mage :
mage »
e la zone

DE LA RECHERCHE À L'INDUSTRIE

cea den

Monte Carlo simulation of gamma and fission transfer reactions using extended R-matrix theory: Application to U-237* system

$$Neutron + target \Longrightarrow C^*$$
$$Projectile + surrogate\ target \Longrightarrow C^* + ejectile$$

Olivier Henri Bouland

DER / SPRC / Physics Studies Laboratory
CEA Cadarache (France)

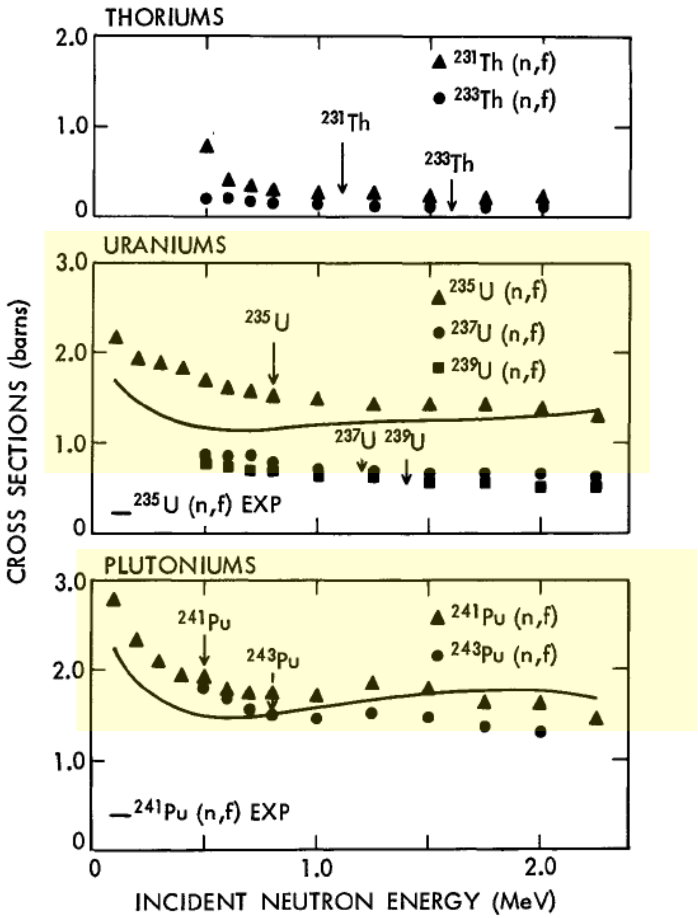
ND2016 Conference, September, the 13th

OUTLINE

- Context and objectives
- Monte Carlo *R*-Matrix simulation as a nice substitute to standard Hauser-Feshbach calculations
- Challenge overview based on 3 factors Hauser-Feshbach equation
- Seeking for agreement with γ and fission surrogate measurements but dropping historical Weisskopf-Ewing frame
- Summary and perspectives

CONTEXT : LONG STANDING DEBATE ON SURROGATE USEFULNESS

Cramer & Britt, NSE 41 (1970) : (t,pf)



Britt & Wilhelmy, NSE 72 (1979): (^{3}He,df), (^{3}He,tf)

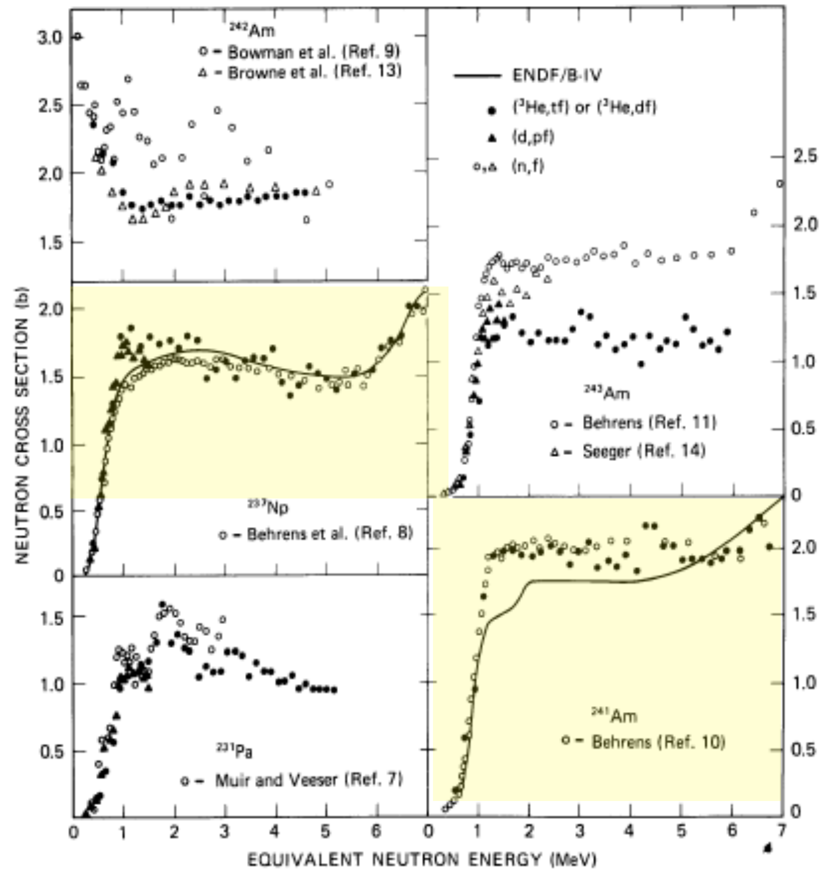


Fig. 2. Simulated neutron cross sections compared to direct neutron measurements and to the ENDF/B-IV cross-section evaluation.

Weisskopf-Ewing (WE) frame

$$\sigma_{n,f}^{WE}(E_n) \approx \sigma_n^{CN}(E_n) \times \mathfrak{P}_{surrogate,f}(E_f)$$

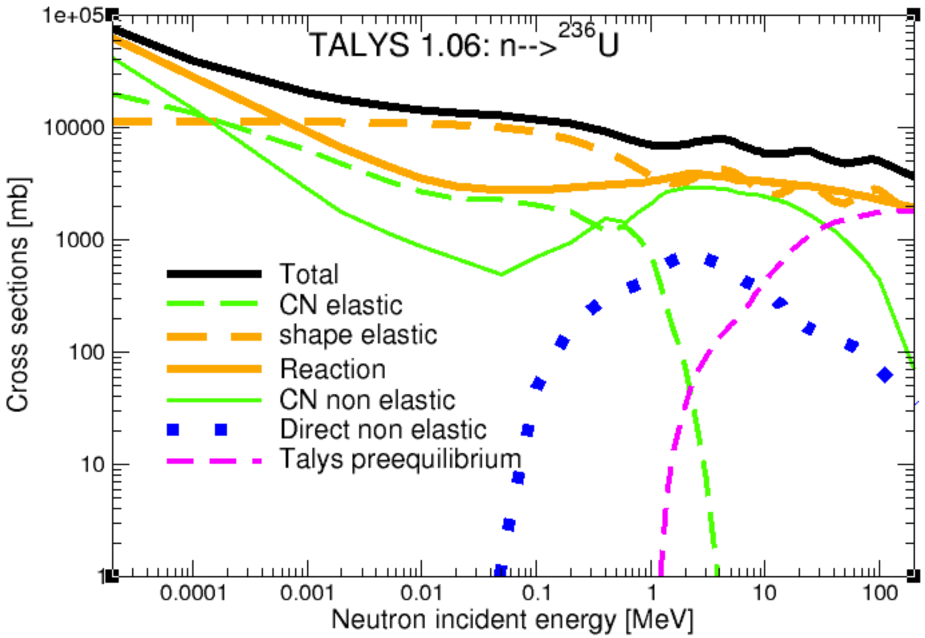
CURRENT CONTEXT AND OBJECTIVES

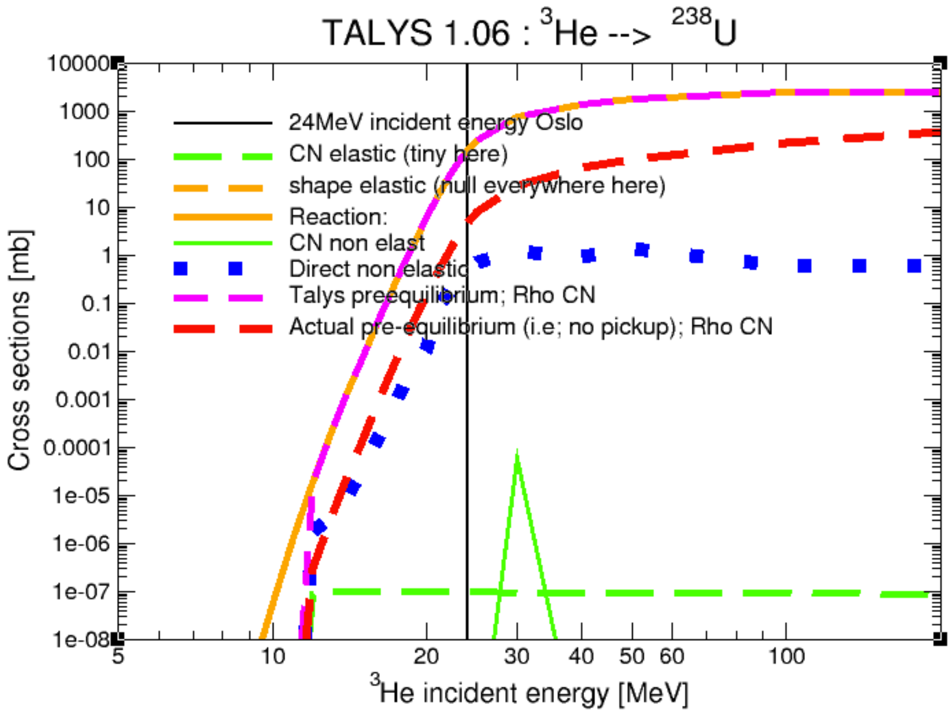
- Can surrogate data actually solve one of our nuclear data evaluator questioning ?
- Nuclear data uncertainty reduction is our top priority since calculation methods accuracy has improved faster than the former
- Neutron cross section evaluation is essentially based on Neutron Physics Spectroscopy (NPS) and surrogate data are a clue to bring more and complementary information during a fit
- Surrogate fission measurements have proved to be helpful for neutron cross section extrapolation (at about 30% accuracy)
  - In a general way, can we afford any type of surrogate data in a neutron cross section fitting procedure as (t,pf), (t,df), (^{3}He,df), (p,p'f), (^{3}He, ^{4}He f), **(^{3}He, ^{4}He gamma)?**

SCHEMATICALLY, WHY TRANSFER DATA STAND OUT FROM NPS ?

Reactor range energy : $\sigma_{n,tot}(E_n) = \sigma_{sh.elas.} + \sigma_{reaction}$
0 – 20 MeV

$$\approx \sigma_{sh.elas.} + \sigma_{Compound\ Nucleus\ (CN)}$$





$$\sigma_{^3He,tot}(E_{inc.} = 24MeV)$$

$$= \sigma_{sh.elas.} + \sigma_{reaction}$$

$$\approx \sigma_{pickup} + \sigma_{actual\ preequilibrium} + \sigma_{direct\ inelastic}$$

EXPANDING EVALUATOR DATABASE IN TERMS OF SURROGATE MEASUREMENTS

- Without WE frame, the corresponding analytical cross section expression is

$$\sigma_{n,c'}(E_n) = \sigma_n^{CN}(E_n) \sum_{J^\pi} \left[\frac{\sigma_n^{CN}(E_n, J, \pi)}{\sigma_n^{CN}(E_n)} \times \mathcal{P}_{c'}^{J^\pi}(E_{c'}) \times W_{n,c'}^{J^\pi} \right]$$

$$\frac{\sigma_n^{CN}(E_n, J, \pi)}{\sigma_n^{CN}(E_n)} = \mathcal{F}_n^{CN}(E_n, J, \pi)$$

- Or in terms of experimental surrogate probability

$$\mathfrak{P}_{surr,c'}(E_x) = \sum_{J^\pi} \left[\mathcal{F}_{surr}^{CN}(E_x, J, \pi) \times \mathcal{P}_{c'}^{J^\pi}(E_{c'}) \times W_{surr,c'}^{J^\pi} \right]$$

- However the AVXSF-LNG (CEA-LANL collaboration) code does not use the analytical route but rather uses Monte Carlo draws of partial widths such that fission sub-barrier effects and width fluctuations are fully mixed together and so

$$\mathfrak{P}_{surr,c'}(E_x) = \sum_{J^\pi} \left[\mathcal{F}_{surr}^{CN}(E_x, J, \pi) \times \mathcal{P}^{\mathcal{MC}}{}_{surr,c'}^{J^\pi}(E_{c'}) \right]$$

SURROGATE DATA SIMULATION CHALLENGE

- Without WE frame and using the Monte Carlo scheme, **we should get the keys for carrying safely** any type of surrogate data in neutron cross section evaluation simultaneously to usual NPS data

- To better understand the challenge we return to the standard 3 factors analytical Hauser-Feshbach formula

$$\sigma_{c,c'}(E_n) = \sigma_c^{CN}(E_n)\left[\sum_{J\pi} \mathcal{F}_c^{CN}(E_c, J, \pi) \times \mathcal{P}_{c'}^{J^\pi}(E_{c'}) \times W_{c,c'}^{J^\pi}\right]$$

Populated CN states are not the same in NPS and surrogate (≠WE frame)

Decay probabilities are J^π sensitive (≠WE hypothesis)

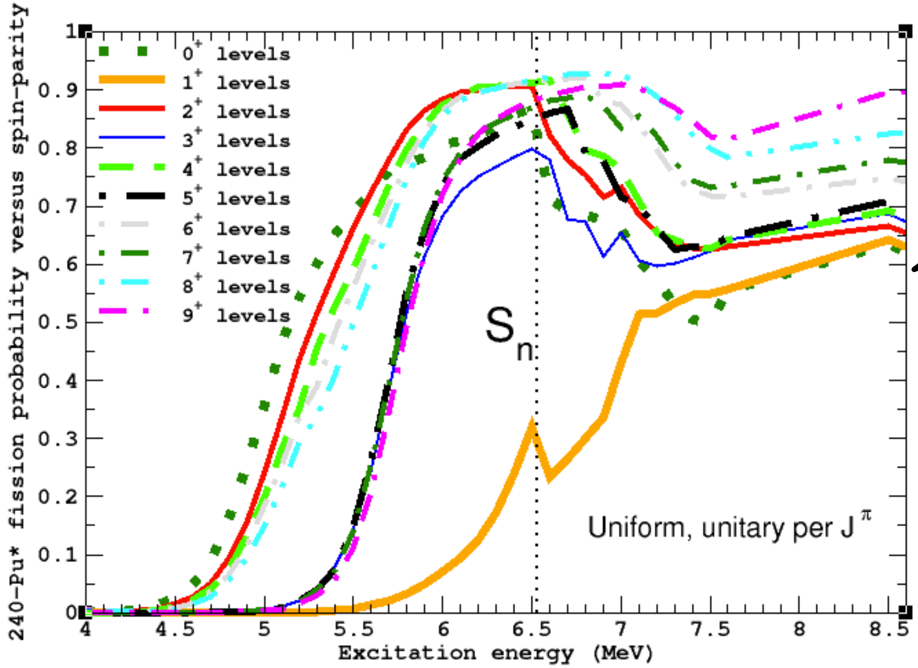
Standard WFCF definition does not apply at low energy (≠ 1 ; WE frame)

DECAY PROBABILITY VS SPIN PARITY

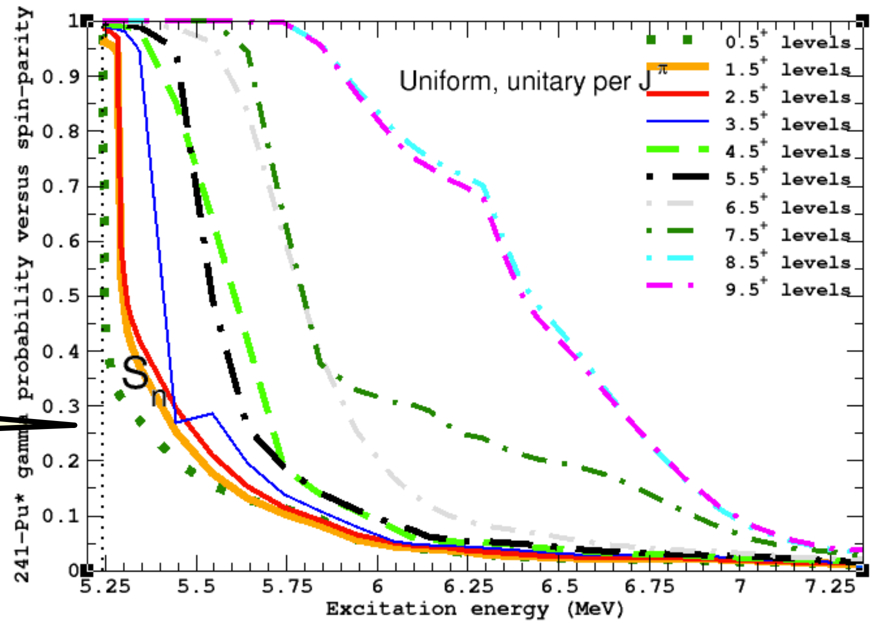
$$\sigma_{c,c'}(E_n) = \sigma_c^{CN}(E_n)\left[\sum_{J^\pi}\mathcal{F}_c^{CN}(E_c,J,\pi)\times\mathcal{P}_{c'}^{J^\pi}(E_{c'})\times W_{c,c'}^{J^\pi}\right]$$

Decay probabilities are J^π sensitive (≠WE frame)

Fissile nucleus : $^{240}Pu^*$ fission decay

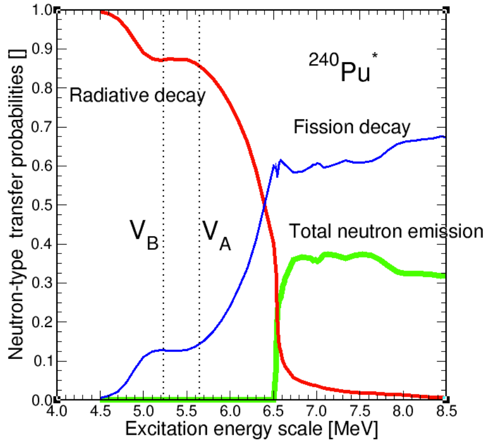


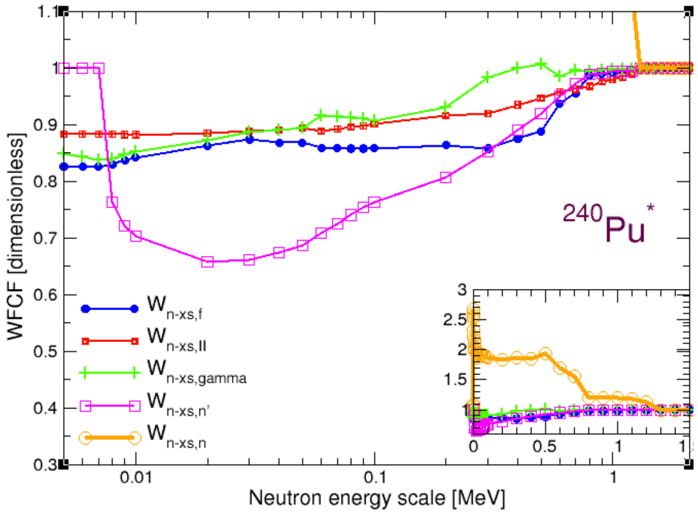
Fertile nucleus : $^{241}Pu^*$ radiative decay

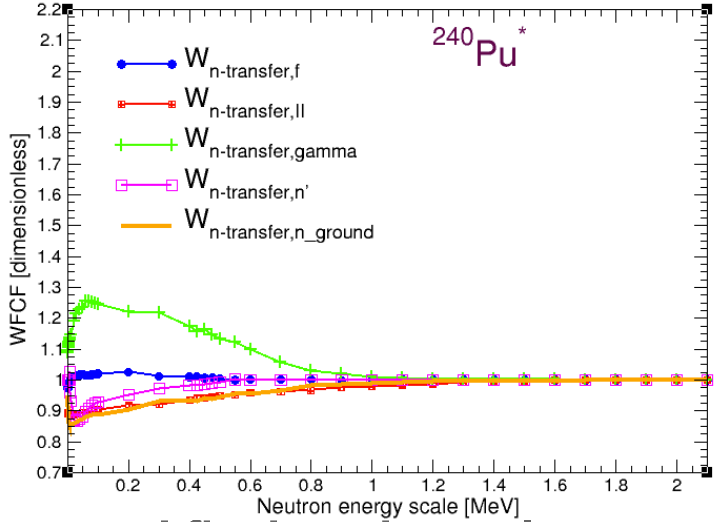


WE hypothesis validity is unlikely at low excitation energy [U* < 8 MeV]

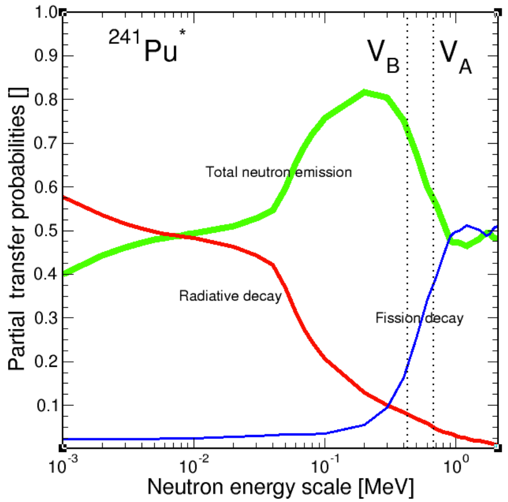
NPS WIDTH FLUCTUATION CORRECTION FACTOR (WFCF) VS. SURROGATE WFCF

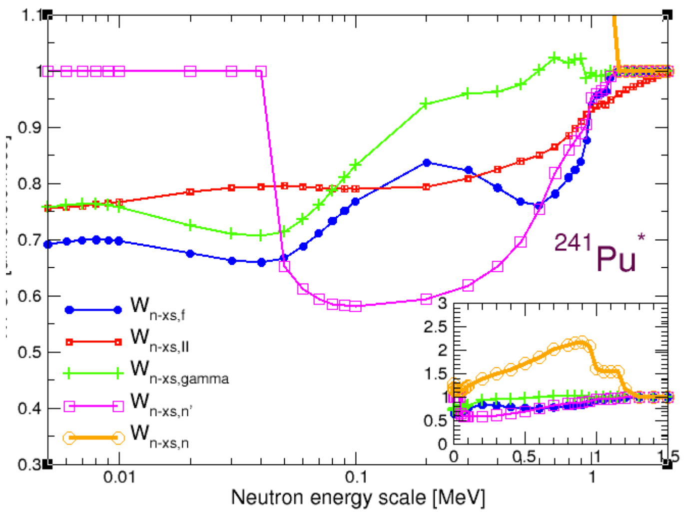


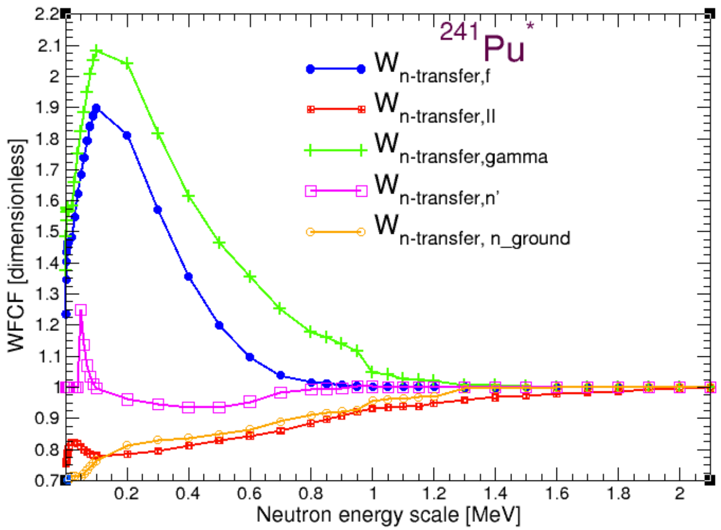




Standard WFCF behaviour does not apply anymore : γ- and fission channels now endorse the role of the enhanced channel (> +100% in case of ^{241}Pu, Sn<En<Sn+1MeV)





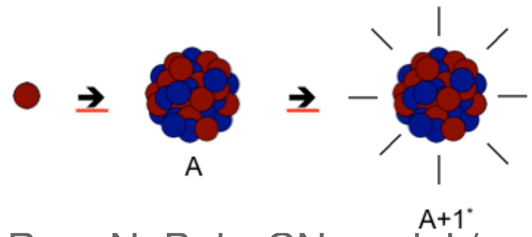


SIMPLICATION EXPECTED IN SURROGATE WFCF FORMULATION

$$\sigma_{c,c'}(E_n) = \sigma_c^{CN}(E_n)\left[\sum_{J\pi} \mathcal{F}_c^{CN}(E_c, J, \pi) \times \mathcal{P}_{c'}^{J^\pi}(E_{c'}) \times W_{c,c'}^{J^\pi}\right]$$

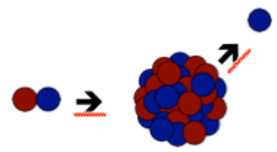
- Standard in/outgoing channel WFCF that satisfies to NPS is

$$\left\langle \frac{\Gamma_c^{J^\pi(ls)}\Gamma_{c'}^{J^\pi(l's')}}{\sum_{c''}\Gamma_{c''}^{J^\pi(l''s'')}} \right\rangle = \frac{\left\langle \Gamma_c^{J^\pi(ls)} \right\rangle \left\langle \Gamma_{c'}^{J^\pi(l's')} \right\rangle}{\left\langle \sum_{c'' \in [in+out]} \Gamma_{c''}^{J^\pi(l''s'')} \right\rangle} \times W_{c,c'}$$



Pure N. Bohr CN model / strong coupling

- Since surrogate reactions are especially sensitive to direct transfer reaction features, little correlation is expected between in and out-going channel widths


Single-particle model / Weak coupling

- More likely in (t,p) stripping reaction cases where a di-neutron is transferred on a s.p. orbital of the target A; then

$$\left\langle \frac{\Gamma_{c'}^{J^\pi(l's')}}{\sum_{c''}\Gamma_{c''}^{J^\pi(l''s'')}} \right\rangle = \frac{\left\langle \Gamma_{c'}^{J^\pi(l's')} \right\rangle}{\left\langle \sum_{c'' \in [out]} \Gamma_{c''}^{J^\pi(l''s'')} \right\rangle} \times W_{surr,c'}$$

CN SPIN-PARITY POPULATION CALCULATION REMAINS THE GENUINE CHALLENGE

$$\mathcal{F}_n^{CN}(E_n, J, \pi) = \left[\frac{\sigma_n^{CN}(E_n, J, \pi)}{\sigma_n^{CN}(E_n)}\right]; \mathcal{AVXSF} \text{ approach or}$$

$$\mathcal{F}_{surr}^{CN}(E_{surr}, J, \pi) = \rho(J, \pi, U_x) \sum_{j=|J-I_0|}^{J+I_0} \sum_{l=|j-i|}^{j+i} \frac{P_l \times \delta(\pi_J, \pi_i \pi_{I_0}(-1)^l)}{\sum_{j=|J-I_0|}^{J+I_0} \sum_{j=|j-i|}^{j+i} 1};$$

and P_l from Back et al.; PRC 9,5 (1974)

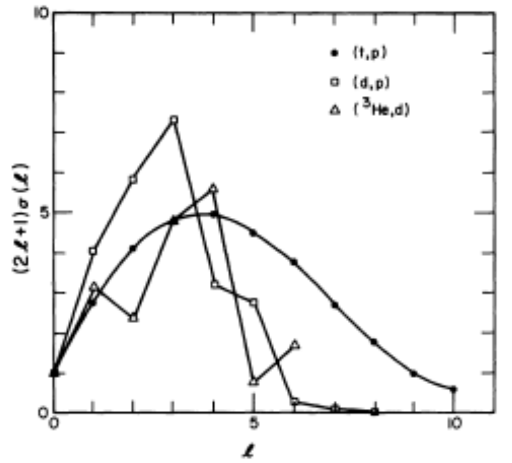
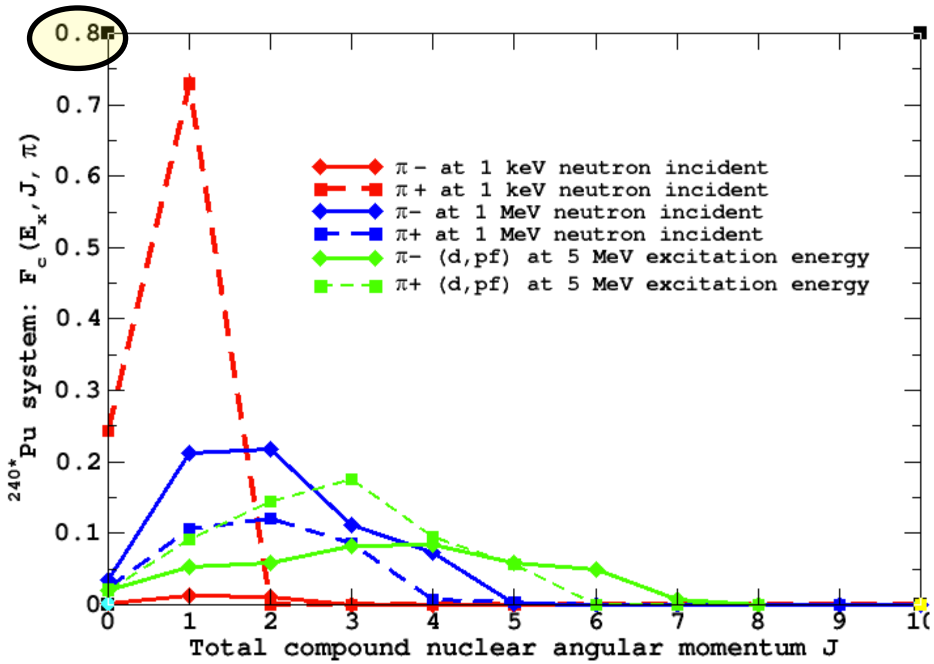
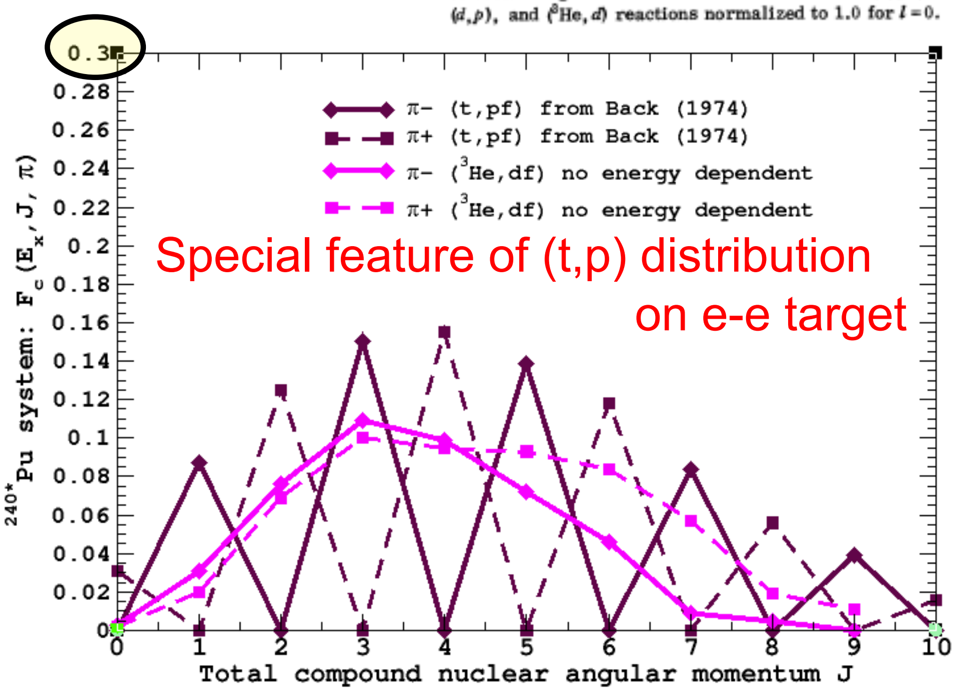


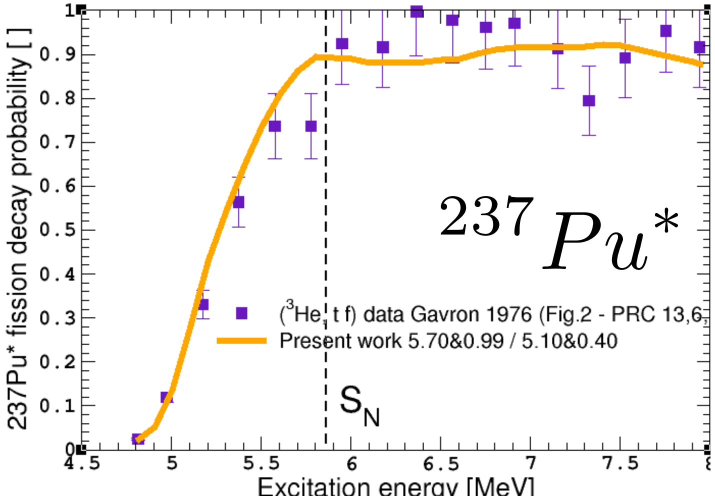
FIG. 7. Differential cross sections at 90° as a function of orbital angular momentum transfer l for the (t,p), (d,p), and $(^3He, d)$ reactions normalized to 1.0 for $l=0$.

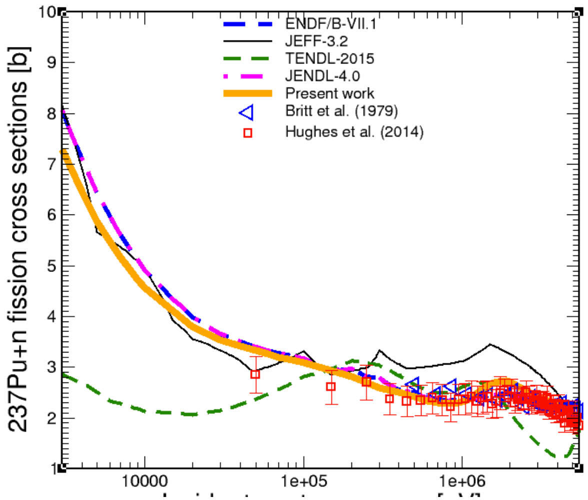


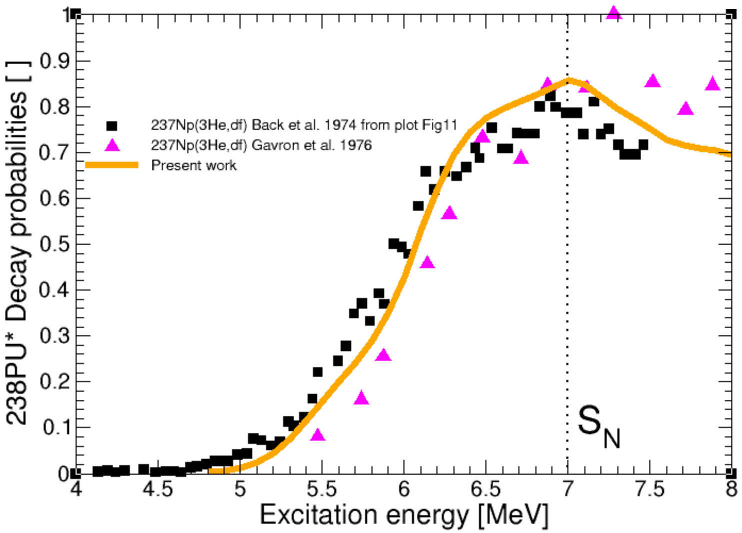


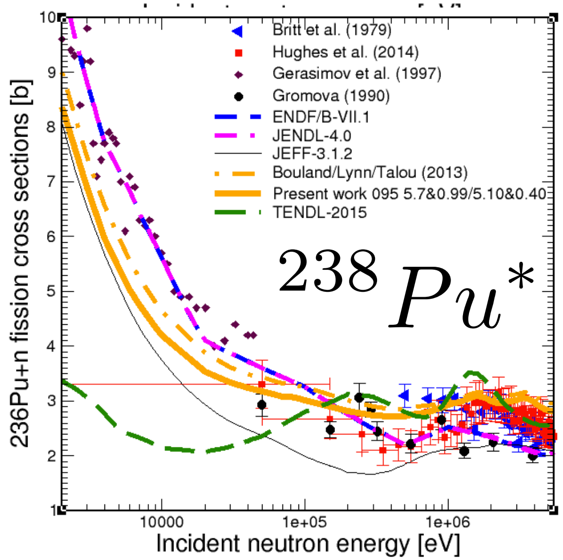
DEMONSTRATED PERFORMANCES OUTSIDE W.E. FRAME

- Iterating on common parameters of neutron reaction cross sections and a set of fission surrogate measurements for a range of Pu isotopes, proof was made of the validity of our method (*PRC 88 054612 (2013) and 2016 paper to be submitted*)







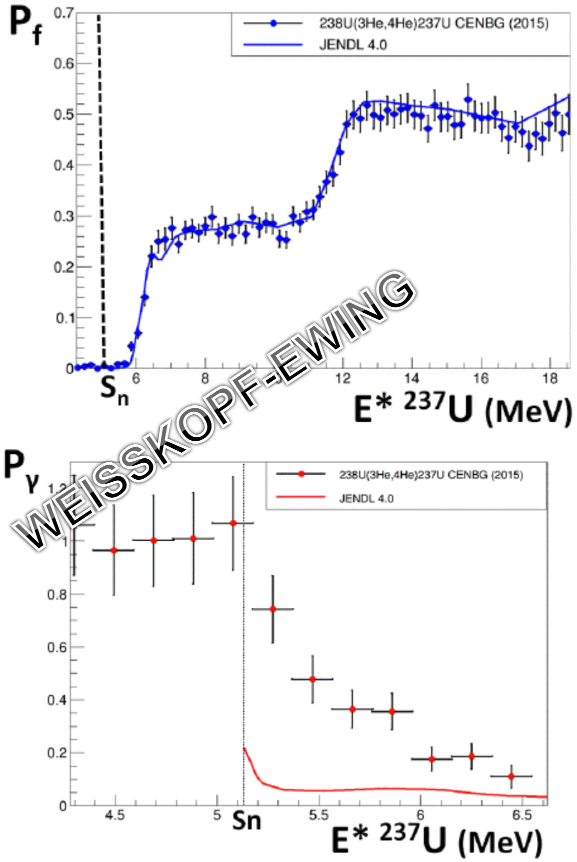


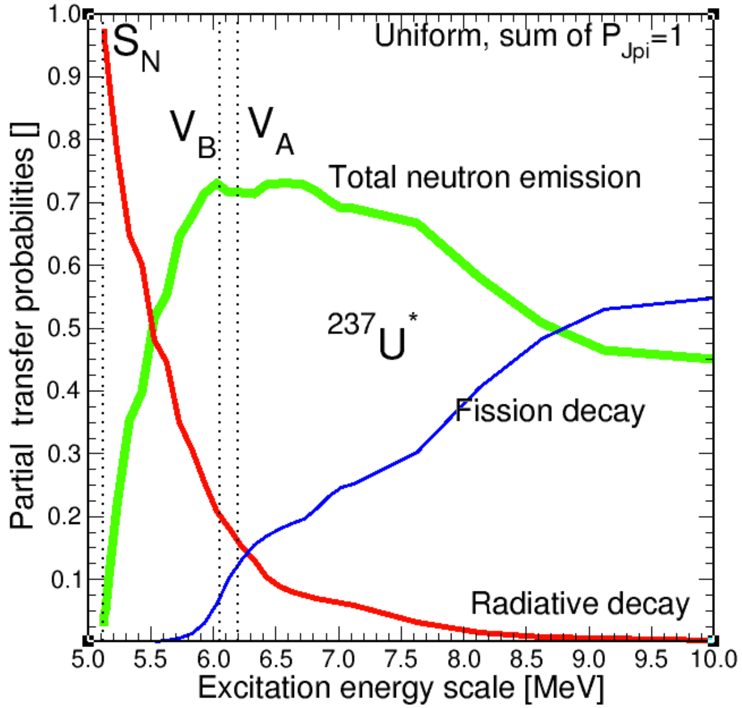
Fission surrogate measurements are obviously of great help for fission threshold assessments on fissile isotopes

A MORE DIFFICULT CHALLENGE: γ-SURROGATE FISSION PROBABILITIES

- Agreement in terms of fission surrogate probabilities with measurements was expected since already 'working' within the W.E frame **and thus the true challenge is to make it happens with γ-surrogate probabilities too …**

- Recent surrogate probability measurements both in γ and fission channels give the opportunity to test (non-exhaustively) that Monte Carlo *R*-matrix-based simulation

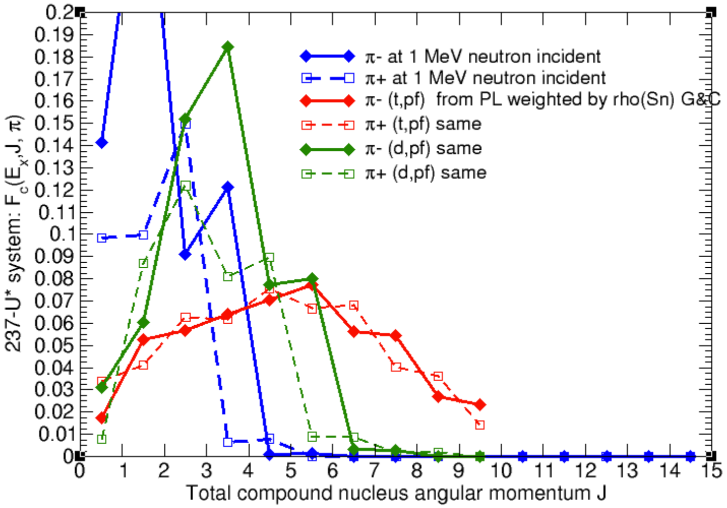


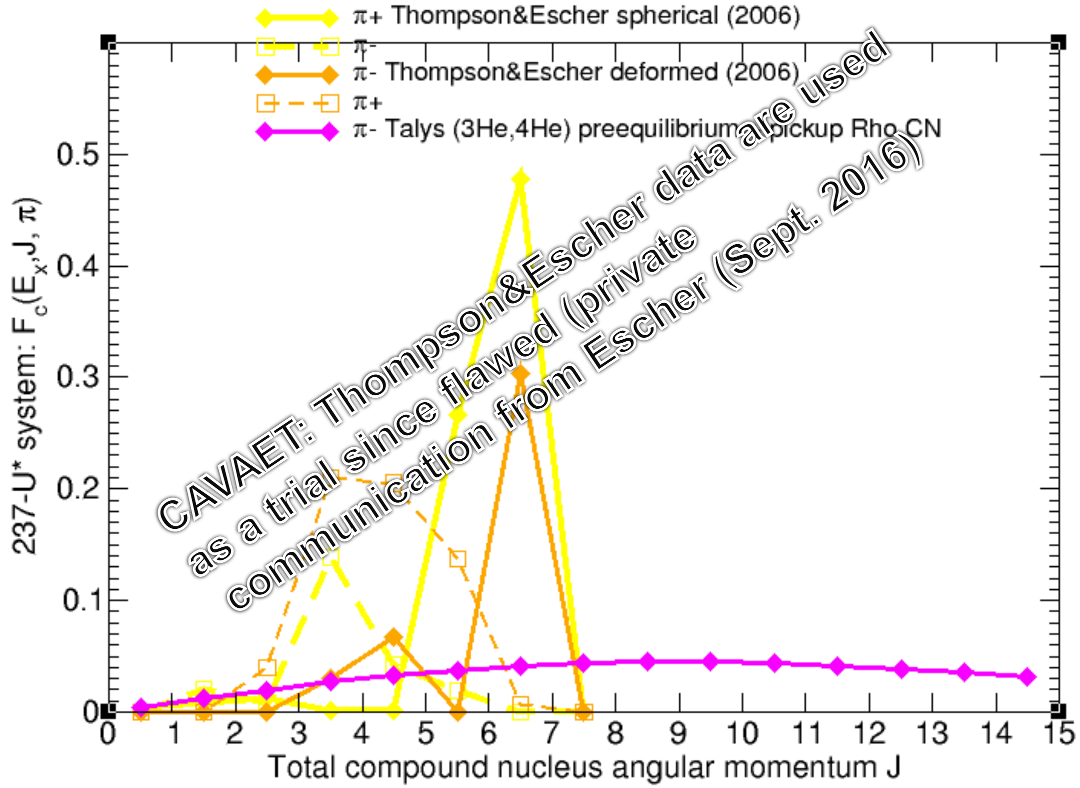


- **$^{238}U(^{3}He,^{4}He)^{237}U^{*}$ pickup reaction at 24 MeV (Oslo)**
  Q.Ducasse PhD thesis, CENBG (2015).
  B. Jurado – ND2016 – I366 paper

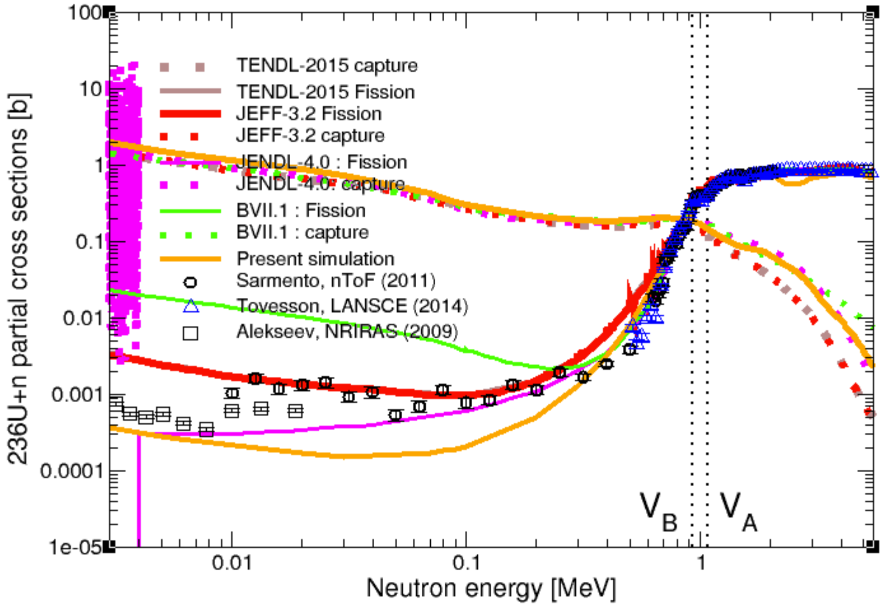
ASSUMED PRIOR TO DECAY SPIN-PARITY POPULATION

Reactions	Exp. data	Population fraction
$^{238}\mathrm{U}(^3He,^4Hef)\mathrm{U}^{237*}$	Jurado, Ducasse et al. (2015)	Thompson and Escher (2006-TR-225984)
$^{238}\mathrm{U}(^3He,^4He\gamma)\mathrm{U}^{237*}$		Talys 1.06 calculations
$^{235}\mathrm{U}(t,pf)\mathrm{U}^{237*}$	Britt and Cramer (1970)	P_l from Back et al.; PRC 9,5 (1974)
$^{236}\mathrm{U}(d,pf)\mathrm{U}^{237*}$	Britt and Cramer (1970)	P_l from Back et al.; PRC 9,5 (1974)





BEST THOMPSON-FEEDED AVXSF-LNG SIMULATIONS



$\sigma^{236U}_{(n,f)}$

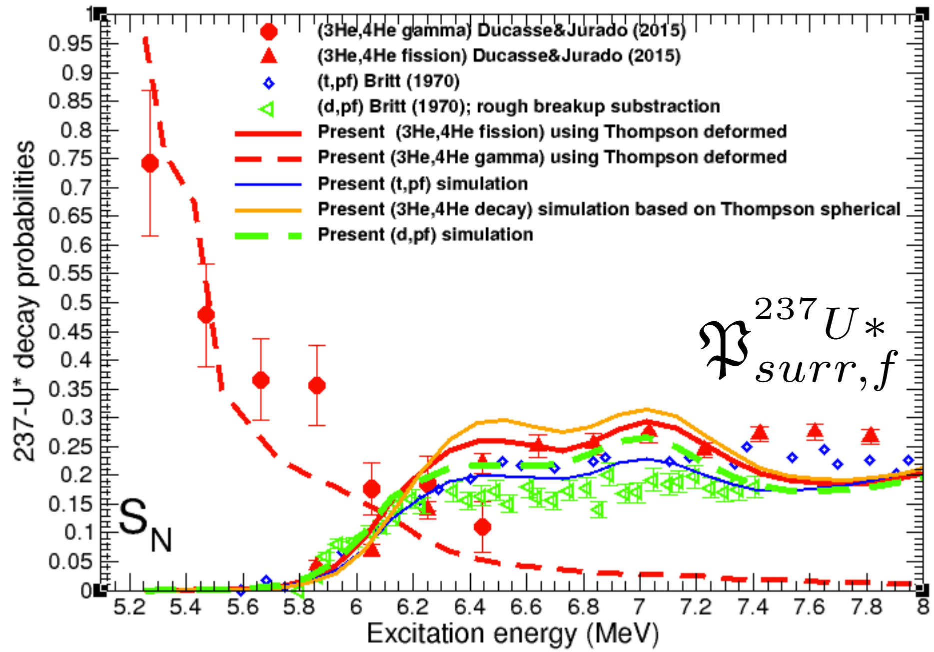
$\sigma^{236U}_{(n,\gamma)}$

✧ The simulated fission subthreshold cross section is lower on magnitude than the measurements,

✧ Simulated capture is satisfactory and easy to reproduce.

✧ Promising results for the simulated gamma probability are obtained without any correction of the population distribution from Thompson and Escher (deformed nucleus).

$\mathfrak{P}^{237U*}_{surr,\gamma}$



$\mathfrak{P}^{237U*}_{surr,f}$

SUMMARY AND PERSPECTIVES

- Promising (outside Weisskopf-Ewing frame) results were obtained for simultaneous cross section and surrogate probability simulations both in fission (Pu isotope family) and γ channels ($^{237}U^*$),

  - AVXSF to AVXSF-LNG integrated new structure

- Several TALYS options for $^{237}U^*$ prior to decay population fraction calculations were tested but results were not conclusive yet (some feedback however)

- Forthcoming integration of the spirit of this method is expected in a near future in the *CONRAD* code at CEA Cadarache across a necessary change of frame (NPS to CN) [new PhD work]

- Larger γ-decay surrogate probability database is welcome for actinides. In particular, we are eagerly waiting any new data related to the Pu family !

  - Special acknowledgments to Back et al. for early DWBA calculations and to Thompson & Escher for recent pickup results on deformed ^{237}U nucleus (caveat: those data happened to be flawed)