# Progress and challenges toward the microscopic description of nuclear fission

D. Regnier[1]

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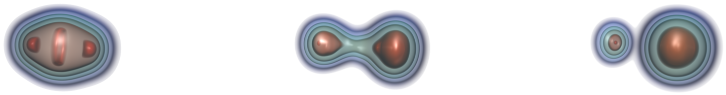
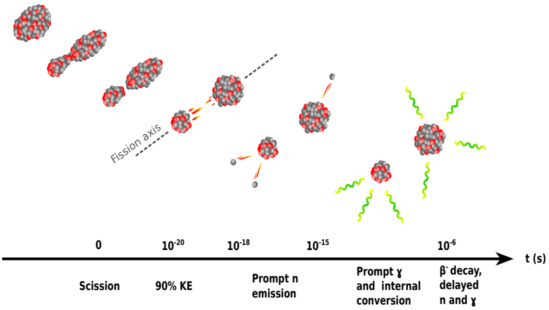
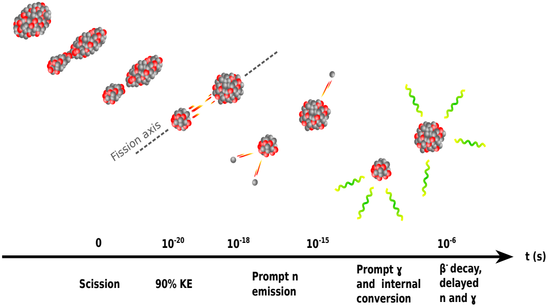


# The impacts and challenges of nuclear fission

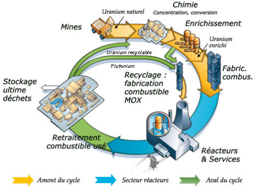


# The impacts and challenges of nuclear fission



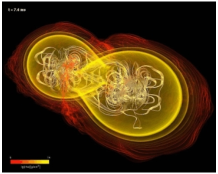

## Nuclear energy

D. Rochman *et. al.* Ann. Nucl. Energy **95**, 125-134 (2016)




## Nucleosynthesis

S. Goriely *et. al.* PRL **111**, 242502 (2013)

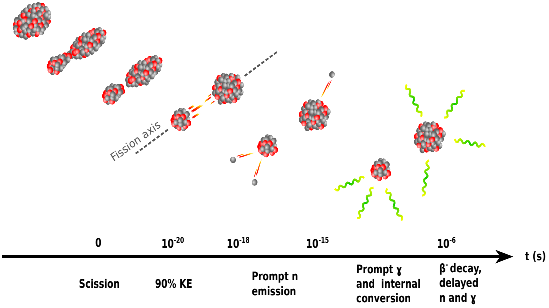


# The impacts and challenges of nuclear fission

Fission time scale ?
R. Rodrıguez-Guzmán *et. al.* Eur. Phys. J. A **52**, 348 (2016)

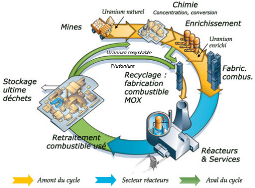
Scission neutron ?
R. Capote *et. al.* PRC 93, 024609 (2016)

Primary fragments characteristics ?
A. Bulgac *et. al.* PRL **116**, 122504 (2016)




Many body pb, dynamics, open system, entanglement:
- heavy ions collisions A. S. Umar et. al., PRC 94, 024605 (2016)
- quantum chemistry C. L. Zhang *et. al.*, PRC **94**, 064323 (2016)

Nuclear energy
D. Rochman *et. al.* Ann. Nucl. Energy **95**, 125-134 (2016)

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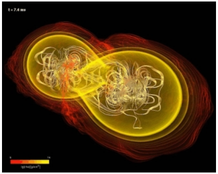
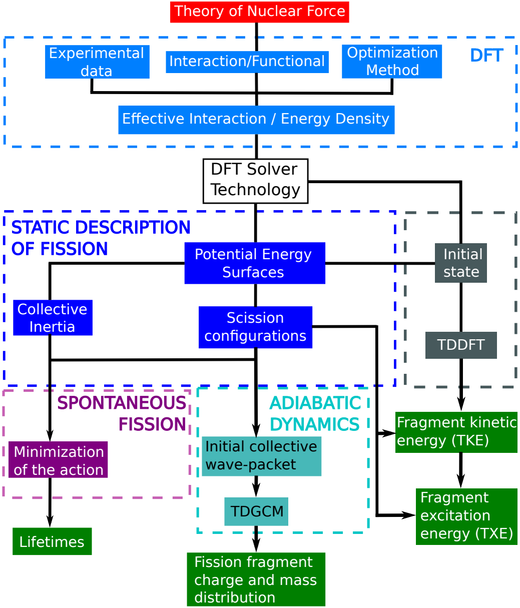


# Schematic workfow of microscopic theory of fission




'Microscopic' ≡ based on energy density functional

## A usefull review

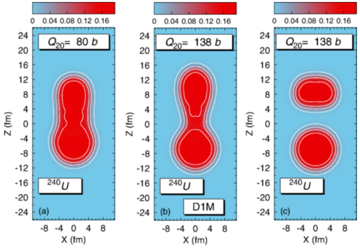
N. Schunck *et al.*, Rep. Prog. Phys. 79 (2016)

**Table of contents:**

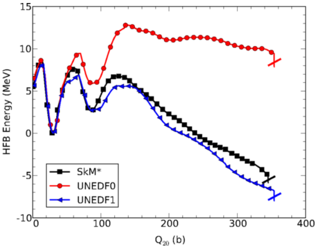
# Static meand field (HFB)

From a density functional (Skyrme, Gogny, RMF,...) to the energy and nucleon density of a nuclear ground state

**Constraints on the deformation**:




R. Rodríguez-Guzmàn *et al.*, Eur. Phys. J. A 52 (2016)




N. Schunck *et al.*, PRC 90 (2014)

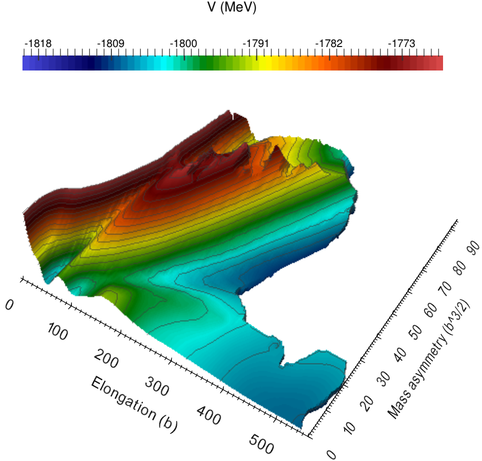
## Continuous efforts towards

1. Speed and stability of HFB solvers at high deformations
2. Better and better density functionals

# Adiabatic dynamics (TDGCM+GOA, ATDHB)

Dynamics in a few dimensional space of deformations

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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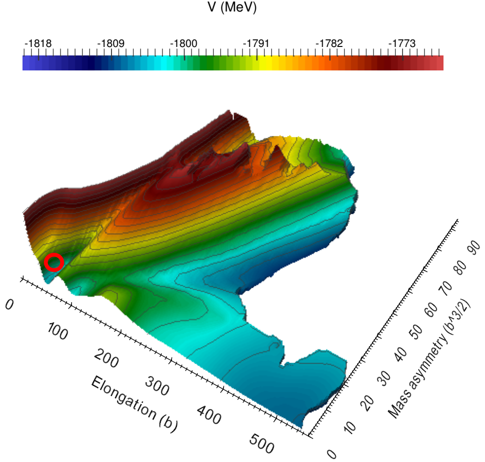


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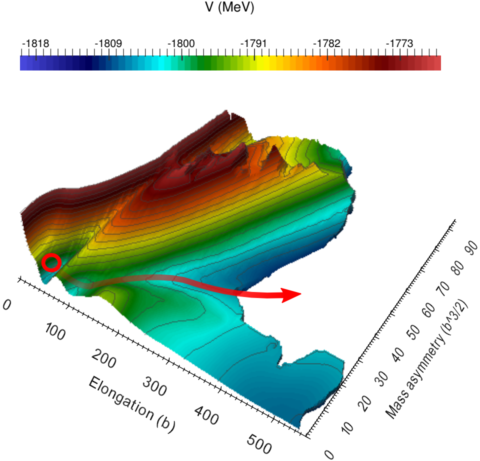


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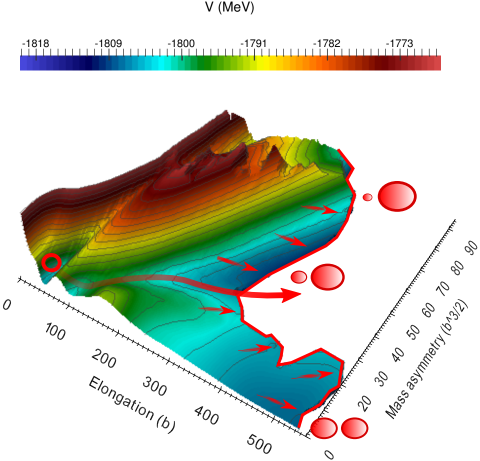



Interpolated potential energy surface for ($n+^{239}Pu$) fission

# Development of the adiabatic dynamics for fission

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

H. Goutte *et al.*, PRC **71**, 024316

- High numerical costs

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

Upgrade numerical methods

**2018:** FELIX-2.0

D. Regnier *et al.*, in press in CPC.

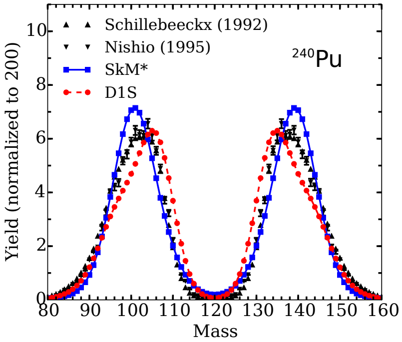
New applications

**2016-2017:** Fission of $^{240}$Pu, $^{252}$Cf, $^{226}$Th

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

A. Zdeb *et al.*, PRC **95**, 054608 (2017)

H. Tao *et al.*, PRC **96**, 024319 (2017)




Mass distribution of the primary fragments for $n+^{239}$Pu

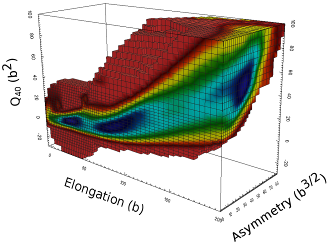
Qualitative agreement with experiments for a few fissioning systems

# Limitations and challenges

Two major limitations:

1. Mapping of the full pb in a low dimensional space → discontinuities
2. Adiabatic picture → no description of the dynamics around scission

**Adding collective variables**




A numerical challenge, $\simeq 1.10^6$ cpu.h for a full 3D PES.

D. Regnier *et al.*, EPJ Web of Conferences **146**, 04043 (2017)

**Adding some intrinsic excitation**

- SCIM method, R. Bernard *et al.*, PRC **84** (2011)
- Fully-fledged TDGCM M. Verrière *et al.*, EPJ Web of Conferences **146**, 04034 (2017)
- Finite temperature EDF N. Schunck *et al.*, PRC **91** (2015)

Drastic increase of the number of degrees of freedom

# Time dependent mean field (TDHF, TDBCS, TDHFB)

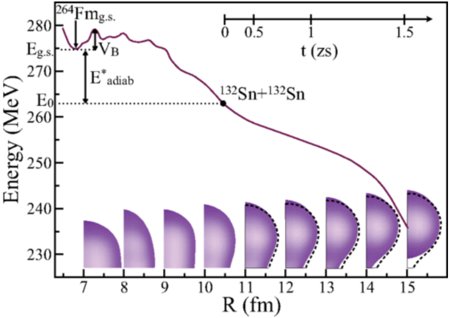
Evolution of one trajectory in the space of mean field states

The dynamics is governed by a system of $k$ non linear differential equations coupled by $h, \Delta$:

$$i\hbar\partial_t \begin{bmatrix} U \\ V \end{bmatrix} = \begin{bmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda^* \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix}$$

Diabatic dynamics up to two 'separated fragments'

- Nucleon density
- Excitation energies
- Kinetic energies
- Evaporation of nucleons




C. Simenel *et al.*, PRC **89**, 031601(R) (2014)

# Development of this microscopic approach

Two lines of improvements in the last few years:

- Unrestricted spatial symmetries
- Inclusion of the pairing correlations

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

C. Simenel *et al.*, PRC **89**, 031601(R) (2014)

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

G. Scamps *et al.*, PRC **92**, 011602(R) (2015)

$\simeq$ 1 week on a few CPU

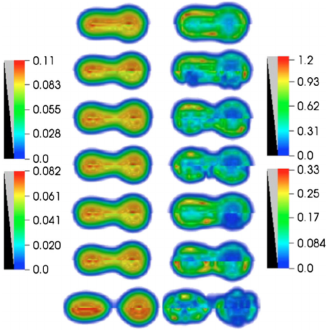
- 60 to 80% of the TXE is generated during the rapid descent to scission

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

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

$\simeq$ 10h on 1700 GPU

- TKE reproduction within 3%




Dynamics of the scission of $^{240}$Pu

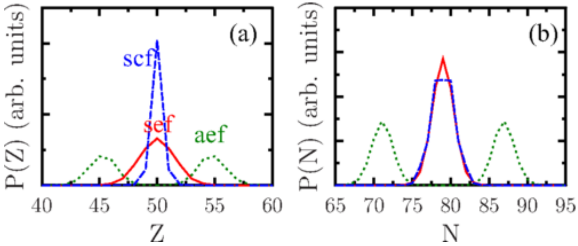
# To do list and major limitation

Up to now, only a few applications of this method to fission. Need for further investigations:

- Dependency with the energy density functional
- More comparison with experimental data
- Scission neutrons
- Fragments spin ?

Major limitation: mean field approximation

1. Too sharp distributions for the fragment observables (no yields)
2. No tunneling through the fission barrier

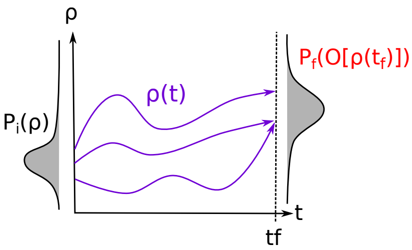


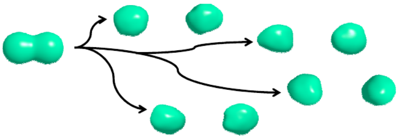

Particle distribution in the fragments G. Scamps *et al.*, PRC **92**, 011602(R) (2015)

# Stochastic mean field

Method:

1. Generate an ensemble of one body-densities that mimic the fluctuations of one mean field state
2. Evolve each density with the TDHFB equation
3. Recover distributions of final observables by classical average



Y. Tanimura *et al.*, PRL **118** (2017)

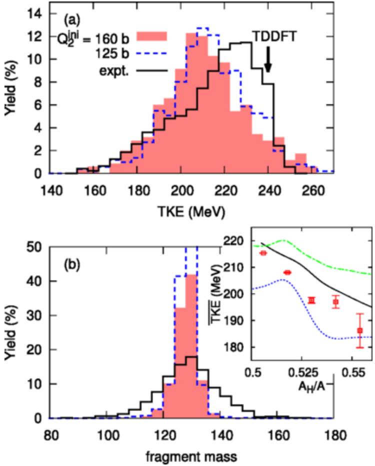
- Possibility to compute fission fragments yields
- No tunneling through the fission barrier

# First application

Spontaneous fission of $^{258}$Fm: Y. Tanimura *et al.*, PRL **118** (2017)

Calculations based on 400 independent TDBCS trajectories.

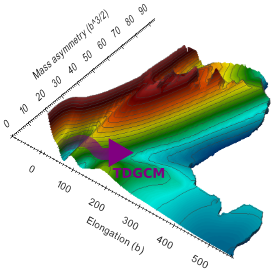
- Promising recovery of fission fragments distributions
- Application to other fissionning systems ?
- Bifurcations between fission valleys ?




Total kinetic energy and mass yields of $^{258}$Fm

# Outlook & Perspectives

Improvement of numerical methods and leveraging modern computers provides new opportunities




To do with the current methods:

- More comparisons with sound experimental data
  → range of validity
- Large scale applications (astrophysics)
- Nuclear data applications ? (few % precision required)

## Big challenges:

- Build a theoretical framework containing both collective fluctuations and diabatic dynamics
  → Predict correlated observables *e.g.* Y(A,Z,TKE)
- Link it with the entrance channel (initial excitation energy, spin...)

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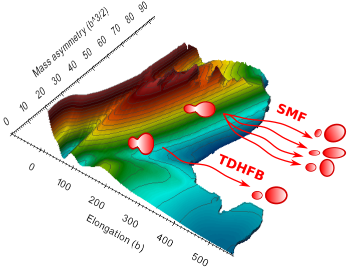


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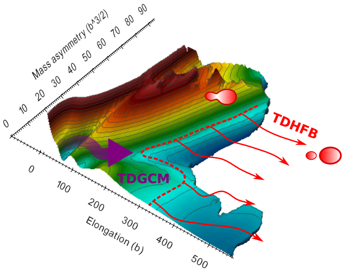


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# Thank you for your attention !