Probing the evolution of the fission modes with a microscopic approach

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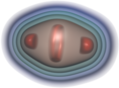
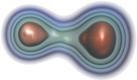
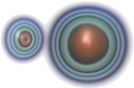




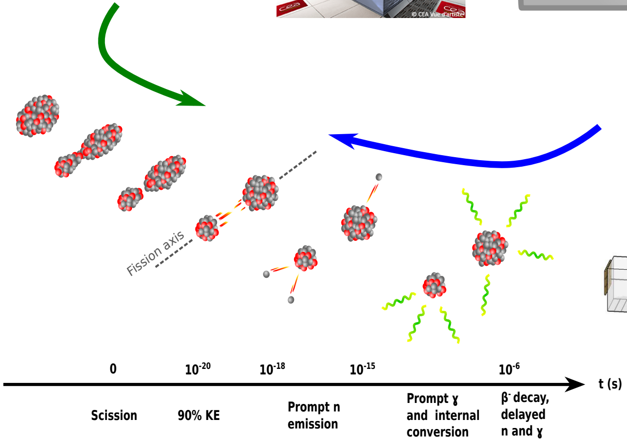


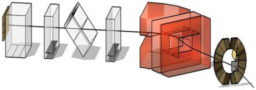
Probing the fission dynamics

Many-body calculations based on energy density functional

Fission time scale ?
Scission neutron ?
Fragments characteristics ?
Fragments deexcitation ?

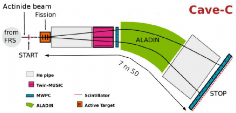
VAMOS@GANIL
SOFIA@GSI
SPIDER@LANL
Fission@ALTO
...

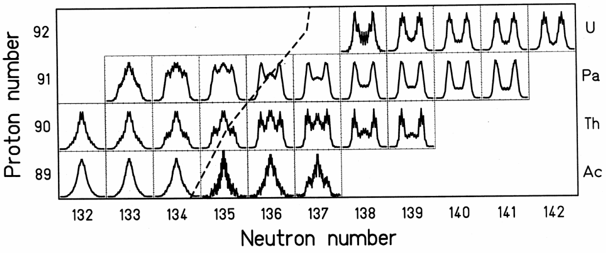




Symmetric/asymmetric yields transitions

Systematic studies of fission yields with inverse kinematics measurements sheds light on numerous yields transitions.





Fragment charge distribution measured by inverse kinematics at GSI, K.H Schmidt *et al.*, Nucl. Phys. A 665, 221-267 (2000)

- How well can EDF based approaches reproduce these yields transitions ?
- What fission modes do these approaches predict in the SHE region ?

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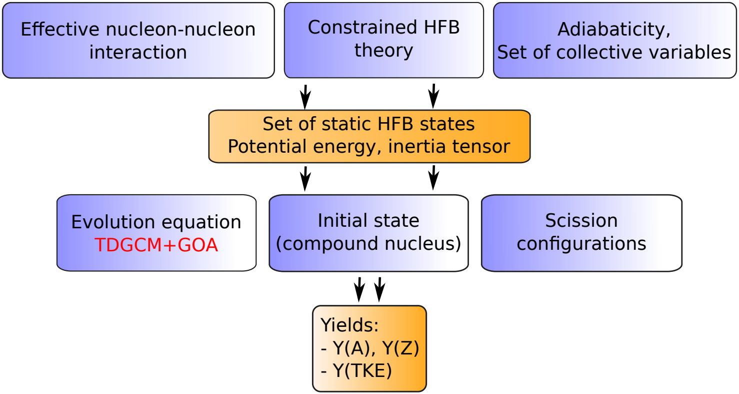
Time Dependent Generator Coordinate Method (Multi-reference DFT)



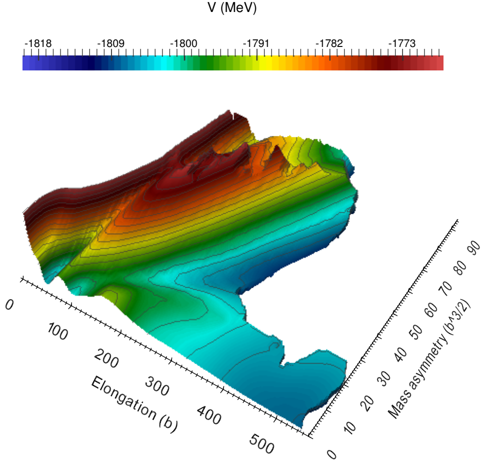
A fully quantum-mechanical description of the time evolution

Gives the amplitude of probability for the nucleus to have a given shape at time t.

Time Dependent Generator Coordinate Method (TD-GCM)

Example of a n + ^{239}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



Interpolated potential energy surface for (n+^{239}Pu) fission

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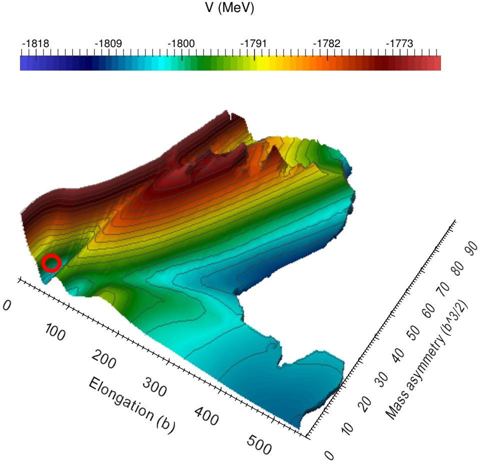

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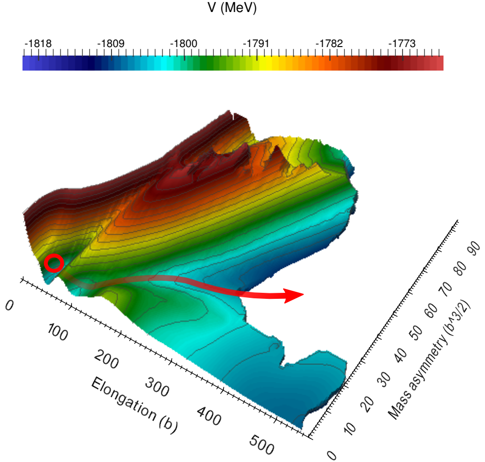

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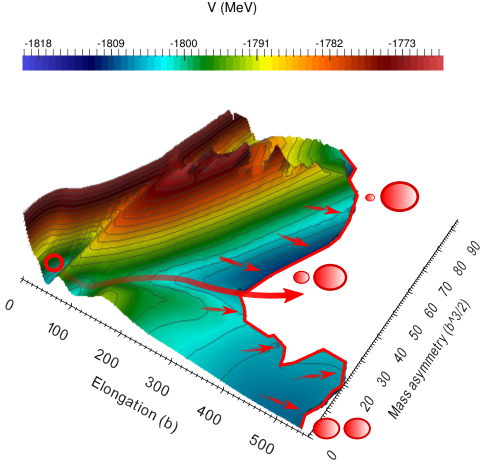


Interpolated potential energy surface for (n+^{239}Pu) fission

Development of this microscopic approach

2005: First calculation for ^{238}U

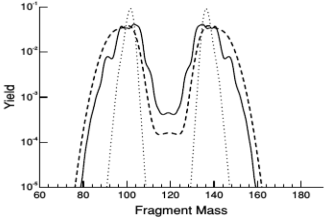
H. Goutte *et al.*, Phys. Rev. C **71**, 024316

2012: Fission yields of ^{236}U and ^{240}Pu

W. Younes *et al.*, LLNL-TR-586678

- Promising results
- High numerical costs

2D PES	40000 HFB states
Dynamics	10 zs ($10^{-21}s$)



Pre-neutron mass yields for ^{238}U at 2.4 MeV above the fission barrier (H. Goutte *et al.*).
solid line: dynamics calculation
dashed line: Whal evaluation (2002)

Upgrade numerical methods

FELIX-1.0 D. Regnier *et al.*, Comput. Phys. Commun. **122**, 350-363 (2016)

FELIX-2.0 D. Regnier *et al.*, Comput. Phys. Commun. **225**, 180-191 (2018)

Machine learning for PES N. Martin *et al.*, work in progress

Recent applications

Fission of ^{240}Pu, ^{252}Cf, ^{226}Th

D.Regnier *et al.*, Phys. Rev. C **93**, 054611 (2016)

A. Zdeb *et al.*, Phys. Rev. C **95**, 054608 (2017)

H. Tao *et al.*, Phys. Rev. C **96**, 024319 (2017)

FELIX: a generic solver for the TDGCM+GOA

Features:

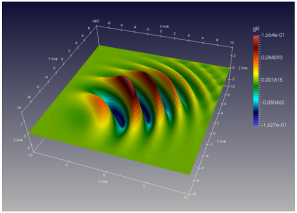
- Capable of handling N≥2 collective variables
- Arbitrary collective degree of freedom
- Scalable numerical methods
- Solving the static GCM+GOA

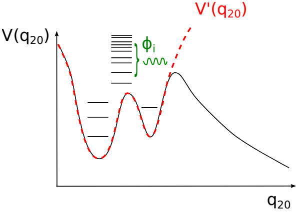
Numerical methods for 2.0:

- Spectral finite element (space)
- Krylov propagator (time)

Validation

- Unitary tests
- Analytical benchmarks





x20 speedup

Developments

FELIX-1.0 released (Open Source GPL-2)

FELIX-2.0 released (Open Source GPL-3)

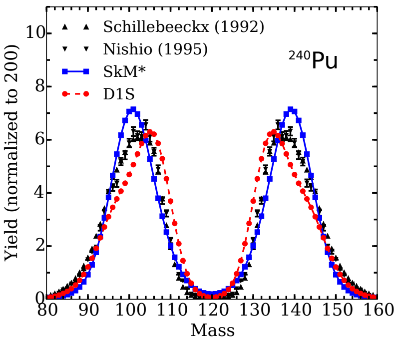
FELIX

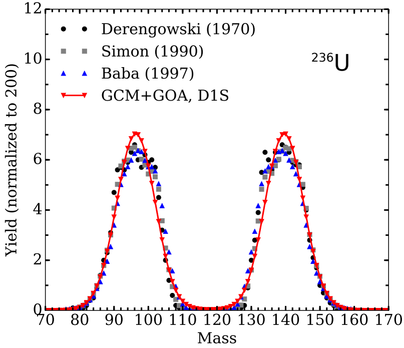
2014 — 2015 — 1.0 — 2016 — 2017 — 2.0 — 2018

D. Regnier, *et. al.* CPC **122** (2016)

D. Regnier, *et. al.* CPC **225** (2018)

Primary fragments mass yields for low energy fission of actinides





- The initial energy is taken 1 MeV above the fission barrier.
- The raw flux results are convoluted with a Gaussian of width $\sigma = 4$.

- The qualitative reproduction of the asymmetric fission of actinides is robust.
- A better modeling of several physics effects (initial state, fragment separation) is necessary to reach a $\simeq$10% accuracy.

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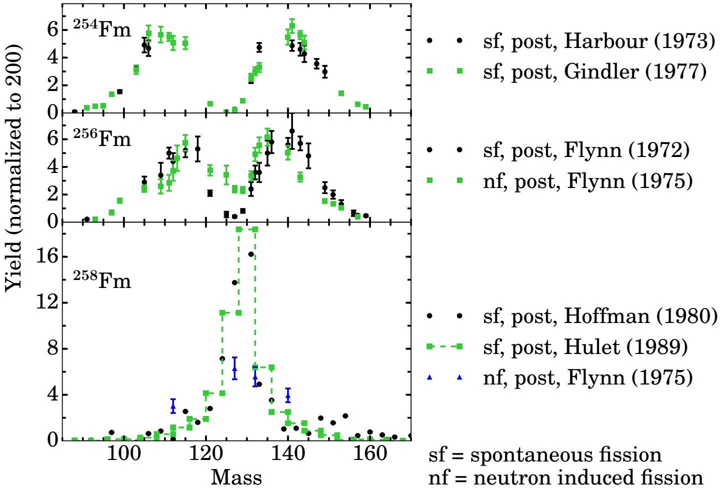
Fission yields in neutron rich Fermium isotopes



	^{253}Fm	^{254}Fm	^{255}Fm	^{256}Fm	^{257}Fm	^{258}Fm
T1/2	3.00 d	3.240 h	20.07 h	157.6 min	100.5 d	370 μs
SF (%)		0.0592	$2.4.10^{-5}$	91.9	0.210	
$\sigma(n,f)$ (b)			3200		2950	

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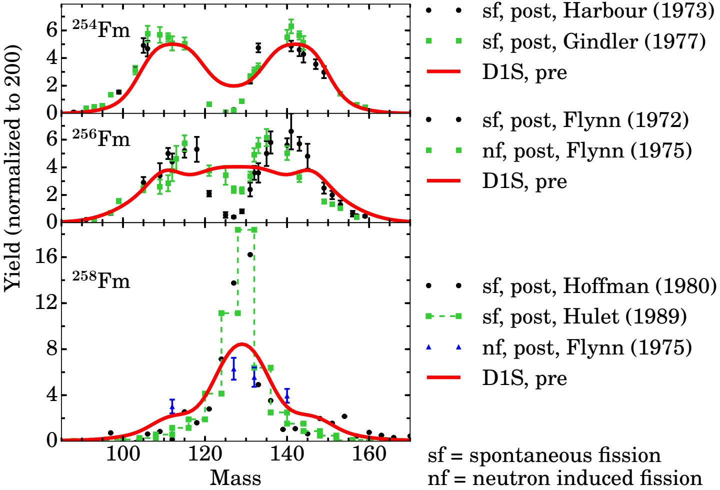

sf = spontaneous fission
nf = neutron induced fission

	^{253}Fm	^{254}Fm	^{255}Fm	^{256}Fm	^{257}Fm	^{258}Fm
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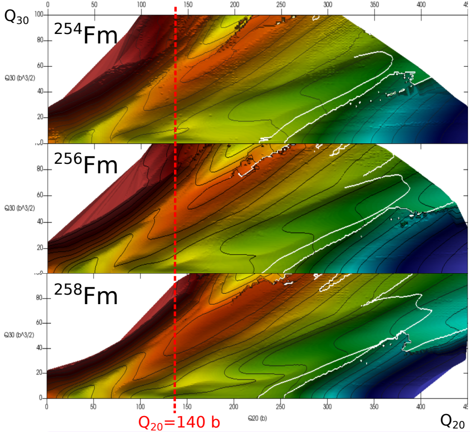
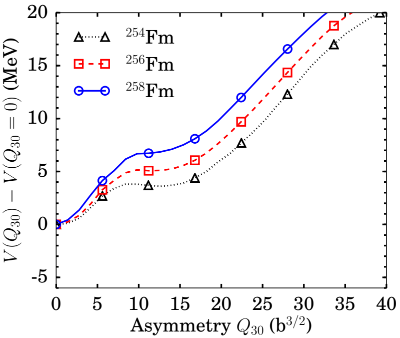
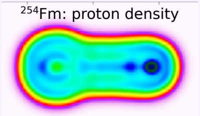
Competition between collective potential valleys





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



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

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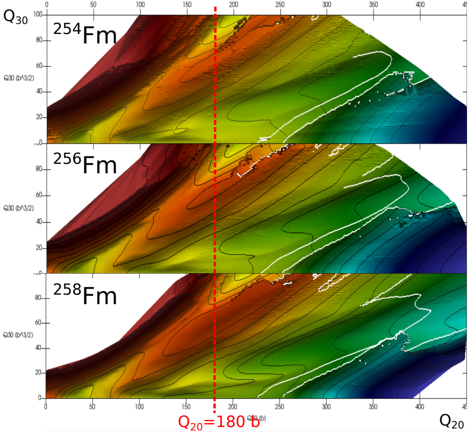

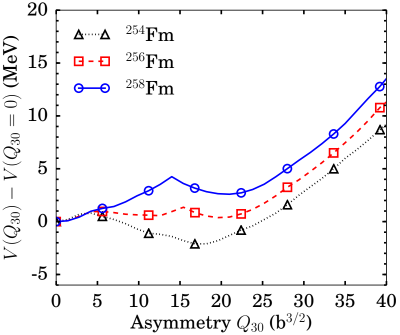

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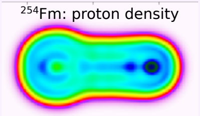

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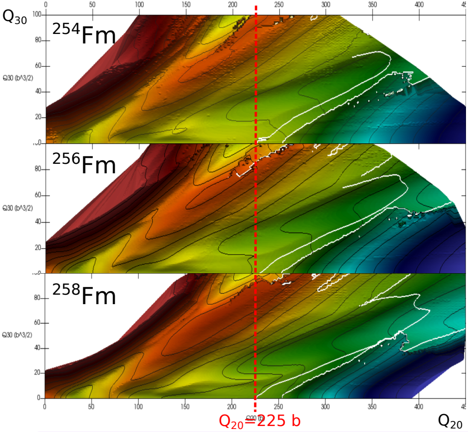

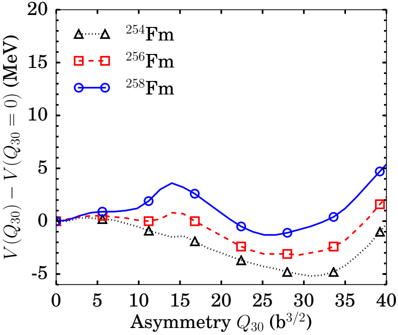

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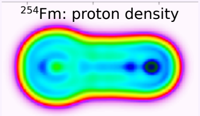

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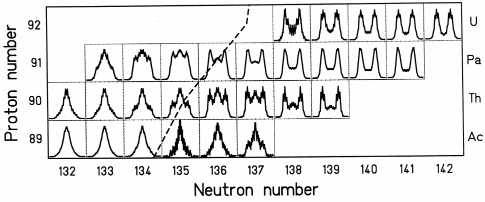
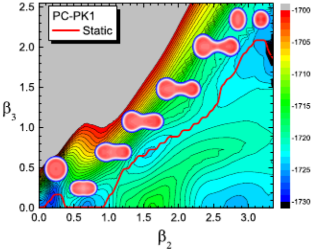
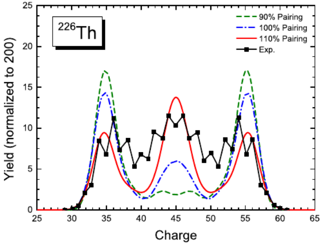
Fission yields in proton rich Thorium isotopes

- Fragment charge distribution, K.H Schmidt *et al.*, Nucl. Phys. A 665, 221-267 (2000)



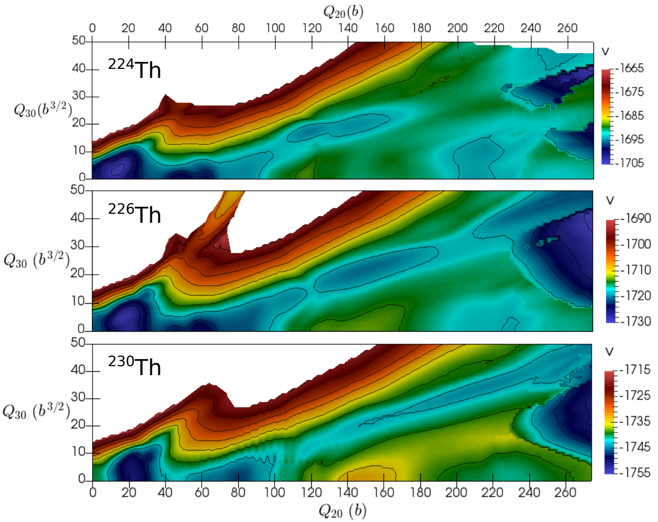
- First TDGCM+GOA calculation performed with relativistic density functional PC-PK1 H. Tao *et al.*, Phys. Rev. C **96**, 024319 (2017)





- Difficulty to get the correct ratio between modes
- Important sensitivity to the pairing strength

Preliminary Thorium PES obtained with D1S



- Main modes of the fission yields driven by the static potential energy
- Clear change of topology around $Q_{20} \simeq 200$

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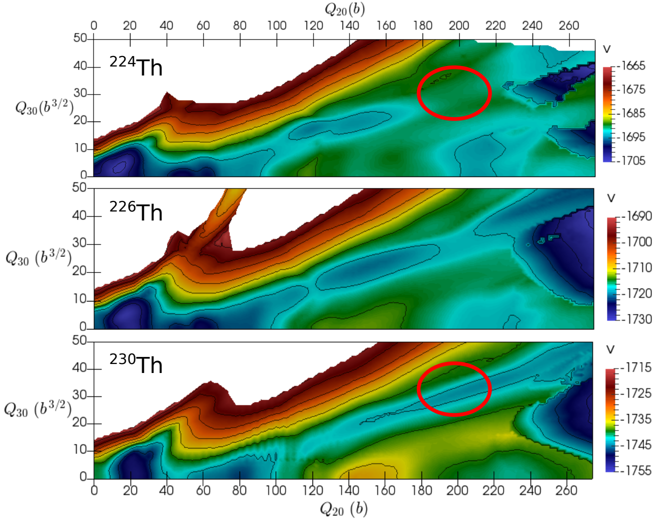

- Main modes of the fission yields driven by the static potential energy
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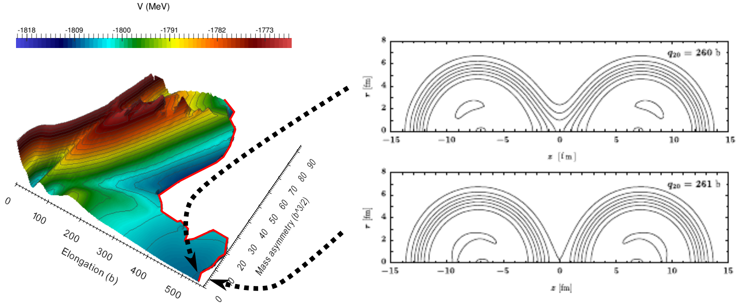
Discontinuities in the set of generator states

Each point of the PES:

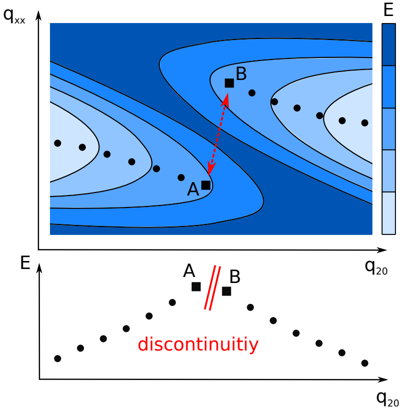
- is a solution of the constrained Hartree Fock Bogoliubov (HFB) equation,
- is determined by minimization of the energy among a set of deformed states



Problem

1. Two solutions close in the collective subspace are not close in the full deformation space.

Origin of the problem



Exemple of a discontinuity in a 1D Potential Energy Surface (PES) for the collective variable q_{20}:

- Point A and B may represent very different systems
- Point A and B energy are close to each other
- Due to the energy minimization involved, they are neighboors in the 1D potential energy surface

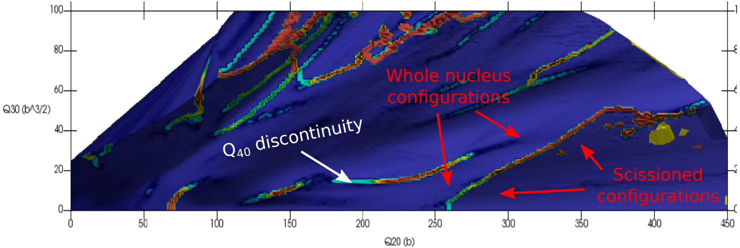
Consequence

- The 1D PES is missing a part of the physics: underestimated barriers.
- In principle, the system should not cross a discontinuity during the dynamics

Pinpoint the discontinuities: example of ^{256}Fm

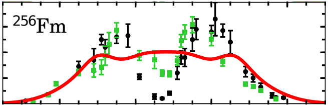
Simple criteria to detect discontinuities:

$$d(\rho, \rho') = \int_{\mathbf{r}} d\mathbf{r} |\rho(\mathbf{r}) - \rho'(\mathbf{r})|$$



Maximum density distance between closest neighboors

- A higher potential ridge should separate the symmetric and asymmetric valleys (Q_{40} discontinuity)
- States around scission are missing in the GCM description

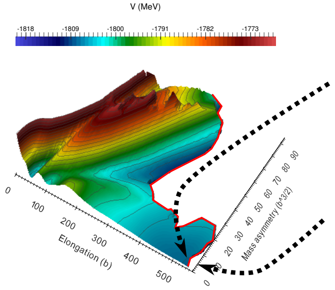


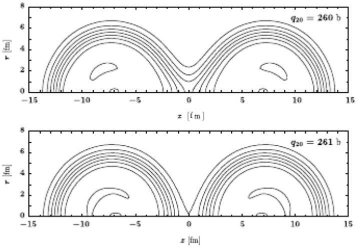
Discontinuity around scission

Consequences:

- The dynamics has to be stopped before scission
  $\Longrightarrow$ Prevent predictions of a number of observables (*e.g.* TKE)
- Presence of a neck in the final states
  $\Longrightarrow$ The number of particles in the fragments are defined up to the number of particles in the neck (Q_{neck}).

Actinides	$Q_{neck} \simeq 4$
Proton rich Th	$Q_{neck} \simeq 12$



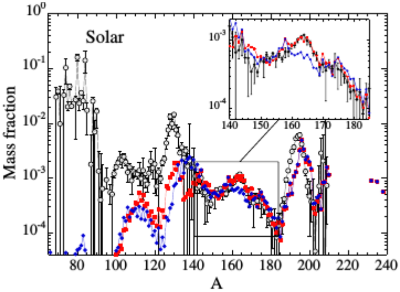


Discontinuities in the neutron rich ^{278}Cf

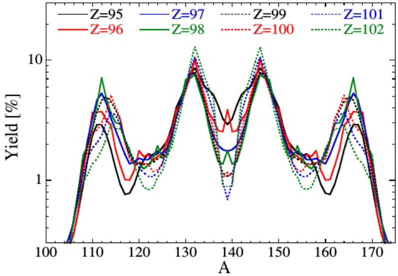
Motivation:

Prediction of a very asymmetric fission modes with a static approach (SPY) that impacts the element abundances in the rare earth region.

S. Goriely et. al., PRL **111** (2013)

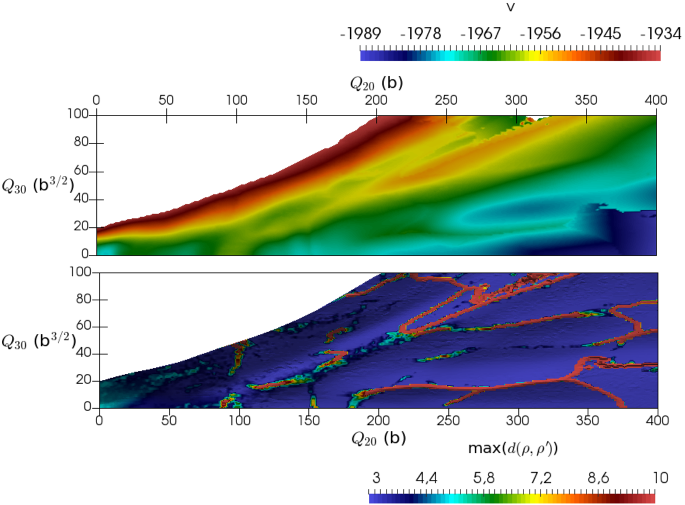


Impact of the fission yields model on r-process abundances. Blue= GEF, Red= SPY.



Mass yields of exotic systems with mass $A_{CN} = 278$ obtained with SPY

Discontinuities in the neutron rich ^{278}Cf



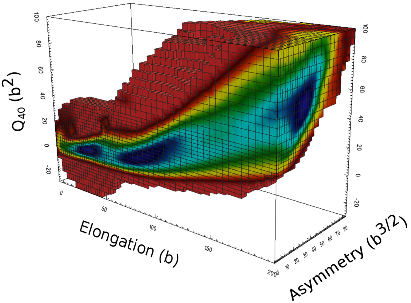
Patchwork of PES that are disconnected

$\Longrightarrow$ The 2D TDGCM+GOA approach cannot predict the yields

Adding collective variables to remove some discontinuities

Including the additional variable Q_{40} (partly related to the neck size)

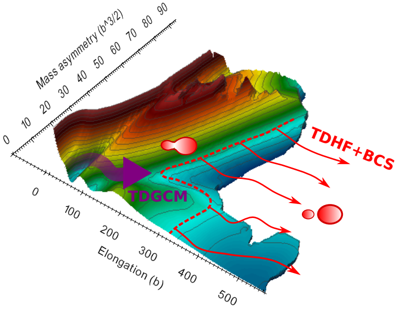
- would involve roughly 2.10^6 constrained HFB calculations,
- imply a numerical cost $\simeq 1.10^6$ cpu.h for a full 3D PES.



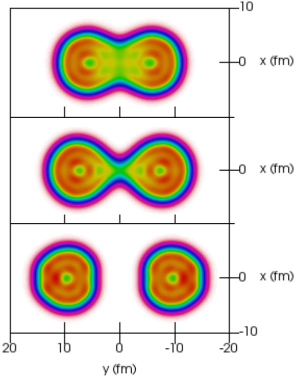
One third of the full potential energy surface for a n+^{239}Pu fission in the collective space $(\hat{Q}_{20}, \hat{Q}_{30}, \hat{Q}_{40})$

- Current bottleneck: generation of the potential energy surface.
- Work in progress: machine learning for HFB optimization and PES generation

Using TDHFB to describe the diabatic dynamics through scission



Hybrid approach to fission dynamics



Density of protons for a symmetric fission of ^{258}Fm

Requires:

- TDBCS starting from octupolar deformed densities
- Proper connection between the two theories

Impact: a variety of new charachteristics of the fission fragments

- Improved resolution of for $Y(A), Y(Z)$
- Distribution of kinetic and excitation energies
- Emission of neutrons at scission

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Outlook & Perspectives

Improved numerical methods and increased computational power provides new opportunities to bridge theory with the state of the art experiments.

Fission dynamics with TDGCM+GOA

- Development of a new generation of numerical tools
- Reproduction of the dominant mode of fission yields in neutron rich Fermium isotopes
- 2-dimensional description seems insufficient to describe transition nuclei and explore the SHE region

Challenge: merging the benefits of TDGCM+GOA with TDHFB

- Include diabatic dynamics through scission
- Prediction of new observables *e.g.* Y(A,TKE)
- Impact far beyond the fission process (heavy ion reactions, *etc*)

Thank you for your attention !