Fully Microscopic Description of Fission with Three Degrees of Freedom

Third edition of the FIESTA School & Workshop 11/19/2024

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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

LLNL-PRES-848409

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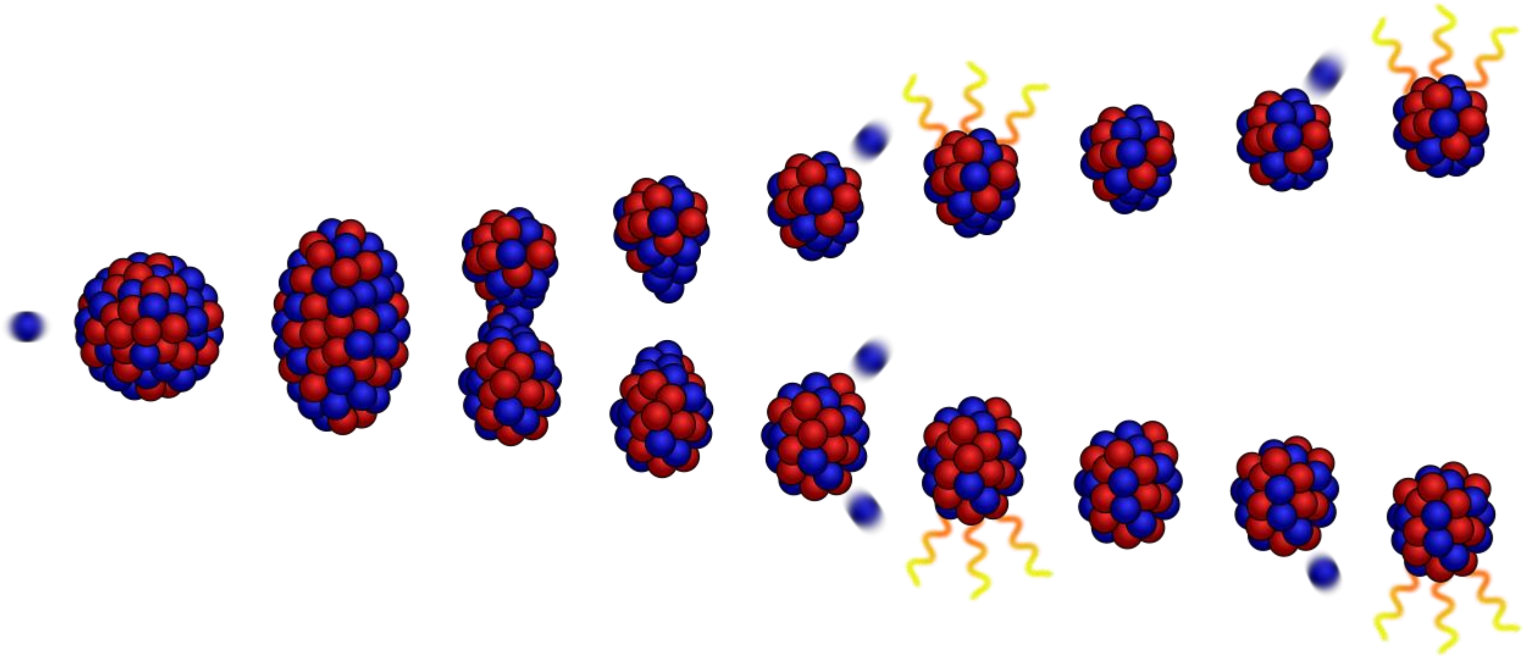
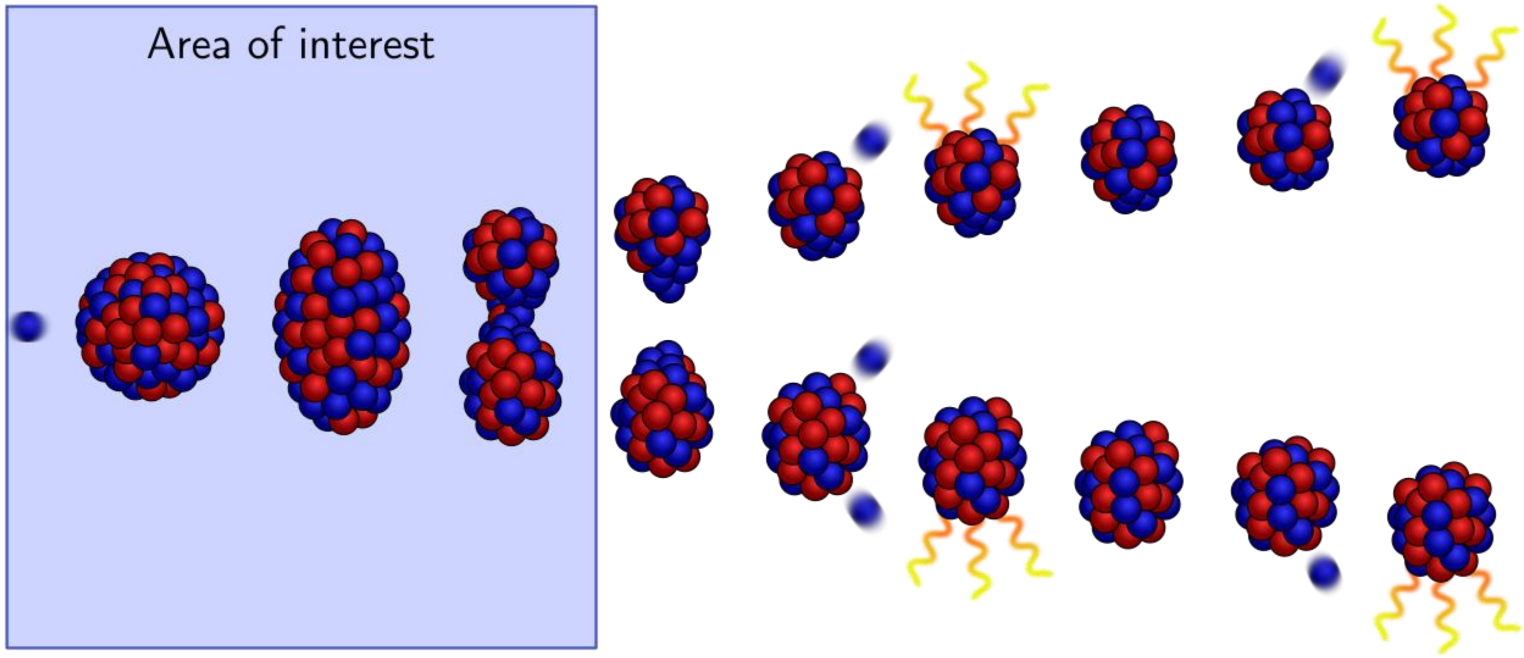
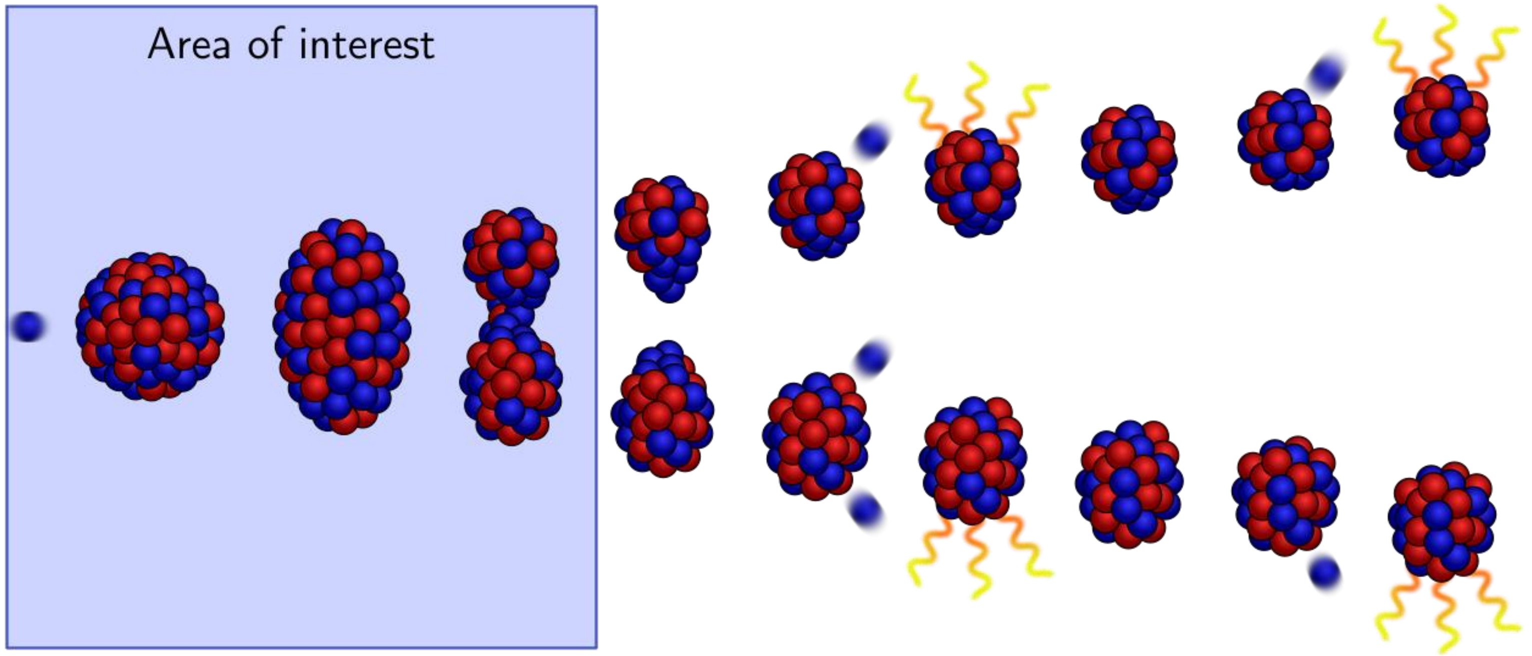
We describe the fission process using a fully microscopic approach.



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



Our theoretical framework leads to Schrodinger-like equation.

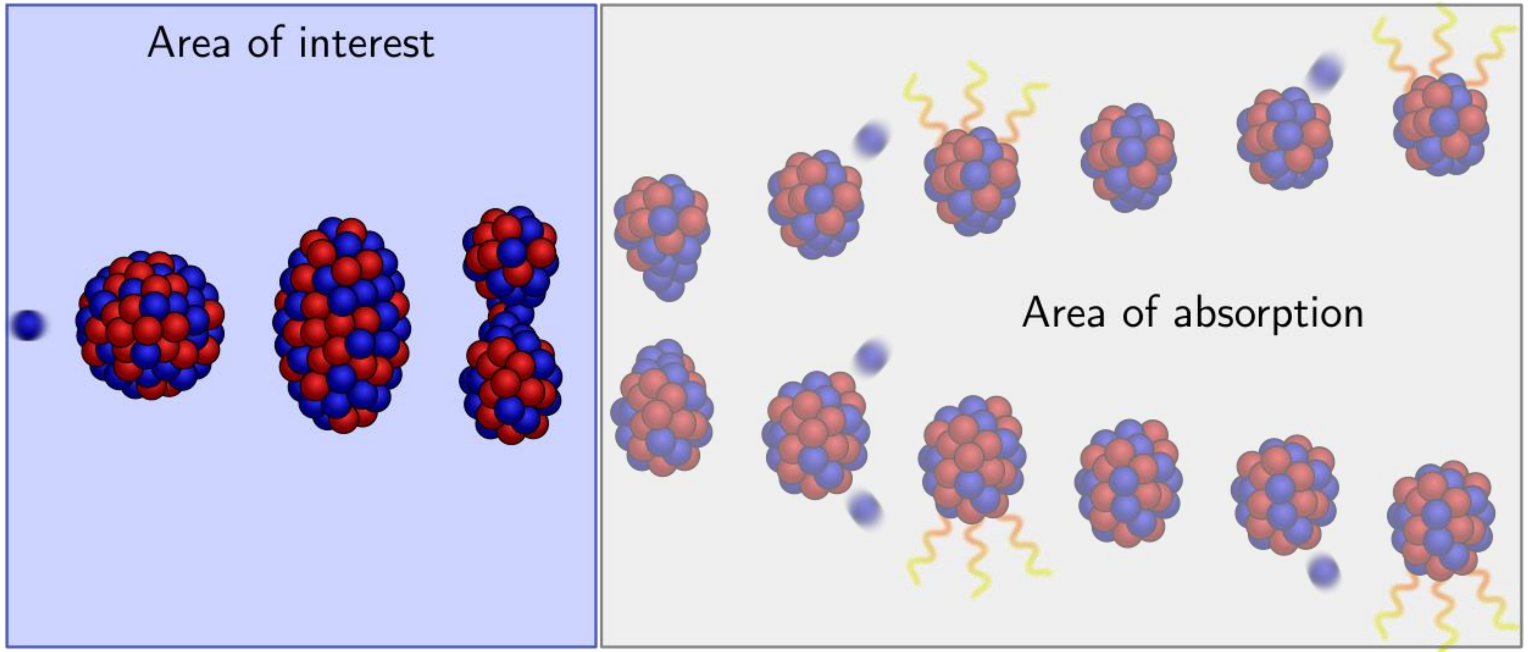


$$i\hbar \frac{\partial g(\boldsymbol{q},t)}{\partial t} = \left[-\frac{\hbar^2}{2} \gamma^{-\frac{1}{2}}(\boldsymbol{q}) \nabla \cdot \gamma^{\frac{1}{2}}(\boldsymbol{q}) B(\boldsymbol{q}) \nabla + V(\boldsymbol{q}) \right] g(\boldsymbol{q},t)$$

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

- local **complex-valued** diffusion equation with real-valued $\boldsymbol{q}$-dependent coefficients $\gamma^{\pm\frac{1}{2}}$, B and V.
- $\boldsymbol{q}$: collective degrees of freedom describing the nucleus' deformation (2-D → **3-D**).
- $g(\boldsymbol{q},t)$: nucleus' probability amplitude to be in $\boldsymbol{q}$ at time t (complex-valued).

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



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We developed a new MFEM-based solver able to tackle three collective degrees of freedom.

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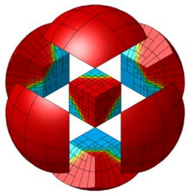


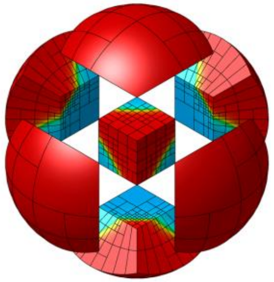
1. We discretize the collective space using the Finite Element Method with MFEM.

2. We developed a high-order (≥ 10) numerical time-discretization scheme.

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

https://lc.llnl.gov/gitlab/verriere/felix3D

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



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Partition space

Collective space (infinite size)

Q_{21}	Q_{22}	Q_{25}	Q_{26}	Q_{37}	Q_{38}	Q_{41}	Q_{42}
Q_{20}	Q_{23}	Q_{24}	Q_{27}	Q_{36}	Q_{39}	Q_{40}	Q_{43}
Q_{19}	Q_{18}	Q_{29}	Q_{28}	Q_{35}	Q_{34}	Q_{45}	Q_{44}
Q_{16}	Q_{17}	Q_{30}	Q_{31}	Q_{32}	Q_{33}	Q_{46}	Q_{47}
Q_{15}	Q_{12}	Q_{11}	Q_{10}	Q_{53}	Q_{52}	Q_{51}	Q_{48}
Q_{14}	Q_{13}	Q_{8}	Q_{9}	Q_{54}	Q_{55}	Q_{50}	Q_{49}
Q_{1}	Q_{2}	Q_{7}	Q_{6}	Q_{57}	Q_{56}	Q_{61}	Q_{62}
Q_{0}	Q_{3}	Q_{4}	Q_{5}	Q_{58}	Q_{59}	Q_{60}	Q_{63}

Define basis functions

The $g(\boldsymbol{q},t)$ scalar field is smooth:

➔ H1-conformal real basis,

➔ piecewise p-degree polynomials.

➔ Basis function noted φ_i

Project the equation

Orthogonal projection on the basis functions using the scalar product:

$$(\phi,\psi) = \int \phi^*(\boldsymbol{q})\psi(\boldsymbol{q})\,\gamma^{\frac{1}{2}}(\boldsymbol{q})\,\mathrm{d}\boldsymbol{q}$$

$$i\hbar \mathrm{M}\frac{\partial G(t)}{\partial t} = (\mathrm{D}+\mathrm{V}-\mathrm{iA})G(t)$$

$$\mathrm{M}_{ij} = \left(\varphi_i, \gamma^{\frac{1}{2}}\varphi_j\right),$$

$$\mathrm{V}_{ij} = \left(\varphi_i, \gamma^{\frac{1}{2}}V\varphi_j\right),$$

$$\mathrm{A}_{ij} = \left(\varphi_i, \gamma^{\frac{1}{2}}A\varphi_j\right),$$

$$D_{ij} = (\varphi_i, -\nabla\cdot\Lambda\nabla\varphi_j)$$
$$= \left(\nabla\varphi_i, \Lambda\nabla\varphi_j\right) + \cancel{\partial B}.$$

➔ Sparse & partially assembled!

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

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

First-order linear differential equation:

$G(t) = U(t)\, G_0$

$\mathrm{U}(t) = \exp\left(-\frac{it}{\hbar}\mathrm{M}^{-1}(\mathrm{K} - i\mathrm{A})\right)$

- Inverting M is **expensive**,
- M^{-1} and $\mathrm{U}(t)$ are **not sparse**,
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➔ **Only compute the action** of $\mathrm{U}(t)$.

Step 1: Taylor-expand $\mathrm{U}(t)$

$$\mathrm{U}(t) \approx \sum_{n=0}^{N} \frac{1}{n!} \left(-\frac{it}{\hbar} \mathrm{M}^{-1} (\mathrm{K} - i\mathrm{A})\right)^n$$

➔ Only valid around $t = 0$.

Step 2: Discretize time

$$t = \delta t + \cdots + \delta t$$
$$\mathrm{U}(t) = \mathrm{U}(\delta t) \ldots \mathrm{U}(\delta t)$$

$$\mathrm{U}(\delta t) \approx \sum_{n=0}^{N} \frac{1}{n!} \left(-\frac{i\delta t}{\hbar} \mathrm{M}^{-1} (\mathrm{K} - i\mathrm{A})\right)^n$$

Step 3: Evaluate action of $\mathrm{U}(t)$

$$\mathrm{U}(\delta t) G \approx \sum_{n=0}^{N} \frac{1}{n!} \mathrm{F}^n G$$

$$\mathrm{F} = -\frac{i\delta t}{\hbar} \mathrm{M}^{-1} (\mathrm{K} - i\mathrm{A})$$

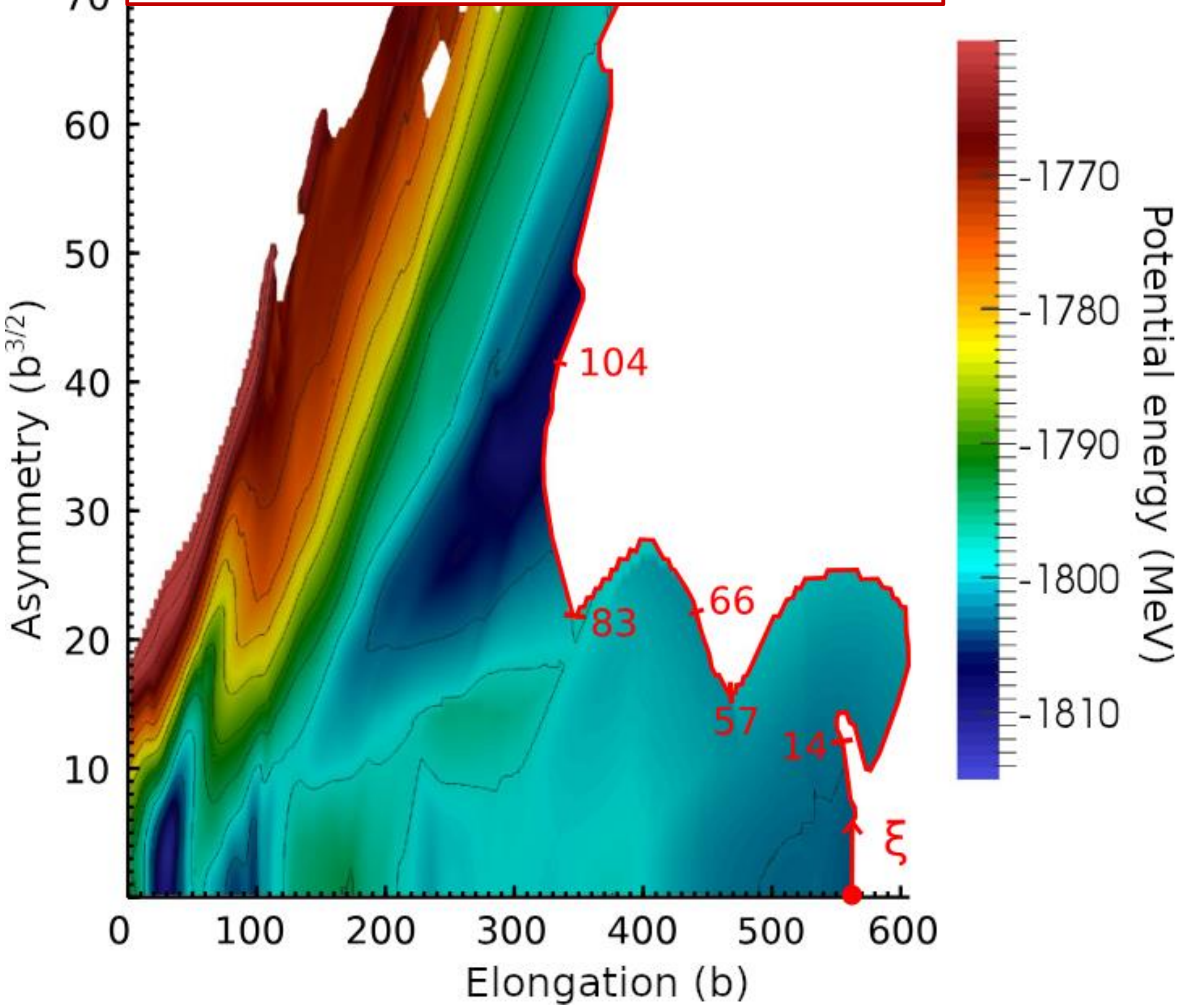
Determine $\mathrm{F}^n G$ by recurrence:

$$\mathrm{F}^0 G = G$$

$$M(\mathrm{F}^{n+1} G) = -\frac{\mathrm{i}\delta t}{\hbar} (\mathrm{K} - i\mathrm{A})\, (\mathrm{F}^n G)$$

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

FORMER APPROACH



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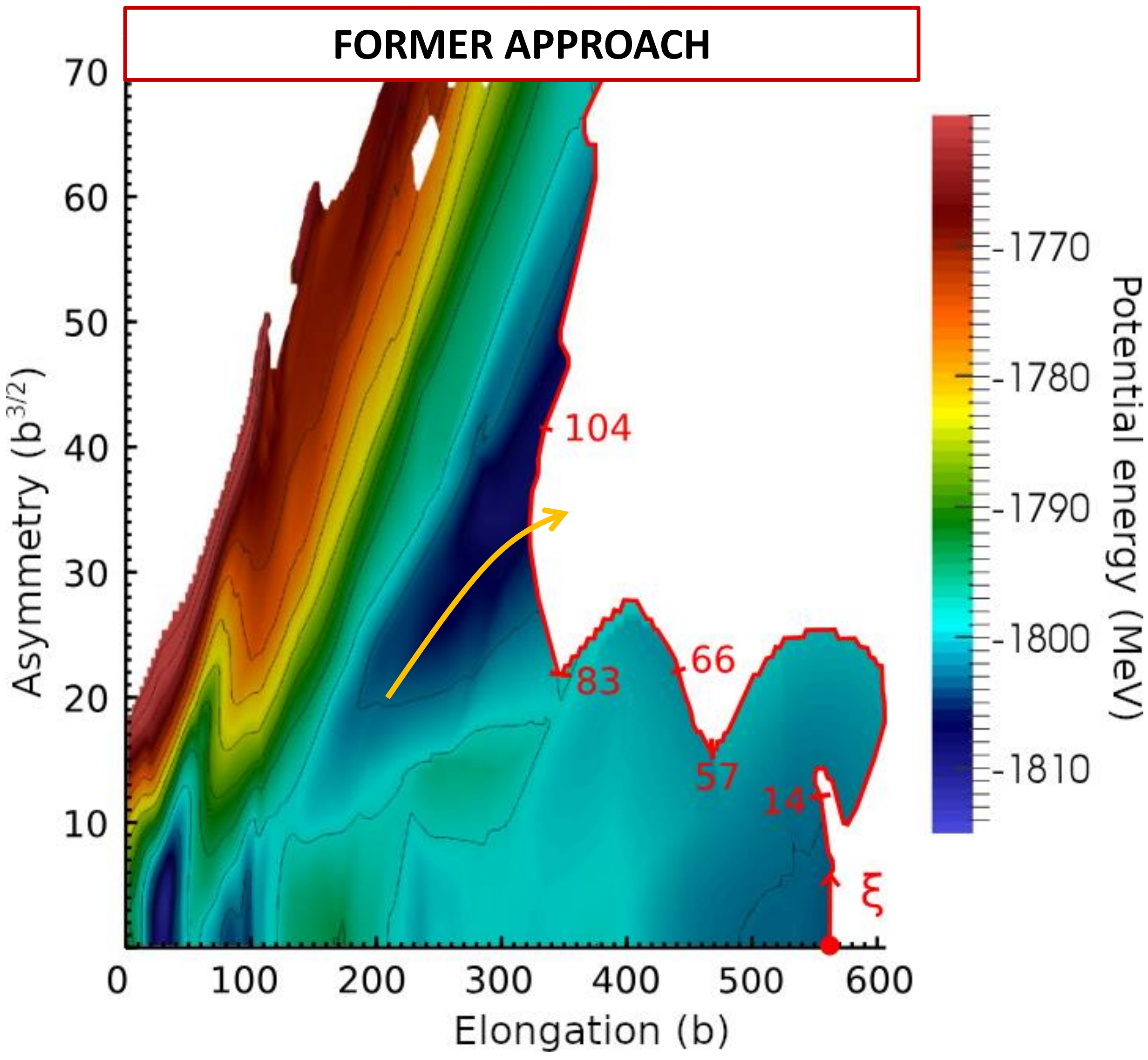

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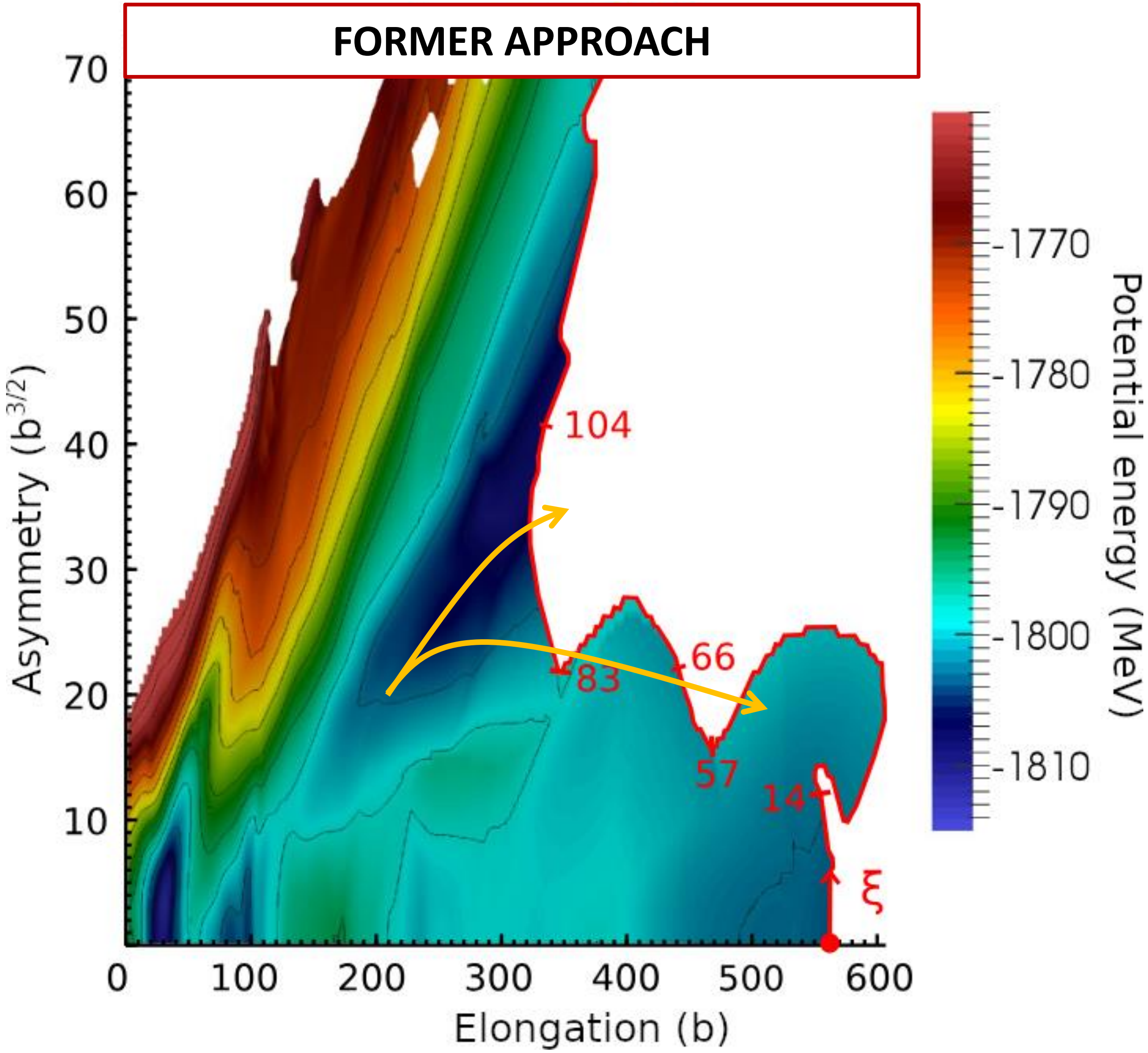

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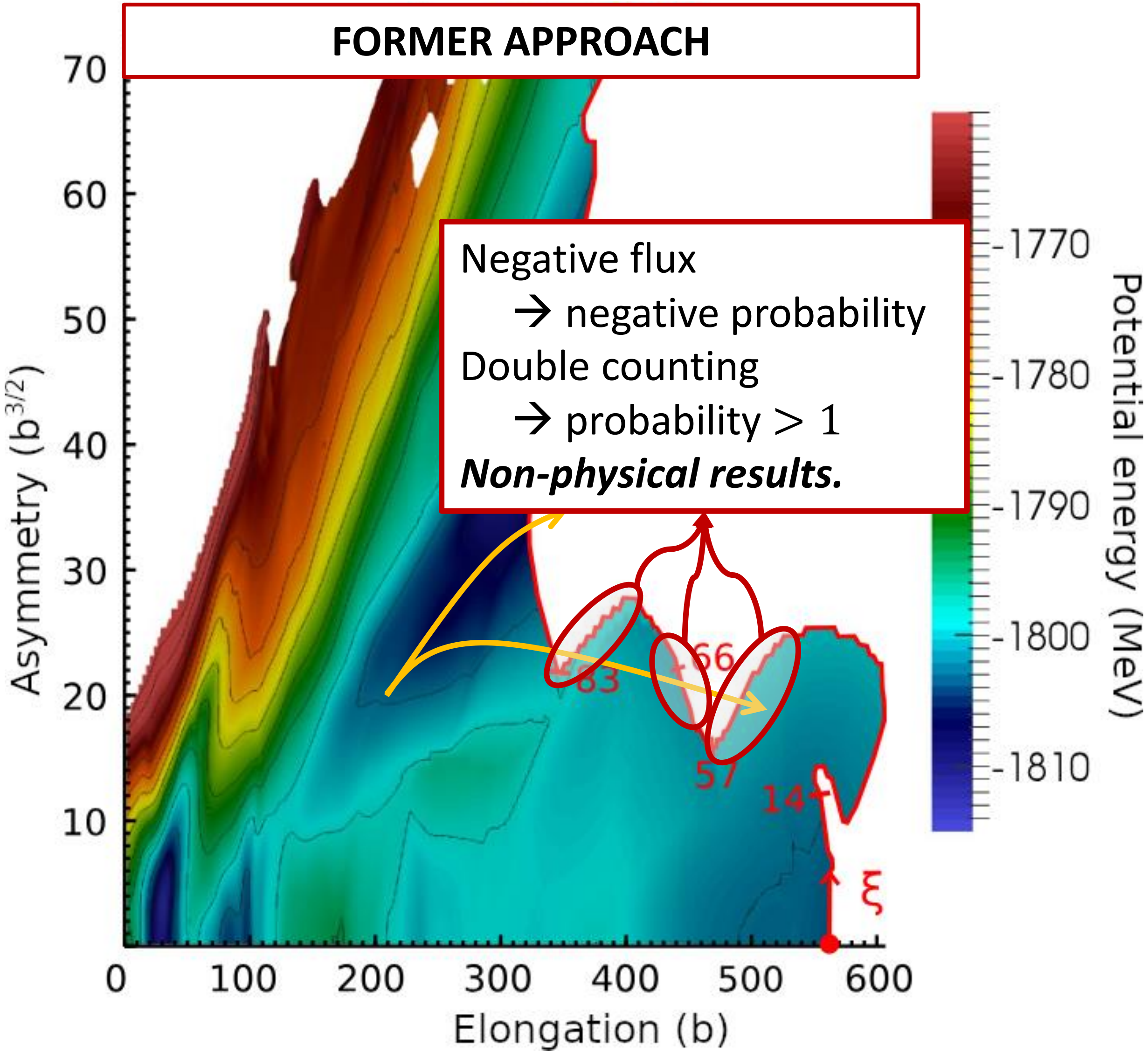

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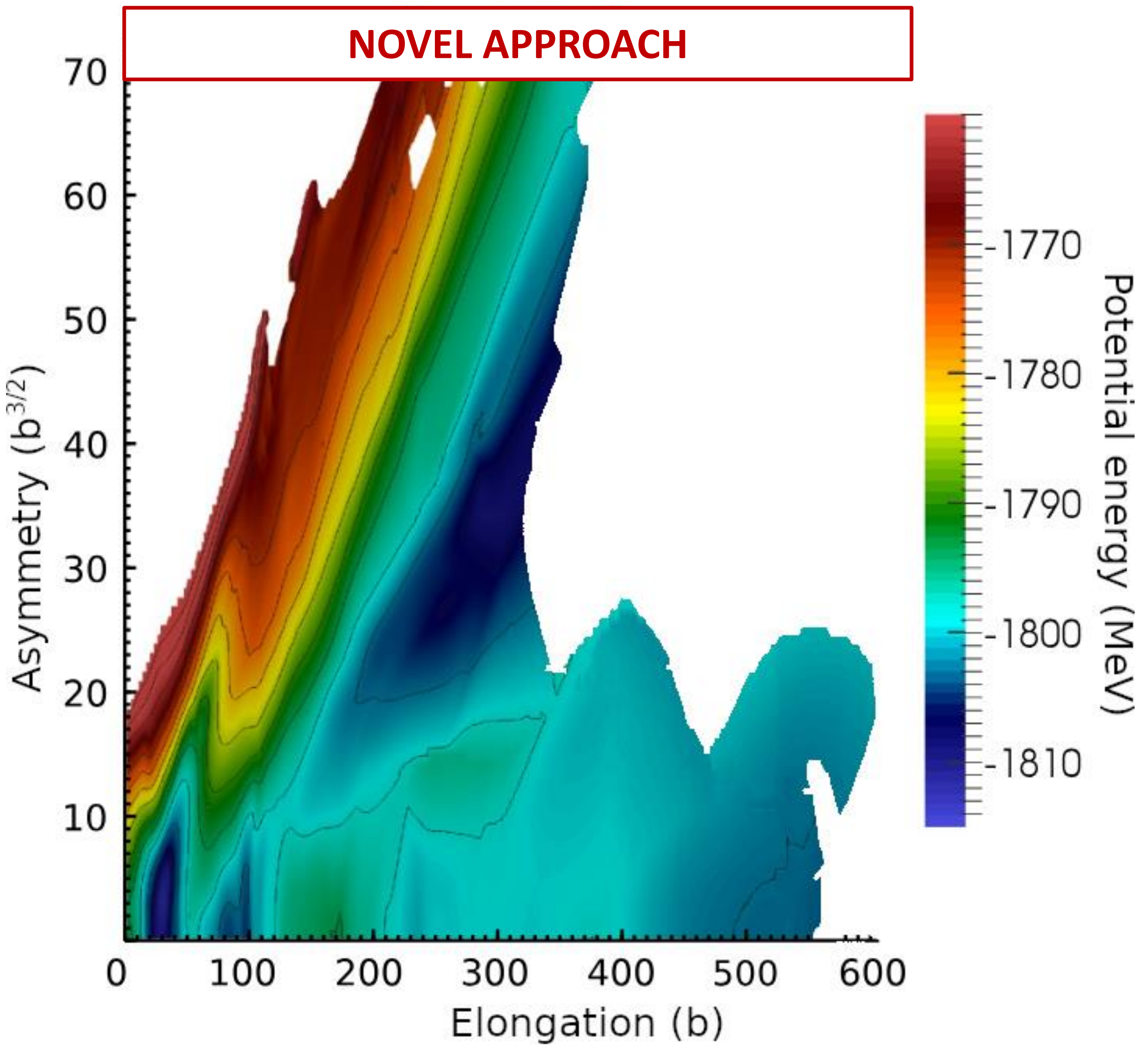

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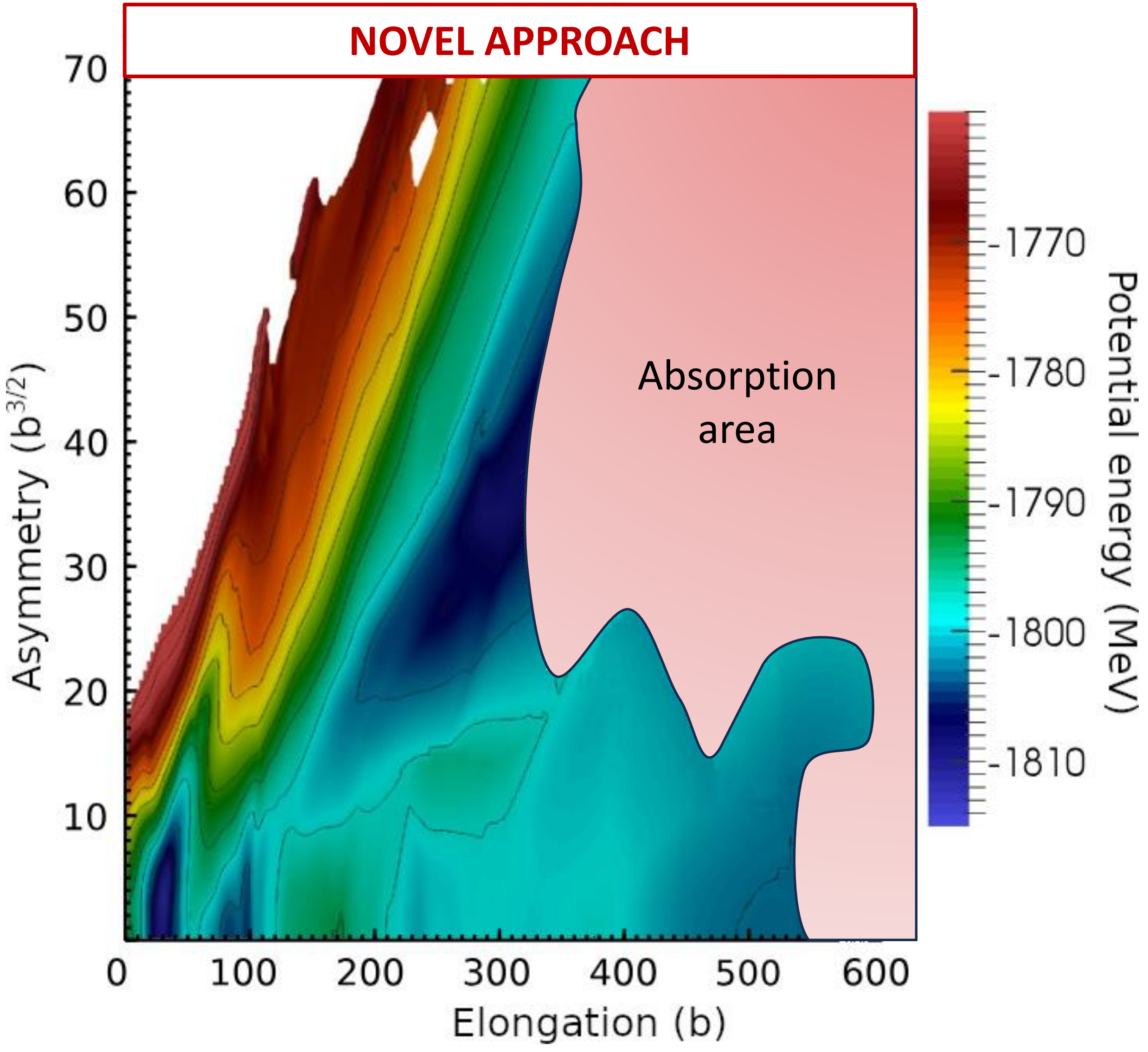

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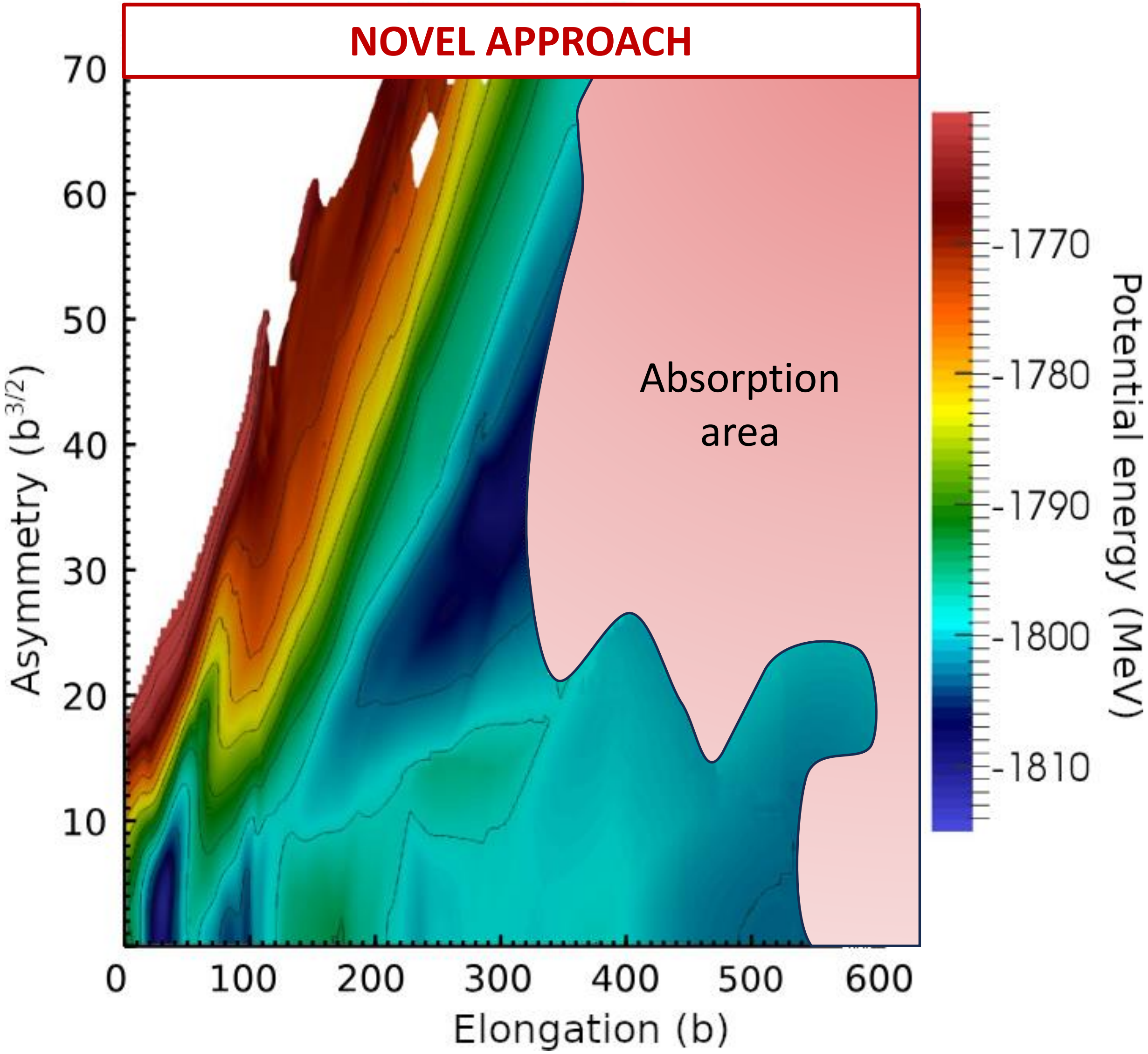


Probability $\rho_{\text{abs}}(\boldsymbol{q})$ to be absorbed in $\boldsymbol{q}$:

$$\rho_{\text{abs}}(\boldsymbol{q}) = \left(1 - e^{-\frac{\delta t}{\hbar}A(\boldsymbol{q})}\right) |g(\boldsymbol{q},t)|^2\, \gamma^{\frac{1}{2}}(\boldsymbol{q})$$

Probability to measure a fragment with N particles at a given $\boldsymbol{q}$:

$$P(X \mid \boldsymbol{q}) \approx \int_{X-\frac{1}{2}}^{X+\frac{1}{2}} e^{-\frac{1}{2}\frac{\left(x-\bar{X}(\boldsymbol{q})\right)^2}{\sigma_X^2}} \frac{\mathrm{d}x}{\sqrt{2\pi\sigma_X^2}}$$

→ Probability of a fragment with X particles:

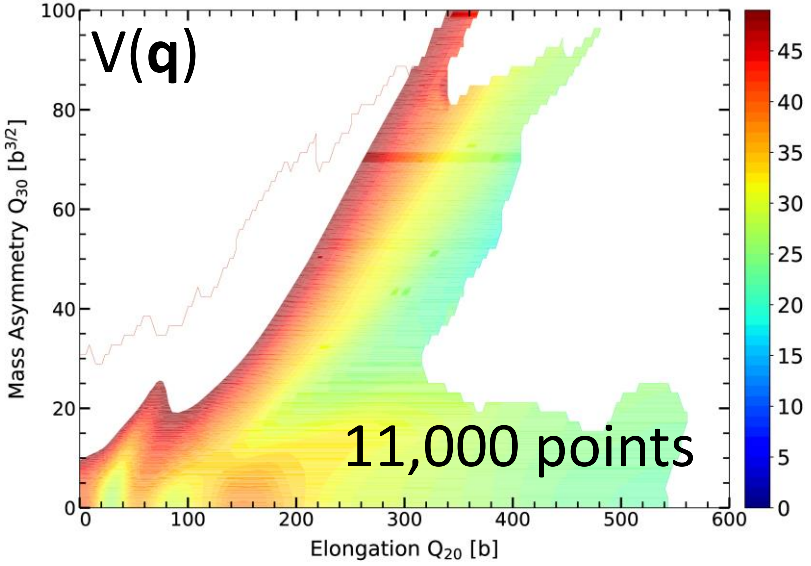
$$Y(X) \approx \int P(X \mid \boldsymbol{q})\, \rho_{\text{abs}}(\boldsymbol{q})\, \mathrm{d}\boldsymbol{q}$$

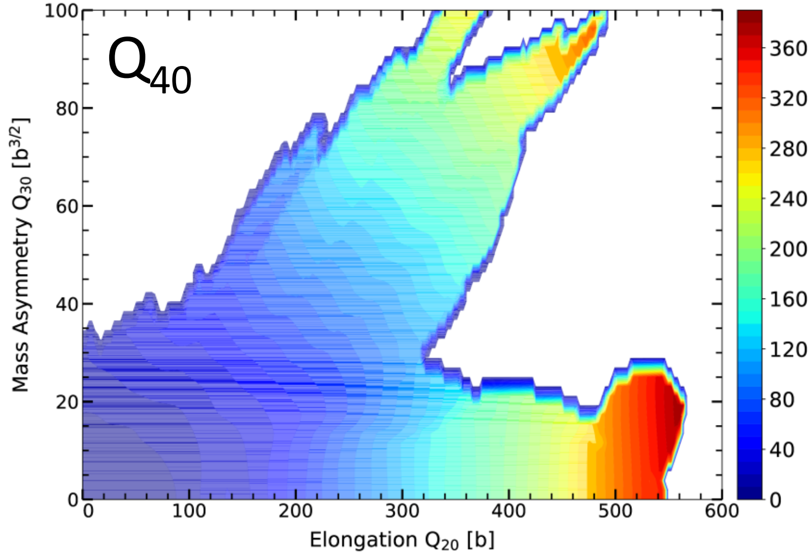
$$X = A_{\mathrm{f}}, Z_{\mathrm{f}}$$

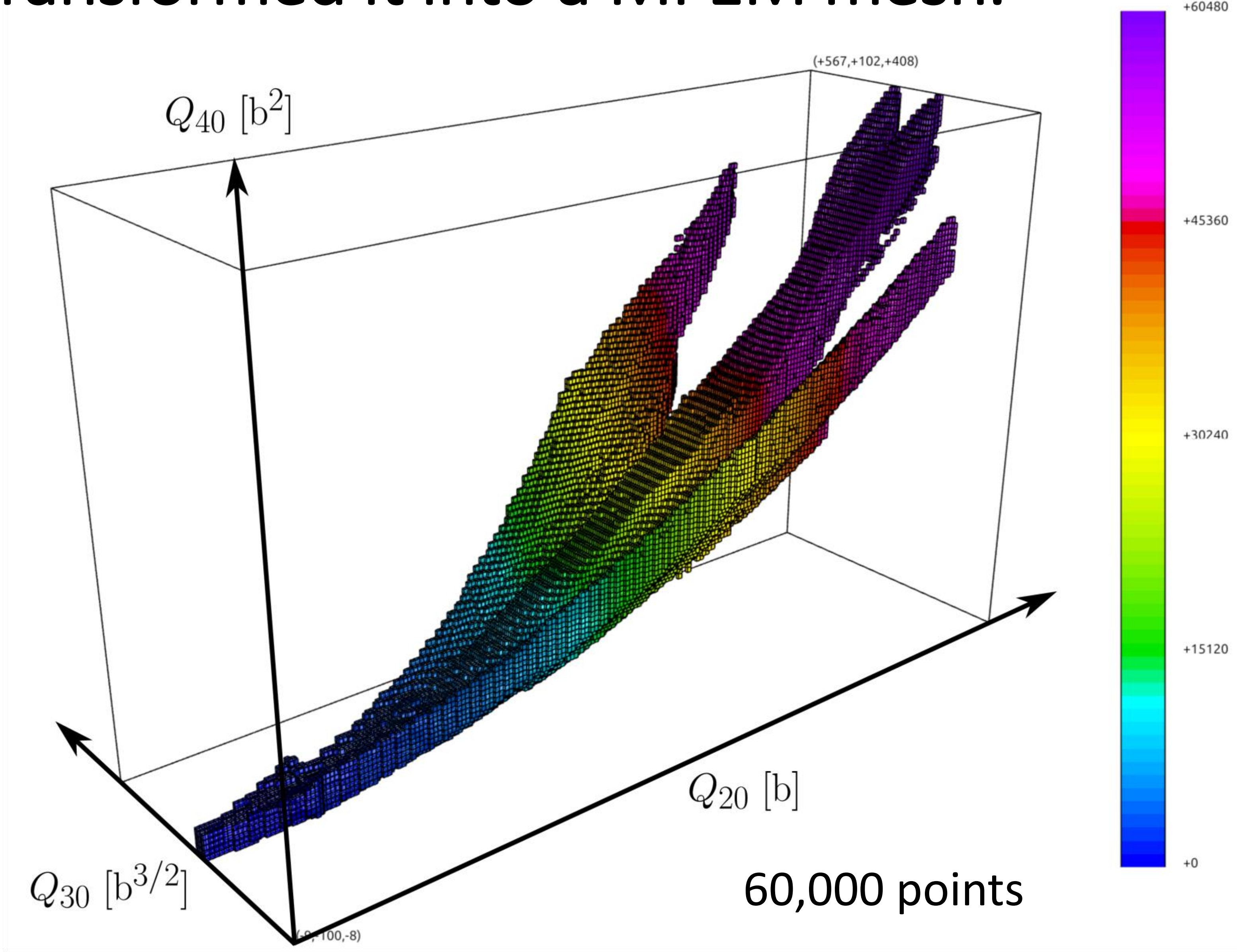
Partial assembly w/ MFEM

→ ≈ **300 kernels** loaded at the same time!

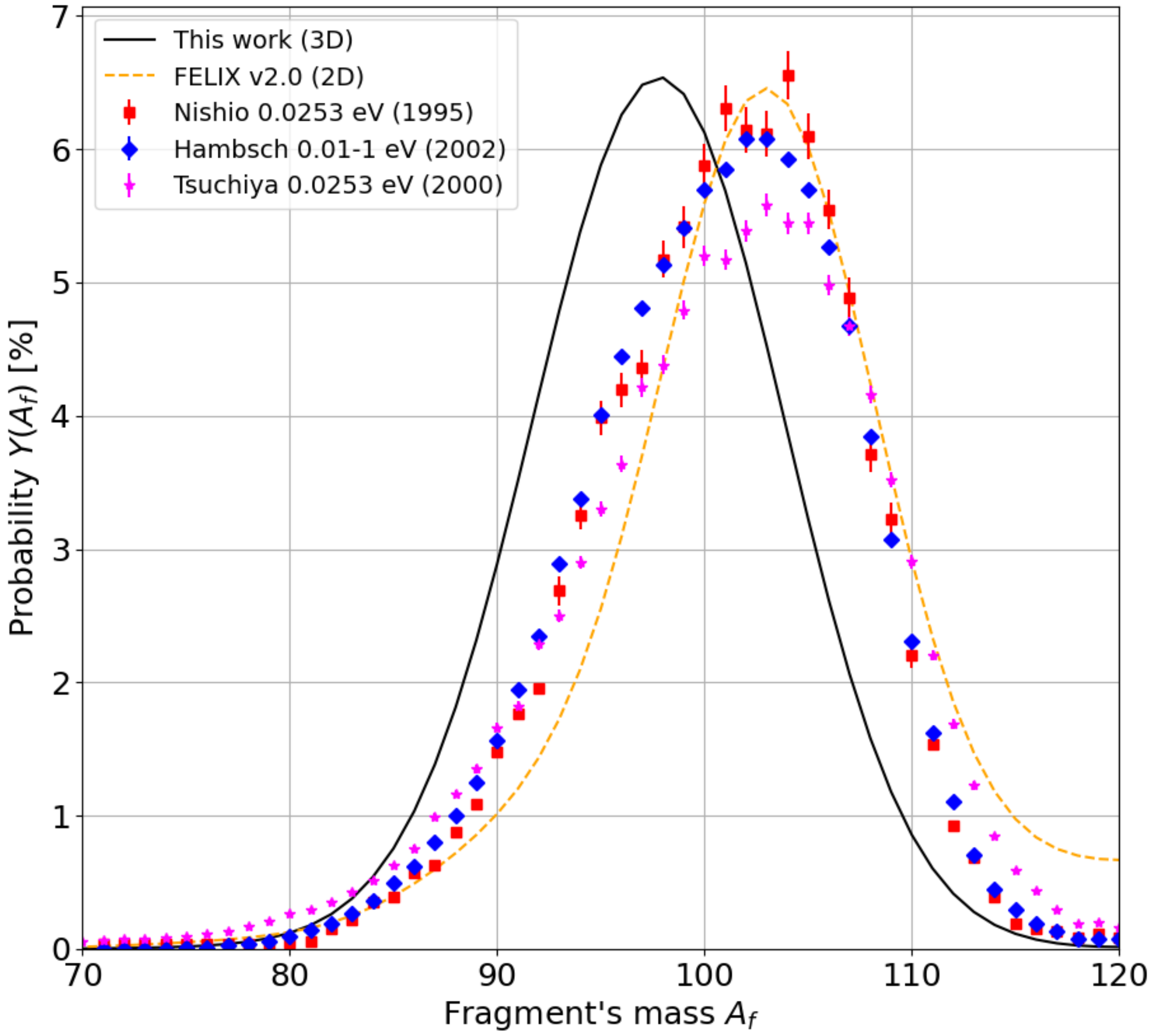
We generated a 3D potential energy surface using a Skyrme functional on ^{240}Pu and transformed it into a MFEM mesh.

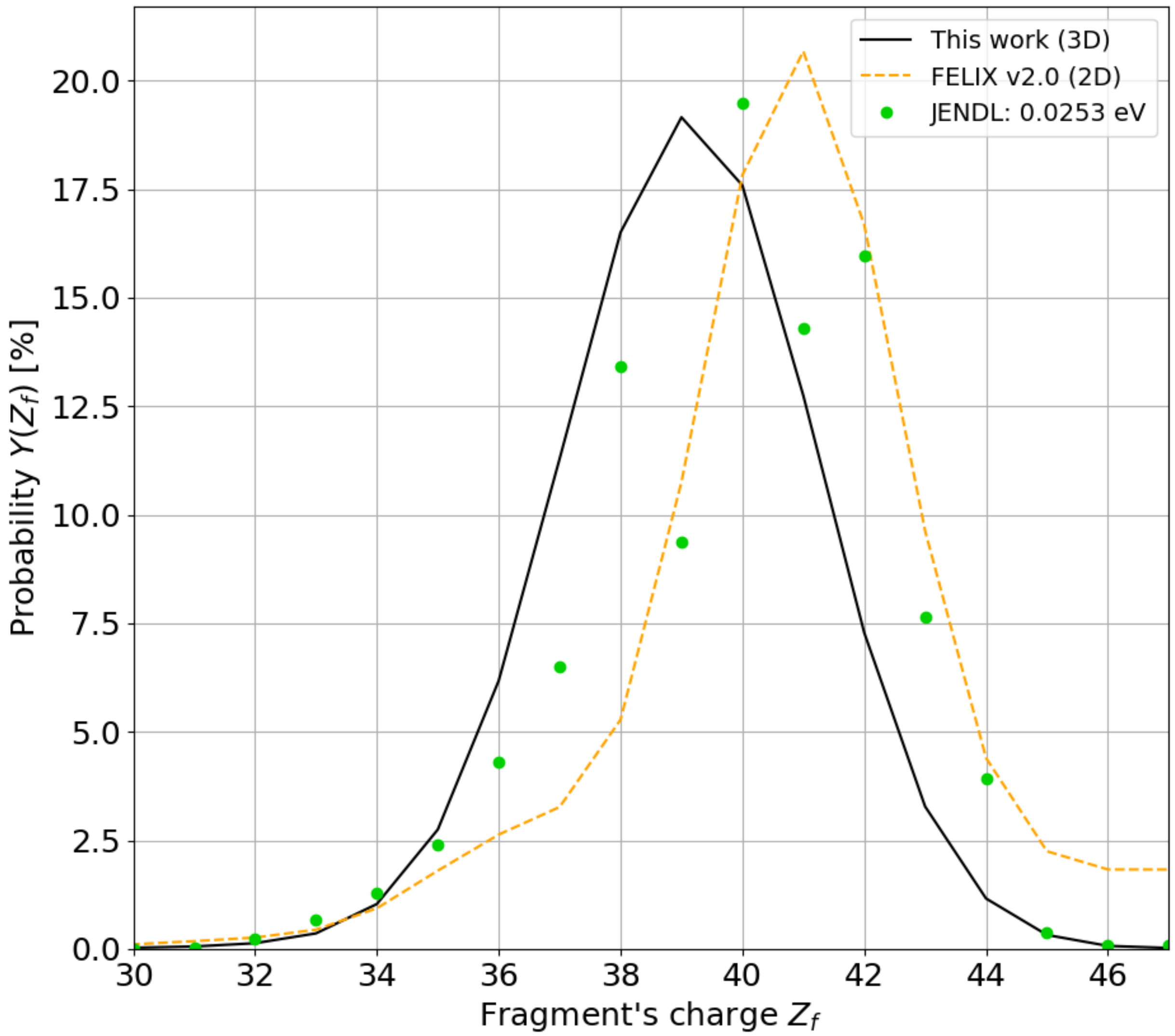




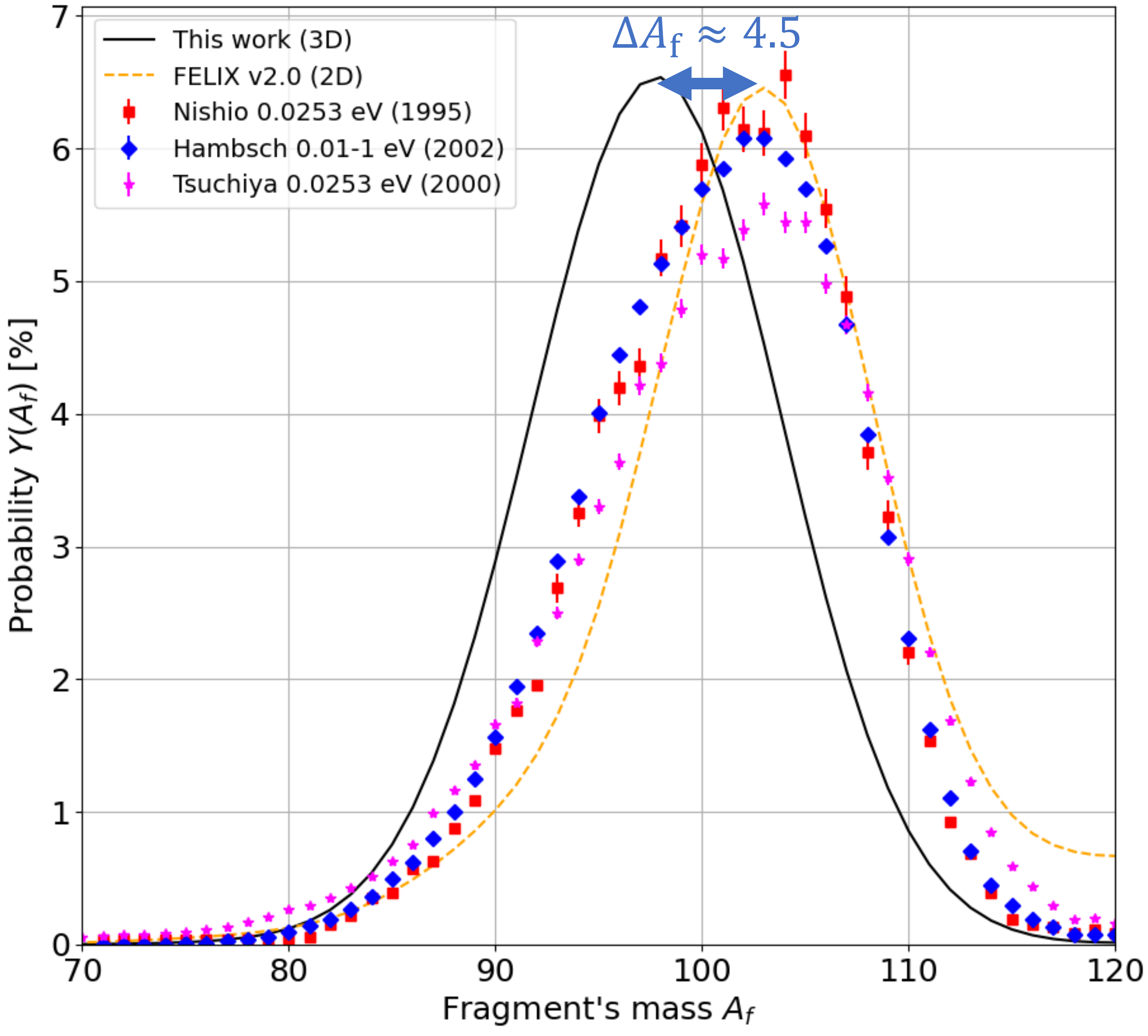


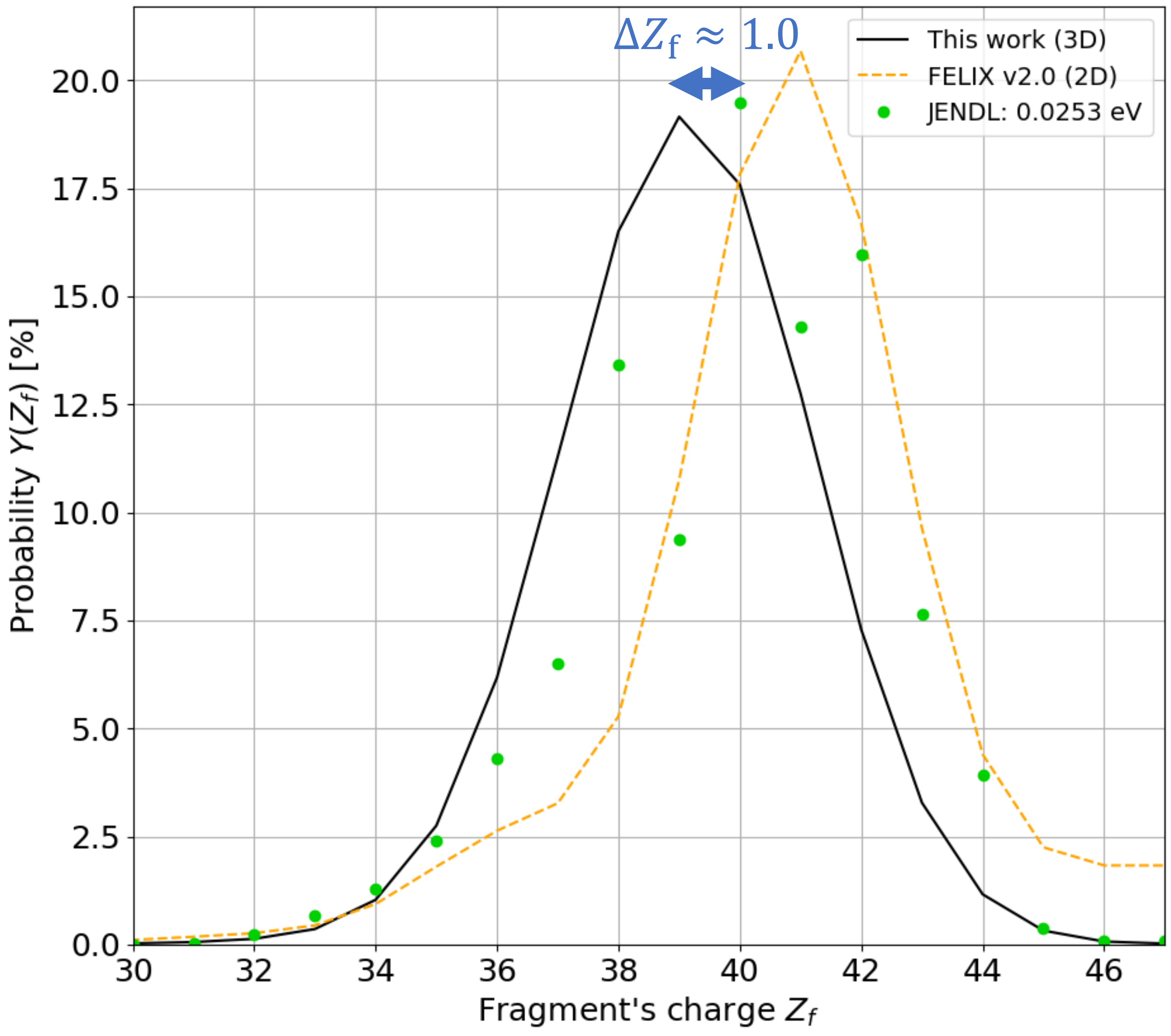
Finally, we extracted fission fragment mass and charge yields using our new pipeline.





Our (very) preliminary results are encouraging: symmetric fission is better reproduced, but the mass yields show a bigger deviation.





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.
- Strengthen the 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 (CMake, Pybind11, Doxygen, etc).
- …

Thank you

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