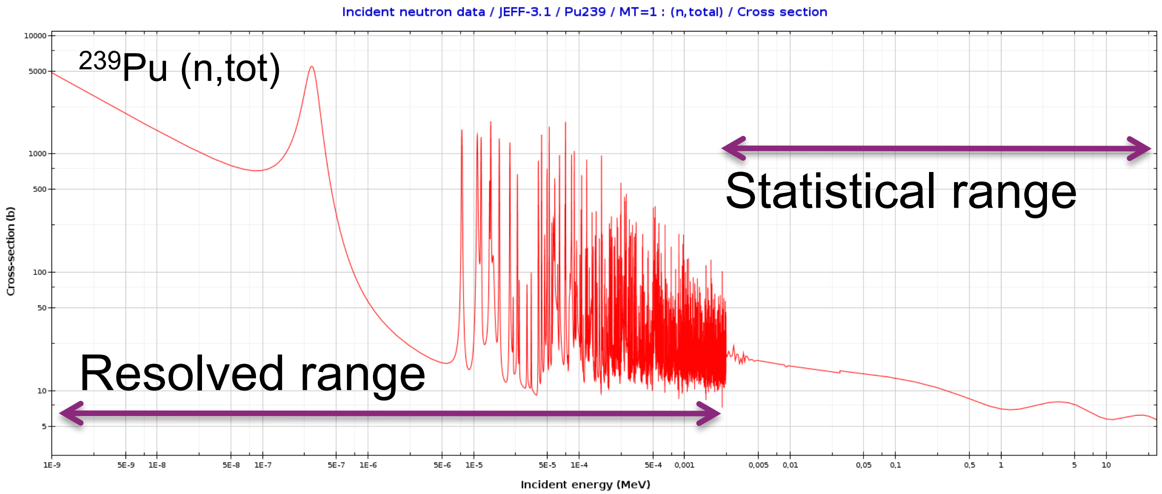
DE LA RECHERCHE À L'INDUSTRIE

TOWARDS IMPROVED METHODS FOR FISSION CROSS SECTION EVALUATION IN STATISTICAL ENERGY RANGE



DER/SPRC/LEPh

FIESTA-2014
Santa Fe

SEPTEMBER 10 2014

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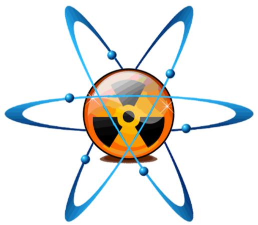
OUTLINE

State of the art of evaluated fission cross sections and evaluation models

Undergoing developments in the Conrad* code and numerical validation

Physics underneath



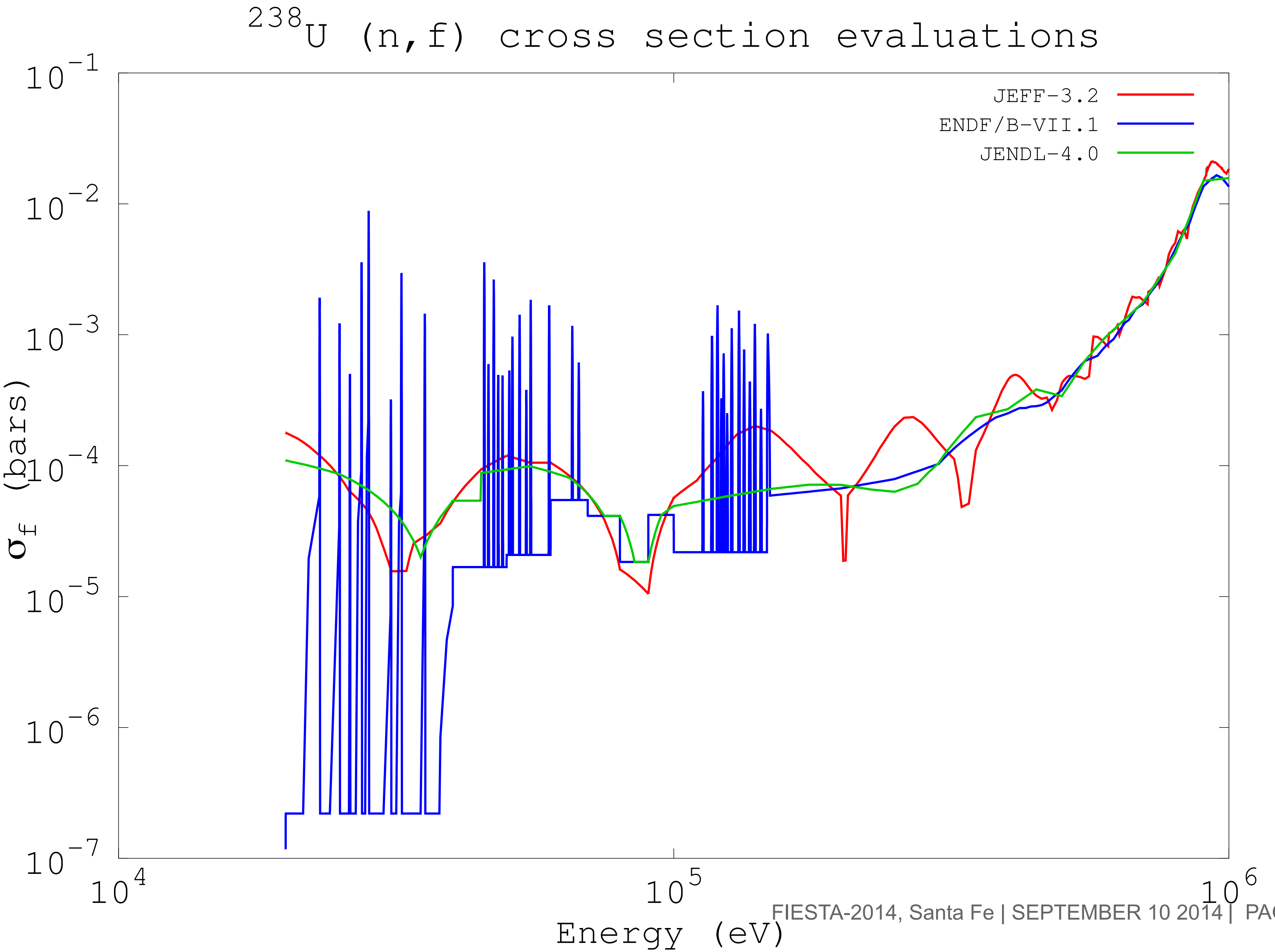
Conclusion and outlook

*C. De Saint Jean et al., International Conference on Nuclear Data for Science and Technology 2007

STATE OF THE ART OF EVALUATED FISSION CROSS SECTIONS AND EVALUATION MODELS

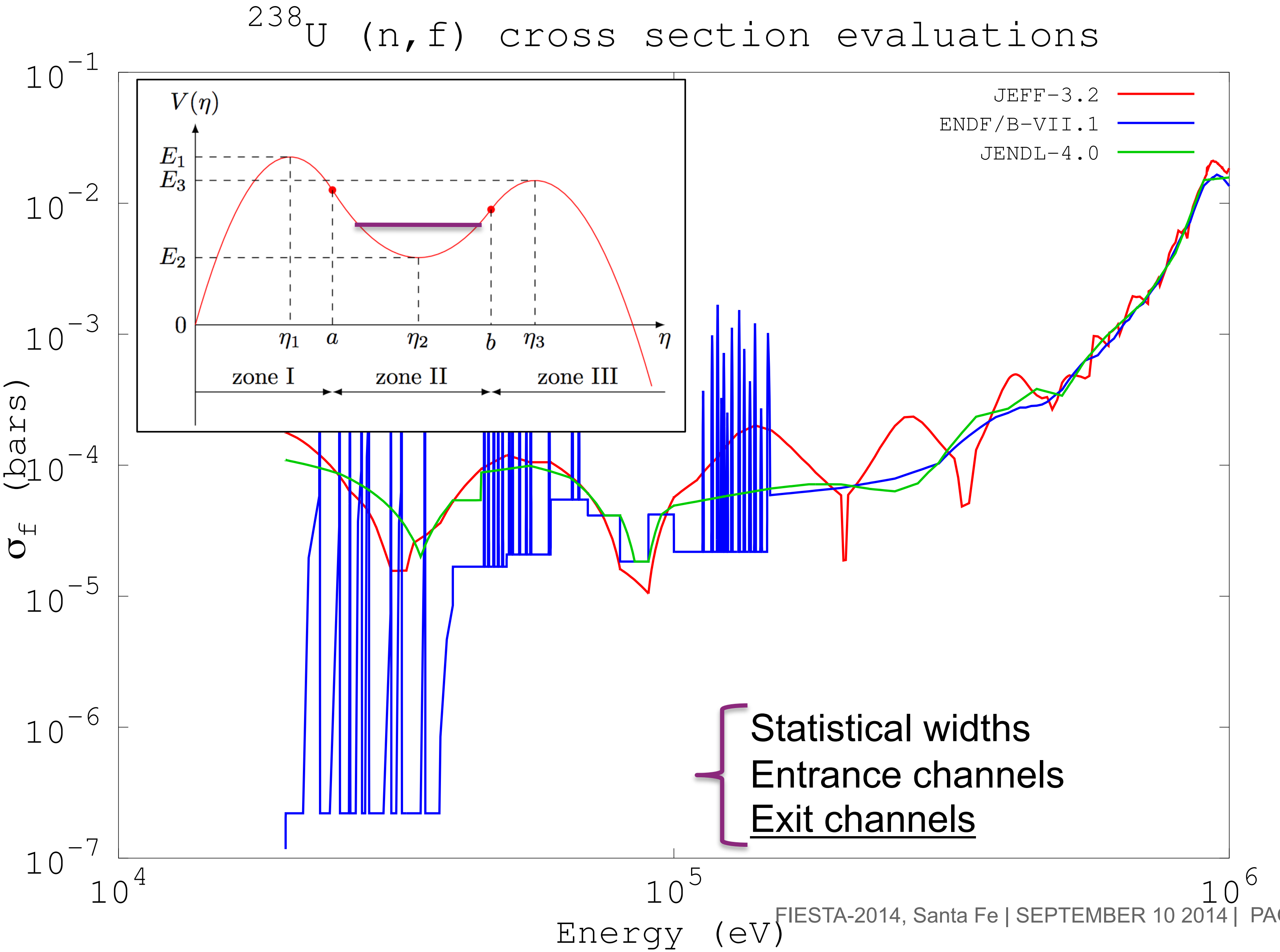
WHAT ARE WE TALKING ABOUT?

state of the art



CURRENT CROSS SECTIONS SHOW FLUCTUATIONS

state of the art

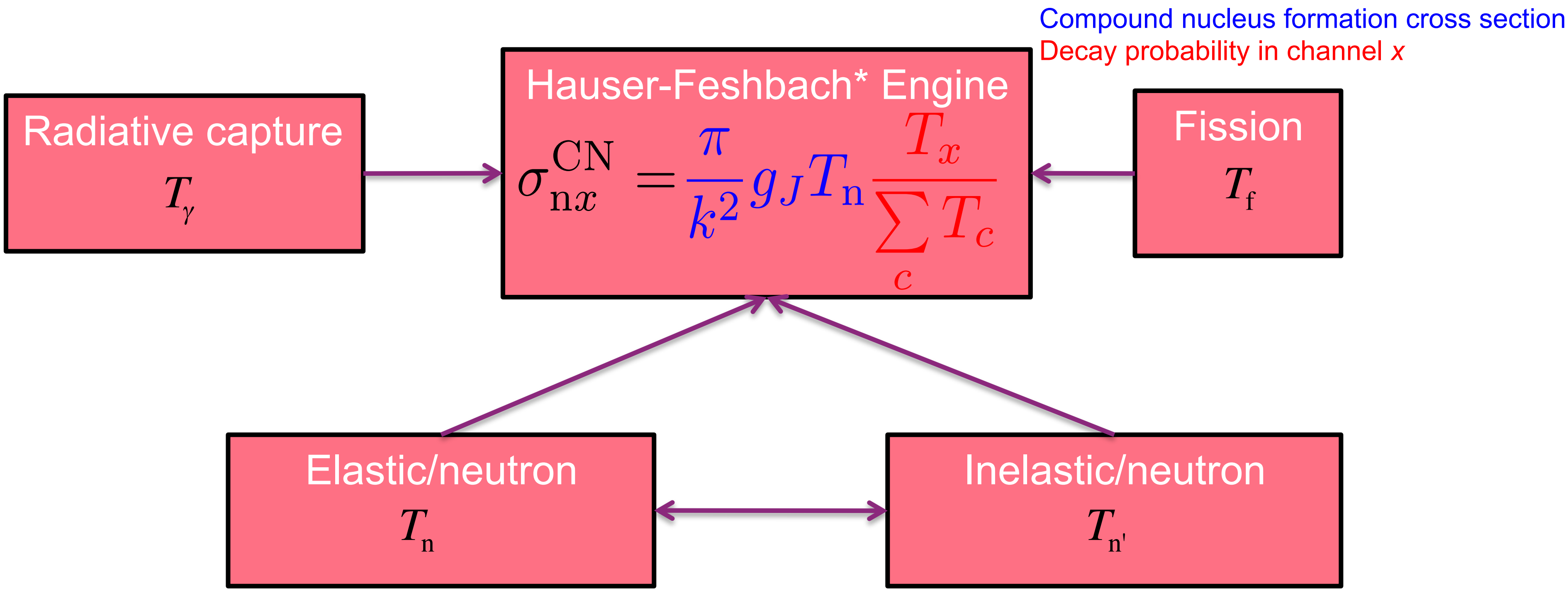


- Statistical widths
- Entrance channels
- Exit channels

MODEL FOR STATISTICAL ENERGY RANGE (NO WIDTH FLUCTUATION FACTOR)

$$\sigma_{nx} = \sigma_{nx}^{dir} + \sigma_{nx}^{CN}$$

Each type of reaction is treated by a sub-model



The formalism intrinsically correlates the calculated cross sections

* W. Hauser, H. Feshbach, Phys. Rev. 87, 366 (1952)

STANDARD MODELS FOR FISSION TRANSMISSION COEFFICIENT

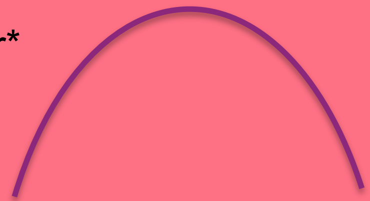
state of the art

Fission T_f

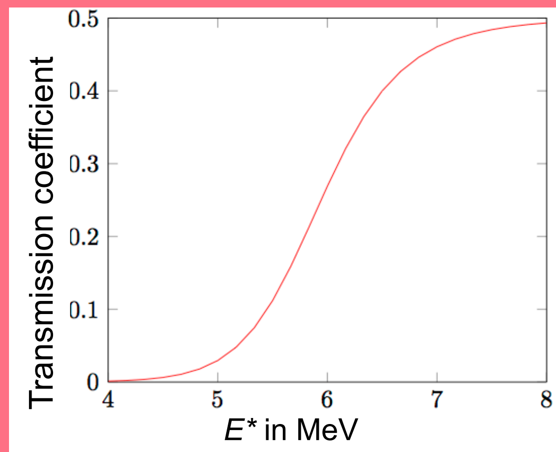
Fission process modeled as particle passing through parabolic potential barrier

$$T_f = \frac{1}{1 + \exp\left(-2\pi \frac{E^* - V}{\hbar\omega}\right)}$$

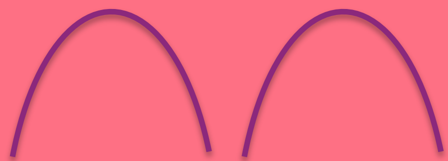
Hill-Wheeler* analytical solution



Or passing through two barriers with statistical equilibrium



$$T_{\mathrm{eff}} = \frac{T_A T_B}{T_A + T_B}$$



Possibility of local enhancements

$$T_{\mathrm{eff}} = \frac{T_A T_B}{T_A + T_B} F_{AB}(E)$$

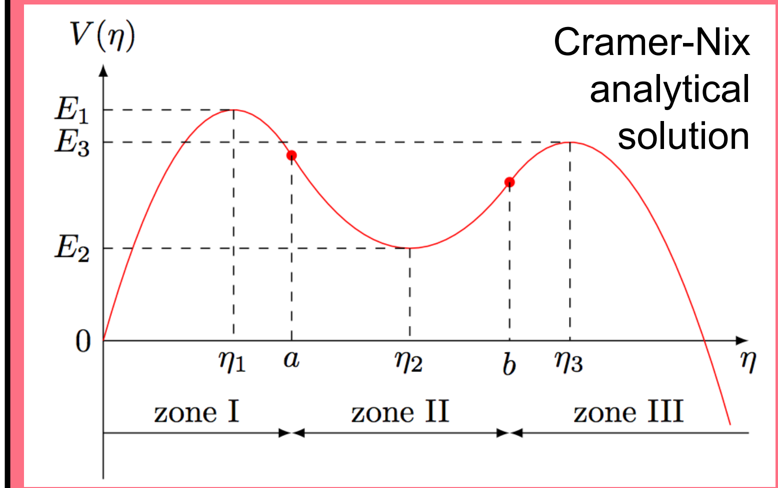
Intermediate state

$$F_{AB}(E) = 1 + \sum_{\text{class } II} \left[\frac{4}{T_A + T_B} + \left(\frac{E - E_{II}}{\Gamma_{II}/2}\right)^2 \left(1 - \frac{4}{T_A + T_B}\right) - 1 \right] \delta_{E \in [E_{II} \pm \Gamma_{II}/2]}$$

*D. L. Hill and J. A. Wheeler, Phys. Rev. 89, 1102 (1953)

IMPROVED TRANSMISSION COEFFICIENT REQUIRED

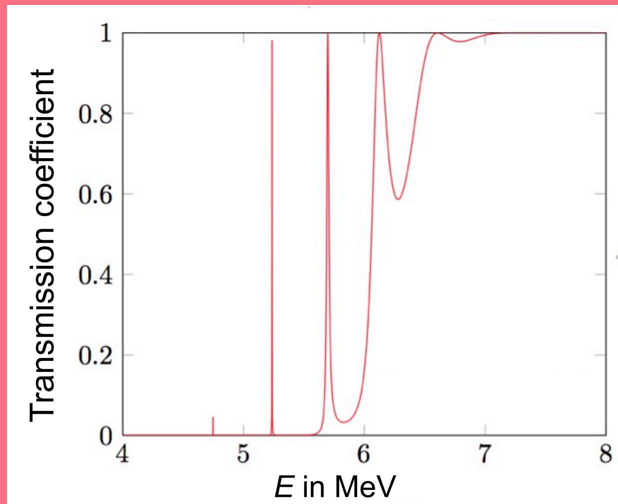
Fission T_f



Cramer-Nix potential*

$$V(\eta) = \begin{cases} E_1 - \frac{1}{2}\mu\omega_1^2(\eta-\eta_1)^2, & \eta \le a \\ E_2 + \frac{1}{2}\mu\omega_2^2(\eta-\eta_2)^2, & a \le \eta \le b \\ E_3 - \frac{1}{2}\mu\omega_3^2(\eta-\eta_3)^2, & \eta \ge b \end{cases}$$

$$T_\mathrm{f} = \sqrt{\frac{\omega_3}{\omega_1}}\left|\frac{T}{A}\right|^2$$



$$\frac{T}{A} = \frac{v'u'2i\sqrt{2/\pi}}{\det M}$$

$$u = \sqrt{2\mu\omega_1/\hbar}(\eta-\eta_1)$$
$$v = \sqrt{2\mu\omega_2/\hbar}(\eta-\eta_2)$$
$$w = \sqrt{2\mu\omega_3/\hbar}(\eta-\eta_3)$$

$$\alpha_1 = (E_1-E)/\hbar\omega_1, \quad \alpha_2 = (E_2-E)/\hbar\omega_2, \quad \alpha_3 = (E_3-E)/\hbar\omega_3$$

$$M = \begin{bmatrix} E_a(\alpha_1,-u) & -V_a(\alpha_2,v) & -U_a(\alpha_2,v) & 0 \\ -u'E_a^{(-u)}(\alpha_1,-u) & -v'V_a^{(v)}(\alpha_2,v) & -v'U_a^{(v)}(\alpha_2,v) & 0 \\ 0 & V_b(\alpha_2,v) & U_b(\alpha_2,v) & -E_b(\alpha_3,w) \\ 0 & v'V_b^{(v)}(\alpha_2,v) & v'U_b^{(v)}(\alpha_2,v) & -w'E_b^{(w)}(\alpha_3,w) \end{bmatrix}$$

* J. D. Cramer and J. R. Nix, Phys. Rev. C 2, 1048 (1970)

UNDERGOING DEVELOPMENTS IN THE Conrad CODE AND NUMERICAL VALIDATION

EVALUATION = MODEL + EXPERIMENTS + ADJUSTMENTS + COVARIANCE DATA

Development and validation

The CEA/Cadarache code Conrad was created for such evaluation

->originally developed for the resolved resonances range

- (Reich-Moore & multi-level Breit-Wigner)

->few statistical range capabilities

- Average R-matrix only

->New developments using the Talys* code as guideline

Hauser-Feshbach

$$\sigma_{\mathrm{n}x}^{\mathrm{CN}} = \frac{\pi}{k^2} g_J T_{\mathrm{n}} \frac{T_x}{\sum_c T_c}$$

Radiative capture

T_γ

Fission

T_{f}

Inelastic/neutron

$T_{\mathrm{n'}}$

Elastic/neutron

T_{n}

* A.J. Koning, S. Hilaire, M.C. Duijvestijn, Proceedings of the International conference on nuclear data for science and Technology, April 2007

NEUTRON AND GAMMA TRANSMISSION COEFFICIENTS

Development and validation

Neutron T_n $T_{n'}$

- Coupled channels calculation performed by the ECIS* code
- Average R-matrix

Gamma T_γ

$$T_\gamma^{J\Pi}(E^*) = 2\pi \sum_{X\ell} \sum_{I'=|J-\ell|}^{J+\ell} \int_0^{E^*} d\epsilon_\gamma \epsilon_\gamma^{2\ell+1} f_{X\ell}(\epsilon_\gamma, E^*) \rho(E^* - \epsilon_\gamma, I', \Pi(-1)^{\ell+\delta_{MX}})$$

Strength function for the electromagnetic transition

Level density for the nucleus after emission of gamma

→ Several available models for both level densities and gamma strength functions thanks to library sharing with the FIFRELIN** code

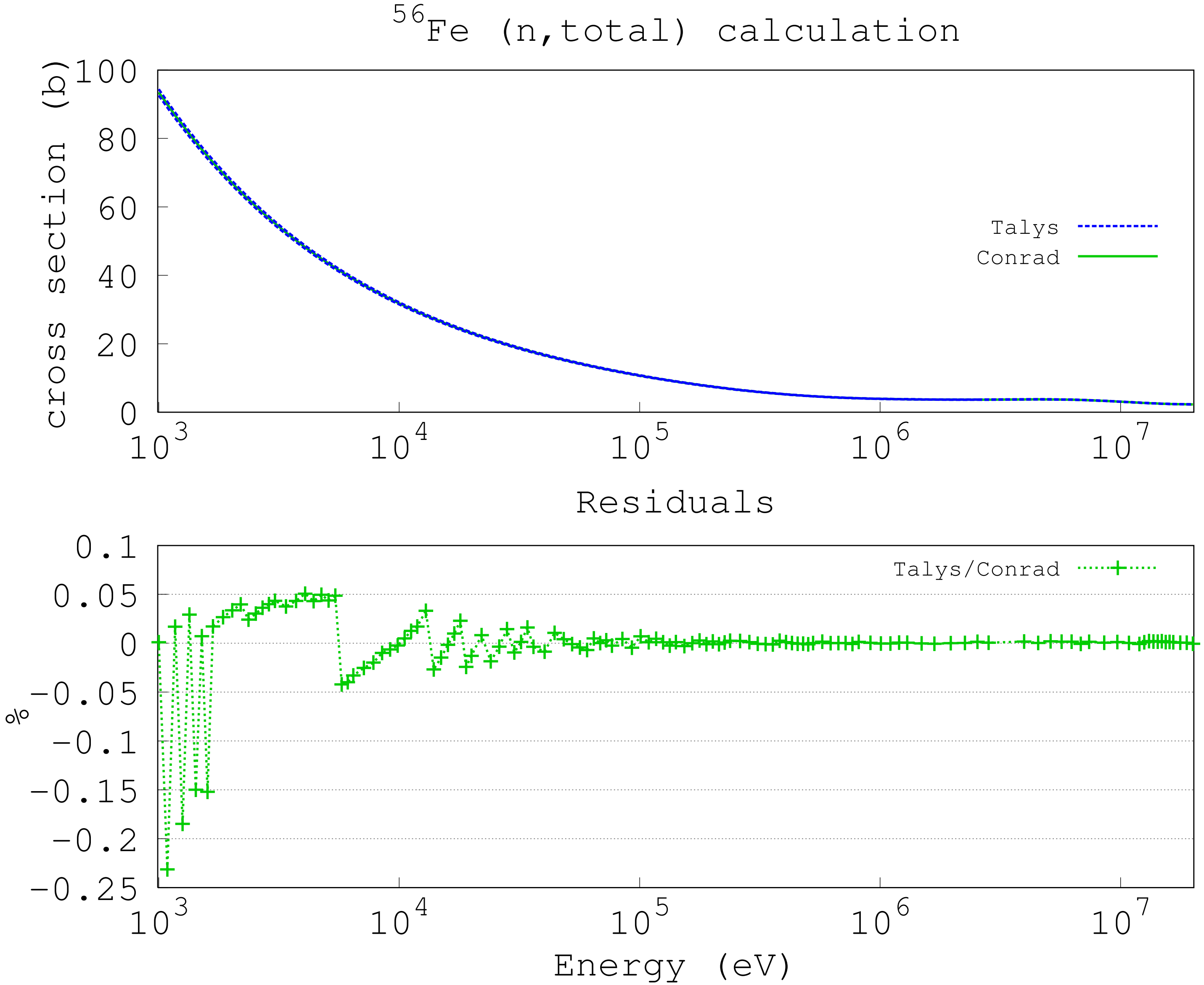
$$\sigma_{nx} = \sigma_{nx}^{dir} + \sigma_{nx}^{CN}$$

For inelastic levels not taken into account in the coupled channels scheme:
->DWBA calculation performed either by ECIS or internally by Conrad

*J. Raynal, Notes on ECIS94, CEA Saclay report No. CEA-N-2772 (1994)
**O. Litaize, O. Serot, Phys. Rev. C 82, 054616 (2010)

RESULTS FOR EVEN-EVEN SPHERICAL NUCLEUS ^{56}Fe

Development and validation

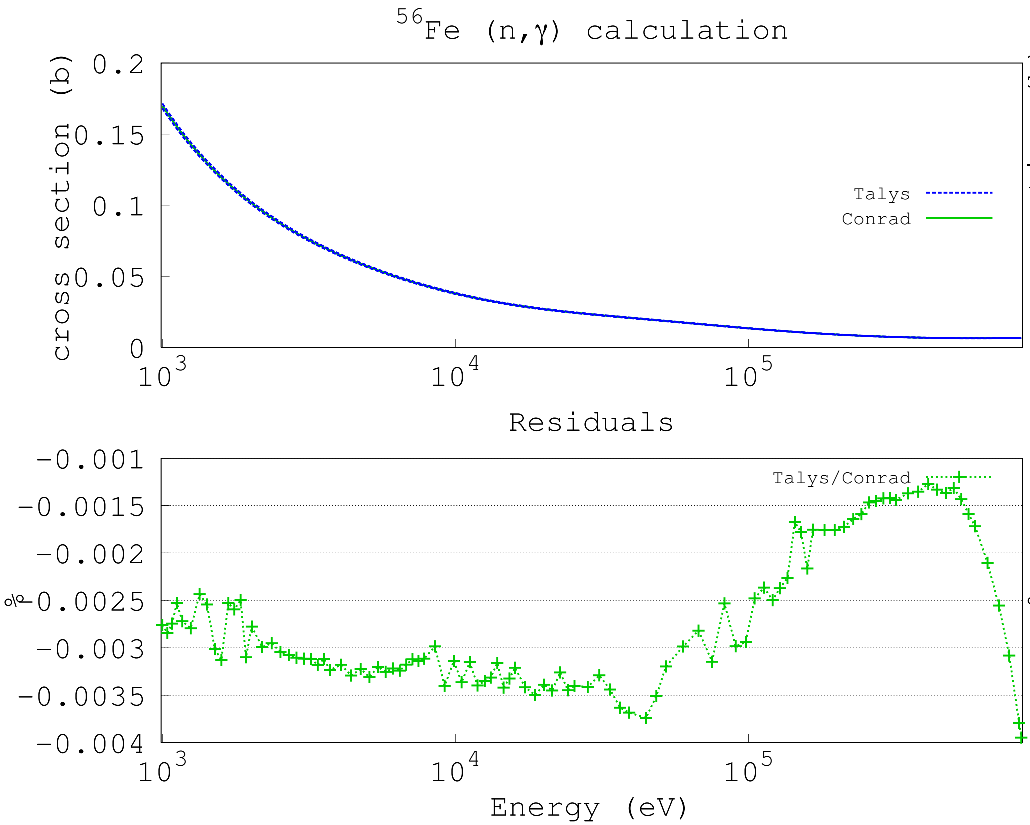


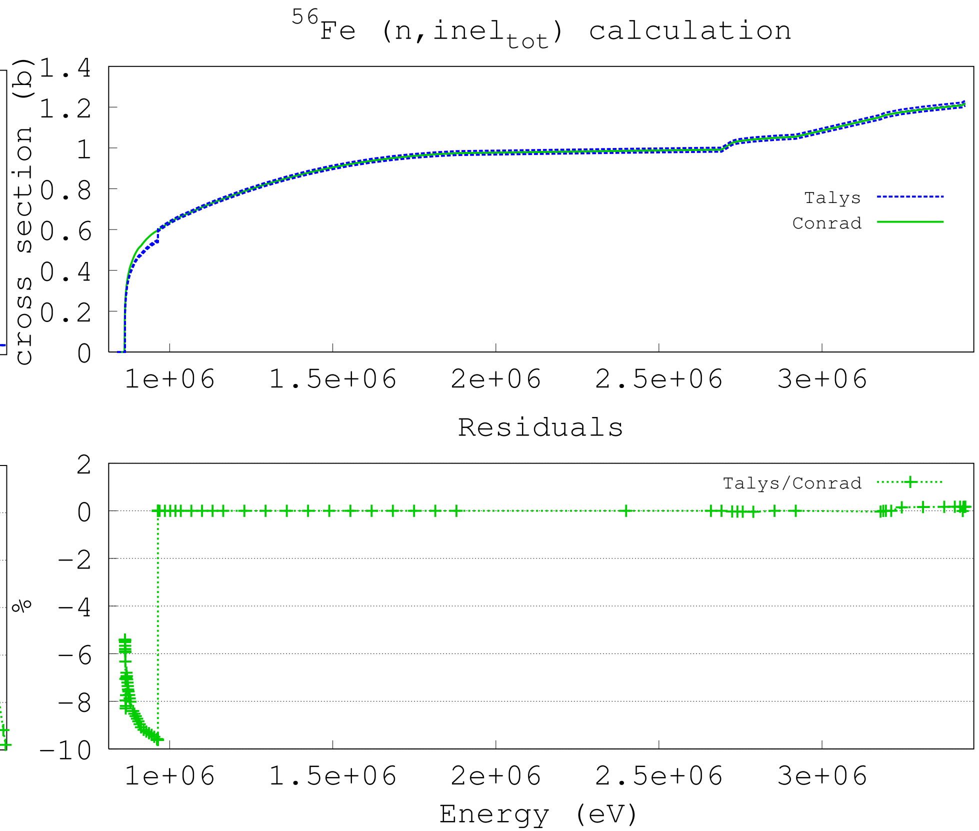
$$\sigma_{n,\mathrm{tot}} \propto T_n$$

Validation of T_n

RESULTS FOR EVEN-EVEN SPHERICAL NUCLEUS ^{56}Fe

Development and validation





$$\sigma_{n\gamma} \propto \frac{T_n T_\gamma}{T_n + T_\gamma}$$

Validation of T_γ

$$\sigma^{\mathrm{CN}}_{nn'} \propto \frac{T_n T_{n'}}{T_n + T_\gamma + T_{n'}}$$

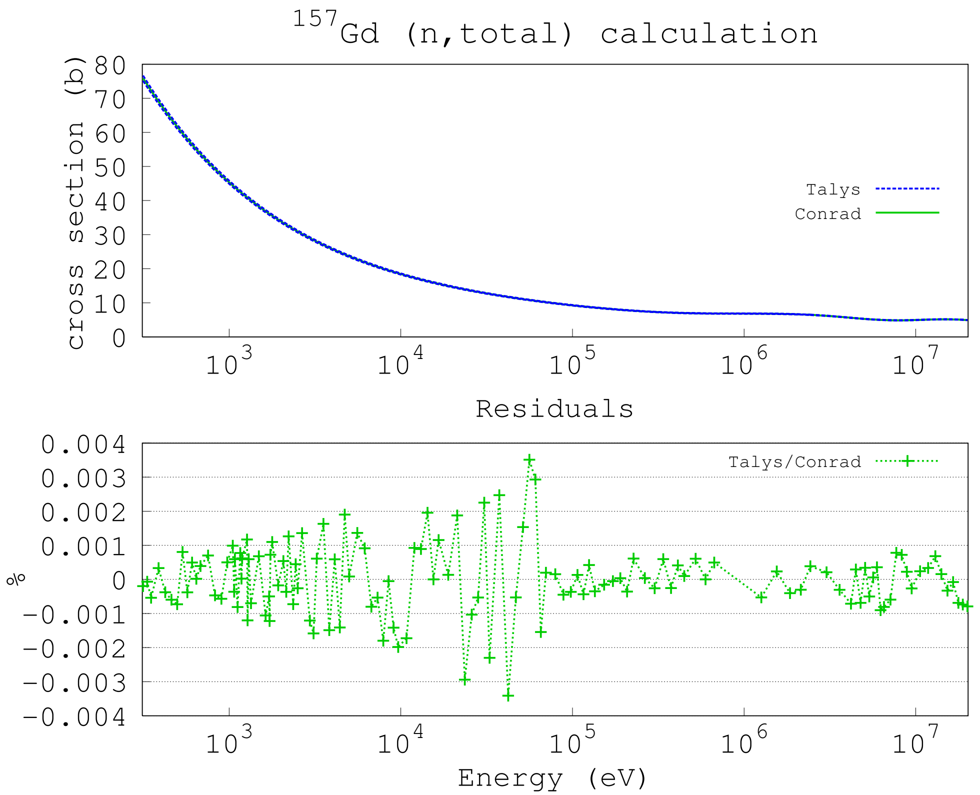
Validation of $T_{n'}$

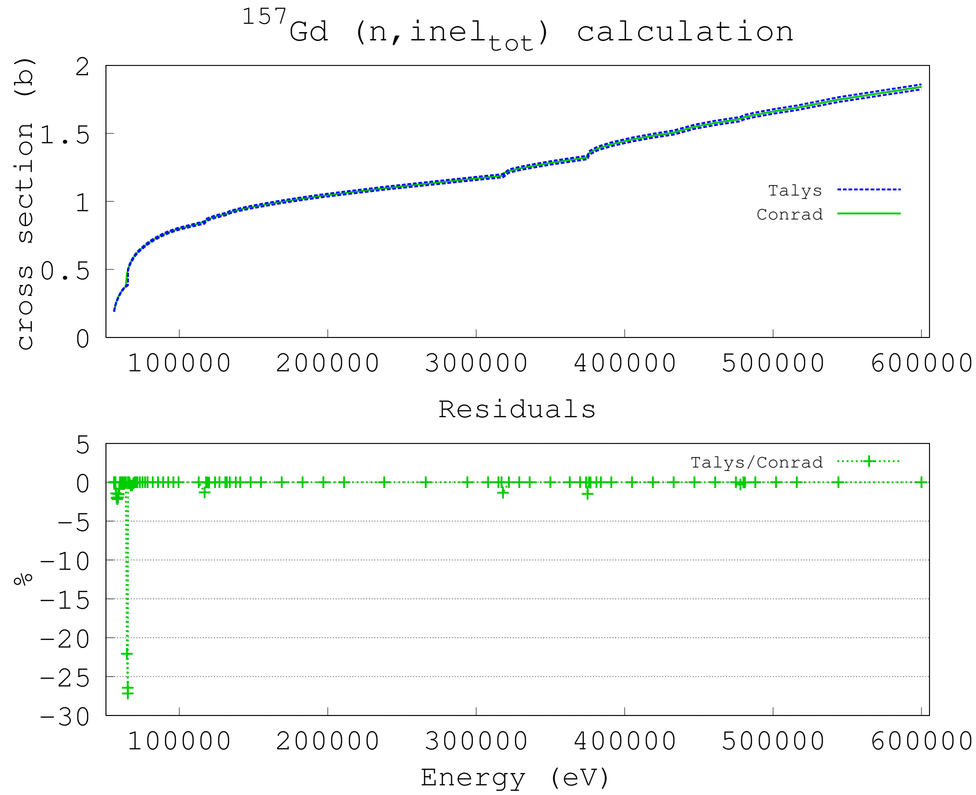
$$\sigma^{\mathrm{dir}}_{nn'} = \sigma^{\mathrm{DWBA}}_{nn'}$$

Validation of DWBA calculation

RESULTS FOR DEFORMED ODD NUCLEUS ^{157}Gd

Development and validation



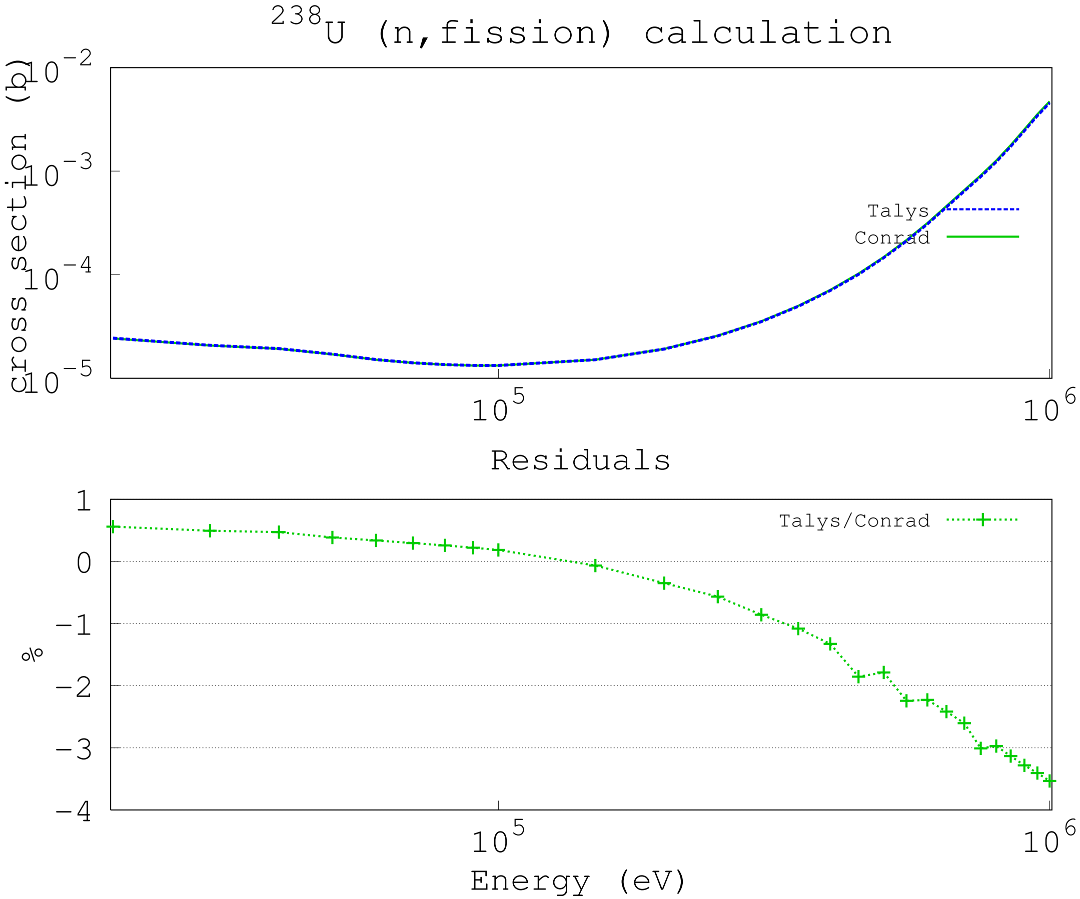


Validation of the coupled channels calculated $T_{j\ell}^{J\Pi}$

$\sigma_{nn'}^{\mathrm{dir}}$, is given by the coupled channels calculation

Other reaction are verified, what about fission?

ACTINIDES WITH STANDARD FISSION TRANSMISSION COEFFICIENT ^{238}U

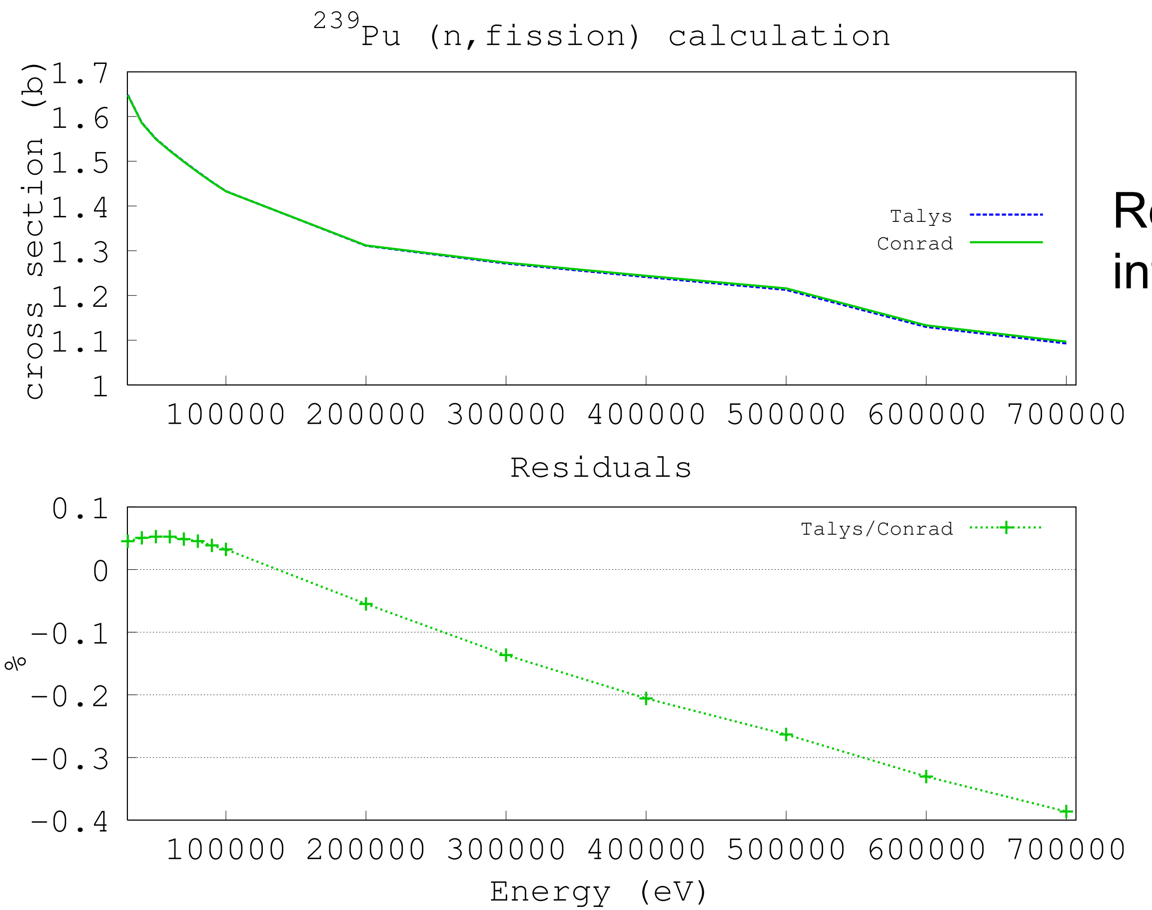


Remaining differences due to integration method

$$T_{\text{barrier } i}(E^*) = \sum_{\text{disc. trans. states } t_i} T^{\text{Hill-Wheeler}}(E^* - \epsilon_{t_i}) + \int_{E_i^{\text{limit}}}^{E^*} \rho_i(J, \Pi, E^* - \epsilon) T^{\text{Hill-Wheeler}}(E^* - \epsilon) \mathrm{d}\epsilon$$

ACTINIDES WITH STANDARD FISSION TRANSMISSION COEFFICIENT ^{238}U, ^{239}Pu

Development and validation

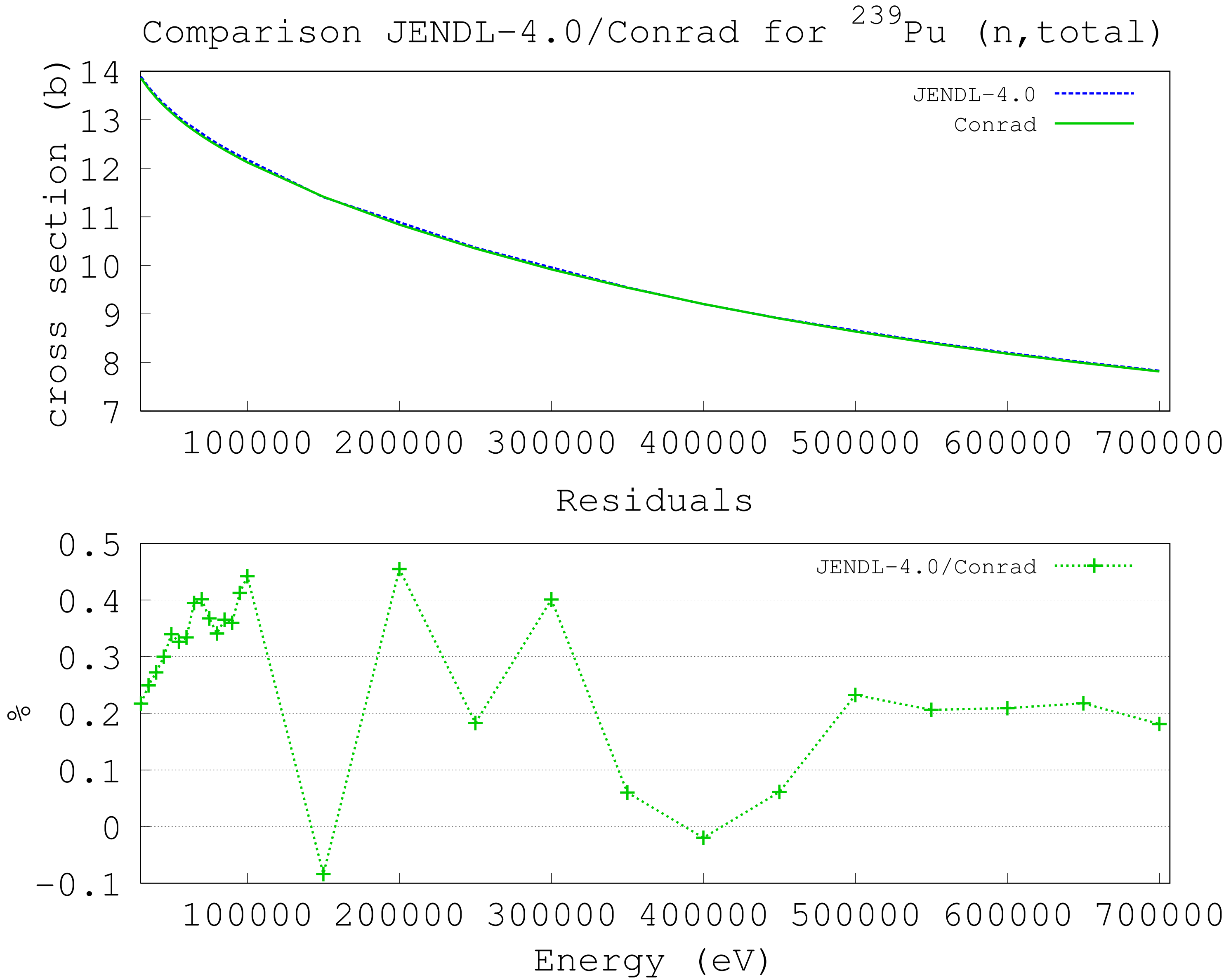


Remaining differences due to integration method

$$T_{\text{barrier } i}(E^*) = \sum_{\text{disc. trans. states } t_i} T^{\text{Hill-Wheeler}}(E^* - \epsilon_{t_i}) + \int_{E_i^{\text{limit}}}^{E^*} \rho_i(J, \Pi, E^* - \epsilon) T^{\text{Hill-Wheeler}}(E^* - \epsilon) \mathrm{d}\epsilon$$

COMPARISON WITH EVALUATIONS

Development and validation

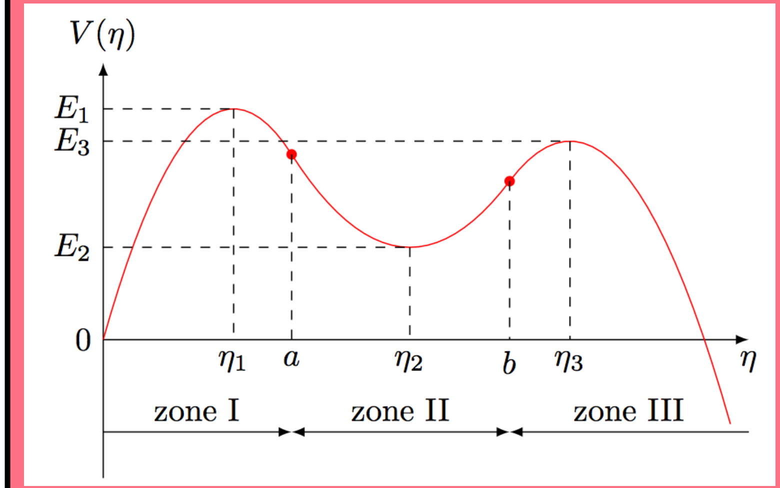


Numerical validation is achieved.

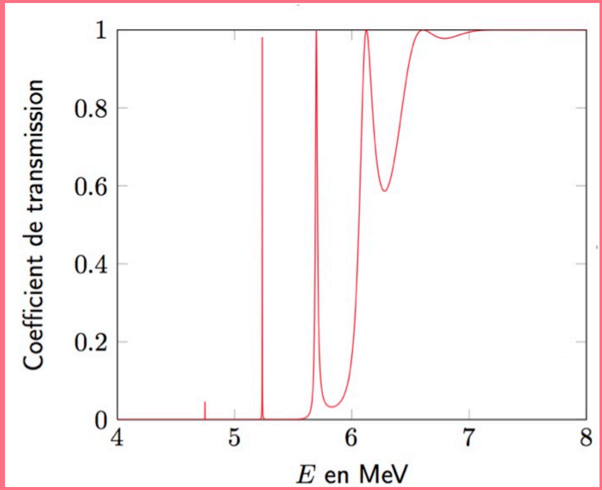
Comparison with evaluations is possible when parameters are known.

CRAMER NIX APPROACH STILL LIMITED

Fission T_f



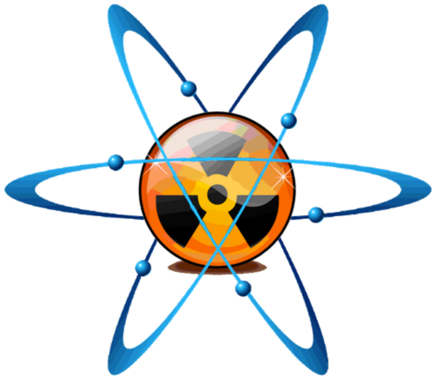
$$V(\eta) = \begin{cases} E_1 - \frac{1}{2}\mu\omega_1^2(\eta-\eta_1)^2, & \eta \le a \\ E_2 + \frac{1}{2}\mu\omega_2^2(\eta-\eta_2)^2, & a \le \eta \le b \\ E_3 - \frac{1}{2}\mu\omega_3^2(\eta-\eta_3)^2, & \eta \ge b \end{cases}$$



6 adjustable parameters per "global transition states" (continuous potential) ⇒ Too many for adjustments

6 adjustable parameters identical for all "global transition states" ⇒ Section enhancements occur at similar energies and accumulate (too much)

Need for distinct – not one-by-one adjustable – parameters for each « global transition states »



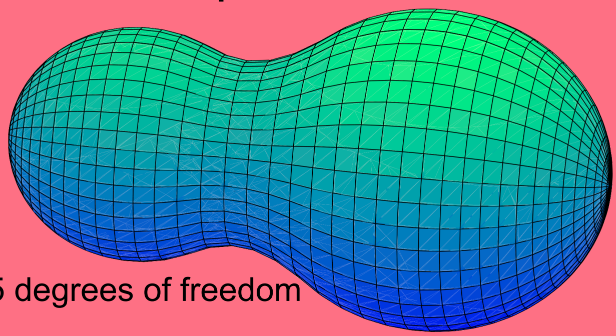
PHYSICS UNDERNEATH

MACRO-MICROSCOPIC APPROACH TO DESCRIBE FISSION BARRIER SHAPES : FRDM & FRLDM*

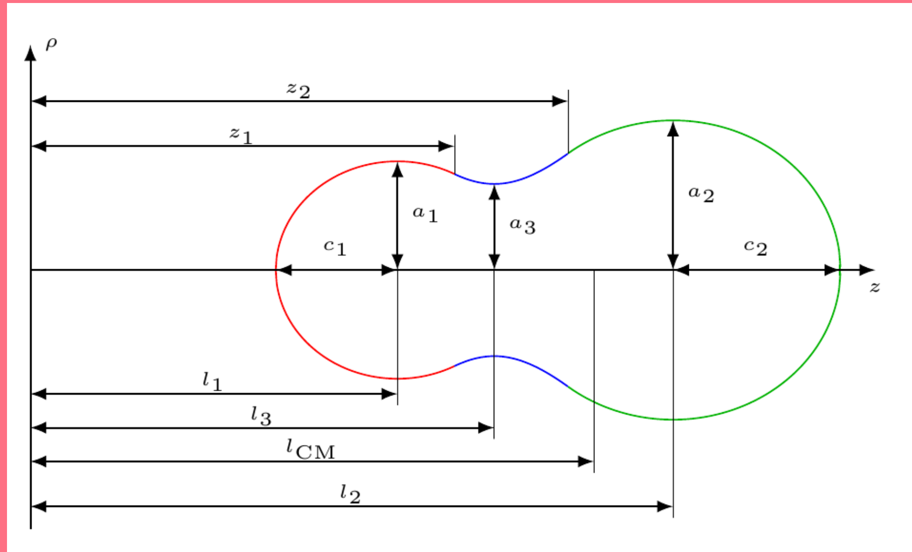
Physics underneath

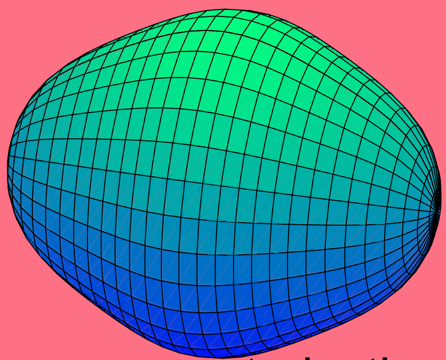
Fission T_{f}

Three quadratic surfaces



5 degrees of freedom

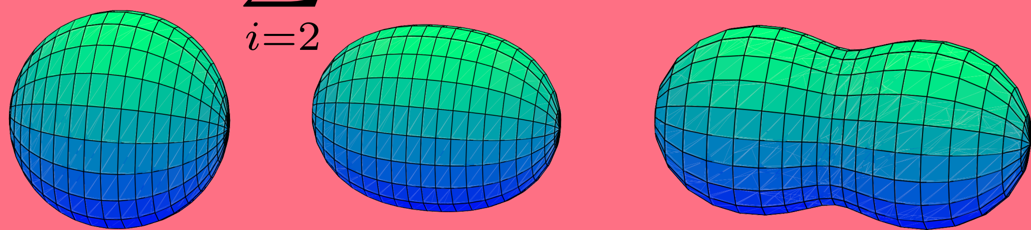




ε parameterization

Legendre polynomials expansion

$$r(\theta) = R_0[1 + \sum_{i=2}^{\infty} \beta_i P_i(\cos\theta)]/\lambda(\beta_2, \beta_3, ...)$$



1) Provide $\rho(z)$ or $r(\theta)$

* P. Moller et al, At. Data Nucl. Data Tables 59 185 (1995)

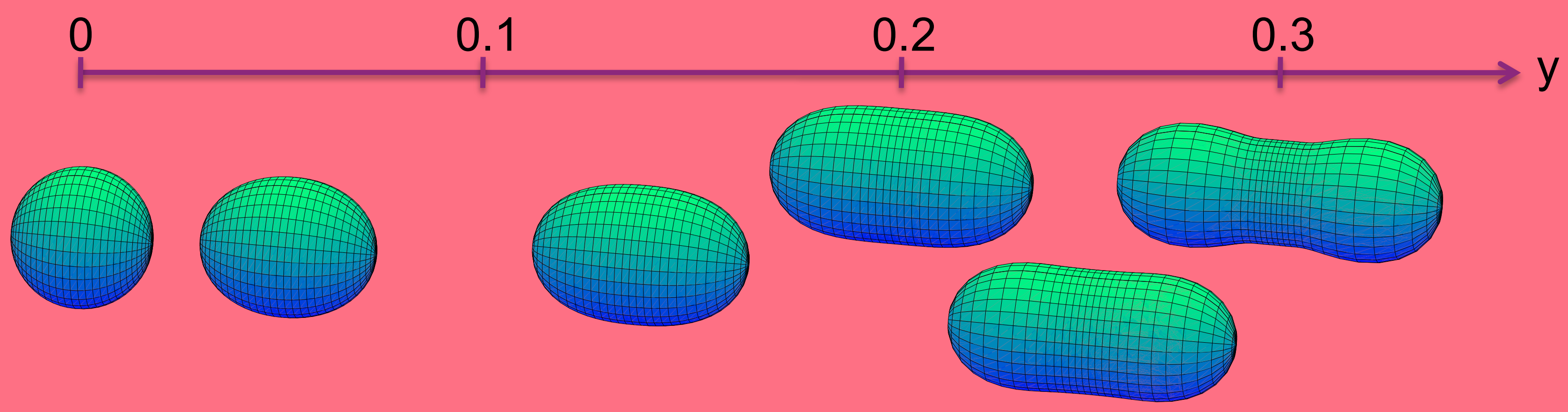
HILL-WHEELER LIQUID DROP MODEL SHAPE PARAMETERIZATION*

Physics underneath

Fission T_f

$$r(\cos\theta) = a_0(y)\left[1 + \sum_{i=1}^{4} a_{2i}(y) P_{2i}(\cos\theta)\right]$$

Numerical expression



1 parameter = a “reasonable” shape description

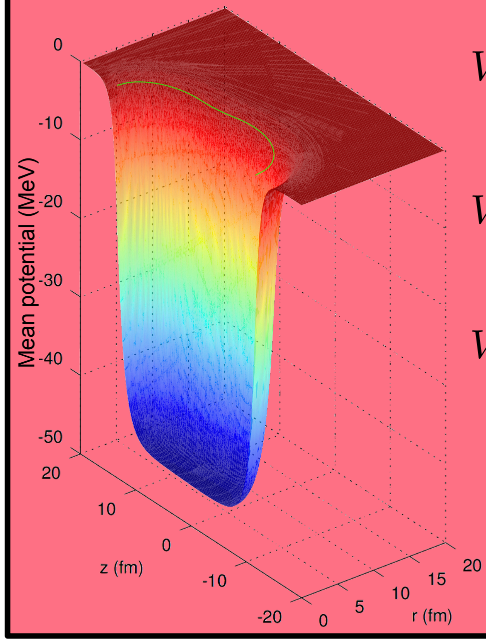
*D. L. Hill and J. A. Wheeler, Phys. Rev. 89, 1102 (1953)

LIQUID DROP/DROPLET CONTRIBUTIONS

Fission T_f $\quad V(\text{shape}) = V_{\text{macro}}(\text{shape}) + \Delta V_{\text{micro}}(\text{shape})$

$$E_\mathrm{C}(\text{shape}) = \frac{1}{2}\int_V \mathrm{d}^3\vec{r}_1 \int_V \mathrm{d}^3\vec{r}_2 \frac{\rho(\vec{r}_1)\rho(\vec{r}_2)}{\|\vec{r}_1 - \vec{r}_2\|} \qquad E_\mathrm{S}(\text{shape}) = \gamma \int_S \mathrm{d}^2 S$$

2) $\quad V_{\text{macro}}(\text{shape}) \overset{*}{=} E_\mathrm{C}(\text{shape}) + E_\mathrm{S}(\text{shape})$



$$V_1(\vec{r}) = -\frac{V_0}{4\pi a_{\text{pot}}^3}\int_V \frac{e^{-\|\vec{r}-\vec{r'}\|/a_{\text{pot}}}}{\|\vec{r}-\vec{r'}\|/a_{\text{pot}}}\mathrm{d}^3\vec{r'}$$

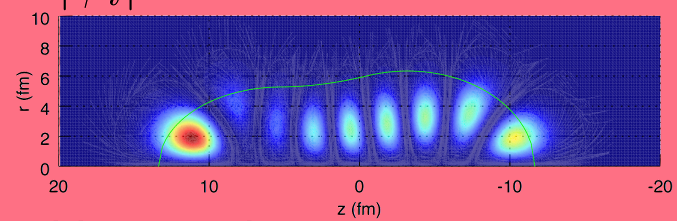
$$V_\mathrm{C}(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{e^2 Z}{V}\int_V \frac{\mathrm{d}^3\vec{r'}}{\|\vec{r}-\vec{r'}\|}$$

$$V_{\text{s.o.}}(\vec{r}) = -\lambda\left(\frac{\hbar^2}{2mc}\right)^2 \frac{\vec{\sigma}\cdot\vec{\nabla}V_1 \times \vec{p}}{\hbar}$$

Independent particle equation

$$\left[\hat{T} + \hat{V}_1 + \hat{V}_\mathrm{C} + \hat{V}_{\text{s.o.}}\right]\psi_i = \epsilon_i \psi_i$$

$|\psi_i|^2$



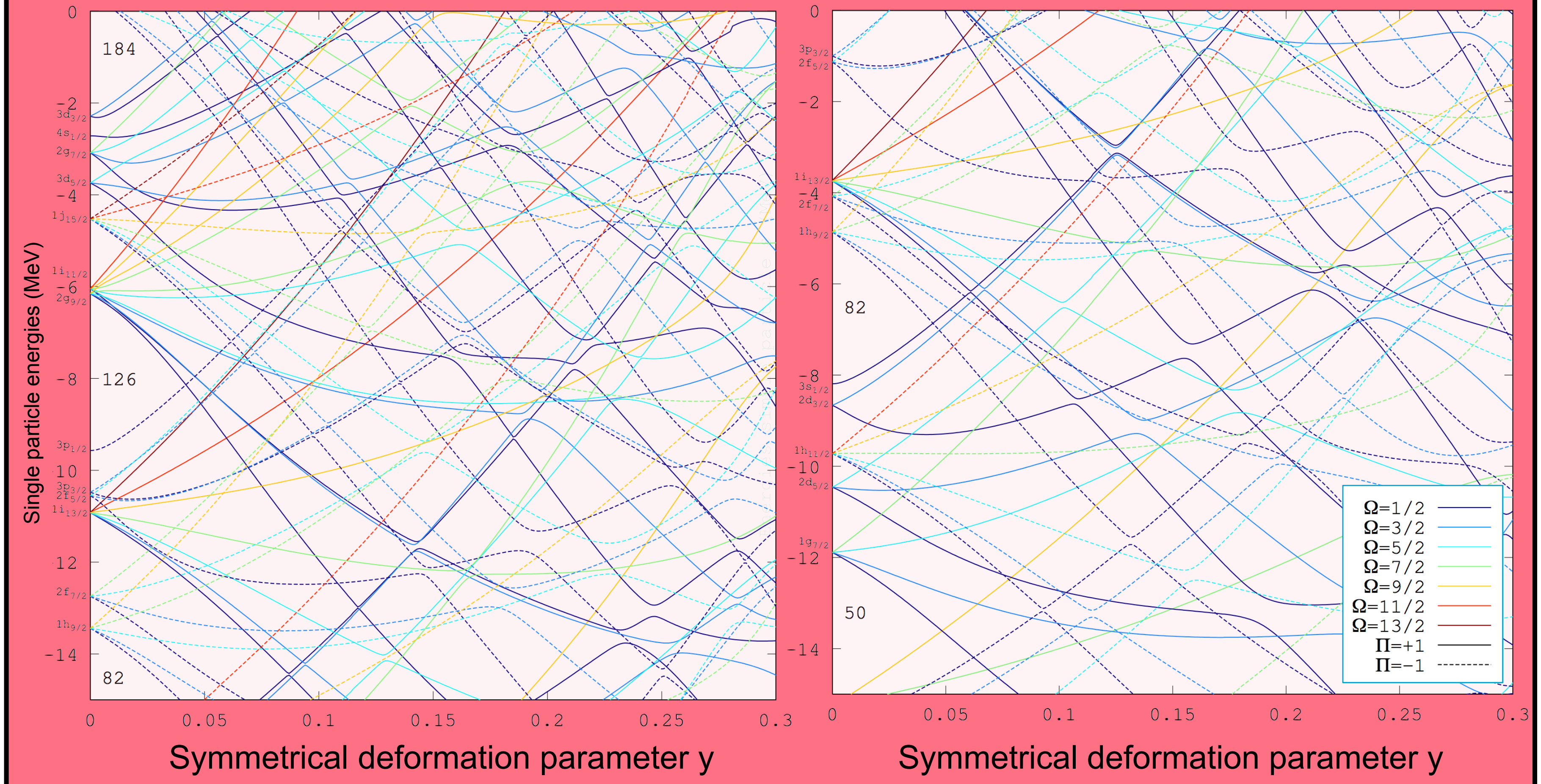
Resolution using deformed harmonic oscillator base functions** $|n_r, n_z, \Lambda, \Sigma\rangle$

•P. Moller et al, At. Data Nucl. Data Tables 39 225 (1988)
P. Moller et al, At. Data Nucl. Data Tables 39 213 (1988)
** J. Damgaard et al., Nucl. Phys. A 135, 432 (1969)

SINGLE PARTICLE ENERGIES AS A FUNCTION OF NUCLEUS DEFORMATION : ^{240}Pu

Physics underneath

Fission T_f — Neutrons — Protons



3) $\epsilon_i(\text{shape}) \longrightarrow$ Extraction* of $\Delta V_{\text{micro}}(\text{shape})$

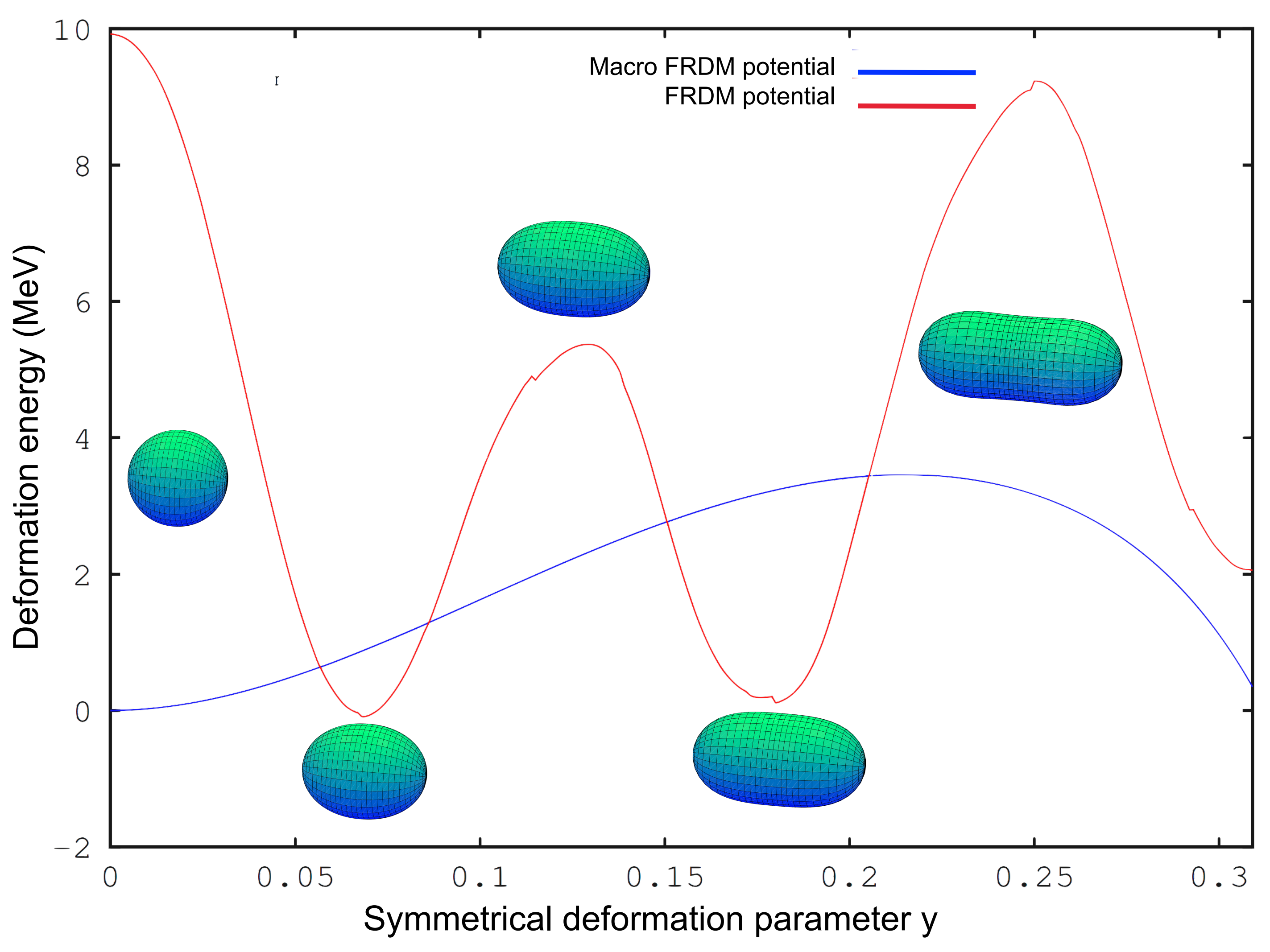
* M. Bolsterli et al., Phys. Rev. C 5, 1050 (1972)

RESULTS FOR SYMMETRICAL BARRIER IN ^{240}Pu

Physics underneath

Fission T_f

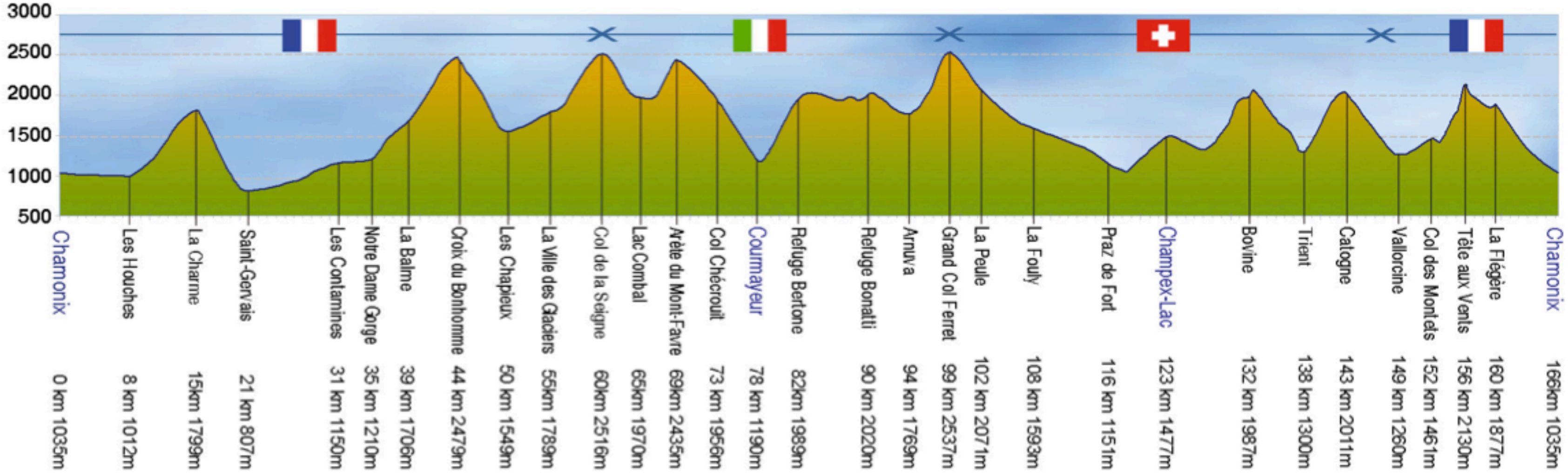
Reasonable values* for symmetric fission



* M. Bolsterli et al., Phys. Rev. C 5, 1050 (1972)

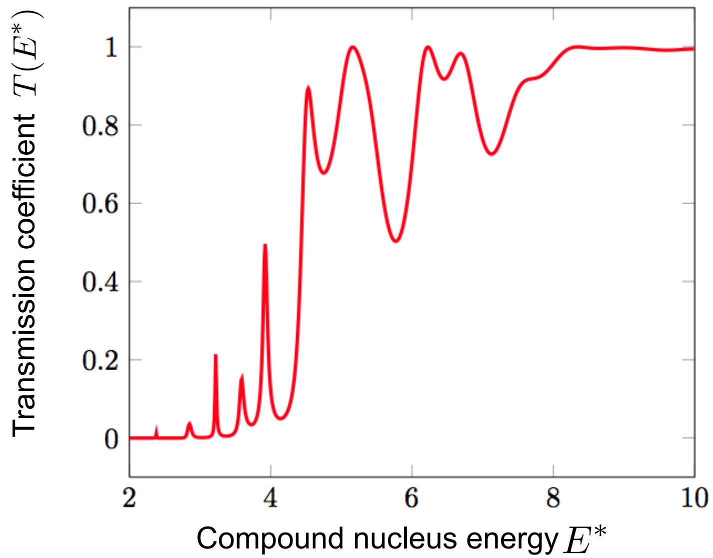
ARBITRARY SHAPE OF ENERGY POTENTIAL FOR TRANSMISSION CALCULATION

Physics underneath



Topologic profile of the Tour du Mont-Blanc (150km)

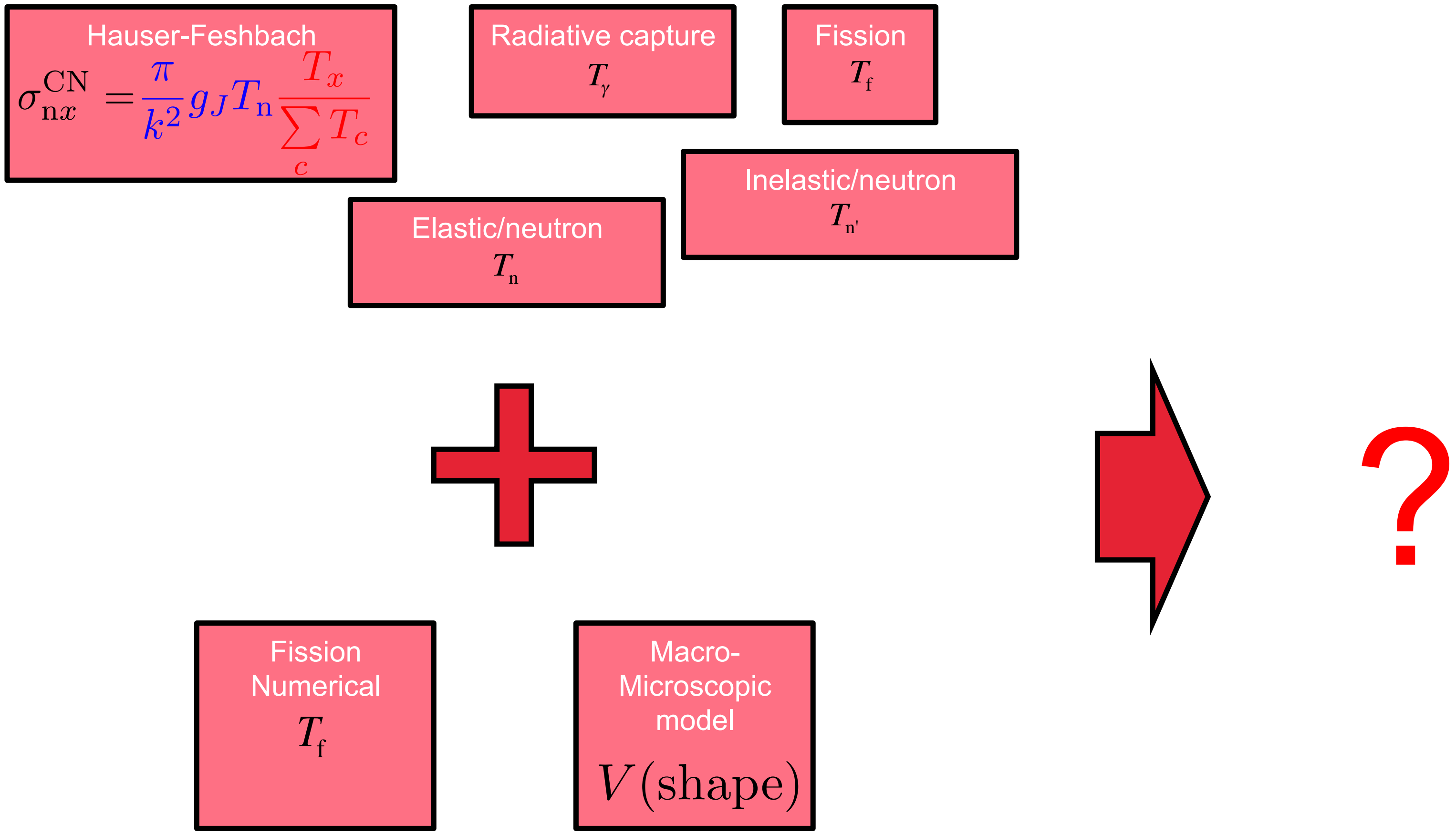
Implementation of the Numerov numerical method* for the calculation of fission transmission coefficients



*H. Durate, B. Morillon, P. Romain, CEA/(DAM/DEN/DSM) seminar (2013)

CONCLUSION AND OUTLOOK

GATHERING ALL PIECES TOGETHER : ON GOING



Actual evaluated fission cross section calculated on some selected nuclei

REMAINING POINTS

conclusion

Determination of a single dimension path for fission (mass asymmetry exploration)

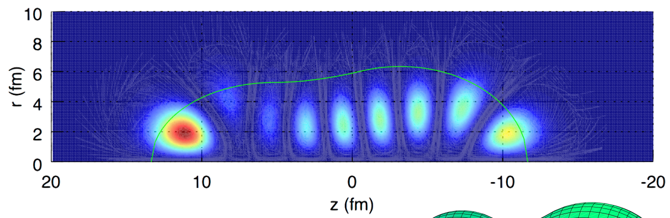
Axially asymmetric shapes (gamma deformations)

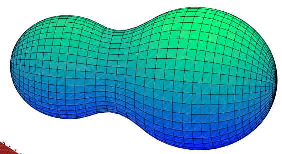
Dependence of the inertial parameter on deformation

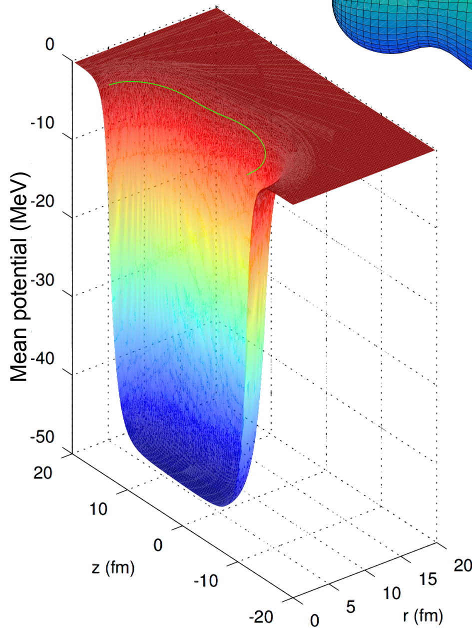
Degree of freedom in the width fluctuation factor for fission*

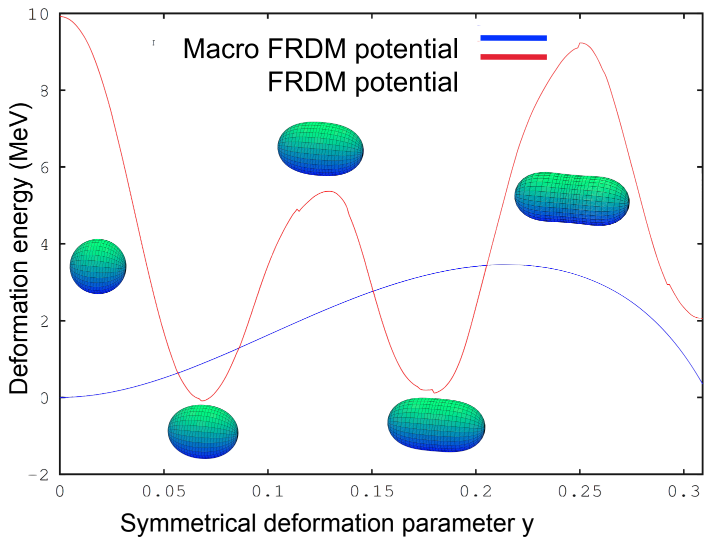
Comparison with the AVXSF** code

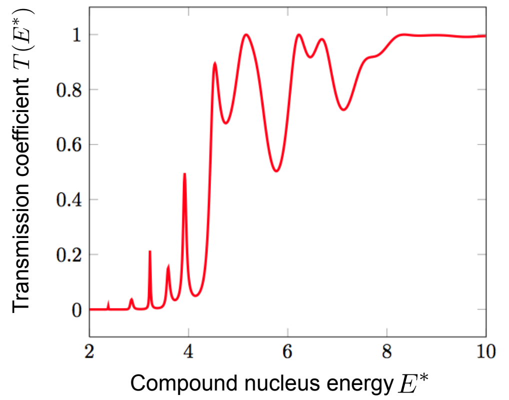
* O. Bouland, J.E. Lynn and P. Talou, Phys. Rev. C 88, 054612 (2013)
**J. E. Lynn, Harwell Report AERE-R 7468 (1974)

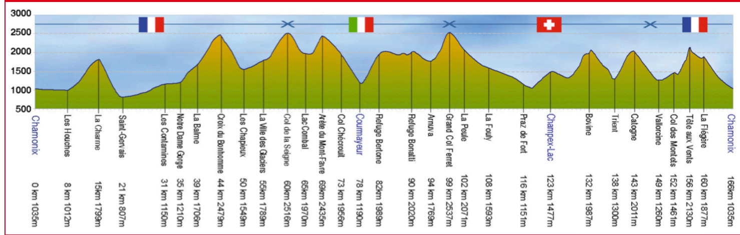




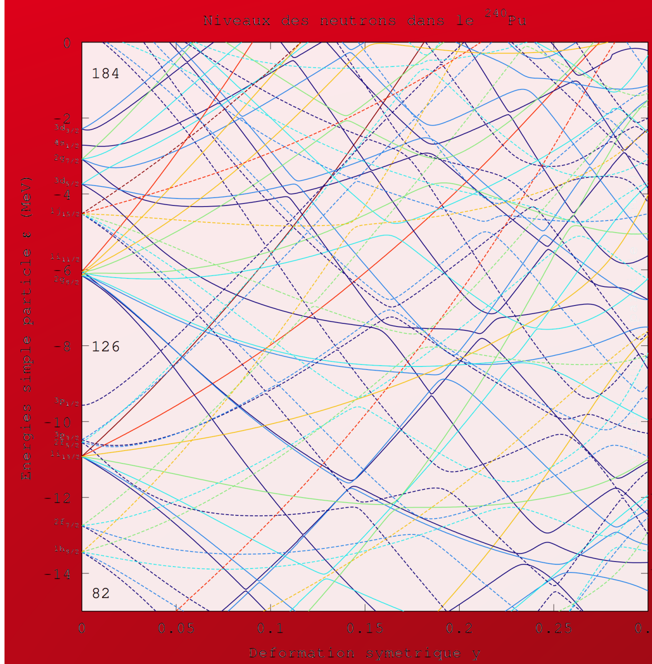


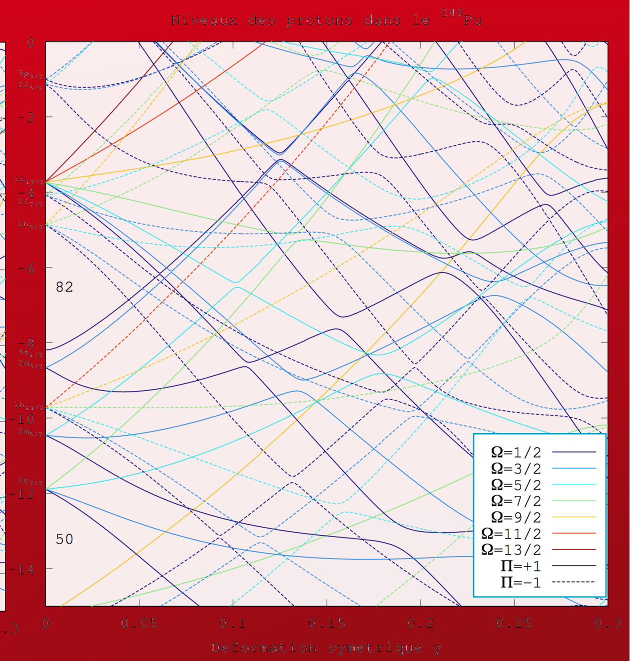






Thank you for your attention





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