DE LA RECHERCHE À L'INDUSTRIE

Validation of the Nuclear Data Evaluation Code CONRAD

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Plan

- Introduction
- Cross sections : Pu239(n,f),(n,n), Xe131(n,n)
- Observables : calculation vs. measurement
- Transmissions : Xe129, U238
- Capture Yields : U238, Au197, Mn55
- Conclusion , Outlook

Introduction

CONRAD is a nuclear data evaluation code.

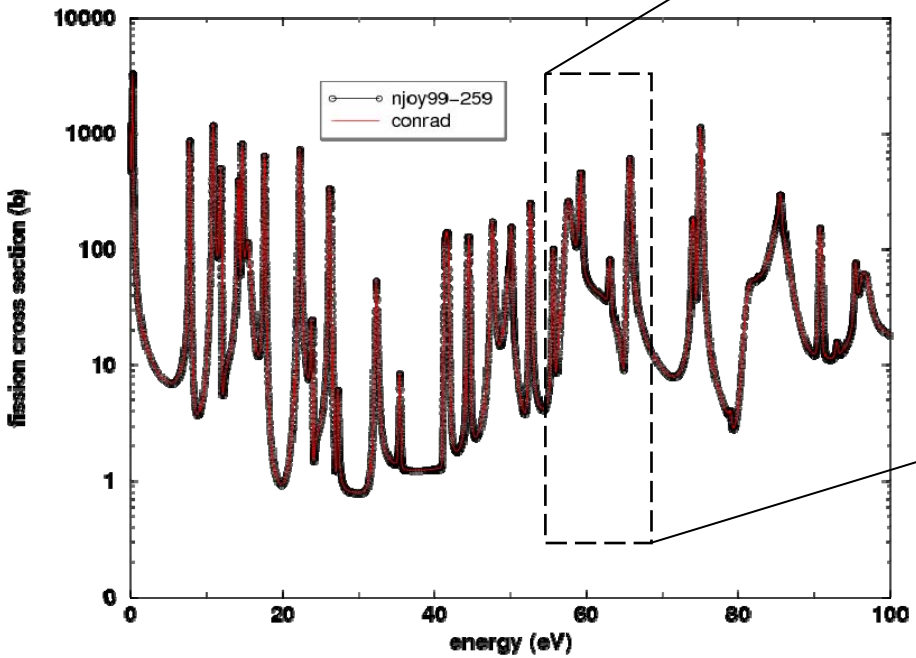
Adjustment of nuclear reaction parameters (RP, OMP, …) for the calculation of cross sections and variance-covariance matrices from thermal range to several MeV.

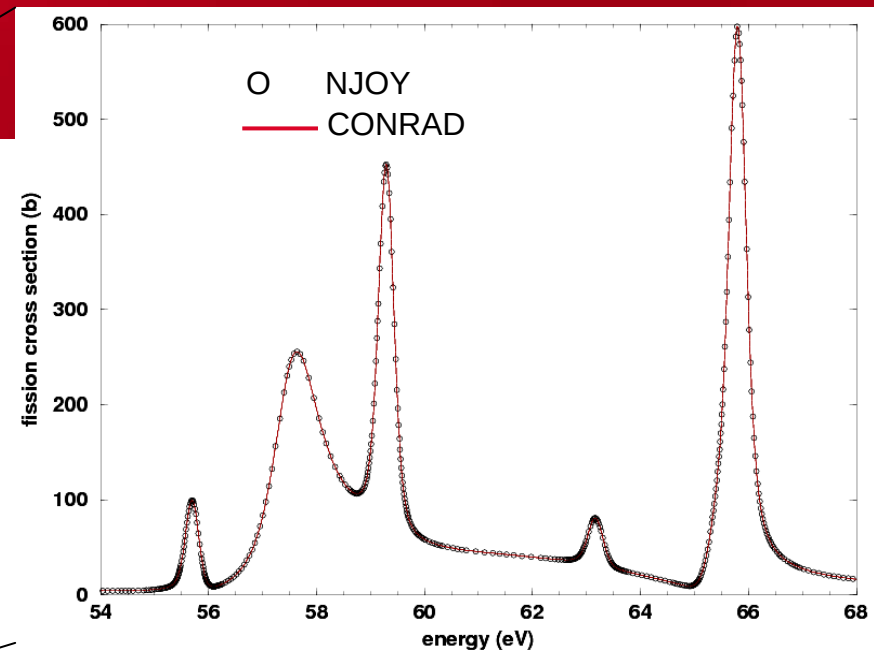
Production of evaluated nuclear data files (JEFF).

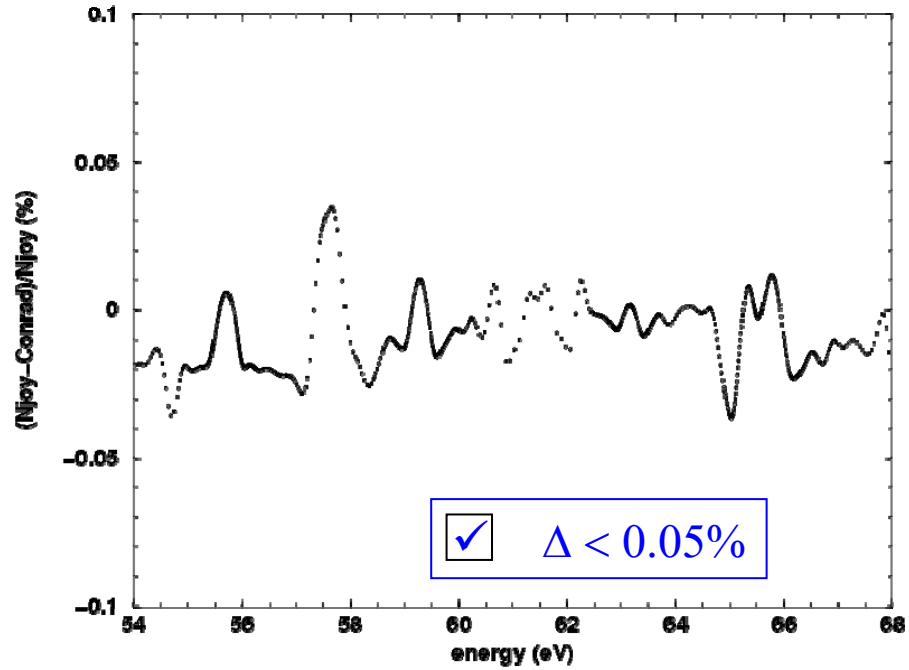
Among others, use of differential and integral experiments for RLSF using marginalization (analytic or Monte Carlo) techniques.

In this short study, we will focus on the validation of theoretical cross sections and related observables (transmission, capture yield).

^{239}Pu fission cross section

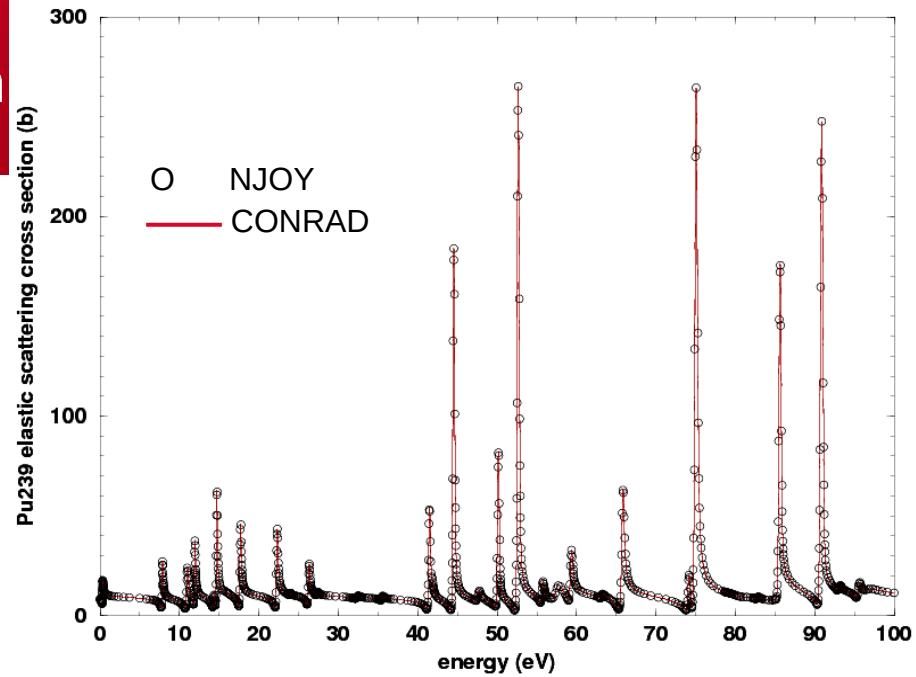




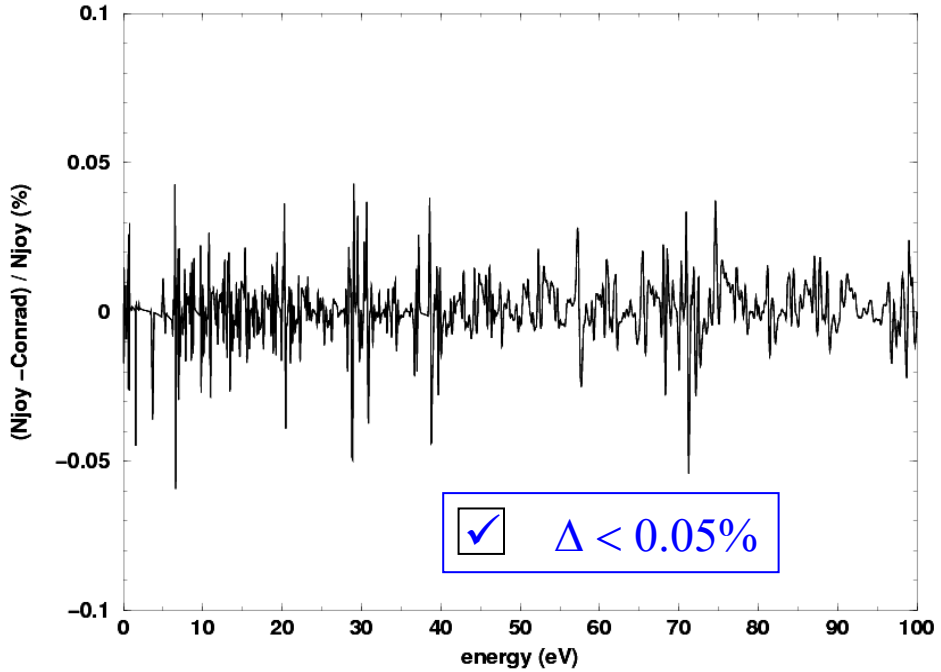


^{239}Pu in RRR
- Fission cross section
- Reich Moore
- Doppler broadening @294K

^{239}Pu elastic cross section



^{239}Pu in RRR
- Elastic cross section
- Reich Moore
- Doppler broadening @294K



A bias is observed if the required accuracy in NJOY is set to 0.1%

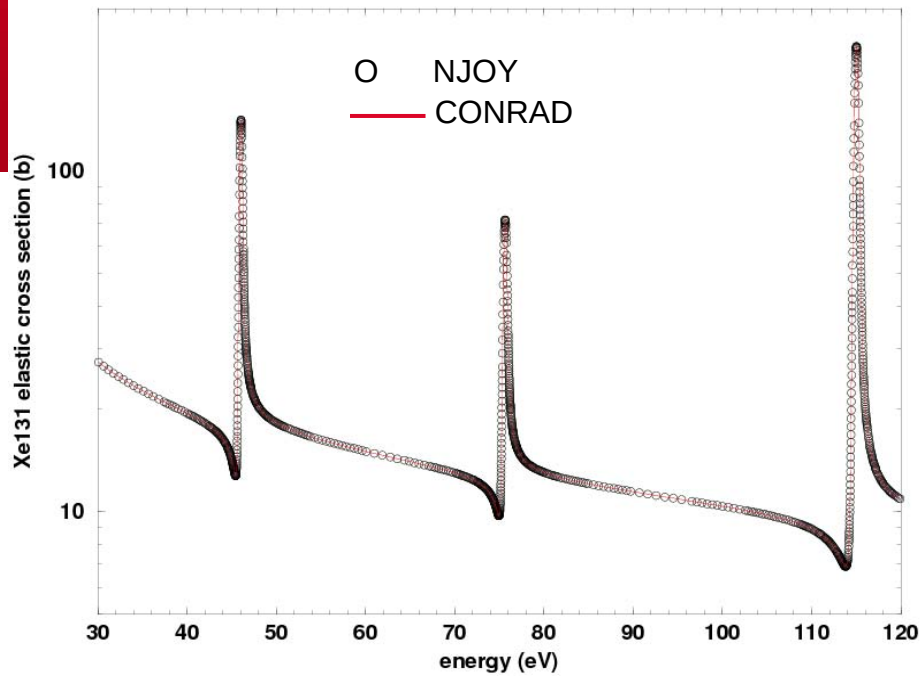
No bias if the criteria is set to 0.01%

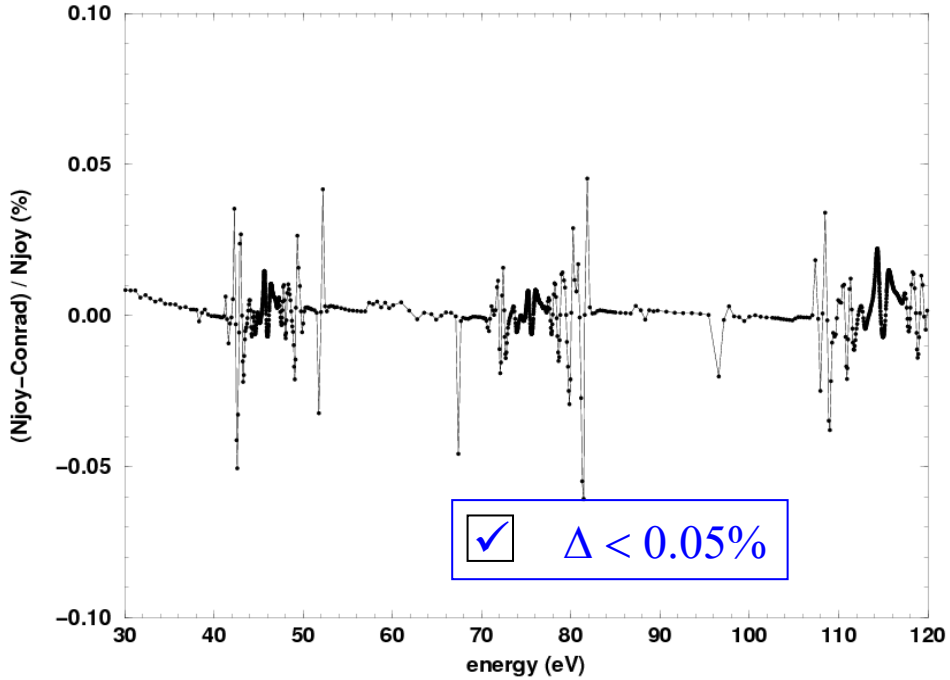
^{131}Xe elastic cross section

^{131}Xe in RRR
- Elastic cross section
- Multi Level Breit Wigner
- Doppler broadening @294K

$\sigma^{CONRAD} = \sigma^{NJOY}$

☑ σ^{CONRAD}





☑ $\Delta < 0.05\%$

Transmissions + Capture yields : calculation

- Observables (transmission, capture yields) are functions of cross sections

Transmission : $T(E) = e^{-n\sigma_t(E)} = e^{-\Sigma_t(E)L}$ ✓

Capture yield : $Y(E) = Y_0(E) + Y_1(E) + Y_n(E)$

$N = n/L$ [at/b] [cm]

$\Sigma = N\sigma$ [cm-1] [b/at]

Primary capture yield | *Single scattering correction* | *"double-plus" scattering correction*

$$Y_0(E) = \left(1 - e^{-n\sigma_t(E)}\right)\frac{\sigma_\gamma(E)}{\sigma_t(E)}$$ ✓

E → E' (target@rest (0.K scatt. Kernel)

$$Y_1^\infty(E) = \int_{-1}^{0} d\mu \left[\frac{1-e^{-\Sigma_t(E)L}}{\Sigma_t(E)} - \frac{1-e^{-(\Sigma_t(E)L-\Sigma_t(E')L/\mu)}}{\Sigma_t(E)-\Sigma_t(E')/\mu}\right]\frac{\Sigma_c(E')}{\Sigma_t(E')}\Sigma_s(E)p(\mu_c)\left|\frac{d\mu_c}{d\mu}\right|$$
$$+ \int_{0}^{1} d\mu \left[\frac{1-e^{-\Sigma_t(E)L}}{\Sigma_t(E)} - \frac{e^{-(\Sigma_t(E')L/\mu)}+e^{-(\Sigma_t(E)L)}}{\Sigma_t(E)-\Sigma_t(E')/\mu}\right]\frac{\Sigma_c(E')}{\Sigma_t(E')}\Sigma_s(E)p(\mu_c)\left|\frac{d\mu_c}{d\mu}\right|$$

Single scattering correction (for infinite sample)

$$Y_1(E) = \frac{\iint dxdy}{S} N\int dz \exp\left(-N\sigma_t(E)z\right)\int d\Omega \frac{d\sigma}{d\Omega}\sigma_c(E')N\int dq \exp(-N\sigma_t(E')q$$

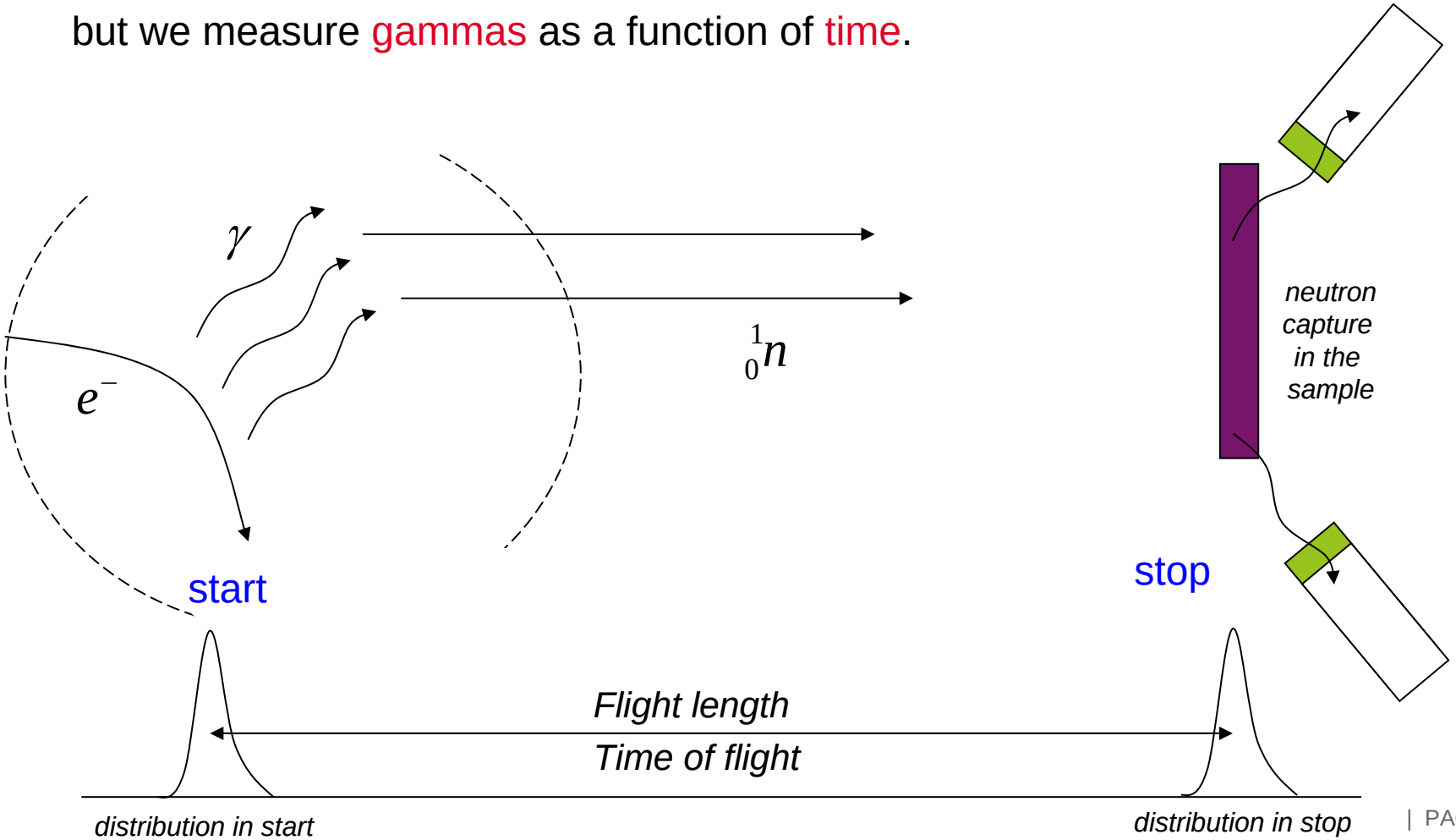
Single scattering correction (from SAMMY manual)

$Y_n(E)$ *Not trivial ; requires approximations (uniform+ isotropic distribution of neutrons after 2 or more scatterings.*

Transmissions + Capture yields : measurement

- **Time of Flight** technique ($e^- \rightarrow \gamma \rightarrow {}^1_0n$)

We would like to record) neutrons as a function of energy
but we measure gammas as a function of time.



Transmissions + Capture yields : measurement

- In this kind of experiment (tof), we know “when” (time of flight) but not “where” (collision site) then the time spectrum is transformed in an energy spectrum using a fixed distance (the flight path F.P.).

- The experimental resolution function (detector, moderator,…) is used in the calculations to reproduce the experimental results.

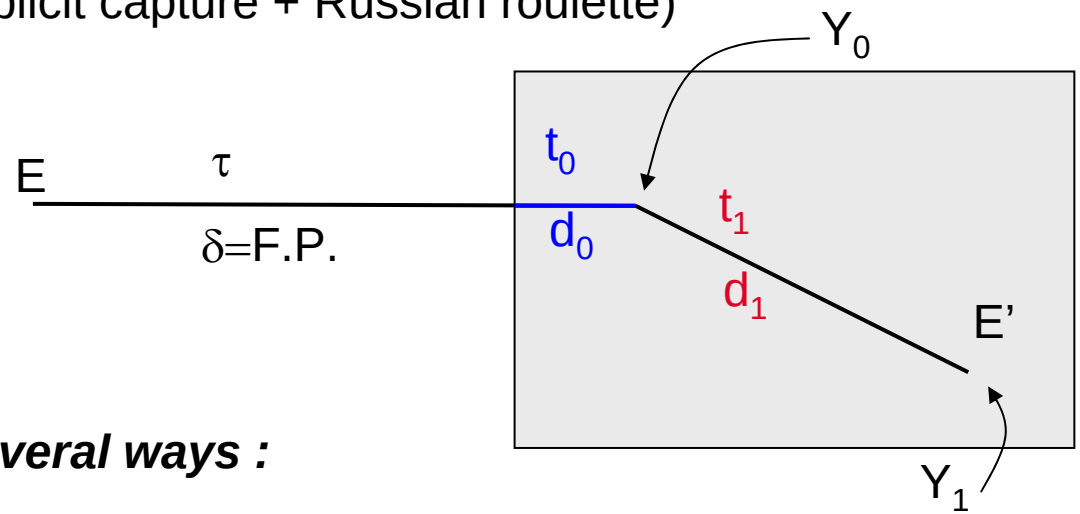
- If we leave aside the experimental resolution (which can be neglected for various configurations), we must be able to calculate as precisely as possible the response (T(E), Y(E), …).

Transmissions + Capture yields : calc. / meas.

- **Monte Carlo** simulation

Neutron transport in the sample (Implicit capture + Russian roulette)

$$E = \mathrm{E}(\tau, \delta)$$
$$= \mathrm{E}(\tau + t_0, \delta + d_0)$$



Simulation can be performed in several ways :

1. in time (Tof Varying with actual distance in the sample → actual energy E')
2. in time (Tof Varying with constant fixed distance, e.g. the flight path δ)
3. in time (Tof fixed with constant fixed distance, e.g. the flight path δ)
4. in energy (tally at energy just before capture E')
5. in energy (tally at incident energy E)

1. ≡ 4. : identical to simulation in energy with MC transport codes (Tripoli4, Mcnp5, …)

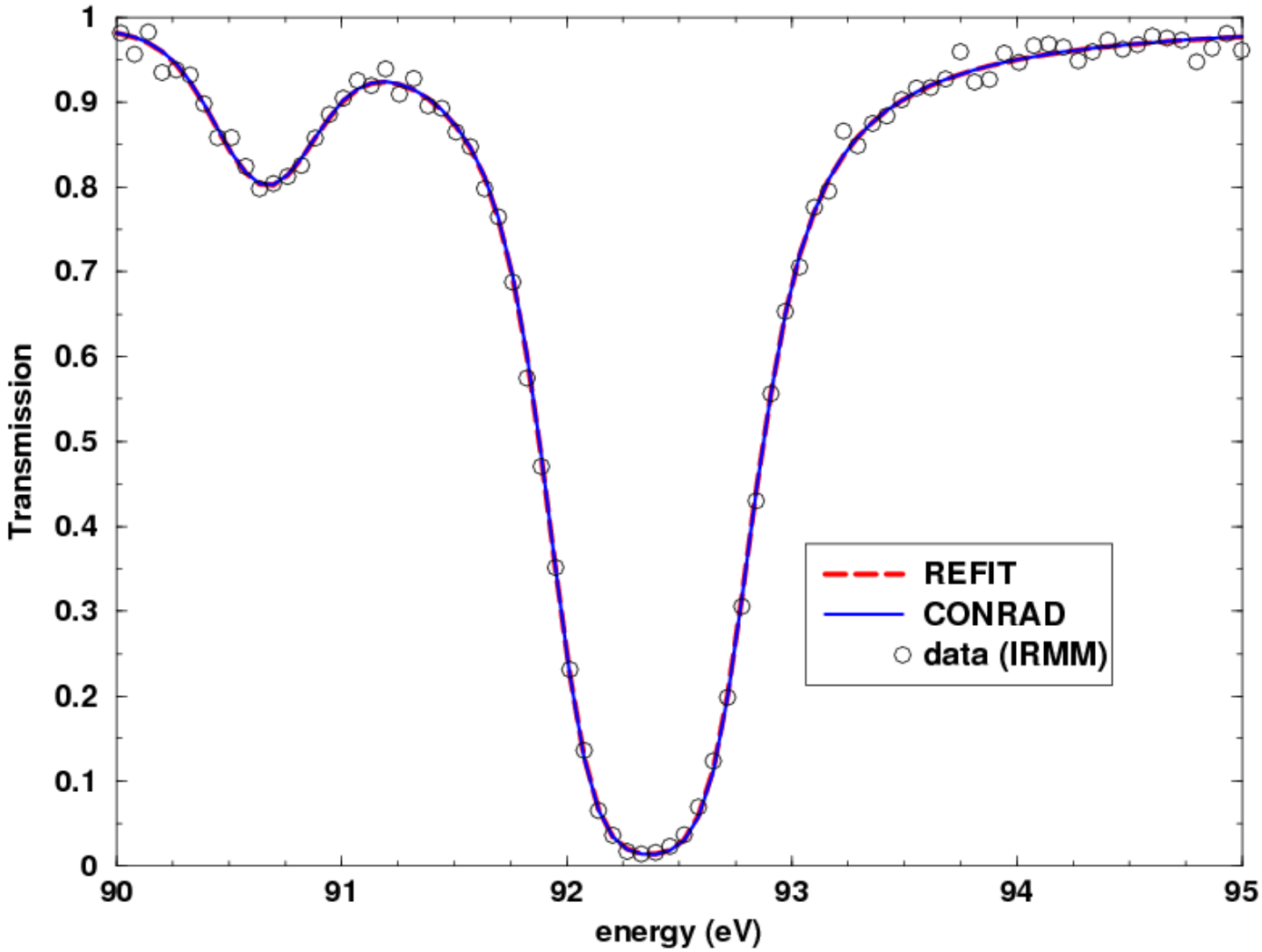
2. ≈ Experimental result
3. = 5. = Analytical (p.7)

2. and 3. are difficult to distinguish (experimentally)
→ effect observed for unusually thick targets !!

^{129}Xe transmission

✓ T^{CONRAD}

$T^{CONRAD} = T^{REFIT}$

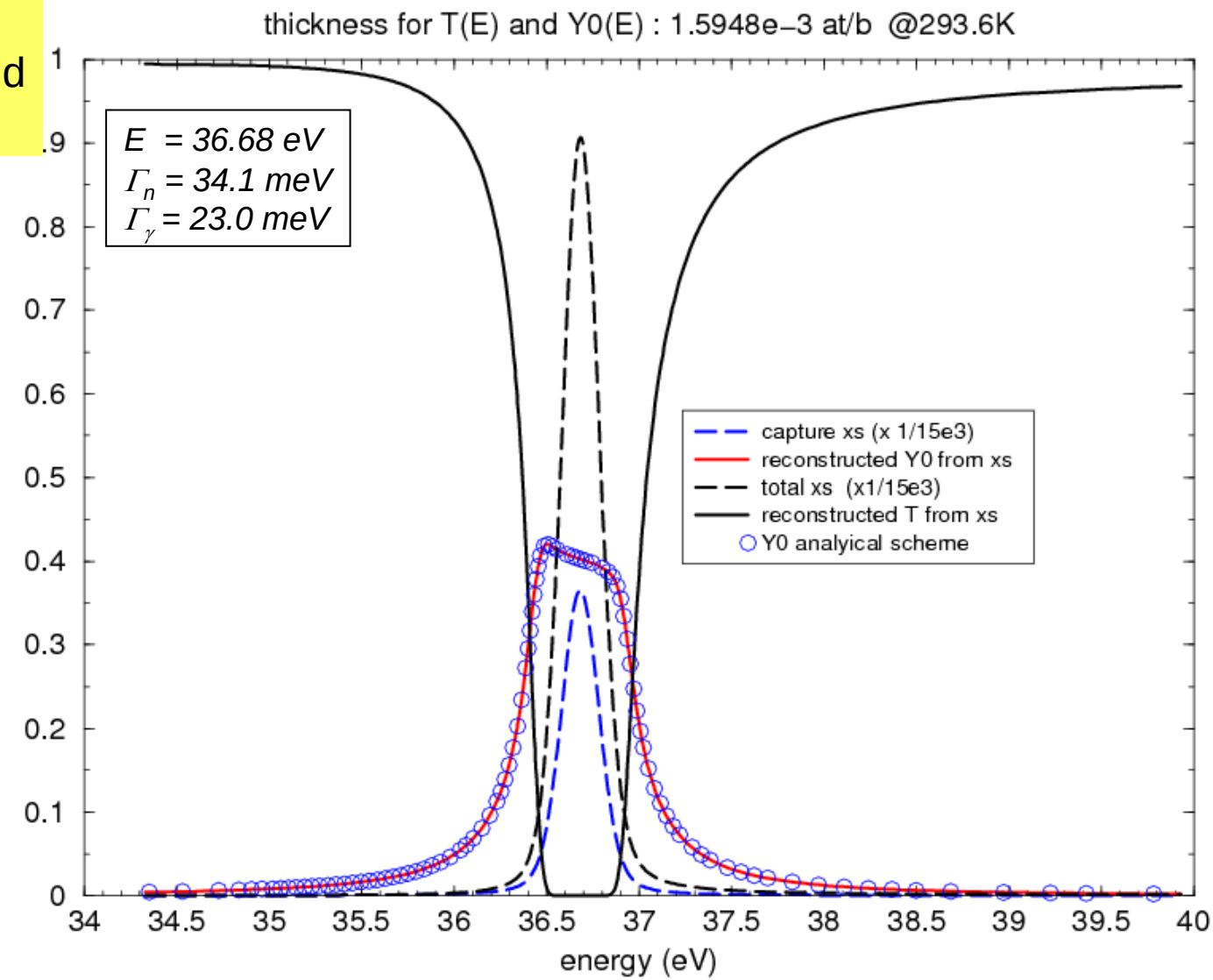


^{238}U *primary* capture yield (analytical scheme)

^{238}U @36.6eV
- Primary capture yield
- T = 294 K

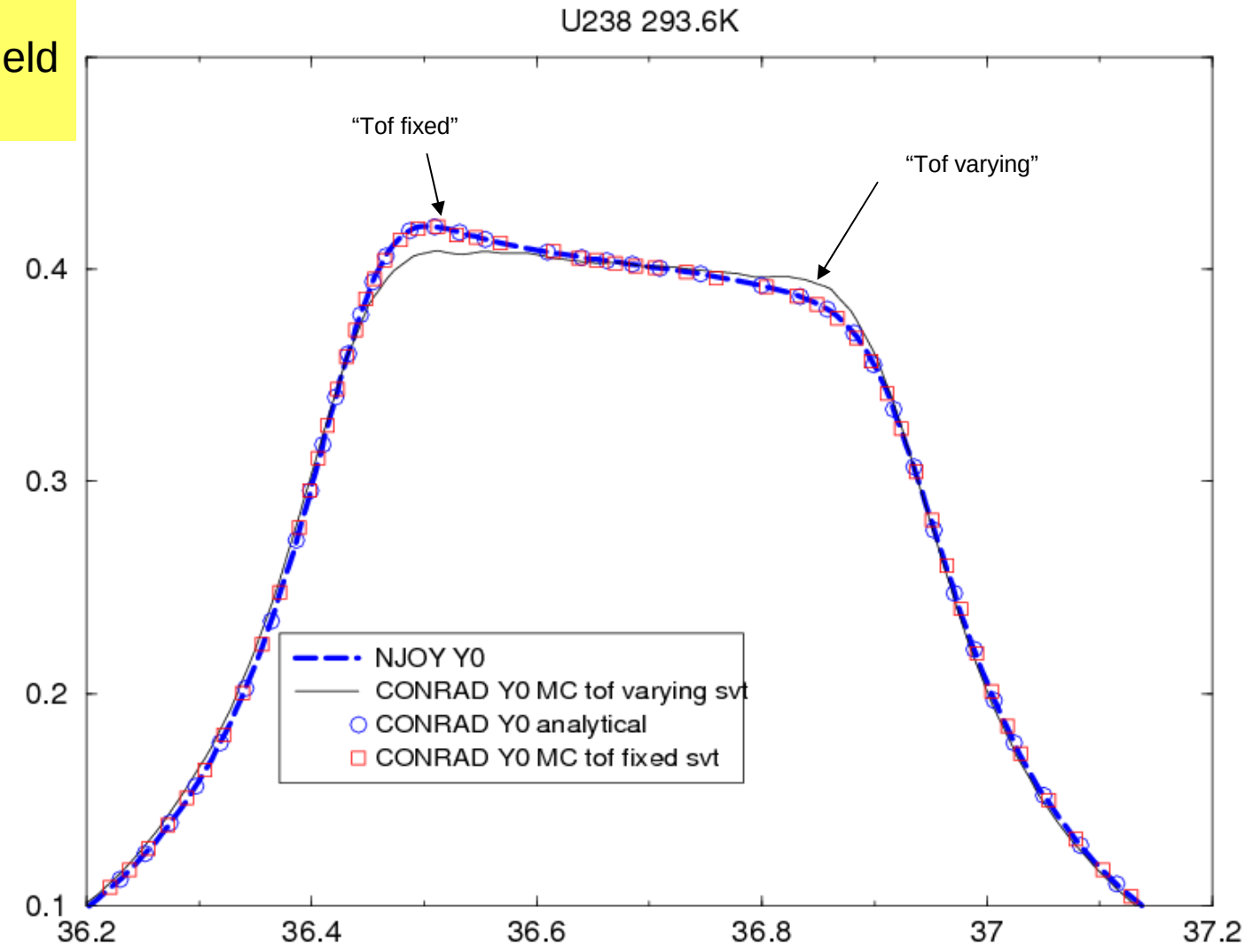
n ≈ 1.595 10^{-3} at/b
e = 0.5 cm

☑ $Y_0^{CONRAD,AN.}$



^{238}U *primary* capture yield (ANalytical / MC schemes)

^{238}U @36.6eV
- Primary capture yield
- T = 294 K



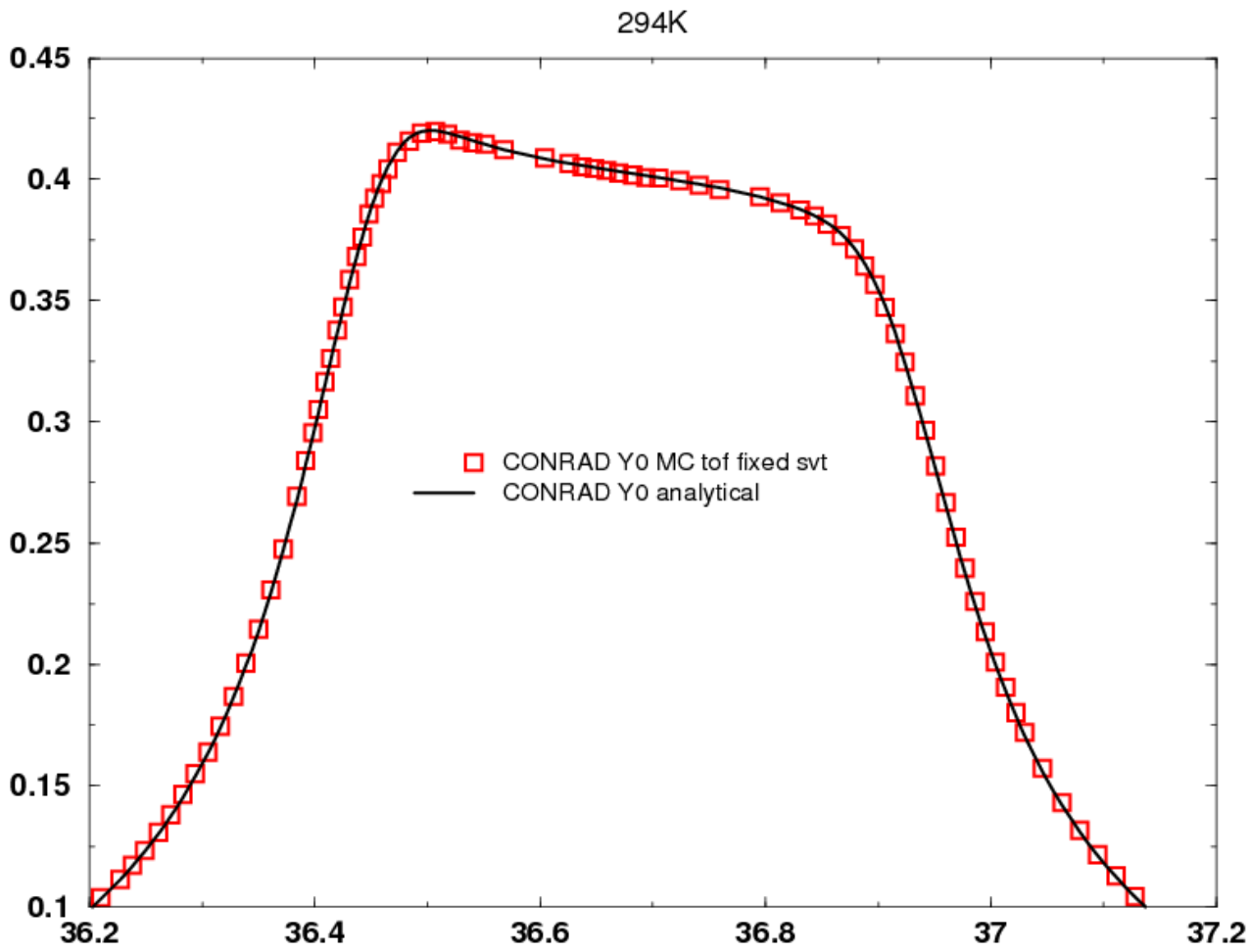
$Y_0^{AN.} = Y_0^{MC}$

✓ $Y_0^{CONRAD,MC.}$

^{238}U *primary* capture yield (ANalytical / MC schemes)

^{238}U @36.6eV
- Primary capture yield
- T = 294 K

$Y_0^{AN.} = Y_0^{MC}$



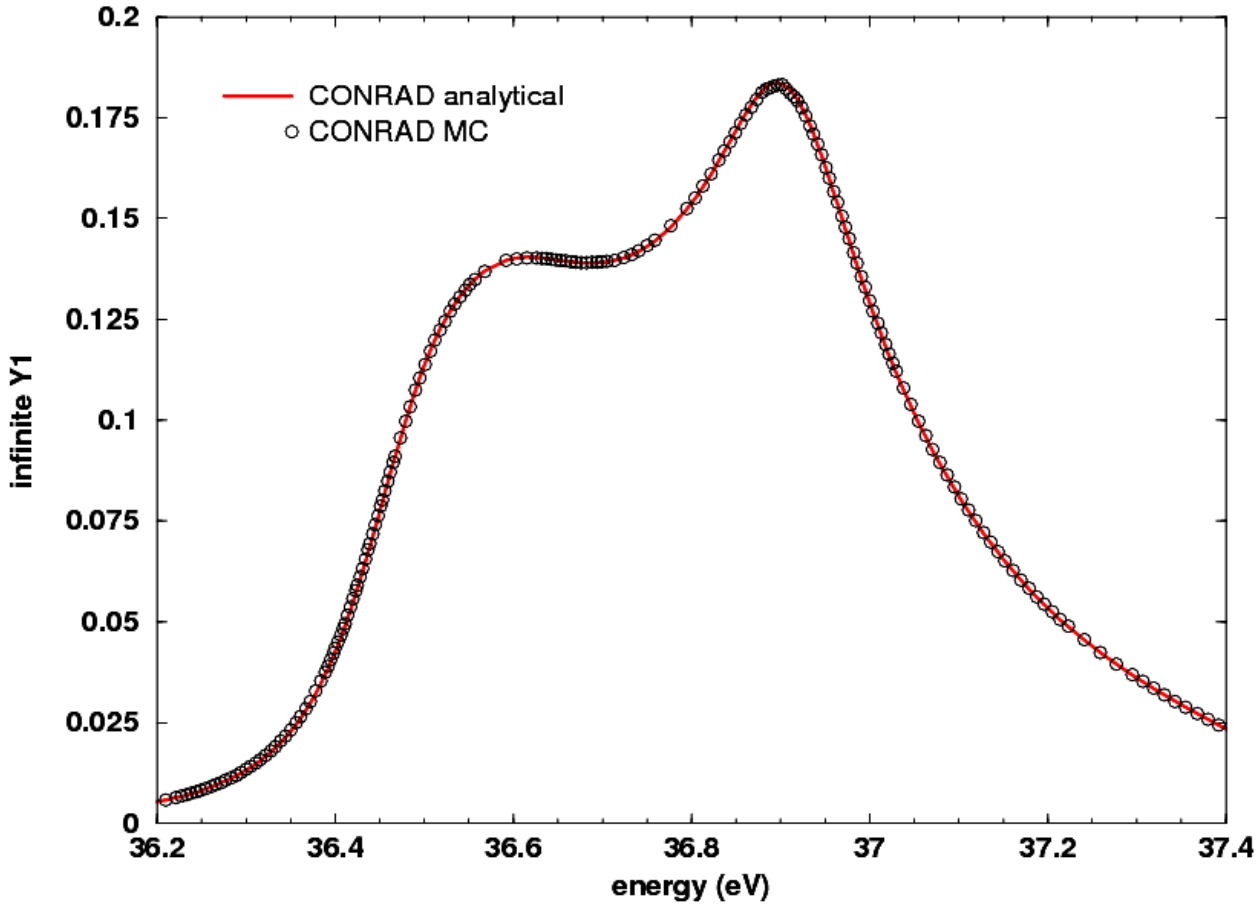
^{238}U *single* scattering correction (infinite sample) (ANalytical / MC schemes)

^{238}U @36.6eV @294K
- Single scattering correction Y_1

$$Y = Y_0 + \mathbf{Y_1} + Y_n$$

"infinite sample approximation for single scattering correction $R_S >> R_B$"

$$Y_{1,\infty}^{AN.} = Y_1^{MC}$$

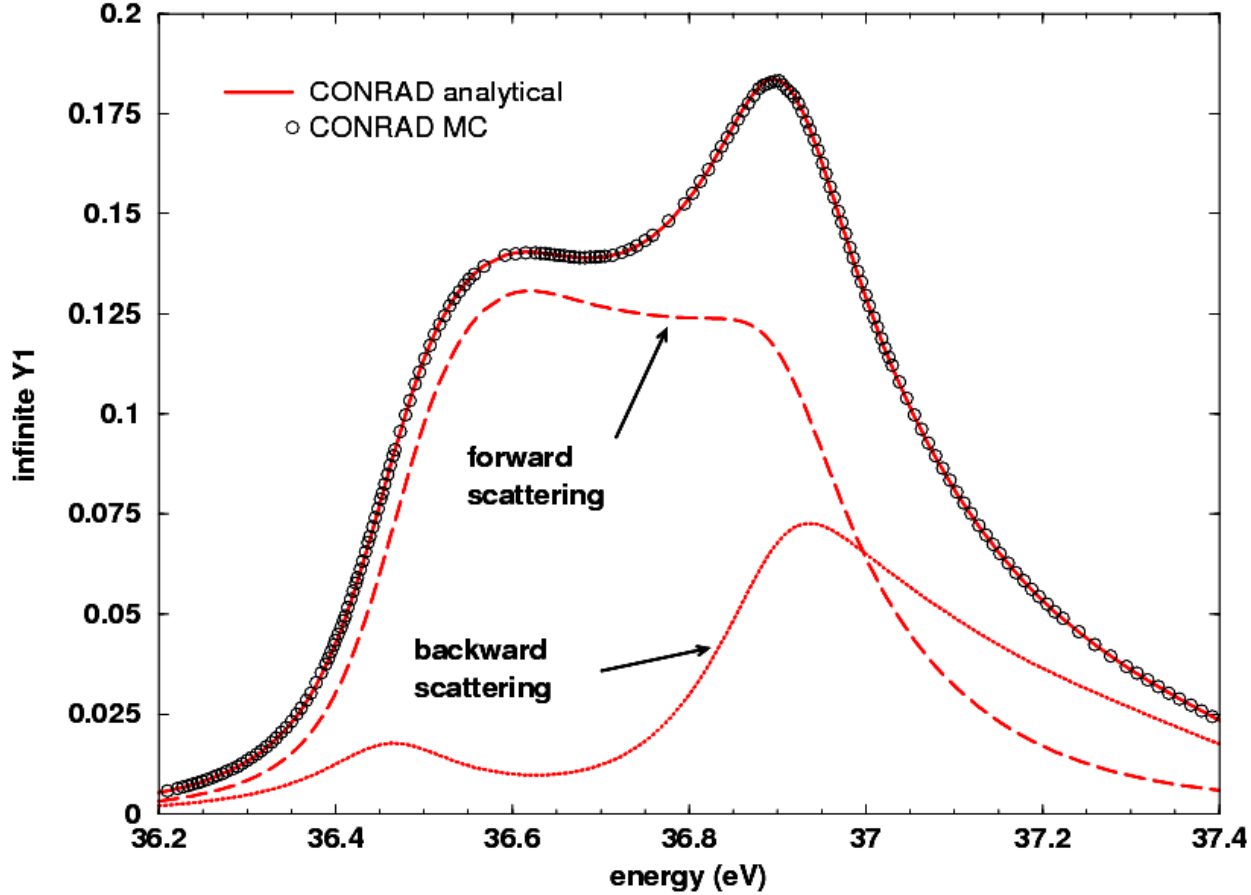


^{238}U single scattering correction (backward and forward contributions)

^{238}U @36.6eV @294K
- Single scattering correction Y_1

$$Y_1 = Y_1^f + Y_1^b$$

backward and forward contributions



^{238}U single scattering correction (backward and forward contributions)

$E'(E=37.4, \mu=+1)=37.4\,\text{eV}$

$\rightarrow \sigma_t \approx 120\,b$: 'low' proba. of interaction

$\rightarrow$ capture after forward scattering $\downarrow$

$E'(E=37.4, \mu=-1)=36.8\,\text{eV}$

$\rightarrow \sigma_t \approx 6800\,b$: 'high' proba. of interaction

$\rightarrow$ capture after backward scattering $\uparrow$

$E'(E=36.8, \mu=+1)=36.8\,\text{eV}$

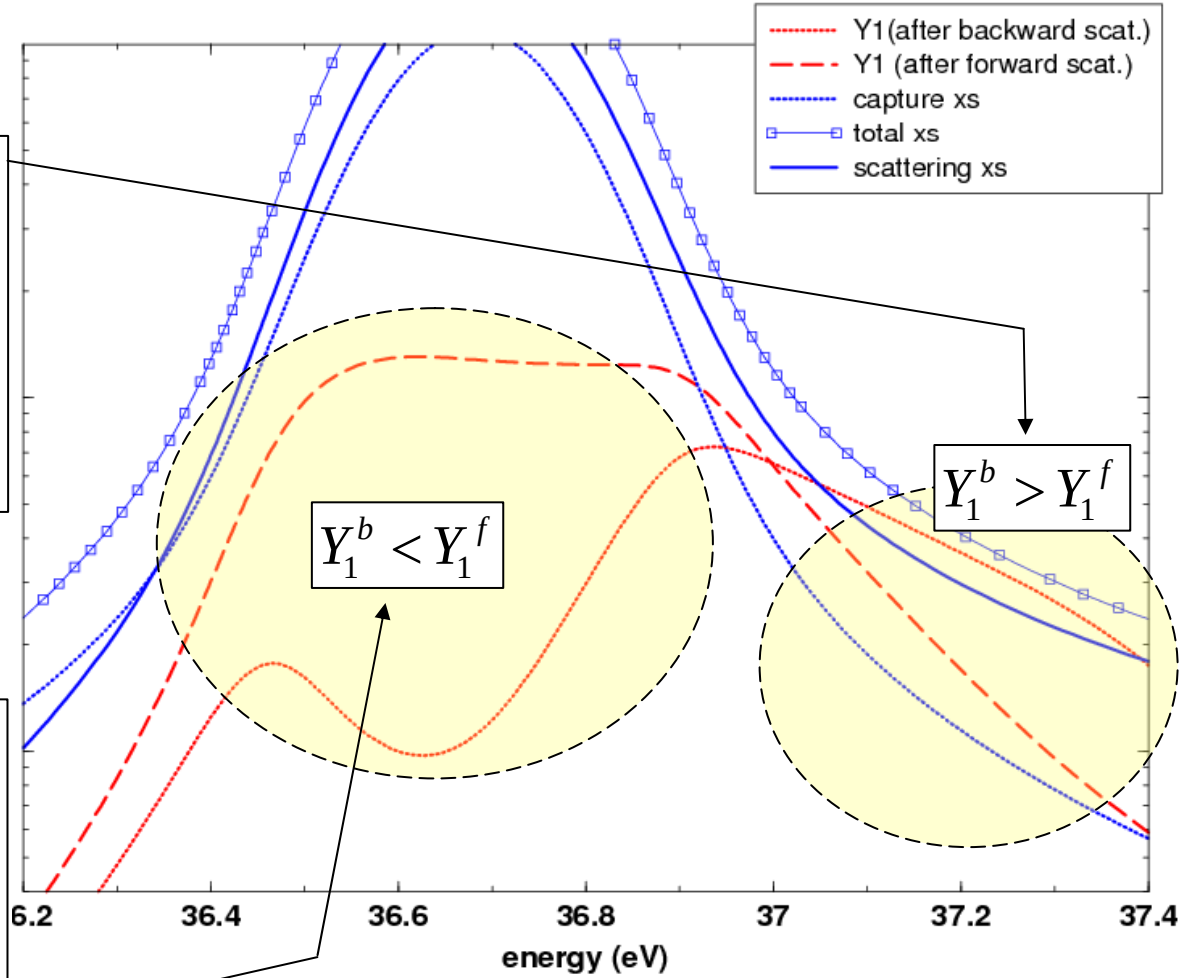
$\rightarrow \sigma_t \approx 6800\,b$: 'high' proba. of interaction

$\rightarrow$ capture after forward scattering $\uparrow$

$E'(E=36.8, \mu=-1)=36.2\,\text{eV}$

$\rightarrow \sigma_t \approx 120\,b$: 'low' proba. of interaction

$\rightarrow$ capture after backward scattering $\downarrow$



^{197}Au multiple scattering corrections (infinite sample) (Sammy ANalytical / Conrad ANalytical / MC schemes)

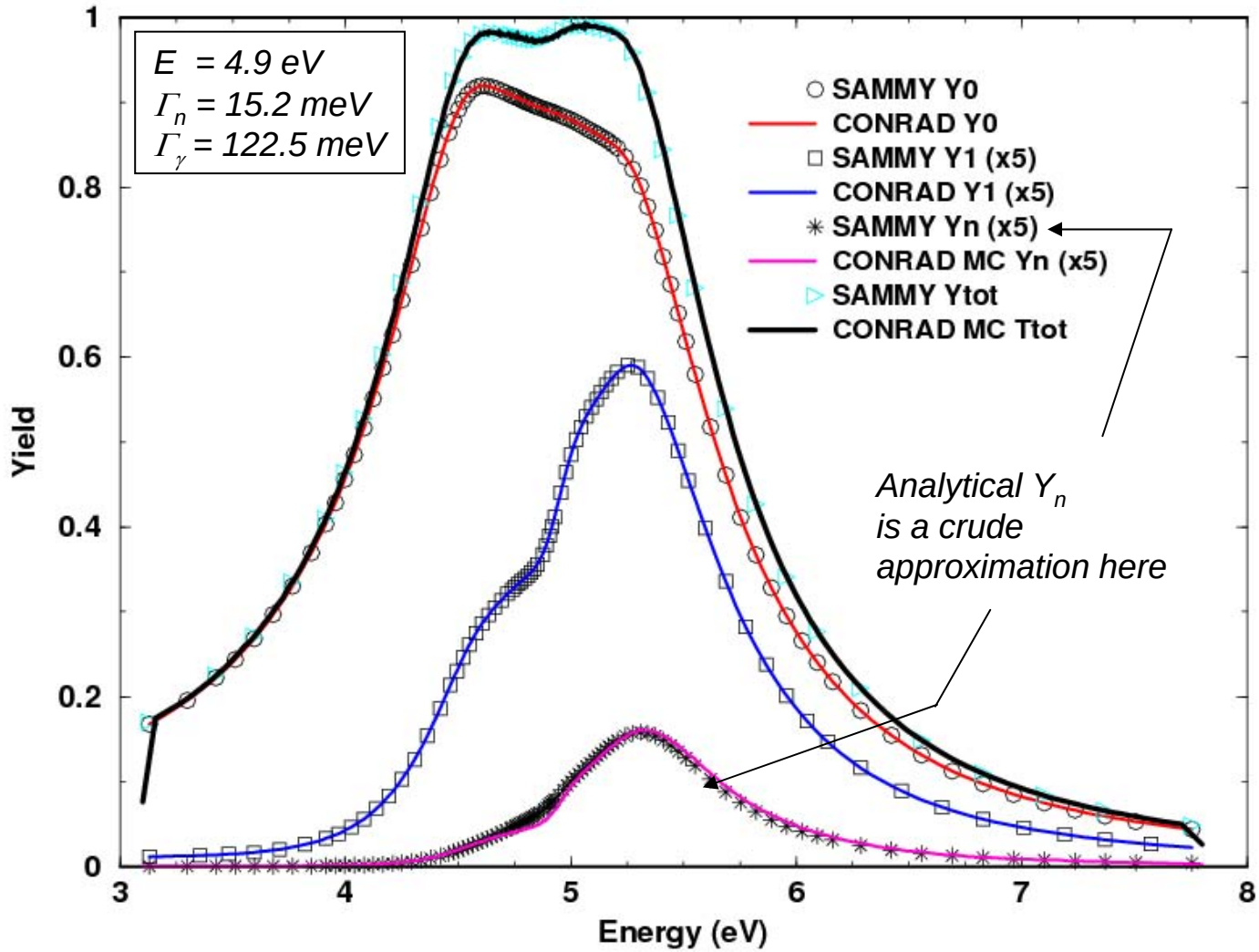
^{197}Au @4.9 eV
- Capture yields
- T = 294 K

"not so usual sample"
n ≈ 2.9 10^{-3} at/b
e = 5. cm !!
Rs = 40. cm …

… to check Y_1^{∞} against SAMMY

Compared with SAMMY:

- ✓ Y_0 CONRAD, AN
- ✓ Y_1^{∞}, CONRAD, AN
- ✓ Y_{tot} CONRAD, MC.

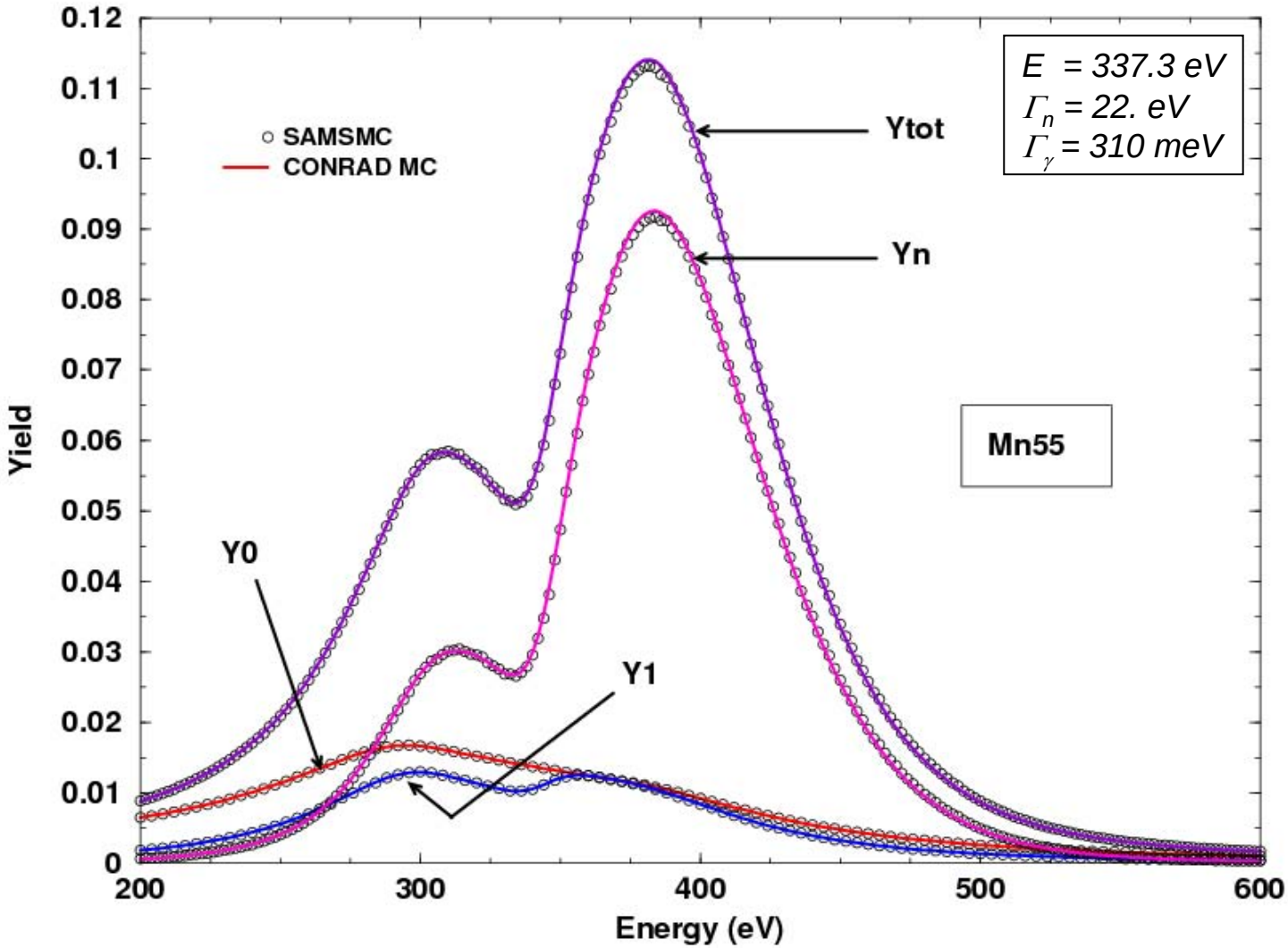


^{55}Mn multiple scattering corrections (SAMSMC / CONRAD MC schemes)

^{55}Mn @ 337.3 eV
- Capture yields
- T = 294 K

Compared with SAMSMC:

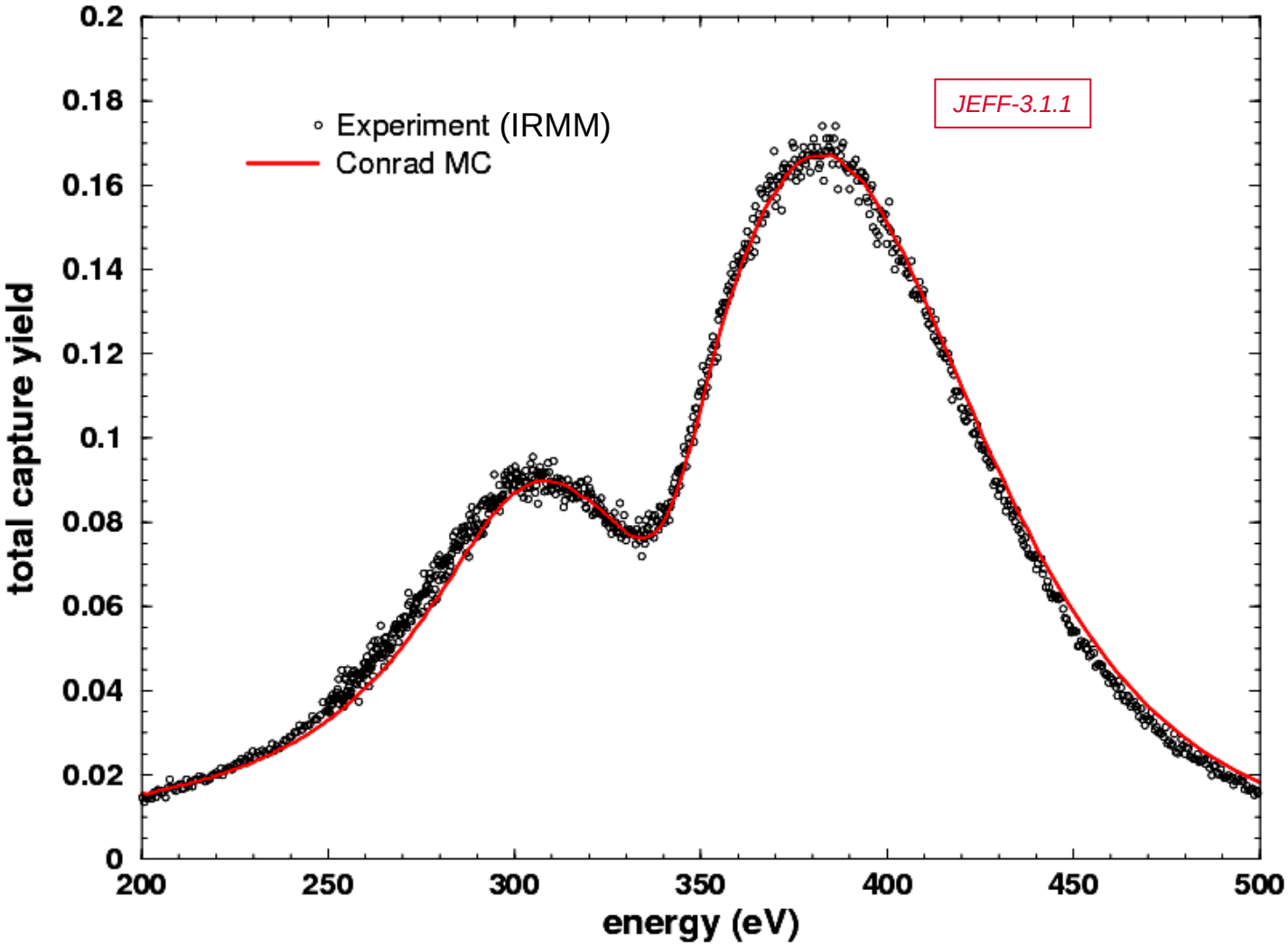
- ✓ Y_0 CONRAD,MC.
- ✓ Y_1 CONRAD,MC.
- ✓ Y_n CONRAD,MC.
- ✓ Y_{tot} CONRAD,MC.



^{55}Mn multiple scattering corrections (CONRAD MC / Experiment)

✓ *not so bad compared with experiment without any resolution function*

(analyt. solution fails (Y_n, zero K Scatt. Ker., ...), See WG36, WPEC may 2011, P. Schillebeeckx)



Conclusion

CONRAD code is validated for the calculation of doppler broadened

- cross sections (RM, MLBW) in the RRR but also at higher energy (not discussed here).
- transmissions
- capture yields : Y_0, Y_1^{∞} (analytical), Y_0, Y_1, Y_n, Y_{tot} (Monte Carlo)

through NJOY, REFIT, SAMMY, SAMSMC codes.

Outlook

Additional comparisons have to be performed, especially :

- test the SVT and DBRC target velocity sampling methods (in preparation),
- find a target candidate as thick as possible to disentangle the different MC simulations/analytical calculations compared with experiment.

Thank you for your attention

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