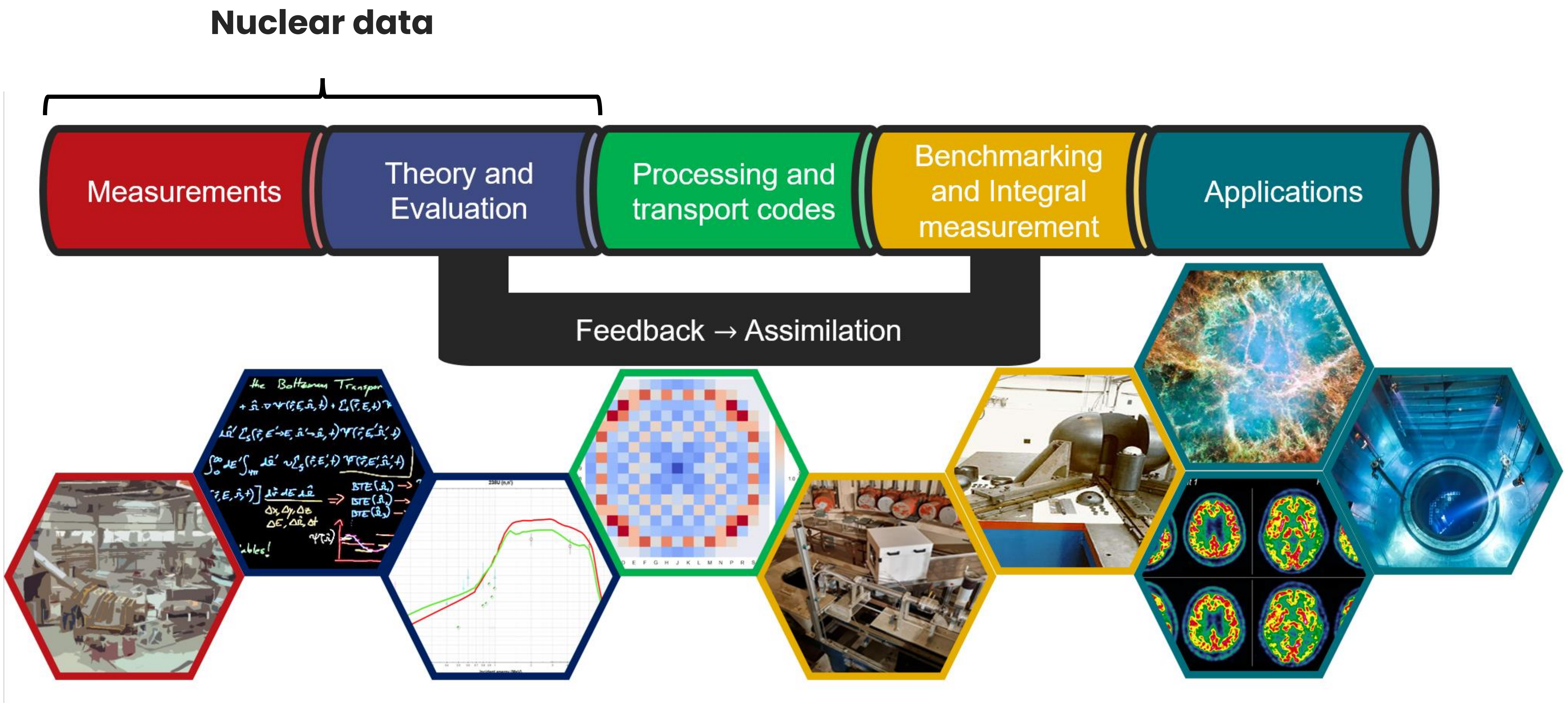
Bayesian optimization on FIFRELIN Monte-Carlo code to fit neutron and gamma multiplicities

G. BAZELAIRE[1], A. CHEBBOUBI[1], D. BERNARD[1],
G. DANIEL[2], J.-B. BLANCHARD[2]

[1]CEA, DES, IRESNE, DER, SPRC, Cadarache, Physics Studies Laboratory, Saint-Paul-lès-Durance, 13108, France

[2]Université Paris-Saclay, CEA, Service Génie Logciel pour la simulation, 91191, Gif-sur-Yvette, France

Context : nuclear data



A. CHEBBOUBI, HDR (2023)

Contents

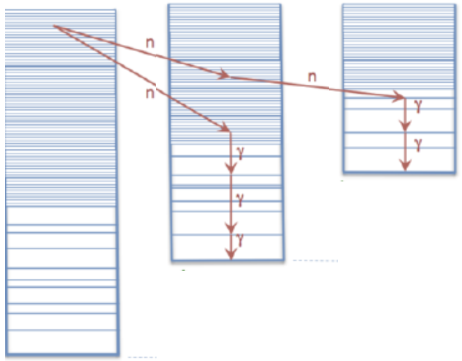
1. FIFRELIN

FIFRELIN : simulation of the de-excitation process of fission fragments

A FIFRELIN calculation is done in two steps :

STEP 1 Determination of the physical caracteristics A, Z, KE, E^*, J^π for both the light and the heavy fragment

STEP 2 De-excitation of those fragments by the emission of prompt particules n, γ, e^-



O. Litaize, O. Serot, and L. Berge, Eur. Phys. J. A 51, 177 (2015)

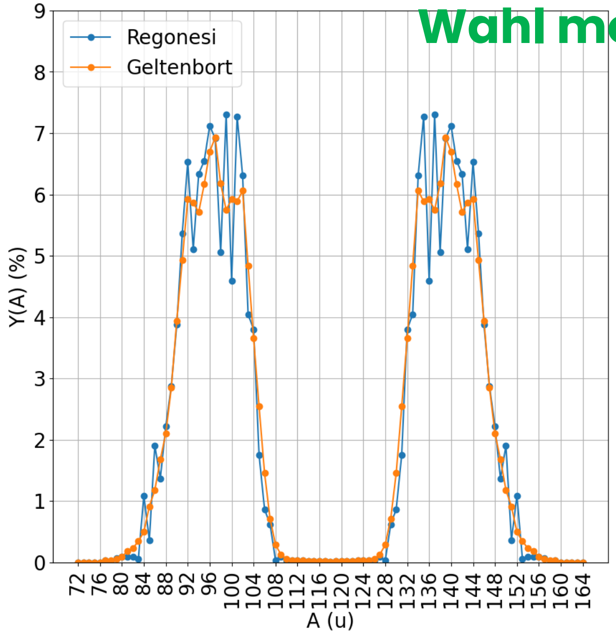
FIFRELIN step 1 : generation of fission fragments

Caracteristics are defined through a sampling over experimental data and phenomenological models

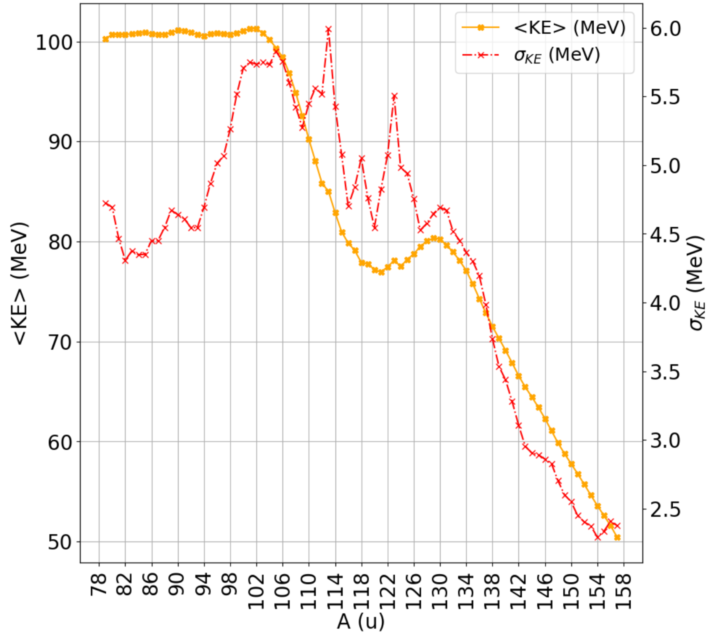
$$Y(A,Z,E^*,KE,J,\pi) = Y(A) \times P(Z|A) \times P_{\theta_1}(E^*|A,Z) \times P(KE|A) \times P_{\theta_2}(J|A,Z,E) \times P(\pi)$$

Experimental data **Phenomenological models**

Wahl model



$^{235}U(n_{th}, f)$

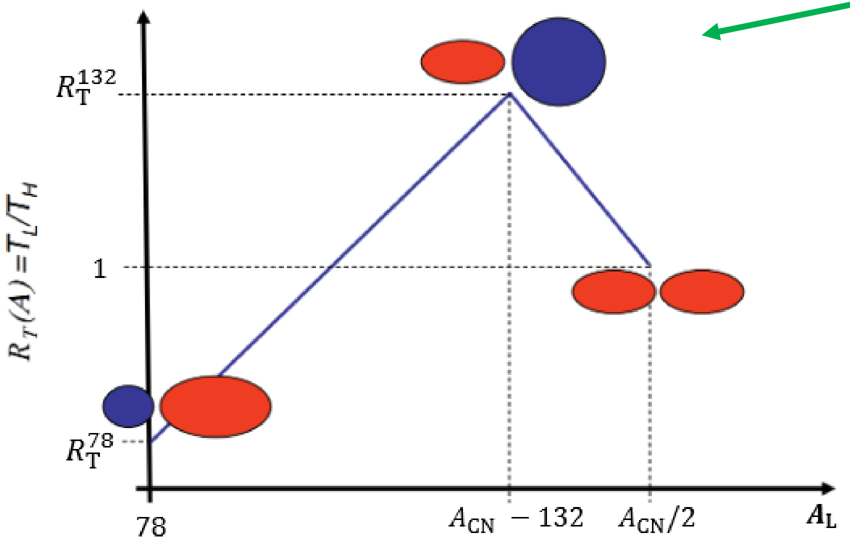


$^{235}U(n_{th}, f)$

FIFRELIN step 1 : generation of fission fragments

$$Y(A,Z,E^*,KE,J,\pi) = Y(A) \times P(Z|A) \times P_{\theta_1}(E^*|A,Z) \times P(KE|A) \times P_{\theta_2}(J|A,Z,E) \times P(\pi)$$

Phenemenological models



Excitation energy sharing based on mass-dependant temperature ratio law

Default model $R_T(A) = \begin{cases} R_T^{78} + (A-78)\dfrac{R_T^{132} - R_T^{78}}{120 - 78} & \text{if } 78 \le A < 120 \\ R_T^{132} + (A-120)\dfrac{1 - R_T^{132}}{126 - A} & \text{if } 120 \le A < 126 \\ 1 & \text{if } A = 126 \end{cases}$

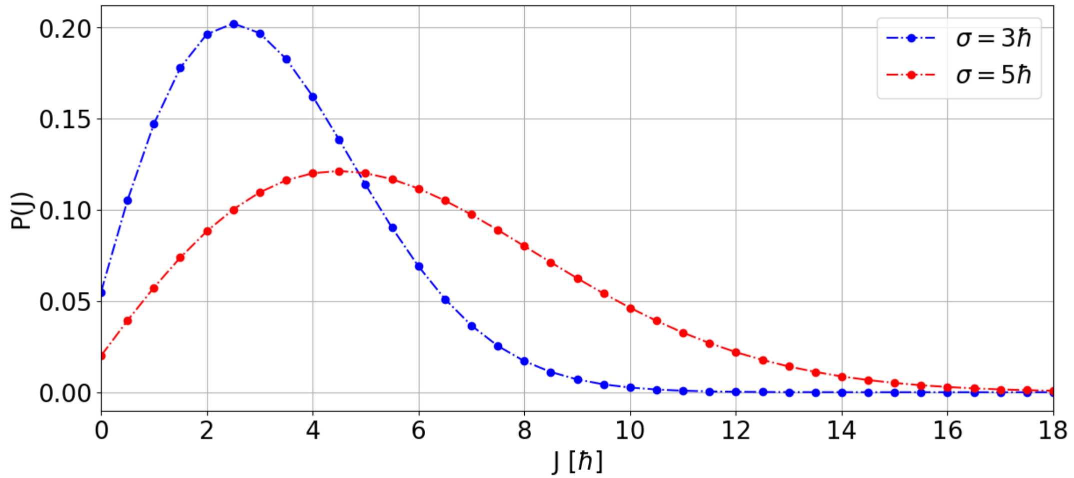
Second model $R_T(A) = \begin{cases} \text{adjusted by the user} & \text{if } 78 \le A < 126 \\ 1 & \text{if } A = 126 \end{cases}$

$\boldsymbol{\theta_1} = (\boldsymbol{R_T^{78}}, \boldsymbol{R_T^{132}})$ or $\boldsymbol{\theta_1} = (\boldsymbol{R_T(A)})$ are ***adjustement*** parameters to better fit experimental data.

FIFRELIN step 1 : generation of fission fragments

$$Y(A,Z,E^*,KE,J,\pi) = Y(A) \times P(Z|A) \times P_{\theta_1}(E^*|A,Z) \times P(KE|A) \times P_{\theta_2}(J|A,Z,E) \times P(\pi)$$

$$P(J) = \frac{2J+1}{2\sigma(E)^2} \exp \frac{-\left(J+\frac{1}{2}\right)^2}{2\sigma(E)^2}$$



Phenemenological models

Total angular momentum definition

The parameter $\sigma^2(E)$ is dependent on the excitation energy of the fragment.

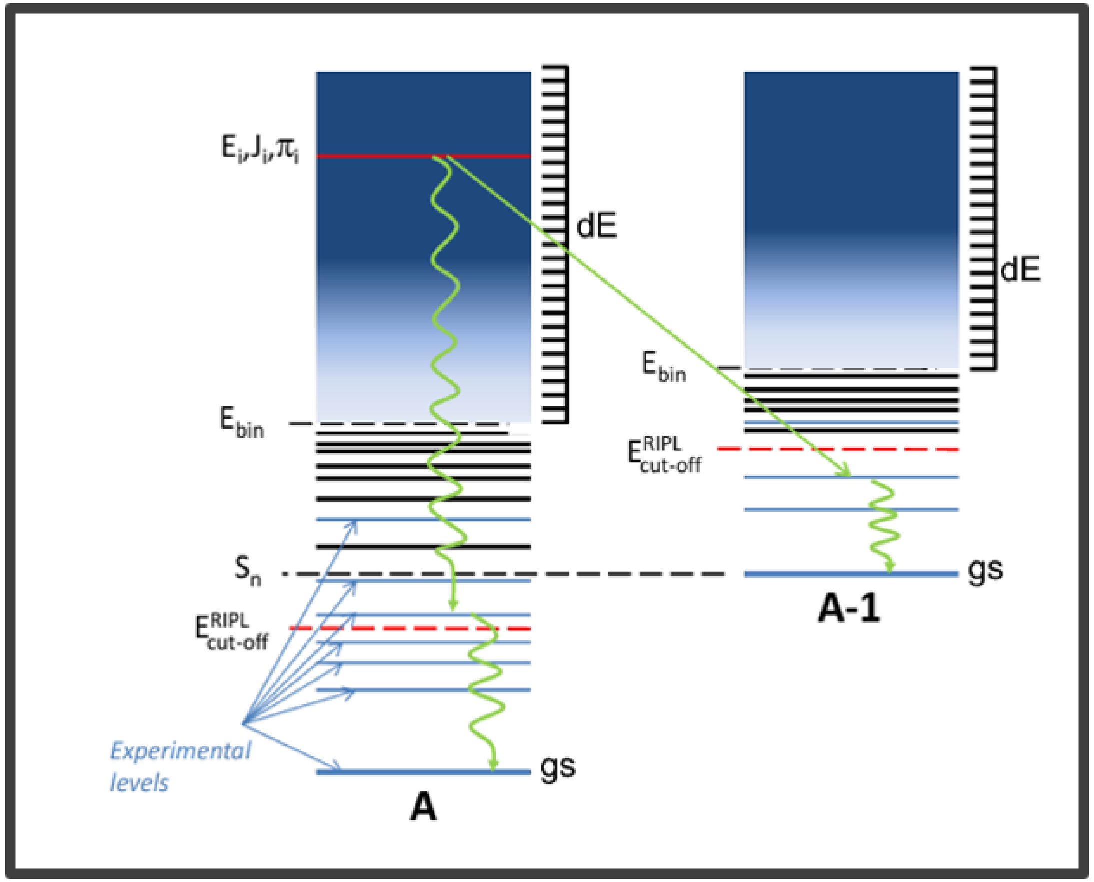
For $E \geq S_n : \sigma_S^2(E) = f_\sigma^2 g \frac{a}{\tilde{a}} \sqrt{\frac{U}{A}}$

$\theta_2 = (f^2_{\sigma(L)}, f^2_{\sigma(H)})$ are ***adjustement*** parameters to better fit experimental data.

FIFRELIN step 2 : de-excitation process

De-excitation process based on Hauser-Feshbach formalism and nuclear realization.

No more interference from the selected free parameters.



Physical outputs per masse A :

1. $\overline{\nu}(A)$: neutron multiplicity
2. $\overline{M}_{\gamma}(A)$: gamma multiplicity
3. $Y(A)_{\mathrm{post}}$: post-emission yields
4. etc.

W. Hauser, H. Feshbach, Phys Rev 87.2, 366-373 (1952)
D. Regnier, Thesis (2013)

FIFRELIN : black-box

Experimental data

Models

Free parameters : x

FIFRELIN

Fissile nucleus

$y = FIF(x)$

→

Output files : y with uncertainties

$\approx$

Experimental data with uncertainties

Usually $\bar{\nu}$ and $\bar{M}_\gamma$

Goal : optimization. Knowing Y_{data}, find $\boldsymbol{x}$ such that $|\boldsymbol{FIF}(\boldsymbol{x}) - \boldsymbol{Y}_{\boldsymbol{data}}| \leq \boldsymbol{\epsilon}$
This operation can take **several hours** done manually.

How about bayesian optimization ?

2. Gaussian Process regressor & Bayesian Optimization

Gaussian Process regressor (GPR)

GPR : used mainly when the function f is costly to evaluate, based on conditionning.

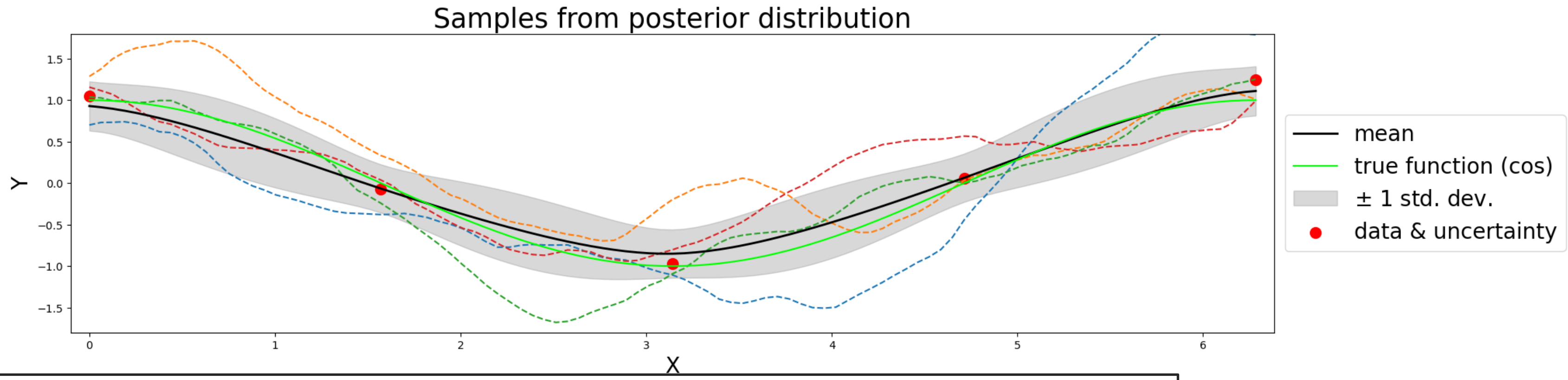
Given $\{\boldsymbol{x_i}, y_i\}_{i=1,\dots,n}$ a database of n evaluations of f. The *hypothesis* is that those evaluations form a Gaussian Process :

$$f(\boldsymbol{X}) = \boldsymbol{f} \sim N(\boldsymbol{\mu}, \boldsymbol{K})$$

with well chosen functions of mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{K}$.

After some tricks we arrive to *key-equations* for predictions at unseen point $\boldsymbol{x}_*$:

$$\mathrm{E}[f_* \,|\boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}] = \mathbf{k}_*^T[\boldsymbol{K} + \sigma^2\mathbf{I}_\mathrm{n}]^{-1}\mathbf{y}$$
$$\mathrm{V}[f_* \,|\boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}] = k(\boldsymbol{x}_*, \boldsymbol{x}_*) - \mathbf{k}_*^T[\boldsymbol{K} + \sigma^2\mathbf{I}_\mathrm{n}]^{-1}\mathbf{k}_*$$



C. E. Rasmussen, C. K. I. Williams, Gaussian Process for Machine Learning (2006)

Bayesian Optimization (BO)

BO : generally used for minimizing stochastic, costly to evaluate functions.

General Design of Experiment using bayesian optimization

- Generate initial sampling with f
- Fit GPR on $\{\boldsymbol{X}, \boldsymbol{Y}\}$
- While some criteria not reached
  - Find $\boldsymbol{x}_{\min}$ that maximizes *acquisition function (depends on GPR)*
  - Evaluate $f(\boldsymbol{x}_{\min})$
  - Fit GPR on $\{\boldsymbol{X}, \boldsymbol{Y}\}$ with $\{\boldsymbol{x}_{\min}, f(\boldsymbol{x}_{\min})\}$ added to the database

J.-H Snoek et al., IEEE Transactions of Information Theory 58.5 (2012)

3. Adjustement of experimental data

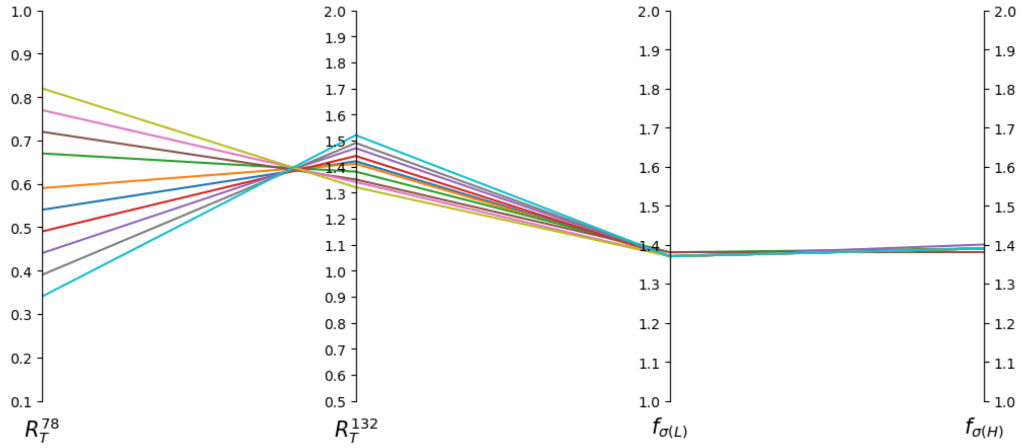
Fitting the saw-tooth

Goal : create an algorithm to adjust $R_T(A)$ and $f_{\sigma(L)}$ & $f_{\sigma(H)}$ in order to fit $\bar{\nu}(A)$ (*experimental saw-tooth*) and gamma multiplicities.

$R_{T(A)}$ → excitation energy for fragments of the corresponding fragmentation → neutron multiplicities $\bar{\nu}(A_L)$ & $\bar{\nu}(A_H)$

$f_{\sigma(L)}$ & $f_{\sigma(H)}$ → total angular momentum → $\bar{M}_{\gamma,L}$ & $\bar{M}_{\gamma,H}$

From previous work we know that f_σ is around **1.40** fort light and heavy fragment for both $^{235}\mathrm{U}(\mathrm{n}_{th},\mathrm{f})$ and $^{252}\mathrm{Cf(sf)}$



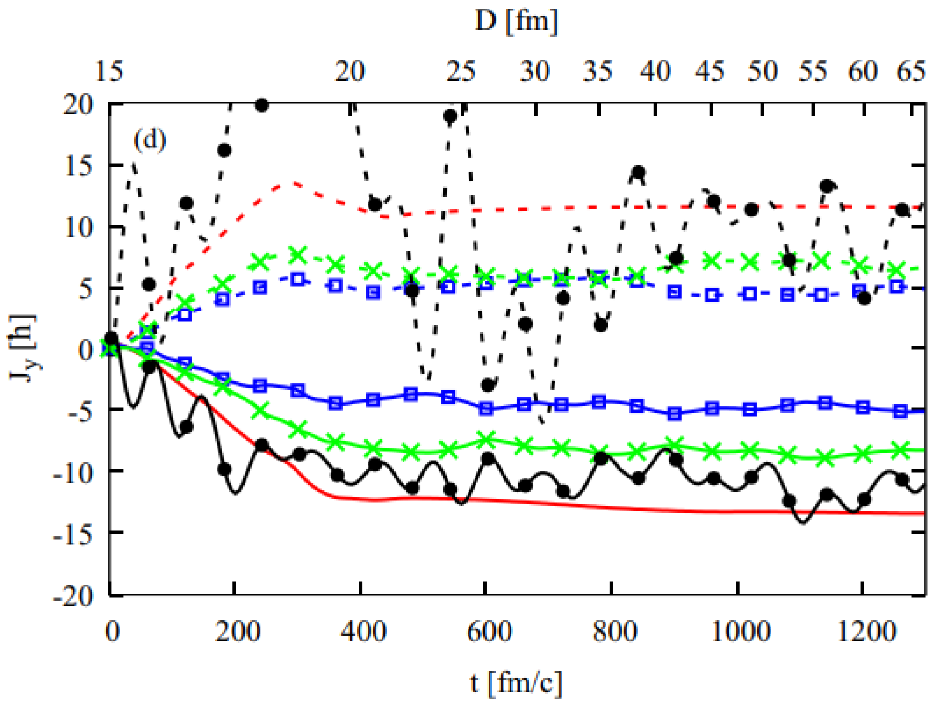
Adjustement parameters $f_{\sigma(L)}$ and $f_{\sigma(H)}$

f_σ are used as adjustement parameters to define total angular momentum ***at scission*** while they are used to reproduce γ multiplicites, which are defined ***long time after***.

Reminder : $\sigma_S^2(E) = f_\sigma^2 \mathcal{g} \frac{a}{\tilde{a}} \sqrt{\frac{U}{A}}$

$P(J) = \frac{2J+1}{2\sigma(E)^2} \exp \frac{-\left(J+\frac{1}{2}\right)^2}{2\sigma(E)^2}$ and $f_\sigma \approx 1.40$

Seems that $\sigma_S^2(E)$ should be upraded by a factor 2, taking into account the increase of total angular momentum of the fragments after scission.

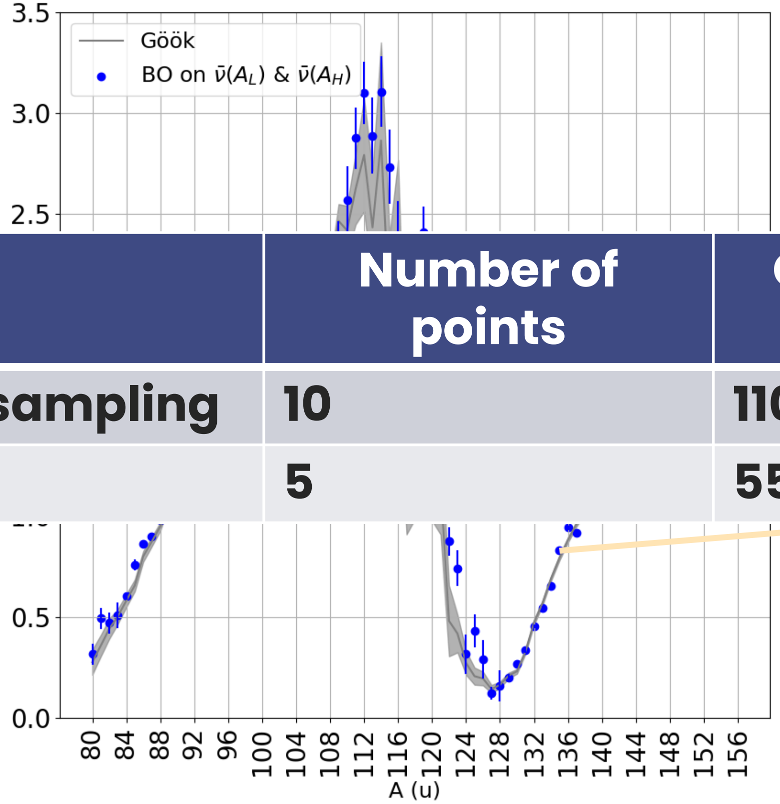


: total angular momentum for light fragment
: total angular momentum for heavy fragment

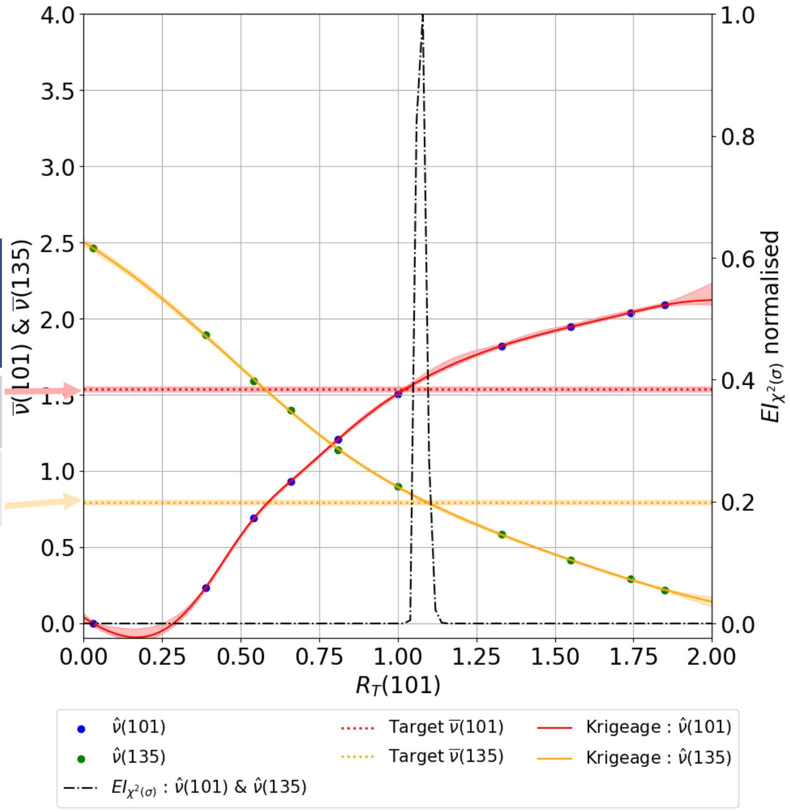
G. Scamps, Physical Review C 106.5 (2022)

Fitting the saw-tooth

Reaction : $^{235}\mathrm{U}(\mathrm{n}_{th}, \mathrm{f})$



	Number of points	Computation time (min)
Initial sampling	10	110
DoE	5	55



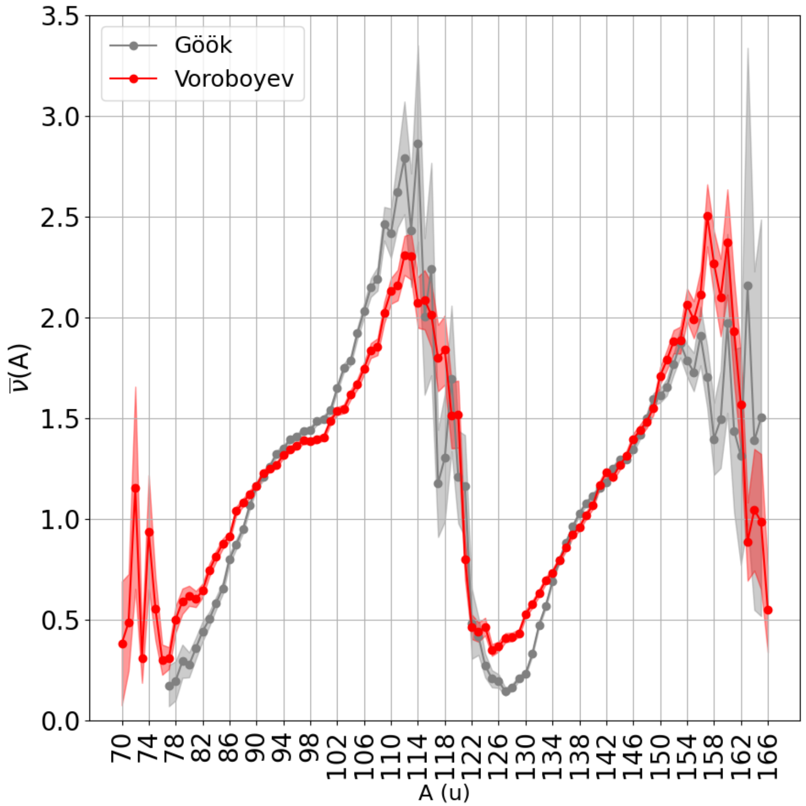
For each mass A : find $R^*_{T(A)} = \min_{R_{T(A)} \in [0,2]} \dfrac{\left(\hat{\nu}(A_L) - \bar{\nu}(A_L)\right)^2}{\sigma^2_{\bar{\nu}(A_L)}} + \dfrac{\left(\hat{\nu}(A_H) - \bar{\nu}(A_H)\right)^2}{\sigma^2_{\bar{\nu}(A_H)}}$

4. Comparaison / results

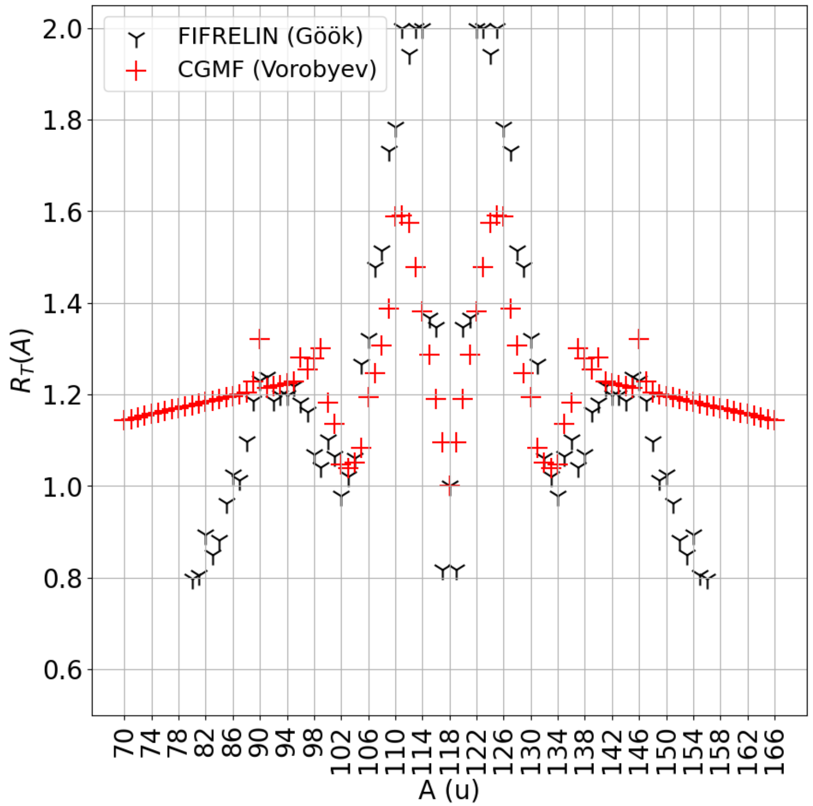
Comparaison with CGMF

Desintegration : $^{235}\mathrm{U}(\mathrm{n_{th}}, \mathrm{f})$

Saw-tooth used : Göök (2018) and Vorobyev (2010)

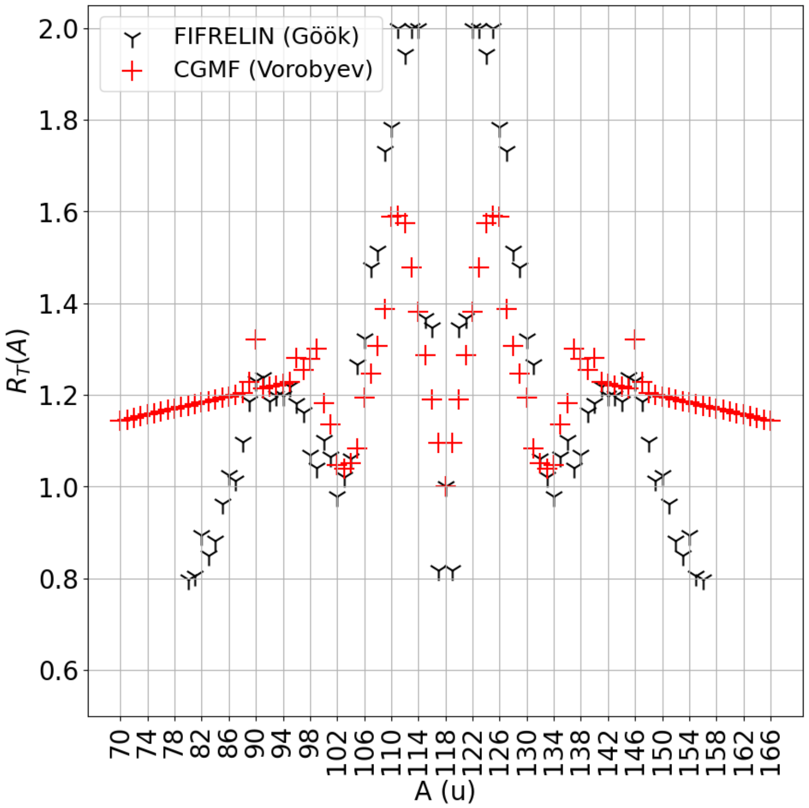


Models $R_T(A)$ produced by optimization for FIFRELIN and CGMF



Comparaison with CGMF

Desintegration : $^{235}\mathrm{U}(\mathrm{n_{th}}, \mathrm{f})$



Structures show-up around :

- Maximum should be aroud $\boldsymbol{A \approx 132}$ $(\mathbf{N = 82, Z = 50})$, since *heavy fragment is double-magic* but instead is around $A = 125$. ***Structure already seen*** by Tudora and Kessedjian (on post emission emission mass yields).

- $\boldsymbol{A \approx 140}$ $(\mathbf{N = 84, Z = 56})$, *where* $Z = 56$ can also be considered *magic* for octupole deformation.

- $\boldsymbol{A \approx 136}$ $(\mathbf{N = 82, Z = 52})$, *where* $Z = 52$ can also be considered *magic* for octupole deformation.

A. Tudora, P. Gogita, Eur. Phys. J. A 60,9, 190 (2024)

Conclusion

- **Bayesian Optimization** is well-suited applied on stochastic codes such as FIFRELIN.
- Automation of the adjustement procedure of the **free parameters** that correctly reproduce experimental data.
- Gives us interesting physical insights to investigate.

Perspectives

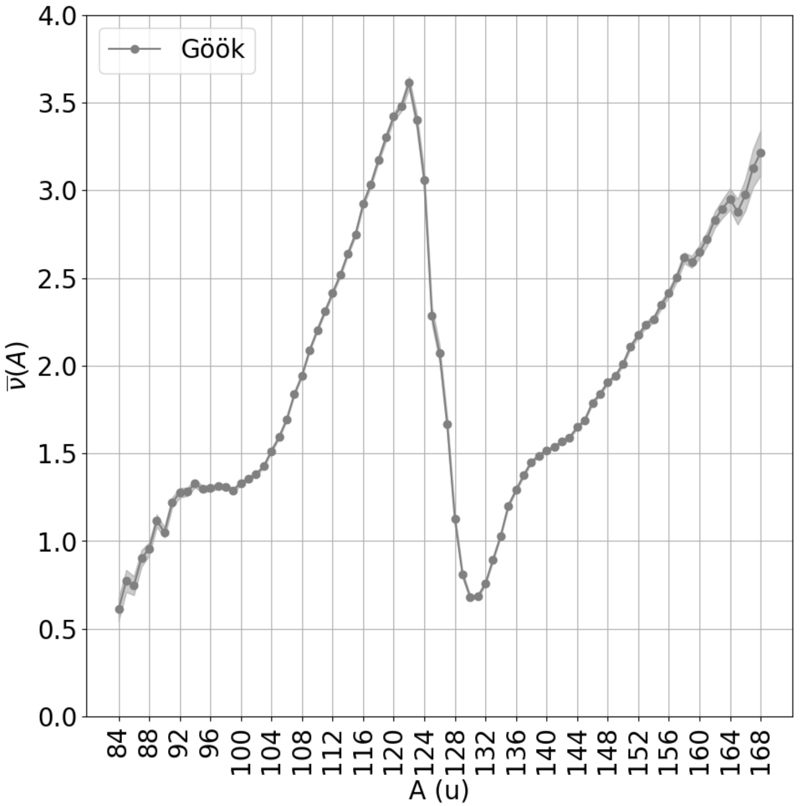
- Differents targets to reproduce
- Different reactions (only two reactions studied now)

Thank you

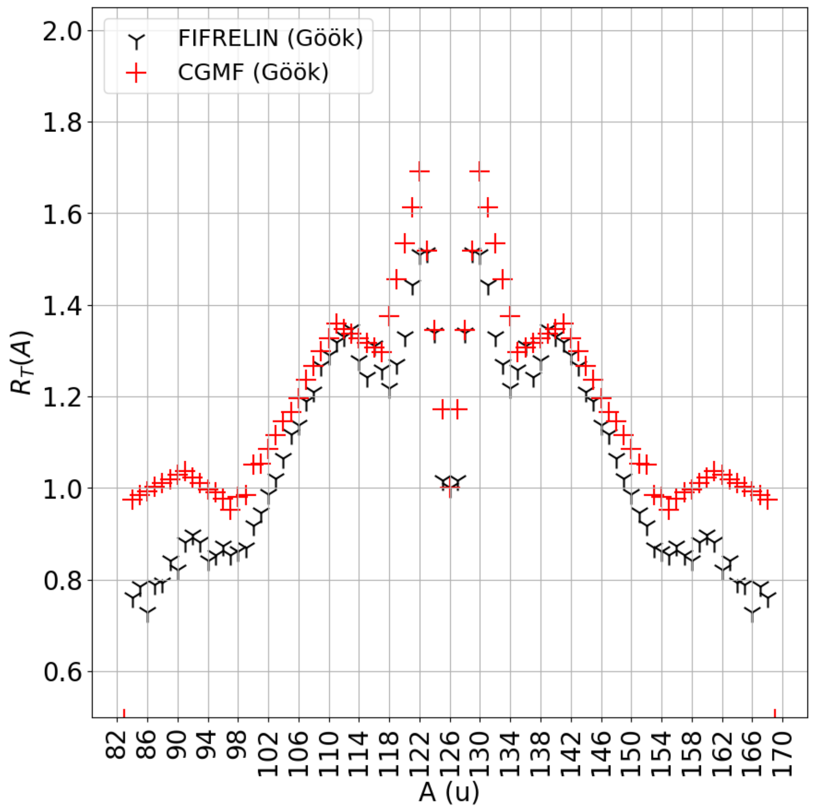
Comparaison with CGMF

Desintegration : $^{252}\mathrm{Cf(sf)}$

Saw-tooth used : Göök (2014)

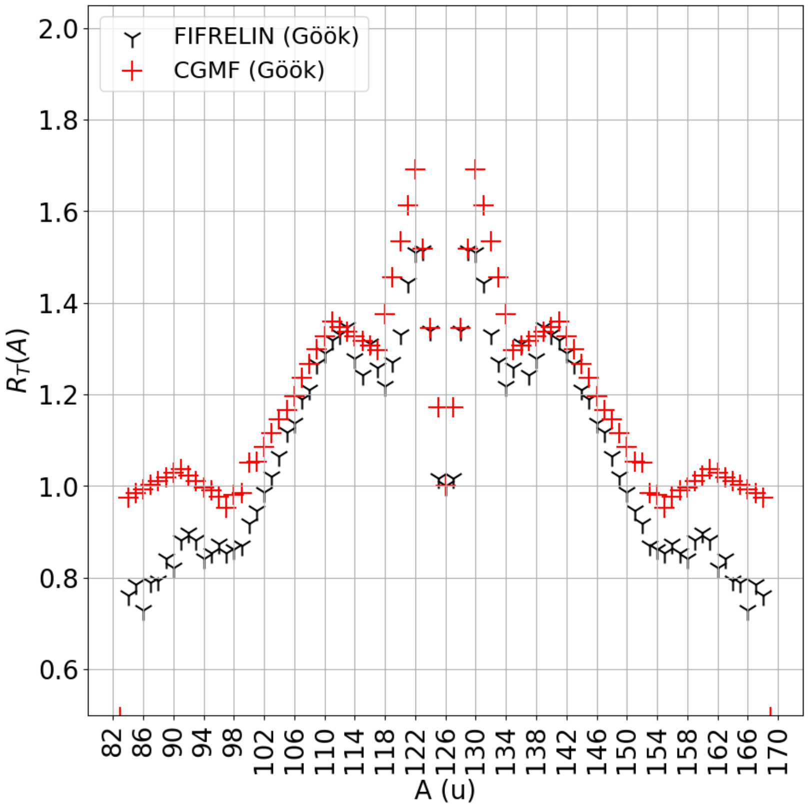


Models $R_T(A)$ produced by optimization for FIFRELIN and CGMF



Comparaison with CGMF

Desintegration : $^{252}\mathrm{Cf(sf)}$



Structures show-up around :

- $\boldsymbol{A \approx 132}$ $(\mathbf{N = 82, Z = 50})$, which seems normal since *heavy fragment is double-magic.*
- $\boldsymbol{A \approx 140}$ $(\mathbf{N = 84, Z = 56})$, *where* $Z = 56$ can also be considered *magic* for octupole deformation.
- $\boldsymbol{A \approx 136}$ $(\mathbf{N = 82, Z = 52})$, *where* $Z = 52$ can also be considered *magic* for octupole deformation.