



## Probing the fission dynamics with time-dependent approaches based on energy density functional

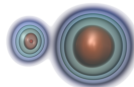
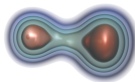
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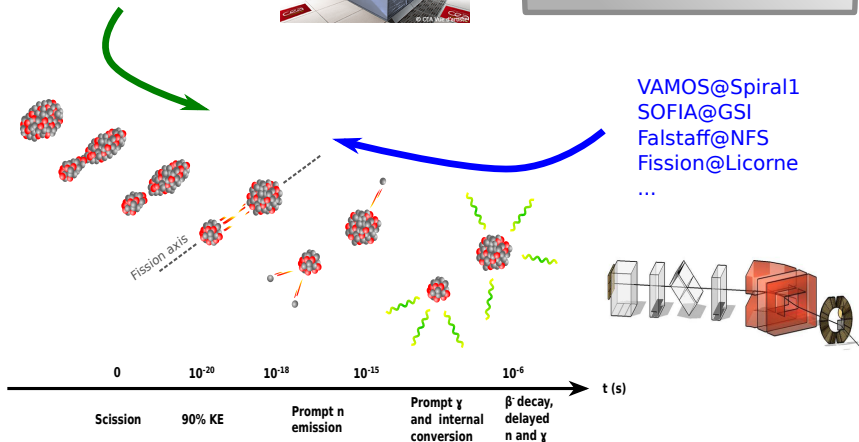


# Probing the fission dynamics

Many-body calculations  
based on energy density  
functional



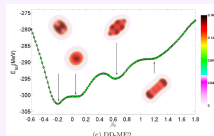
Fission time scale ?  
Scission neutron ?  
Fragments characteristics ?  
Fragments deexcitation ?



# Dynamics from energy density functional

## Basic application of energy density functional theory (EDF)

From a **density functional** (e.g. *Skyrme*, *Gogny*, *RDF*, etc) to the energy and nucleon density of a nuclear **ground state**



(c) DD-ME2  
J.P. Ebran et. al. Phys. Rev. C 90, 054329 (2014)

## Fission dynamics from energy density functional (EDF)

- Generalizing to a time dependent problem
- Dealing with both large collective motions and single particle excitations (close to scission)

### TD-GCM

The system is described by a **mixing of static densities** (e.g. different shapes). The weights associated to each density evolve in time.

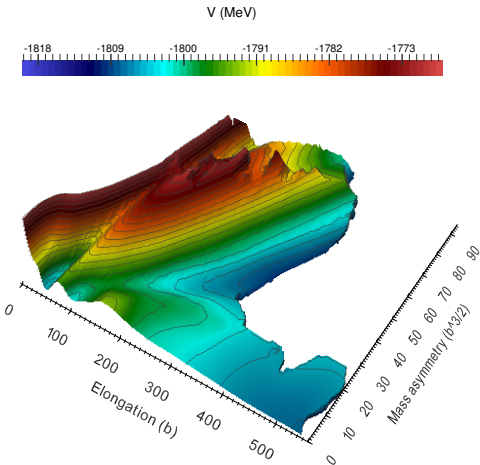
### TD-EDF

The system is described by its nuclear density that can evolve in time

# Time Dependent Generator Coordinate Method (TD-GCM)

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

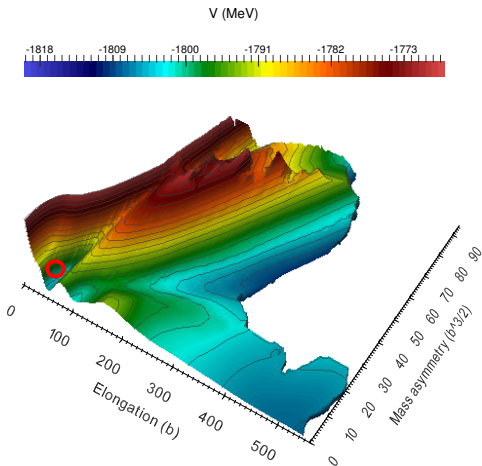


Interpolated potential energy surface for  $(n+{}^{239}\text{Pu})$  fission

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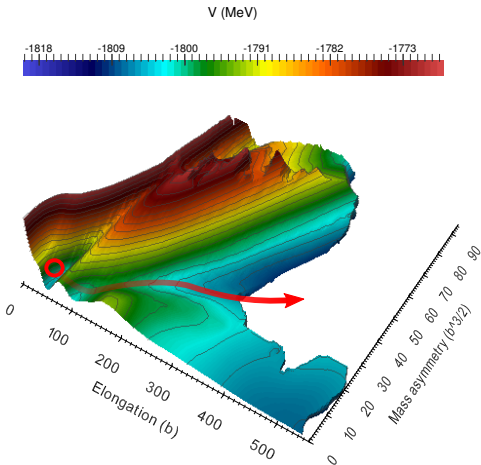


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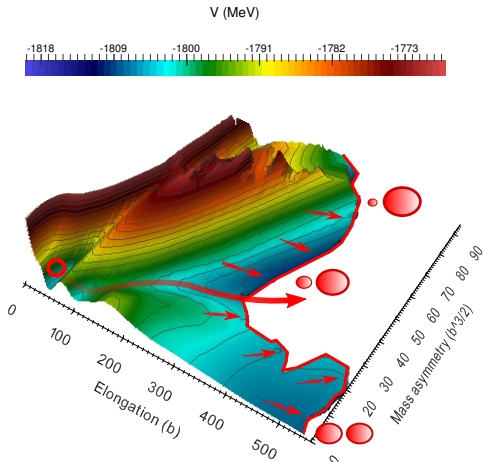


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Interpolated potential energy surface for  $(n+{}^{239}\text{Pu})$  fission

# Development of this microscopic approach

**2005:** First calculation for  $^{238}\text{U}$

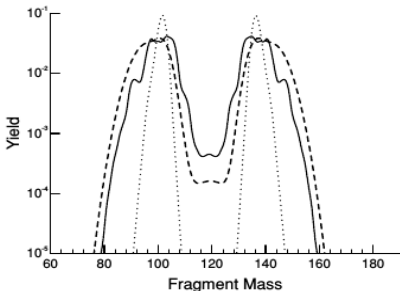
H. Goutte *et al.*, *Phys. Rev. C* **71**, 024316

**2012:** Fission yields of  $^{236}\text{U}$  and  $^{240}\text{Pu}$

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

- Promising results
- High numerical costs

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



Pre-neutron mass yields for  $^{238}\text{U}$  at 2.4 MeV above the fission barrier (H. Goutte *et al.*).

**solid line:** dynamics calculation

**dashed line:** What evaluation (2002)

Upgrade numerical methods

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

FELIX-2.0 accepted in *Comput. Phys. Commun.*

New applications

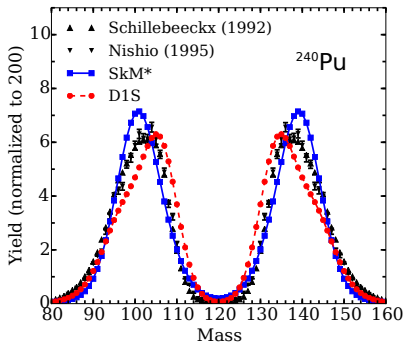
D. Regnier *et al.*, *Phys. Rev. C* **93**, 054611 (2016)

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

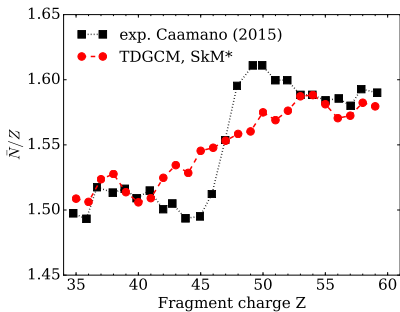
H. Tao *et al.*, *Phys. Rev. C* **96**, 024319 (2017)



# Mass and charge of the primary fragments for a $^{240}\text{Pu}$ fission



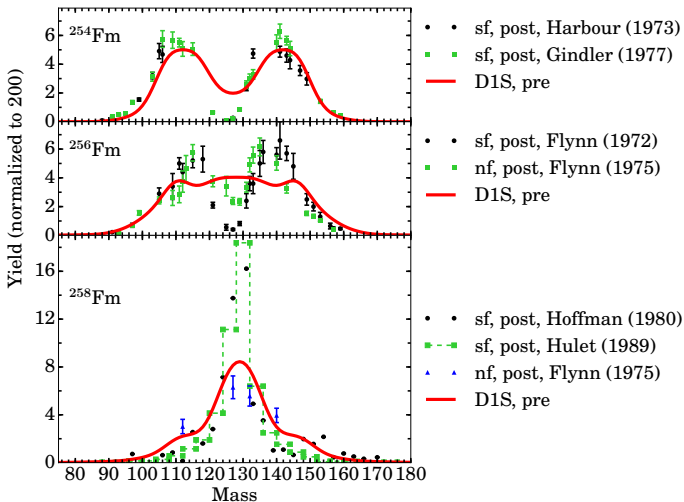
Mass yields of the primary fragments. The initial energy is taken 1 MeV above the fission barrier. *D. Regnier et al., Phys. Rev. C* **93**, 054611 (2016).



Average neutron excess  $\bar{N}/Z$  of primary fragments.

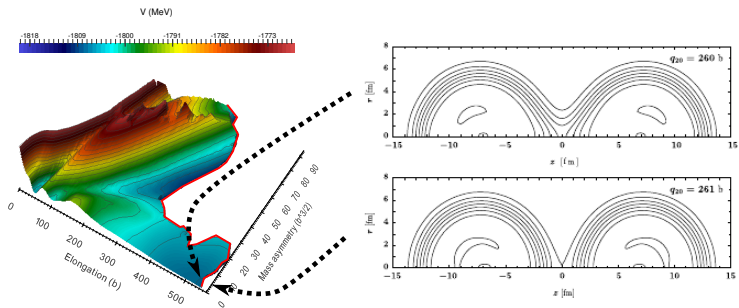
- Qualitative reproduction of the mass yields for actinides
- Missing the non-adiabatic rupture of the neck

## Symmetric/asymmetric yields transitions in Fm isotopic chains



Work in progress on **Th isotopes** for comparison with the last SOFIA campaign

# Major issue: discontinuity at scission



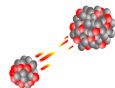
The dynamics must only be computed on a continuous part of the deformation space. In the final configurations:

- masses of the fragments are defined up to the number of particles in the neck,
- the nuclear force is still acting between the two fragments.

Discontinuity at scission prevents us to compute **post-scission fragment observables**

# TD-EDF for the superfluid dynamics in the vicinity of scission

- ① Goal: characterize the primary fragments
- ② Method: Time dependent energy density functional with pairing



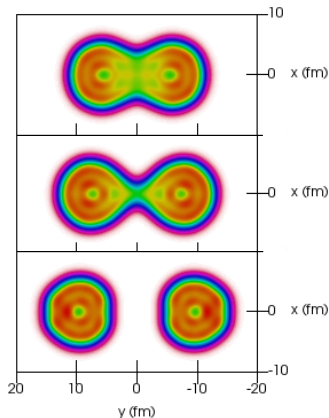
- trajectory of an average fragmentation
- diabatic dynamics

Its recent application to fission enables the prediction of new observables e.g. the **average energy repartition** between the fragments.

It also opens new opportunities concerning:

- scission neutrons
- spin of the fragments ?

Limit: only **averaged observables** over all possible fragmentations (no yields)



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

# Development of this microscopic approach

**2014:**  $^{258}\text{Fm}$   $^{264}\text{Fm}$  (no pairing)

C. Simenel *et al.*, *Phys. Rev. C* **89**, 031601(R)

(2014)

**2015:**  $^{258}\text{Fm}$  with pairing (TDBCS)

G. Scamps *et al.*, *Phys. Rev. C* **92**, 011602(R)

(2015)

$\simeq$  1 week on a few CPU

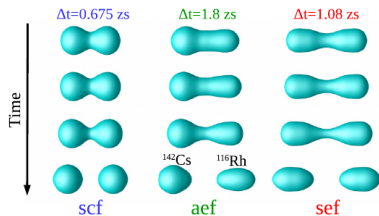
- 60 to 80% of the total excitation energy is generated during the rapid descent to scission

**2016:**  $^{240}\text{Pu}$  with pairing (full TDHFB)

A. Bulgac *et al.*, *PRL* **116**, 122504 (2016)

$\simeq$  10h on 1700 GPU

- TKE reproduction within 3%



Iso-density surfaces for three fission modes of a  $^{258}\text{Fm}$ . G. Scamps *et al.*, *Phys. Rev. C* **92**, 011602(R) (2015).

- Only a few applications up to now
- Rich approach bringing new insight into scission

# Outlook & Perspectives

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

## Perspectives

- TD-GCM: great description of **collective motion** but mostly adiabatic method
  - Test the validity outside of the actinide region
  - Inclusion of additional collective degrees of freedom
  - Systematic calculations for the R-process of nucleosynthesis
- TD-EDF: acces to **new fragment observables** but only one collective trajectory
  - More applications comparable with experiments
  - Investigation on the role of pairing in fission

Big challenge: **merging** the benefits of the two methods

- Correlated fission observables such as  $TKE(A,Z)$
- Impact far beyond the fission process (heavy ion reactions, super-heavy production, *etc*)

Work in progress: SMF to predict pair transfer in heavy ion collisions...

Thank you for your attention !



FELIX

