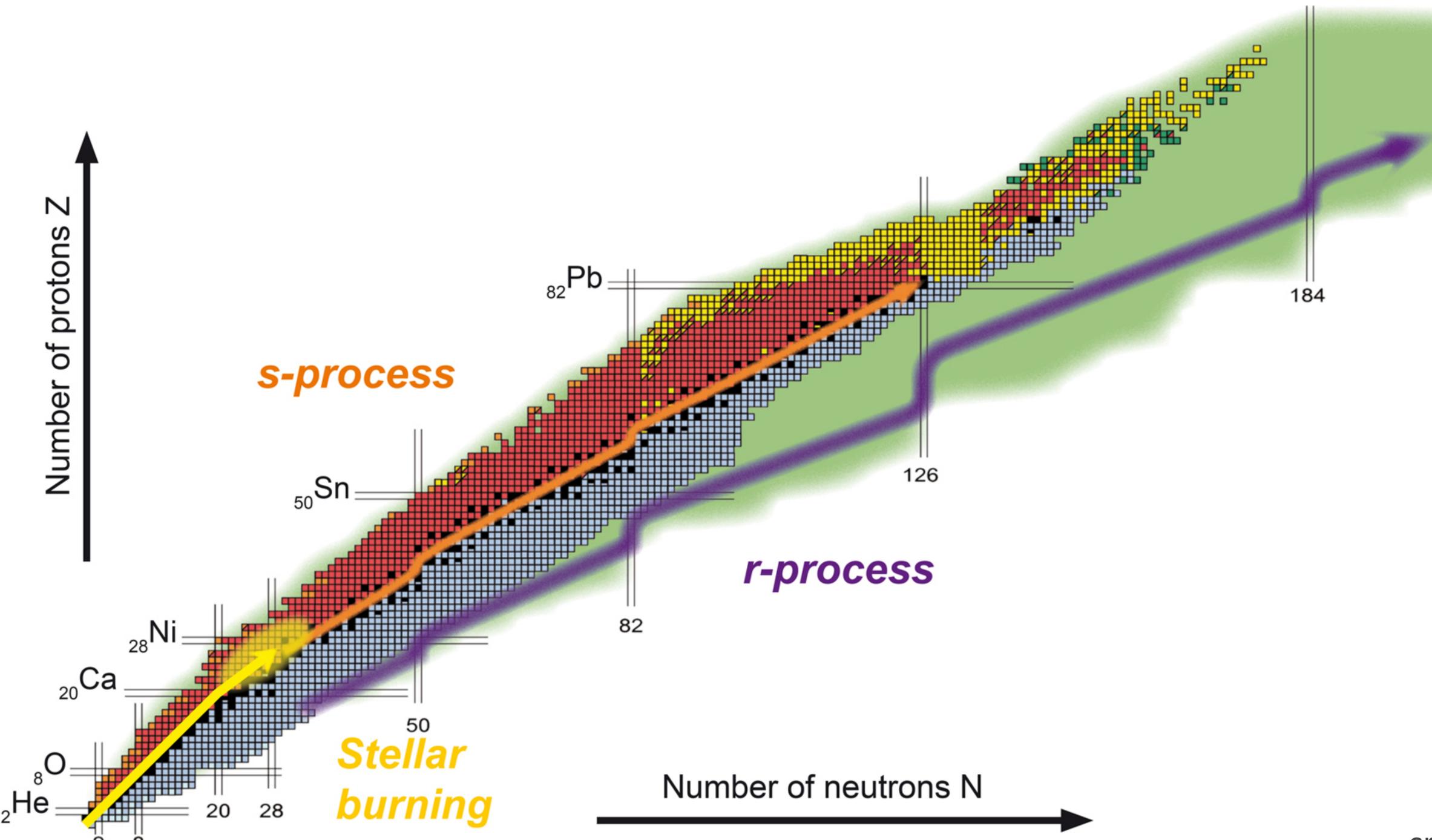


Microscopic large-scale fission calculations with BSkg3

Adrián Sánchez Fernández, Wouter Ryssens and Stéphane Goriely

The origin of the heaviest elements

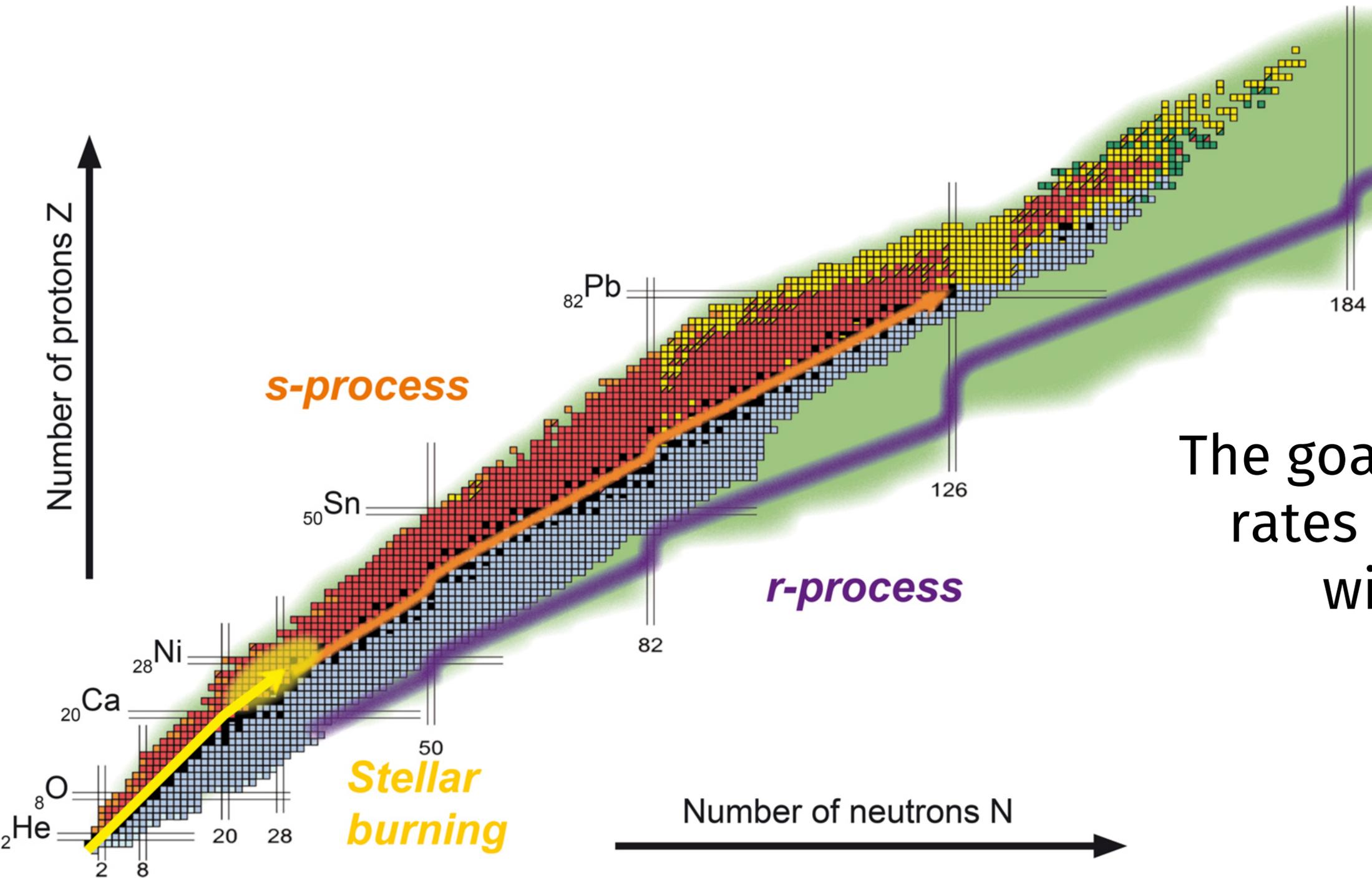
Or at least half of them...



credit: EMMI, GSI/Different Arts

The origin of the heaviest elements

Or at least half of them...



The goal: complete set of fission rates and yields for $Z=[90,118]$ with the same microscopic model (BSkG3 EDF).

credit: EMMI, GSI/Different Arts

Why BSkG3?

Ground state properties

2457 atomic masses
810 charge radii

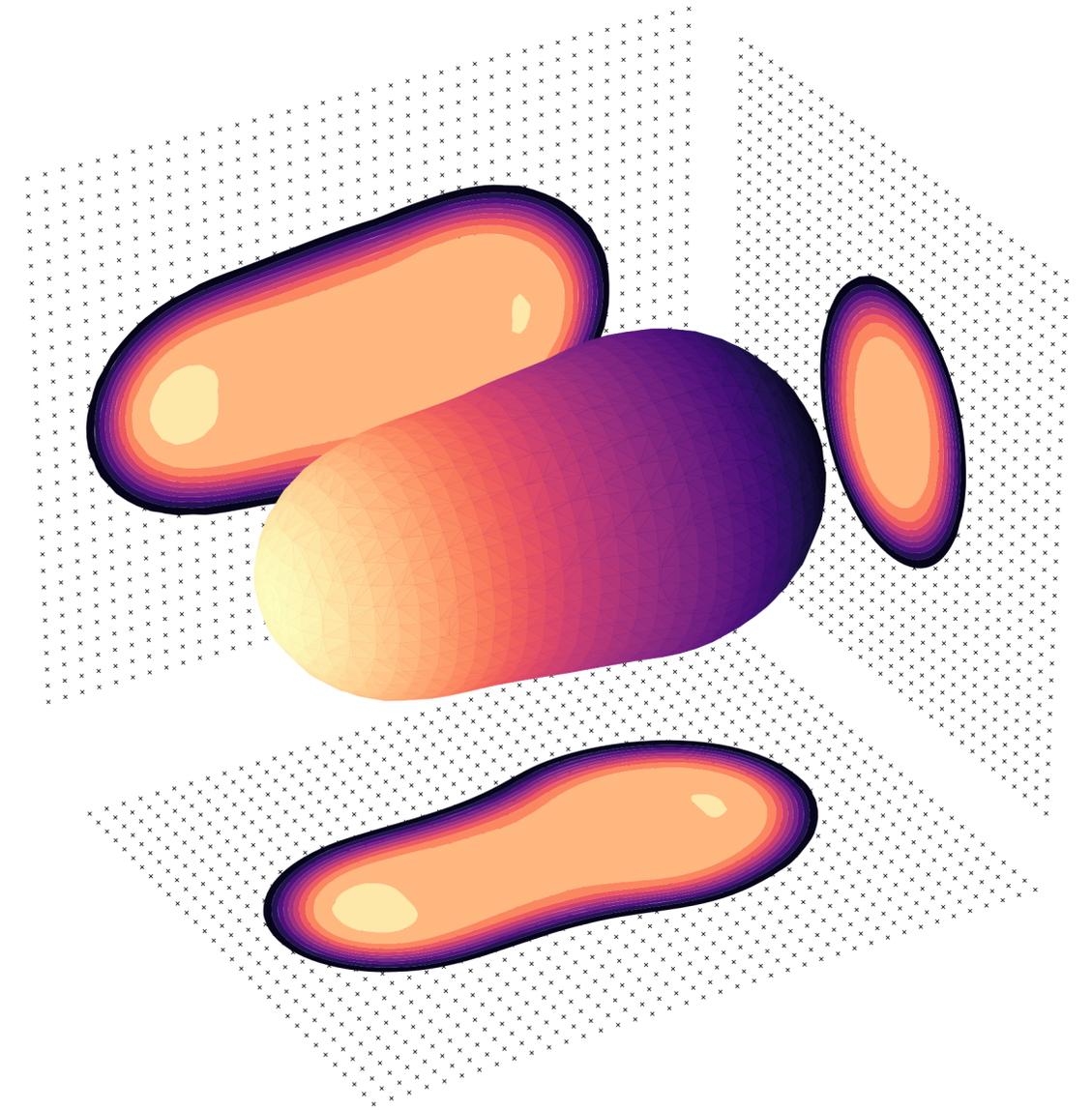
rms deviation

0.631 MeV
0.0237 fm

Fission properties

45 primary fission barriers:
45 secondary fission barriers
28 isomeric excitation energies

0.33 MeV
0.51 MeV
0.34 MeV

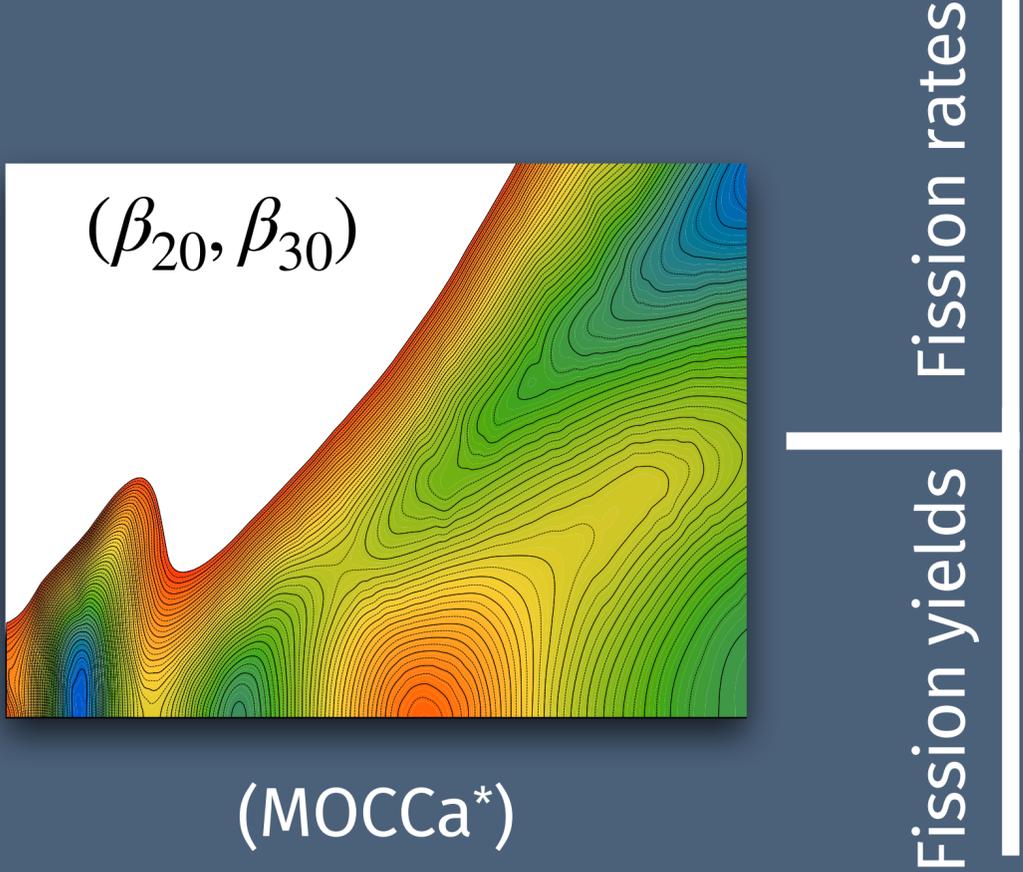


W. Ryssens et al, EPJ A 59(5), 96

Methodology

3

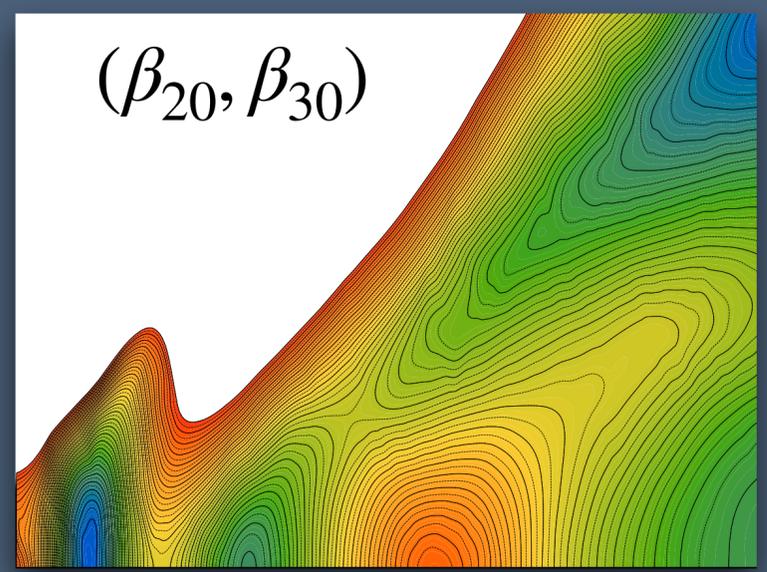
* W. Ryssens, Ph.D. Thesis, ULB (2016)



Methodology

* W. Ryssens, Ph.D. Thesis, ULB (2016)

** E. Flynn et al, Phys. Rev. C 105, 054302

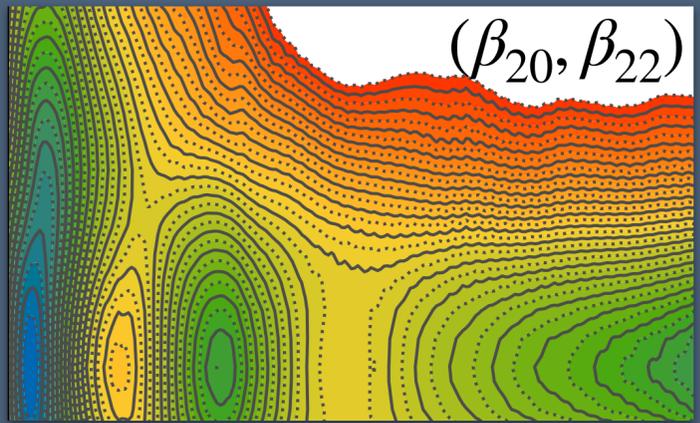


(MOCCa*)

Fission rates

Fission yields

MEP
(PyNEB**)



+ collective inertias

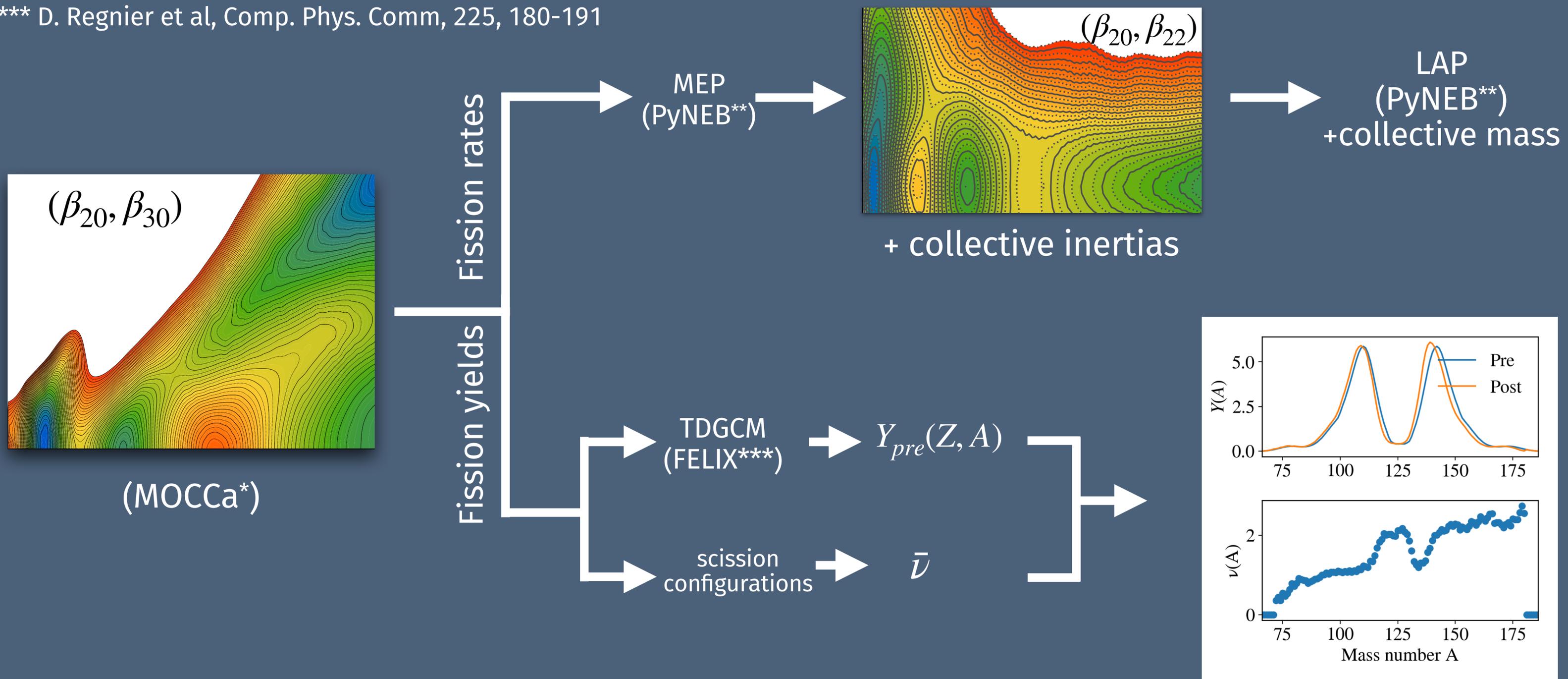
LAP
(PyNEB**)
+ collective mass

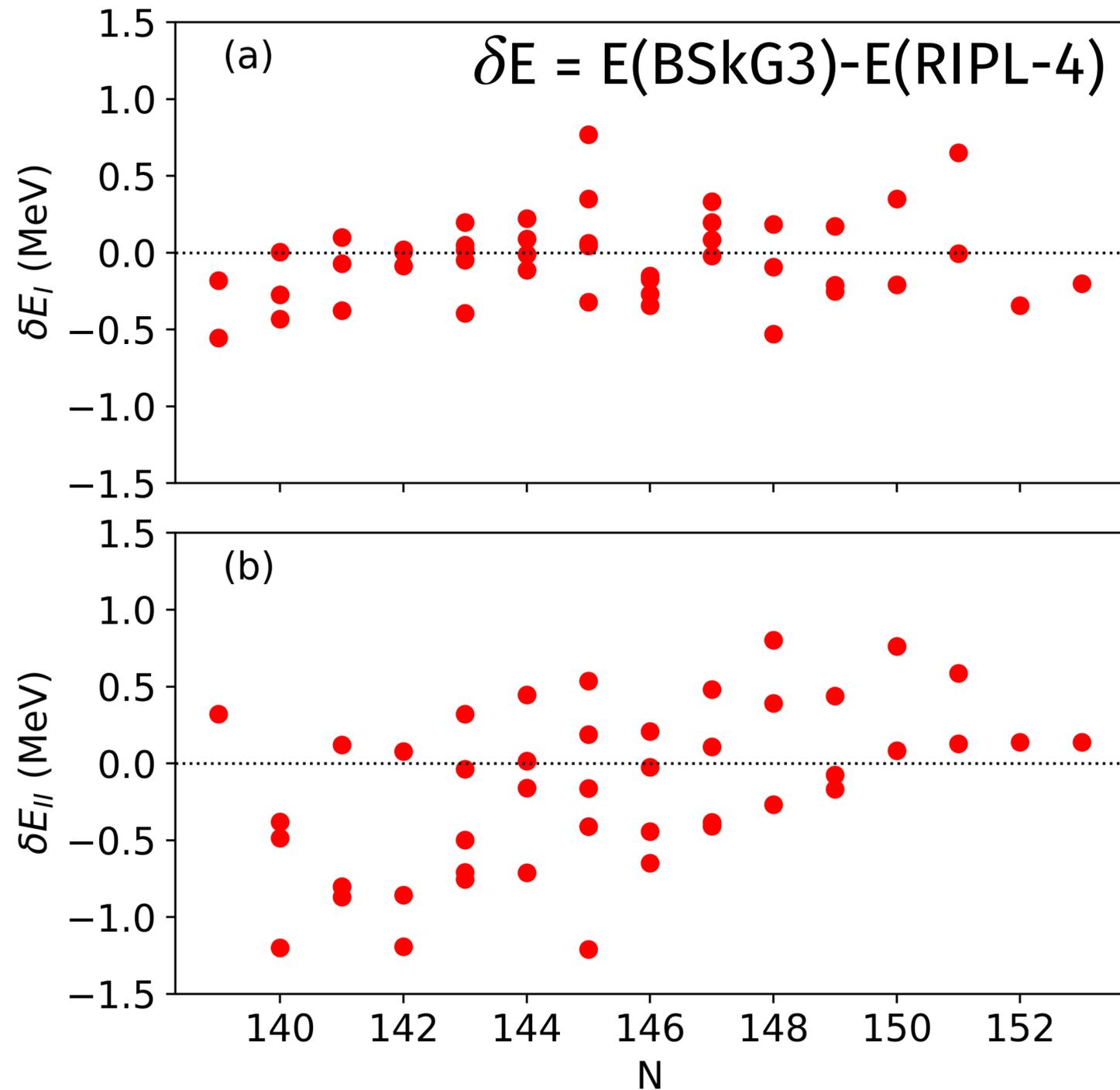
Methodology

* W. Ryssens, Ph.D. Thesis, ULB (2016)

** E. Flynn et al, Phys. Rev. C 105, 054302

*** D. Regnier et al, Comp. Phys. Comm, 225, 180-191





How do we perform?

RIPL-4 empirical fission barriers

Primary barrier (E_I)

rms-deviation: 0.28 MeV
mean deviation: -0.04 MeV

Secondary barrier (E_{II})

rms-deviation: 0.59 MeV
mean deviation: -0.18 MeV

How do we perform?

RIPL-4 empirical fission barriers

Primary barrier (E_I)

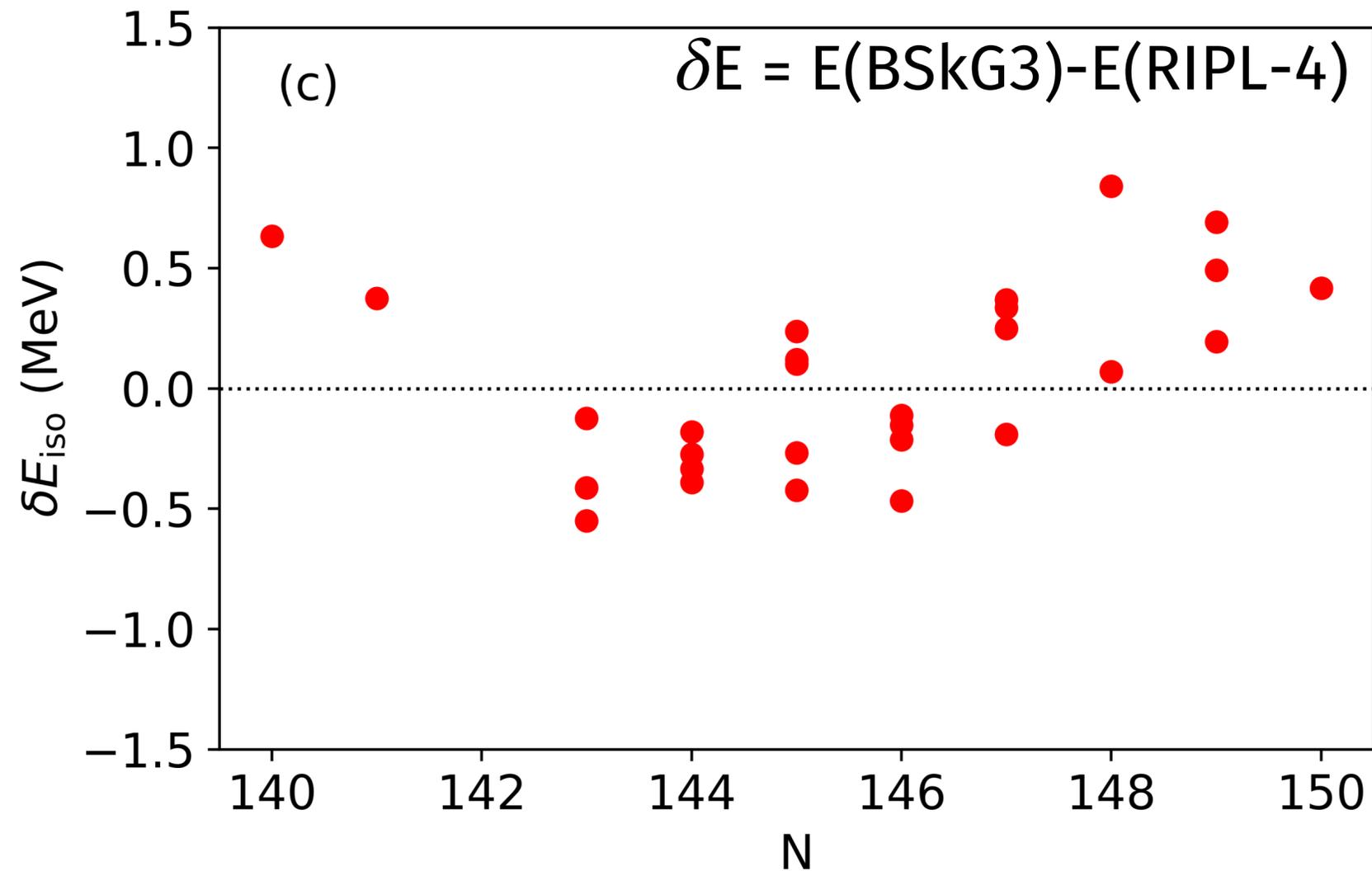
rms-deviation: 0.28 MeV
mean deviation: -0.04 MeV

Secondary barrier (E_{II})

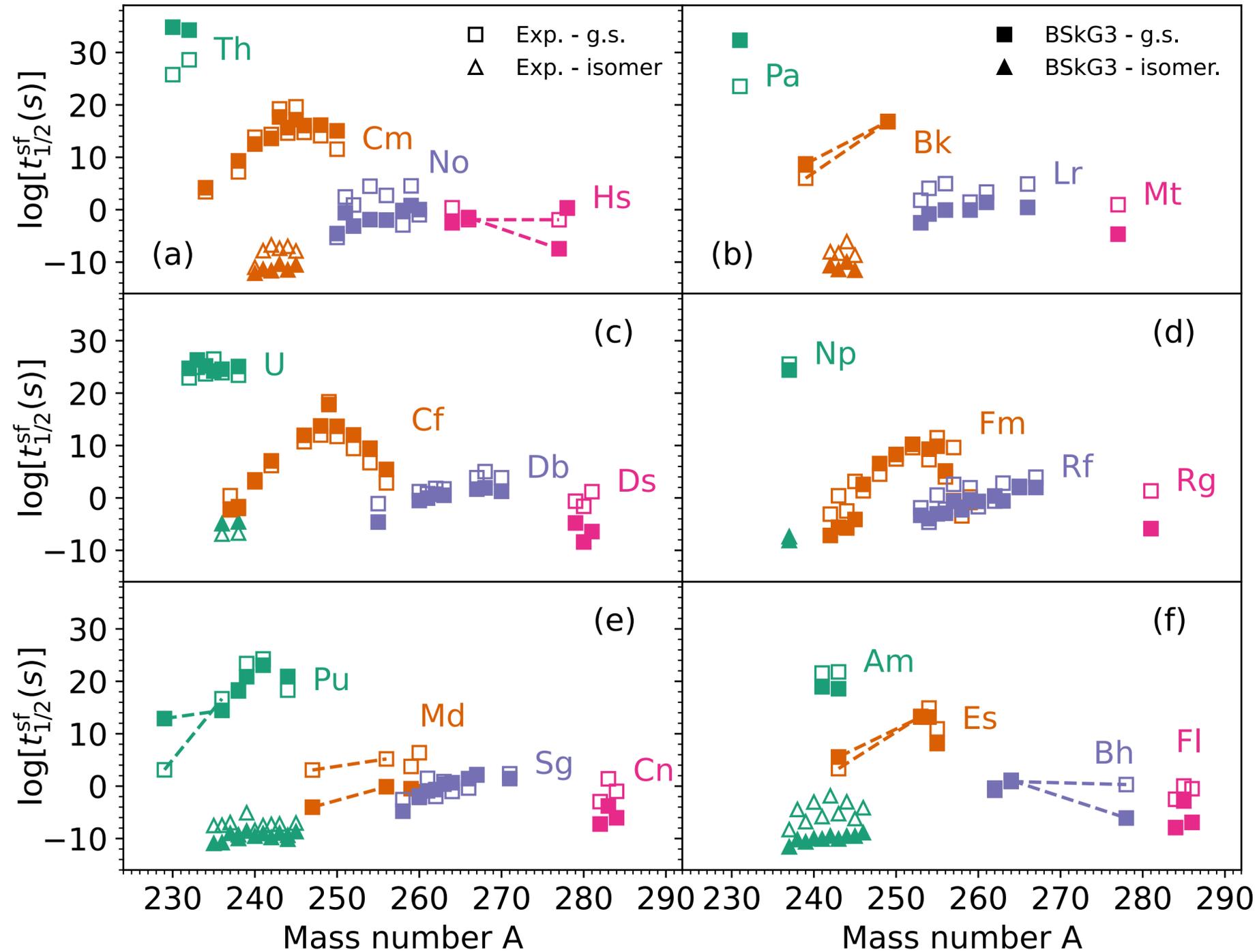
rms-deviation: 0.59 MeV
mean deviation: -0.18 MeV

Isomer excitation energy (E_{iso})

rms-deviation: 0.38 MeV
mean deviation: 0.04 MeV



How do we perform?



Spontaneous fission half-lives

A. Sánchez-Fernández et al., Phys. Lett. B 874 (2026) 140287

GS SF half-lives (107 nuclei):

rms deviation: $1.1 \cdot 10^3$

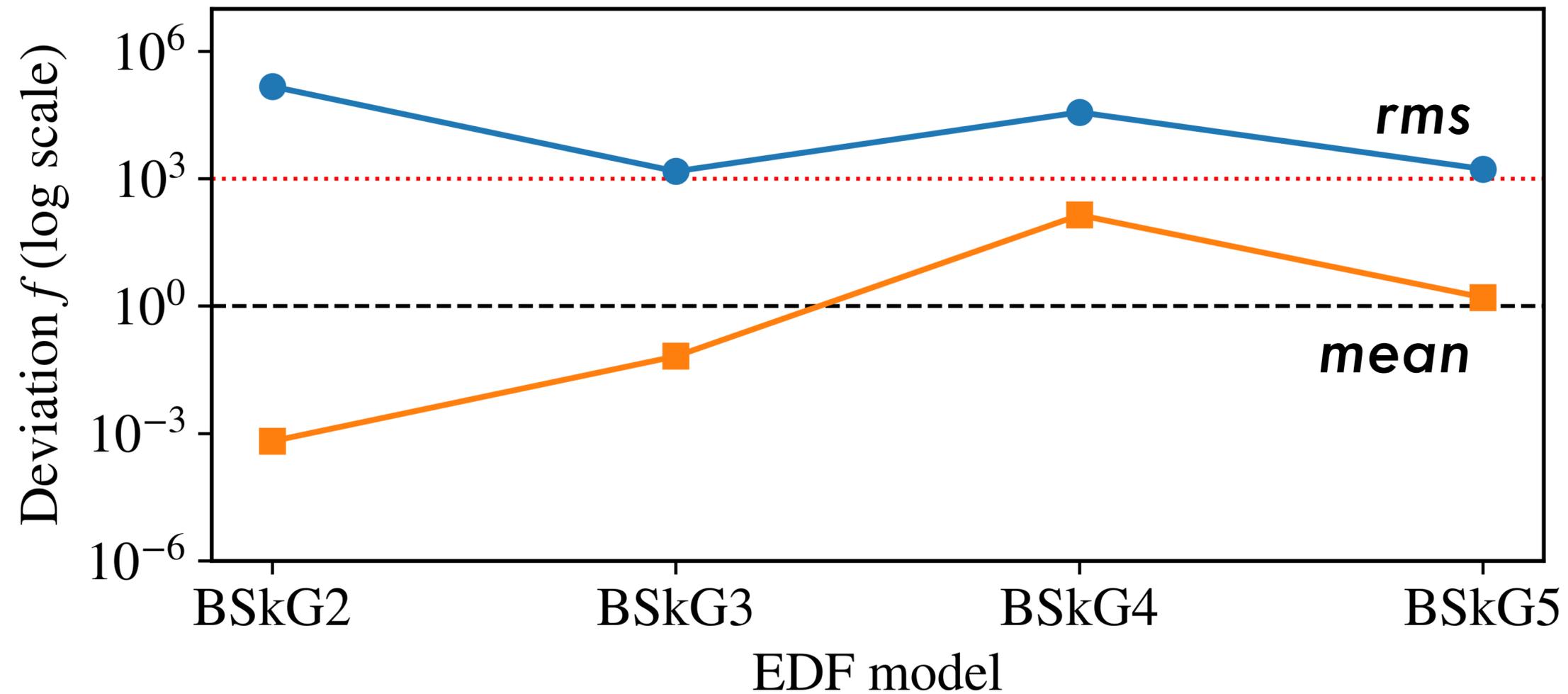
mean deviation: $7.5 \cdot 10^{-2}$

Isomer SF half-lives (29 nuclei):

rms deviation: $5.3 \cdot 10^3$

mean deviation: $7.2 \cdot 10^{-4}$

How do we perform?



Large-scale fission properties I: fission paths and SF half-lives

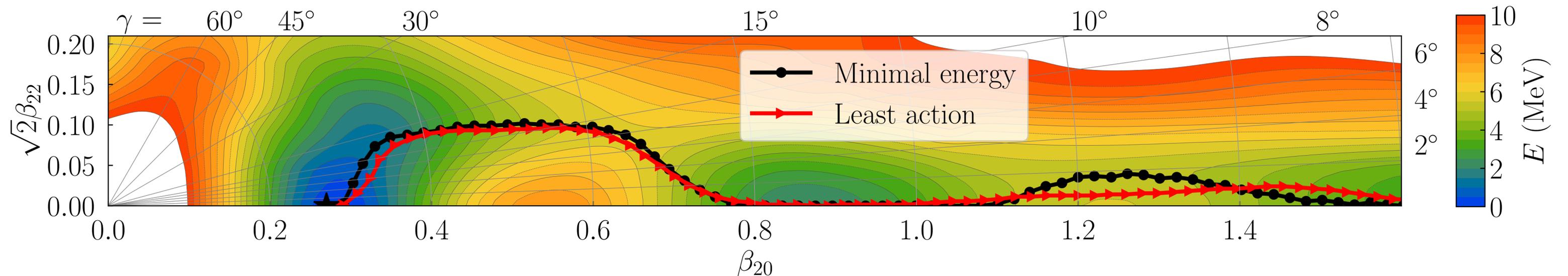
First large-scale HFB study exploring explicitly octupole and triaxial deformations (2.5D) in $Z=[80,118]$.

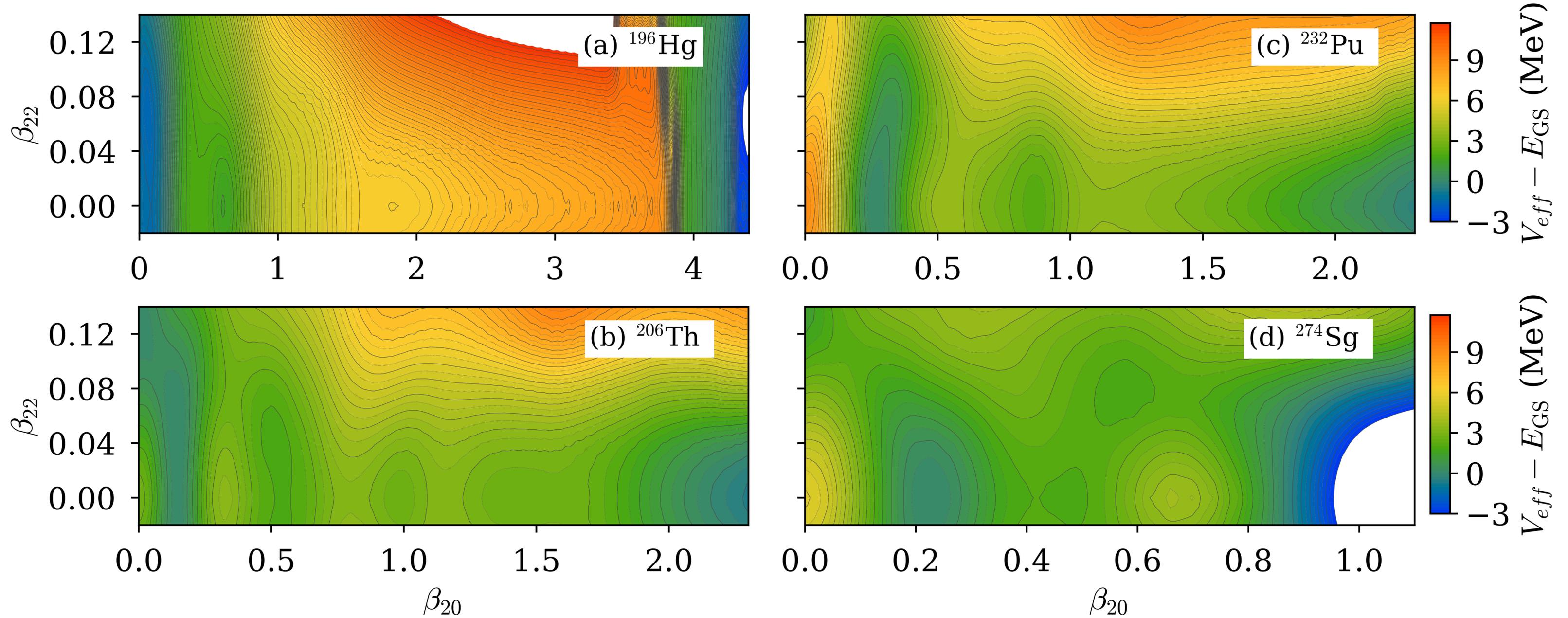
- How common are double-humped paths?
- What are the shapes of the saddle points?
- What is the impact of triaxility on the barrier heights?

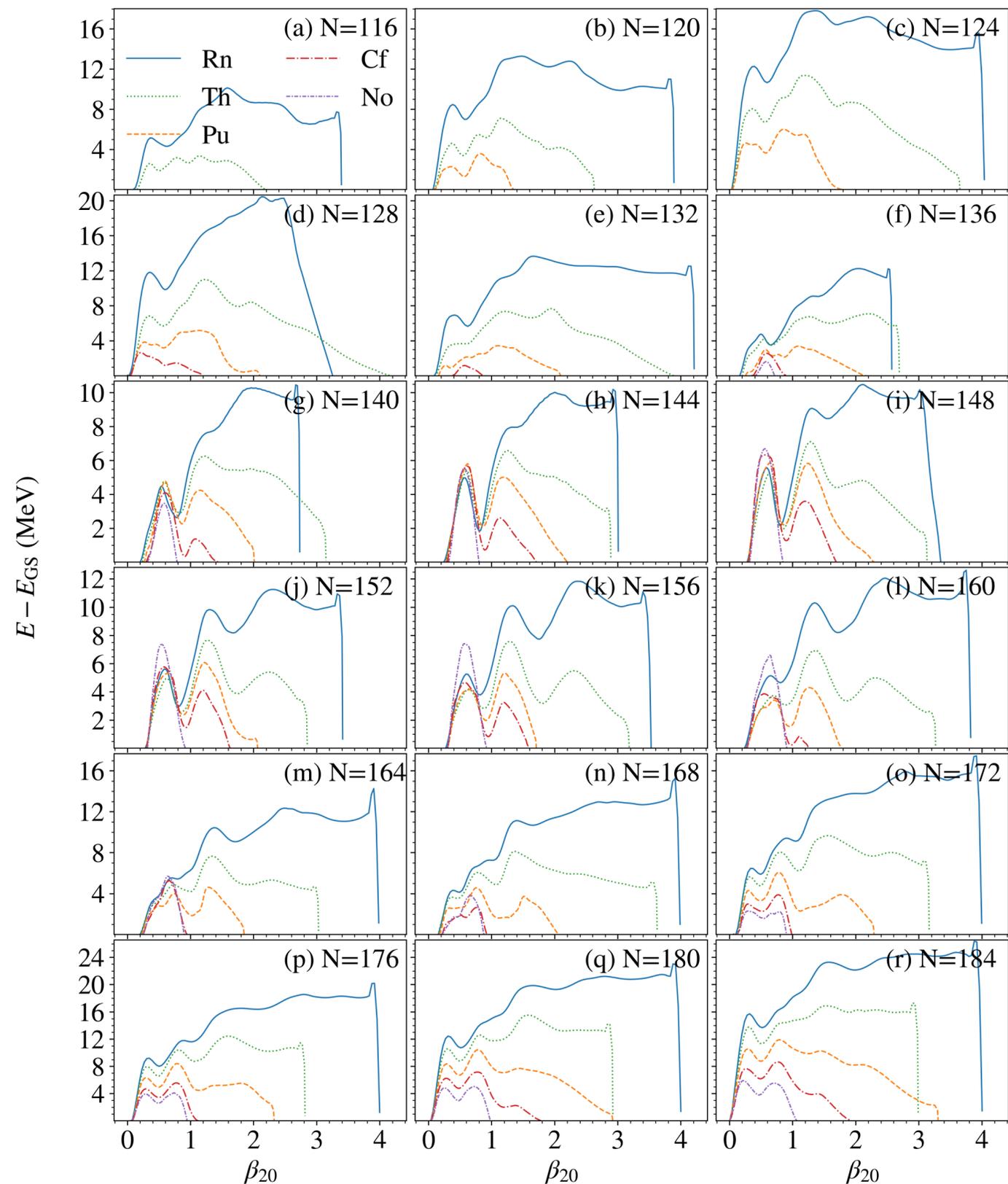
Large-scale fission properties I: fission paths and SF half-lives

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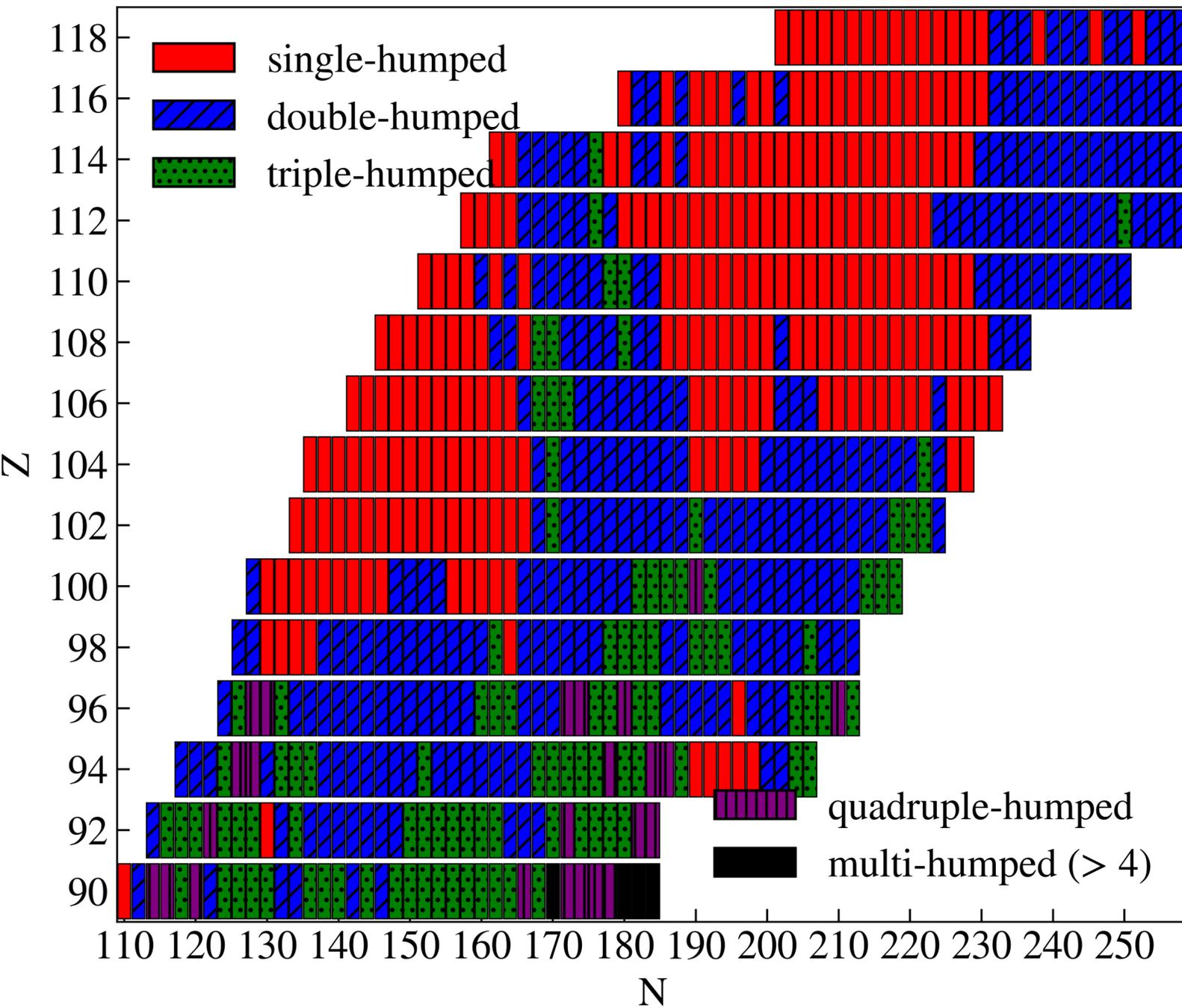




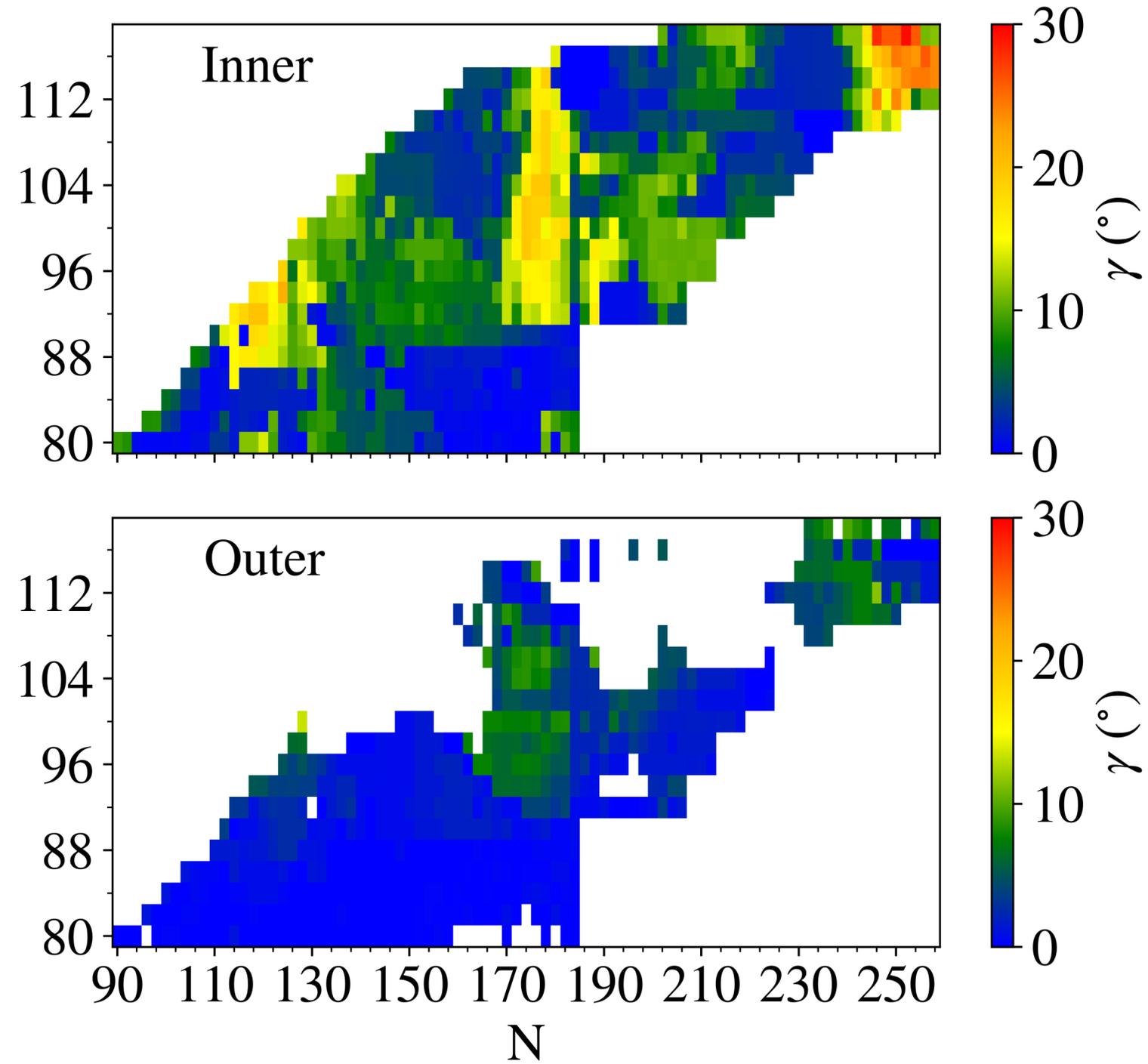
Large-scale fission properties I: fission paths and SF half-lives

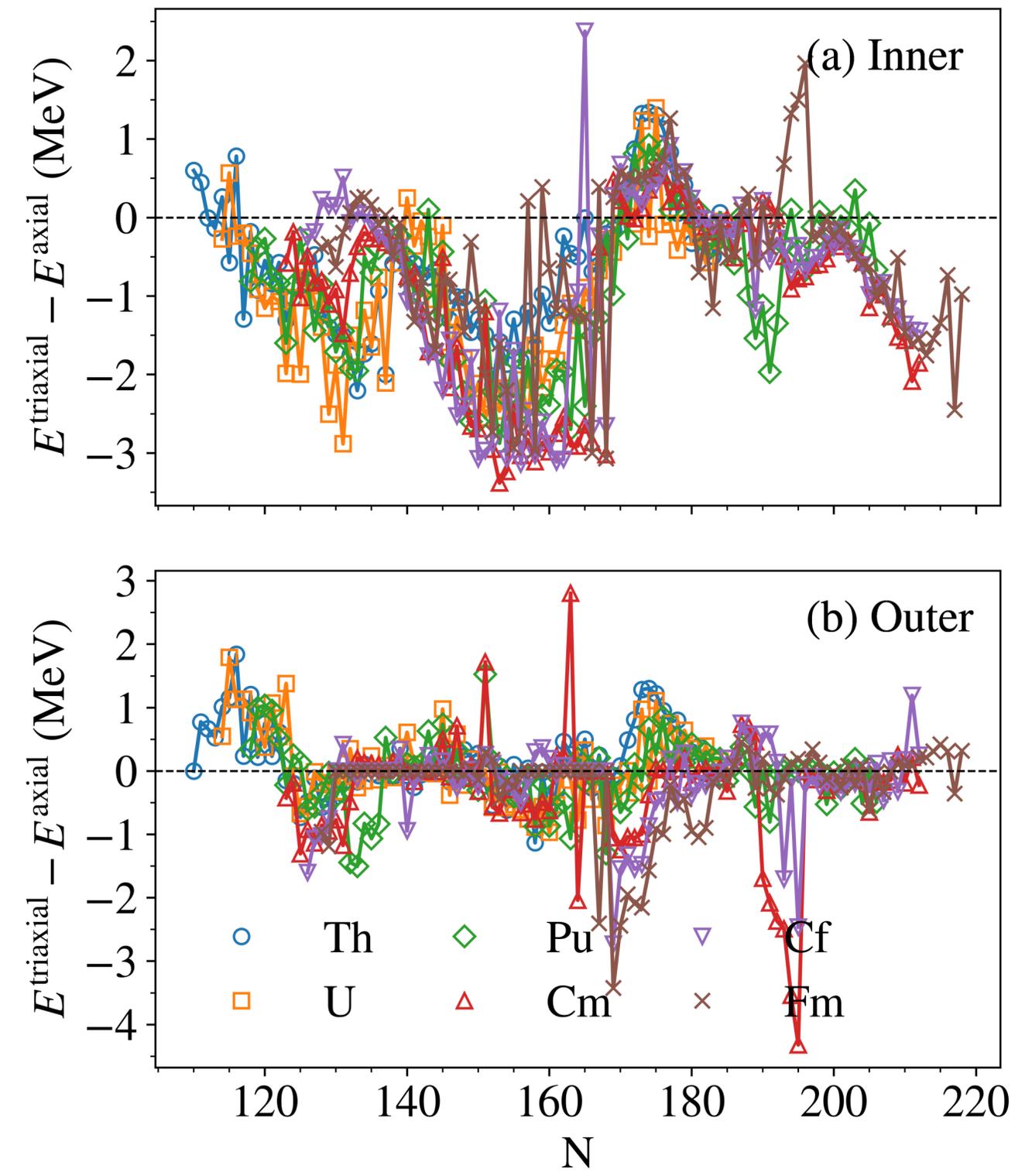
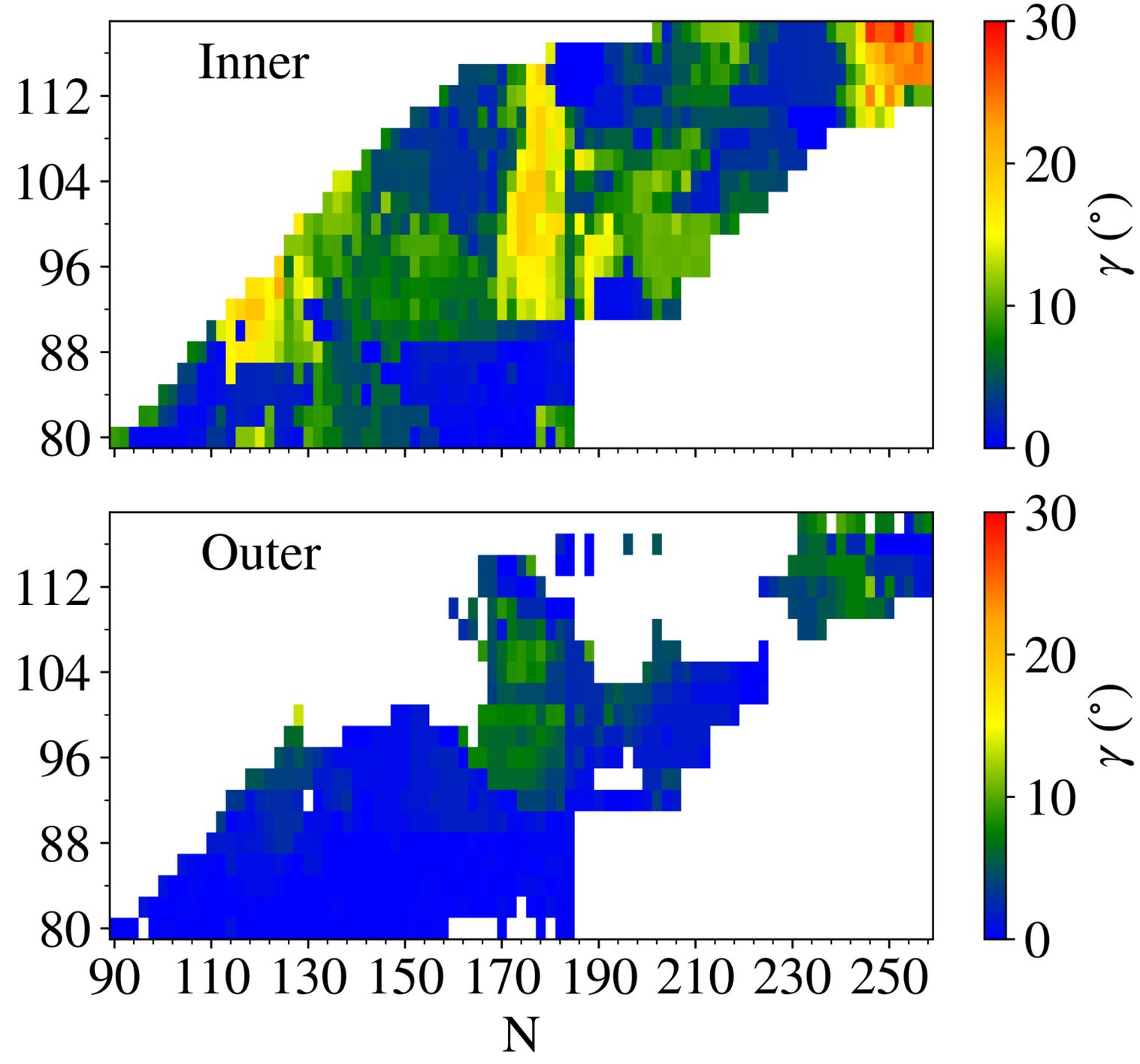
- initial point: GS
- end point: semiclassical outer turning point or scission.

- Position of the barriers remains constant
- Number of humps vary from 1 to 4 (above the GS)

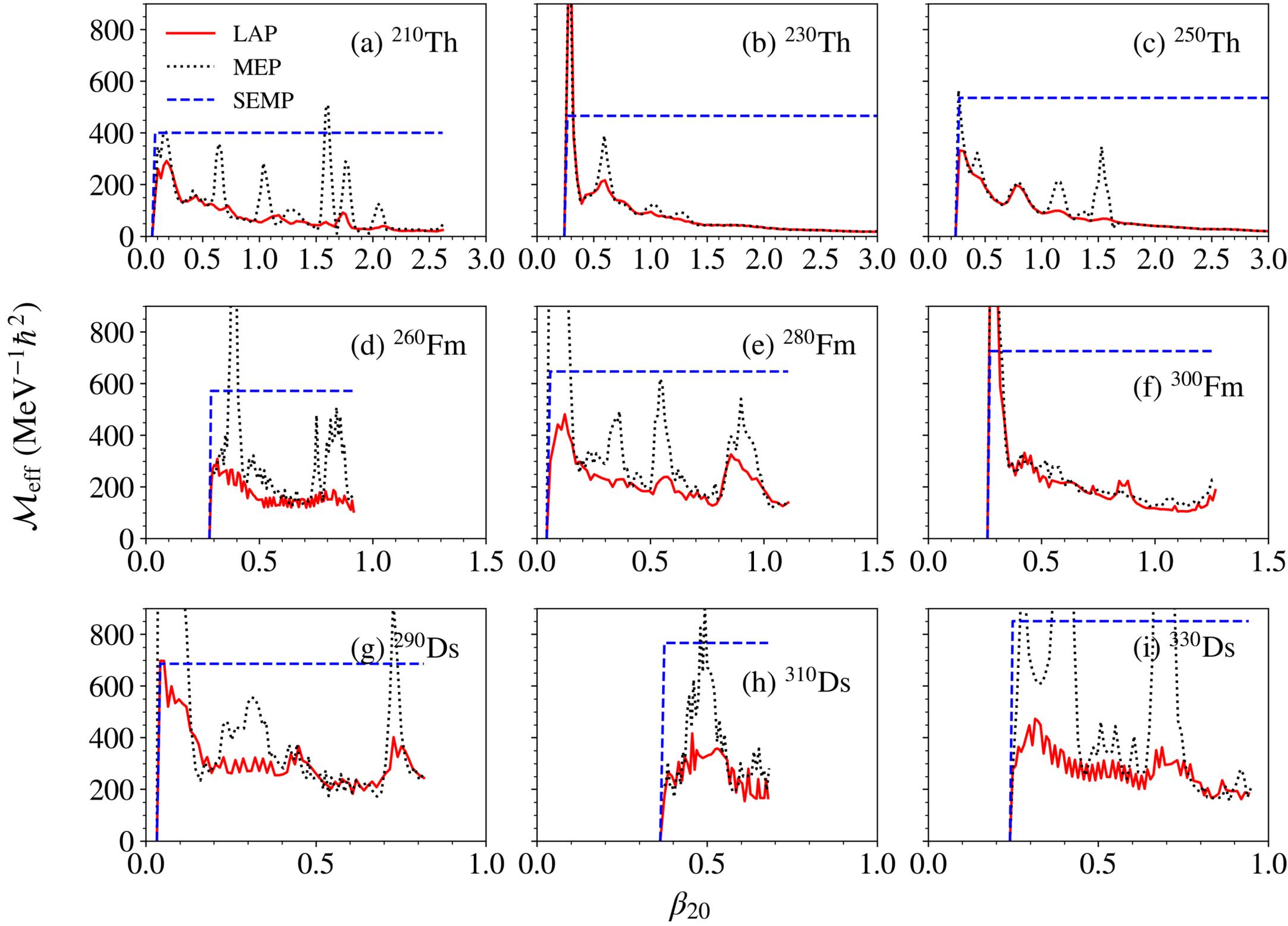


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Large-scale fission properties I: fission paths and SF half-lives

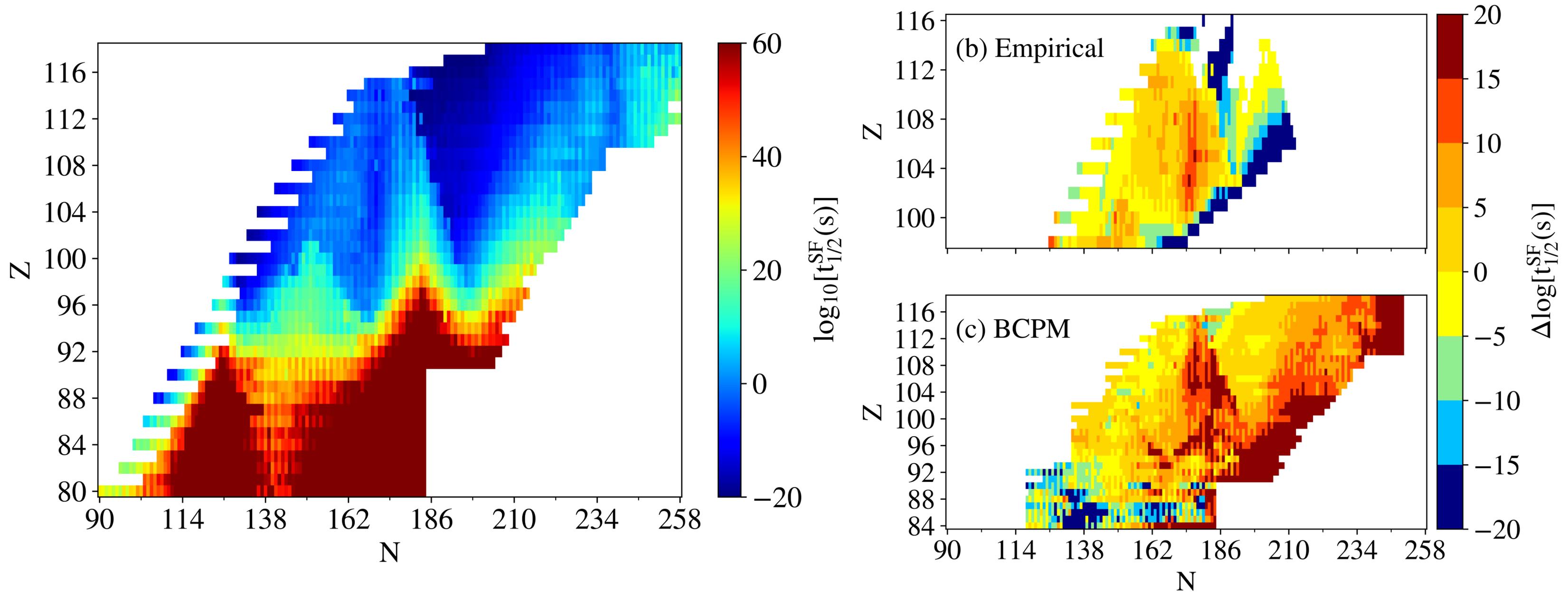


- Minimizing the action smooths out the collective inertial mass along the paths

- the semi-empirical formula can be way off..

$$\mathcal{M}_{\text{eff}}^{\text{SEMP}} = 0.054A^{5/3} \text{ MeV}^{-1}\hbar^2$$

Large-scale fission properties I: fission paths and SF half-lives



ETFSI barriers

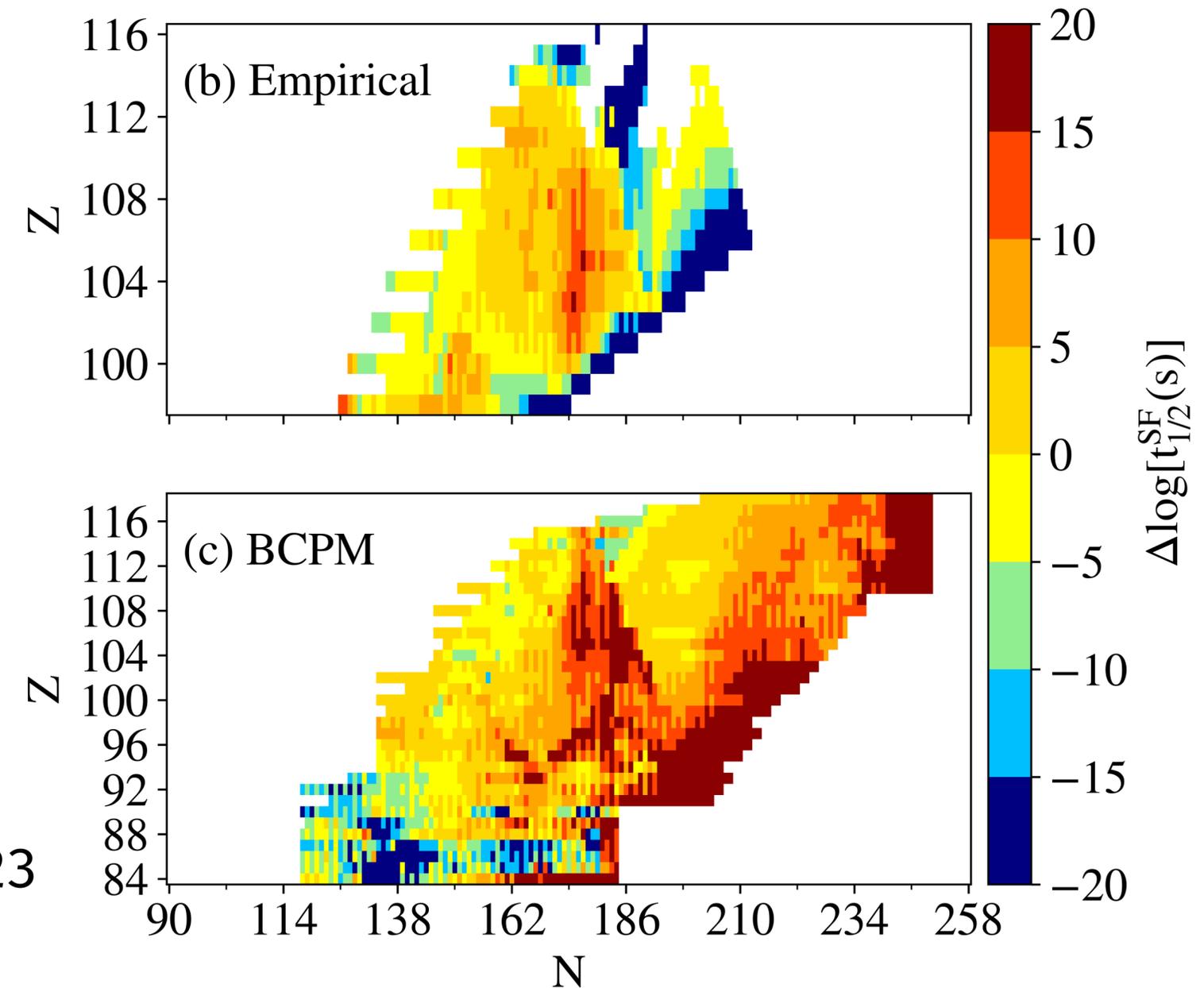
$$\hbar\omega = 0.14025 \cdot Z^2/A - 4.6335$$

FRLDM barriers

$$\hbar\omega = -0.02534(Z^2/A)^2 + 2.10736 \cdot Z^2/A - 42.7659$$

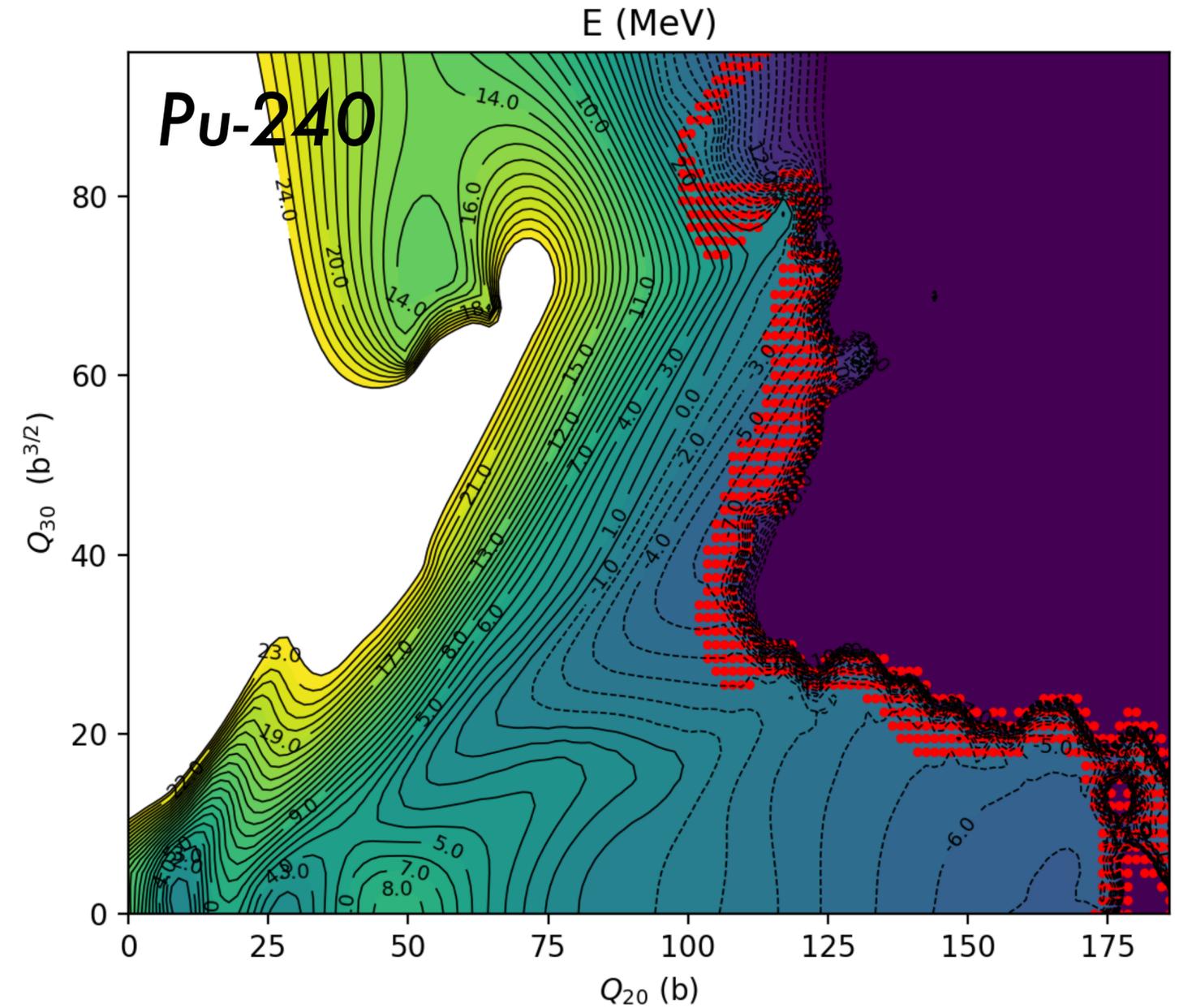
J. Khuyagbaatar. Nuclear Physics A, 1002 (2020) 121958.

S. Giuliani et al. Phys. Rev. C, 97 (3) 034323



Large-scale fission properties II: fission fragments distributions

TDGCM + BSkG3 PESes and collective inertias

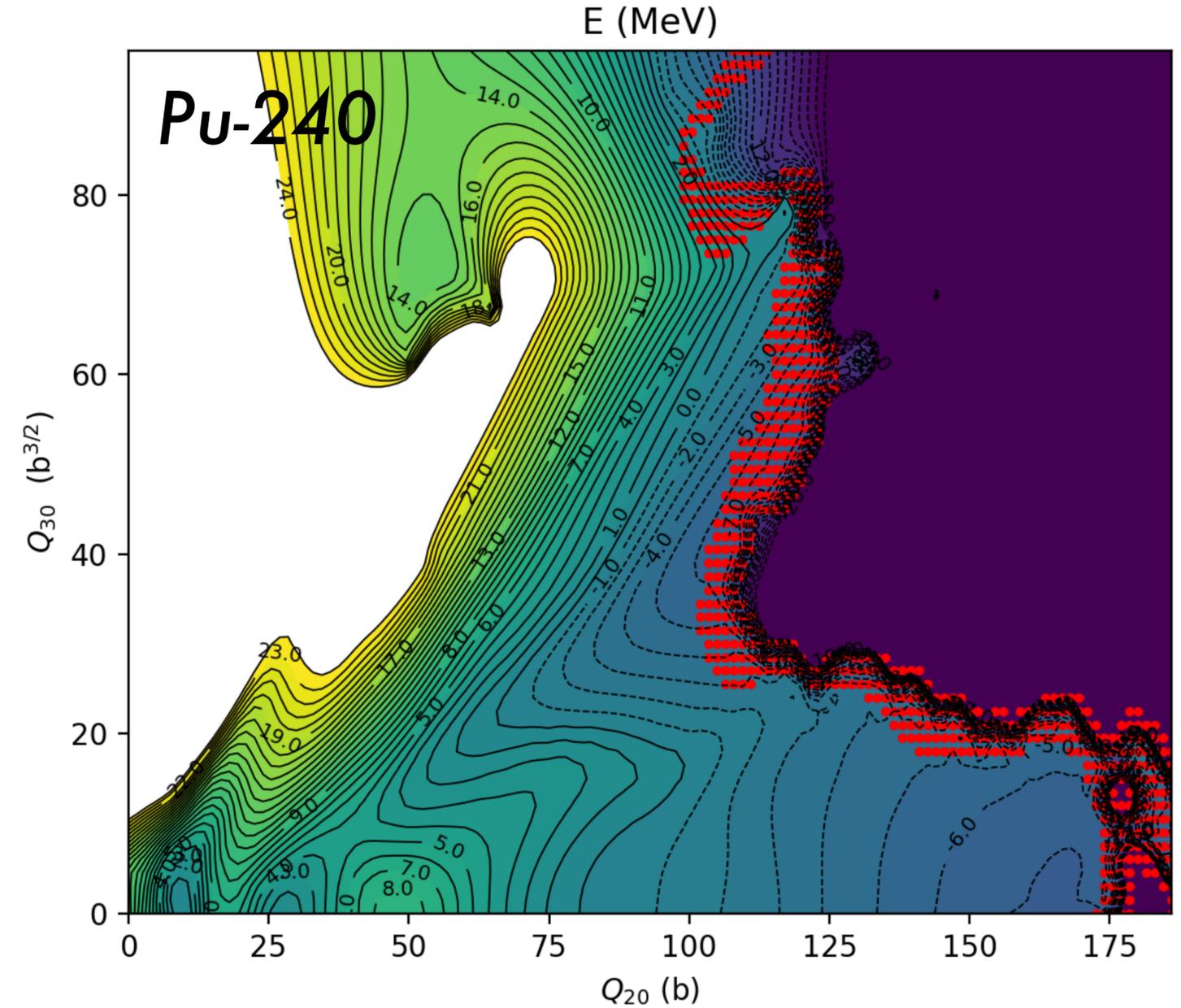


Large-scale fission properties II: fission fragments distributions

TDGCM + BSkG3 PESes and collective inertias

scission configurations $\text{TKE} \approx e^2 \frac{Z_L Z_H}{d_{ch}}$

$$\text{TXE} = \sum_i E_{def}^i + E_{dis}$$



Large-scale fission properties II: fission fragments distributions

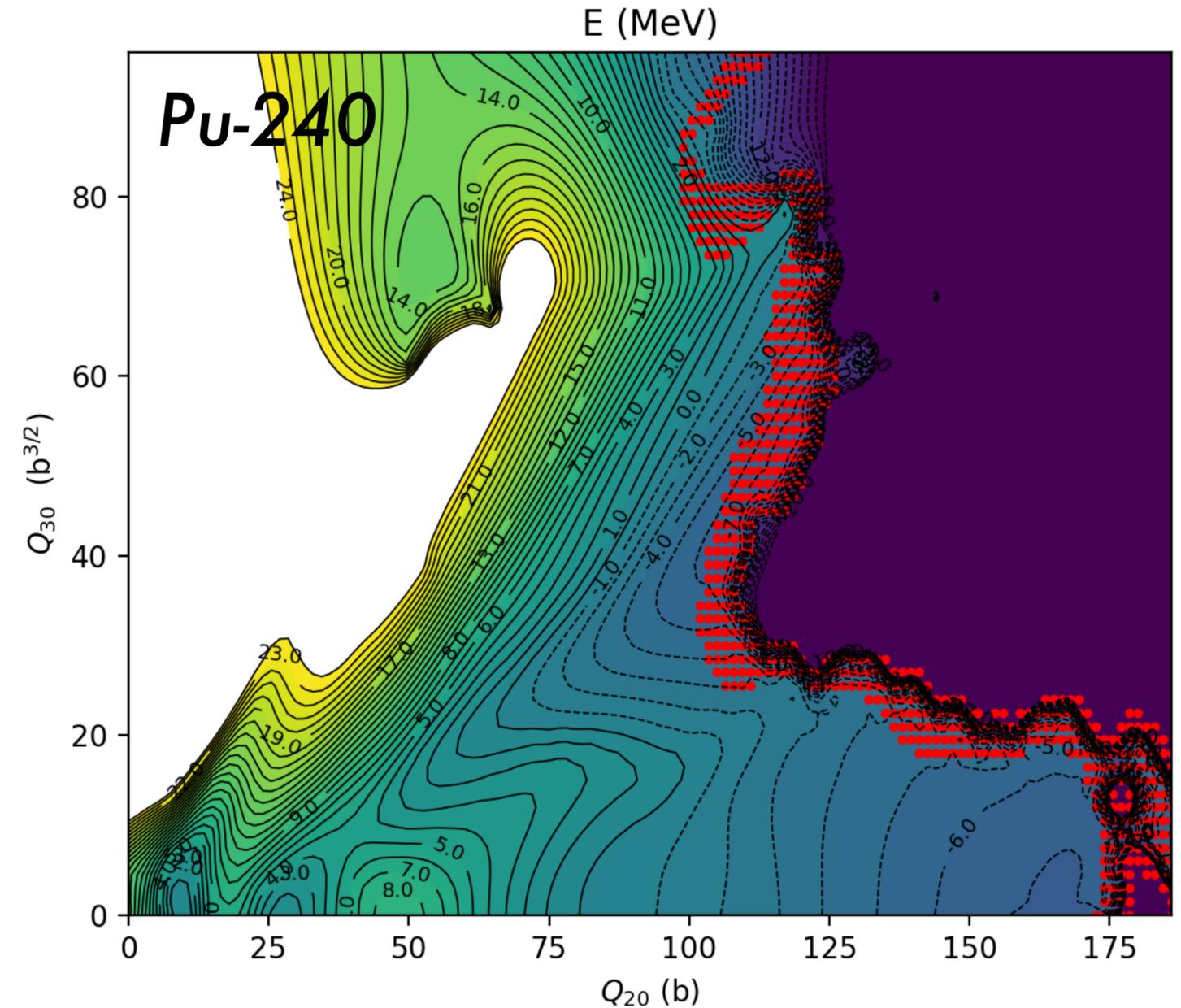
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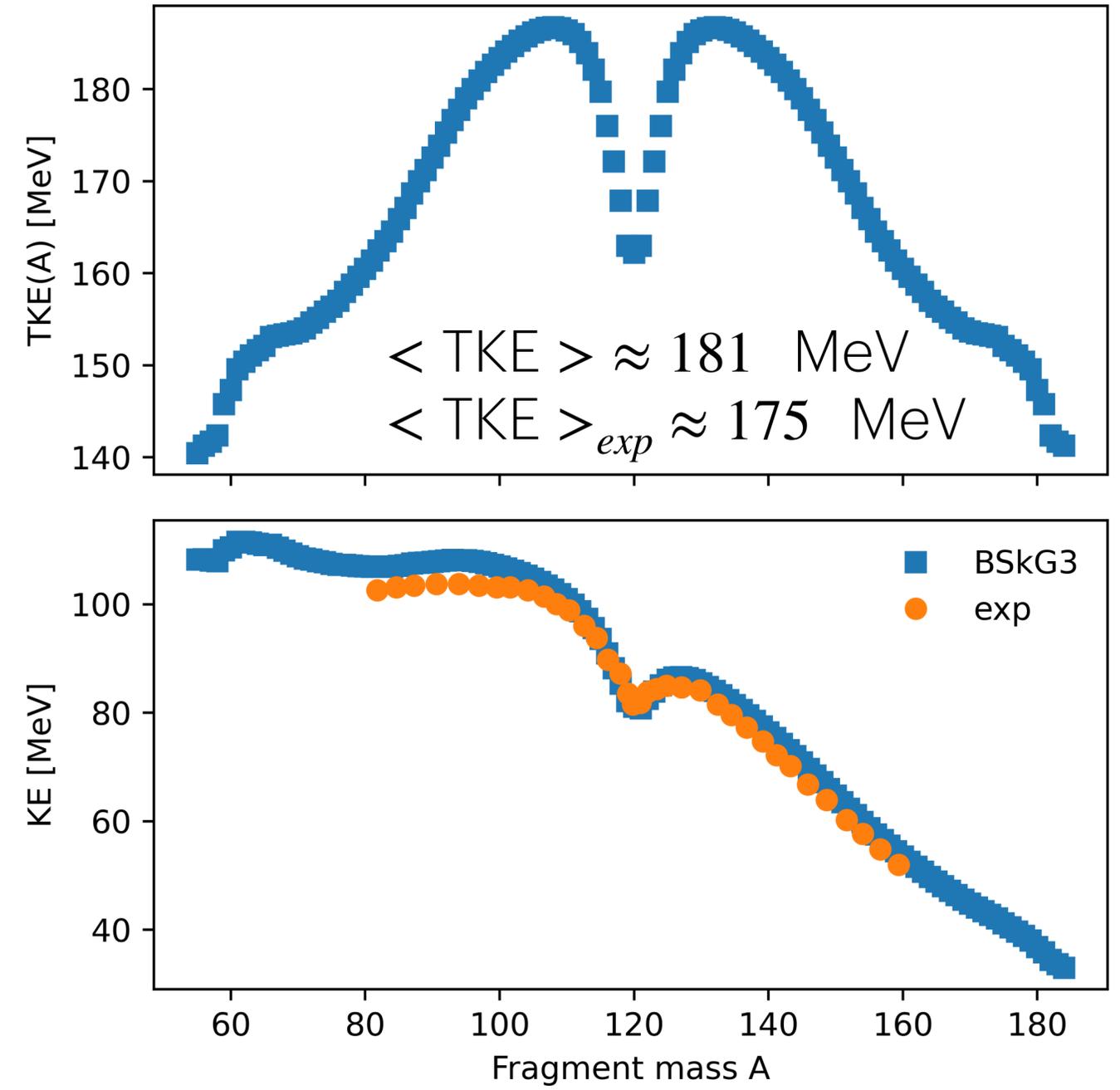
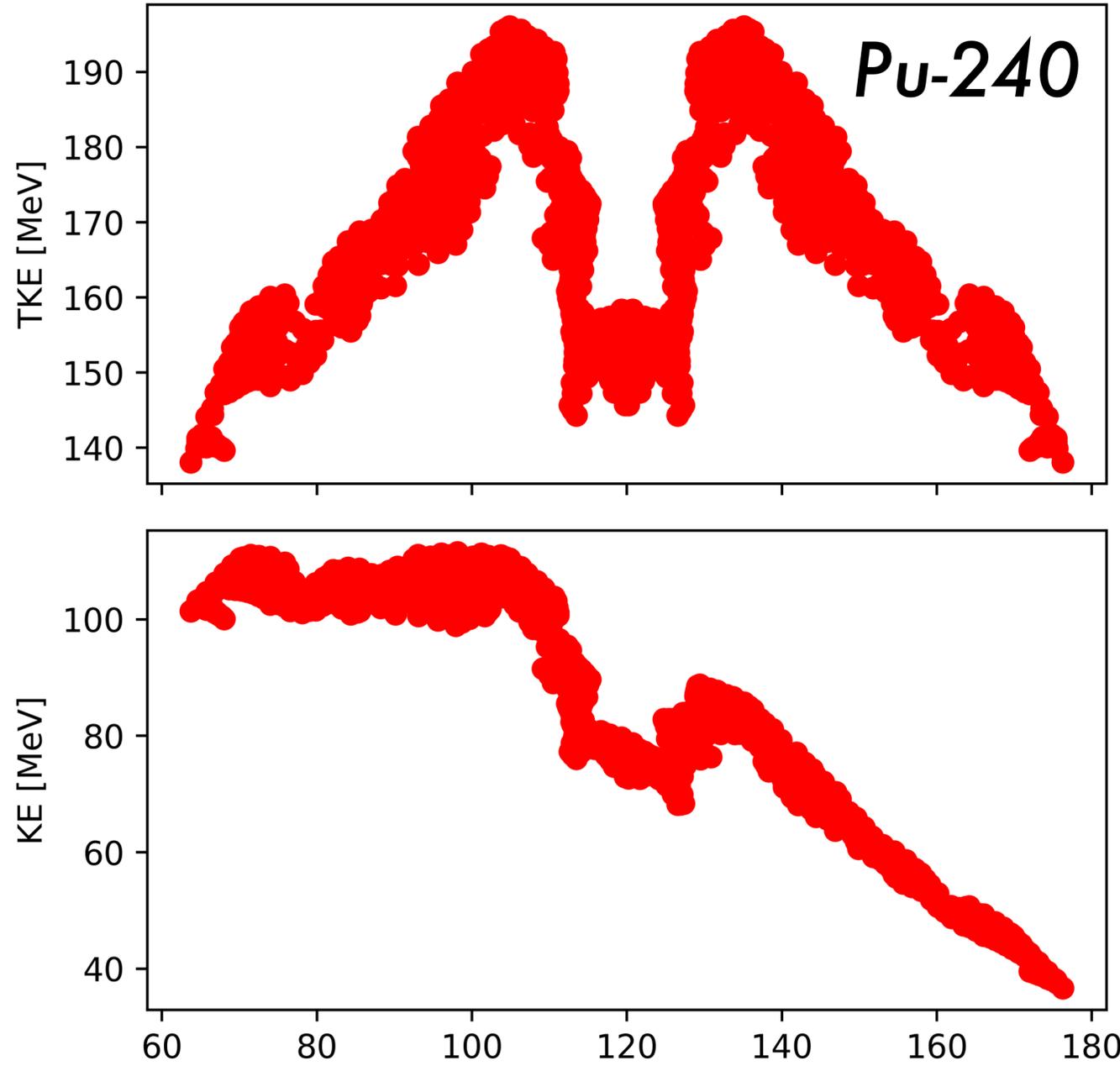
$$TXE = \sum_i E_{def}^i + E_{dis}$$

$$\sum_i E_{def}^i = E_{sc} - \sum_i E_{GS}^i - TKE$$

$$E_{dis} = kE_{free} = k(E_{GS}^{CN} + S_n + e_n - E_{sc})$$



Large-scale fission properties II: fission fragments distributions

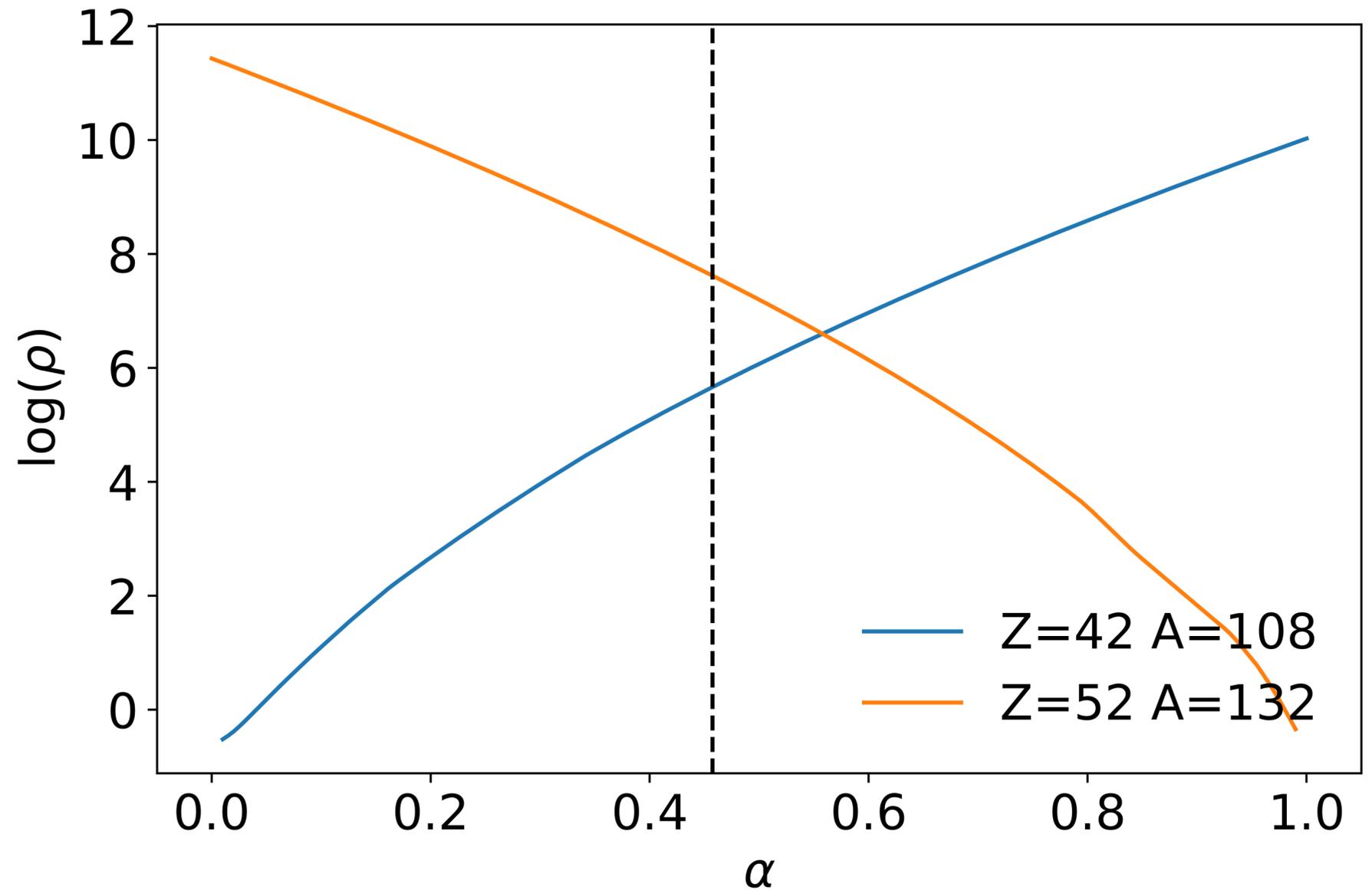


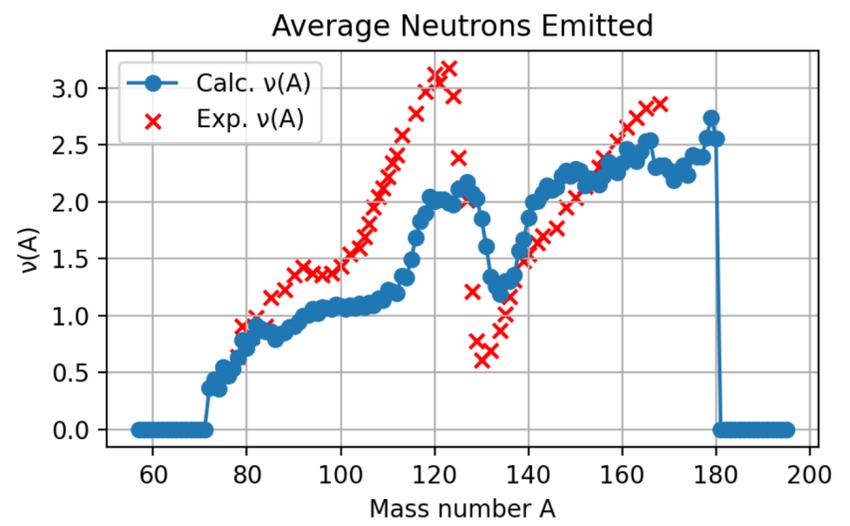
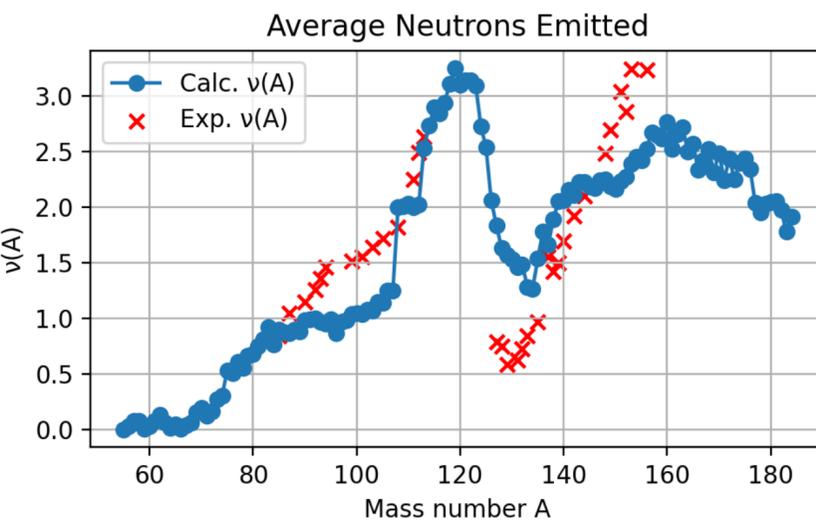
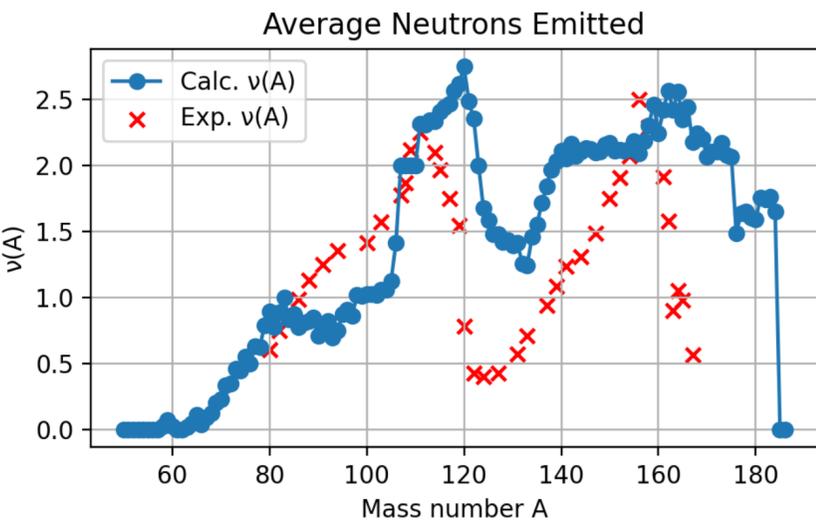
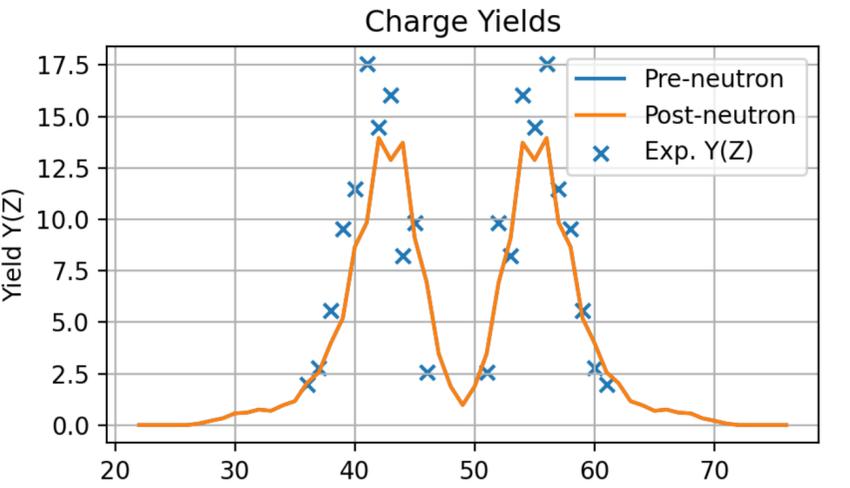
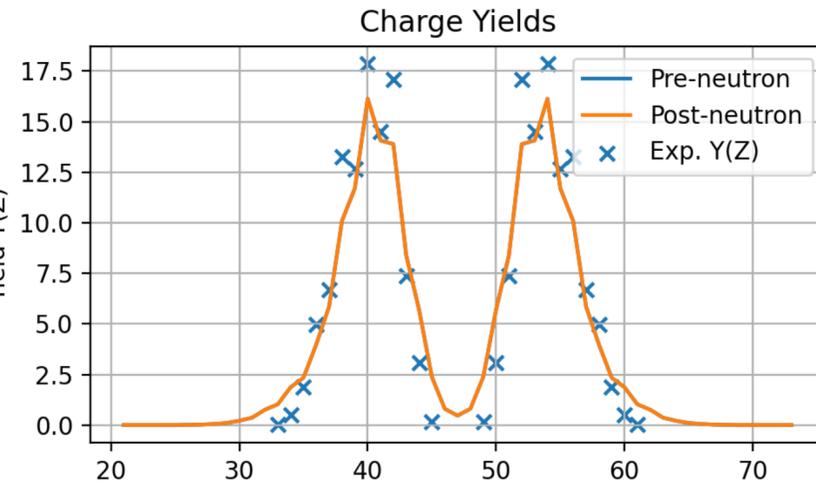
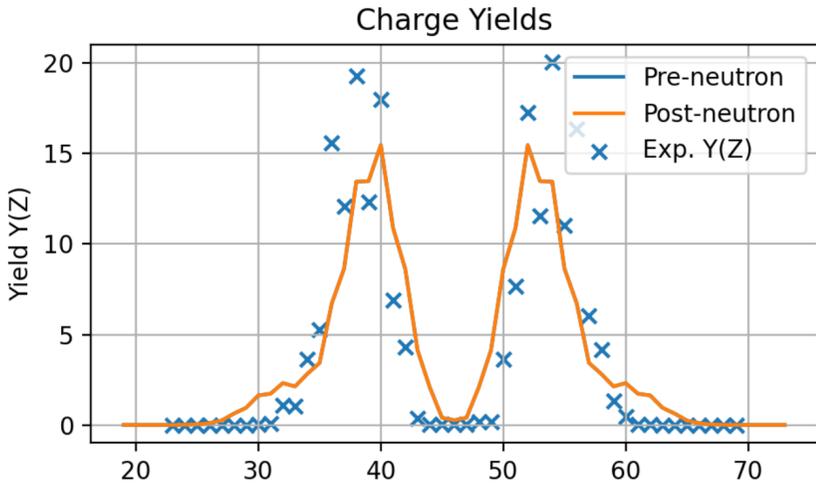
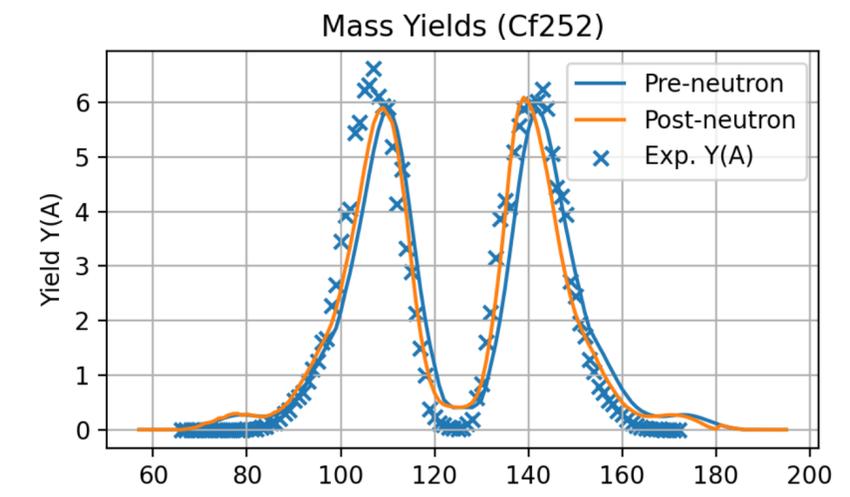
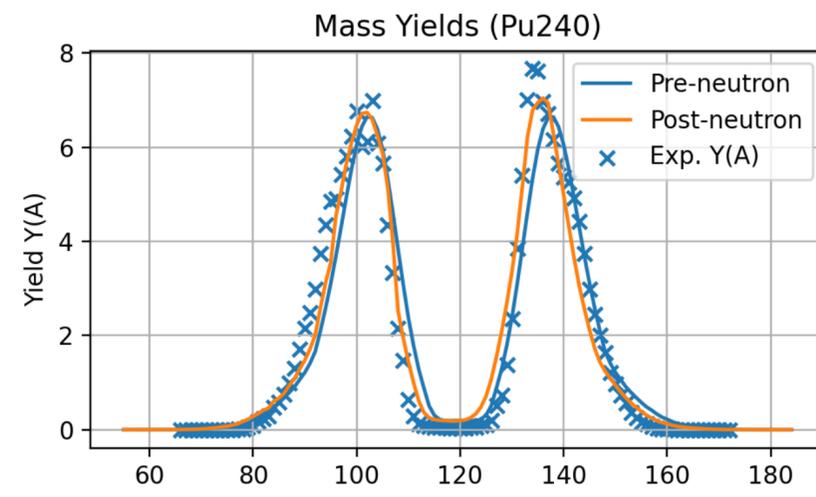
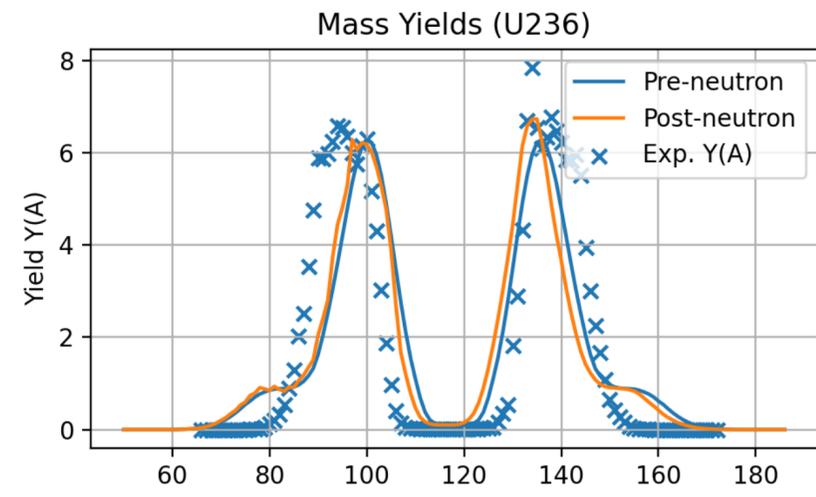
TXE is distributed
maximizing the product of
level densities

$$E_L^* = \alpha \text{TXE}$$

$$E_H^* = (1 - \alpha) \text{TXE}$$

$$\alpha \mid \rho(E_L^*, \beta_{20}^L) \rho(E_H^*, \beta_{20}^H) = \max$$





	$\bar{\nu}$ per fission	
	Exp	BSkG3
<i>U-235 (th.n,f)</i>	2.44	2.48
<i>Pu-239 (th.n,f)</i>	2.88	2.86
<i>Cf-252 (sf)</i>	3.77	3.20

We aim to derive all the nuclear inputs relevant for r-process simulations from the BSkG3 EDF.

*Added to TALYS

- fission paths*
- collective inertias*
- fission rates
- fission fragment distributions

Good agreement with empirical fission barriers, isomers and SF half-lives

-Time per benchmark: ~1 week

Reasonable estimates of post-neutron-emission yields

- A lot of room for improvement...