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* \( \vec{q} \)
- Evolution equation
- Initial state \( \phi_i \) (compound nucleus)

**Results:**
- \( Y(A) \)
- \( Y(TKE) \)
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
- Evolution equation
- Initial state $\phi_i$ (compound nucleus)
- Gaussian Overlap Approximation (GOA)
- Results:
  - $Y(A)$
  - $Y(TKE)$

Set of collective variables $\vec{q}$

$$|\psi(t)\rangle = \int_{\vec{q}} f(\vec{q}, t) \cdot |\phi(\vec{q})\rangle \cdot d\vec{q} \quad \text{(TD-GCM)}$$
The TD-GCM + GOA approach

This framework yields the following time evolution equation:

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

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 asymmetry\((Q_{30})\)
2. Calculation of the collective inertia and potential (largest computational budget)
3. Construction of an initial wave packet \(g(\bar{q}, t = 0)\)
4. Computation of the time evolution

Figure 1: Interpolated potential energy surface for \((n+^{239}\)Pu\) fission
Example of a $n+^{239}\text{Pu}$ fission

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**Figure 1:** Interpolated potential energy surface for ($n+^{239}\text{Pu}$) fission
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Previous studies

Previous work using the TD-GCM approach for fission:

- 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

Finite difference

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

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

- Deduce the linear system

Differential equation 1D:

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

with \( g(x_{\text{min}}) = g(x_{\text{max}}) = 0 \)
Finite element VS Finite difference

**Finite element**

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

\[ g_{\text{approx}} = \sum_i G_i \cdot \psi_i \]

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

\[ \forall i \in [0, \text{dim}] : \int x \psi_i \cdot \left[ b(x) + \frac{\partial^2 g_{\text{approx}}}{\partial x} \right] = 0 \]

**Differential equation 1D:**

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

with \( g(x_{\text{min}}) = g(x_{\text{max}}) = 0 \)

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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: \( g_{\text{approx}} = ax + b \)

After p-refinement: \( g_{\text{approx}} = ax^2 + bx + c \)
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Recent developments

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 ($|g(q_{20}, q_{30}, t)|$)
Preliminary results on a $n + {}^{239}\text{Pu}$ 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

*Figure 5:* Primary mass yields for a $n + {}^{239}\text{Pu}$ fission
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!