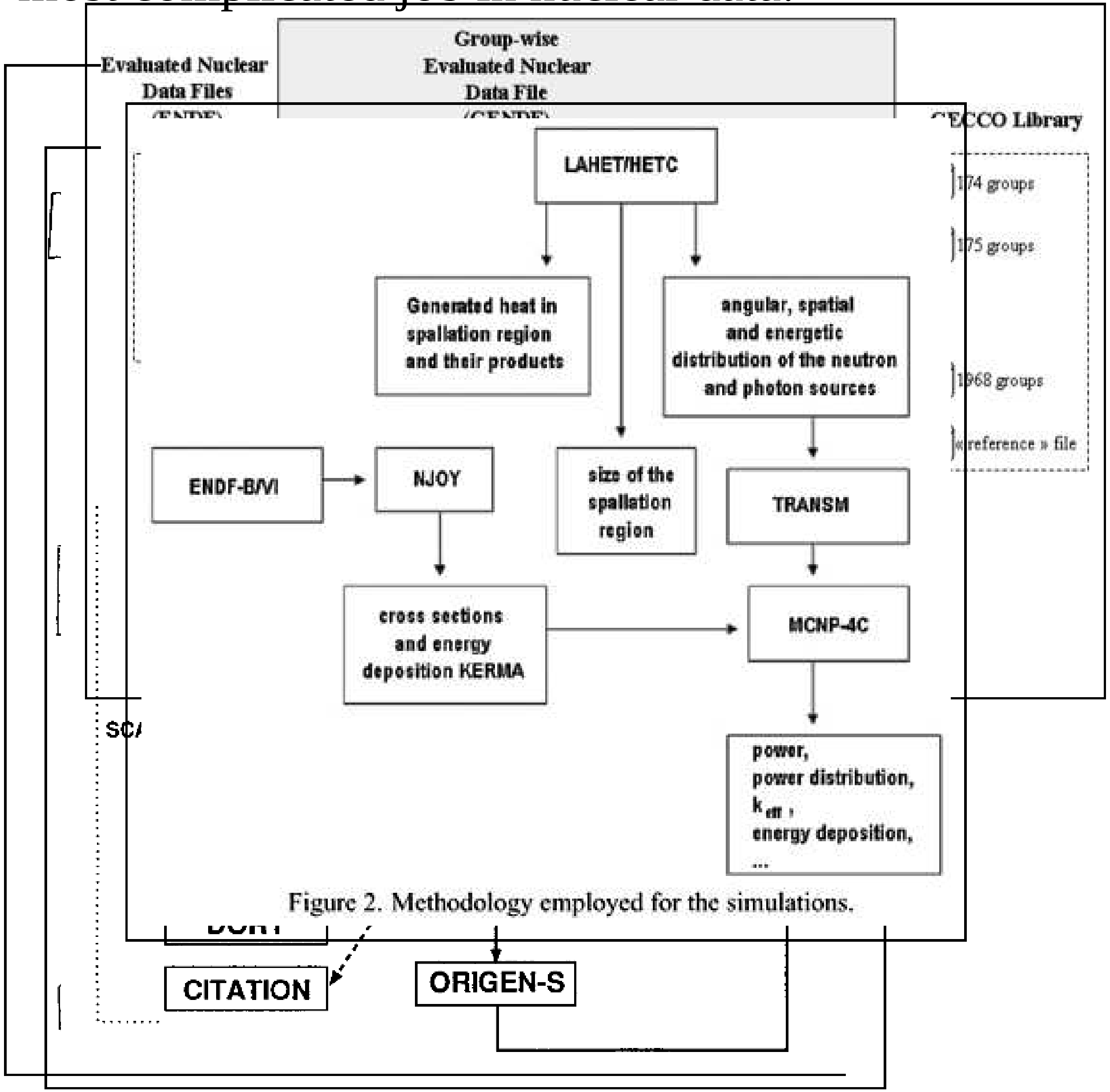
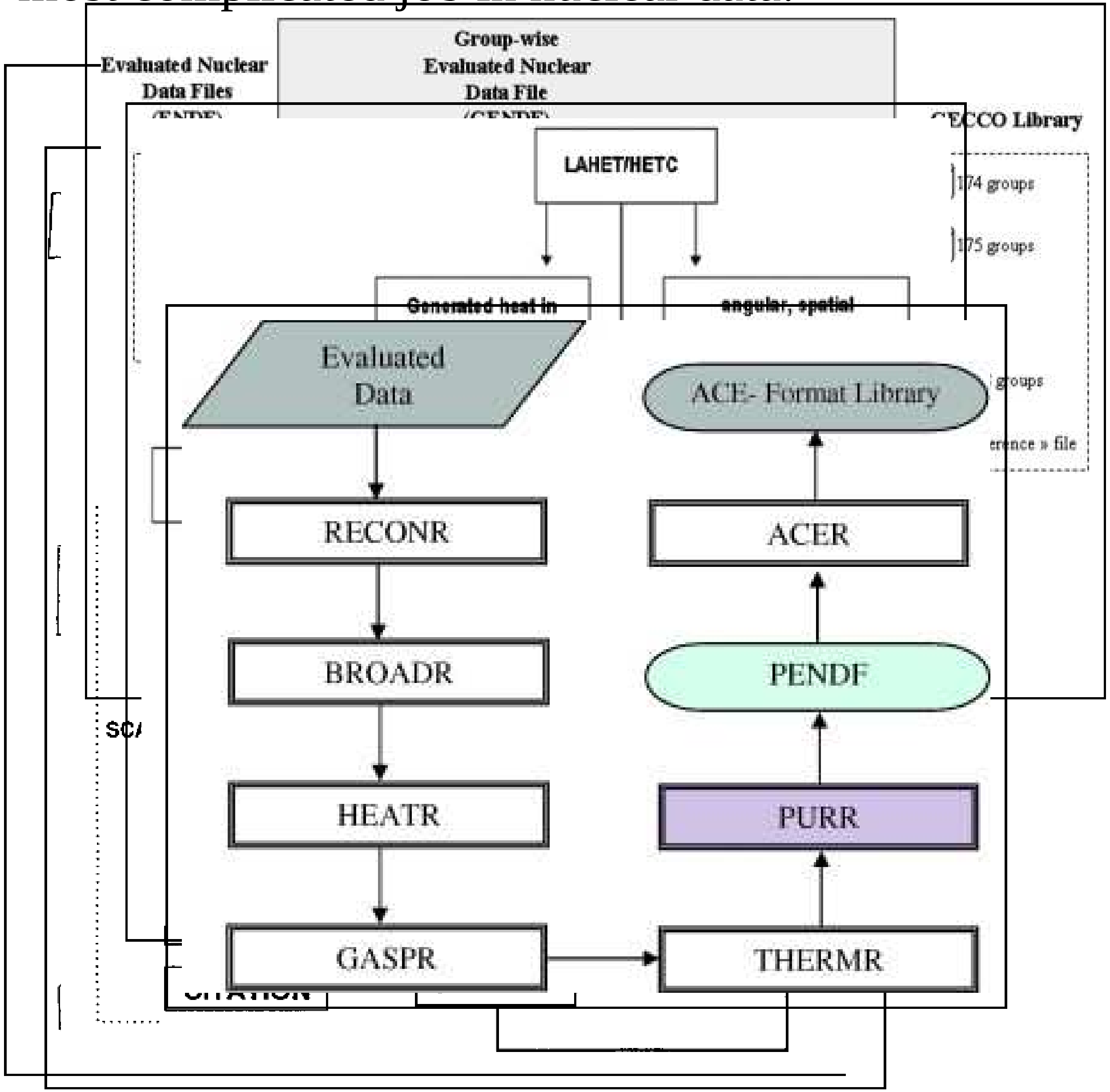


Figure 2. Methodology employed for the simulations.

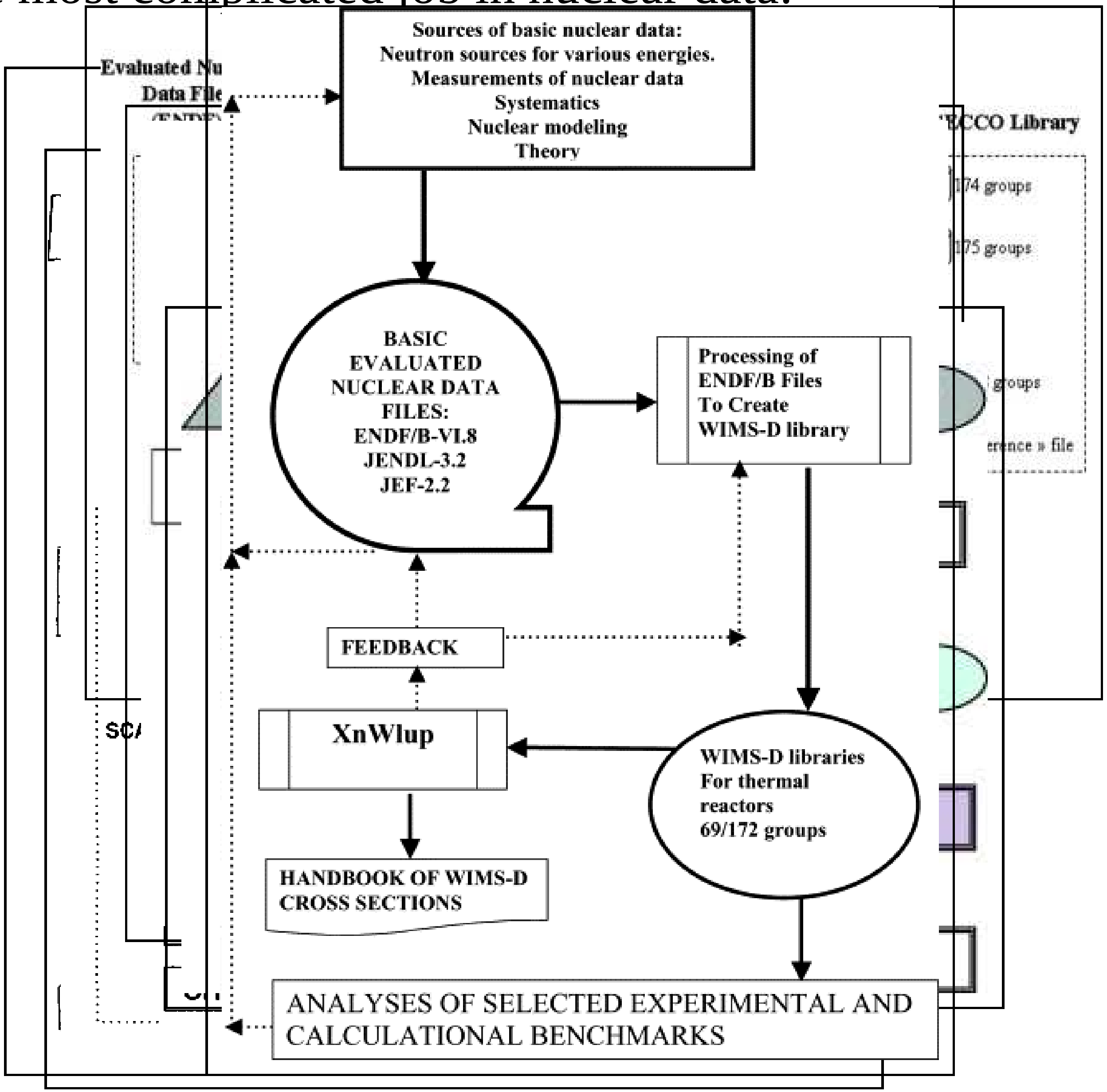
How to process nuclear data ?

One of the most complicated job in nuclear data:



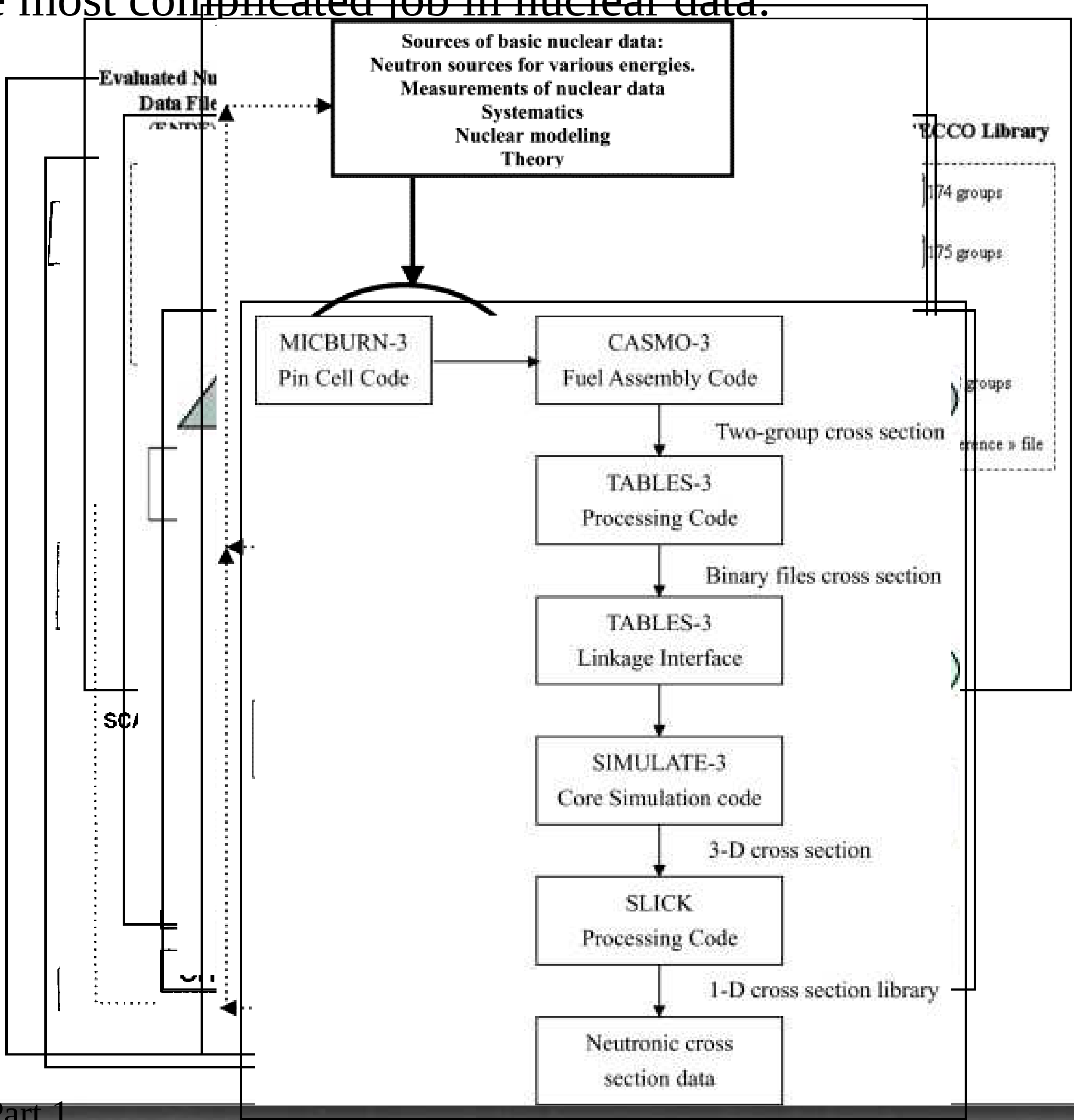
How to process nuclear data ?

One of the most complicated job in nuclear data:



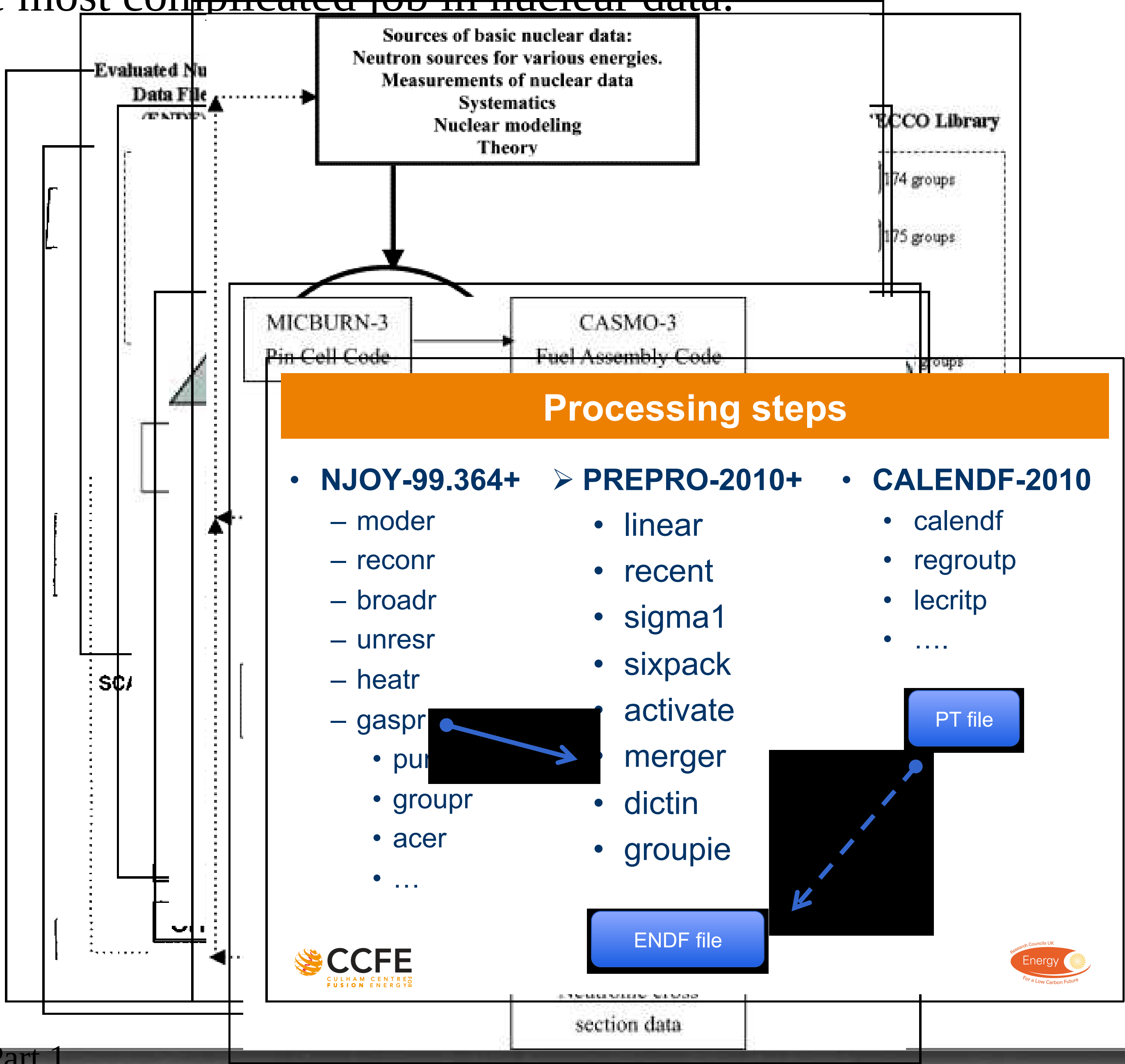
How to process nuclear data ?

One of the most complicated job in nuclear data:



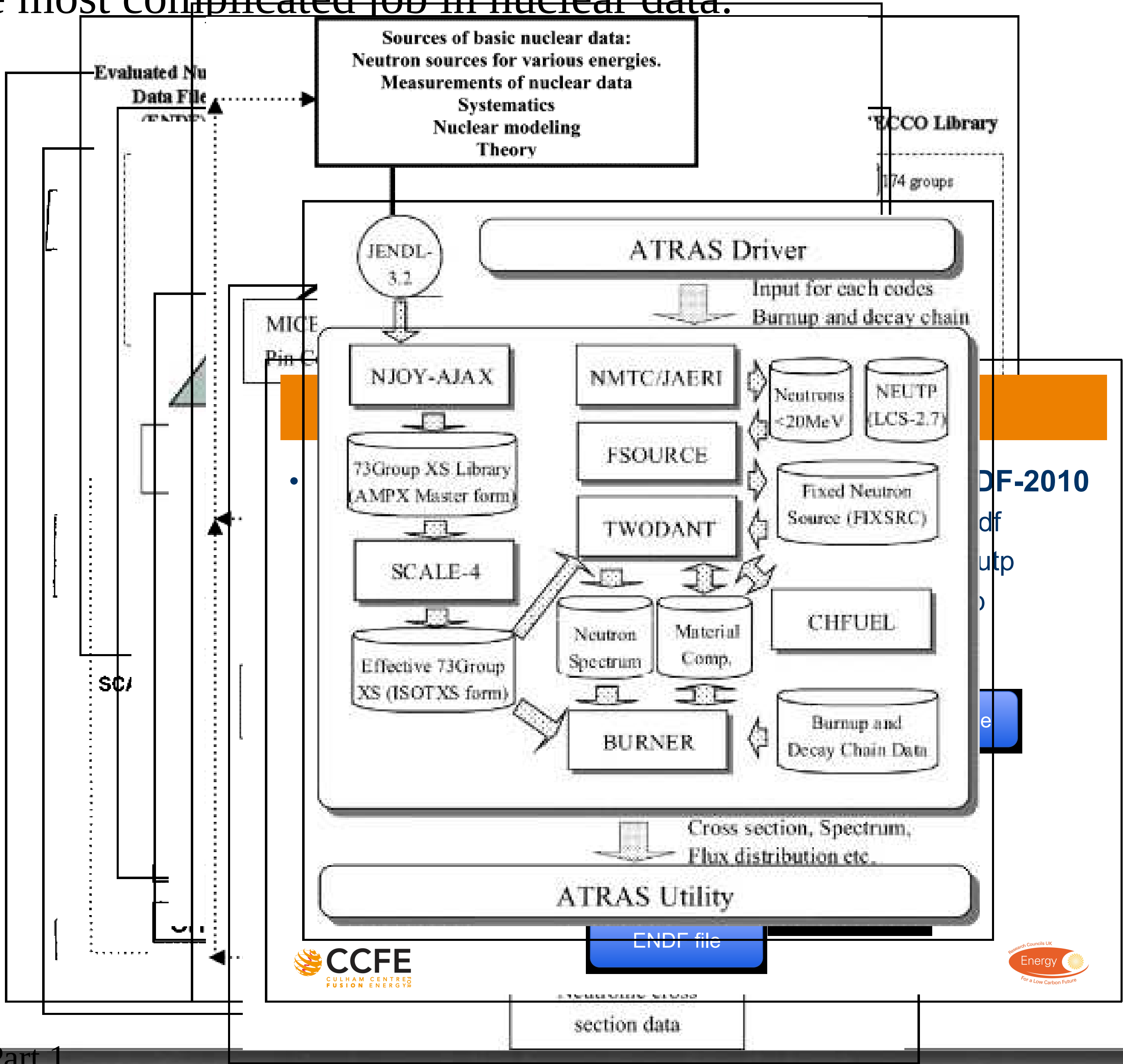
How to process nuclear data ?

One of the most complicated job in nuclear data:



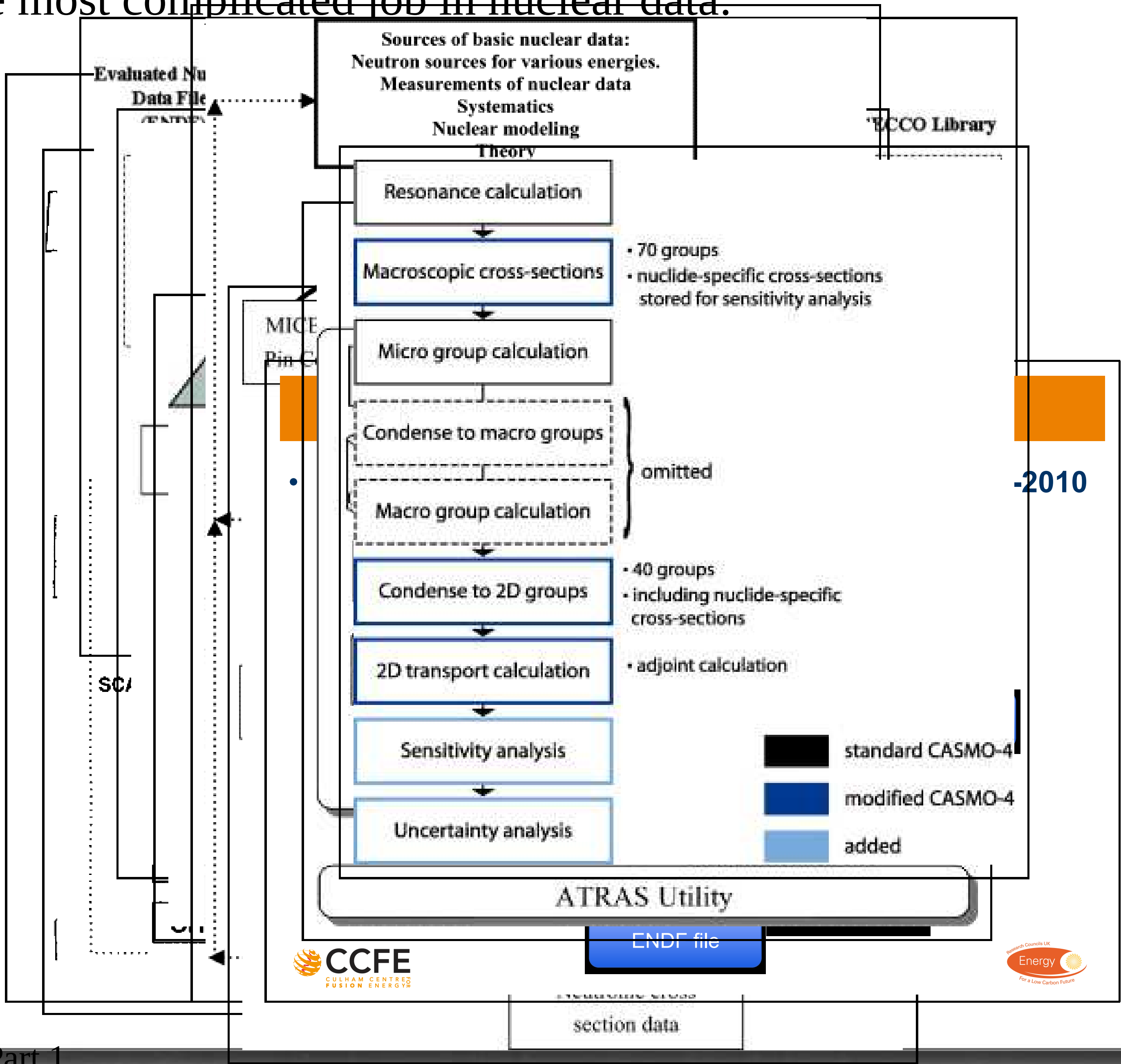
How to process nuclear data ?

One of the most complicated job in nuclear data:



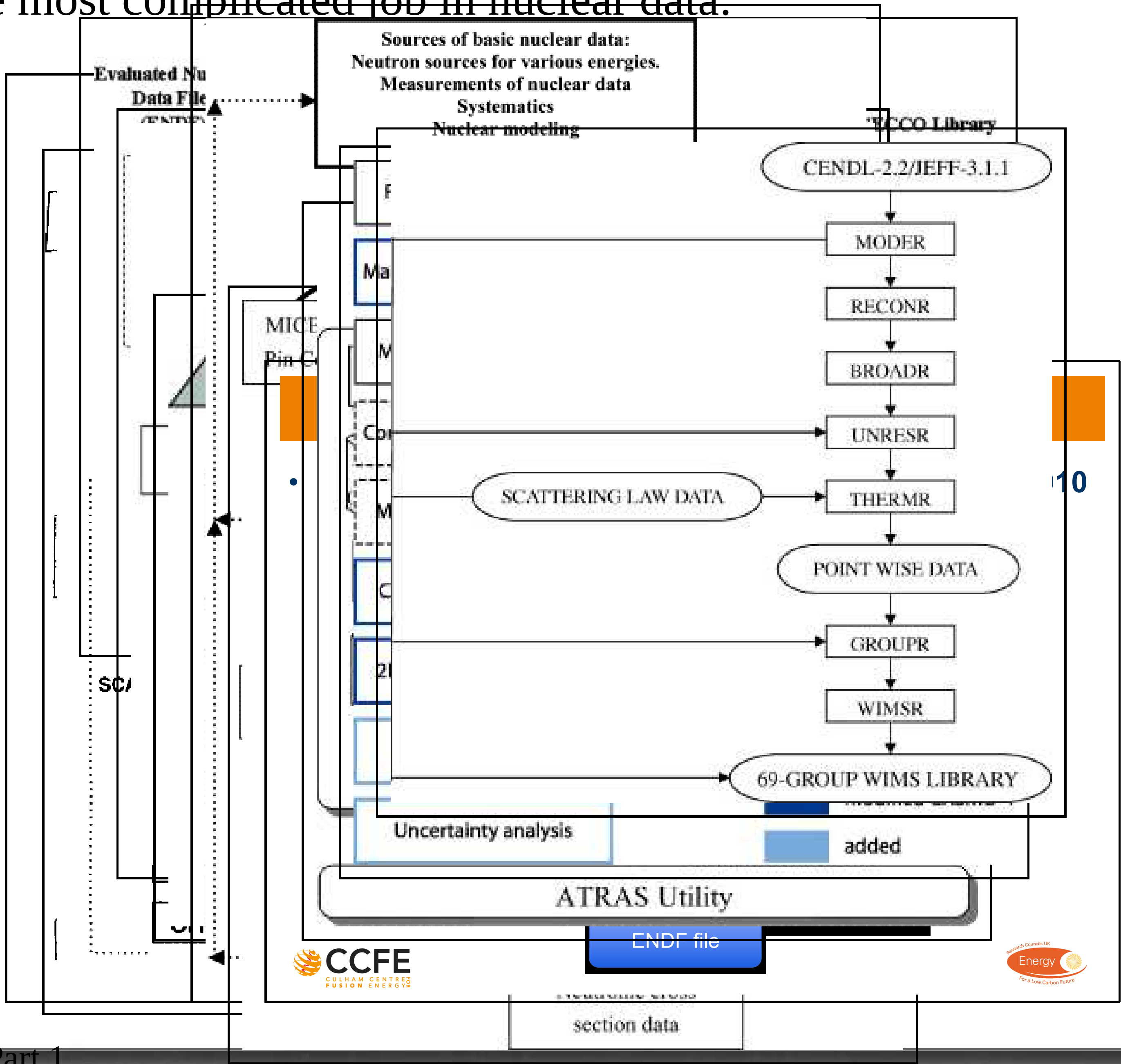
How to process nuclear data ?

One of the most complicated job in nuclear data:



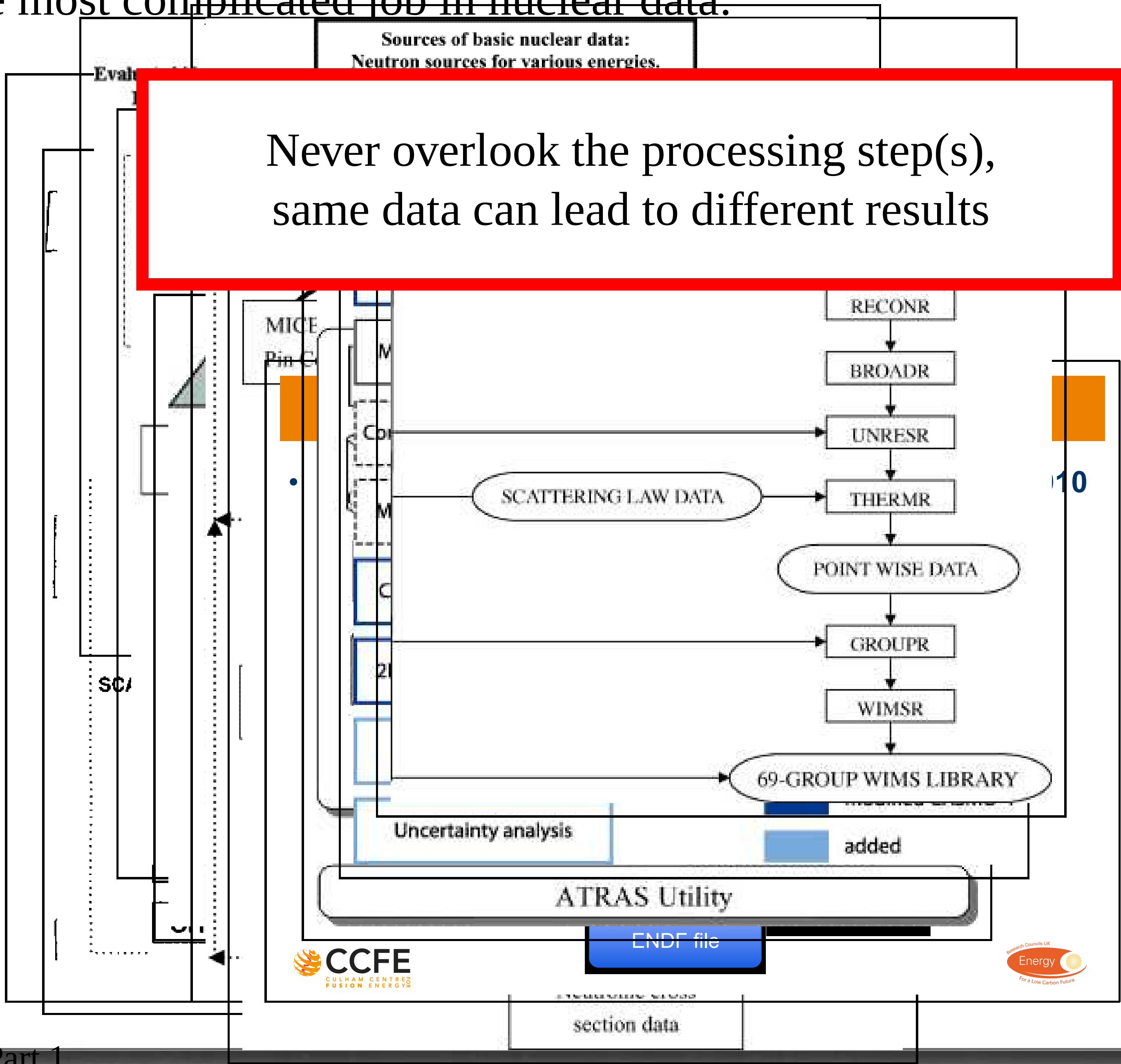
How to process nuclear data ?

One of the most complicated job in nuclear data:



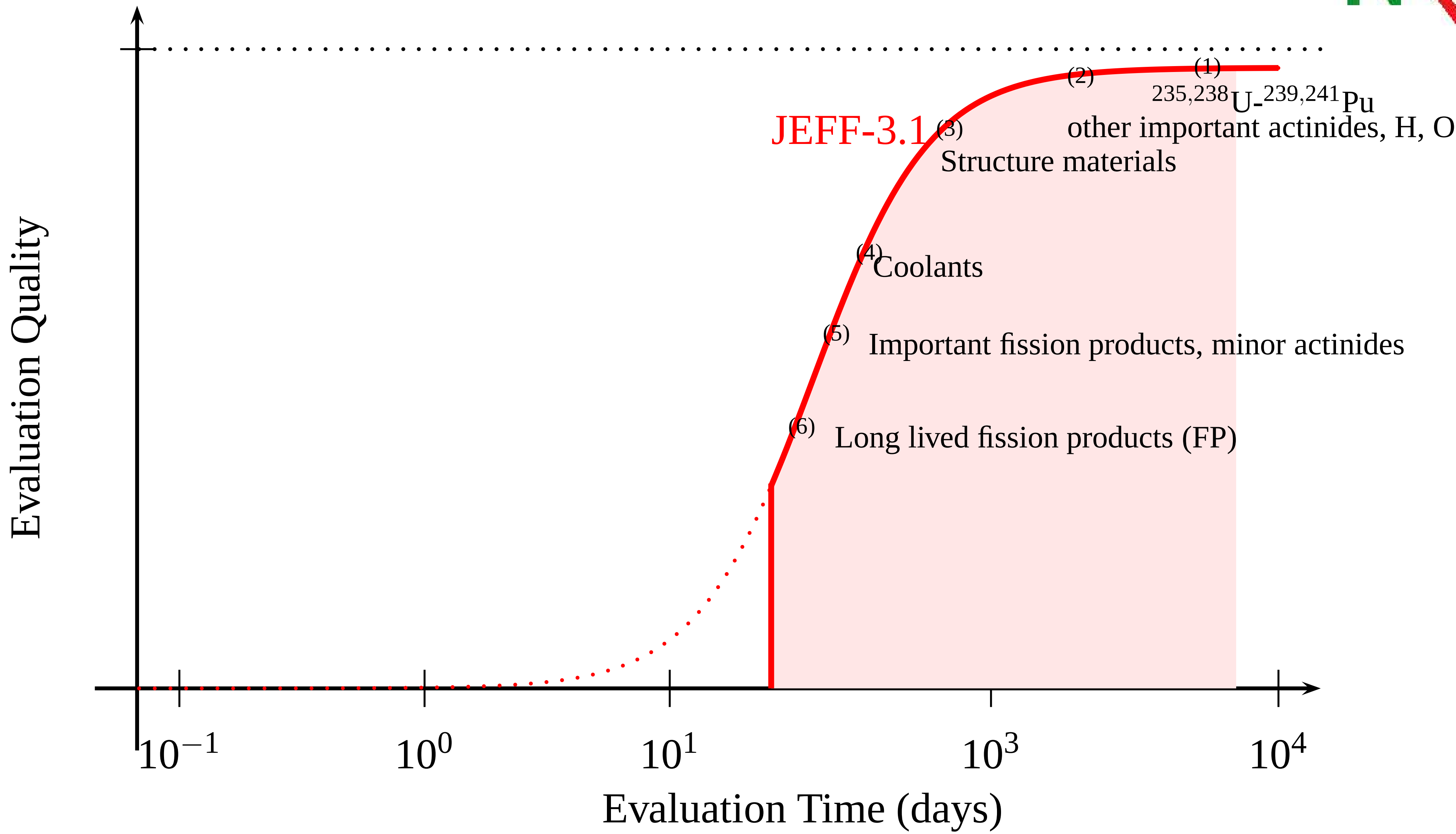
How to process nuclear data ?

One of the most complicated job in nuclear data:

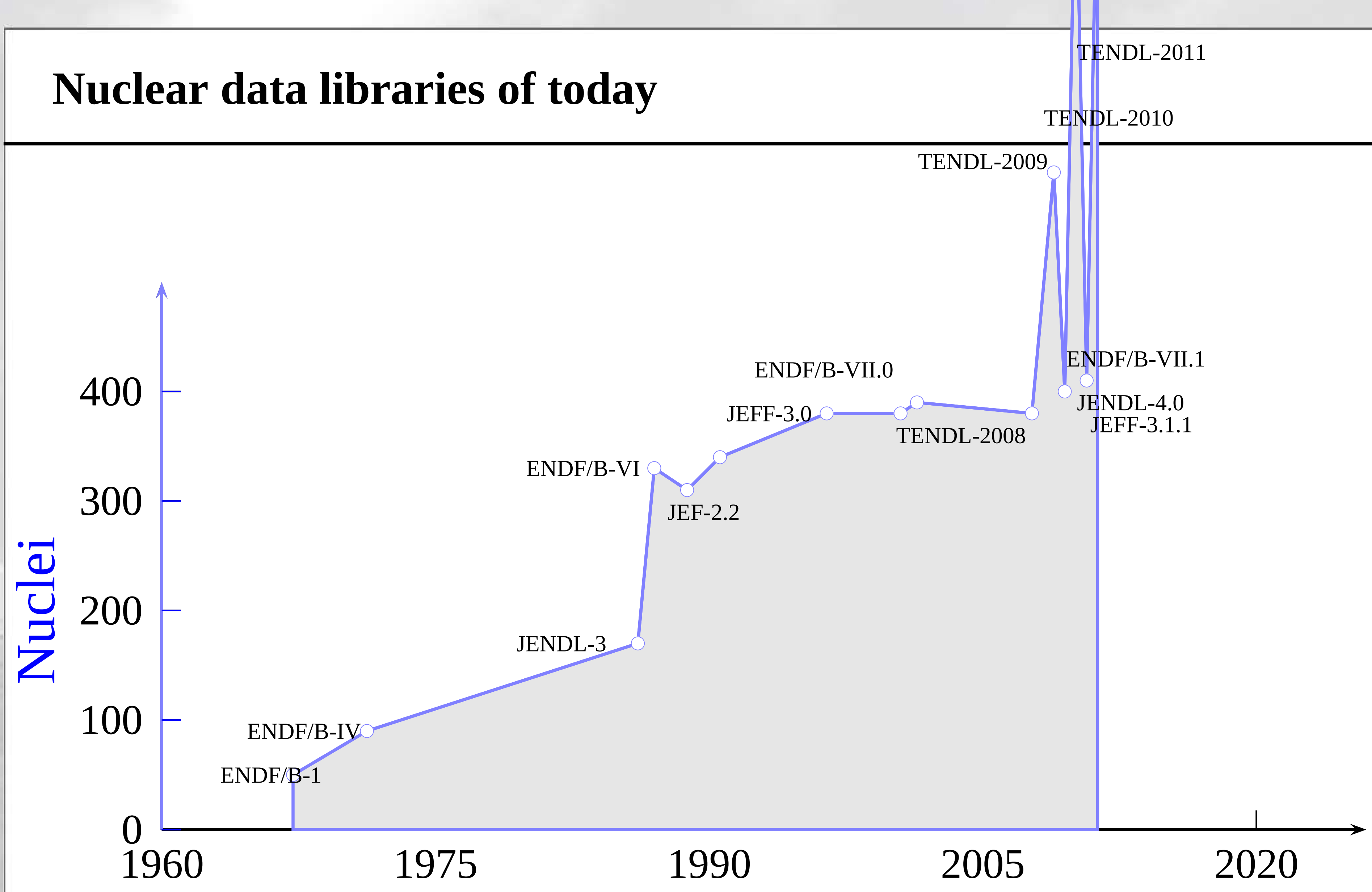


Never overlook the processing step(s), same data can lead to different results

Nuclear data libraries of today



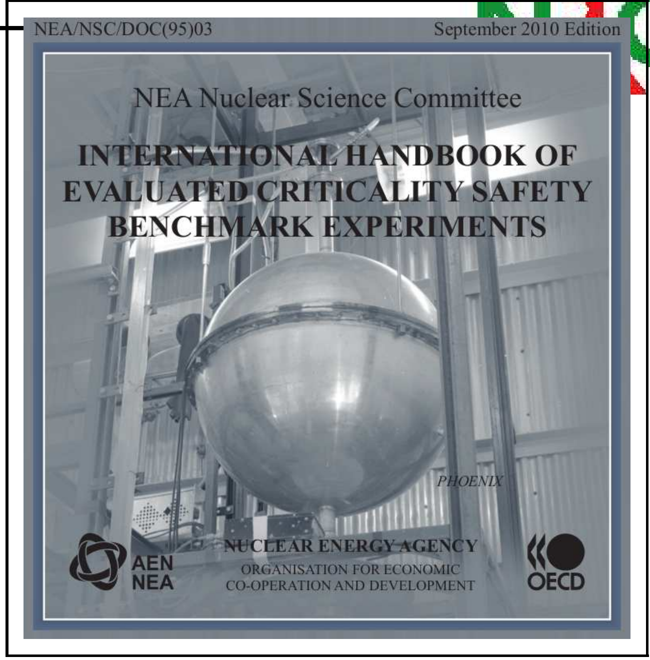
Nuclear data libraries of today

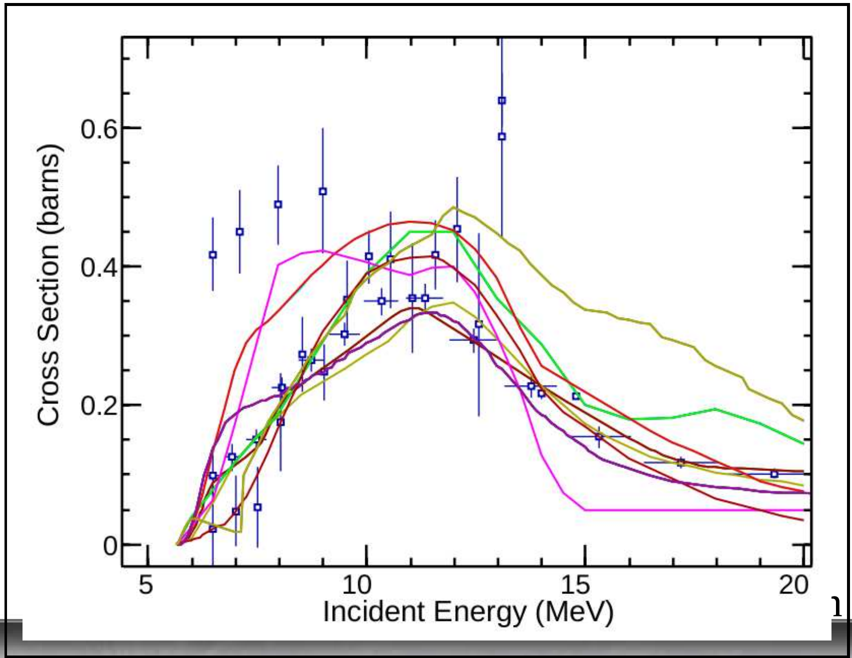


Quality of nuclear data libraries

How to judge the quality of nuclear data ?

- compare with microscopic measurements,
- compare with integral measurements,
  - clean integral experiments,
  - depends on the processing, simulation codes,
  - are adjustments allowed ?
  - is that consistent with microscopic measurements ?
- consistency of the library,
- processability,
- completeness,
- and covariances.

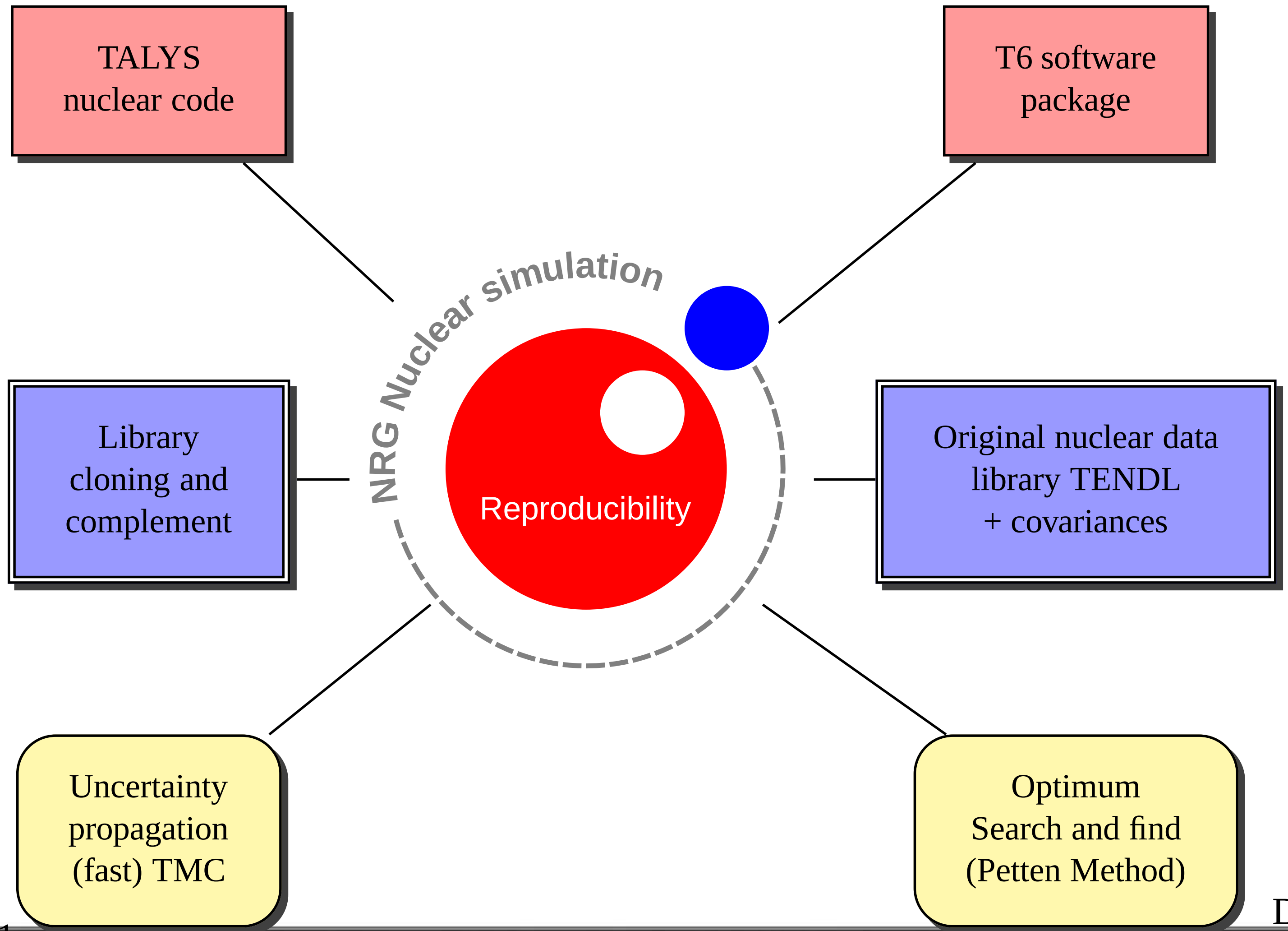




Uncertainty
propagation
TMC

- Started in 2008
- Many publications
- Applied to crit-saf and shielding benchmarks, reactor (k_{eff}, β_{eff}, void, Doppler), burn-up inventory, radiotoxicity
- Still a controversial method

Our mission: improve nuclear simulations



TMC: Motivations for a change

Usual procedures in uncertainty propagation imply:

- ☞ rigid format, fixed libraries of cross sections, simplification of covariances,
- ☞ need for processing, sensitivity and perturbation codes, group scheme,
- ☞ necessity of linearizing inherently nonlinear relationships, and so on. . .

TMC: Motivations for a change

Usual procedures in uncertainty propagation imply:

- ☞ rigid format, fixed libraries of cross sections, simplification of covariances,
- ☞ need for processing, sensitivity and perturbation codes, group scheme,
- ☞ necessity of linearizing inherently nonlinear relationships, and so on. . .

“Researchers should cease trying to be clever in devising refinements to old methods that were developed when computational resources were limited.

TMC: Motivations for a change

Usual procedures in uncertainty propagation imply:

- rigid format, fixed libraries of cross sections, simplification of covariances,
- need for processing, sensitivity and perturbation codes, group scheme,
- necessity of linearizing inherently nonlinear relationships, and so on...

"Researchers should cease trying to be clever in devising refinements to old methods that were developed when computational resources were limited. Instead, their creative instincts should be redirected to unleashing the full potential of computers for **brute** *force analysis"*

D. Smith, Santa Fe 2004

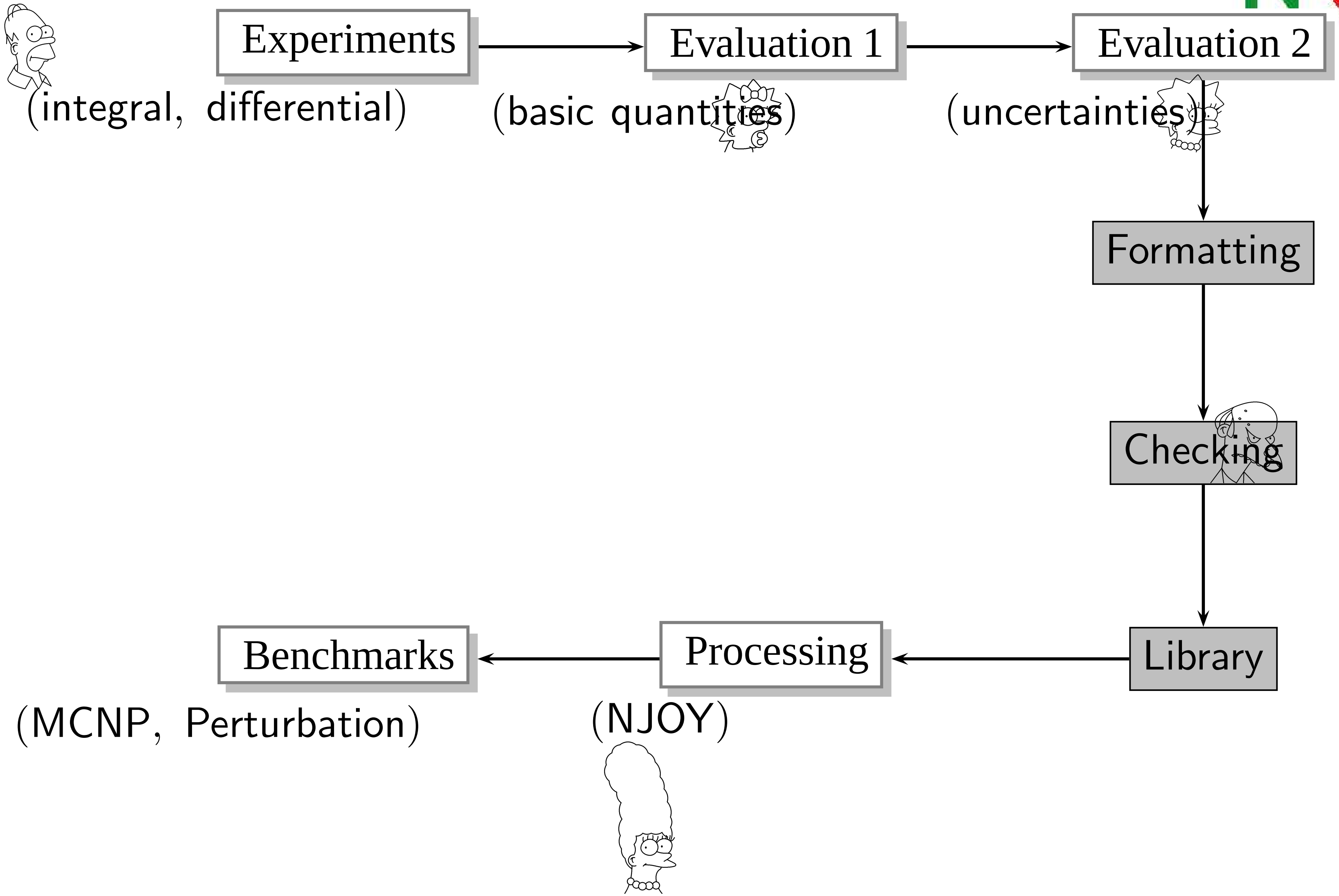
$\Longrightarrow$ Most straightforward way: Total Monte Carlo Approach !

Total Monte Carlo Approach

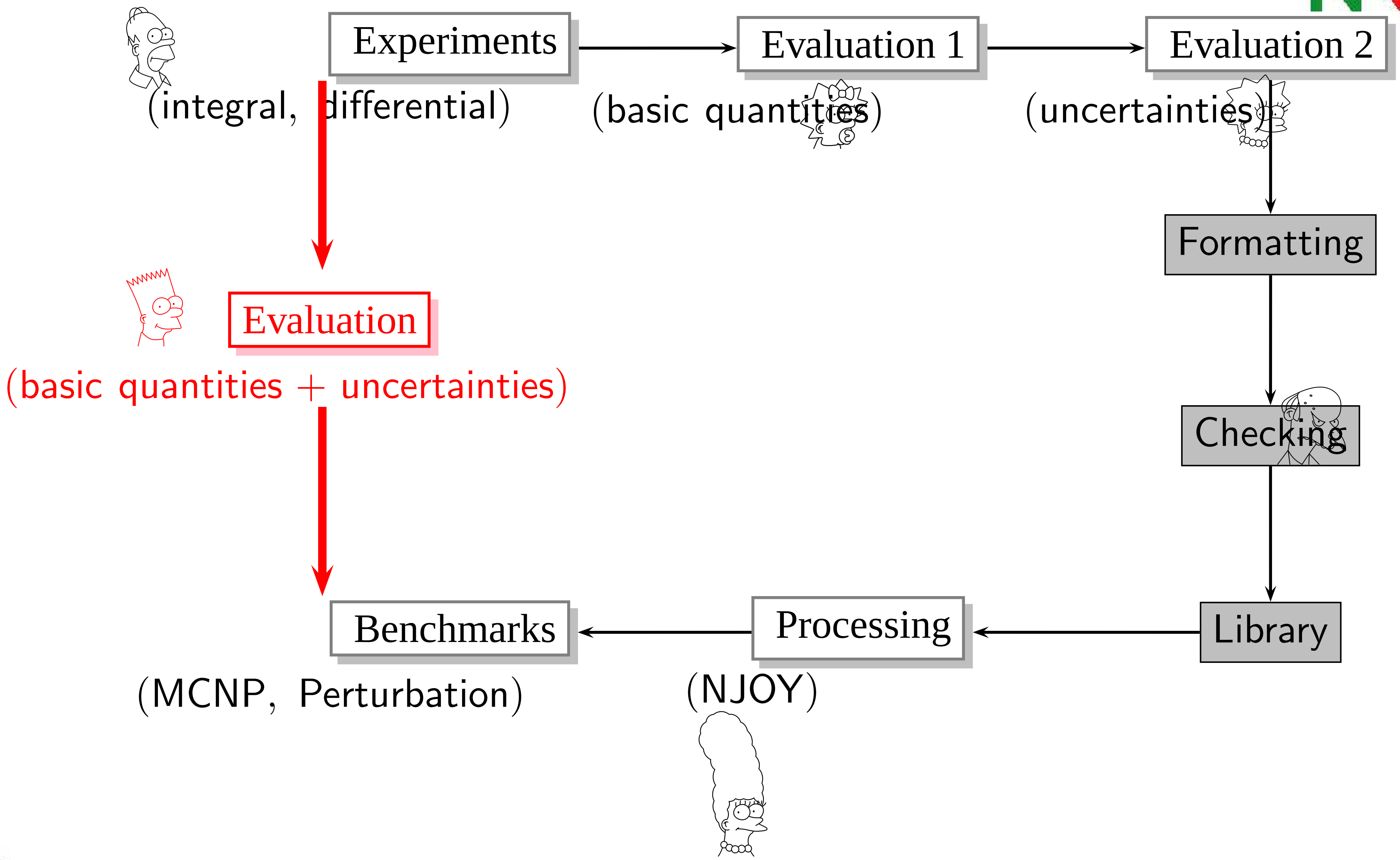
- Stable Nuclear reaction code:**TALYS**
- Talys input parameters + uncertainties
- Resonance parameters + uncertainties

Produce 5000 random, complete ENDF-6 files per isotope

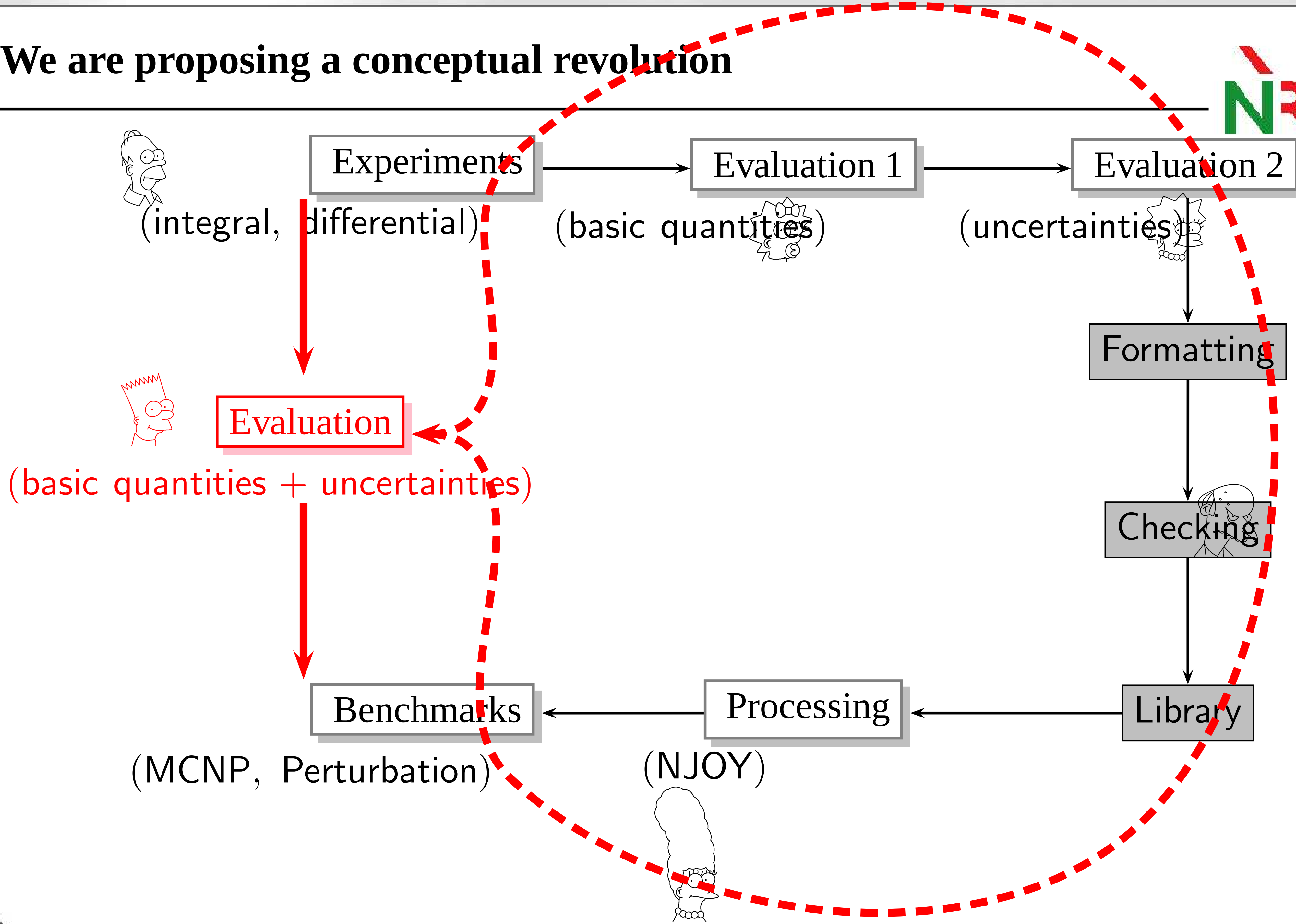
We are proposing a conceptual revolution



We are proposing a conceptual revolution



We are proposing a conceptual revolution



New (and most simple) path

5000 random Talys parameter sets 5000 random resonance parameter sets

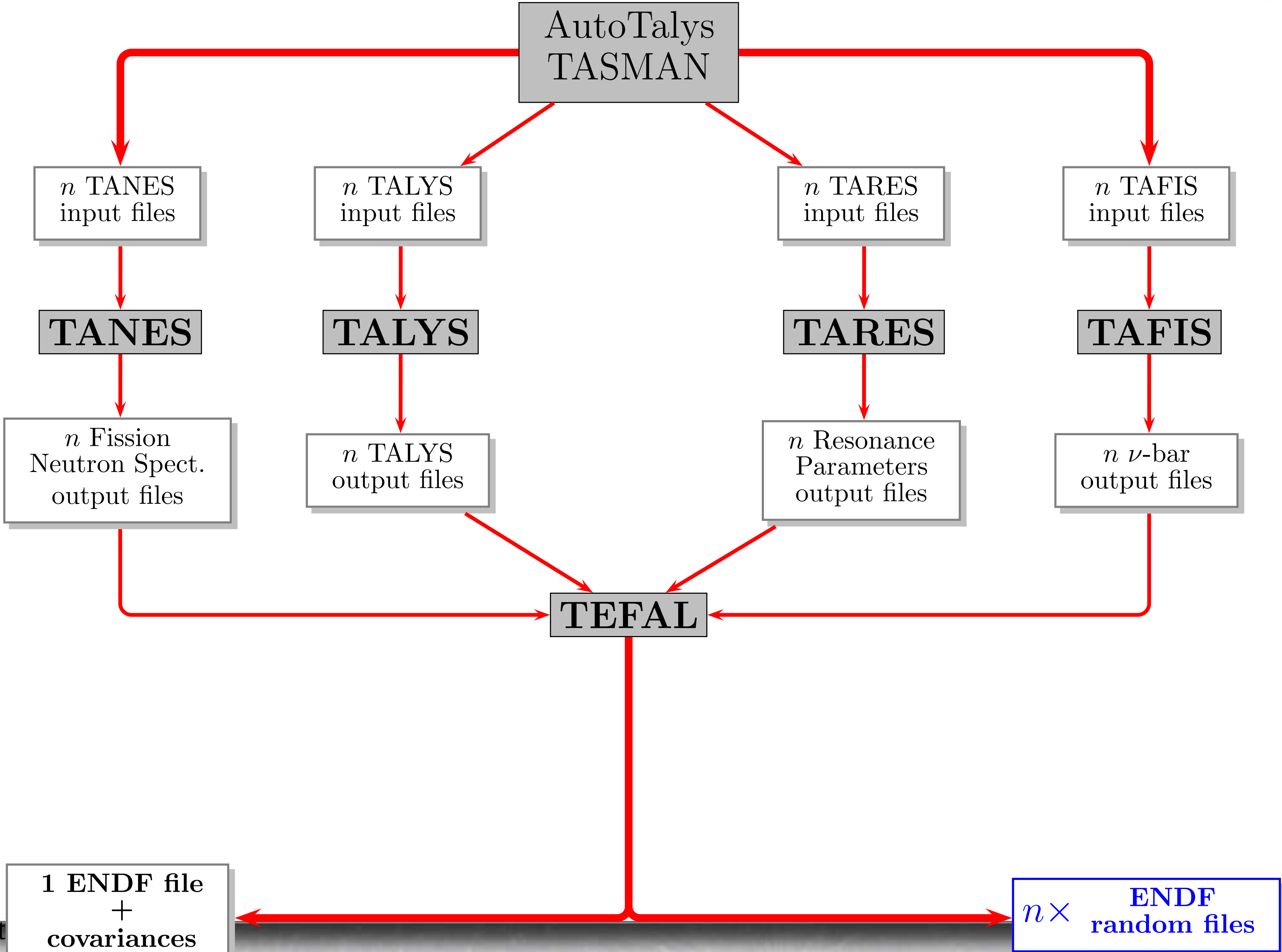
Average to get full covariance matrix MF-32,33,34

5000 random ENDF-6 files
NJOY $\longrightarrow$ 5000 ACE files
5000 MCNP calcs for the same case

Other groups have developed variants: AREVA (NUDUNA), GRS (XSUSA), CIEMAT (ACAB) and PSI, based on covariance files.

No covariances for fission yields, thermal scattering, pseudo-fission products, branching ratios, DDX, γ-production ...

TMC: procedure for the random file production

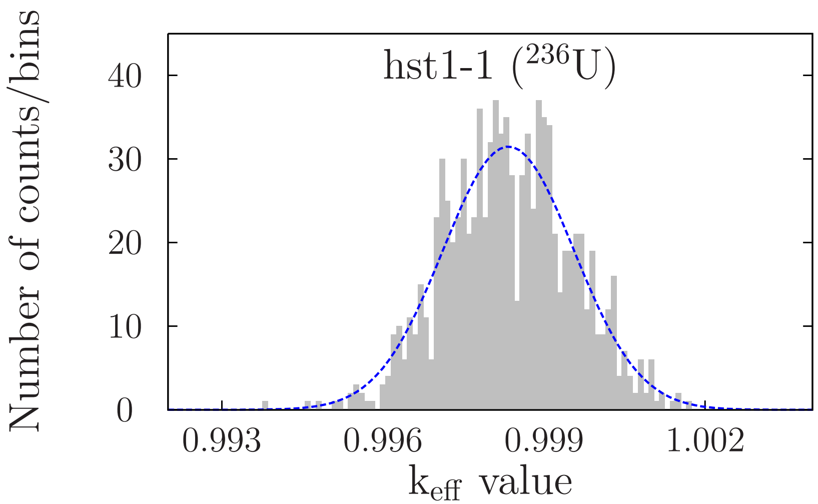


TMC: Total Monte Carlo

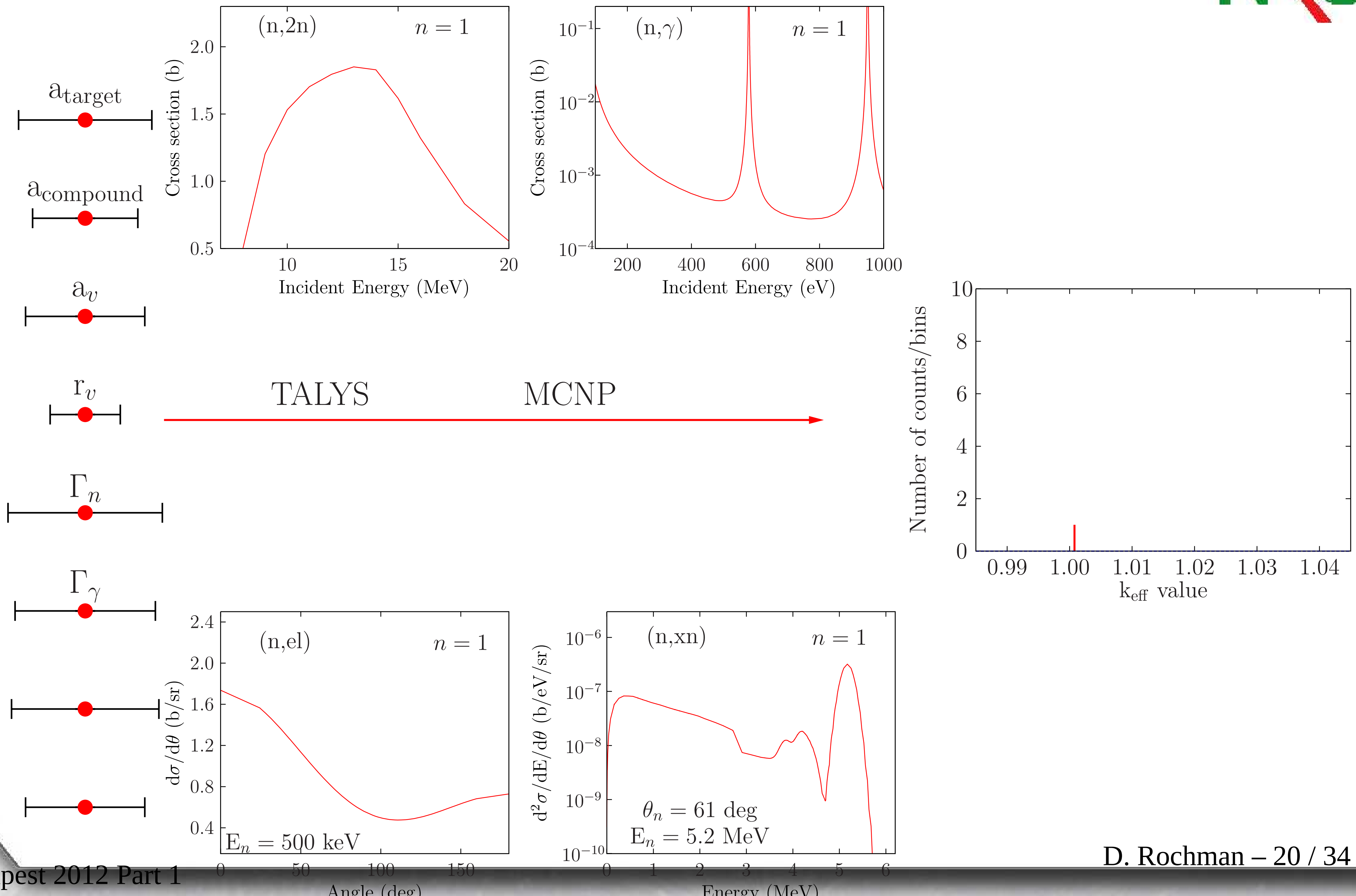
Control of nuclear data (TALYS)
+ simple processing (NJOY)
+ system simulation (MCNP/ERANOS/CASMO...)

1000 times

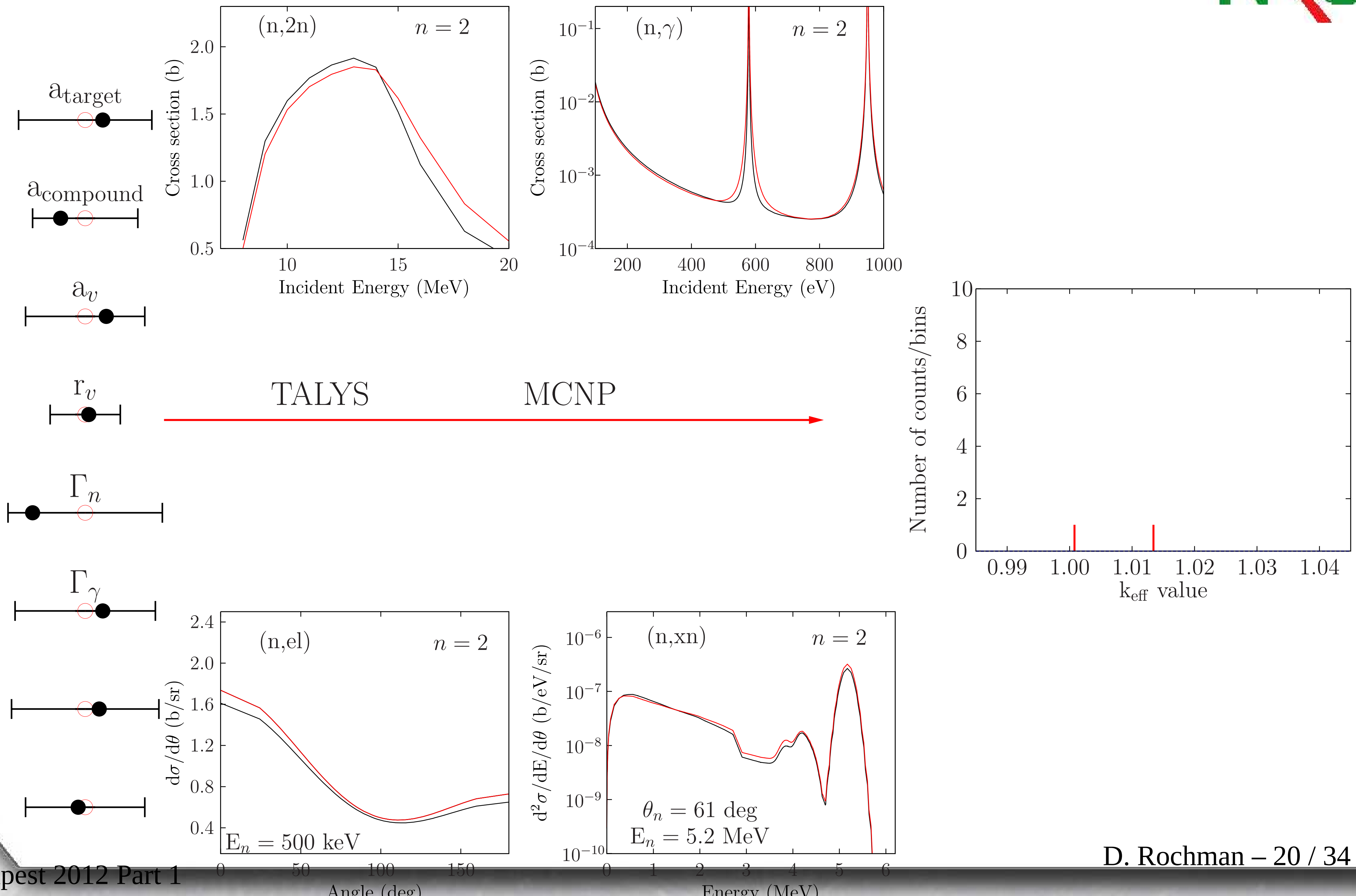
For each random ENDF file, the benchmark calculation is performed with MCNP. At the end of the *n* calculations, *n* different k_{eff} values are obtained. In the obtained probability distribution of k_{eff}, the standard deviation σ_{total} reflects two different effects: $\sigma^2_{total} = \sigma^2_{statistics} + \sigma^2_{nuclear\ data}$.



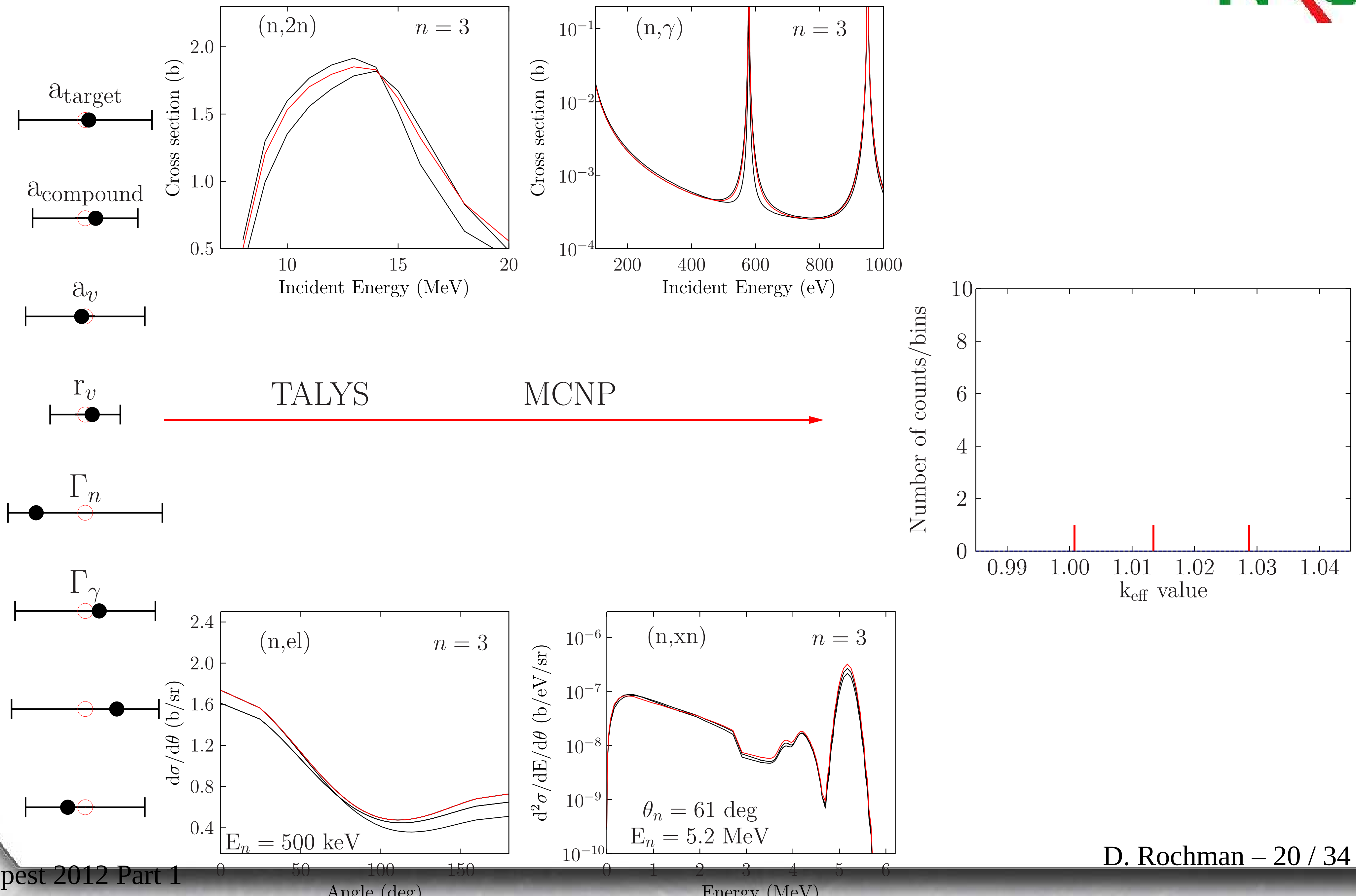
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



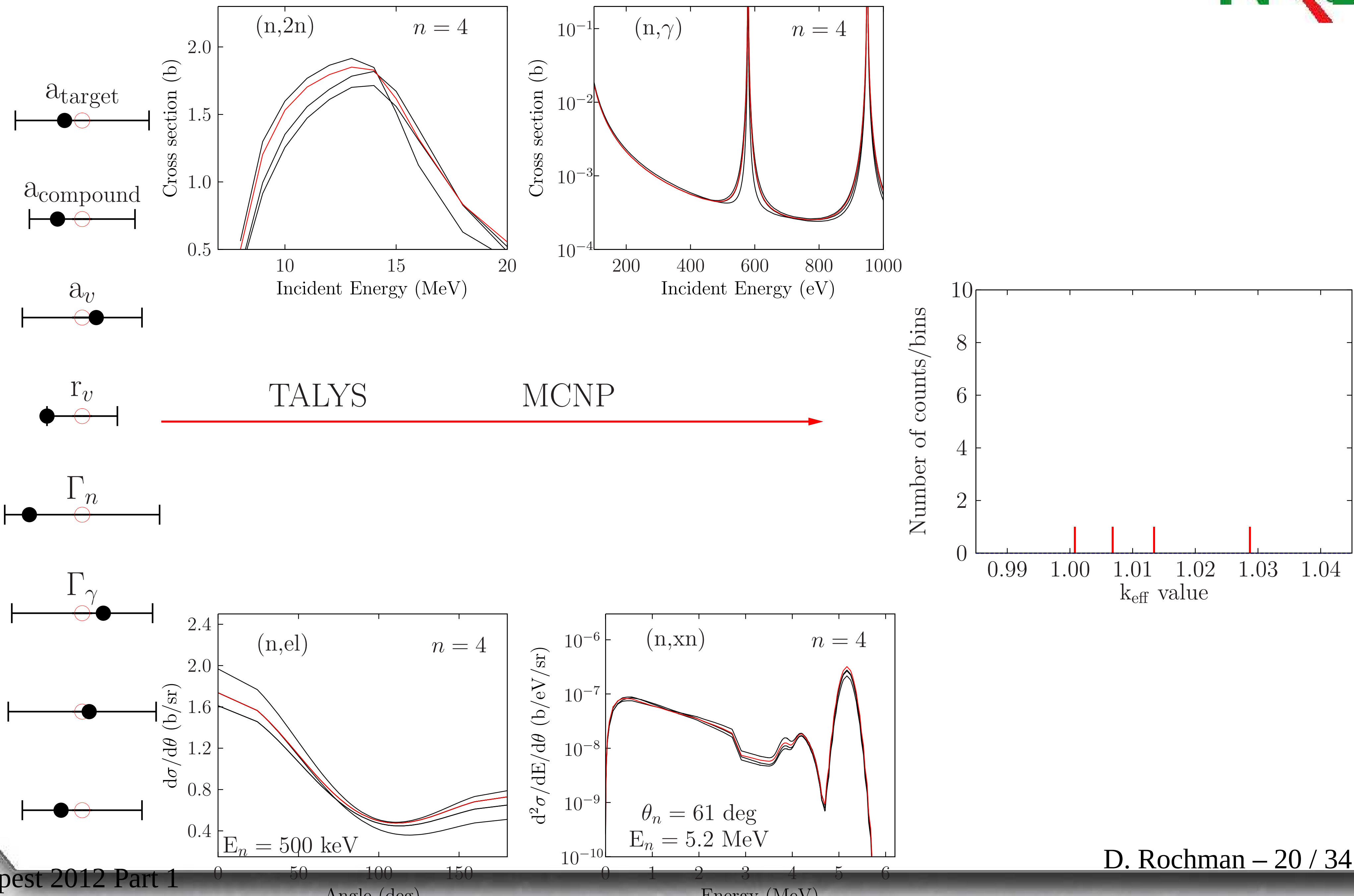
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



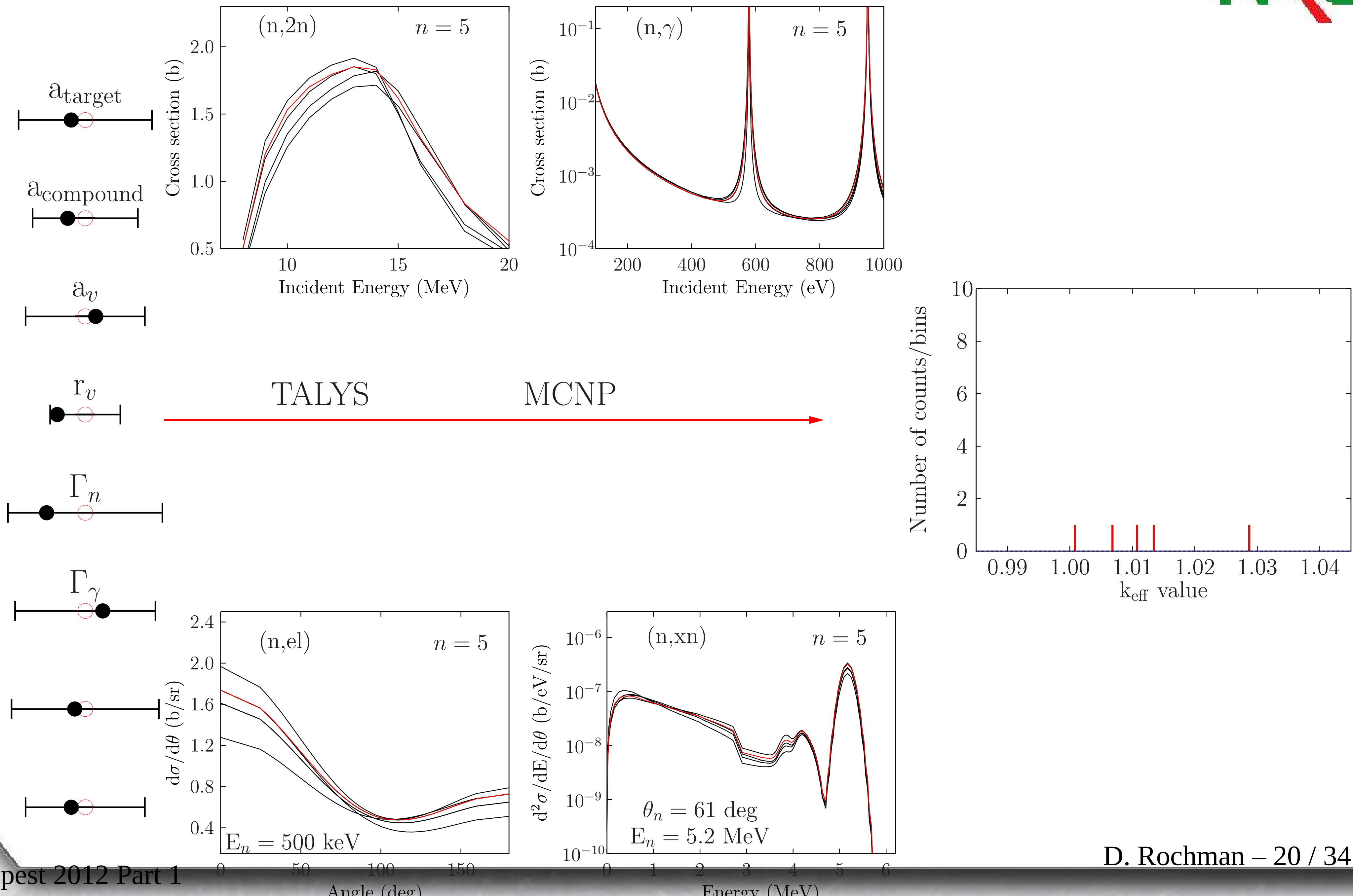
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



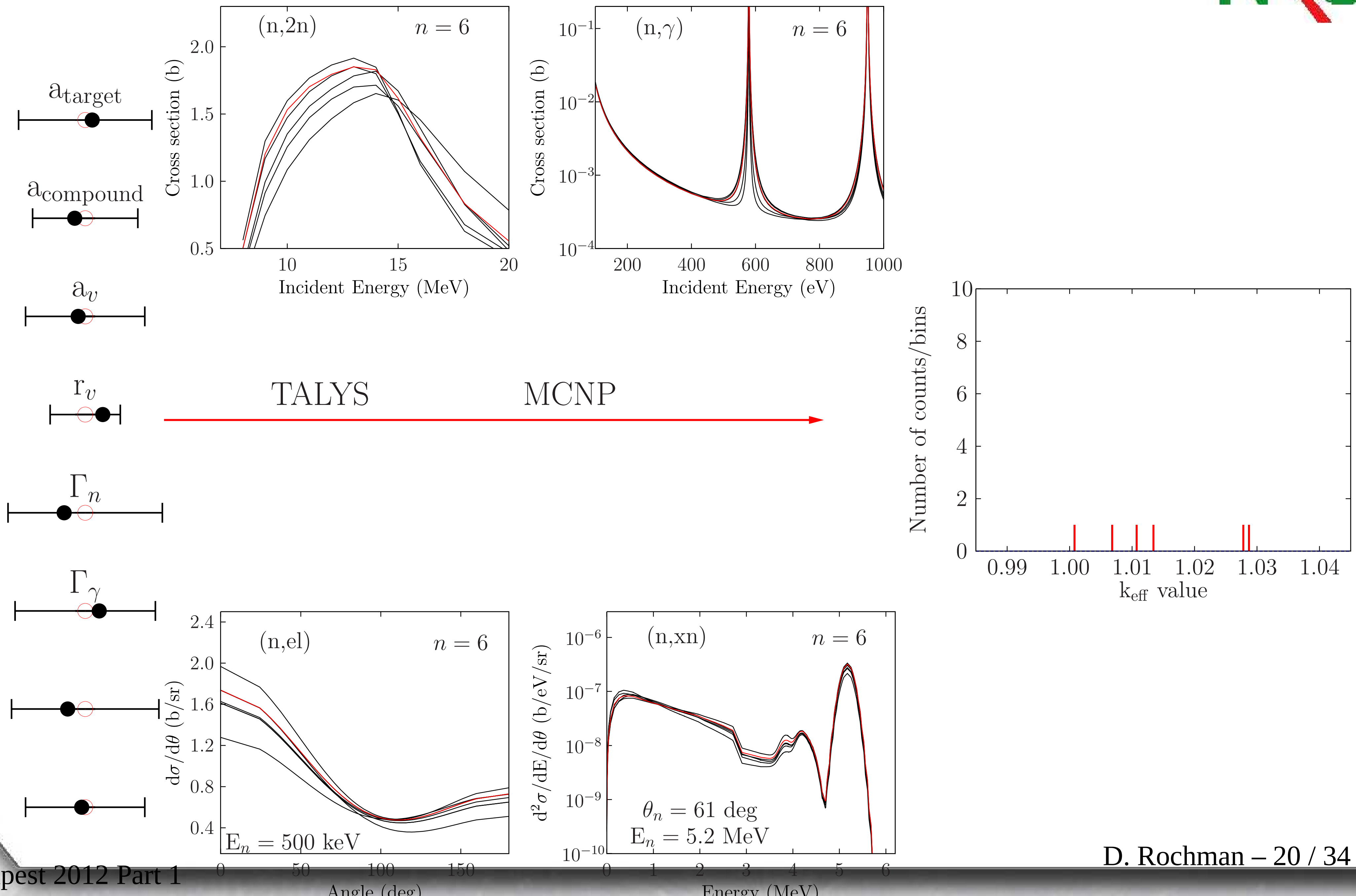
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



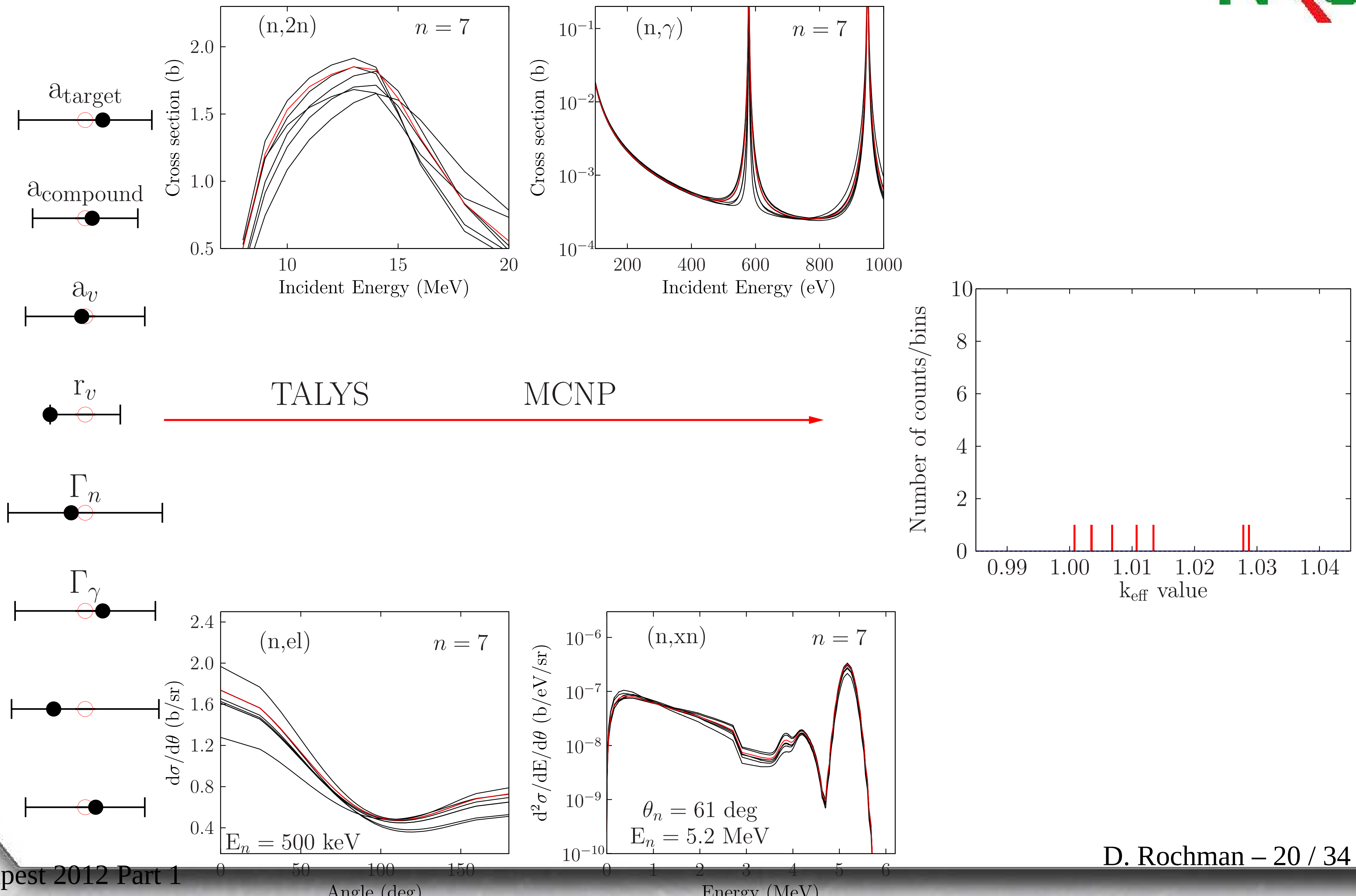
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



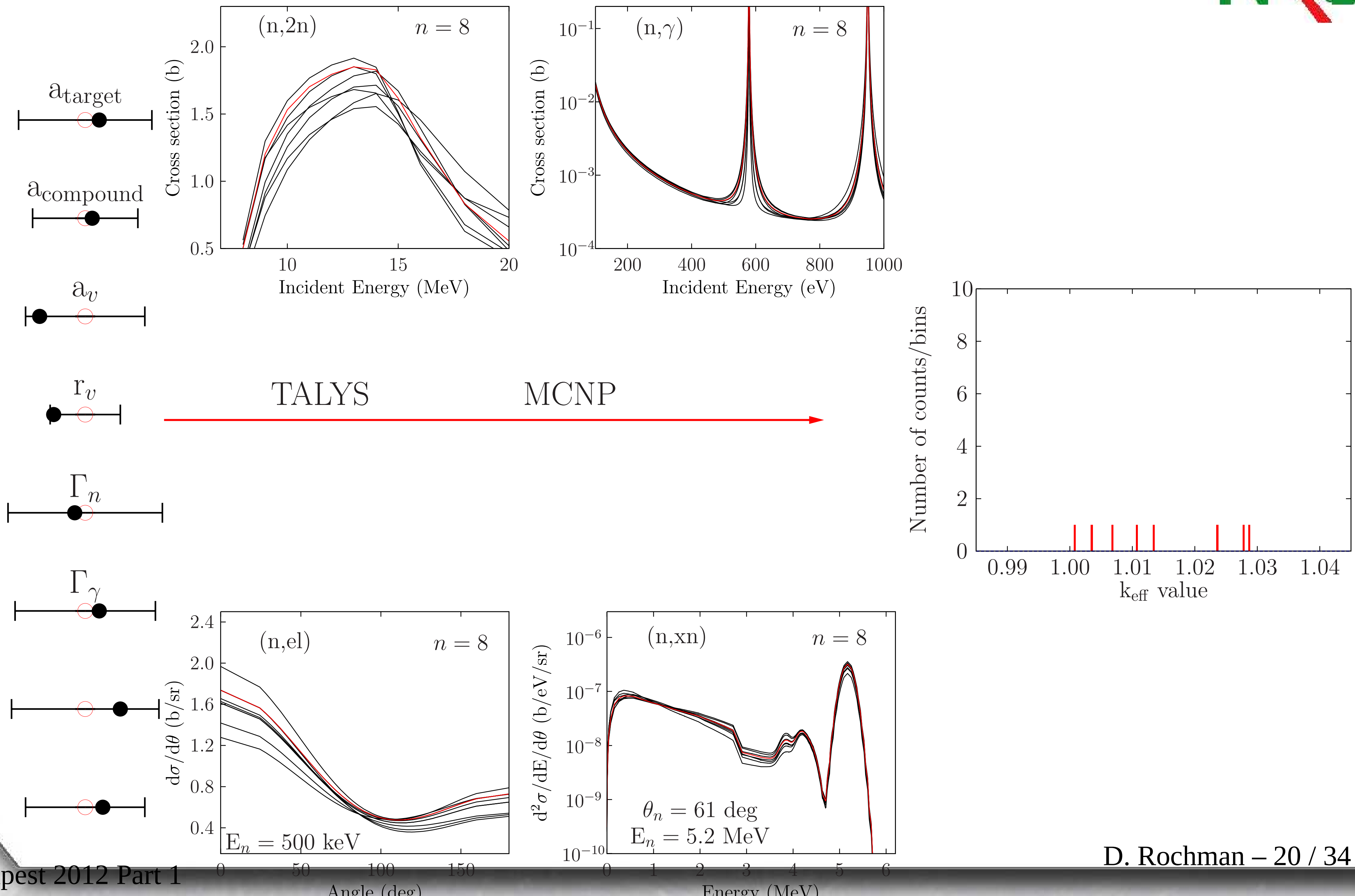
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



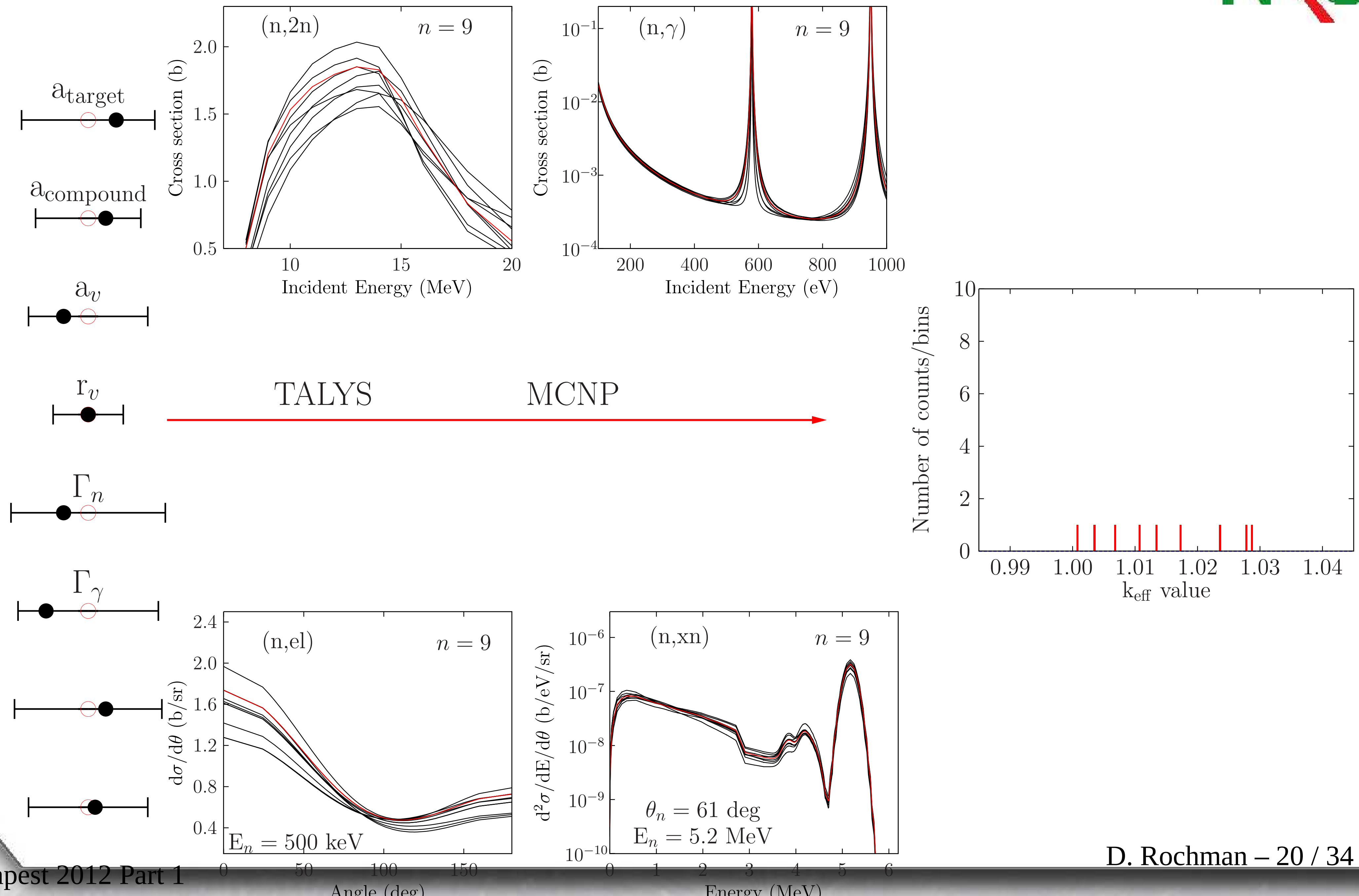
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



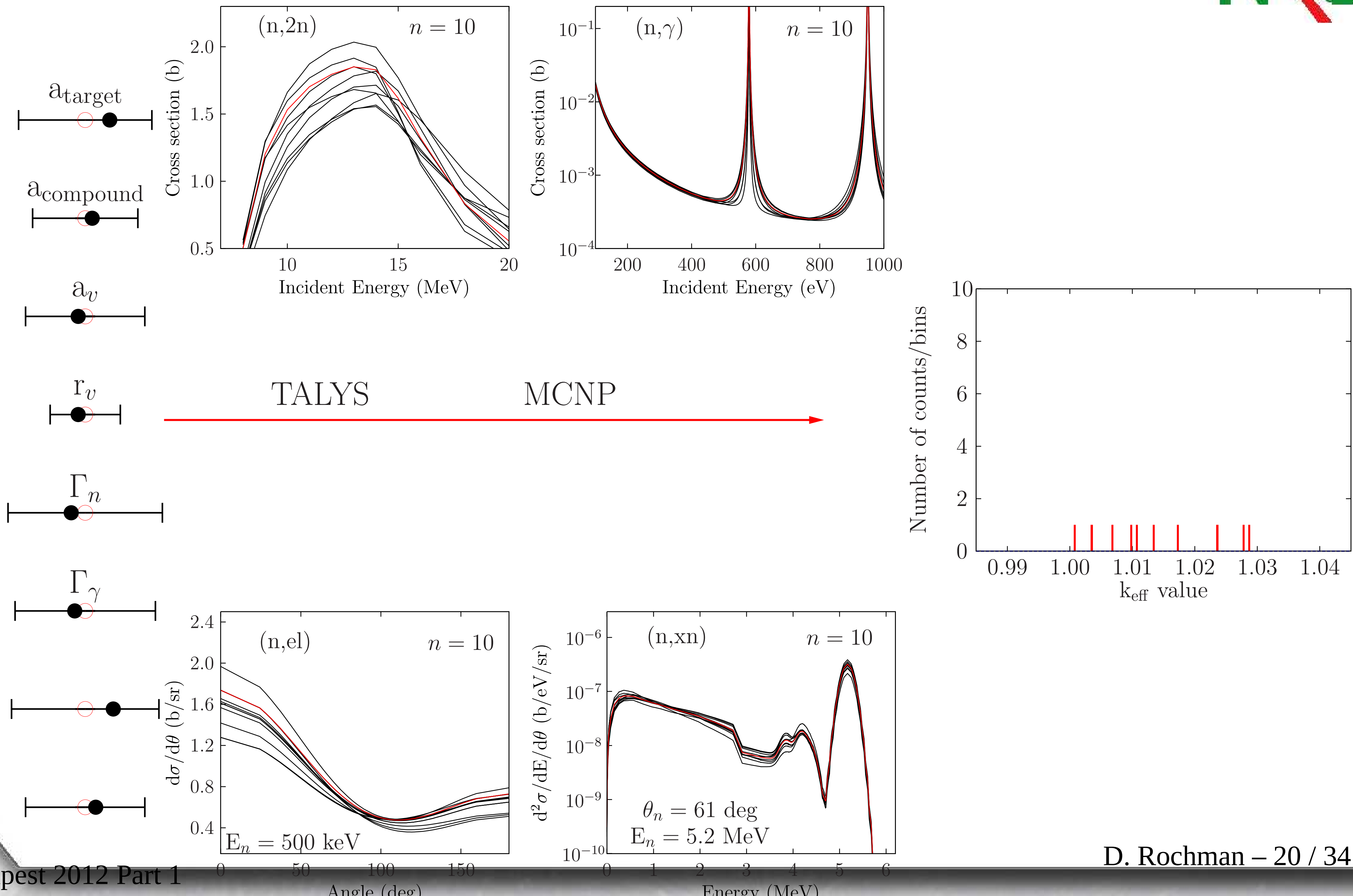
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



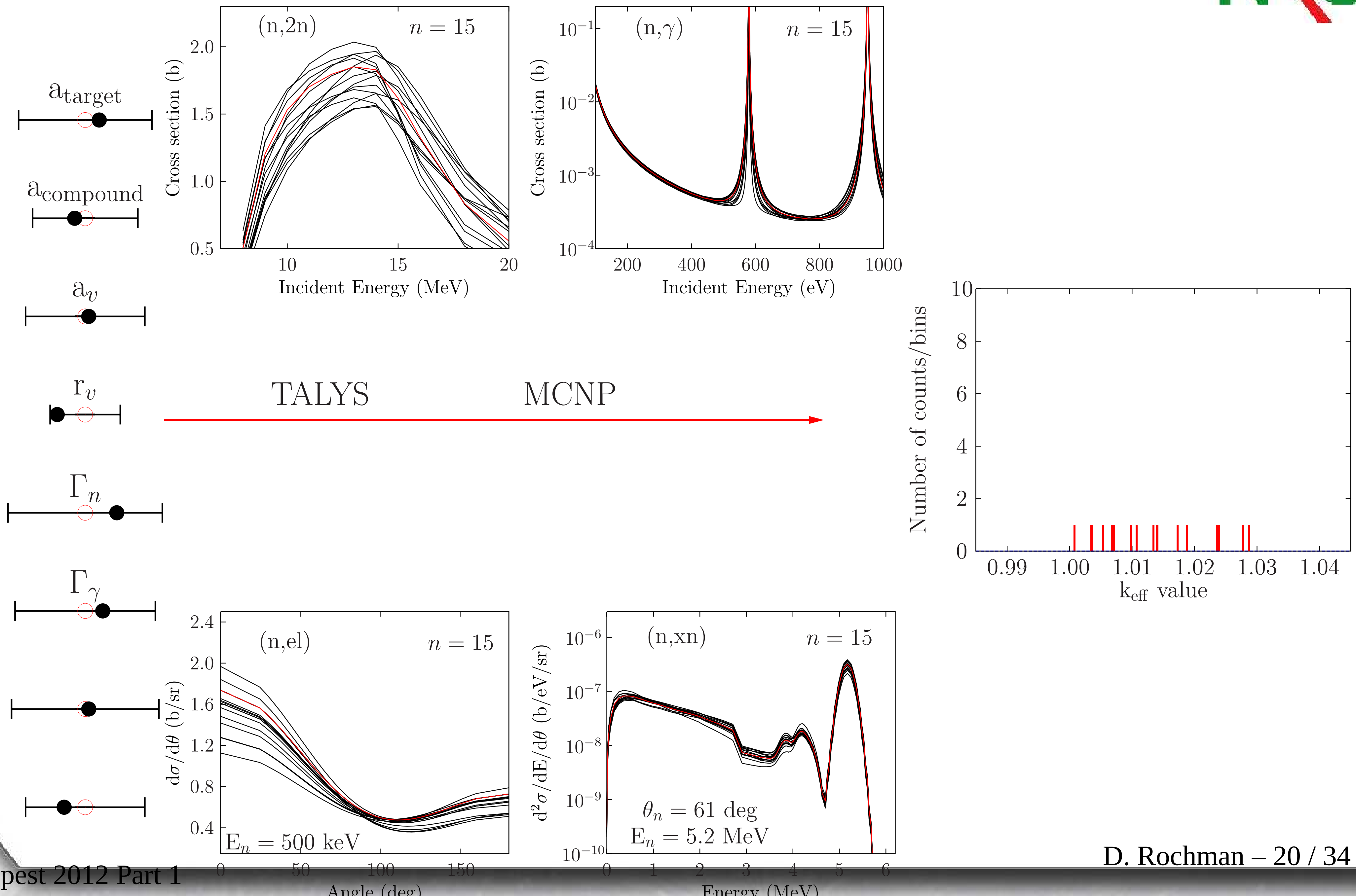
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



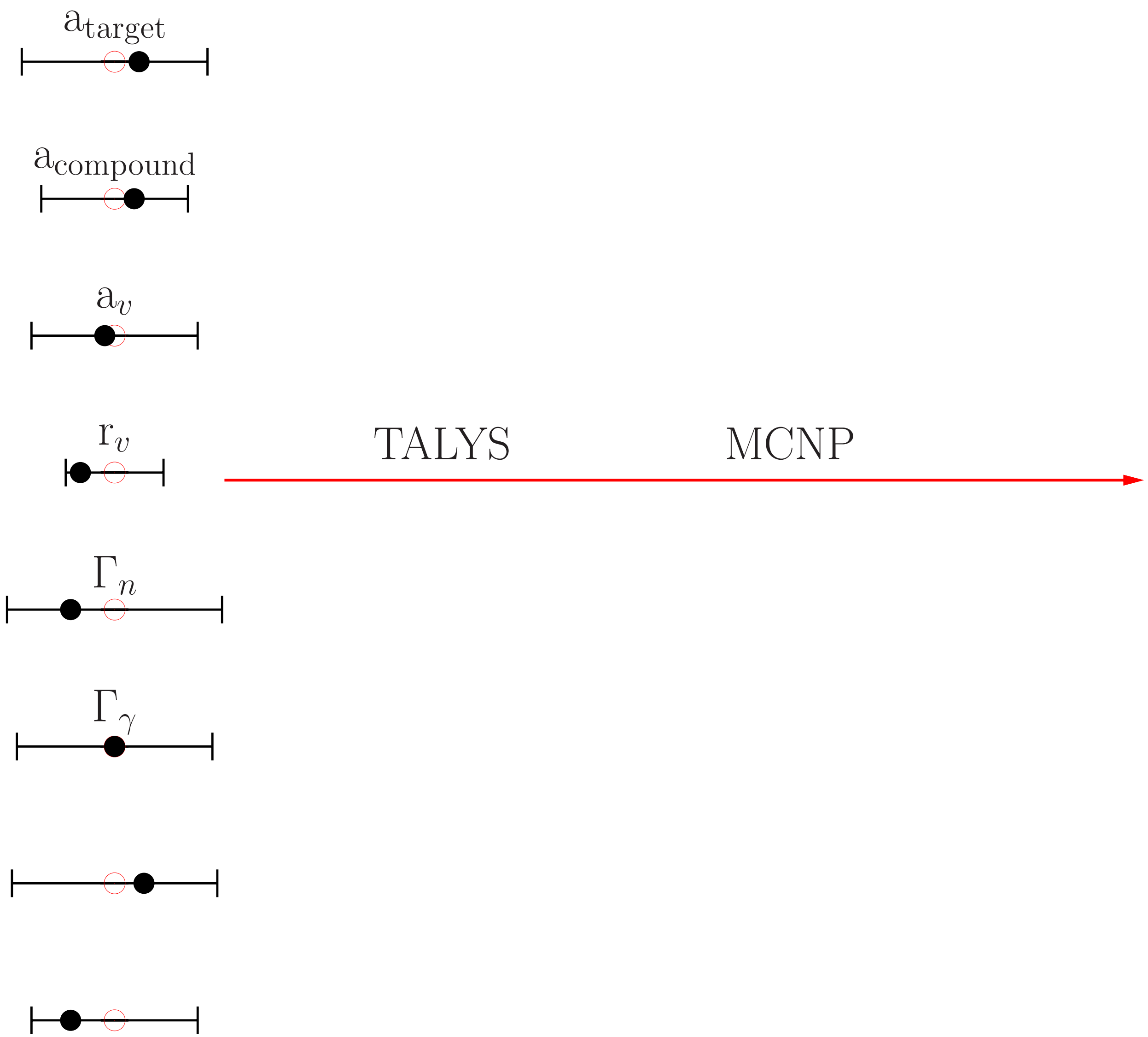
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



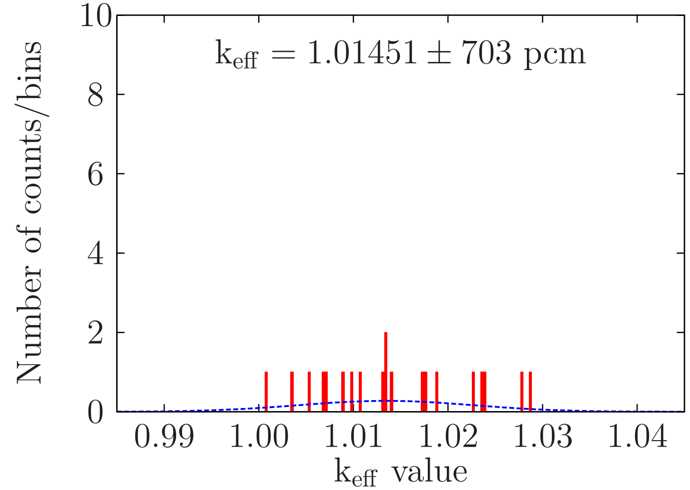
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



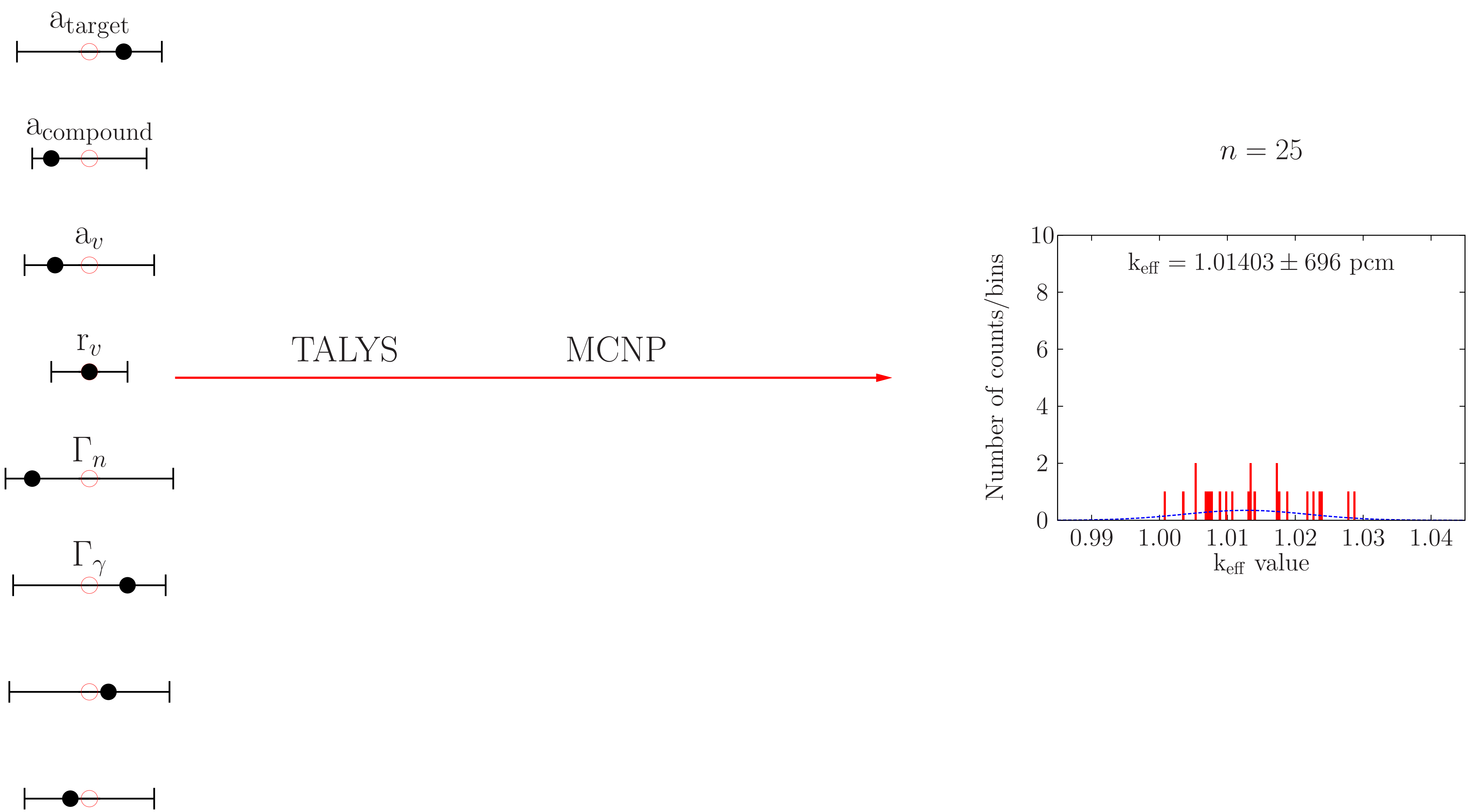
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



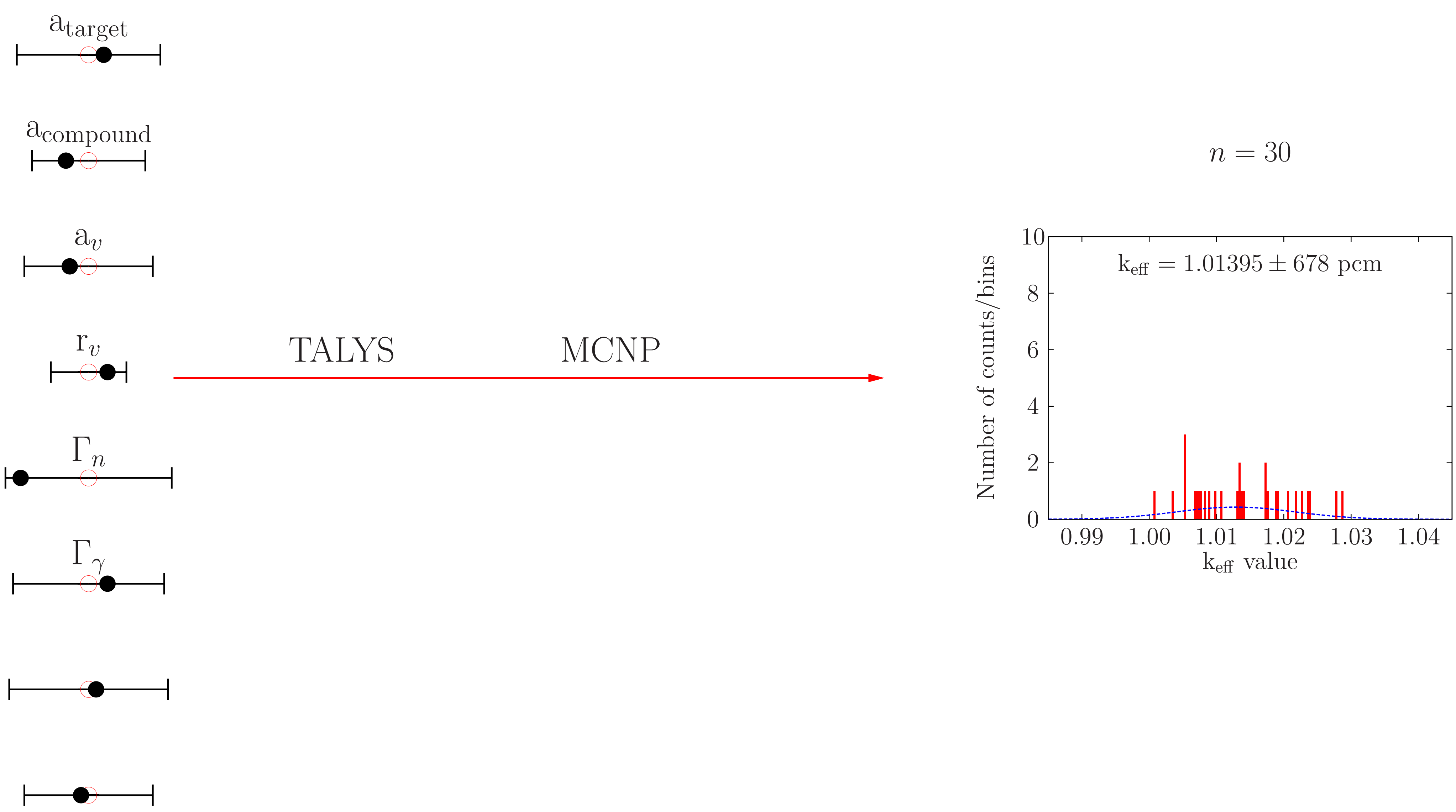
$n = 20$



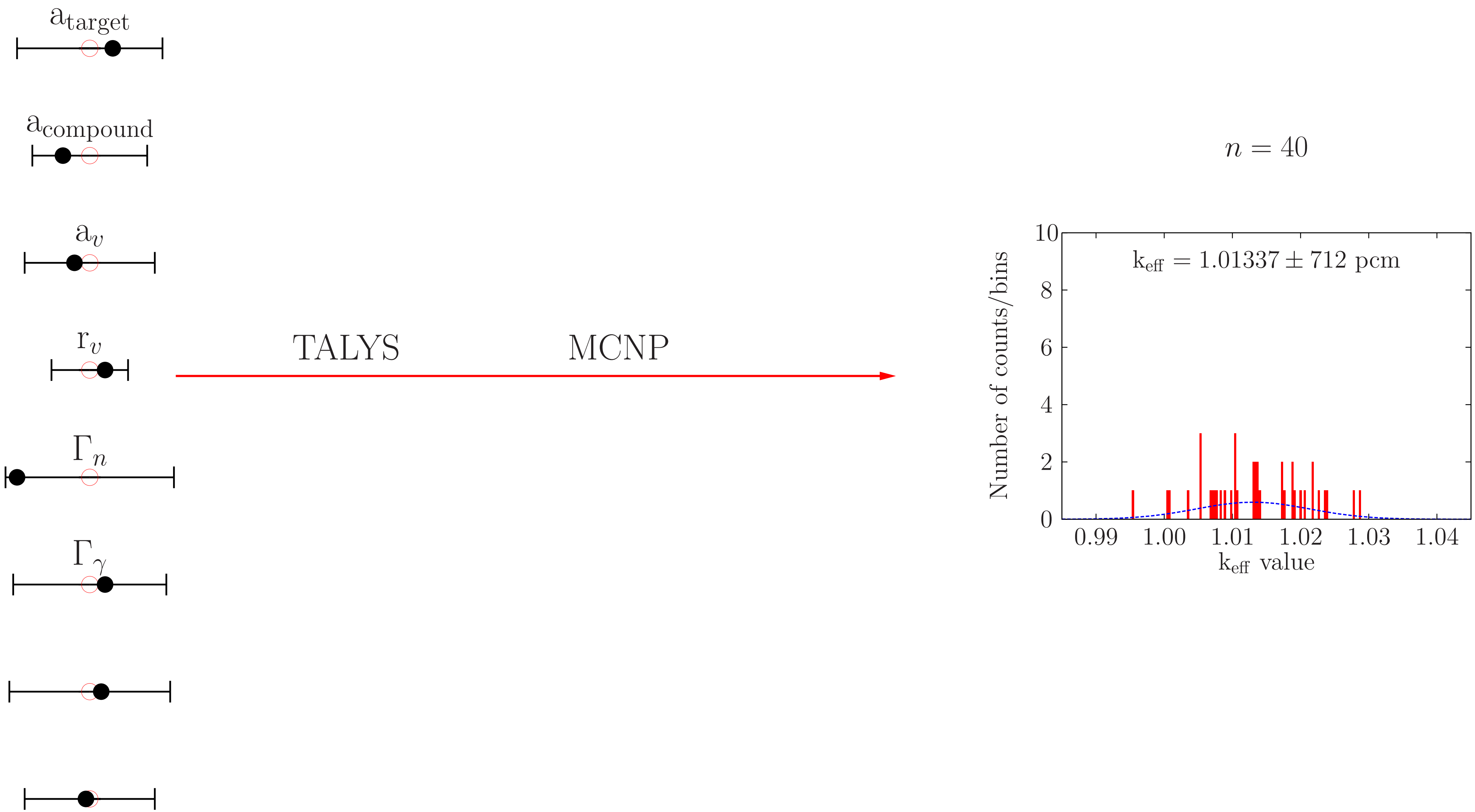
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



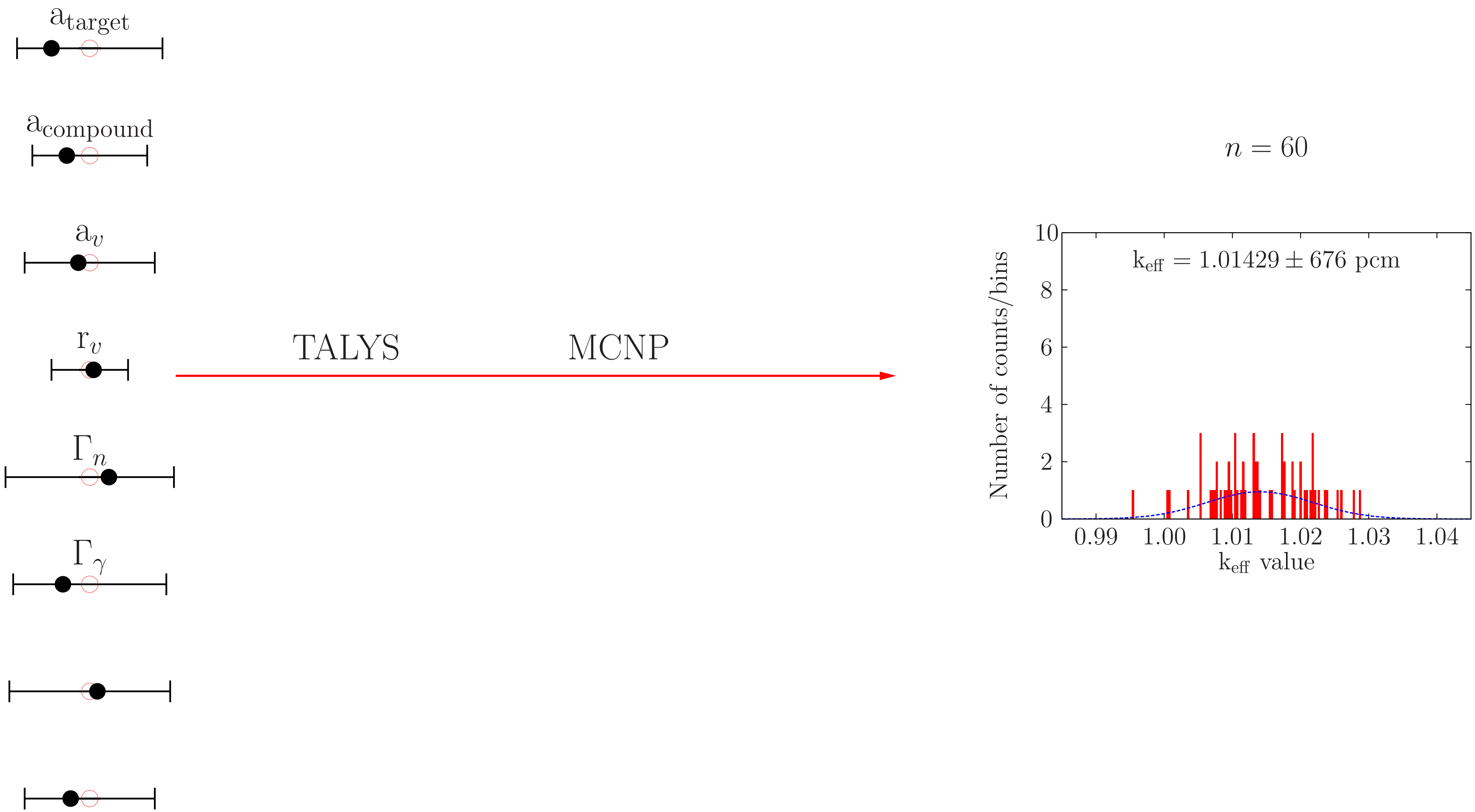
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



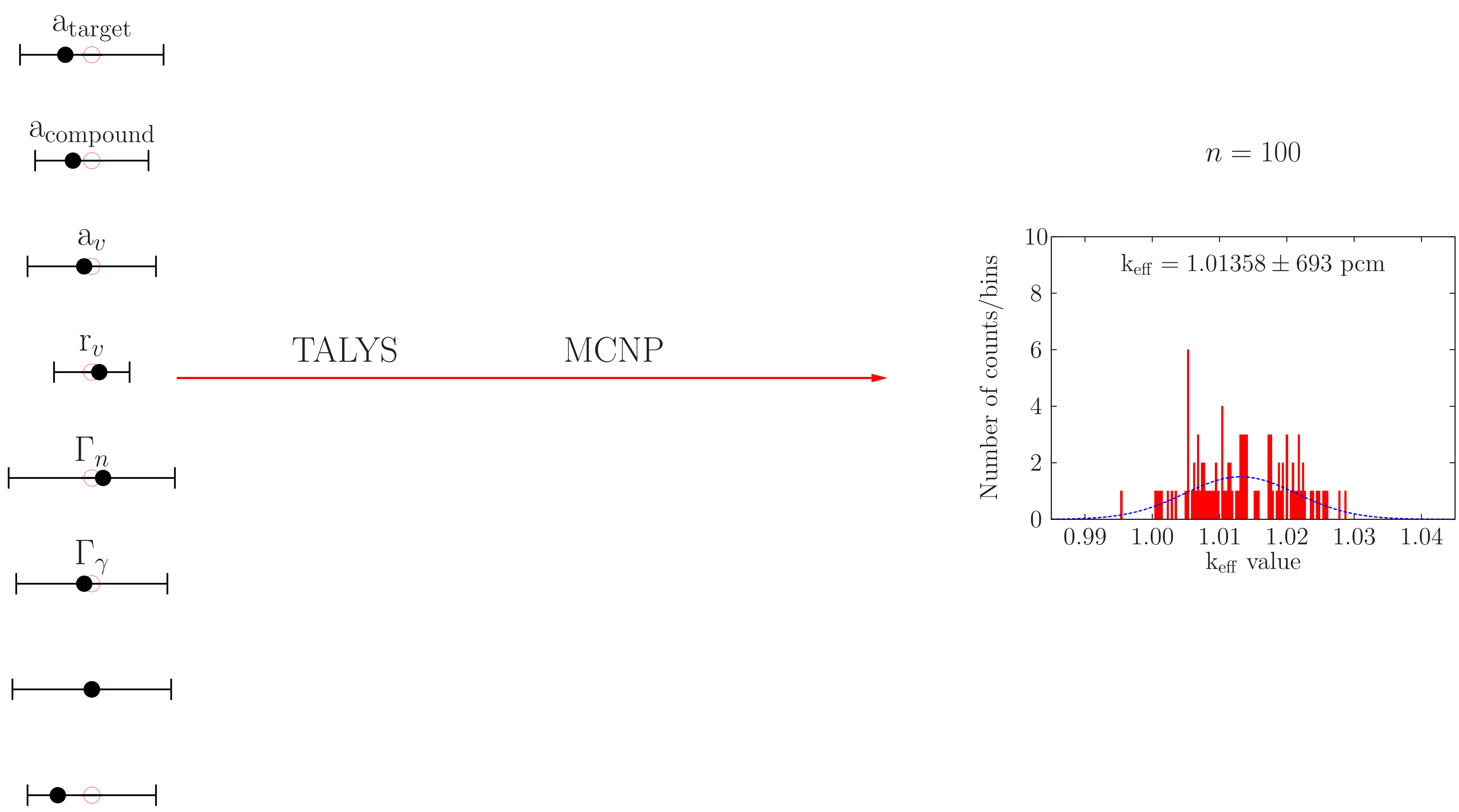
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



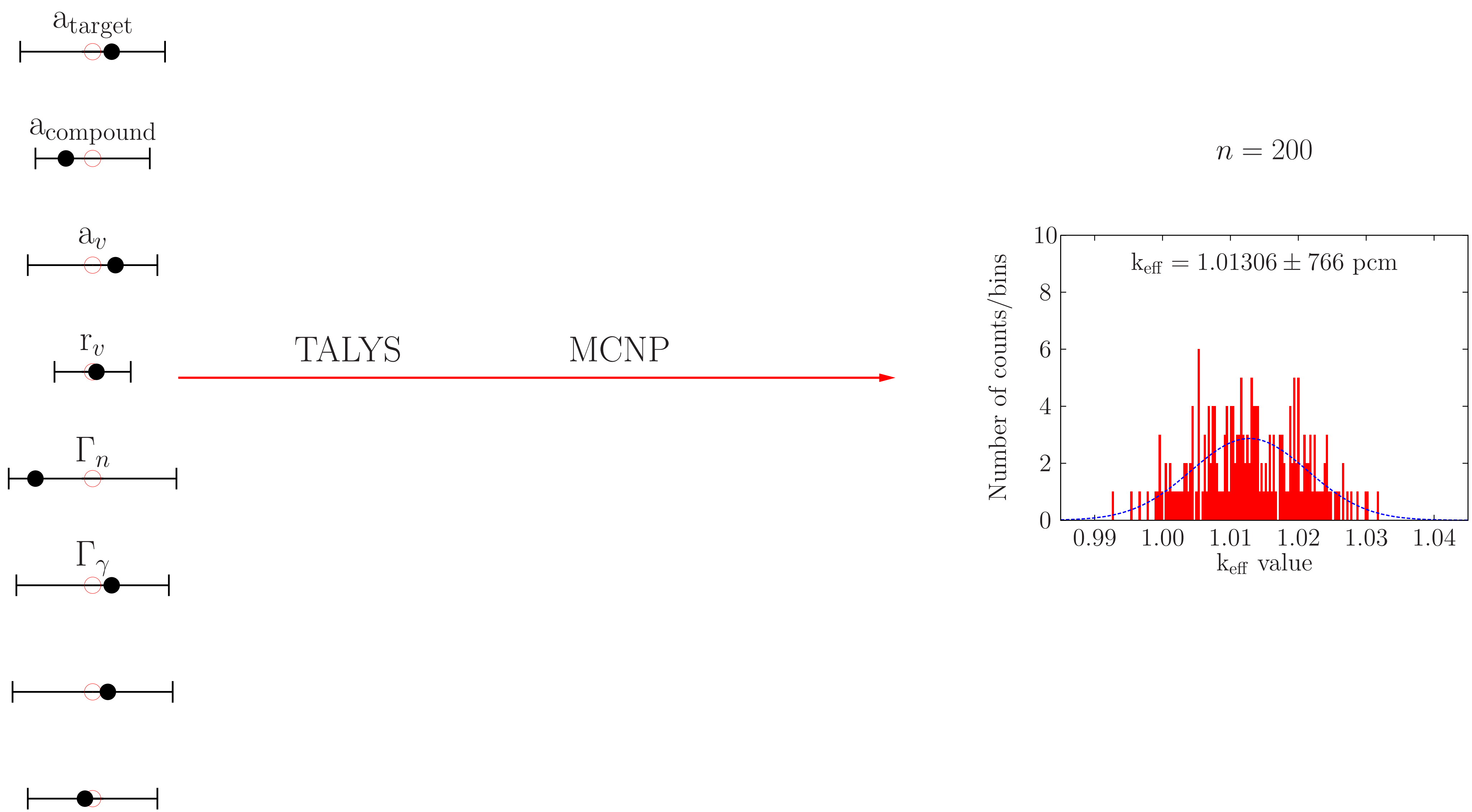
Hands on "1000 ×(Talys + ENDF + NJOY + MCNP) calculations"



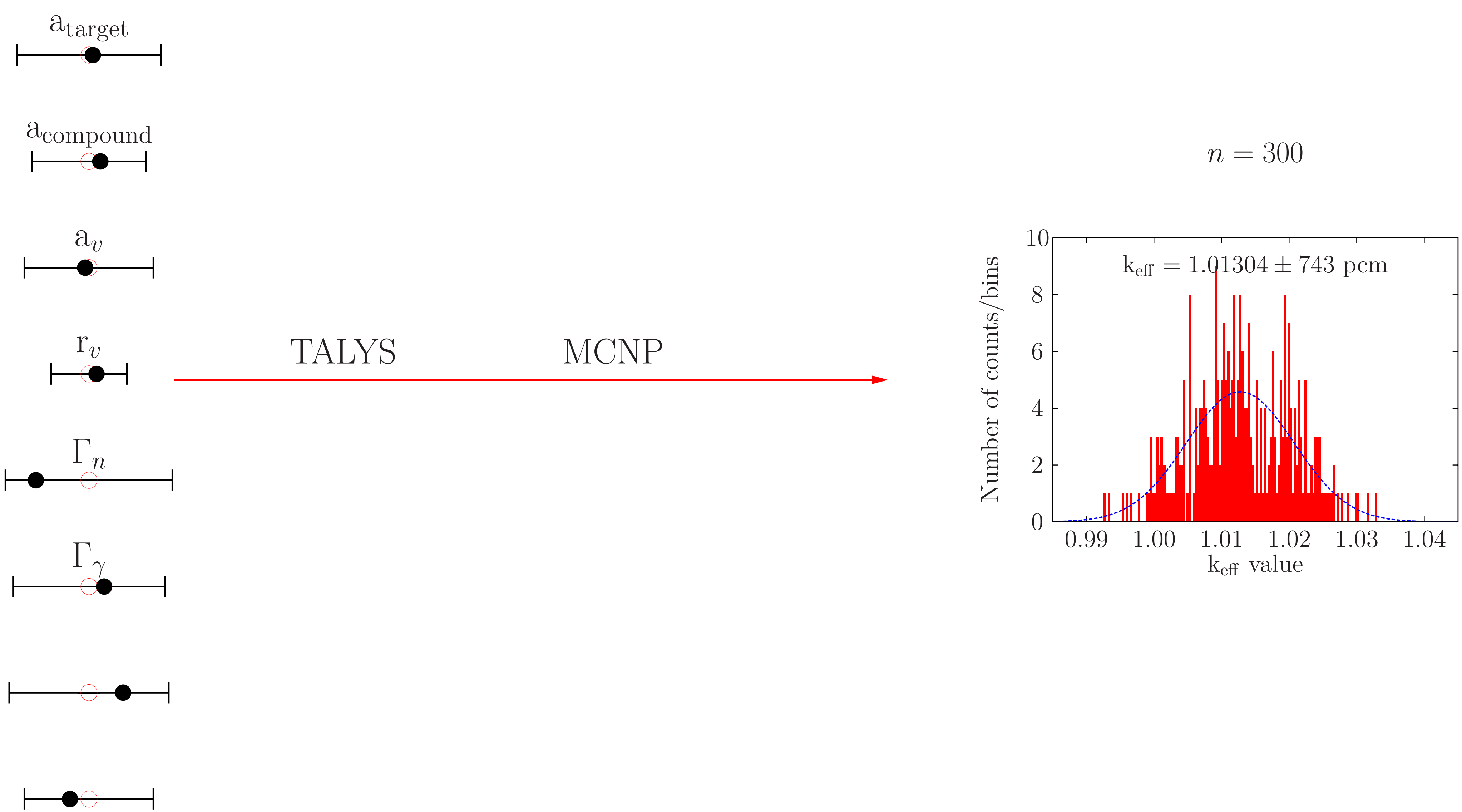
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



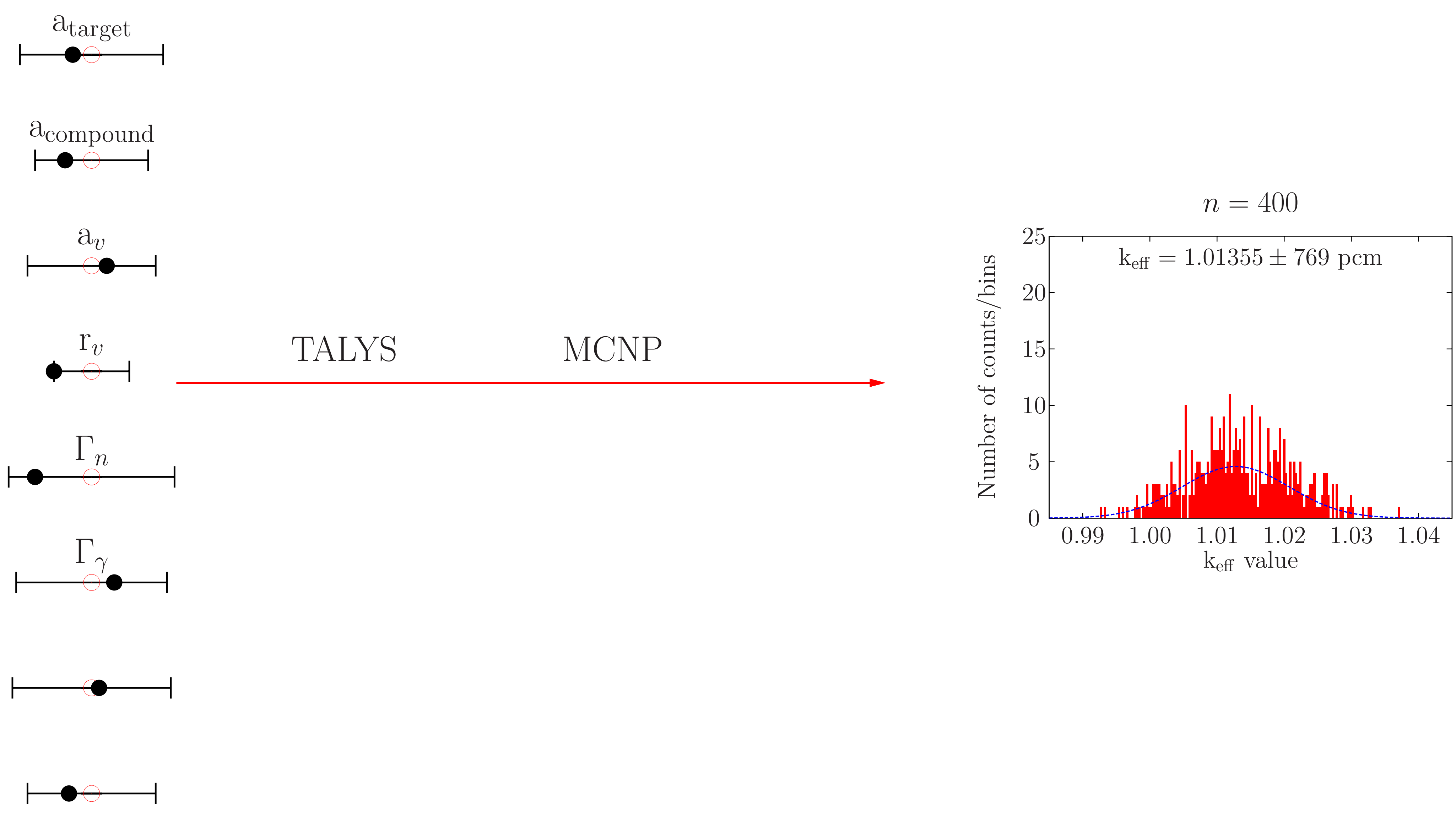
Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



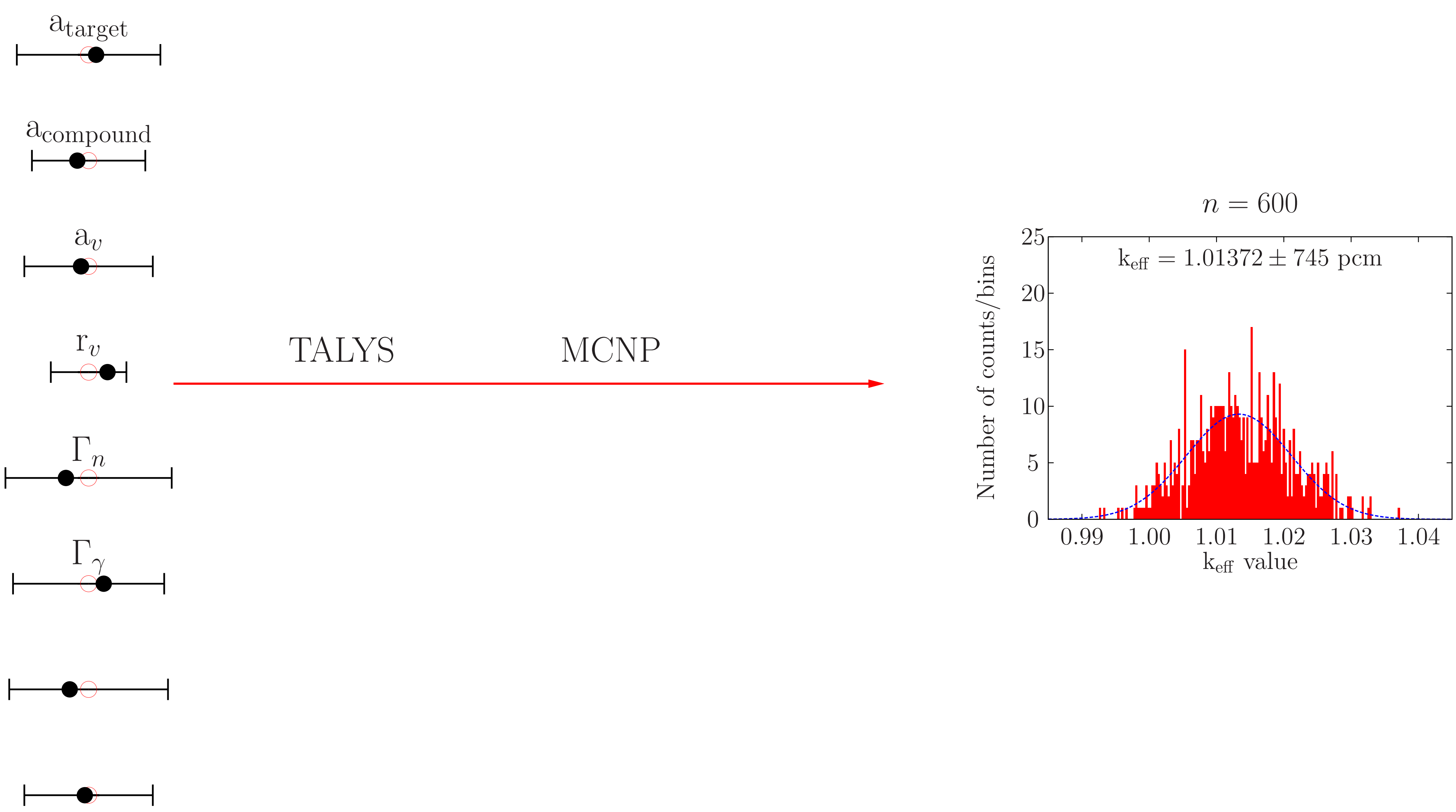
Hands on "1000 ×(Talys + ENDF + NJOY + MCNP) calculations"



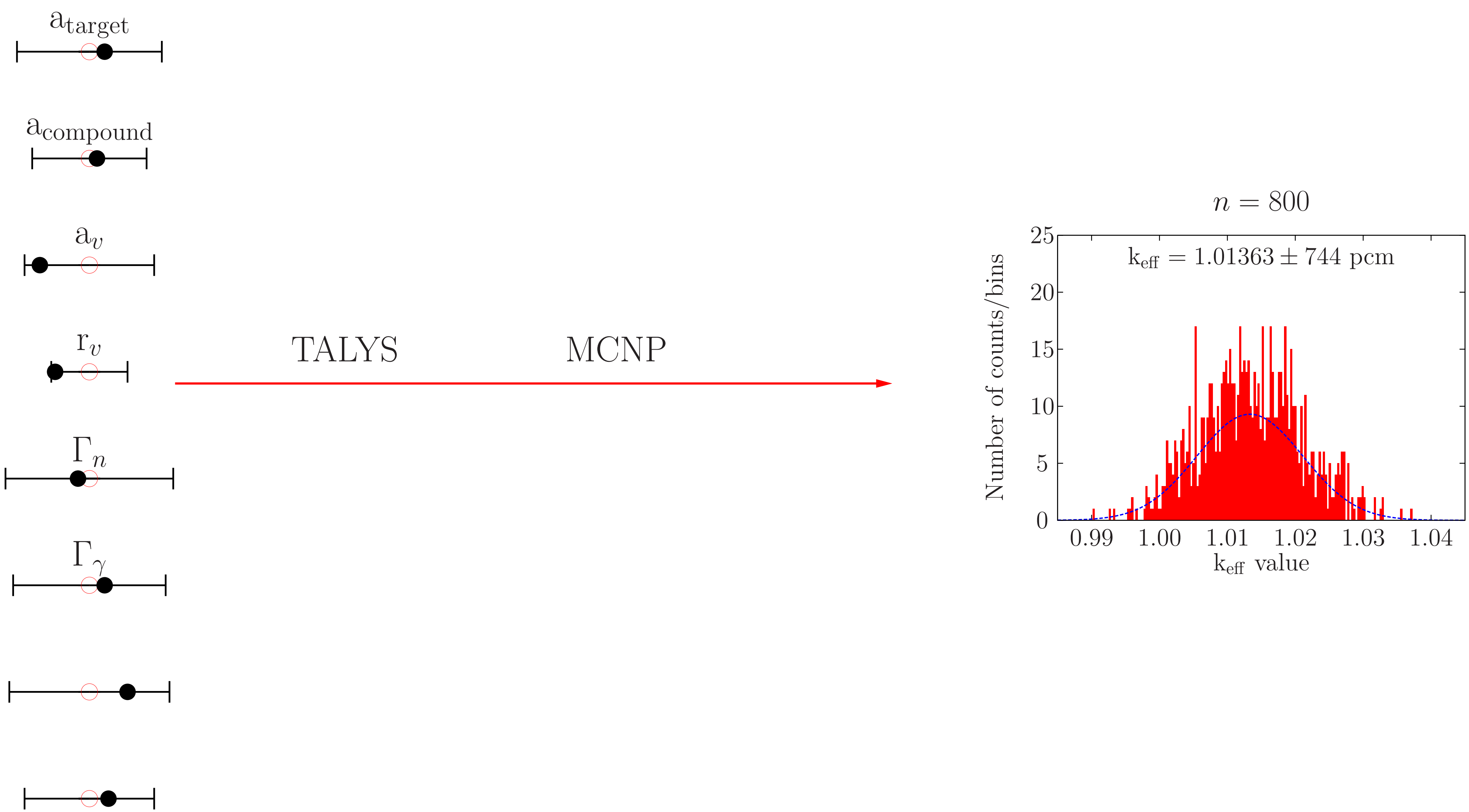
Hands on “1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations”



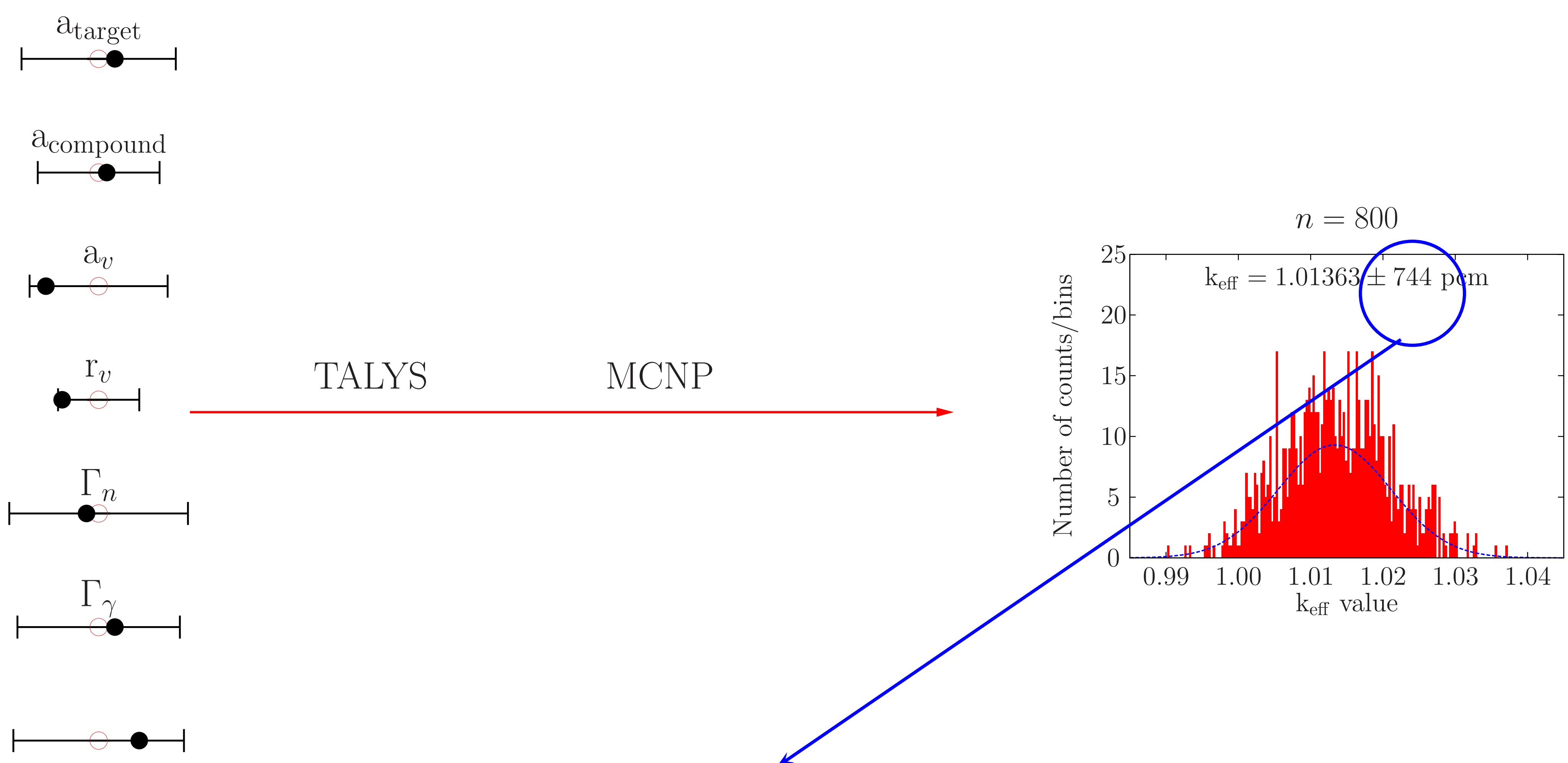
Hands on "1000 ×(Talys + ENDF + NJOY + MCNP) calculations"



Hands on “1000 ×(Talys + ENDF + NJOY + MCNP) calculations”



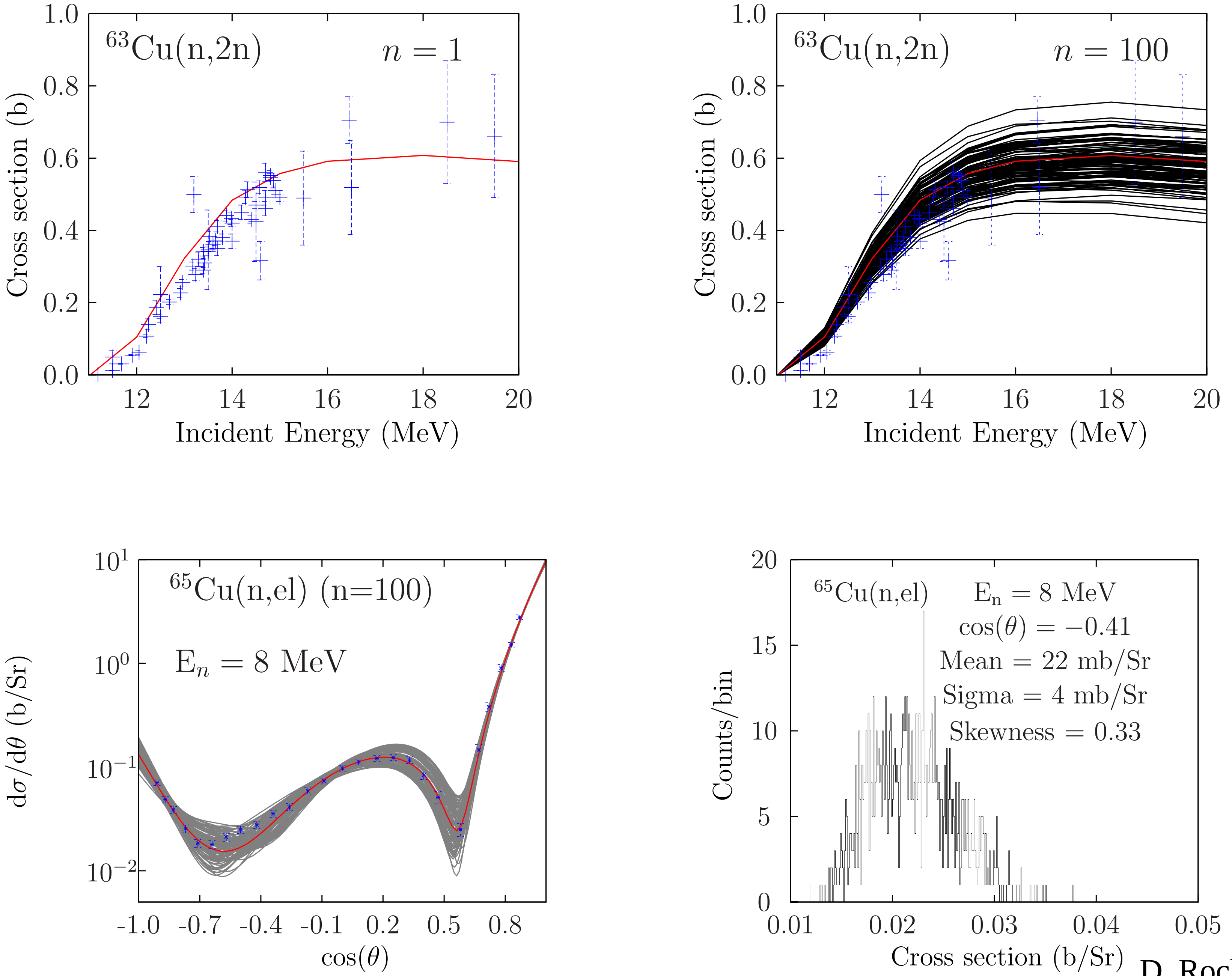
Hands on "1000 $\times$(Talys + ENDF + NJOY + MCNP) calculations"



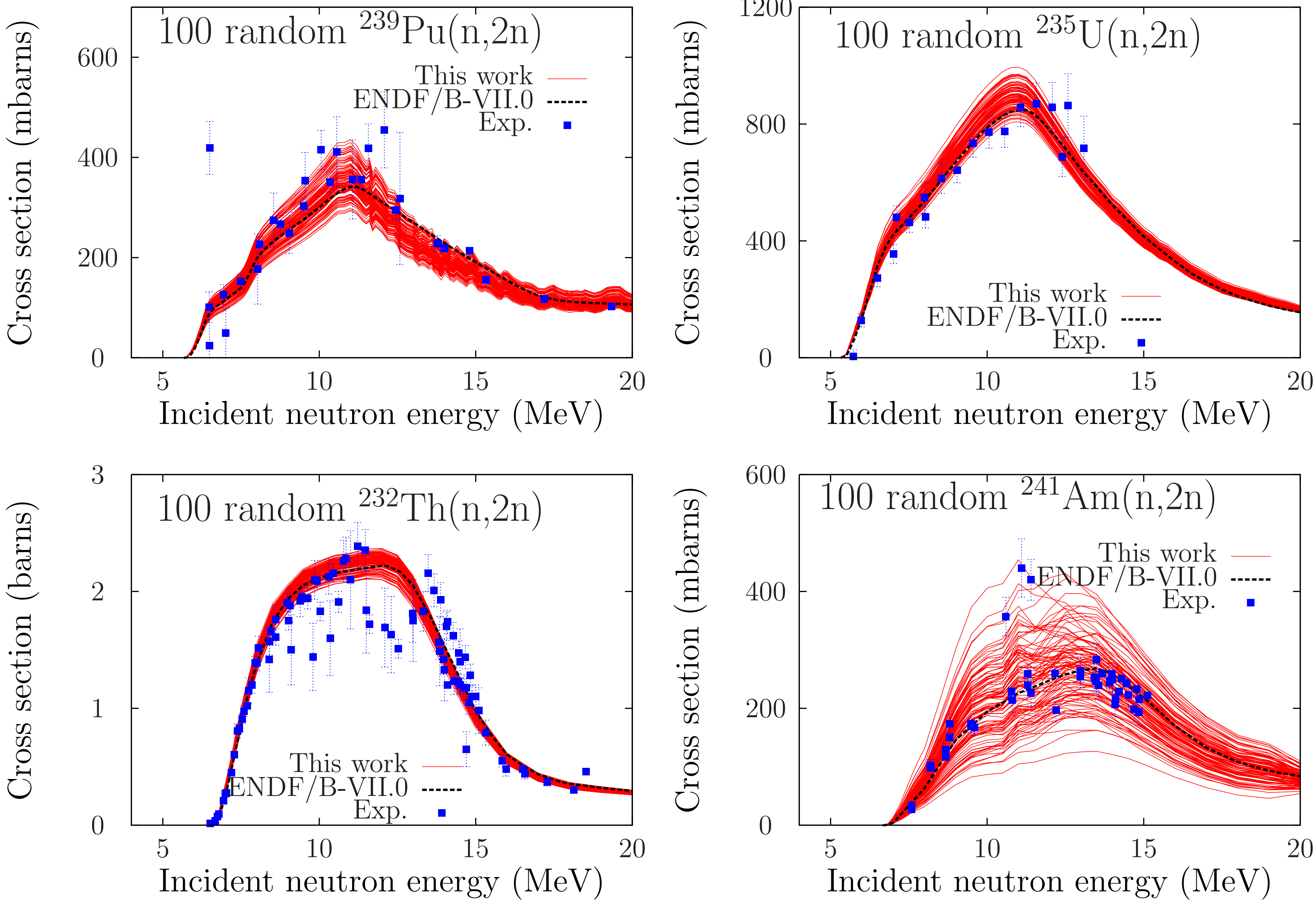
Statistical uncertainty $\simeq$ 68 pcm

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

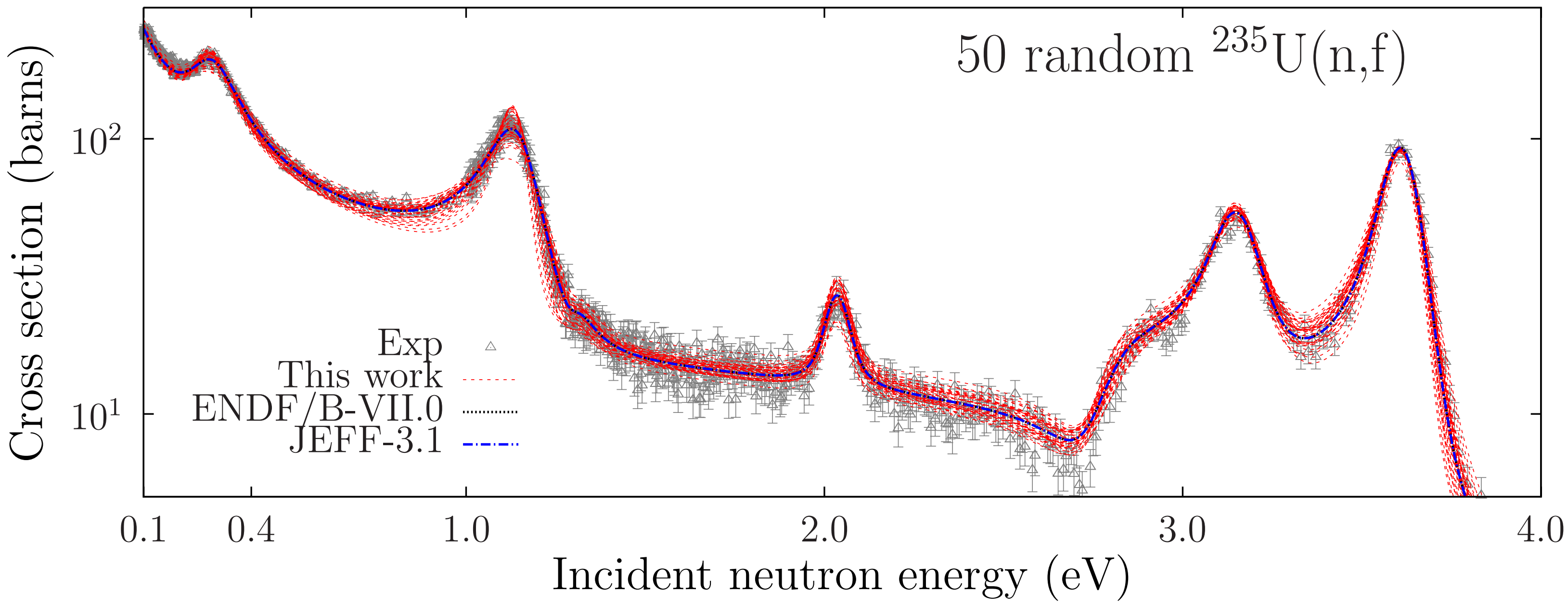
Examples with ^{63}Cu(n,2n) and ^{65}Cu(n,el)

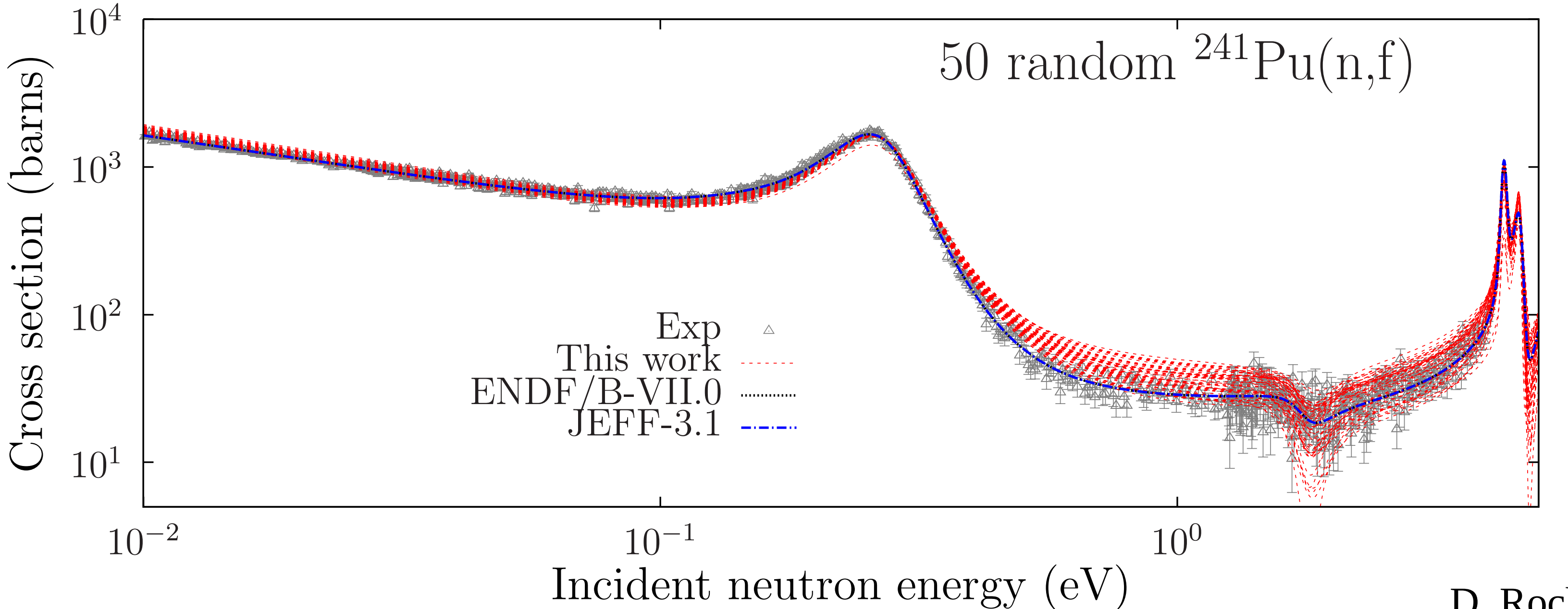


Nuclear data: examples on (n,2n) cross sections



Nuclear data: examples in the resonance region





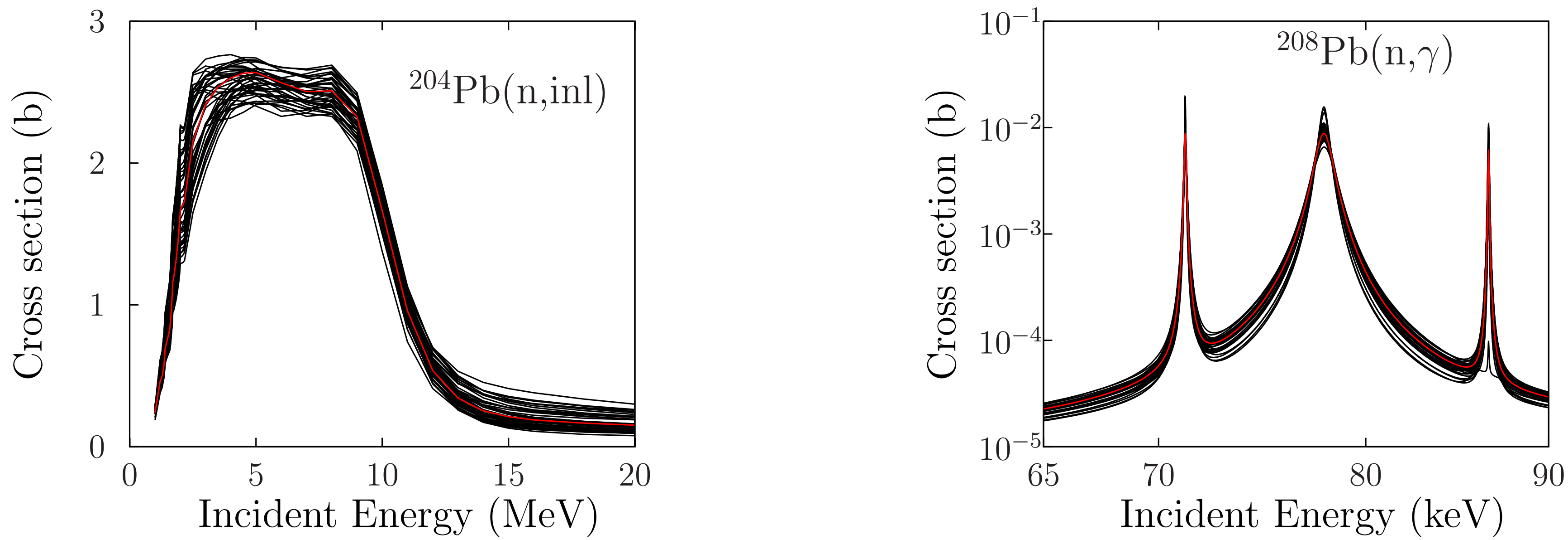
TMC Where can we apply it and examples with Pb isotopes

- Monte Carlo codes (MCNP, Tripoli), Deterministic codes (APOLLO, WIMS)
- Quantities: criticality, flux (+ all from SG-26), shielding and fusion
- Virtually all quantities due to cross sections, fission yields, decay data, thermal scattering...

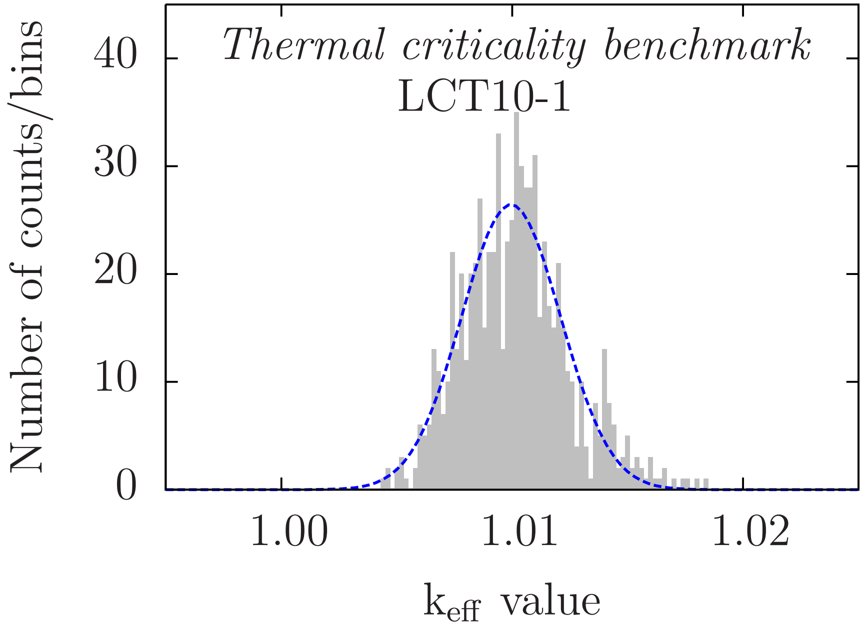
TMC Where can we apply it and examples with Pb isotopes

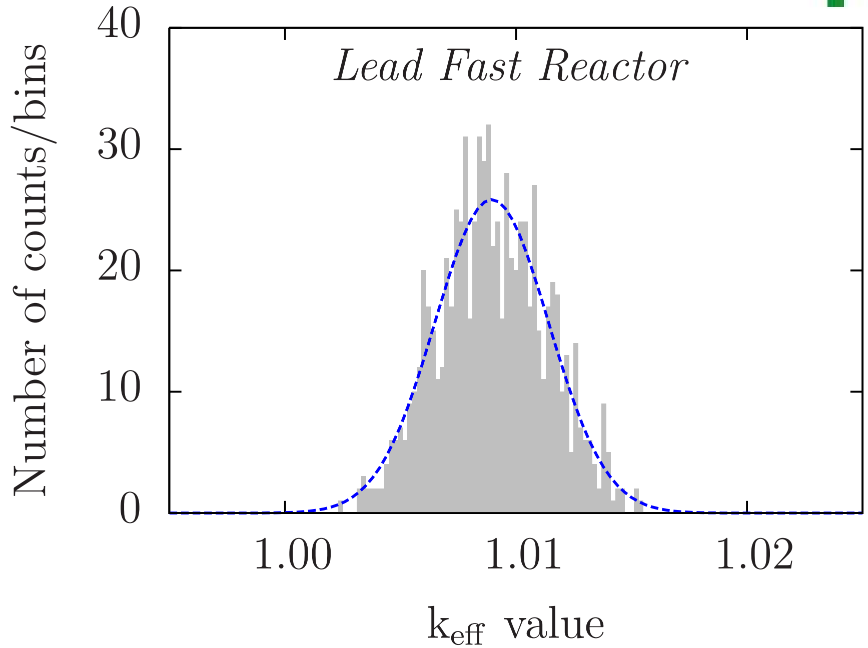
- Monte Carlo codes (MCNP, Tripoli), Deterministic codes (APOLLO, WIMS)
- Quantities: criticality, flux (+ all from SG-26), shielding and fusion
- Virtually all quantities due to cross sections, fission yields, decay data, thermal scattering...

- $^{204-208}$Pb evaluations (NIM A589 (2008) 85) + **5000** random ENDF files
- Applied on k_{eff} and β_{eff} for criticality benchmarks (LCT-10 and HMF-64) and to ADS and LFR

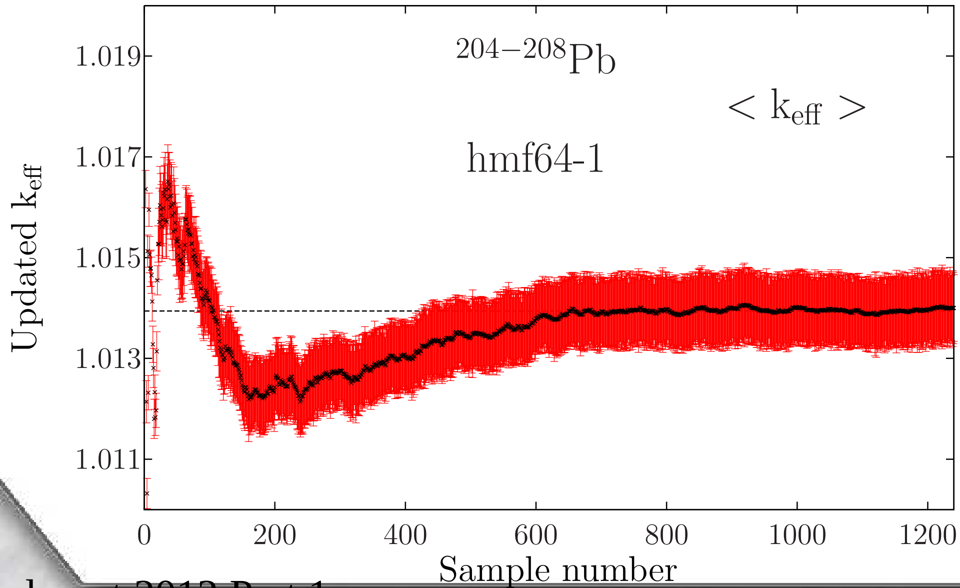


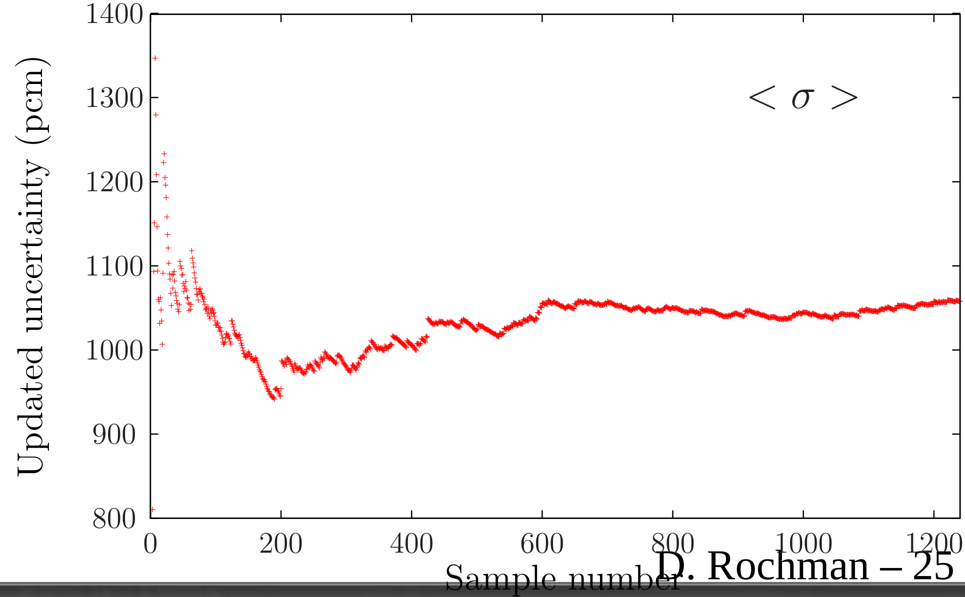
TMC Examples with Pb isotopes



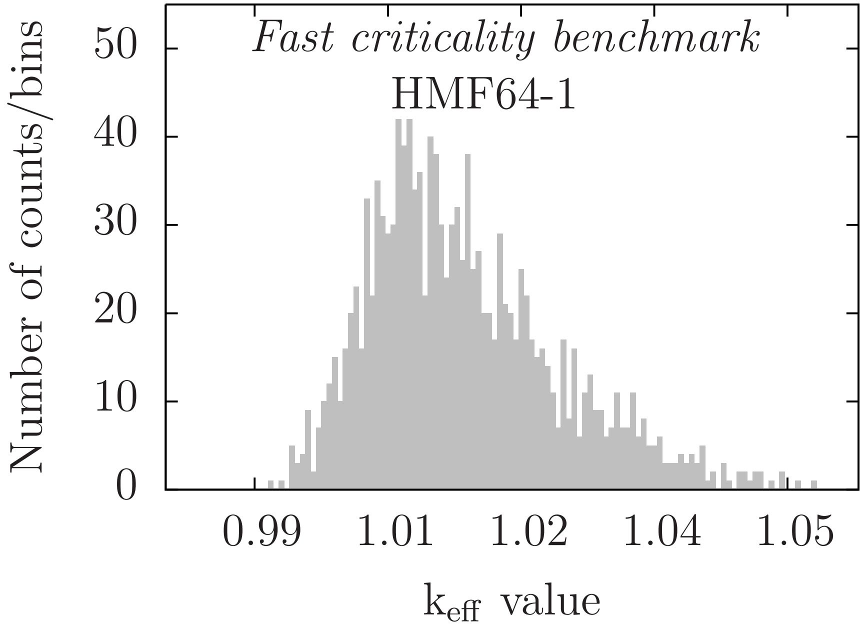


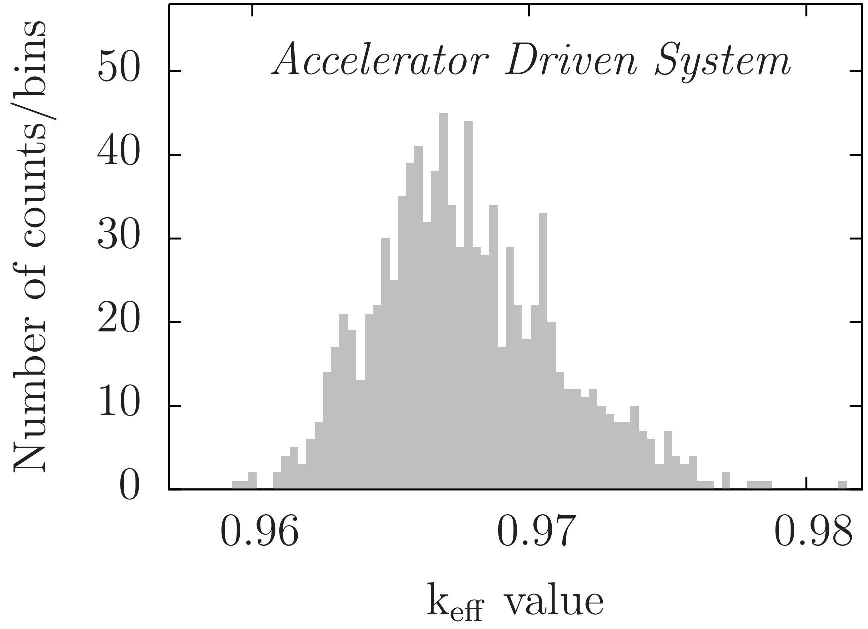
$k_{eff} = 1.01028 \pm (60 \text{ pcm and } 212 \text{ pcm})$ $k_{eff} = 1.00894 \pm (60 \text{ pcm and } 240 \text{ pcm})$



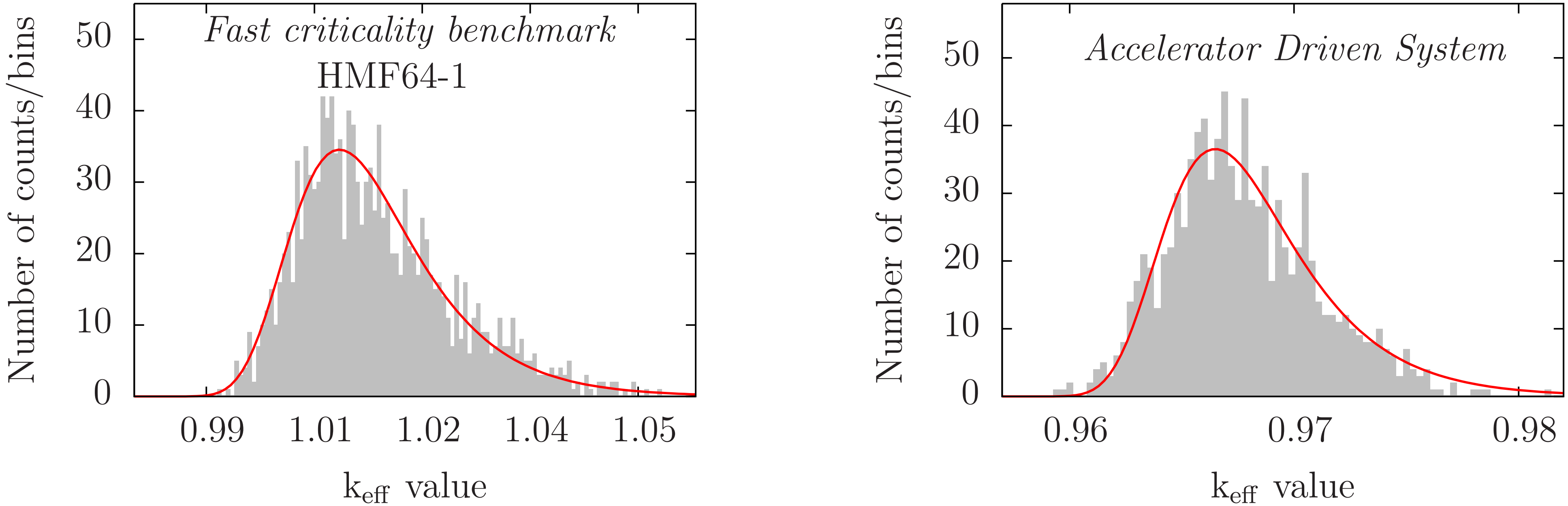


TMC Examples with Pb isotopes





TMC Examples with Pb isotopes



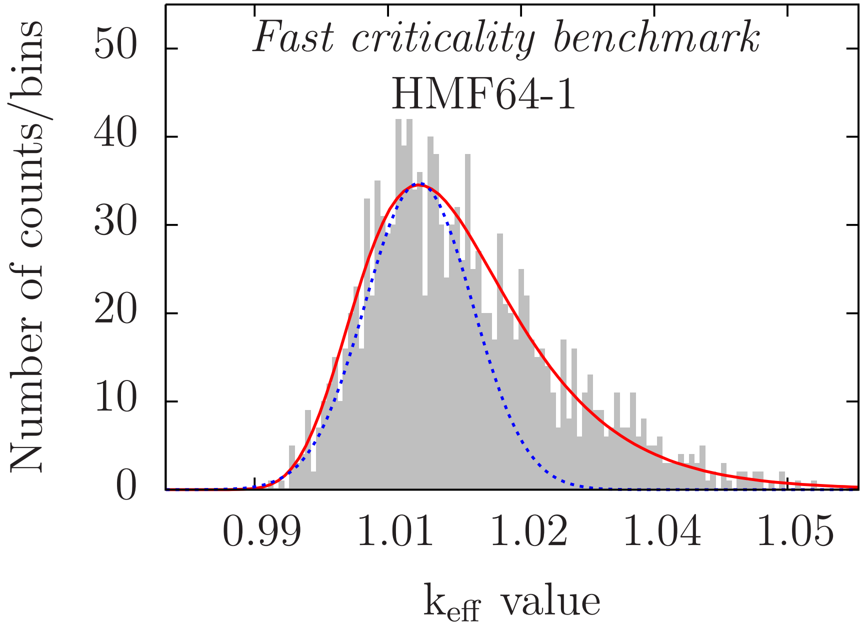
Better fit with the "*Extreme Value Theory*", or EVT:

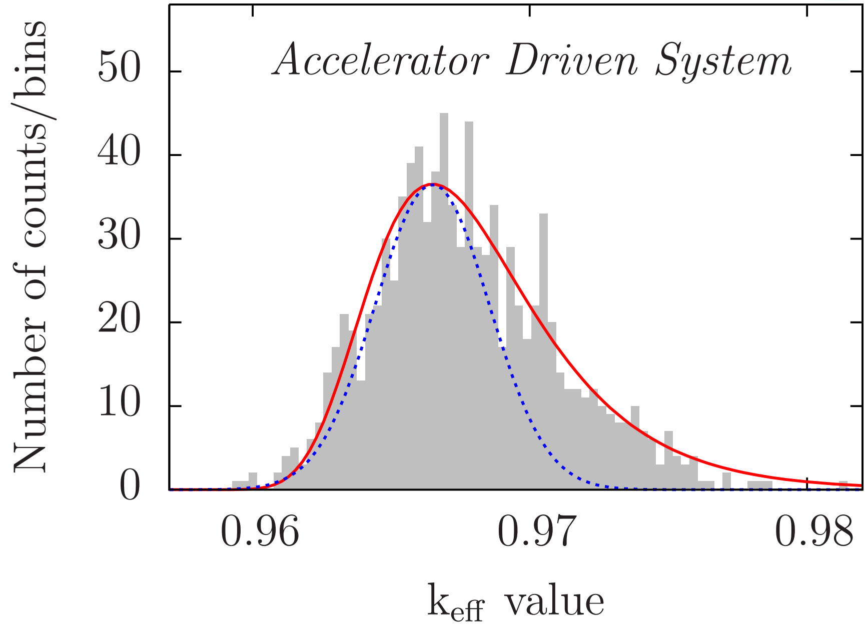
$F(z) = e^{-z-e^{-z}}$ with $z = \frac{X-\mu}{\sigma}$

Mean $\mu' = \mu + \gamma\sigma$

Standard Deviation $\sigma' = \sigma\frac{\pi}{\sqrt{6}}$

TMC Examples with Pb isotopes





Better fit with the "*Extreme Value Theory*", or EVT:

$F(z) = e^{-z-e^{-z}}$ with $z = \frac{X-\mu}{\sigma}$

Mean $\mu' = \mu + \gamma\sigma$

Standard Deviation $\sigma' = \sigma \frac{\pi}{\sqrt{6}}$

	HMF-64.1	ADS
k_{eff}	1.00848	0.96648
	μ'=1.01394	μ'=0.96785
$\sigma_k \times 10^5$	**855**	**291**
	σ'=**1097**	σ'=**345**

In TMC:

If we can do a calculation once, we can also do it a 1000 times, each time with a varying data library.

In TMC:

If we can do a calculation once, we can also do it a 1000 times, each time with a varying data library.

Well, then uncertainty propagation with TMC takes 1000 longer than a single calculation...

In TMC:

If we can do a calculation once, we can also do it a 1000 times, each time with a varying data library.

Well, then uncertainty propagation with TMC takes 1000 longer than a single calculation...
There is a solution with Monte Carlo codes (in fact 2 solutions):

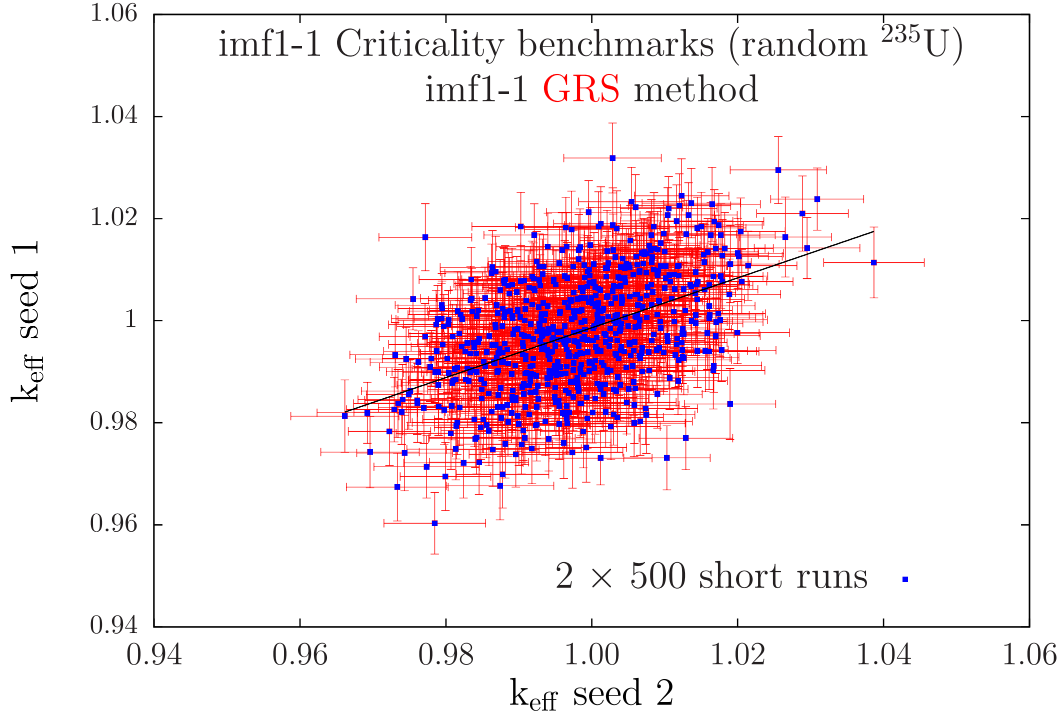
- GRS method,
- and fast TMC.

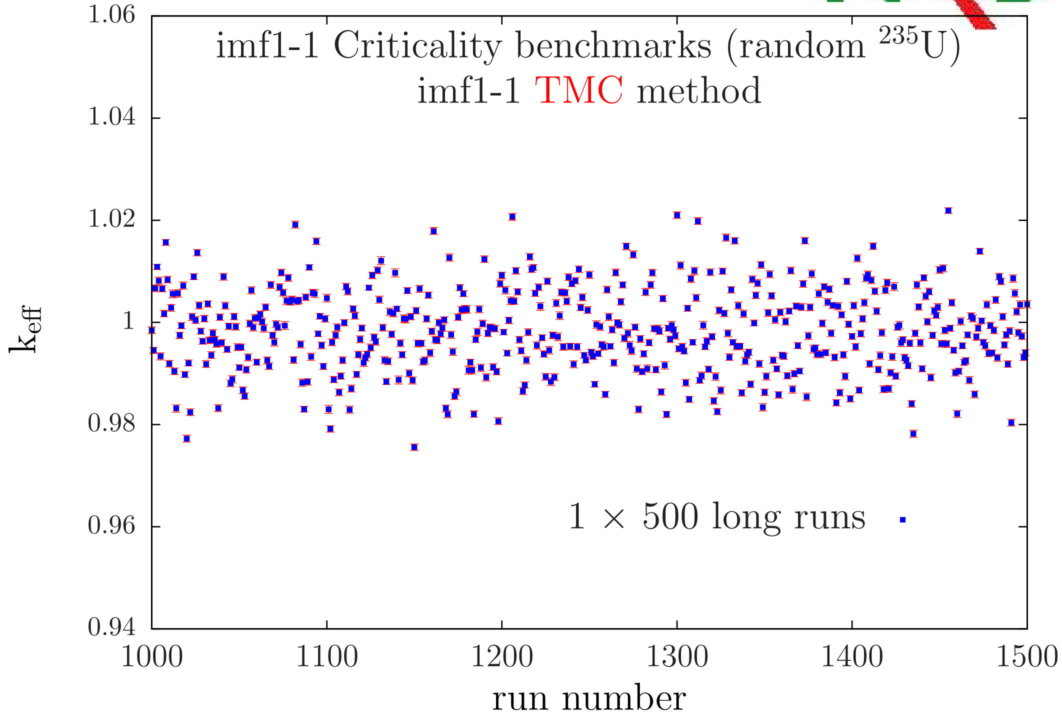
Fast Total Monte Carlo: GRS method

	TMC					GRS method				
	neutron histories	run time	seed	Nuclear data	Observed	neutron histories	run time	seed	Nuclear data	Observed
run 1	m	T	s_0	ND_1	k_1	m/n	T/n	s_0	ND_1	$k_1^\bullet$
run 2	m	T	s_0	ND_2	k_2	m/n	T/n	s_0	ND_2	$k_2^\bullet$
$\vdots$	$\vdots$		$\ddots$		$\vdots$	$\vdots$		$\ddots$		$\vdots$
run n	m	T	s_0	ND_n	k_n	m/n	T/n	s_0	ND_n	$k_n^\bullet$
subTotal										$\overline{k^\bullet} \pm \sigma_1^\bullet$
run $n+1$						m/n	T/n	s_1	ND_1	k_1°
run $n+2$						m/n	T/n	s_1	ND_2	k_2°
$\vdots$						$\vdots$		$\ddots$		$\vdots$
run 2n						m/n	T/n	s_1	ND_n	k_n°
subTotal						m	T			$\overline{k^\circ} \pm \sigma_2^\circ$
Total	m	nT			$\overline{k} \pm \sigma_1$	$2 \times m$	2T			$\sigma_1^\bullet, \sigma_2^\circ$
Method			$\sigma_1^2 = \sigma^2_{\text{statistics}} + \sigma^2_{\text{nucl.data.}}$					$\sigma^2_{\text{nucl.data.}} = \text{cov}(\vec{k}^\circ, \vec{k}^\bullet) = \text{corr}(\vec{k}^\circ, \vec{k}^\bullet) * \sigma_1^\bullet * \sigma_2^\circ$		

<u>GRS method:</u> if two output variables $\vec{k}^\circ$ and $\vec{k}^\bullet$ are identically distributed and conditionally independent given the vector of epistemic input $\vec{ND}$, then their covariance cov($\vec{k}^\circ$,$\vec{k}^\bullet$) is equal to the variance of the conditional expectation.

Fast Total Monte Carlo: GRS method





$$\sigma_{\text{nucl.data}} = \sqrt{\text{cov}(\vec{k_1}, \vec{k_2})} = \sqrt{\text{corr}(\vec{k_1}, \vec{k_2}) \times \sigma_1 \sigma_2}$$
$$= \sqrt{0.48 \times 0.0110 \times 0.0112}$$
$$= 770 \text{ pcm}$$

$$\sigma_{\text{nucl.data}} = \sqrt{\sigma_1^2 - \sigma_{\text{stat}}^2}$$
$$= \sqrt{0.0805^2 - 0.00067^2}$$
$$= 802 \text{ pcm}$$

Fast Total Monte Carlo: NRG method

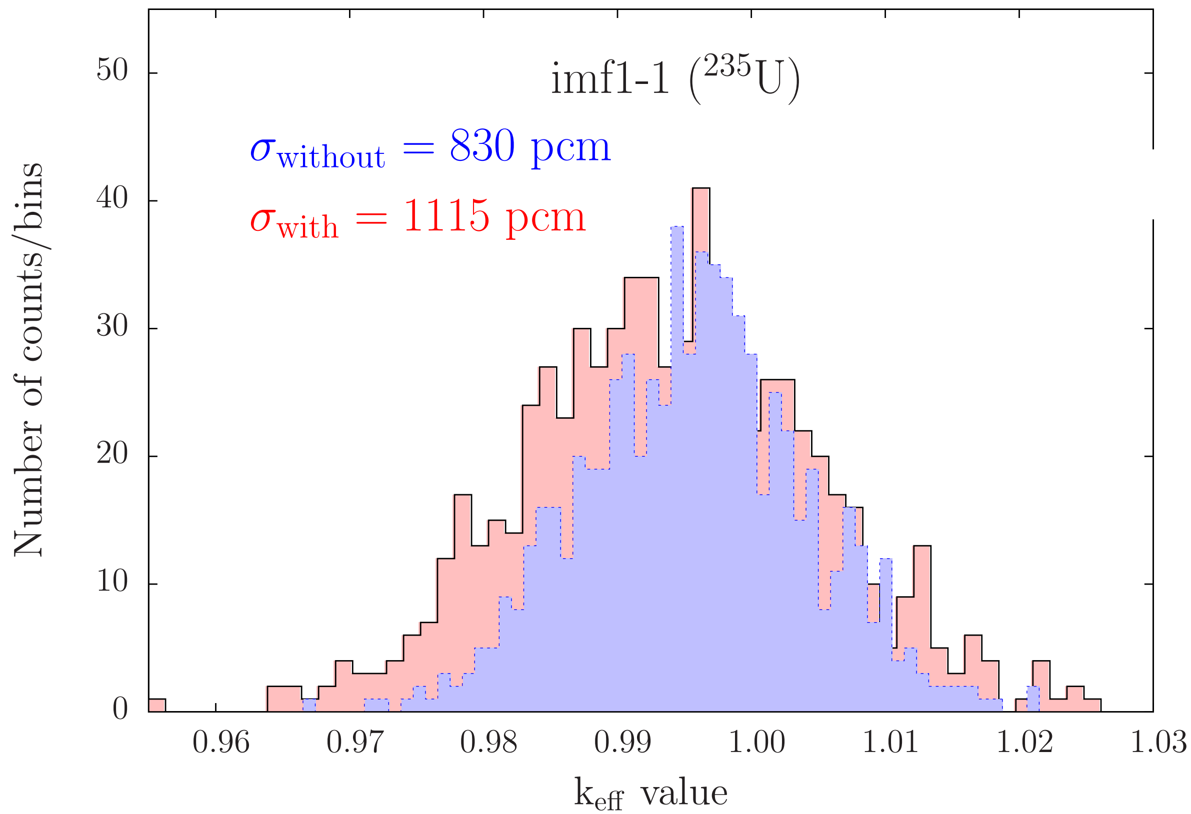
	TMC					NRG fast TMC				
	neutron histories	run time	seed	Nuclear data	Observed	neutron histories	run time	seed	Nuclear data	Observed
run 1	m	T	s_0	ND_1	k_1	m/n	T/n	s_1	ND_1	k^*_1
run 2	m	T	s_0	ND_2	k_2	m/n	T/n	s_2	ND_2	k^*_2
$\vdots$	$\vdots$		$\ddots$		$\vdots$	$\vdots$		$\ddots$		$\vdots$
run n	m	T	s_0	ND_n	k_n	m/n	T/n	s_n	ND_n	k^*_n
subTotal										$\overline{k^*} \pm \sigma_1$
run $n+1$						m/n	T/n	s'_1	ND_0	k'_1
run $n+2$						m/n	T/n	s'_2	ND_0	k'_2
$\vdots$						$\vdots$		$\ddots$		$\vdots$
run 2n						m/n	T/n	s'_n	ND_0	k'_n
subTotal						m	T			$\overline{k'} \pm \sigma_2$
Total	m	nT			$\overline{k} \pm \sigma_1$	$2 \times m$	2T			σ_1, σ_2
Method	$\sigma_1^2 = \sigma^2_{\text{statistics}} + \sigma^2_{\text{nucl.data.}}$					$\sigma_1^2 = \sigma_2^2 + \sigma^2_{\text{nucl.data.}}$				

NRG method: Separate the effect of the nuclear data from the effect of statistics

fast Total Monte Carlo: NRG method

In TMC with MCNP, a single run i takes long so that $\sigma^{(i)}_{\text{statistics}} << \sigma^{(i)}_{\text{nuclear data}}$.
What if we perform:

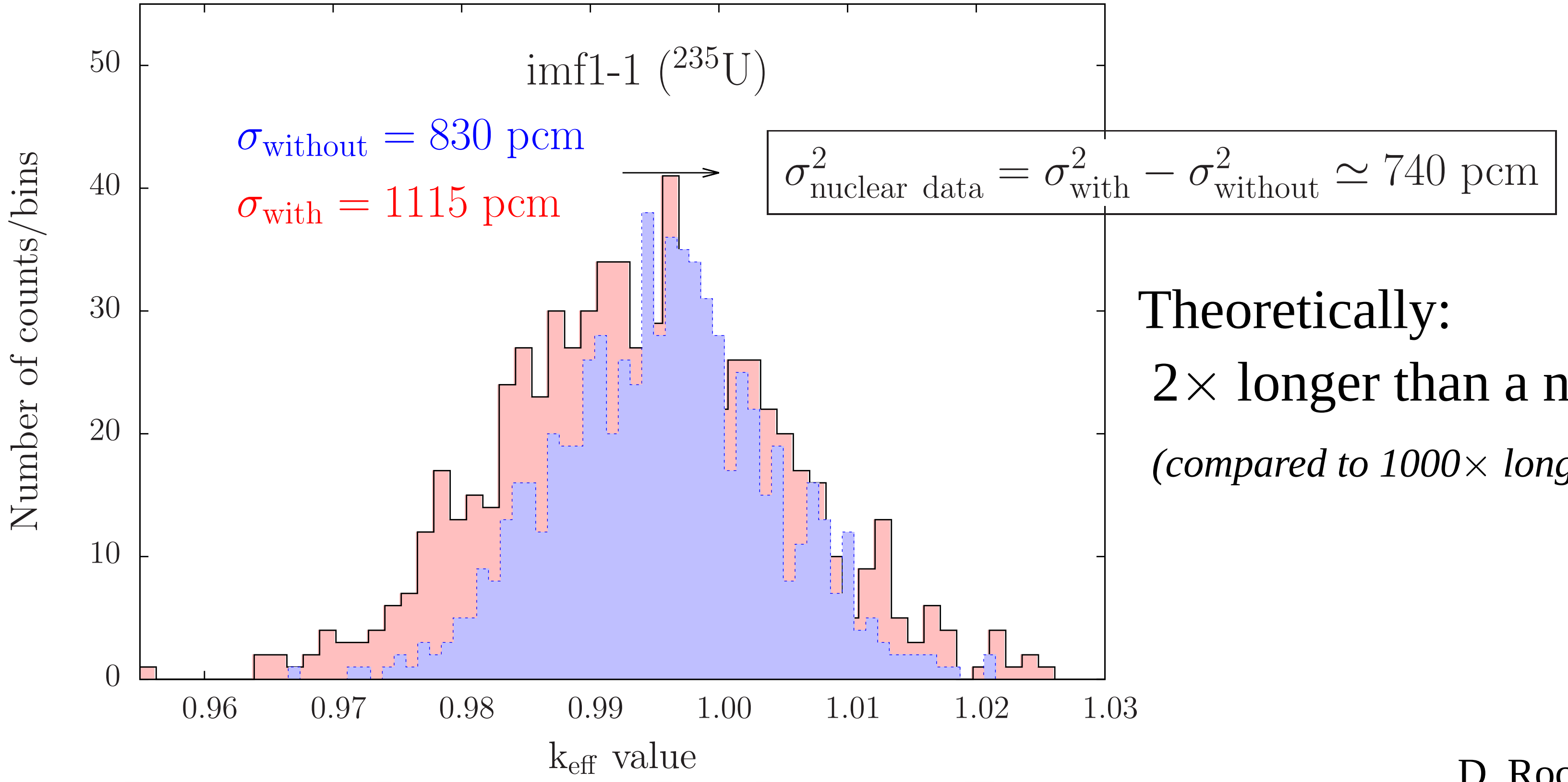
- a 1000 short runs (equivalent in time to one long run) with each time different nuclear data and different seeds ($\sigma^{(i)}_{\text{statistics}} >> \sigma^{(i)}_{\text{nuclear data}}$),
- and 1000 short runs with each time different seeds ?



fast Total Monte Carlo: NRG method

In TMC with MCNP, a single run i takes long so that $\sigma^{(i)}_{\text{statistics}} << \sigma^{(i)}_{\text{nuclear data}}$.
What if we perform:

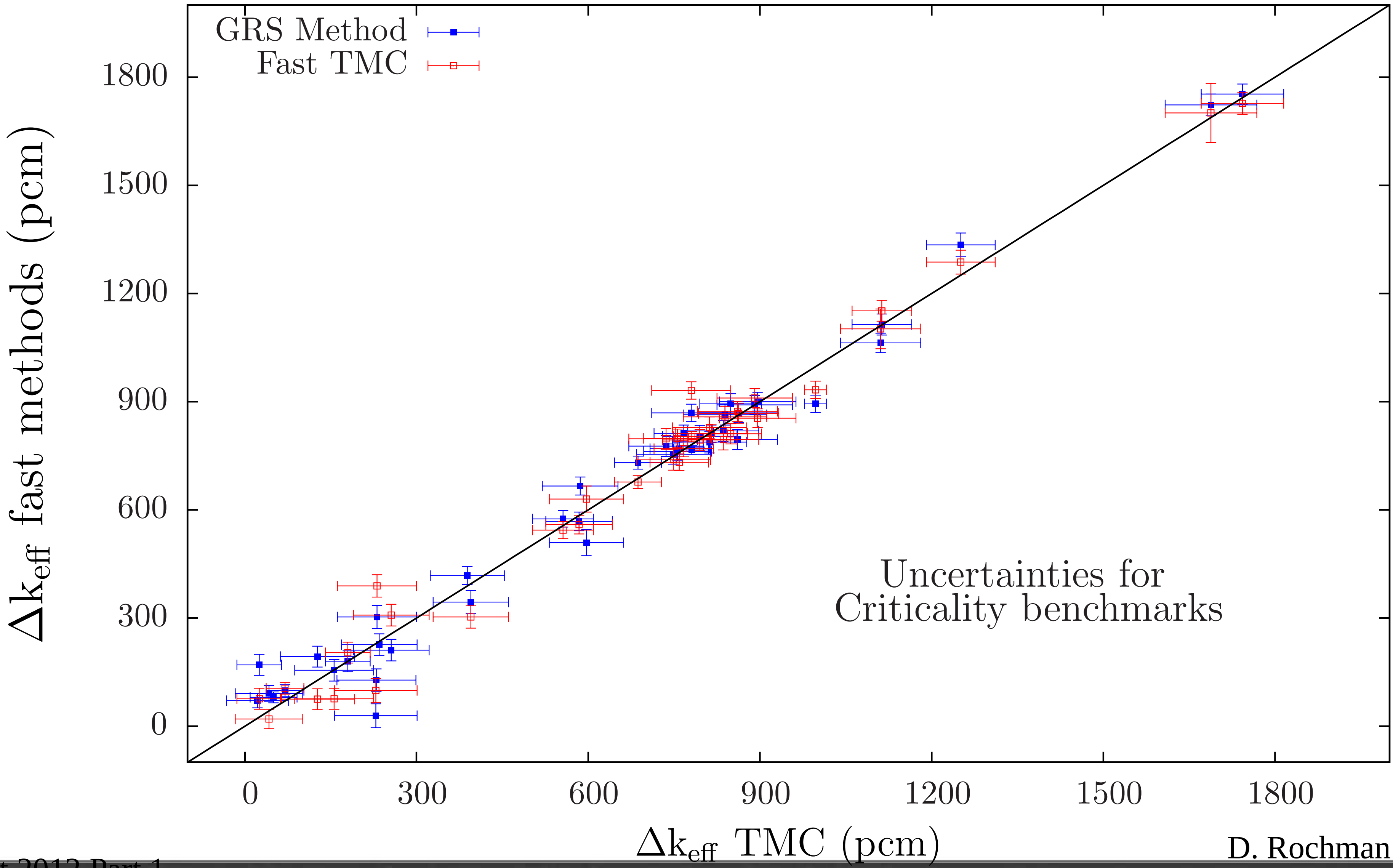
- a 1000 short runs (equivalent in time to one long run) with each time different nuclear data and different seeds ($\sigma^{(i)}_{\text{statistics}} >> \sigma^{(i)}_{\text{nuclear data}}$),
- and 1000 short runs with each time different seeds ?



Theoretically:
2× longer than a normal run
(compared to 1000× longer for TMC)

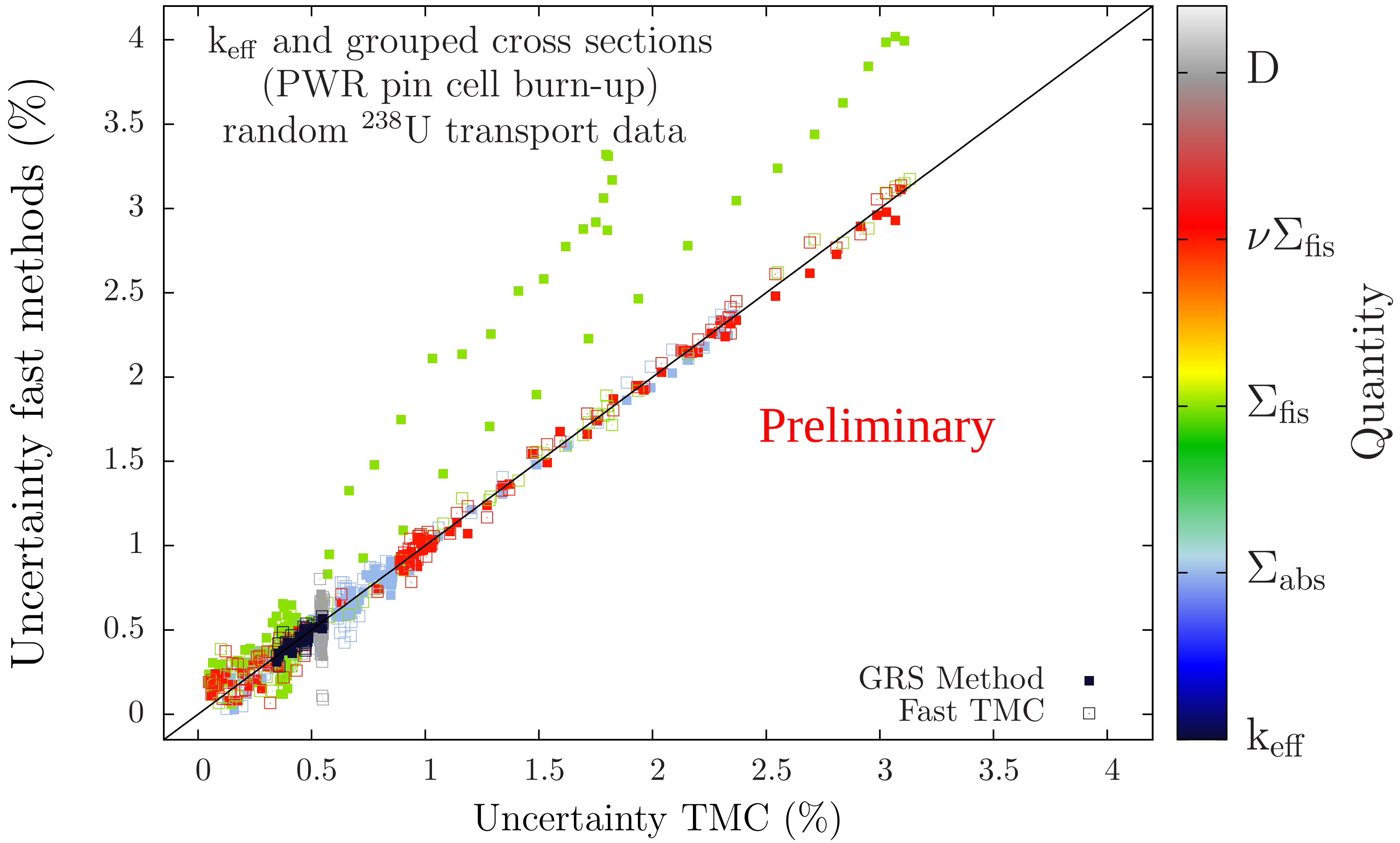
fast TMC: test on k_{eff} criticality benchmarks

Comparison between TMC (considered as reference), fast TMC and the GRS method with 44 benchmarks, changing $^{235,238}U$, $^{239,240}Pu$ and ^{56}Fe.

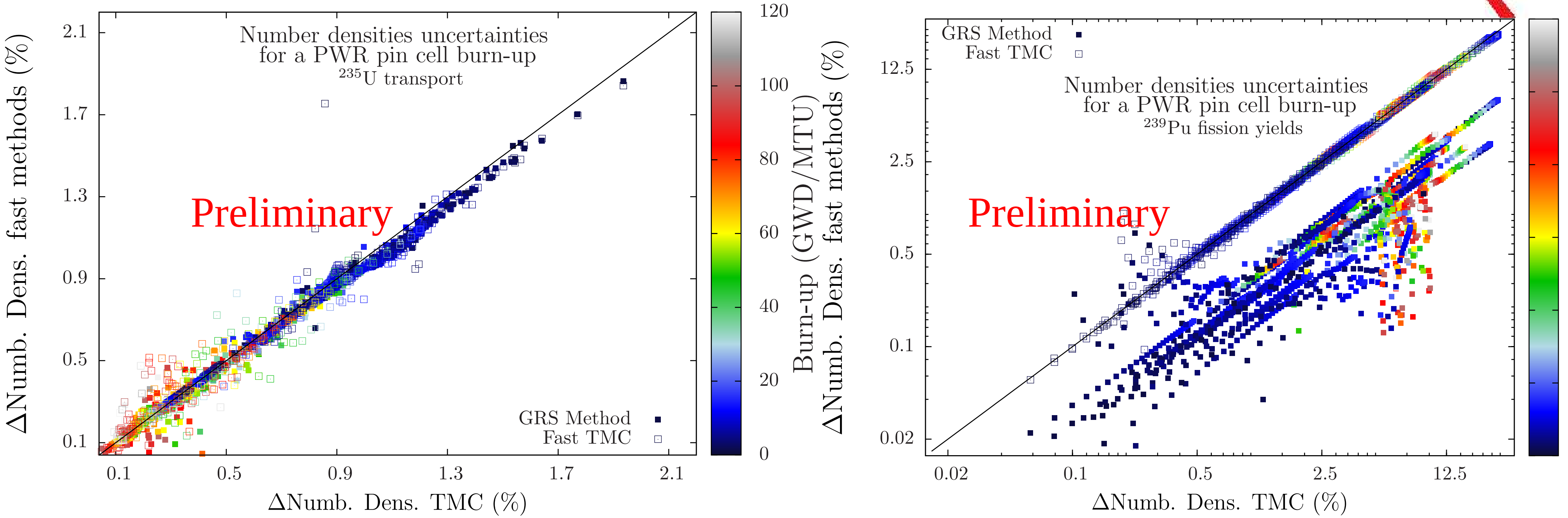


fast TMC: test on burn-up quantities

Comparison between TMC (considered as reference), fast TMC and the GRS method with UAM pin cell model of a PWR, changing $^{235,238}U$ transport data and $^{239,240}Pu$ fission yields.



fast TMC: test on burn-up quantities



The results of the depletion module are relatively not sensitive to the seed of the Monte Carlo transport code, partially due to the normalization to a constant power value. This tends to cancel any existing correlation between two conditionally independent vectors, as used in the GRS method.

Additionally, as a deterministic depletion module is not sensitive to the original random seed of the Monte Carlo.