Fully Microscopic Description of Fission with Three Degrees of Freedom

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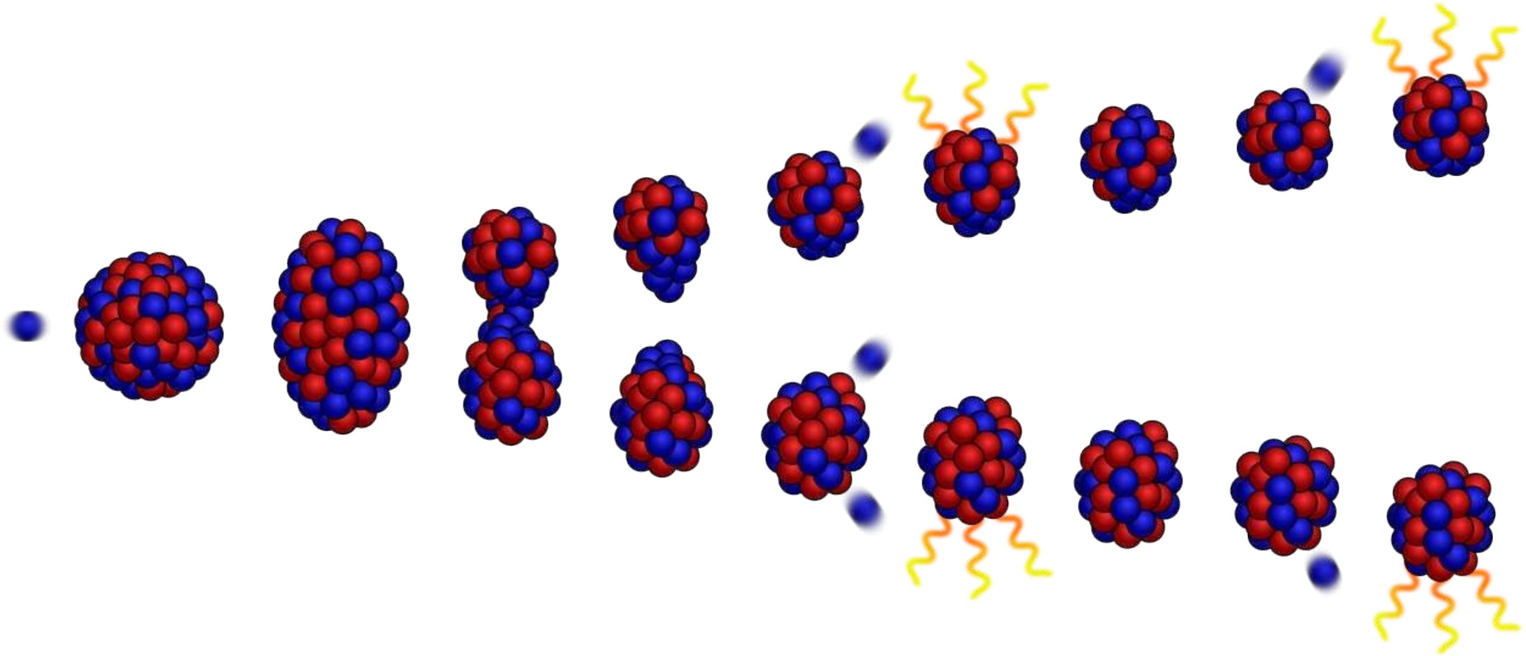
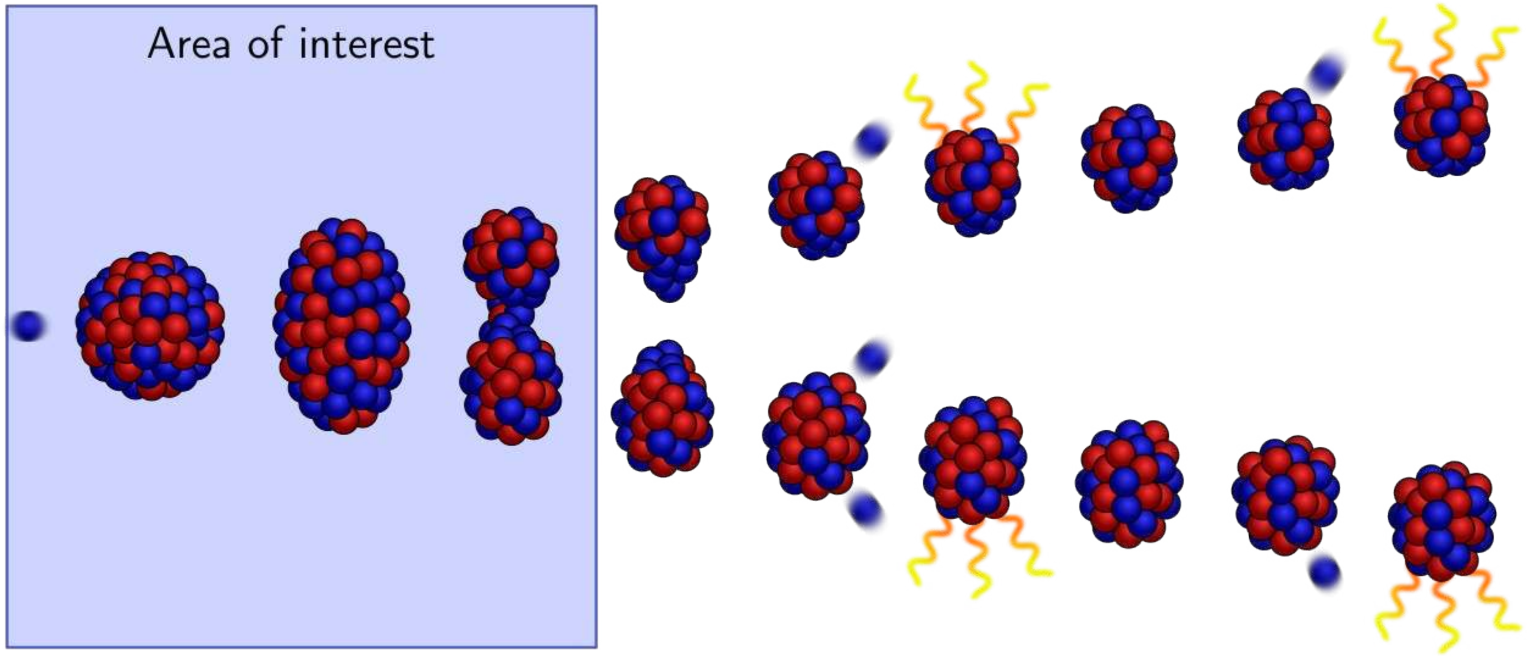
LLNL-PRES-871493

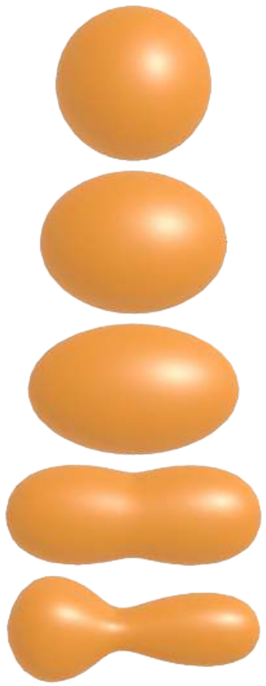
We describe the fission process using a fully microscopic approach.



We simulate the time-evolution of the deformations leading to the formation of the fragments.



Our approach consists in projecting the dynamics on a few relevant collective degrees of freedom.



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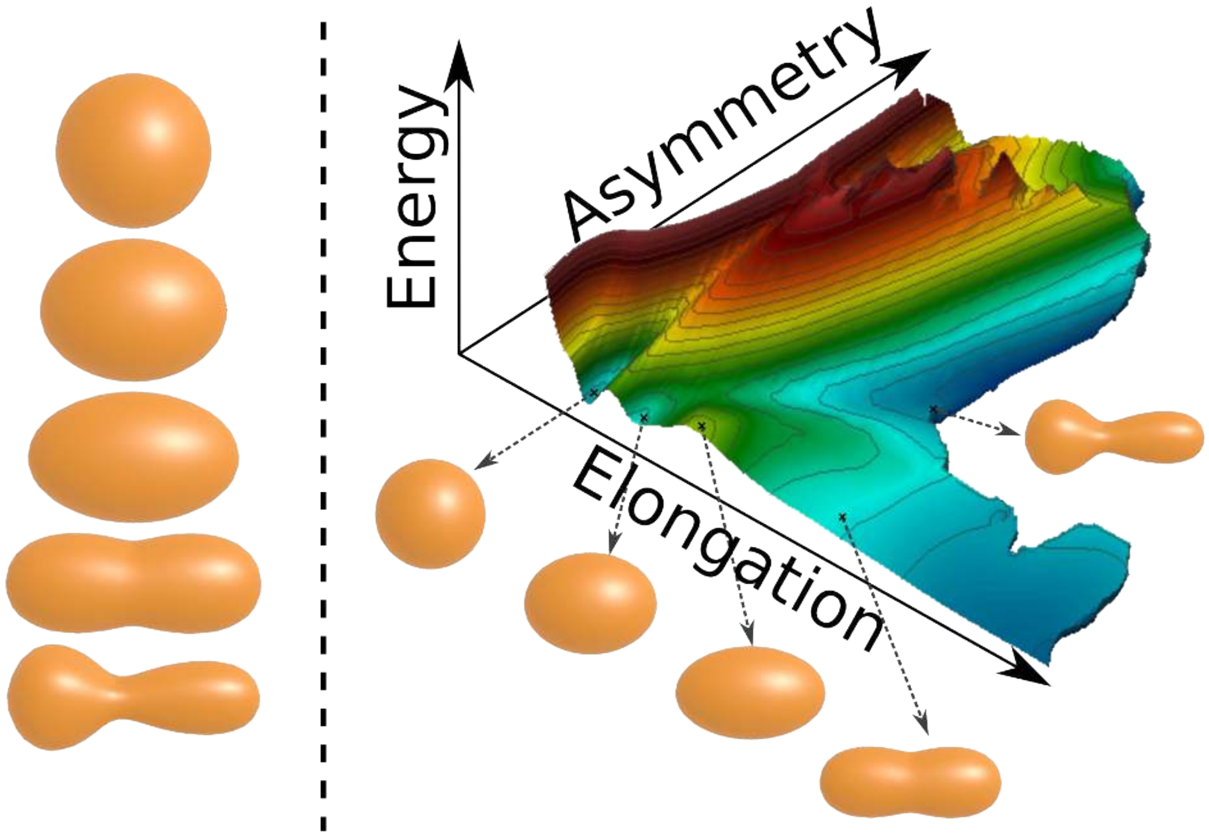

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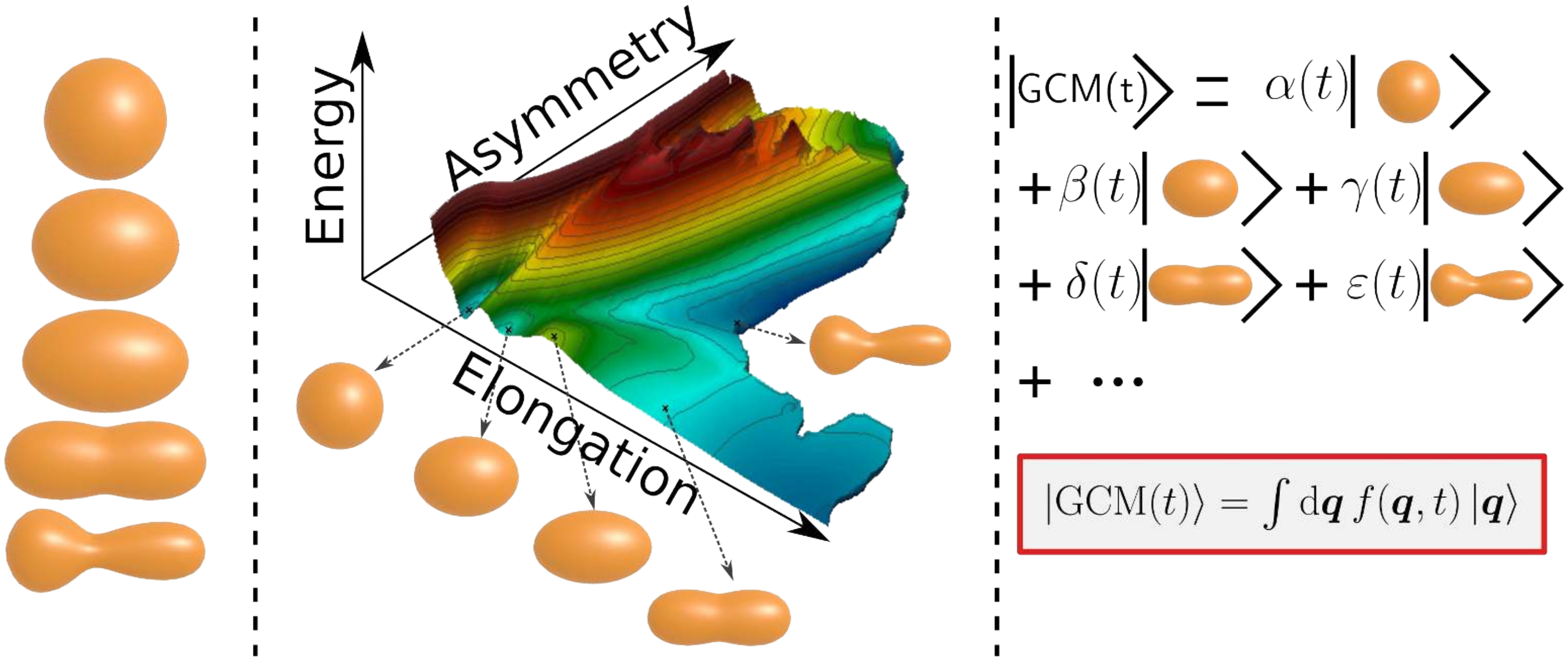

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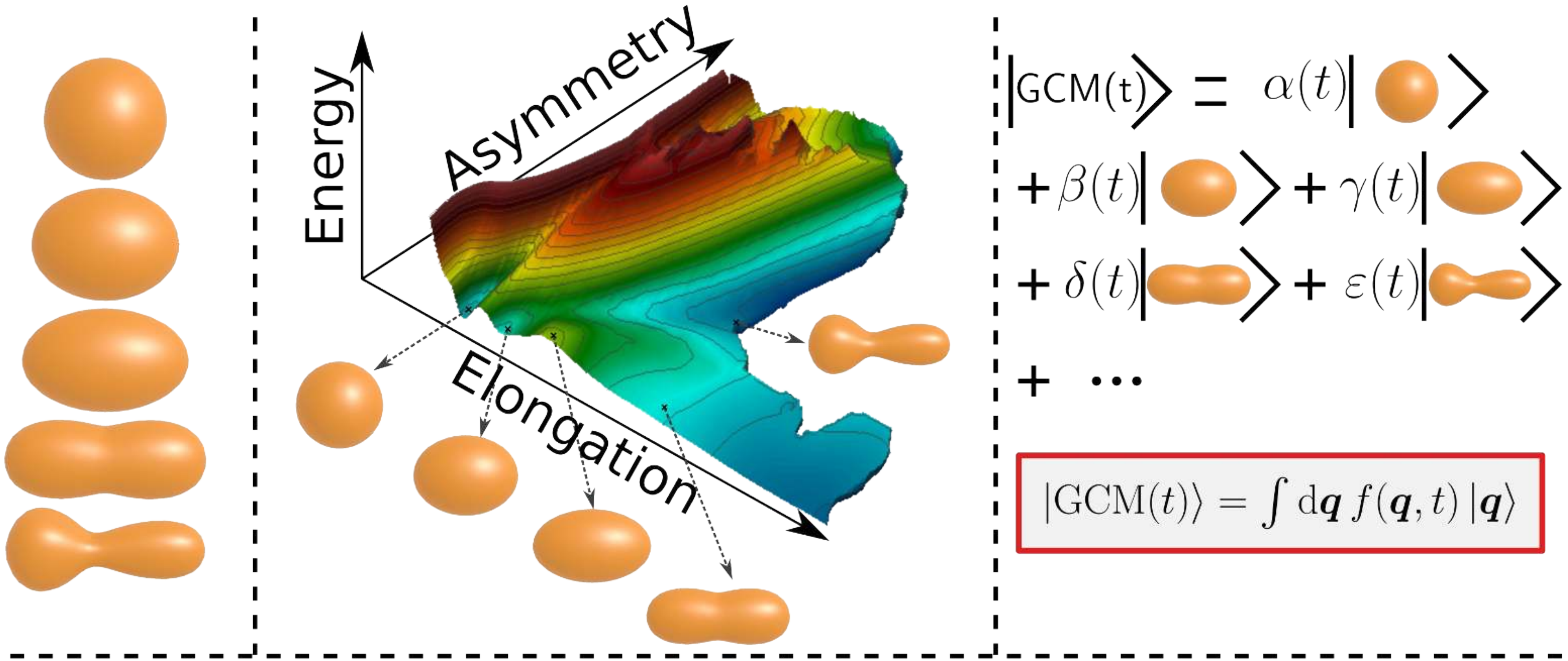

Solve the Schrödinger equation
on the collective subspace:

$$\forall \boldsymbol{q}, \left\langle \boldsymbol{q} \middle| i\hbar \frac{\mathrm{d}}{\mathrm{d}t} - \hat{H} \middle| \mathrm{GCM}(t) \right\rangle = 0$$

Hill-Wheeler-Griffin (non-local, ill-defined)

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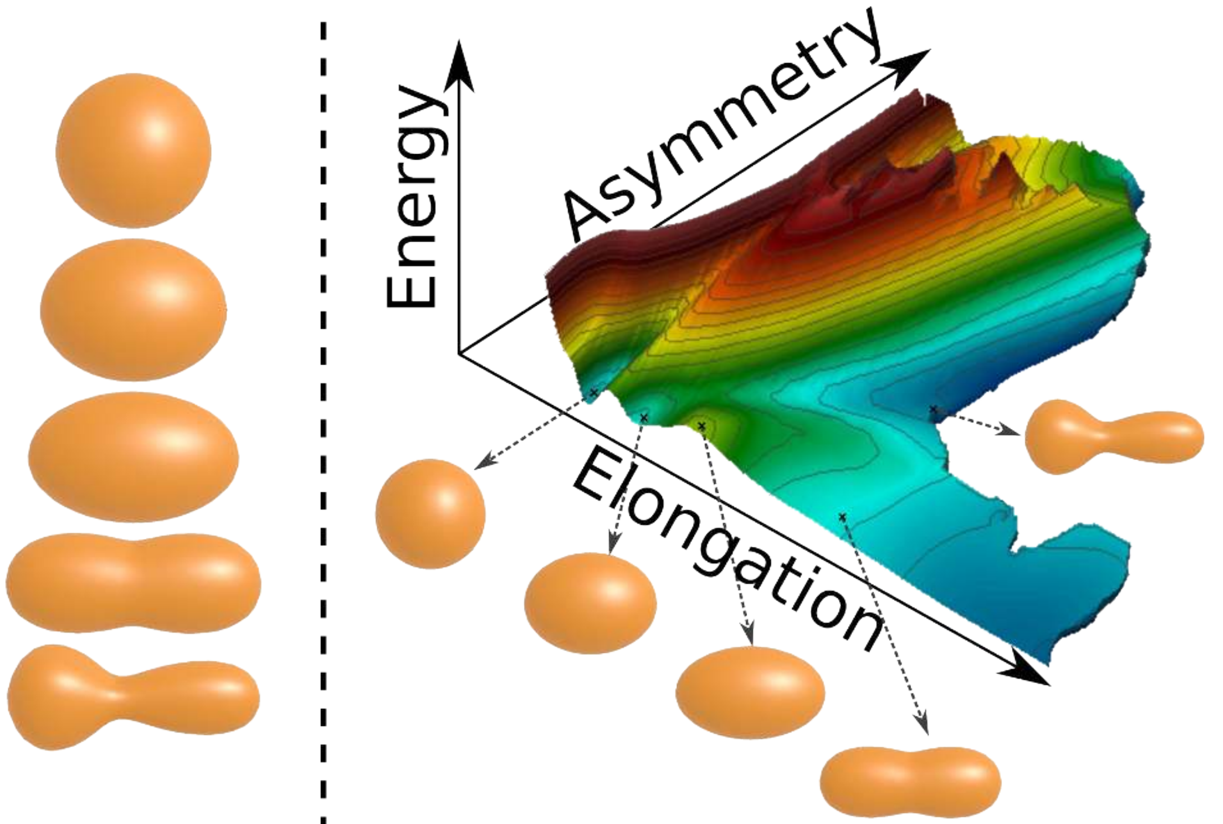

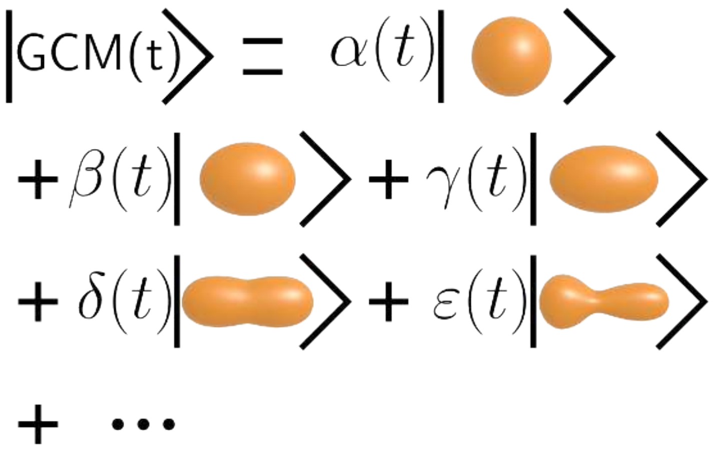

$$|\mathrm{GCM}(t)\rangle = \int \mathrm{d}\boldsymbol{q}\, f(\boldsymbol{q},t)\, |\boldsymbol{q}\rangle$$

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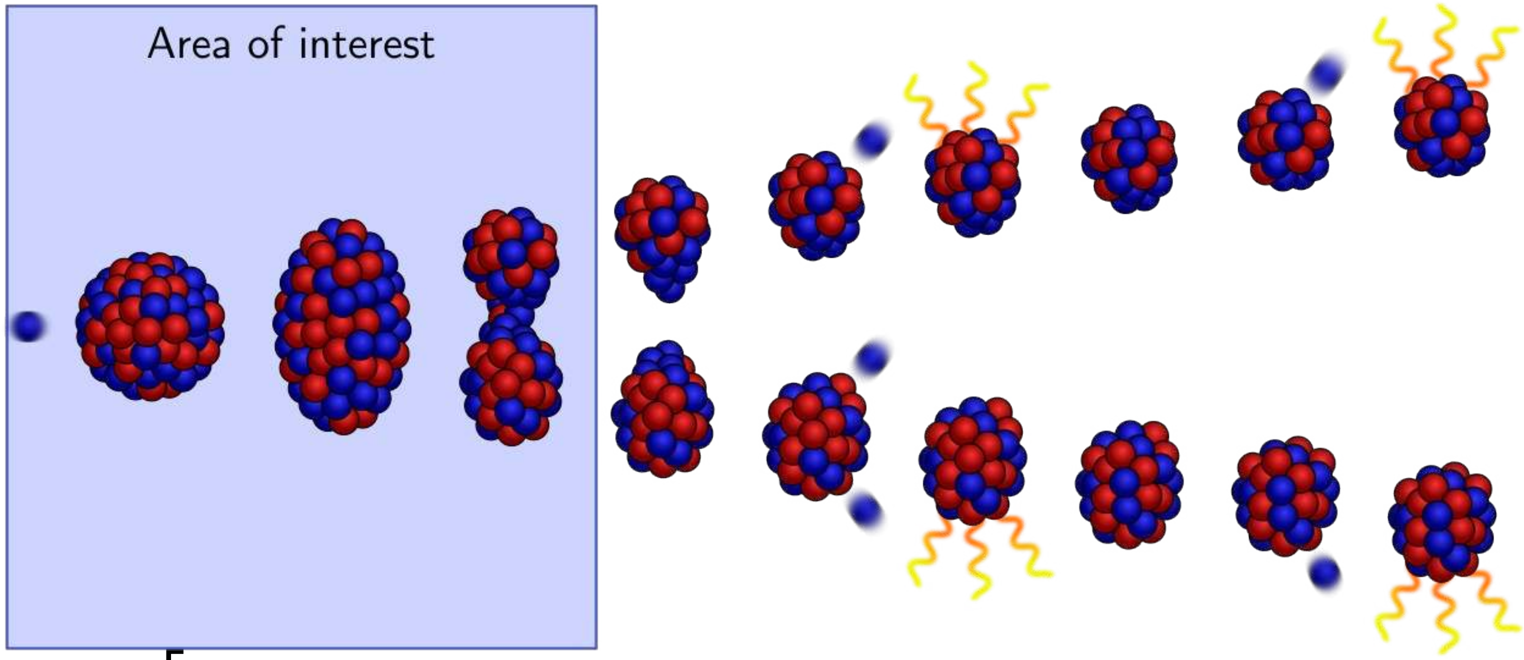
Hill-Wheeler-Griffin (non-local, ill-defined)

Use Gaussian Overlap Approximation:

(reduce HWG to a well-defined local Schrodinger-like equation on the collective space)

Replace $f(\boldsymbol{q},t)$ by $g(\boldsymbol{q},t)$ (same information)

Our theoretical framework leads to Schrodinger-like equation.

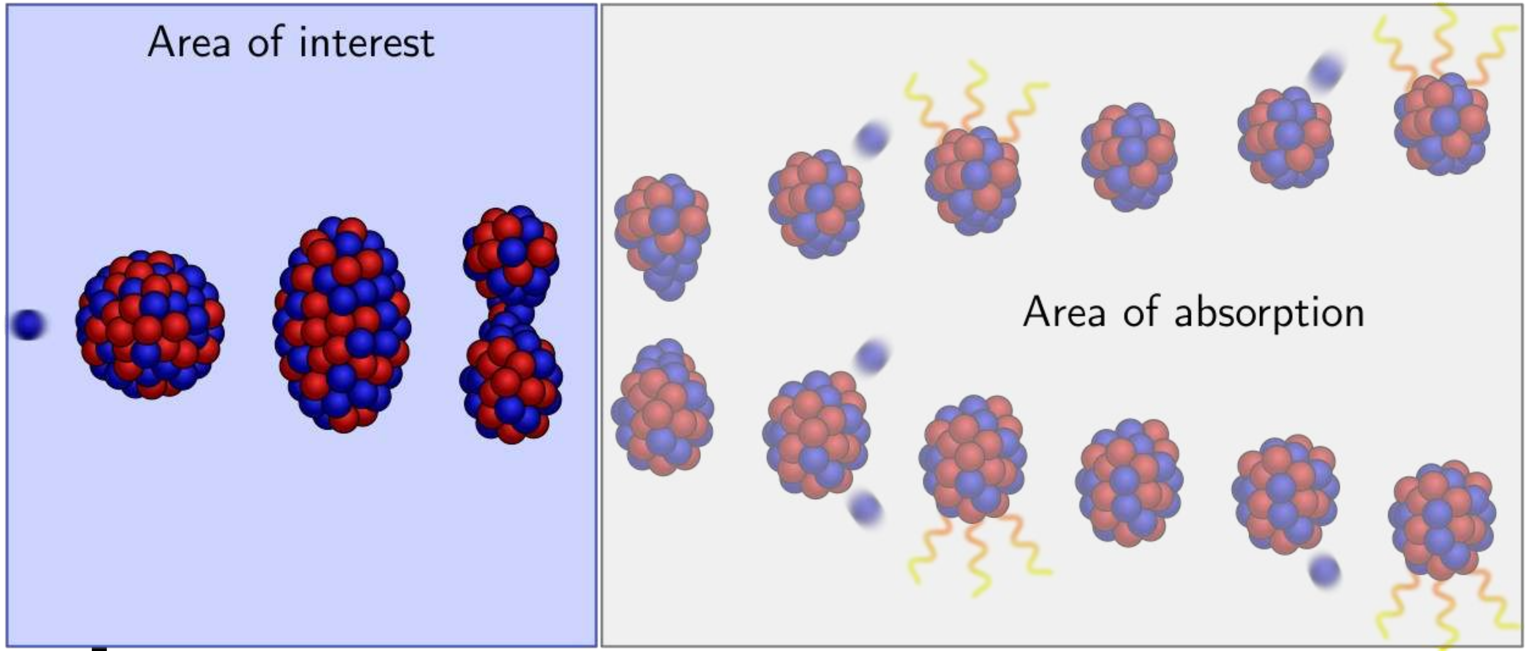


$$i\hbar \frac{\partial g(\boldsymbol{q},t)}{\partial t} = \left[-\frac{\hbar^2}{2} \gamma^{-\frac{1}{2}}(\boldsymbol{q}) \nabla \cdot \gamma^{\frac{1}{2}}(\boldsymbol{q}) B(\boldsymbol{q}) \nabla + V(\boldsymbol{q}) \right] g(\boldsymbol{q},t)$$

Equation describing the fission dynamics at a microscopic level with quantum effects:

- local **complex-valued** diffusion equation with real-valued -dependent coefficients , and .
- : collective degrees of freedom describing the nucleus' deformation (2-D → **3-D**).
- : nucleus' probability amplitude to be in at time (complex-valued).

We add an absorption term to limit our description to the area of interest.



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We developed a new solver, FIDELIS, able to tackle three collective degrees of freedom.

$$i\hbar \frac{\partial g(\boldsymbol{q},t)}{\partial t} = \left[-\frac{\hbar^2}{2} \gamma^{-\frac{1}{2}}(\boldsymbol{q}) \nabla \cdot \gamma^{\frac{1}{2}}(\boldsymbol{q}) B(\boldsymbol{q}) \nabla + V(\boldsymbol{q}) - iA(\boldsymbol{q}) \right] g(\boldsymbol{q},t)$$

1. We discretize the collective space using the Finite Element Method with MFEM.

2. We developed a high-order () numerical time-discretization scheme.

3. We revamped our approach to predict the fission fragment properties.

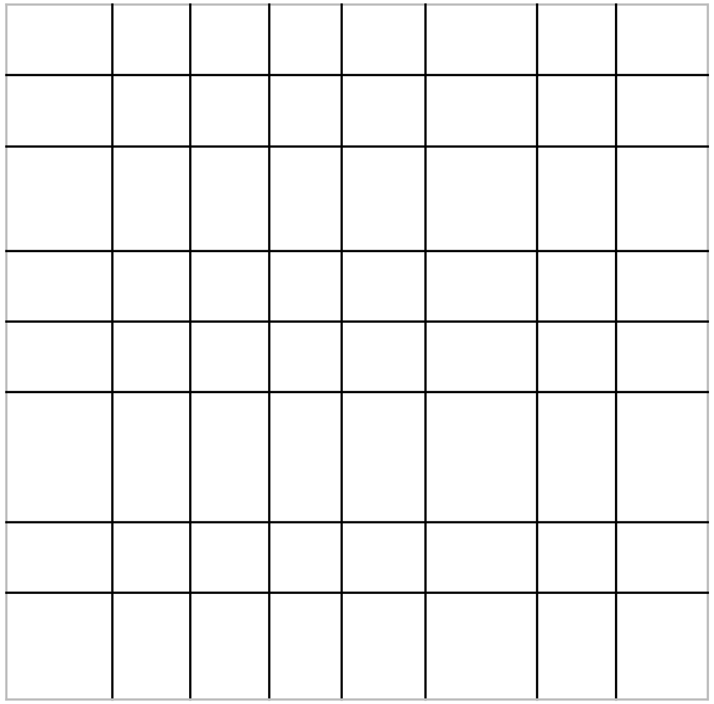
FIDELIS: **FI**nite-element **DE**scription of **L**arge-amplitude collective motion **I**n microscopic **S**ystems

1. We discretize the collective space using the Finite Element Method with MFEM.

$$i\hbar\frac{\partial g(\boldsymbol{q},t)}{\partial t}=\left[-\frac{\hbar^2}{2}\gamma^{-\frac{1}{2}}(\boldsymbol{q})\nabla\cdot\gamma^{\frac{1}{2}}(\boldsymbol{q})B(\boldsymbol{q})\nabla+V(\boldsymbol{q})-iA(\boldsymbol{q})\right]g(\boldsymbol{q},t)$$

Partition space

Collective space (infinite size)



Define basis functions

The scalar field is smooth:

➔ H1-conformal real basis,

➔ piecewise -degree polynomials.

➔ Basis function noted

Project the equation

Orthogonal projection on the basis functions using the scalar product:

,

,

,

.

➔ **Sparse & partially assembled!**

2. We developed a high-order time-discretization scheme.

$$i\hbar M \frac{\partial G(t)}{\partial t} = (K - iA) G(t)$$

First-order linear differential equation:

- Inverting is **expensive**,
- and are **not sparse**,
- Inverting is **not stable**.

➔ **Only compute the action** of .

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➔ **Only compute the action** of .

Step 1: Taylor-expand

➔ Only valid around .

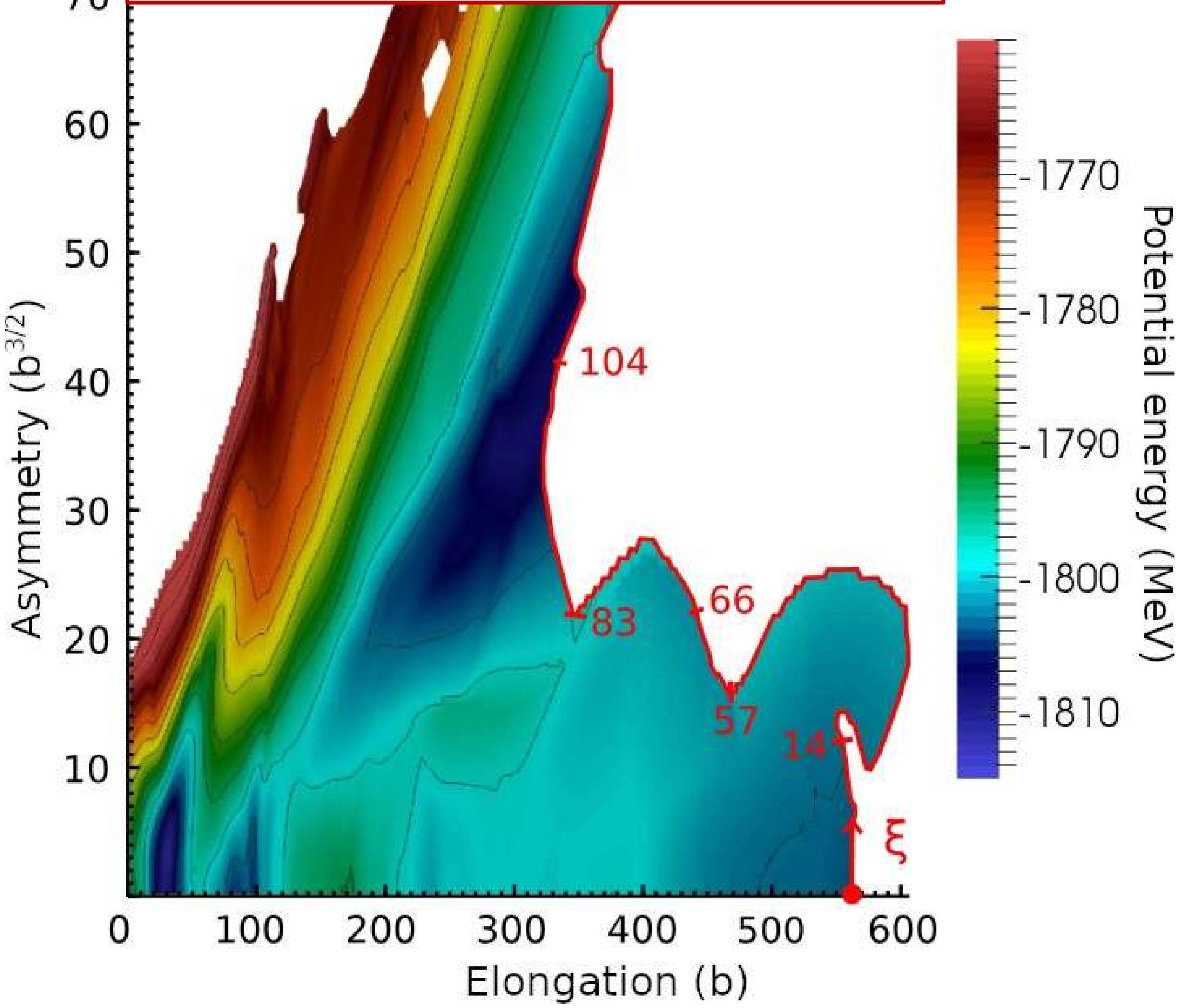
Step 2: Discretize time

Step 3: Evaluate action of

Determine by recurrence:

3. We revamped our approach to predict the fragment properties.

FORMER APPROACH



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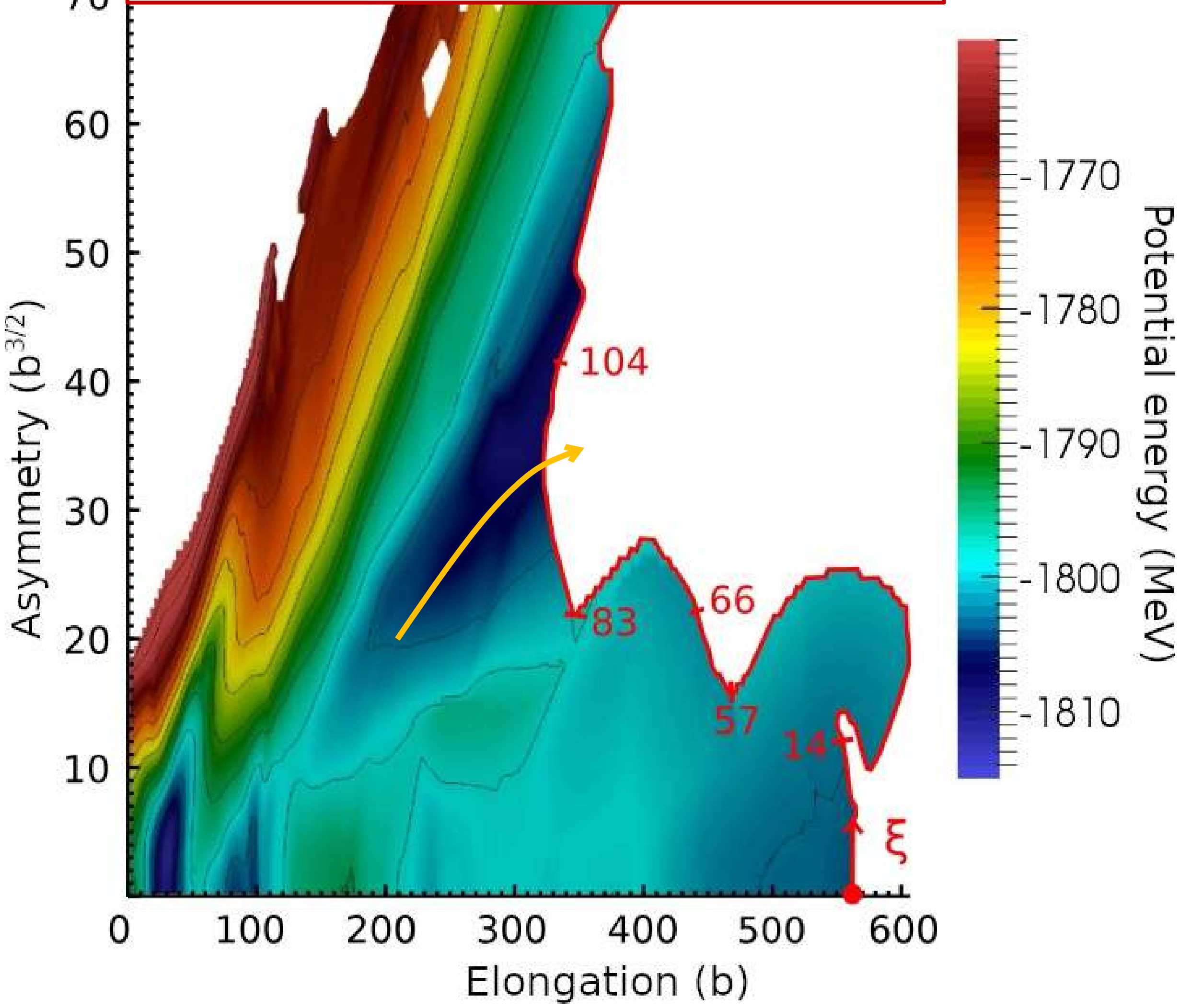

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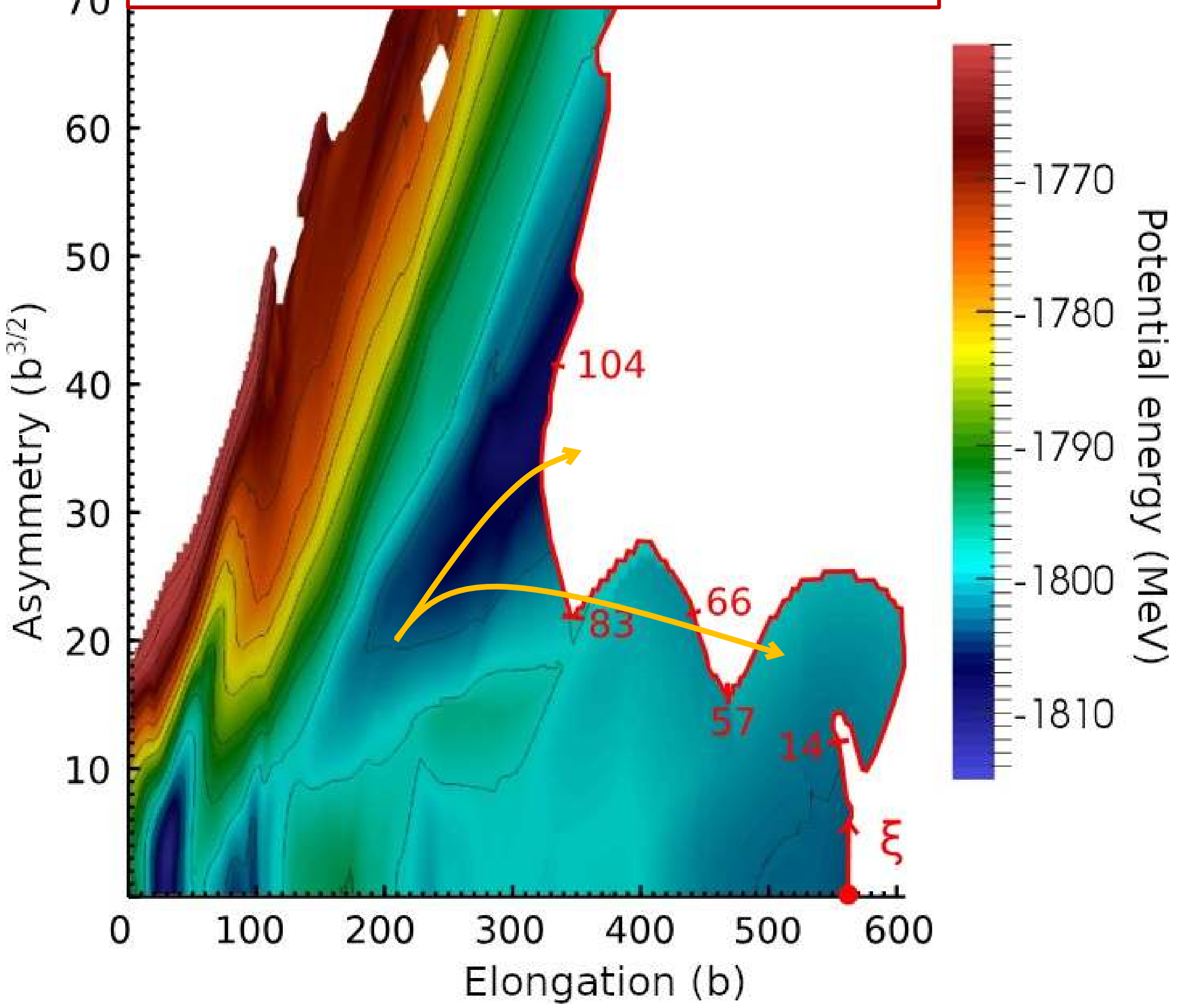

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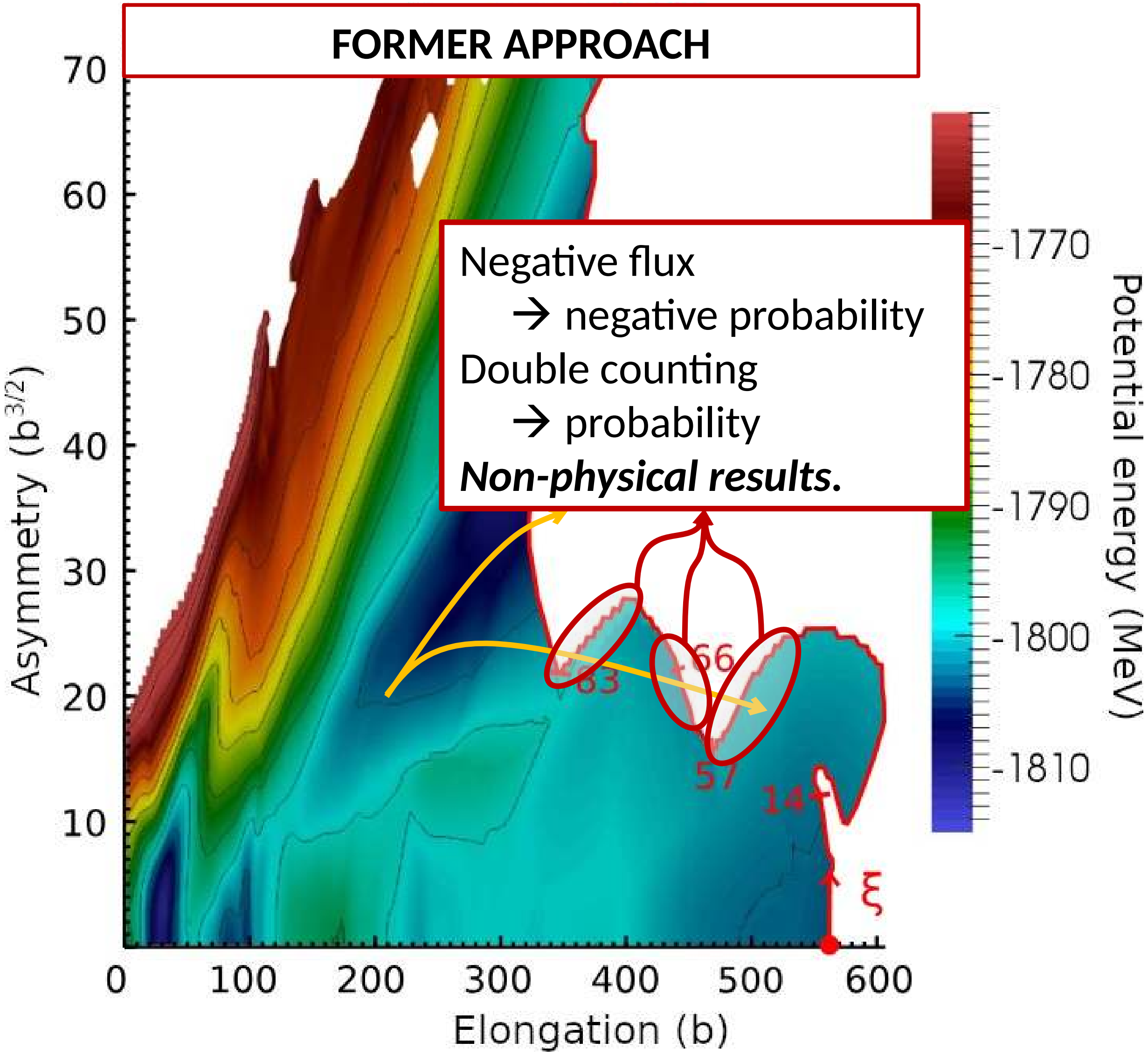

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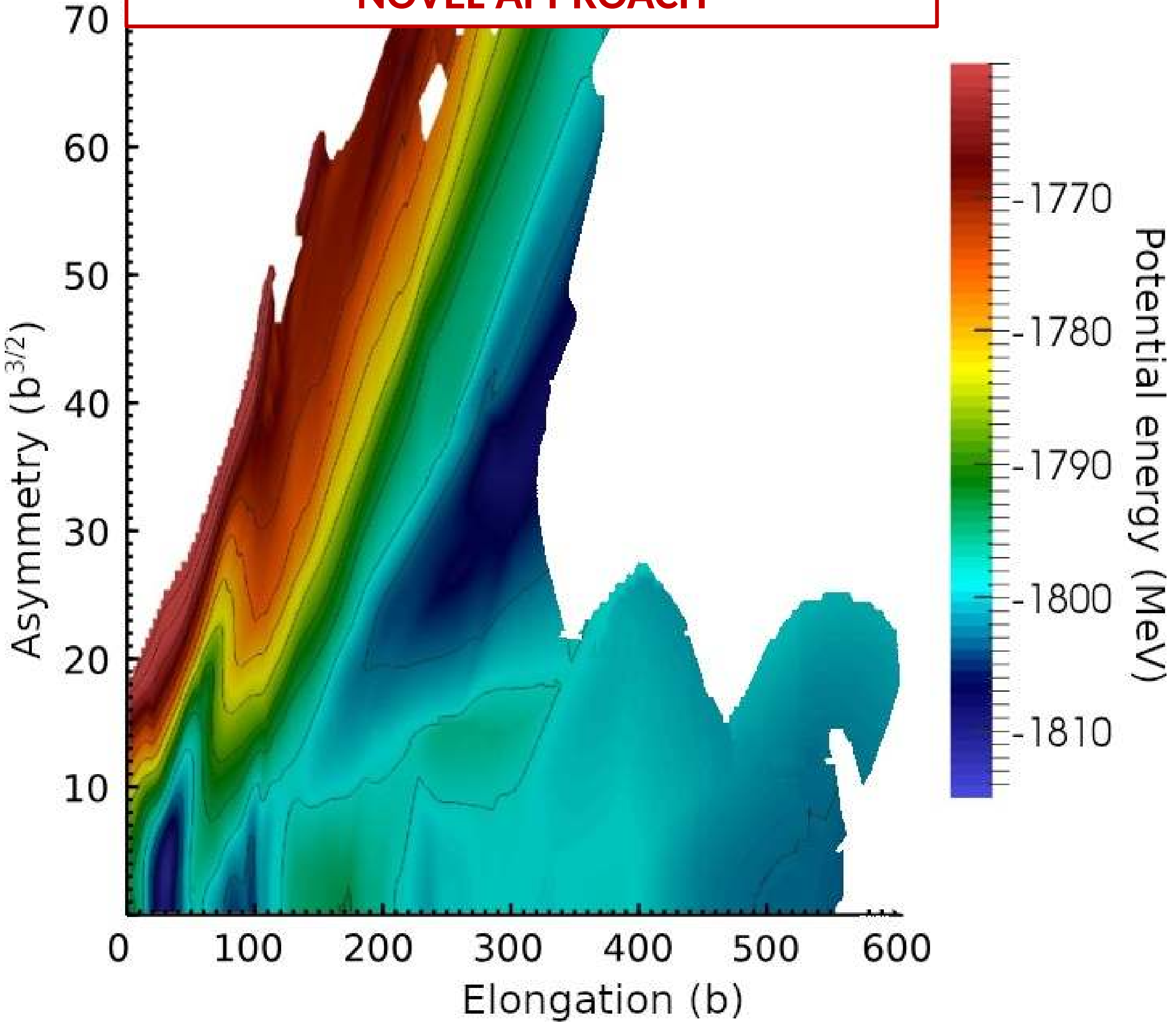
NOVEL APPROACH



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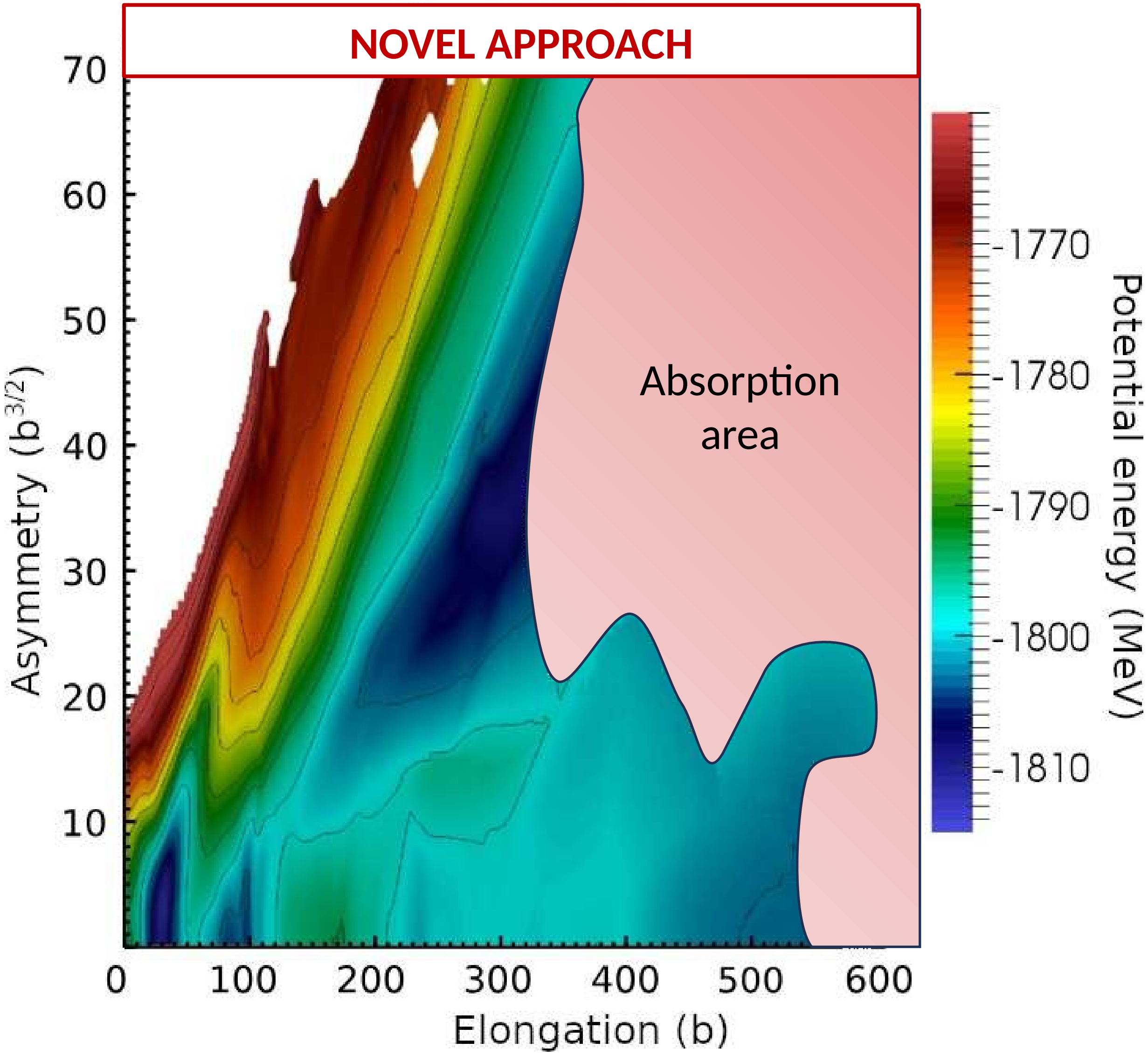

Derivation of the absorption probability:

Evolution operator (non-unitary):

For small , we can approximate by:

The Baker-Campbell-Hausdorff formula gives:

Evolution of the wavefunction after one timestep:

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Evolution of the wavefunction after one timestep:

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W.f. after absorption

Absorbed part of the w.f.

Derivation of the absorption probability:

Evolution operator (non-unitary):

For small , we can approximate by:

The Baker-Campbell-Hausdorff formula gives:

Absorbed part of the wavefunction:

Probability density to be absorbed in at time given by

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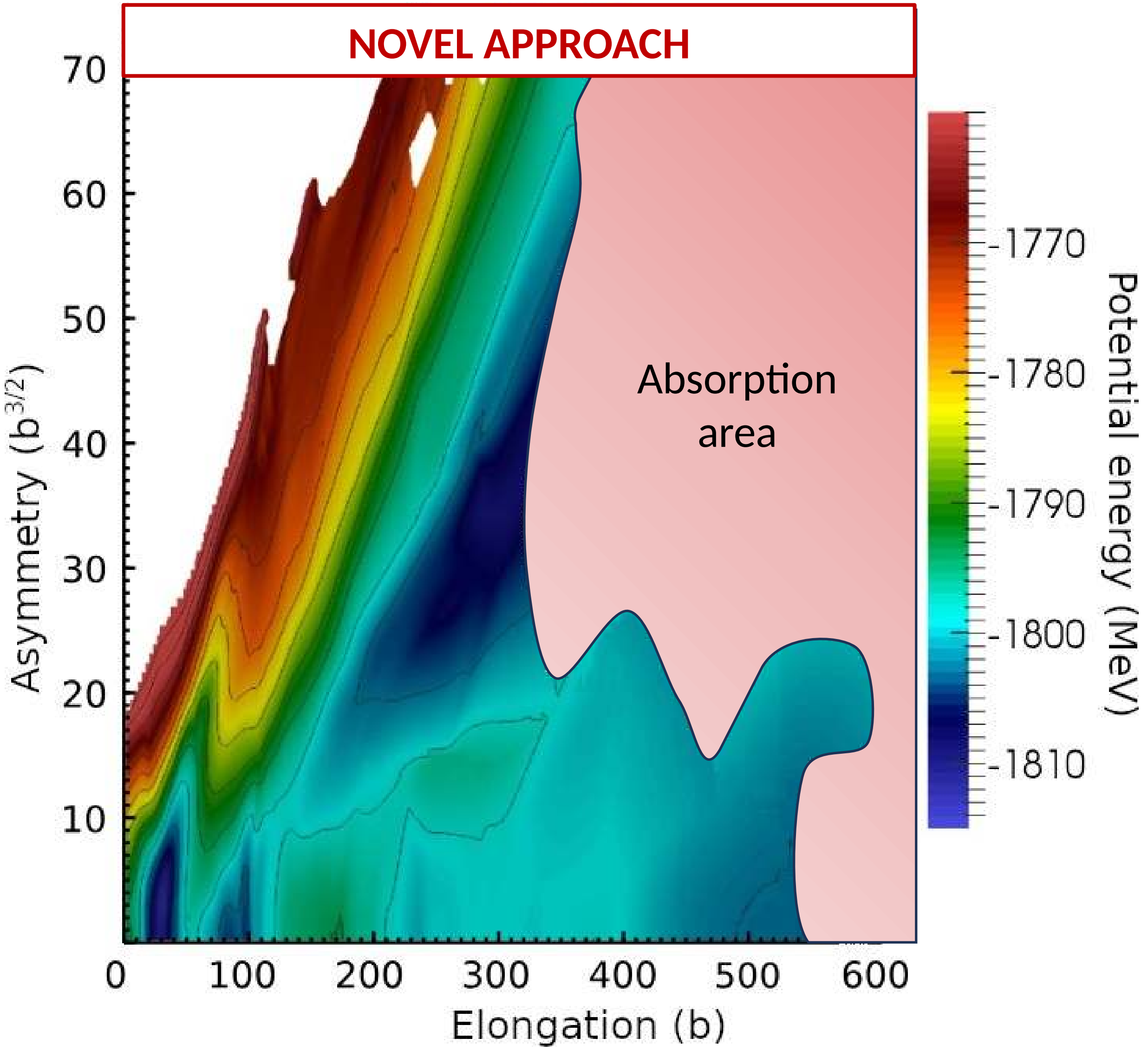


Probability to be absorbed in :

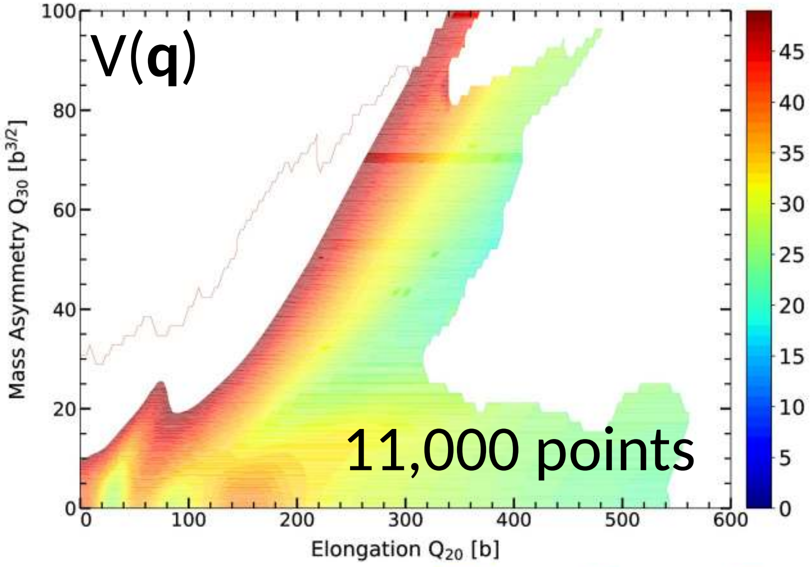
Probability to measure a fragment with particles at a given :

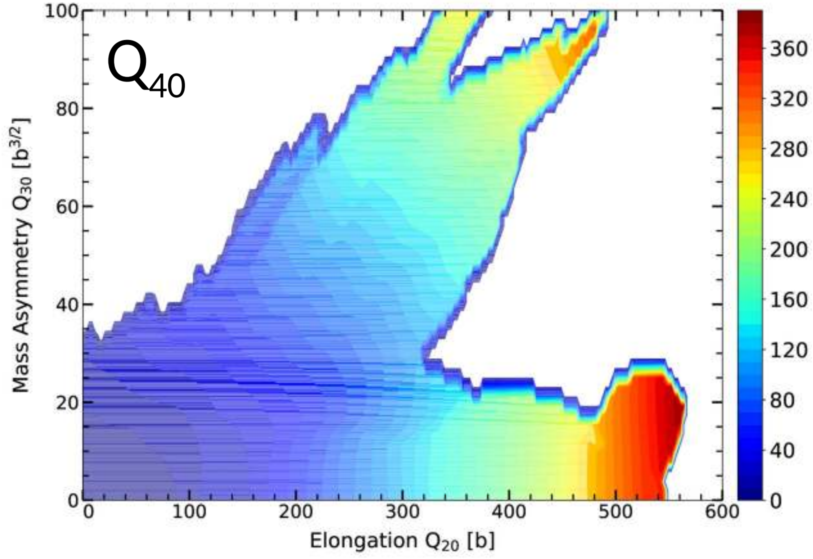
→ Probability of a fragment with particles:

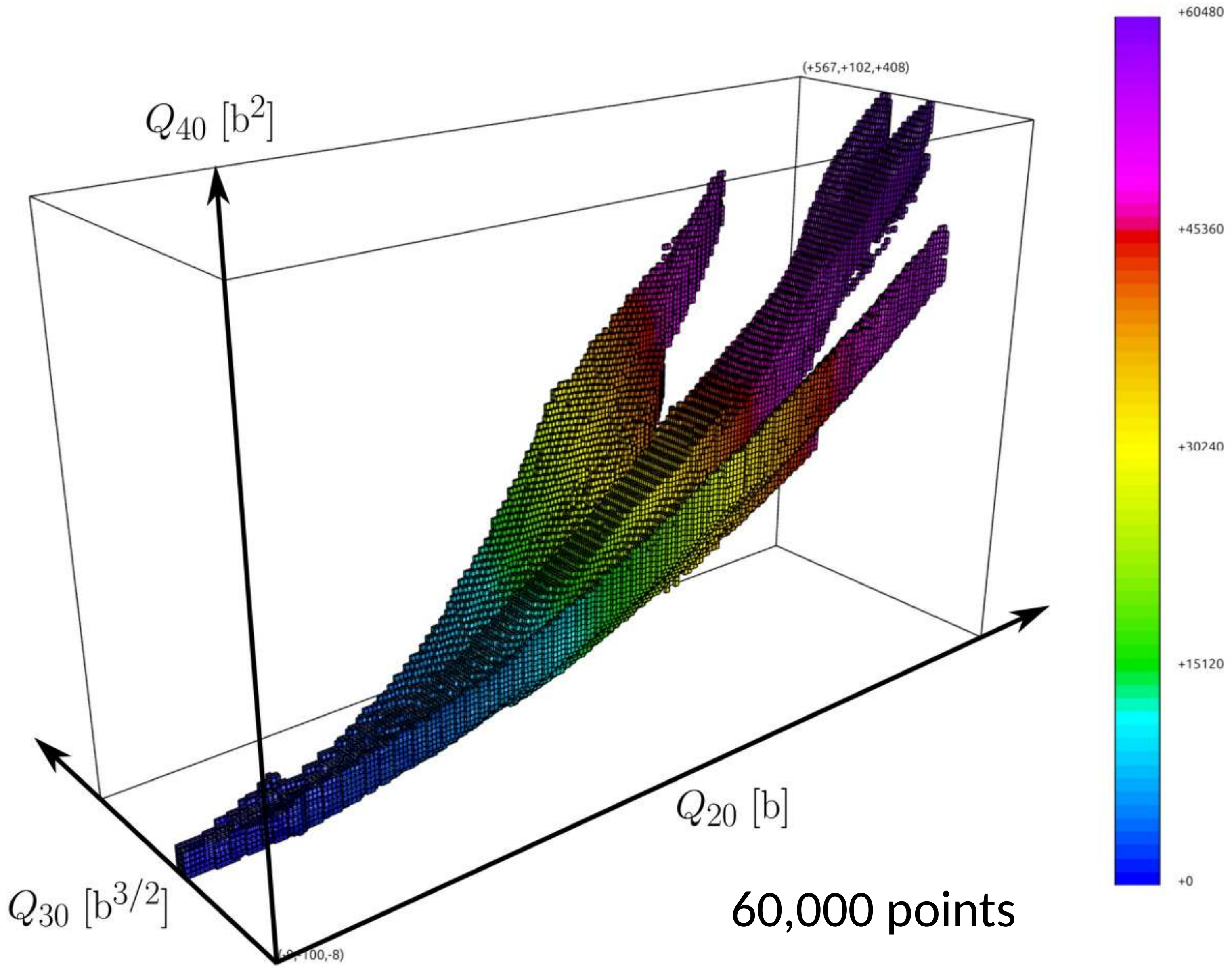
Partial assembly w/ MFEM

→ **kernels** loaded at the same time!

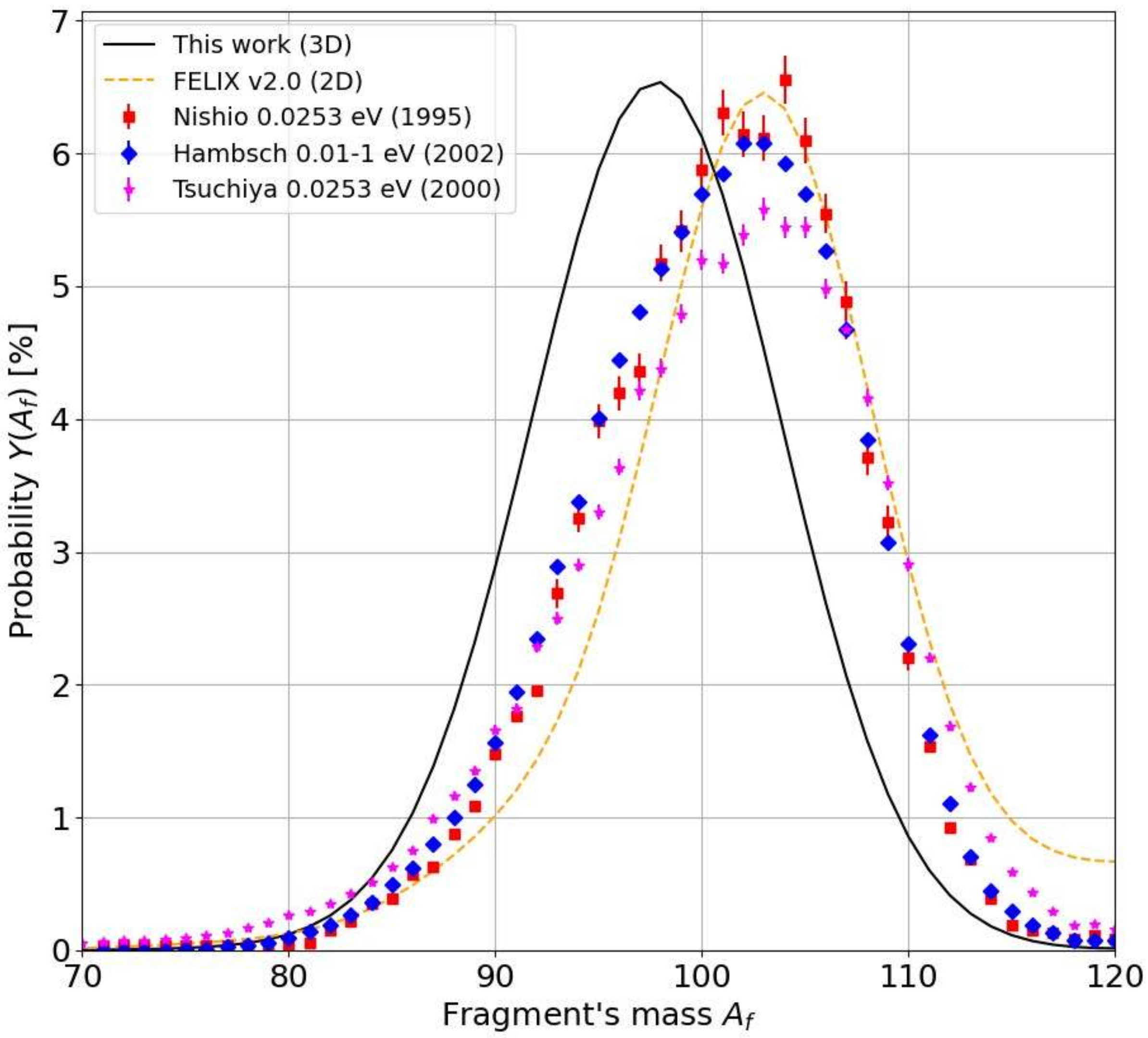
We generated a 3D potential energy surface using a Skyrme functional on ^{240}Pu and transformed it into a MFEM mesh.

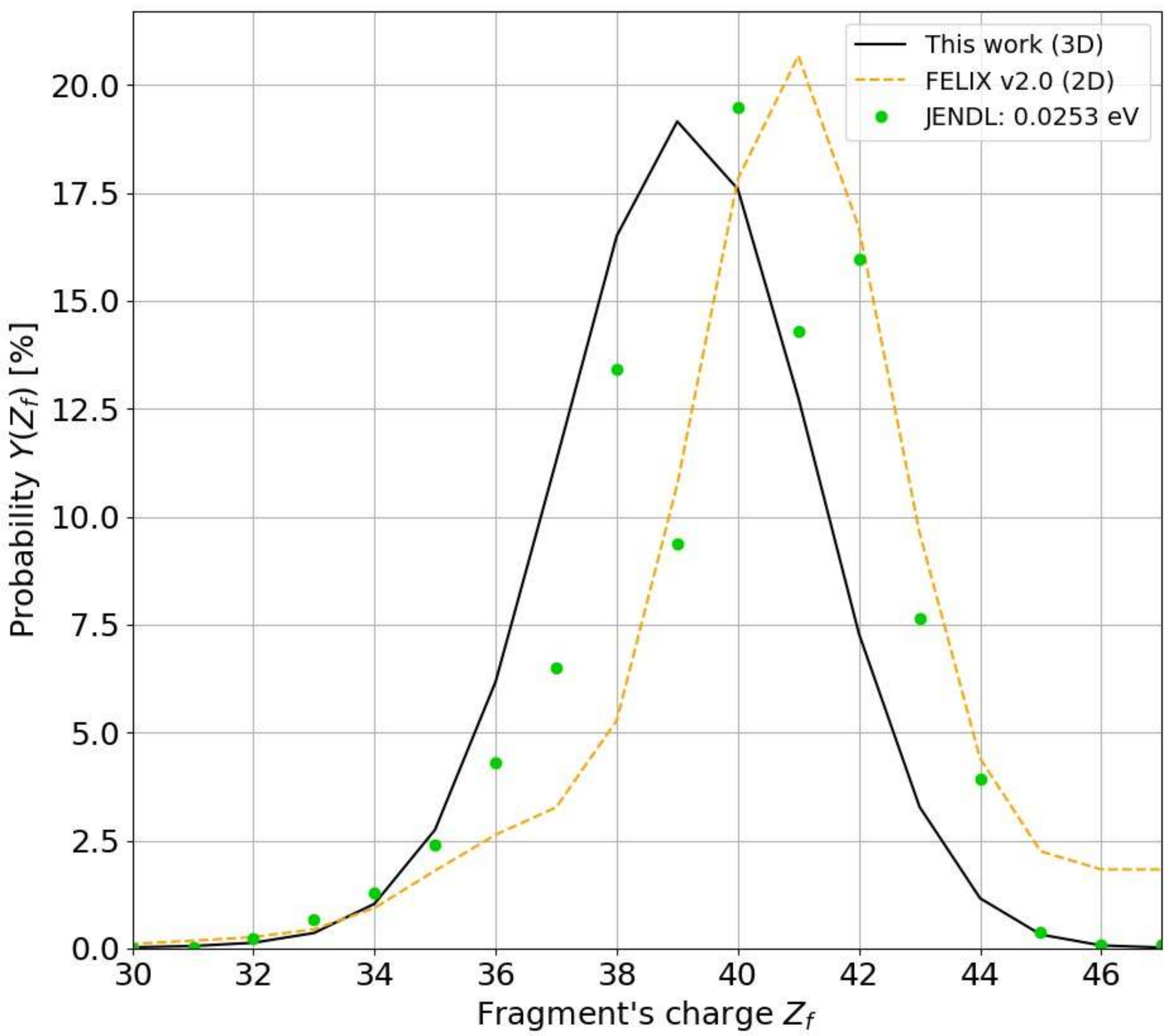




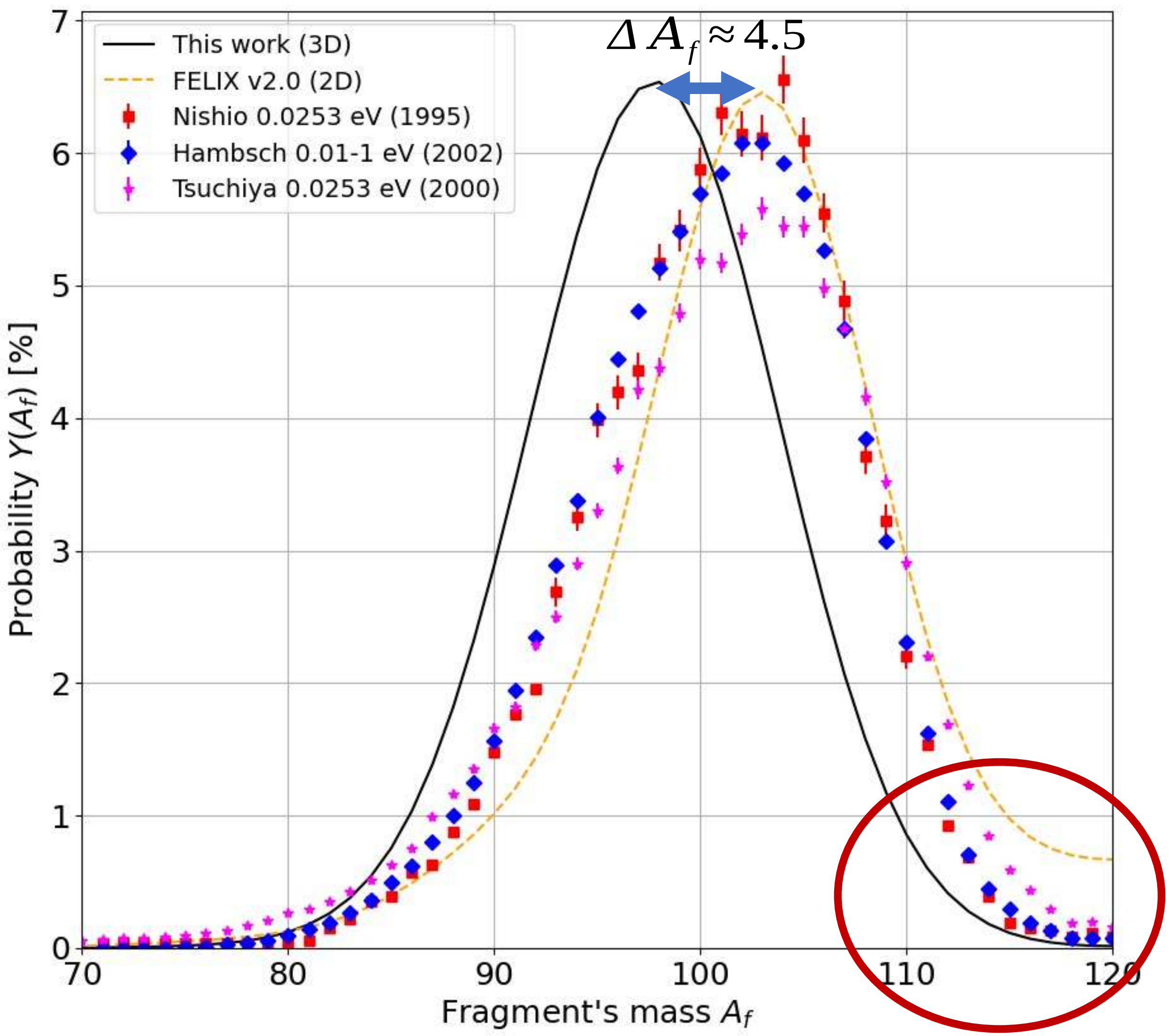


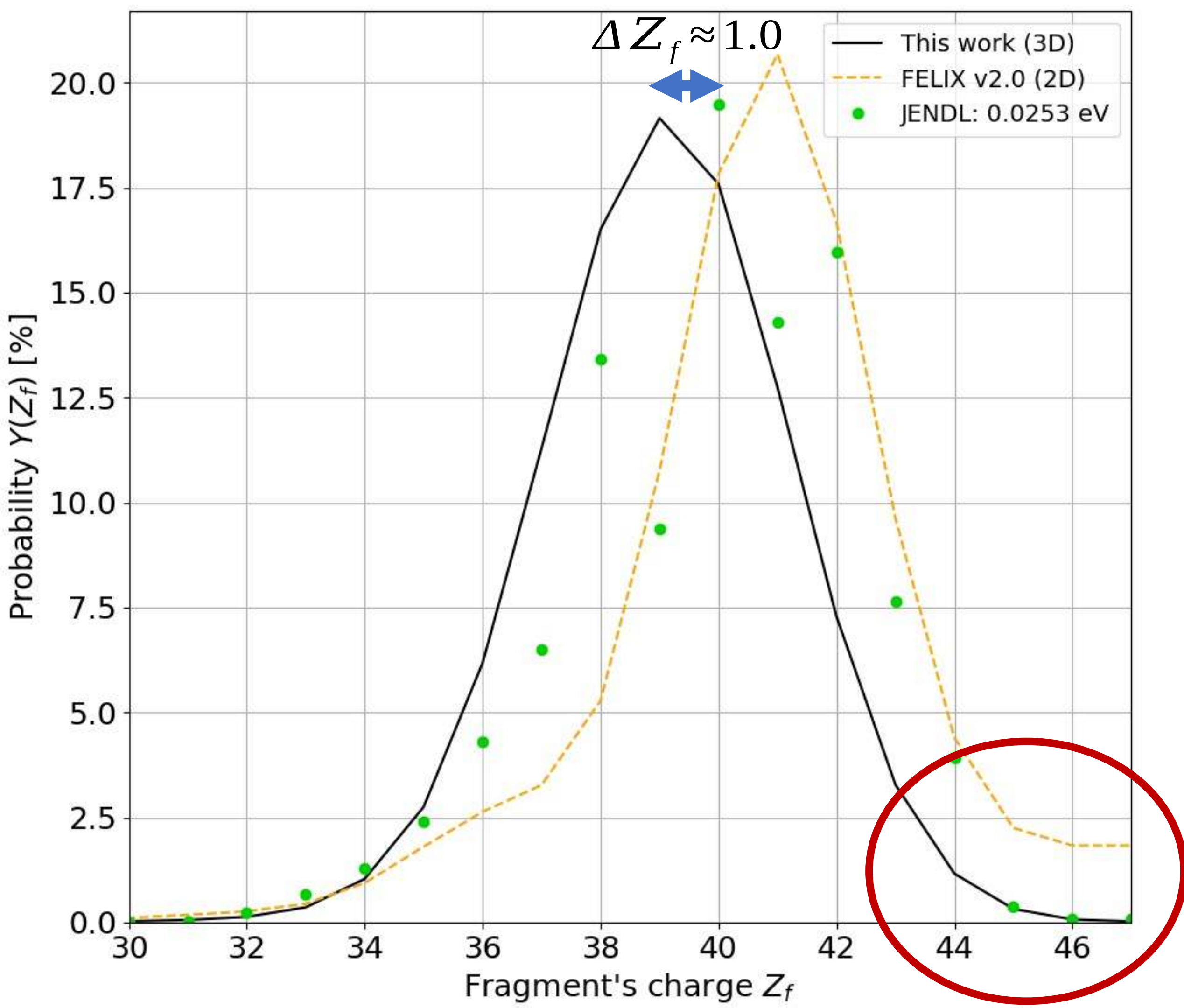
Finally, we extracted fission fragment mass and charge yields using our new pipeline.





Our (very) preliminary results are encouraging, but further work is needed.





These preliminary results are promising, and we are working on many further improvements.

- Improve the handling of the potential energy landscape (interpolation).
- Define the initial state from the eigenstates of the extrapolated potential wells.
- Variable order of the time-propagation approach.
- Enable extrapolation of the potential energy landscape.
- Couple Fidelis with particle-number projection in the fragments.
- Study the impact of three degrees of freedom on several fissioning systems.
- Determine fission observables using a Gogny interaction.
- Package the library (Tests, CMake, Pybind11, Doxygen, etc).
- …

Thank you

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