Why the finite element method could be a powerful tool to model fission dynamic

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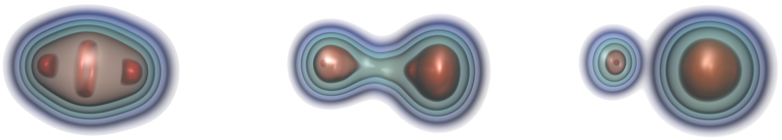
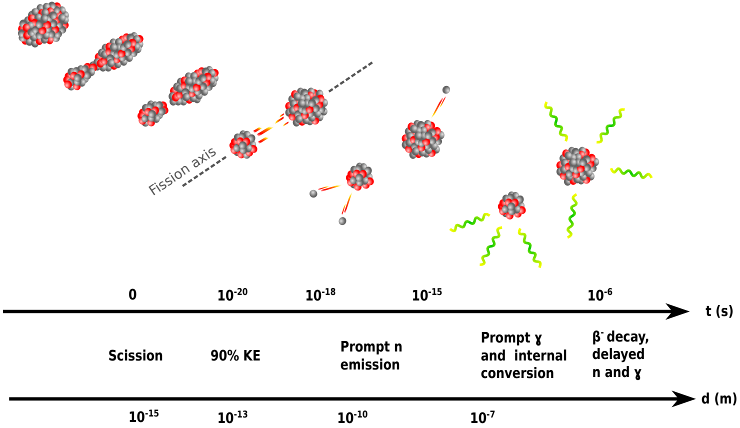


Fission process



What are the properties of the fission fragments after scission ?

Mass yields Y(A), Total Kinetic Energy Y(TKE), spin distribution ...

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The TD-GCM + GOA approach

- Goal: Predict the evolution of the fissioning system from a compound nucleus state.
- Mean: Microscopic approach.

Scheme:

Effective nucleon-nucleon interaction

Set of collective variables $\vec{q}$
$|\psi(t)\rangle = \int_{\vec{q}} f(\vec{q},t) \cdot |\phi(\vec{q})\rangle \cdot d\vec{q}$ (**TD-GCM**)

Evolution equation + initial state ϕ_i (compound nucleus)

Results:
- Y(A)
- Y(TKE)

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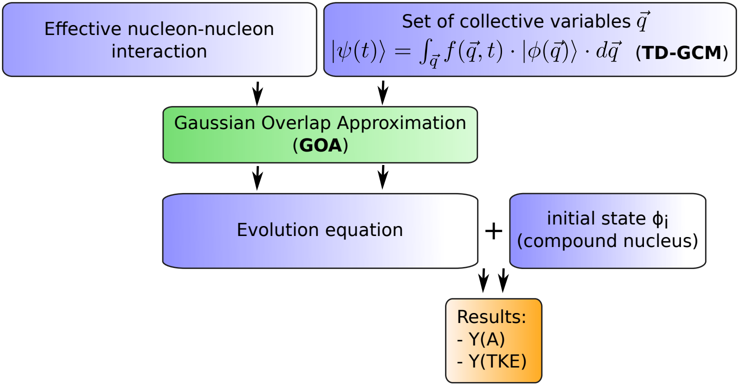

The TD-GCM + GOA approach

This framework yields the following time evolution equation:

Evolution equation

$$i\hbar\frac{\partial}{\partial t}g(\vec{q},t) = \left[-\frac{\hbar^2}{2}\sum_{ij}\frac{\partial}{\partial q_i}B_{ij}^{(\vec{q})}\frac{\partial}{\partial q_j} + V(\vec{q})\right]\cdot g(\vec{q},t) \qquad (1)$$

A diffusion-like equation for the collective variables $\vec{q} = q_1, \cdots, q_n$
With:

- An unknown function $g(\vec{q},t)$, linked to the $f(\vec{q},t)$ coefficients of the $\psi(t)$ expression
- An inertia tensor $B^{-1}(\vec{q})$
- A potential energy surface $V(\vec{q})$

Example of a n+^{239}Pu fission

1. Choice of the collective variables:
   - elongation(Q_{20}),
   - mass assymetry(Q_{30})
2. Calculation of the collective inertia and potential (largest computational budget)
3. Construction of an initial wave packet $g(\vec{q}, t = 0)$
4. Computation of the time evolution

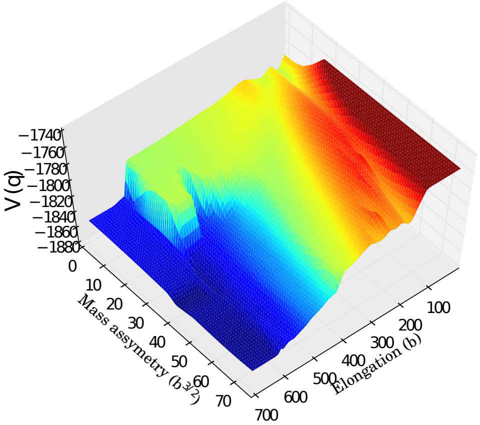

Figure 1: Interpolated potential energy surface for (n+^{239}Pu) fission

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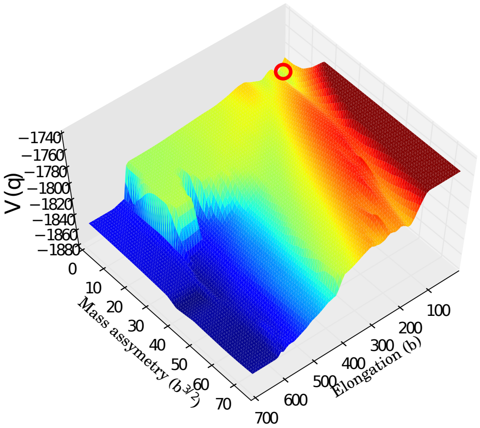

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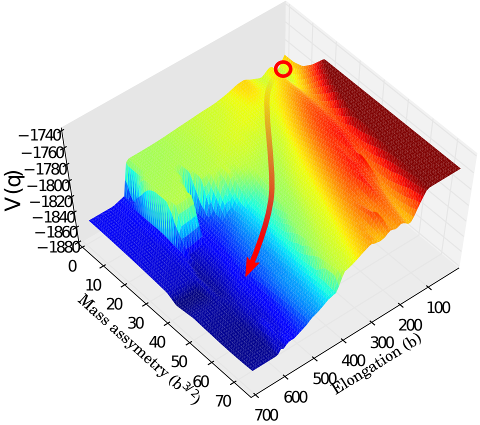

Figure 1: Interpolated potential energy surface for (n+^{239}Pu) fission

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Previous studies

Previous work using the TD-GCM approach for fission:

- J.F Berger *et al.*, Comp. Phys. Comm. 63, 365 (1991)
- H. Goutte *et al.*, Phys. Rev. C 71, 024316 (2005)
- W. Younes *et al.*, LLNL-TR-586678 (2012)

Discretization of the collective variables based on:

1. a finite difference method,
2. a regular mesh.

→ Only 2 collective variables

Can finite element analysis overcome this limitation ?

Finite element VS Finite difference

Differential equation 1D:

$$-\frac{\partial^2 g}{\partial x} = b(x)$$

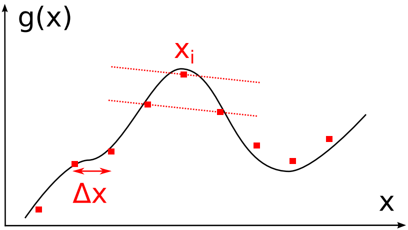
with $g(x_{min}) = g(x_{max}) = 0$

Finite difference

- Generate a mesh
- Compute derivatives based on the neighboor points

$$\frac{\partial g}{\partial x}\Big|_{x_i} = \frac{g(x_{i+1}) - g(x_{i-1})}{2\Delta x}$$

- Deduce the linear system



Finite element VS Finite difference

Finite element

1. Generate a mesh
2. Choose an interpolation inside each element

$$\rightarrow g_{approx} = \sum_i G_i \cdot \psi_i$$

3. Express the variational form

$$\forall \phi : \int_x \phi \cdot \left[b(x) + \frac{\partial^2 g}{\partial x} \right] = 0$$

4. Deduce a linear system $\forall i \in [0, \dim]$:

$$\int_x \psi_i \cdot \left[b(x) + \frac{\partial^2 g_{approx}}{\partial x} \right] = 0$$

Differential equation 1D:

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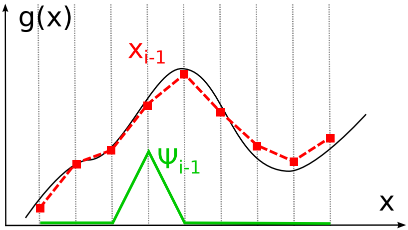
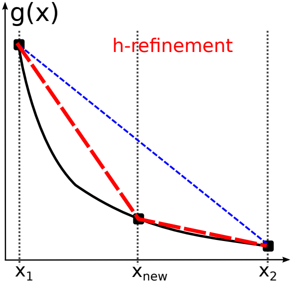
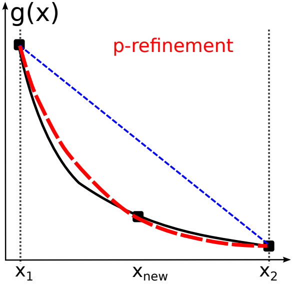


Increasing accuracy with refinement

Two main refinement techniques:

- h-refinement: decrease the maximum size (h) of the elements
- p-refinement: increase the polynomial order (p) of the interpolation function inside the elements





Before p-refinement: $g_{approx} = ax + b$
After p-refinement: $g_{approx} = ax^2 + bx + c$

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Recent developements

December 2013:

- Functional finite element method solver for N collective variables
- Only using polynomial interpolation of degree 1

New capabilities:

- Yield calculation
- Initial wave packet calculation
- Generalization to any degree of polynomial interpolation (p-refinement enabled)

Tests on Toy-models:

- Free wave packet
- Harmonic oscillator 1D, 2D

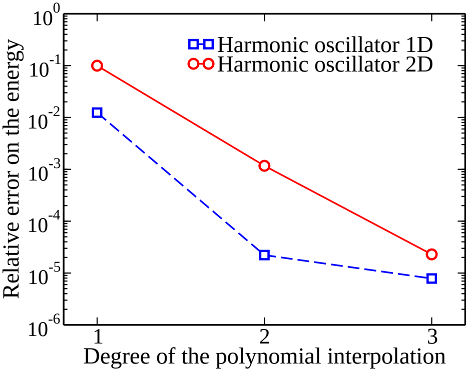

Figure 2: Relative error of the energy of the second solution of an Harmonic Oscillator

Preliminary results on a n+^{239}Pu fission

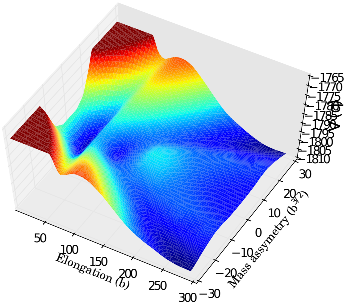

Figure 3: ^{240}Pu potential energy surface for the collective variable q_{20} and q_{30}

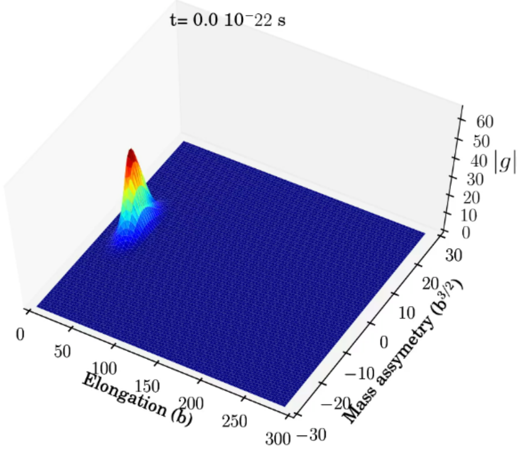

Figure 4: Propagation of the wave packet $(|g(q_{20}, q_{30}, t)|)$

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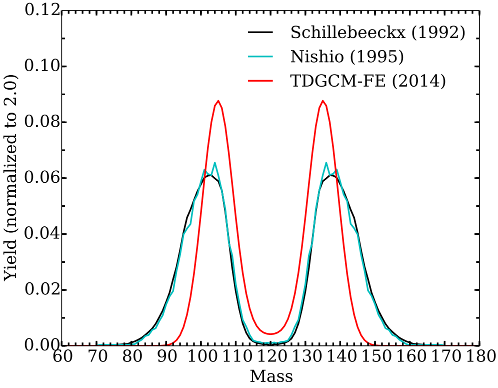

Figure 5: Primary mass yields for a n+^{239}Pu fission

Preliminary calculation:

- Interpolation polynomials of degree 2
- Smoothed yields

To be checked:

- Size of the simulation box
- Numerical accuracy

To be further studied:

- Position of the frontier for the yield calculation
- Fragment masses at the frontier
- Additional collective dimensions

Conclusion & Perspectives

1. Time Dependent Coordinate Generator Method (TD-GCM):
   - Produces a Shrödinger like equation
2. Finite element method:
   - Powerful refinement methods
3. Solver current status:
   - Tested on toy-models
   - Preliminary calculations on n $+^{239}$Pu

Perspectives

- Optimizations $\rightarrow$ N-D calculations
- Production of temperature dependent results (trends of the yields as a function of the incident neutron energy)
- Uncertainty analysis

Thank you for your attention !