



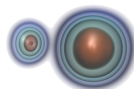
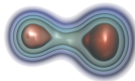
Microscopic calculation of fission fragments distributions with particle-number projection

D. Regnier^{1,2}, M. Verriere³, N. Schunck³, N. Dubray^{1,2}

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³Nuclear and Chemical Sciences Division, LLNL, Livermore, California 94551, USA



Fission modes and yields transition

From experience

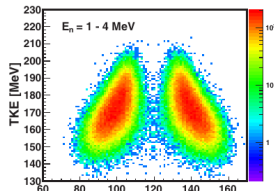
- A few main modes in the yields $Y(A, TKE)$
- Rapid yields transitions

Theoretical approaches

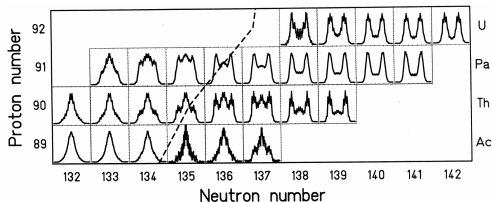
- Scission point models
- Langevin dynamics
- TDGCM+GOA

Challenges

- Prediction of the main fission modes in SHE
- Fission of very n-rich nuclei for r-process



Mass and kinetic energy fission yields for $^{238}\text{U}(n,f)$
D.L. Duke *et al.*, PRC 94, 054604 (2016)



Systematics of fragment charge distributions
K.H Schmidt *et al.*, NPA 665, 221-267 (2000)

How well can we predict yields with the TDGCM+GOA approach ?

Contenu

- 1 Computing fission yields with the TDGCM+GOA
- 2 Application: TDGCM+GOA predictions of fragments mass distribution
- 3 Limitations of the state-of-the-art TDGCM+GOA calculations
- 4 Estimation of the fragments properties at the Q_{neck} isoline

The Time Dependent Generator Coordinate Method

M. Verriere *et al.* Physics. Front. Phys. 8 (2020)

We assume that the system can be described by the ansatz

$$|\psi(t)\rangle = \int_{\mathbf{q}} f(\mathbf{q}, t) |\phi(\mathbf{q})\rangle d\mathbf{q}, \quad (1)$$

with

\mathbf{q} a vector of collective variables,
 $\{|\phi(\mathbf{q})\rangle\}$ the set of generator states.

$$|\psi(t)\rangle = f_1(t) \left| \begin{array}{c} \text{red dots} \\ \text{purple shape} \end{array} \right\rangle + f_2(t) \left| \begin{array}{c} \text{red dots} \\ \text{purple shape} \end{array} \right\rangle + \dots$$

Constrained HFB solutions with \neq shapes,
time independent

A time dependent **variational principle** yields the Hill-Wheeler equation

$$\forall \mathbf{q} : i\hbar \frac{d}{dt} \int_{\mathbf{q}'} \mathcal{N}(\mathbf{q}, \mathbf{q}') f(\mathbf{q}') d\mathbf{q}' = \int_{\mathbf{q}'} \mathcal{H}(\mathbf{q}, \mathbf{q}') f(\mathbf{q}') d\mathbf{q}', \quad (2)$$

with

$$\begin{aligned} \mathcal{N}(\mathbf{q}, \mathbf{q}') &= \langle \phi(\mathbf{q}) | \phi(\mathbf{q}') \rangle, \\ \mathcal{H}(\mathbf{q}, \mathbf{q}') &= \langle \phi(\mathbf{q}) | \hat{H} | \phi(\mathbf{q}') \rangle. \end{aligned}$$

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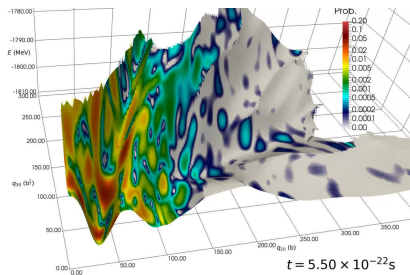
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Fission dynamics with the Hill-Wheeler equation

An attempt to solve the Hill-Wheeler equation numerically:

M. Verriere, PhD thesis, Université Paris-Saclay (2017)



Difficulties:

- Computation of kernels (\neq bases)
- Size of the discretized \mathbf{q} space
- Determination of the yields from the dynamics

No fission yields with this direct method yet.

The Gaussian Overlap Approximation

List of assumptions:

- ① The collective coordinates space is \mathbb{R}^d ,
- ② Generator states are time even,
- ③ The function $\mathbf{q} \rightarrow |\phi(\mathbf{q})\rangle$ is continuous and twice derivable,
- ④ The overlaps can be approximated by

$$\langle \phi(\mathbf{q}) | \phi(\mathbf{q}') \rangle \simeq \exp \left[-\frac{1}{2} (\mathbf{q} - \mathbf{q}')^t G(\bar{\mathbf{q}}) (\mathbf{q} - \mathbf{q}') \right], \quad (3)$$

- ⑤ The Hamiltonian kernel can be approximated by

$$\langle \phi(\mathbf{q}) | \hat{H} | \phi(\mathbf{q}') \rangle \simeq \langle \phi(\mathbf{q}) | \phi(\mathbf{q}') \rangle h(\mathbf{q}, \mathbf{q}'), \quad (4)$$

where $h(\mathbf{q}, \mathbf{q}')$ is a degree 2 polynomial.

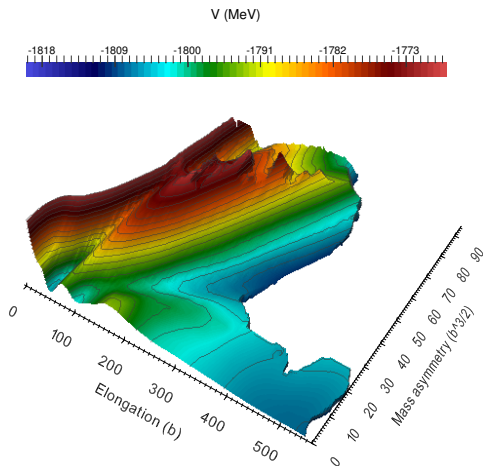
Result: a **local** Schrödinger equation of motion

$$i\hbar \frac{d}{dt} g(\mathbf{q}) = \left[-\frac{\hbar^2}{2\sqrt{\gamma(\mathbf{q})}} \nabla_{\mathbf{q}} \sqrt{\gamma(\mathbf{q})} B(\mathbf{q}) \nabla_{\mathbf{q}} + V(\mathbf{q}) \right] g(\mathbf{q}) \quad (5)$$

TDGCM+GOA: a practical point of view

Example of a $n + {}^{239}\text{Pu}$ fission

- 1 Choose the collective variables:
 - elongation (Q_{20} in b),
 - mass asymmetry (Q_{30} in $b^{3/2}$)
- 2 Calculate potential energy surface and inertia tensor
- 3 Define initial wave packet for the probability amplitude
- 4 Compute time evolution of probability amplitude
- 5 Extract fission fragment distribution by computing the flux of the probability amplitude across the scission line

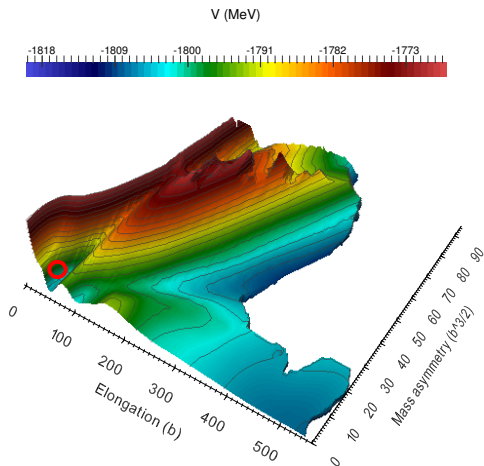


Potential energy surface for $(n + {}^{239}\text{Pu})$ fission

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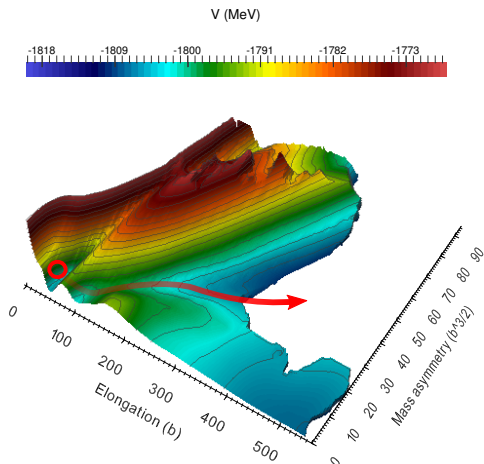


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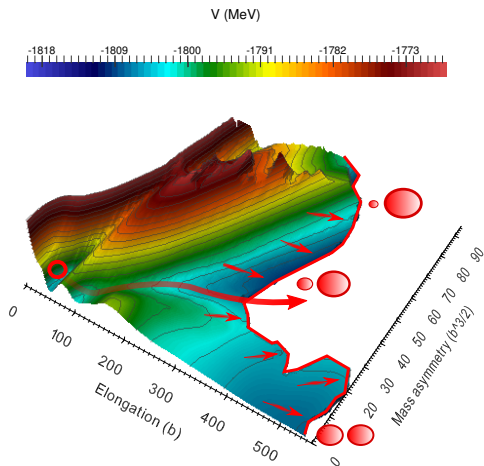


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Potential energy surface for $(n+{}^{239}\text{Pu})$ fission

TDGCM+GOA: technicalities

Computation of the generator states:

- $\simeq 10^4$ constrained HFB states for a 2D calculation
- Codes:
 - HFODD N. Schunck *et al.* CPC 216 (2017),
 - HFBTHO R. Perez *et al.* CPC 220 (2017),
 - etc.
- Harmonic oscillator basis (up to $N_{max} = 30$ shells in 1 center HO)
- Basis parameters optimized at each deformation

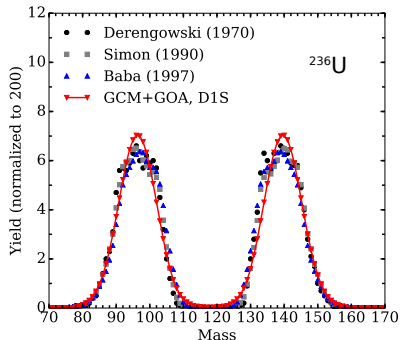
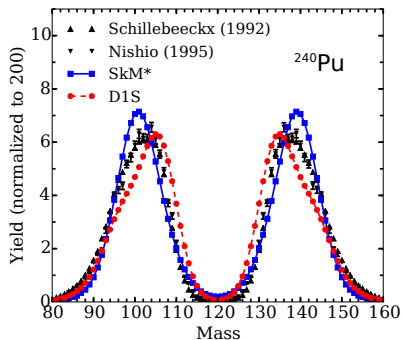
Collective dynamics:

- Excited initial state ($\simeq 1$ MeV above the fission barrier)
- Code: FELIX-2.0 D. Regnier *et al.* CPC 225 (2018)
- Finite element discretization of space, unitary time propagator

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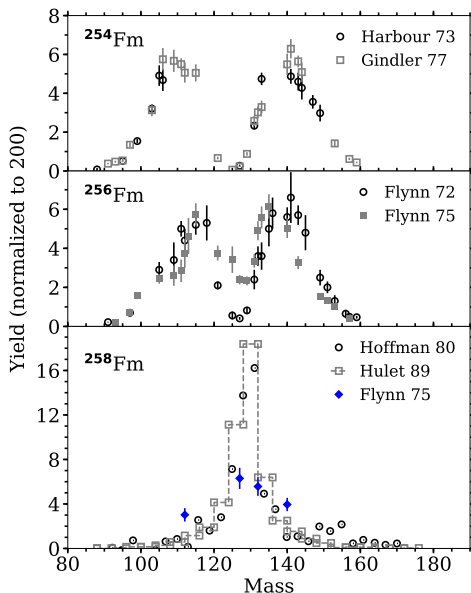
Primary fragments mass yields for low energy fission of actinides



- Robust qualitative reproduction of the asymmetric fission of actinides
- A better modeling of several physics features (initial state, fragment separation) is **necessary to reach better accuracy**.

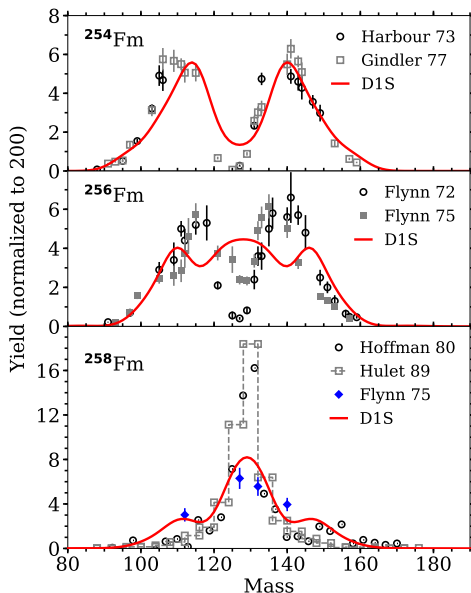
D. Regnier *et al.*, PRC **93**, 054611 (2016)

Fission yields in neutron rich Fermium isotopes



- **Open symbols:**
Spontaneous fission
- **Full symbols:**
Thermal n-induced fission
- **D1S:**
Our calculation starting from 1 MeV above the fission barrier

Fission yields in neutron rich Fermium isotopes



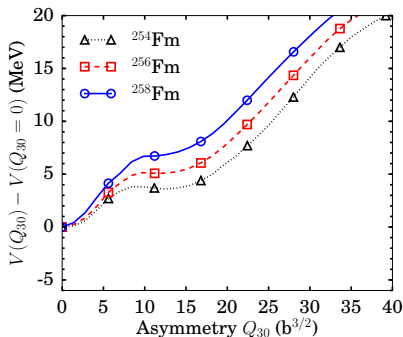
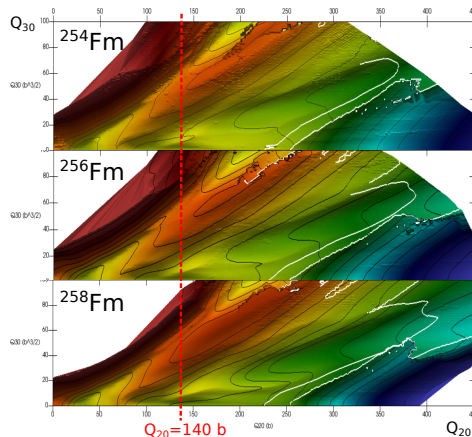
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Results

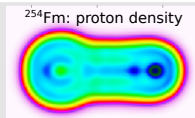
- Transition reproduced
- Difficulty with ^{256}Fm

D. Regnier *et al.* PRC 99 (2019)

Competition between collective potential valleys

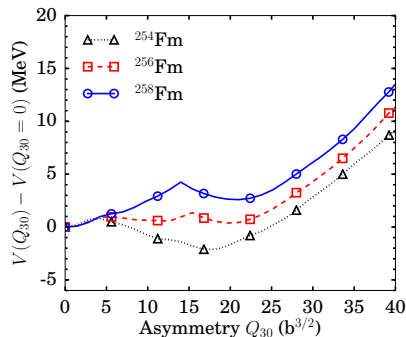
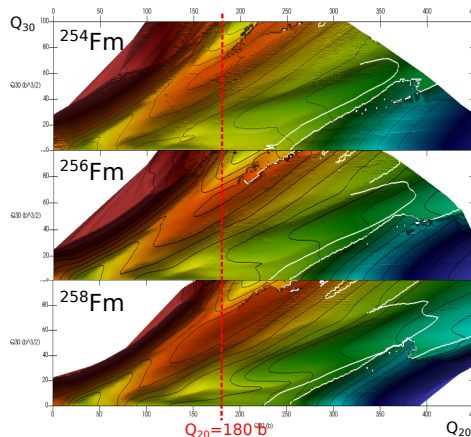


- Main fission modes driven by the static potential energy
- Dominant mode decided at rather **low elongation** $Q_{20} \simeq 180$ b

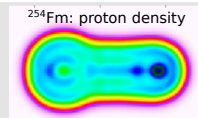


$$Q_{20} = 180 \text{ b}, Q_{30} = 20 \text{ b}^3/2$$

Competition between collective potential valleys

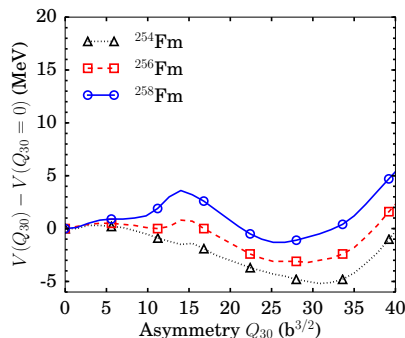
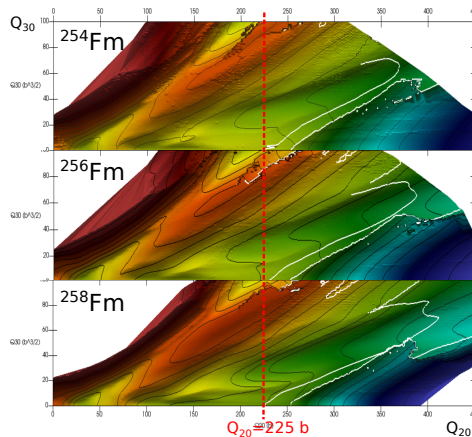


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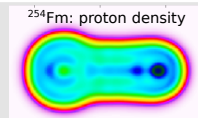


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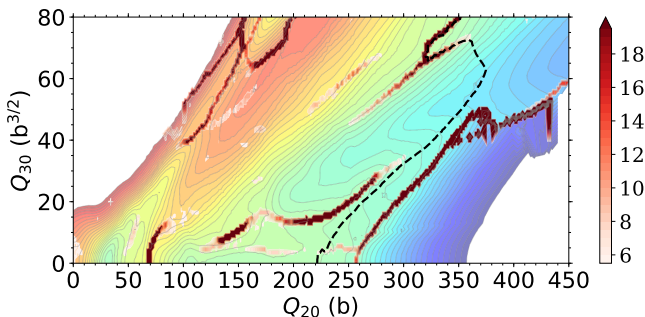
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The weak spots of TDGCM+GOA:

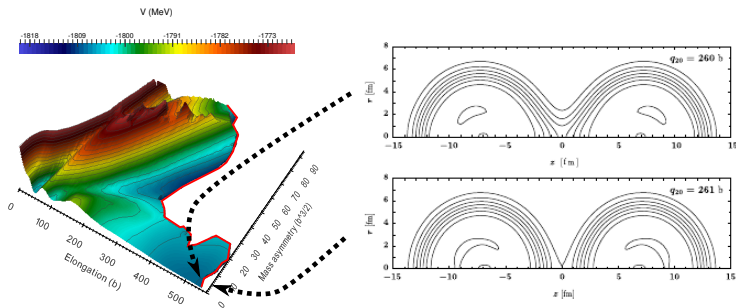
- Hamiltonian kernels are ill-defined when using an EDF.
- The span of the generator states misses some physics (i.e. intrinsic excitation, time odd parts, etc).
- The function $\mathbf{q} \rightarrow |\phi(\mathbf{q})\rangle$ may not be continuous.



Spotting the discontinuities in ^{256}Fm with $d(\rho, \rho') = \int_r dr |\rho(\mathbf{r}) - \rho'(\mathbf{r})|$

Consequences on the prediction of fragments mass/charge distributions

Scission discontinuity: one di-nuclear system versus two cold fragments.



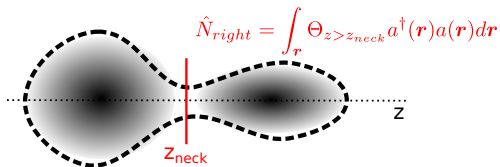
⇒ We retain only di-nuclear configurations in the TDGCM ansatz.

- The flux of probability is estimated through an **isoline of Q_{neck}** .
- This isoline must lie before the scission discontinuity ...
... where typically **4 to 8 nucleons are in the neck**.

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Estimation of the particles number close to scission



For each HFB state on the Q_{neck} isoline considered we compute:

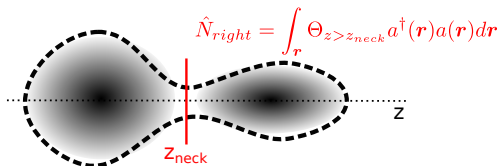
$$\langle \hat{N}_{right}(\mathbf{q}) \rangle = \int_{z > z_{neck}} \int_{\theta \phi} \rho_n(z, \theta, \phi) d\mathbf{r} \quad (6)$$

The final yields are obtained from a Gaussian convolution:

$$Y(N_{right}) \propto \sum_{\mathbf{q} \in isoline} P(\mathbf{q}) \cdot \exp \left(-\frac{1}{2} \frac{(N_{right} - \langle \hat{N}_{right}(\mathbf{q}) \rangle)^2}{\sigma^2} \right) \quad (7)$$

Introduction of a **free parameter** σ , the width of the convolution.

Estimation of the particles number close to scission



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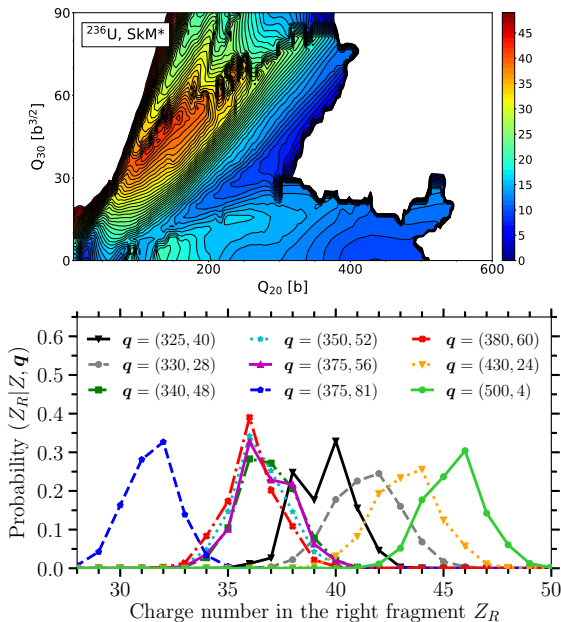
$$P(N_{right}|N, \mathbf{q}) = \frac{\langle \phi(\mathbf{q}) | \hat{P}_n^R(N_{right}) \hat{P}_n(N) | \phi(\mathbf{q}) \rangle}{\langle \phi(\mathbf{q}) | \hat{P}_n(N) | \phi(\mathbf{q}) \rangle} \quad (6)$$

The final yields are obtained from this distribution

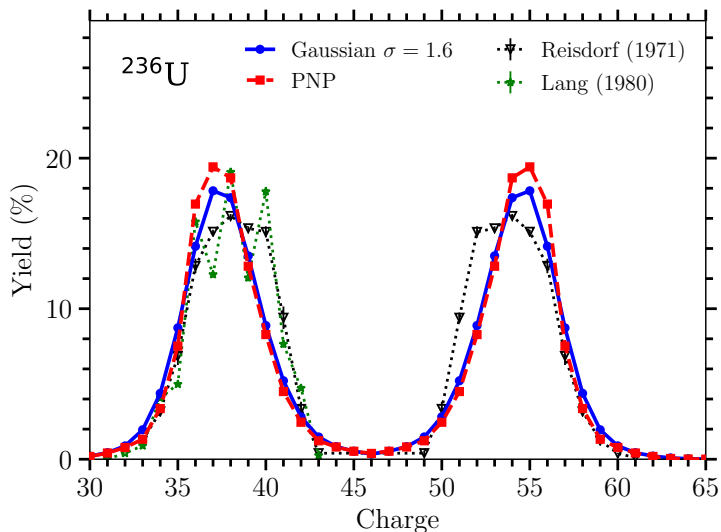
$$Y(N_{right}) \propto \sum_{\mathbf{q} \in isoline} P(\mathbf{q}) \cdot P(N_{right}|N, \mathbf{q}) \quad (7)$$

No more free parameter *M. Verriere et al. PRC 103 (2021)*

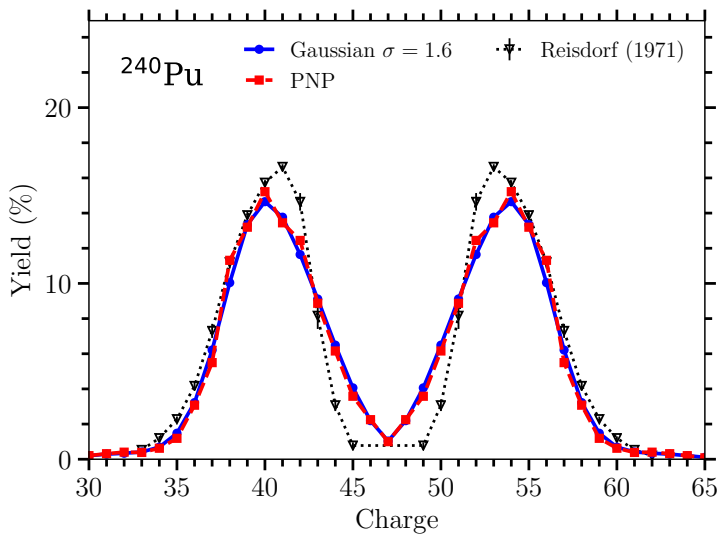
Distribution of the right fragment charge in ^{236}U along the isoline $Q_{neck} = 4$



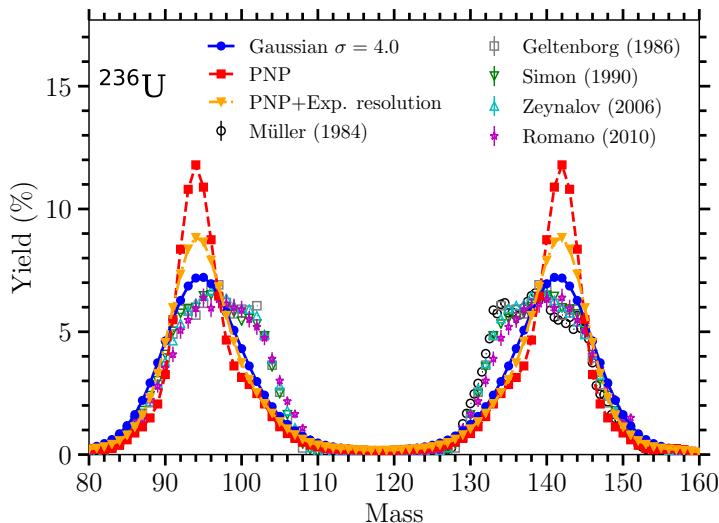
Effect on the charge distribution



Effect on the charge distribution

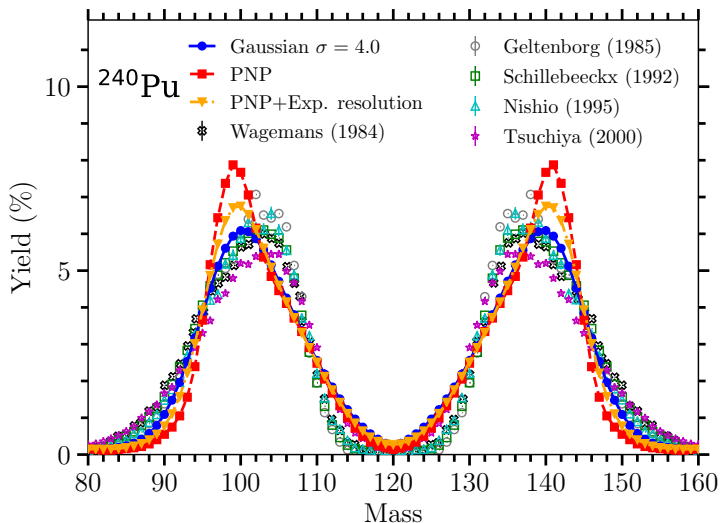


Effect on the mass distribution



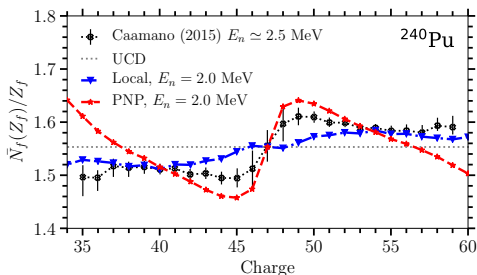
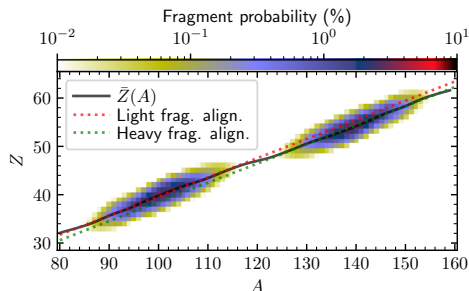
Larger effect than on the charge due to remaining neutrons in the neck

Effect on the mass distribution



Larger effect than on the charge due to remaining neutrons in the neck

First prediction of the mass and charge distribution



- Qualitative reproduction of the 2D width of the distribution
- Prediction of a charge polarization effect

Conclusion & perspectives

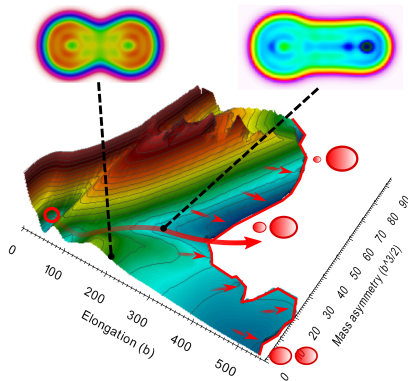
Conclusions

- TDGCM+GOA: an EDF based approach capable of predicting **realistic** fission fragments mass charge distributions
- Long term efforts with many upgrades explored:
 - **particle projection close to scission**,
 - new collective degrees of freedom (pairing, temperature, etc).
- Major flaws:
 - beyond mean-field with EDF,
 - insufficient variational space,
 - discontinuities.

Some related on going work...

- Inclusion of intrinsic excitation within the SCIM approach (**P. Carpentier**)
- Quantum mixing of TDHF trajectories (**P. Marevic**)
- Machine learning families of generator states (**R.-D. Lasserri**)

Thank you for your attention !



N. Schunck and D. Regnier, *Theory of Nuclear Fission*, accepted to Prog. Part. Nucl. Phys.