Microscopic description of fission dynamics: toward a 3D resolution of the time dependent GCM+GOA equation

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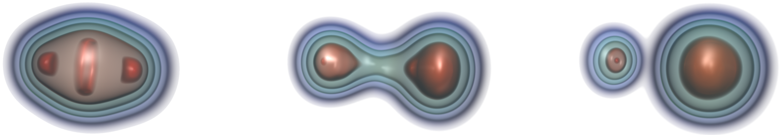

DAM/NNSA project - Dynamics of neutron-induced fission

Start: December 2013

Context

- Build a predictive theory of fission for national security applications
- Use a microscopic approach based on our best knowledge of nuclear forces and quantum many-body methods
- Leverage leadership computing facilities (e.g. the NNSA/ASCR campaigns)

Objectives

1. Deliver a computational framework to predict fission fragment yields
   - Co-developed and shared between CEA and NNSA/ASCR
   - Scalable to next generation of supercomputers
2. Quantify theoretical uncertainties
   - Control numerical errors
   - Estimate sensitivity to model parameters
   - Explore systematic uncertainties

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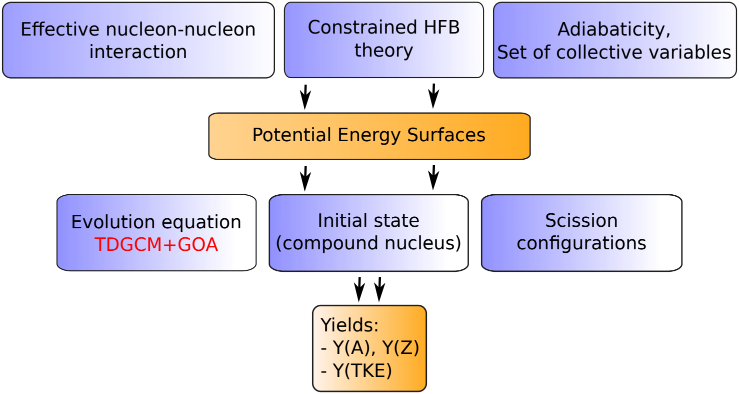
Time Dependent Generator Coordinate Method (TDGCM)



A fully quantum-mechanical description of time evolution

- Gives distribution of probability for the nucleus to have a given shape at time t
- Quantum analog to Kramers equation in classical transport theory

Example of a $n_{th}+\ ^{239}Pu$ 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

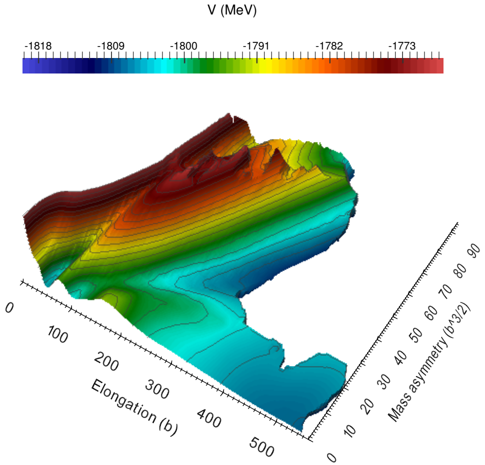


Figure 1 : Interpolated potential energy surface for $(n+^{239}Pu)$ fission

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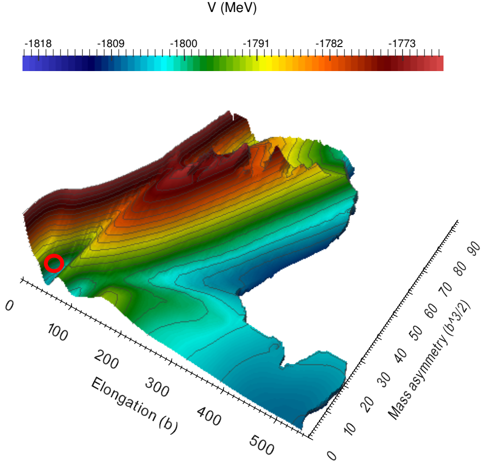

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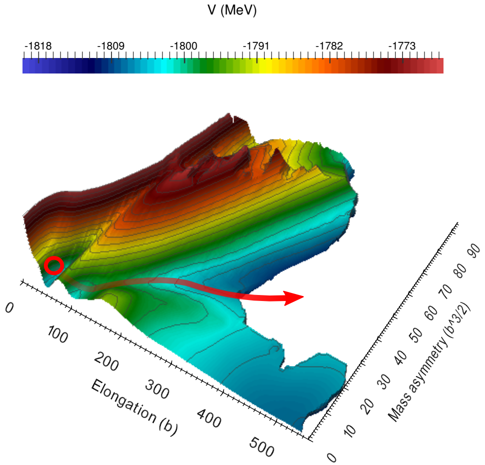

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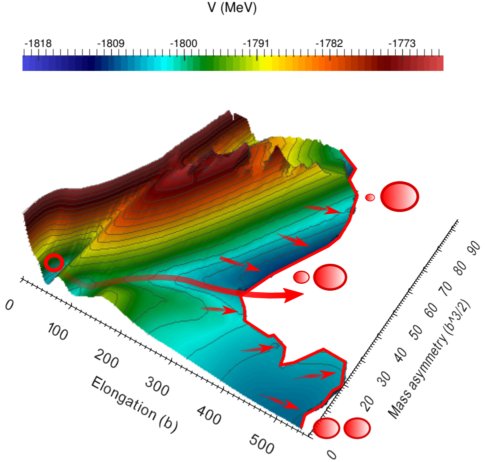

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Fission pre-neutron yields based on the TD-GCM

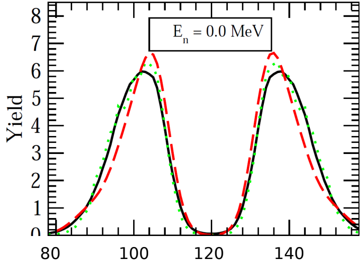

Figure 2 : Pre-neutron mass yields for $n_{th}+{}^{239}$Pu.
Black: experimental data from Schillebeeckx *et al.*(1992).
Red: Microscopic calculation from Younes *et al.*(2012).

2005: First calculation for ^{238}U (n,f)
H. Goutte *et al.*, Phys. Rev. C **71**, 024316

2012: Study of ^{236}U and ^{240}Pu
W. Younes *et al.*, LLNL-TR-586678

Results:

- $\simeq$30% agreement between experiment and theory
- No estimation of uncertainty

Code: tdgcm2d

- Developed and used at CEA and LLNL over last decade
- 2 collective coordinates
- Finite differences, rectangular domain, regular grid

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FELIX: a new solver for the TD-GCM+GOA

Requirements:

- Capable of handling N>2 collective variables for better fidelity
- Full control of numerical precision
- Scalable numerical methods

Numerical methods:

- Finite Element Method (space)
- QMR (sparse matrix inversions)
- Krylov propagation time scheme
- Spectral finite elements

Validation

- Unitary tests
- Analytical benchmarks

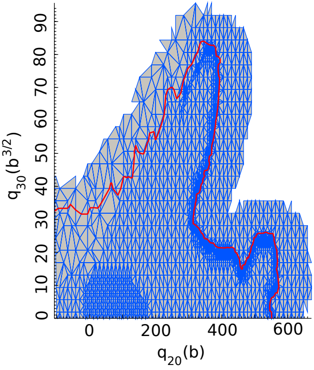
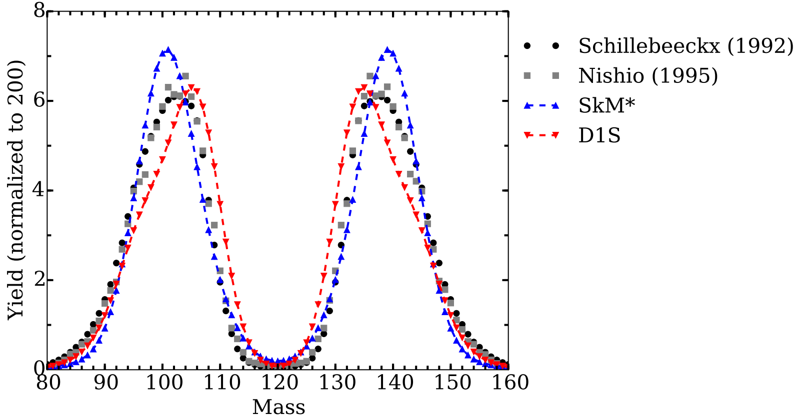


Figure 3 : h-refined mesh of a two-dimensional potential energy surface in ^{240}Pu.

- D. Regnier *et al.*, Comput. Phys. Commun. **122**, 350-363 (2016)
- FELIX-1.0 released under Open Source GPL-2 license

Pre-emission mass yields for $n_{th}+^{239}$Pu fission

Results from FELIX are convoluted with a Gaussian to account for different sources of fluctuations ($\sigma = 4$).



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

Sensitivity analysis

List of the inputs:

1. Form and parameters of the nucleon-nucleon effective interaction
   $\rightarrow$ Potential Energy Surface (PES)
2. Choice and number of the collective variables
3. Definition of the initial state for the time evolution
4. Convolution of the raw flux

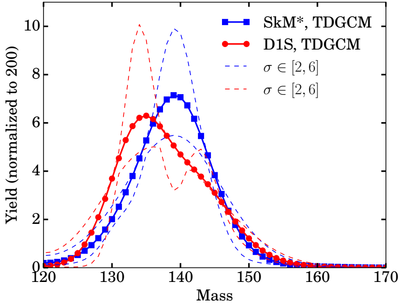


Figure 4 : Variation of the heavy fragments yields for a range of convolution width ($\sigma \in [2, 6]$)

- The qualitative asymetric picture of the the ^{240}Pu fission is robust
- A better modeling of several physics effects (initial state, fragment separation) is necessary to reach quantitative predictions.

Exploration of other fissioning systems

- Is this approach capable of reproducing the yields of various fissioning systems ?
- Is it able to predict a transition from symetric to asymetric fission ?

Series of calculations in progress: ^{236}U,^{256}Fm, ^{258}Fm, ^{260}Fm, ^{226}Th,^{180}Hg

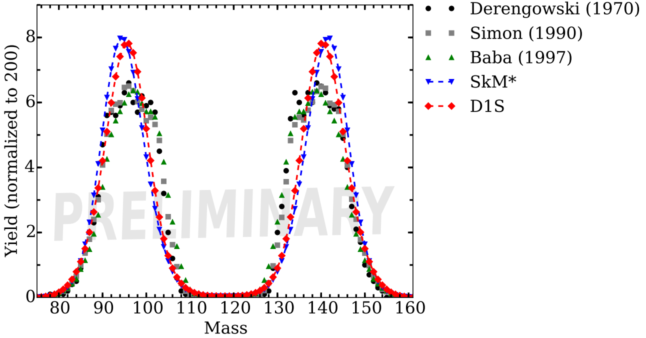


Figure 5 : Pre-emission mass yields for $n_{th}+^{235}$U fission. Results are convoluted with a Gaussian ($\sigma = 4$).

Toward a 3D description

Low dimension → discontinuities issue[a]

- Discontinuities appear in a PES when its dimension is too low to capture the full deformation space topography.
- A dynamic description based on a discontinuous PES is missing a part of the physics (wrong barriers, missing fragmentations . . .).

a: N. Dubray *et al.*, Comput. Phys. Commun. **183**, 2035 (2012)

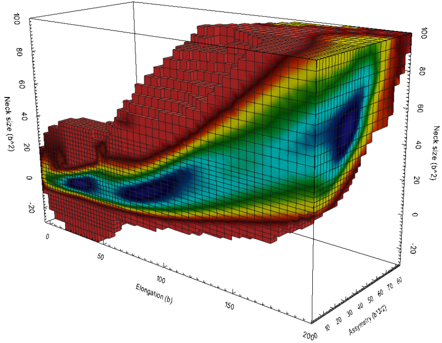


Figure 6 : Potential energy surface for a n+^{239}Pu fission in the collective space ($\hat{Q}_{20}$, $\hat{Q}_{30}$, $\hat{Q}_{40}$).

The first 3D dynamics calculations for a n + ^{239}Pu are on progress...

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Outlook

Results

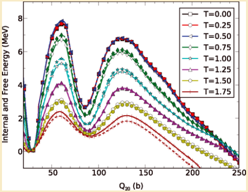
- Deliver a computational framework to predict fission fragment yields
- Fragments yields for a ^{240}Pu fission

Short-term perspectives

- Investigate a variety of fissioning system
- Estimate the benefits of a 3D collective space

Next challenges

- Predict the dynamics through scission
- Step beyond the GOA
- Step beyond the adiabatic approximation



Thank you for your attention !

Related publications:

- N. Dubray *et al.*, Comput. Phys. Commun. **183**, 2035 (2012)
- D. Regnier *et al.*, Comput. Phys. Commun. **122**, 350-363 (2016)
- D. Regnier *et al.*, Phys. Rev. C **93**, 054611 (2016)
- D. Regnier *et al.*, EPJ Web of Conf. **111**, 08005 (2016)