Multidimensional Framework for Modeling Fusion and Fission of Heaviest Nuclei

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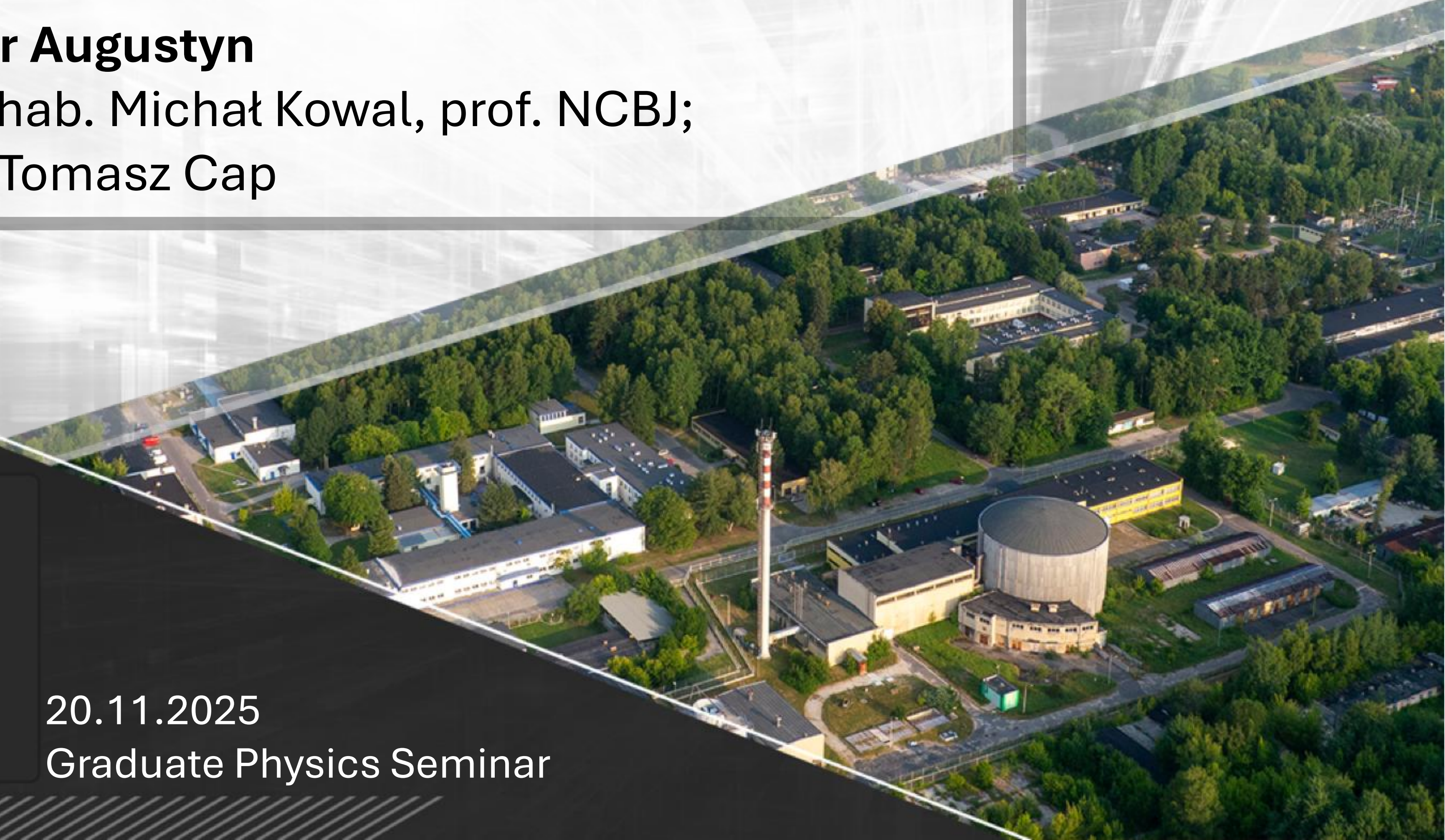

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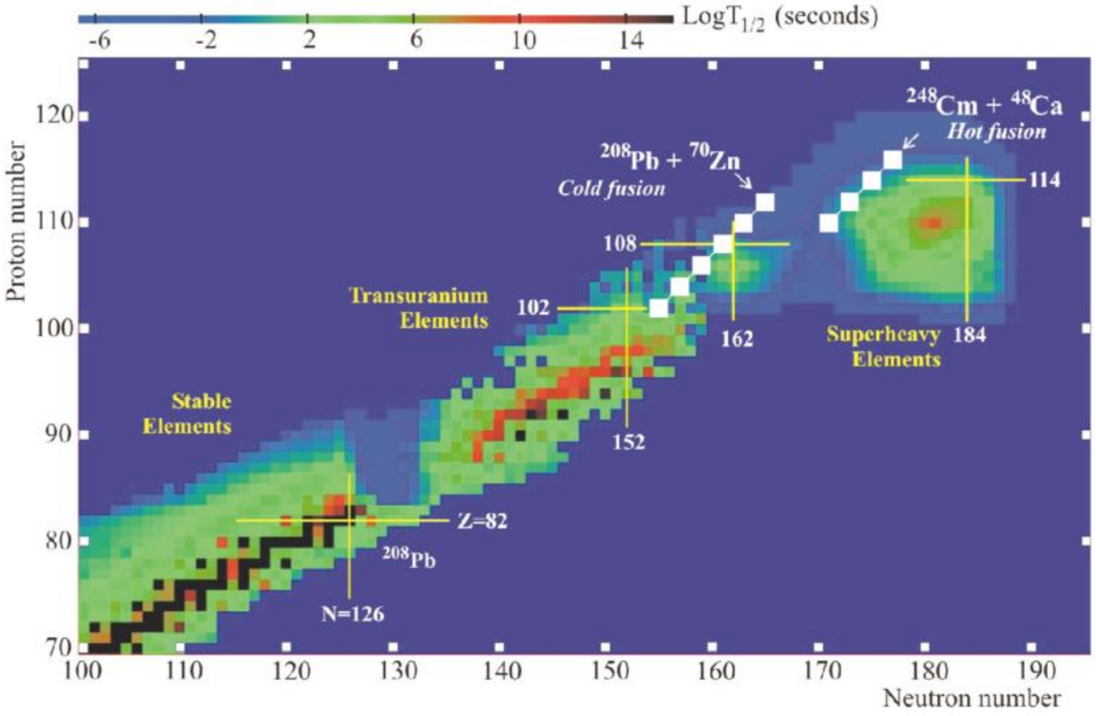
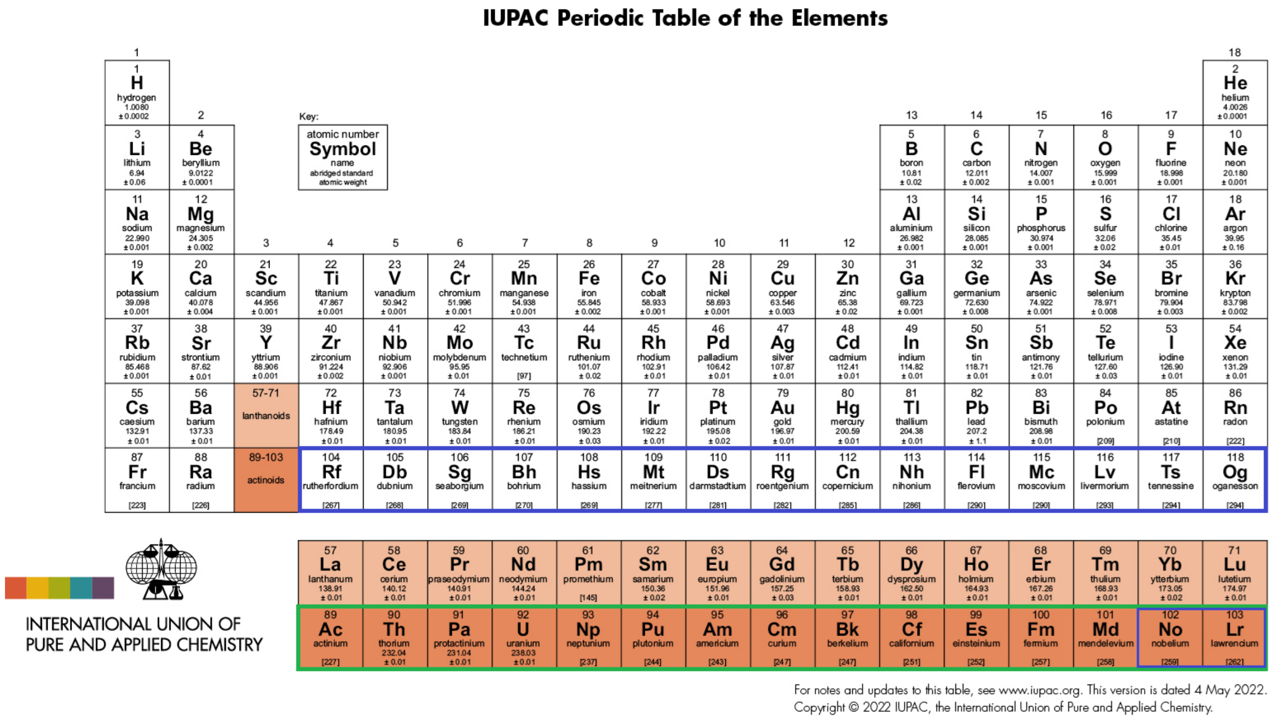
20.11.2025
Graduate Physics Seminar

Research Context

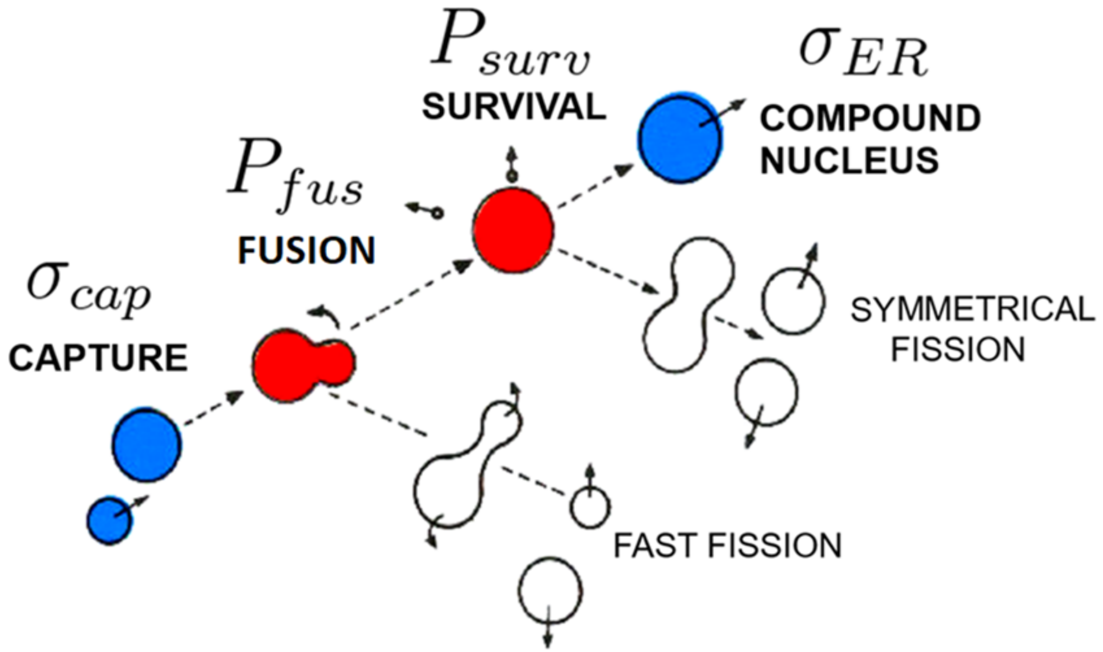
- Low energy, theoretical, nuclear physics
- Heavy (actinides) and superheavy (transactinides) elements – Z ≥ 90
- Nuclear fission and fusion
- Predicting binding energies, masses, cross-sections, mass fragment distributions, etc.

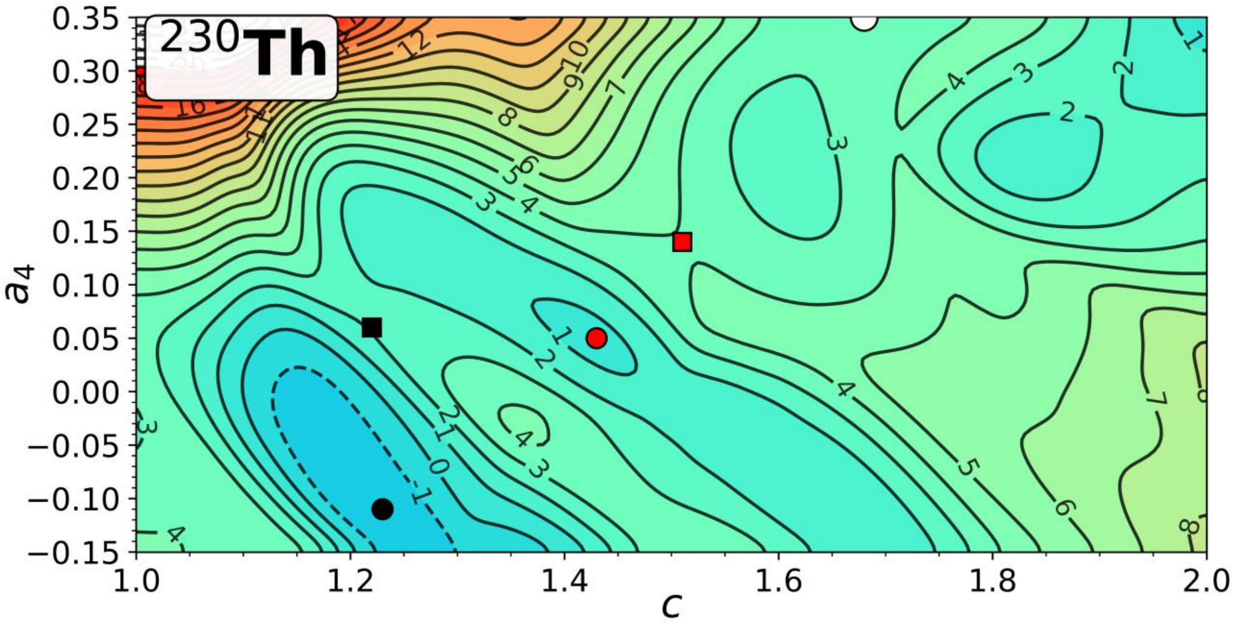




Motivation

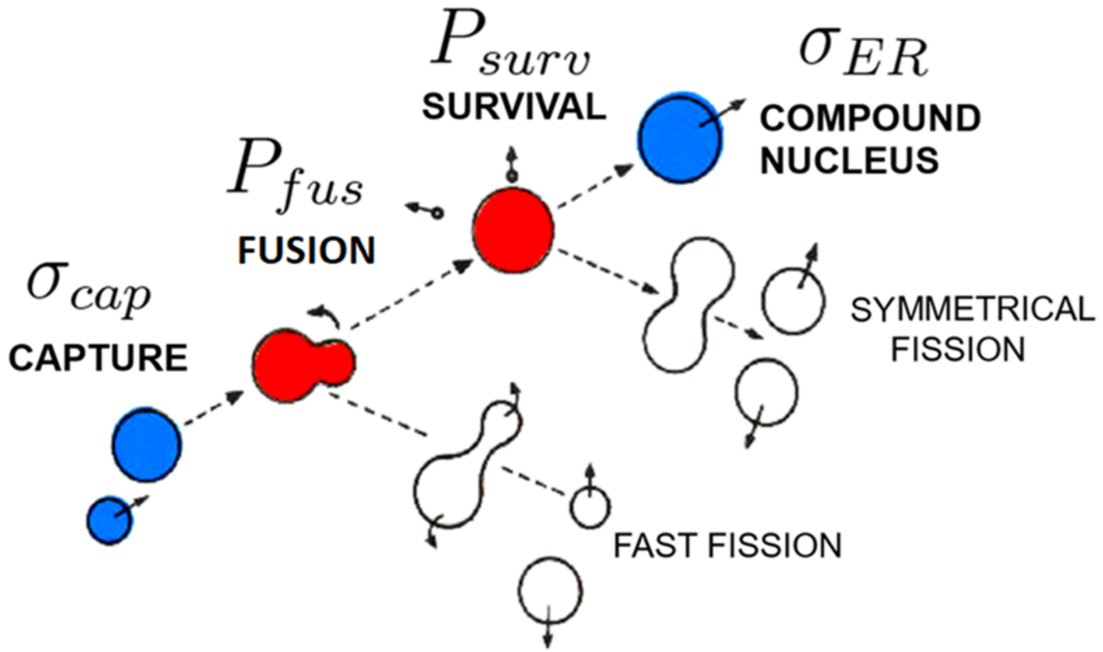
- Unified description of reaction dynamics covering both fusion (elongated →compact) and fission (compact→elongated)
- The system's evolution is governed by the topology of the multidimensional Potential Energy Surface (PES)
- Collective shape variables (parameterization dependent) drive the transformation

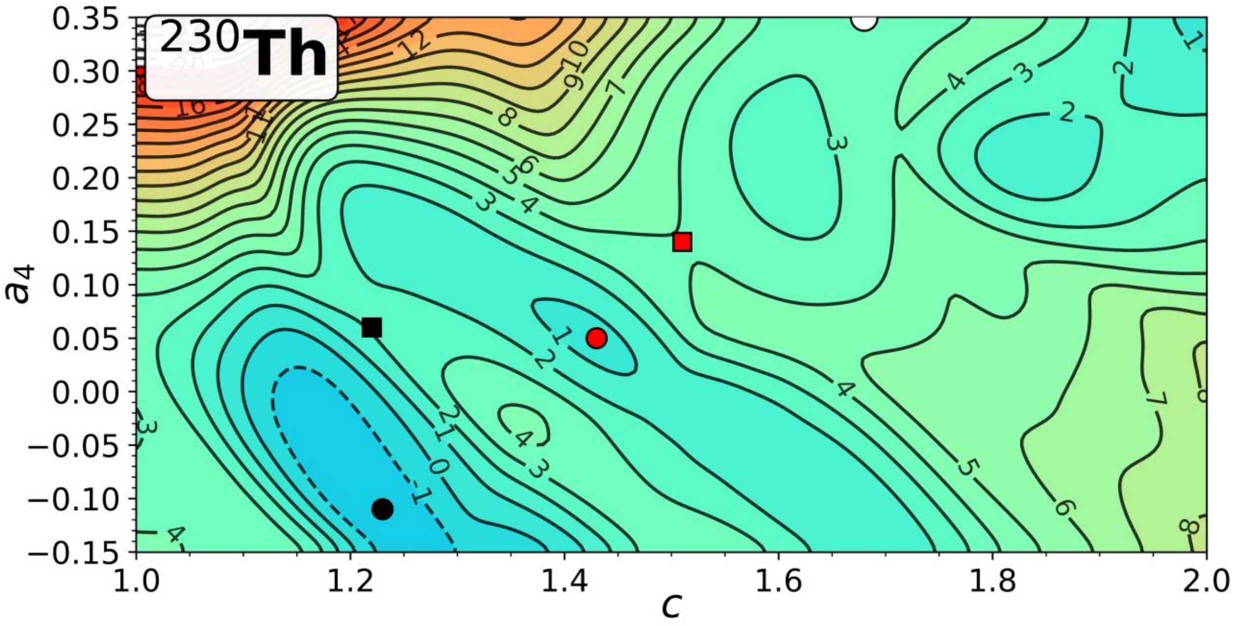




Goals

- The goal was to develop a new framework based on the Warsaw Macroscopic-Microscopic Model (WMMM)
- Use WMMM to calculate potential energy surfaces (PES) using multiple shape parameterizations
- PES can be used directly to reproduce/predict binding energies (ground state masses) and fission barriers
- Employing a stochastic shape evolution procedure (Random Walk, Langevin-plus-Masters) allows for calculating fusion probabilities, mass fragment distributions, decay modes





Plan

- **Tools:**
  - Warsaw Macroscopic-Microscopic Model (WMMM)
  - Beta Shape Parameterization
  - Fourier-over-Spheroid Shape Parameterization
  - Langevin-plus-Masters Model
- **Contributions:**
  - Shape Parameterization Conversion
  - Extending and modifying the WMMM
  - Potential Energy Surfaces Calculations
  - Random Walk Model for Shape Evolution
- **Achievements:**
  - Application I – Fusion Probabilities of Superheavy Elements (T. Cap, A. Augustyn *et al.*, PRC, 2024)
  - Application II – Static Actinide Systematics using Fourier-over-Spheroid Parameterization (A. Augustyn *et al.*, in progress)
  - Application III – Fission Mass Fragment Distributions, Random Walk vs Langevin Formalism (A. Augustyn *et al.*, in progress)

KEY CONCEPTS:
Macro-Micro Model
Shape Parameterization
Potential Energy Surface (PES)
Stochastic Shape Evolution

Warsaw Macroscopic-Microscopic Model*

liquid drop with a Yukawa-plus-exponential model

Strutinsky shell correction + Woods-Saxon potential + BCS

$$E_{\mathrm{tot}}(Z,N,\boldsymbol{q}) = E_{\mathrm{mac}}(Z,N,\boldsymbol{q}) + E_{\mathrm{mic}}(Z,N,\boldsymbol{q})$$

- <u>Allows to obtain the binding energy for a given nuclear shape $\boldsymbol{q}$</u>
- Previously only used with spherical harmonics + beta shape parameterization, with up to 20 deformation parameters
- In current calculations, limited to <u>axially symmetric shapes</u>
- Macroscopic energy normalized with respect to the sphere:

$$E_{\mathrm{mac}} = E_{\mathrm{mac}}(\boldsymbol{q}) + E_{\mathrm{mac}}(\mathrm{sphere})$$

* P. Jachimowicz *et al.*, ADNDT **138**, 101393 (2021).

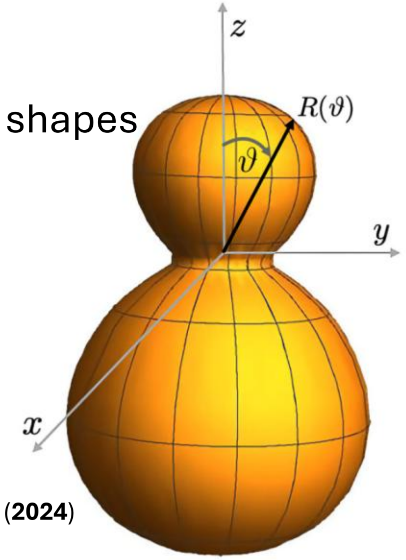
Beta Parameterization*

- Mononuclear shapes can be parameterized via spherical harmonics $Y_l^m(\vartheta,\varphi)$ by the following equation of the nuclear surface:

$$R(\vartheta,\varphi) = c(\{\beta\})R_0\{1 + \sum_{\lambda=1}^{\infty}\sum_{\mu=-\lambda}^{+\lambda}\beta_\lambda^\mu Y_\lambda^\mu\}$$

where c({β}) is the volume-fixing factor and R_0 is the radius of a spherical nucleus

- Used by WMMM
- Unsuited for scission shapes



T. Cap *et al.*,Phys. Rev. C **109**, L061603 (**2024**)

* P. Jachimowicz *et al.*, ADNDT **138**, 101393 (2021).

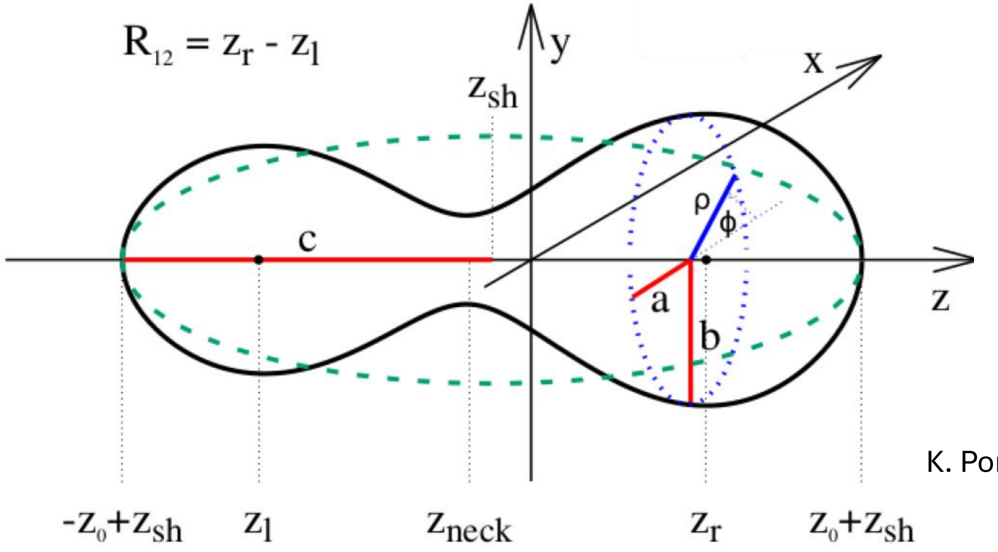
Fourier-over-Spheroid Parameterization**

- The distance from the z-axis to the surface is given by:

$$\rho^2(z,\varphi) = \frac{R_0^2}{c} f\left(\frac{z-z_{\mathrm{sh}}}{z_0}\right)\frac{1-\eta^2}{1+\eta^2+2\eta\cos 2\varphi}$$

where: $f(u) = 1-u^2-\sum_{k=1}^{n}\left\{a_{2k}\cos\left(\frac{2k-1}{2}\pi u\right) \quad +a_{2k+1}\sin(k\pi u)\right\}$

- Able to describe shapes from compact to scission



K. Pomorski

Up to 5 parameters used:
c – elongation
a_3 – asymmetry
a_4 – neck parameter
a_5 – higher order
a_6 – higher order

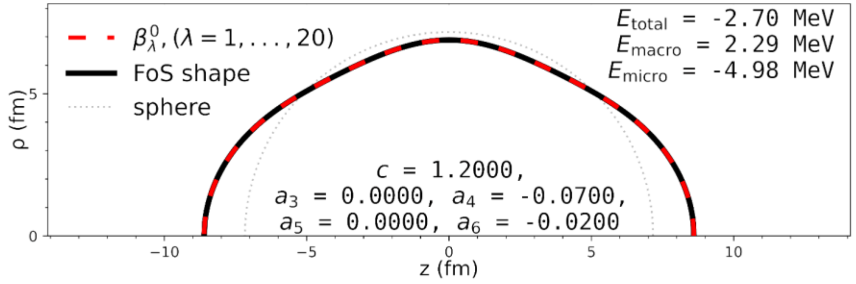
** K. Pomorski *et al.*, Acta Phys. Pol. B Proc. Suppl. **16**, 4-A021 (2023).

Shape Parameterization Conversion

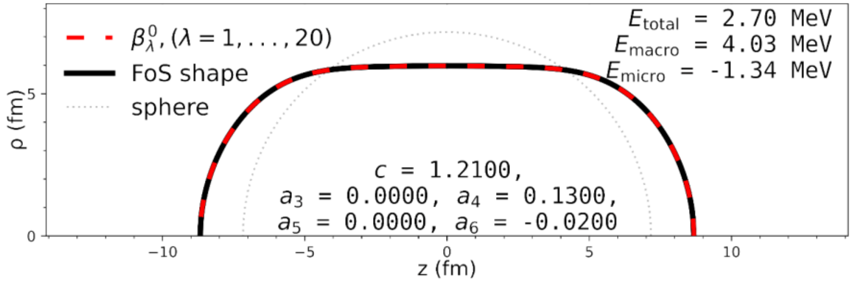
- Convert star-shaped FoS shapes to spherical coordinates
- Given a radius vector R(θ, ϕ) the corresponding β parameters can be calculated from the orthogonality of spherical harmonics:

$$\beta_\lambda^\mu = \sqrt{4\pi}\,\frac{\int \tilde{R}(\vartheta,\varphi) Y_\lambda^\mu \sin\vartheta \mathrm{d}\vartheta\mathrm{d}\varphi}{\int \tilde{R}(\vartheta,\varphi) Y_0^0 \sin\vartheta \mathrm{d}\vartheta\mathrm{d}\varphi}$$

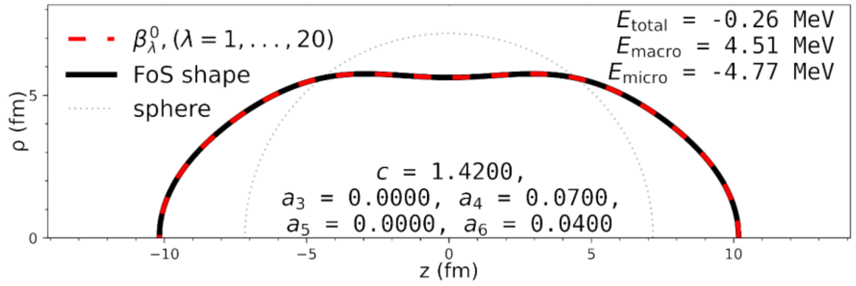
- Any number of β parameters can be fitted (currently up to 20 were used)
- Can be used for other parameterizations as well



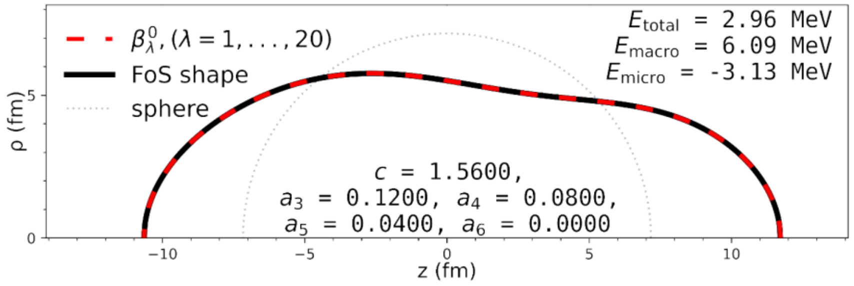
(a) Ground state



(b) Inner saddle point



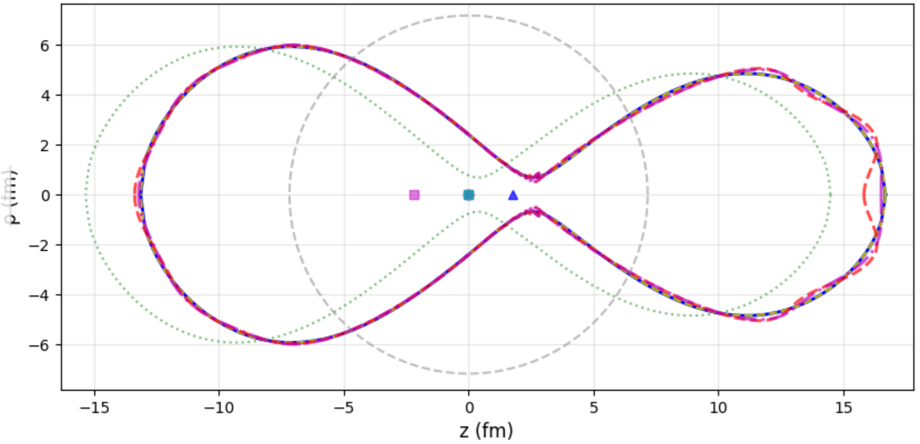
(c) Secondary minimum



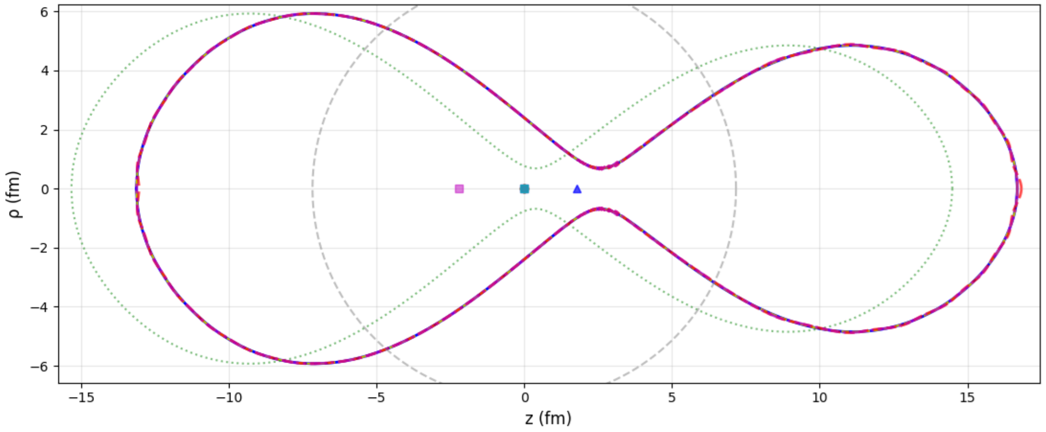
(d) Outer saddle point

Extending and modifying the WMMM

- Extended the model to work with any number of beta parameters, allowing for calculating highly elongated shapes near scission
- Refactored the code developed over 40 years to modern standards (Fortran 2018)
- Clarified logic flow
- Optimized performance
- Created detailed documentation (useful for future users)



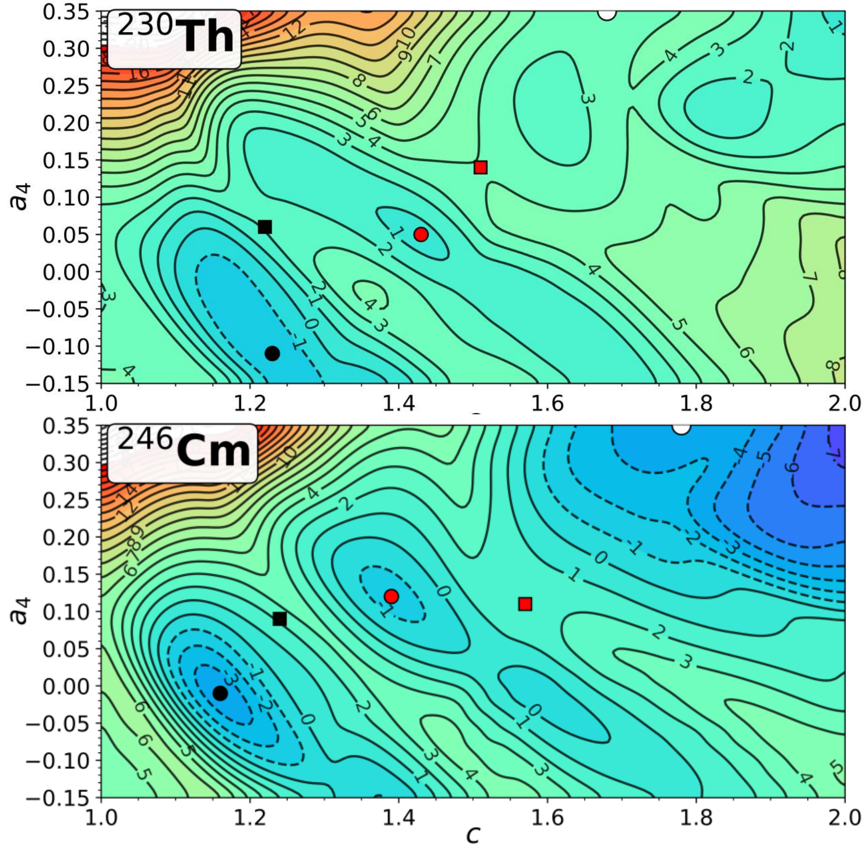
20 β parameters used for fit



64 β parameters used for fit

Potential Energy Surfaces Calculations

- Created scripts for performing large, parallel calculations on the Świerk Computing Centre (CIŚ)
- Performed calculations for PES both in beta and FoS parameterizations (3D and 5D) for many actinide and superheavy nuclei



5D (c, a_3, a_4, a_5, a_6):

Step size 0.01

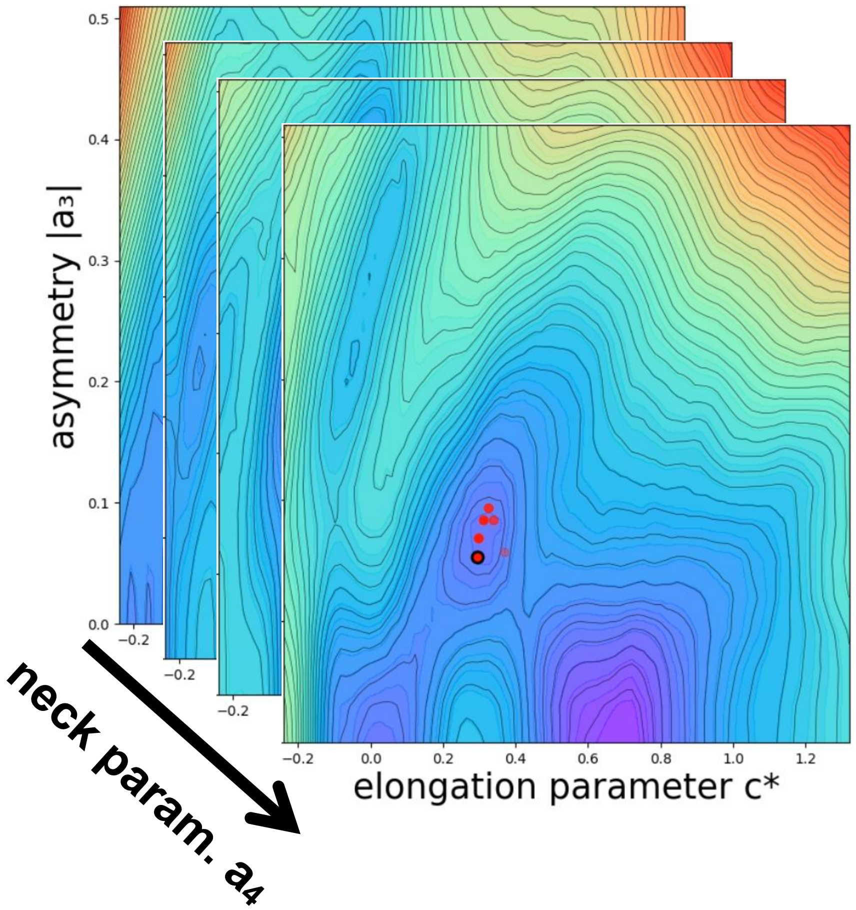
c	(1.00, 2.00)
a_3	(0.00, 0.25)
a_4	(-0.15, 0.35)
a_5	(-0.15, 0.15)
a_6	(-0.15, 0.15)

128 702 886 shape configurations per system

Multidimensionality of the PES

- Full PES cannot be displayed
- Projection on a selected plane are used, while minimizing over other degrees of freedom
- Movement in the multidimensional space requires a stochastic model

Potential Energy Surface (PES)



Langevin-plus-Masters Model*

- Allows for detailed description of shape evolution, accounting for dissipative forces
- Time evolution of collective degrees of freedom **q**(t) and their conjugate momenta **p**(t) is governed by multidimensional Langevin equations:

$$\frac{d\mathbf{q}}{dt} = \mathsf{M}^{-1}(\mathbf{q})\,\mathbf{p},$$

$$\frac{d\mathbf{p}}{dt} = -\nabla_{\mathbf{q}} H(\mathbf{q},\mathbf{p}) - \boldsymbol{\gamma}(\mathbf{q})\mathsf{M}^{-1}(\mathbf{q})\mathbf{p} + \mathsf{G}(\mathbf{q})\boldsymbol{\Gamma}(t)$$

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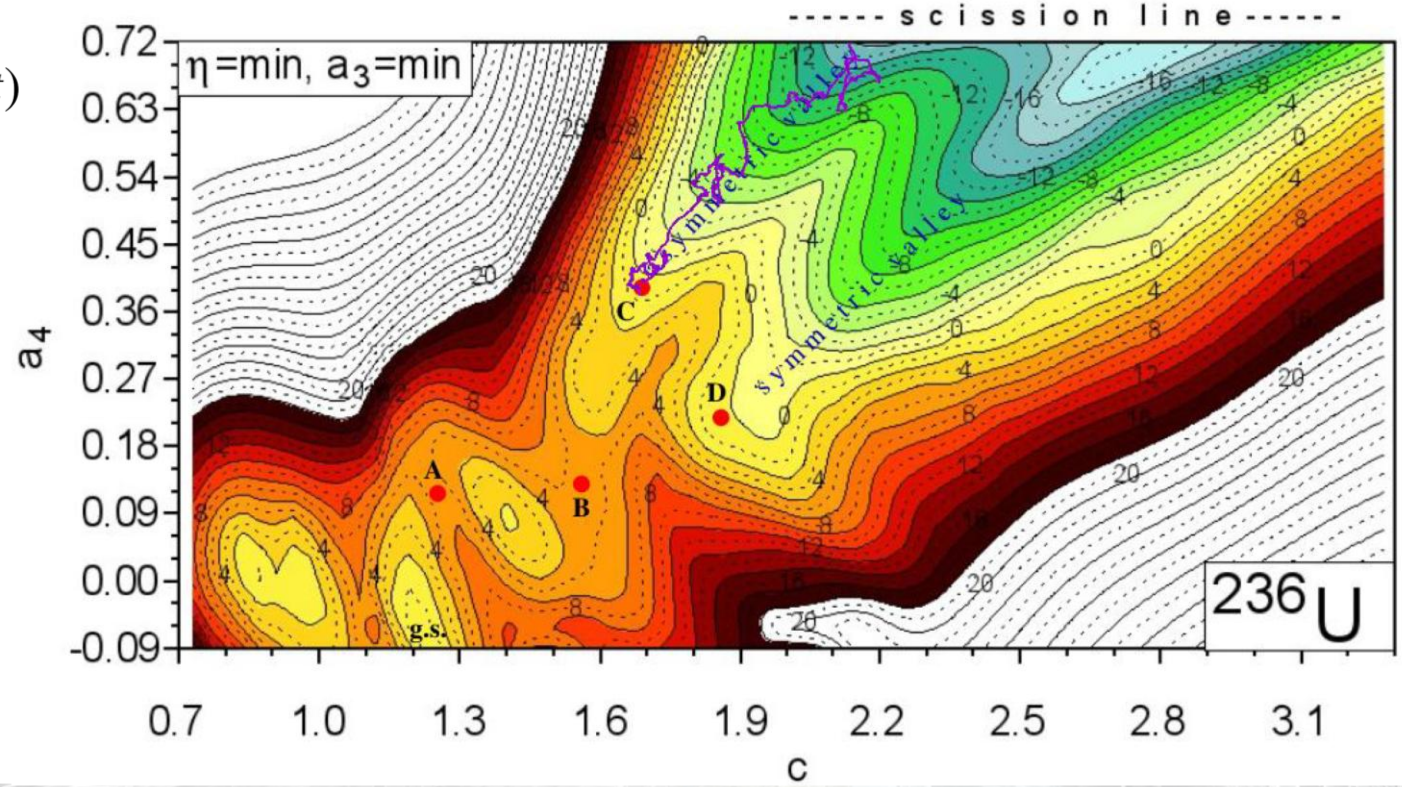


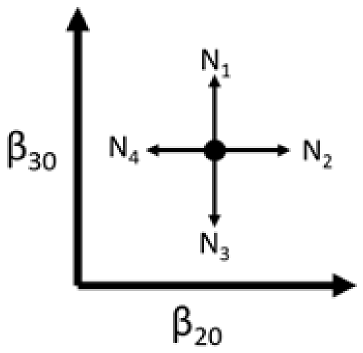
** K. Pomorski *et al.*, PRC **107**, 054616 (2023).

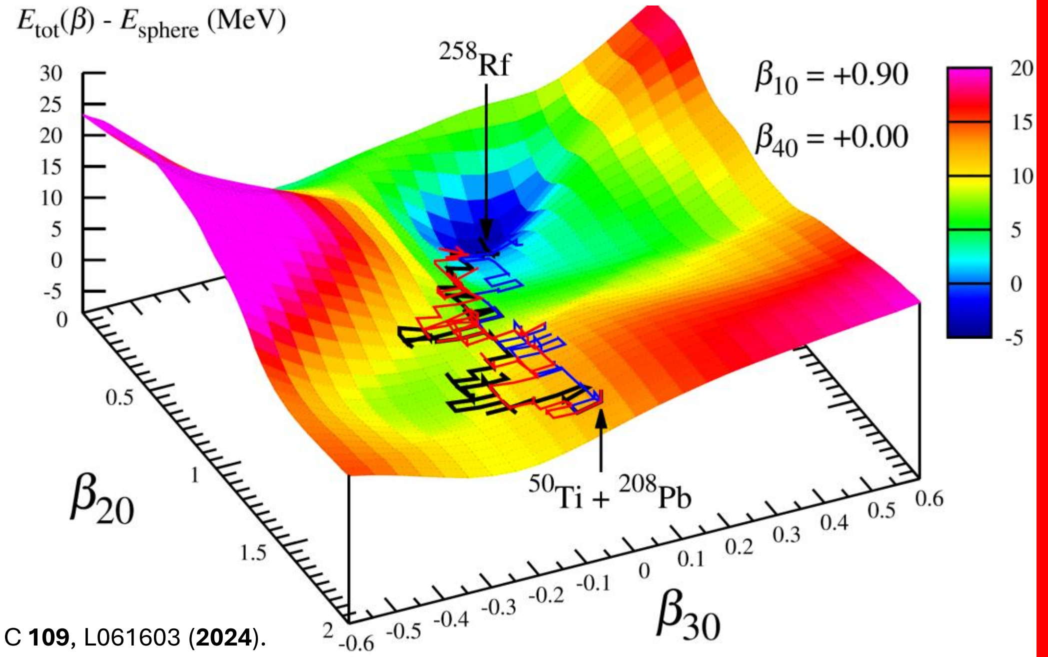
Random Walk Model

- The probability of transitioning from one shape to another is determined by the number of available energy levels for a given shape q

$$\rho(E_{\text{int}}(q)) \propto \exp\left(2\sqrt{aE_{\text{int}}(q)}\right) \quad P_{i\to j} = \frac{N_j}{\sum_k N_k}, \quad \text{where } N_j = \rho(E_{\text{int}}(q_j))$$

- Only one shape parameter changes at a time
- The random walk process continues until an end condition is met





T. Cap *et al.*,Phys. Rev. C **109**, L061603 (**2024**).

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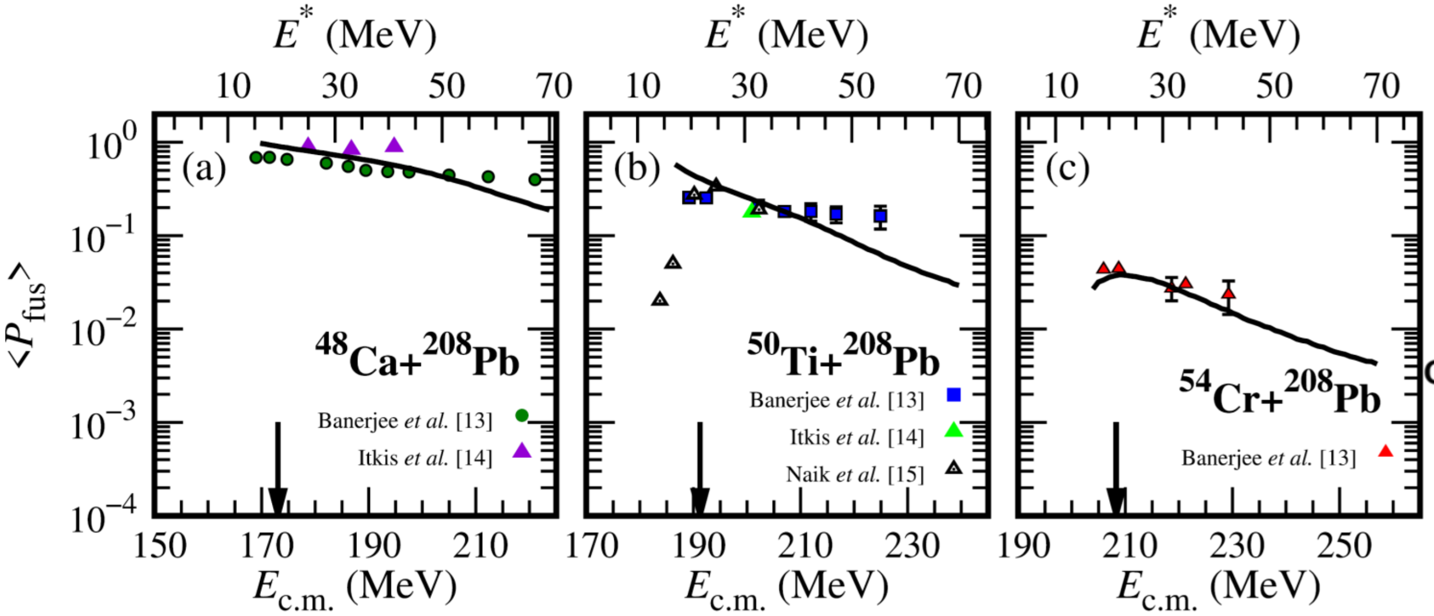
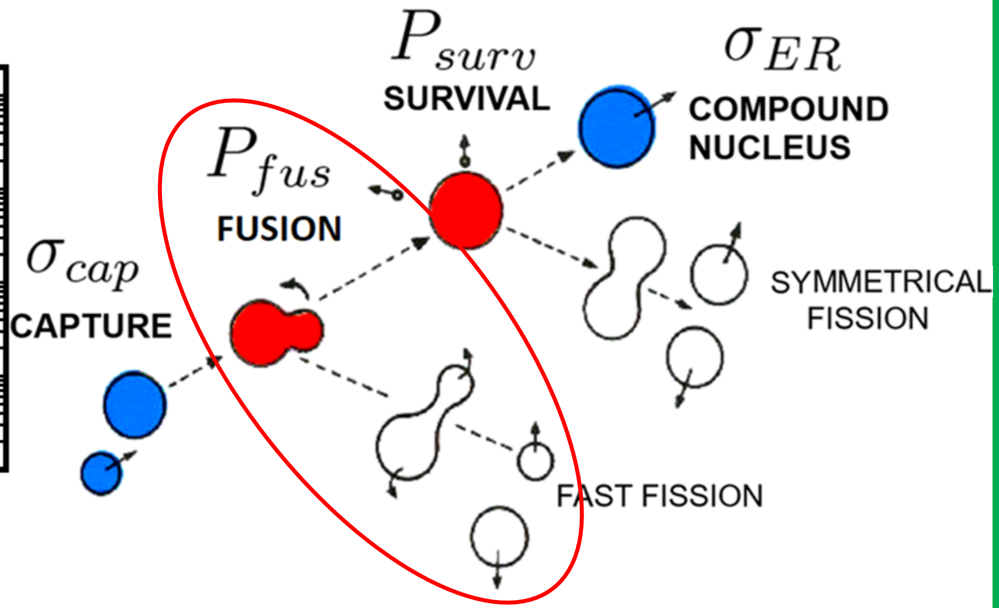
Fusion Probabilities of Superheavy Elements*

- Used Random Walk on 4D β PES
- Calculated the probability of fusion for 3 superheavy systems (^{256}No, ^{258}Rf, ^{262}Sg)
- No fitting of model parameters
- Shows the usefulness of the Random Walk Model



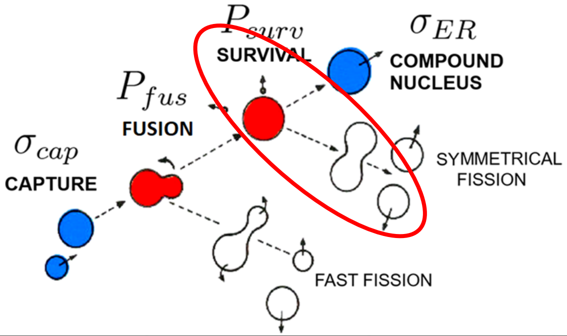


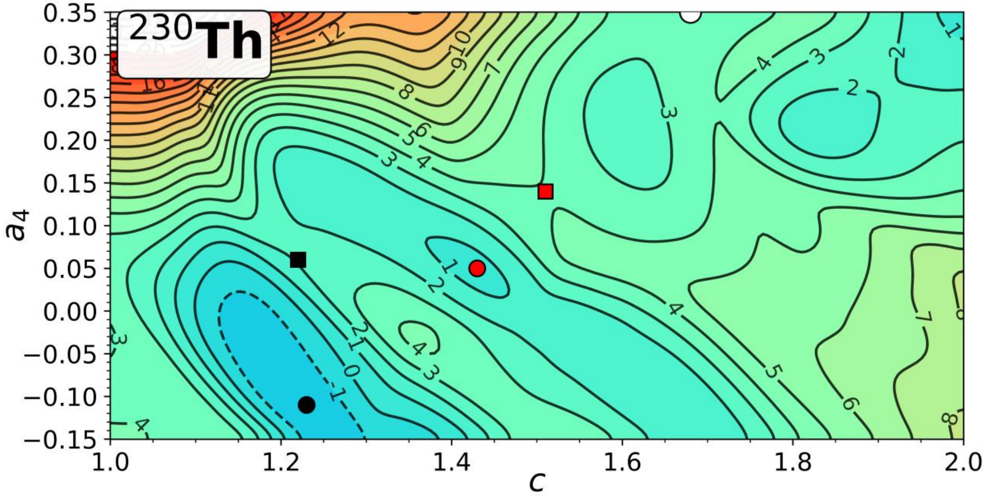
* T. Cap, A. Augustyn *et al.*, PRC, 2024.

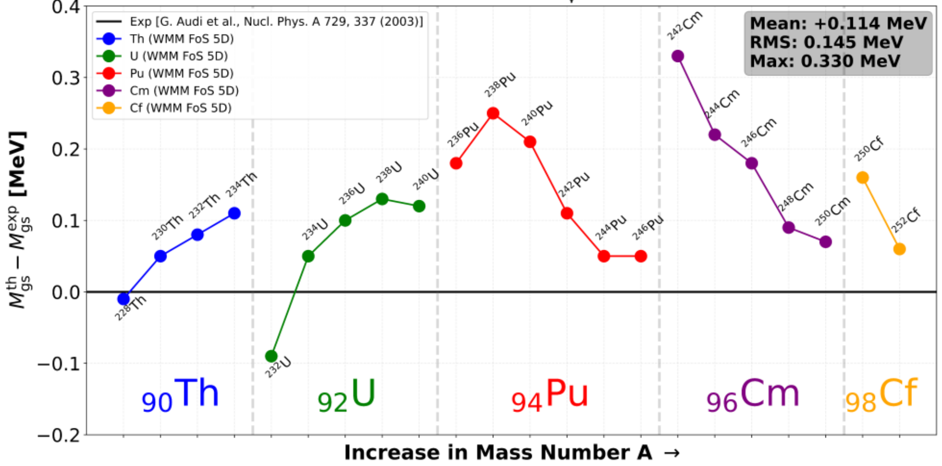
Static Actinide Systematics using FoS*

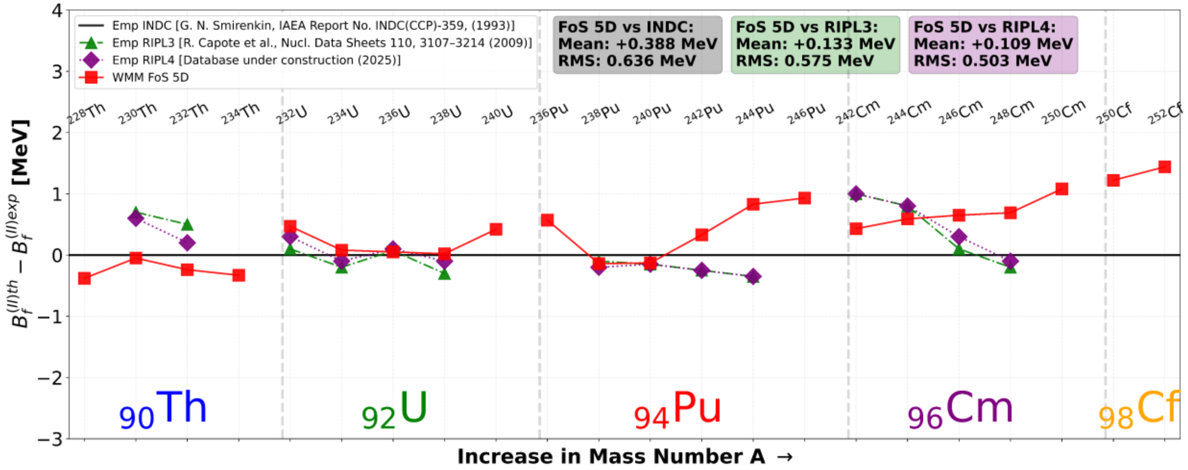
* Used 5D FoS PES
* Calculated ground state masses, inner and outer fission barriers of 22 even-even actinide nuclei
* Shows the effectiveness of the conversion algorithm
* Next step: full PES from ground state to scission

* A. Augustyn *et al.*, PRC, in progress



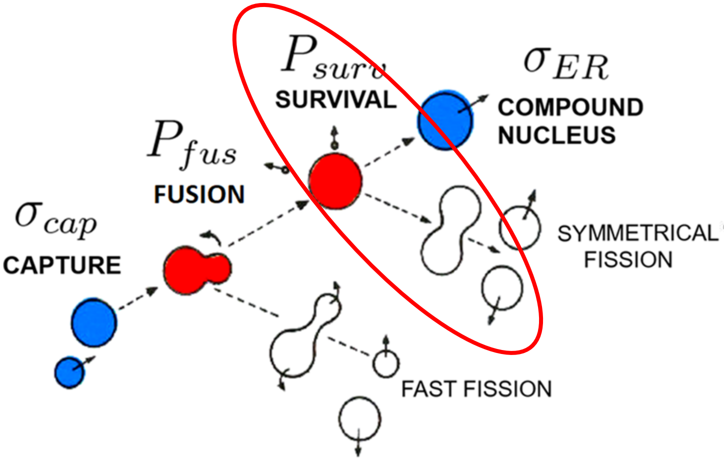


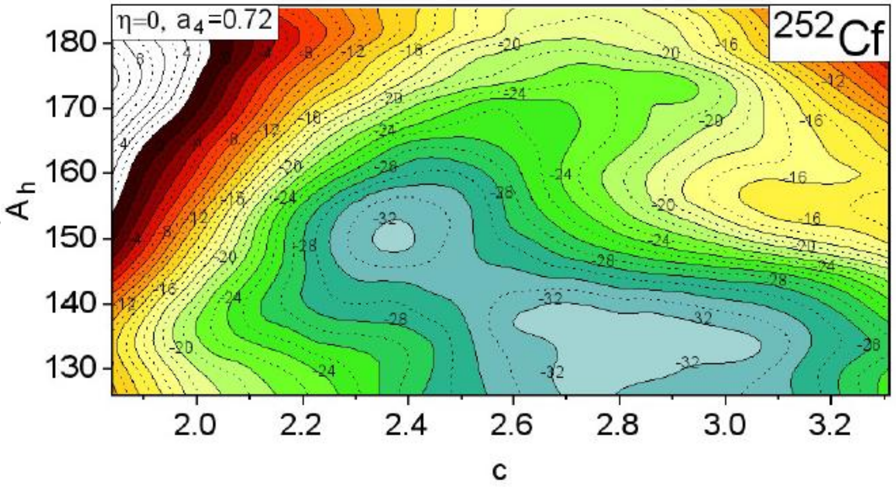


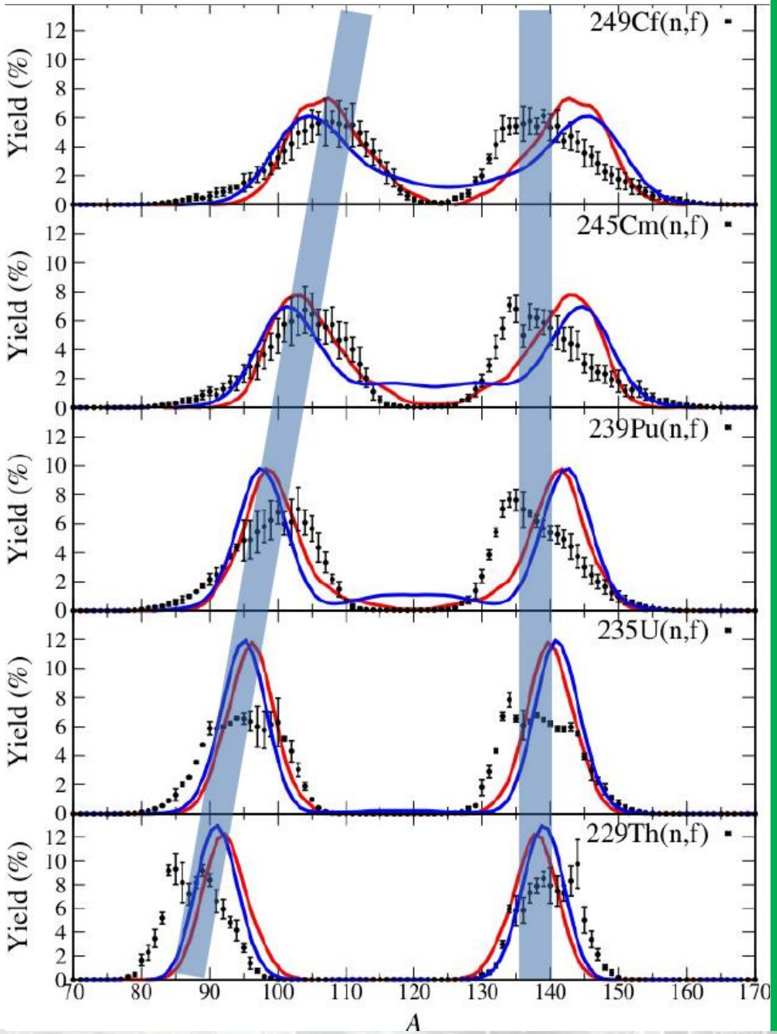


Fission Mass Fragments Distributions, Random Walk vs Langevin Formalism*

- Used Random Walk and Langevin-plus-Masters on 3D FoS PES
- Calculated mass fragment distributions for 5 actinide systems: ^{230}Th, ^{236}U, ^{240}Pu, ^{246}Cm, ^{250}Cf



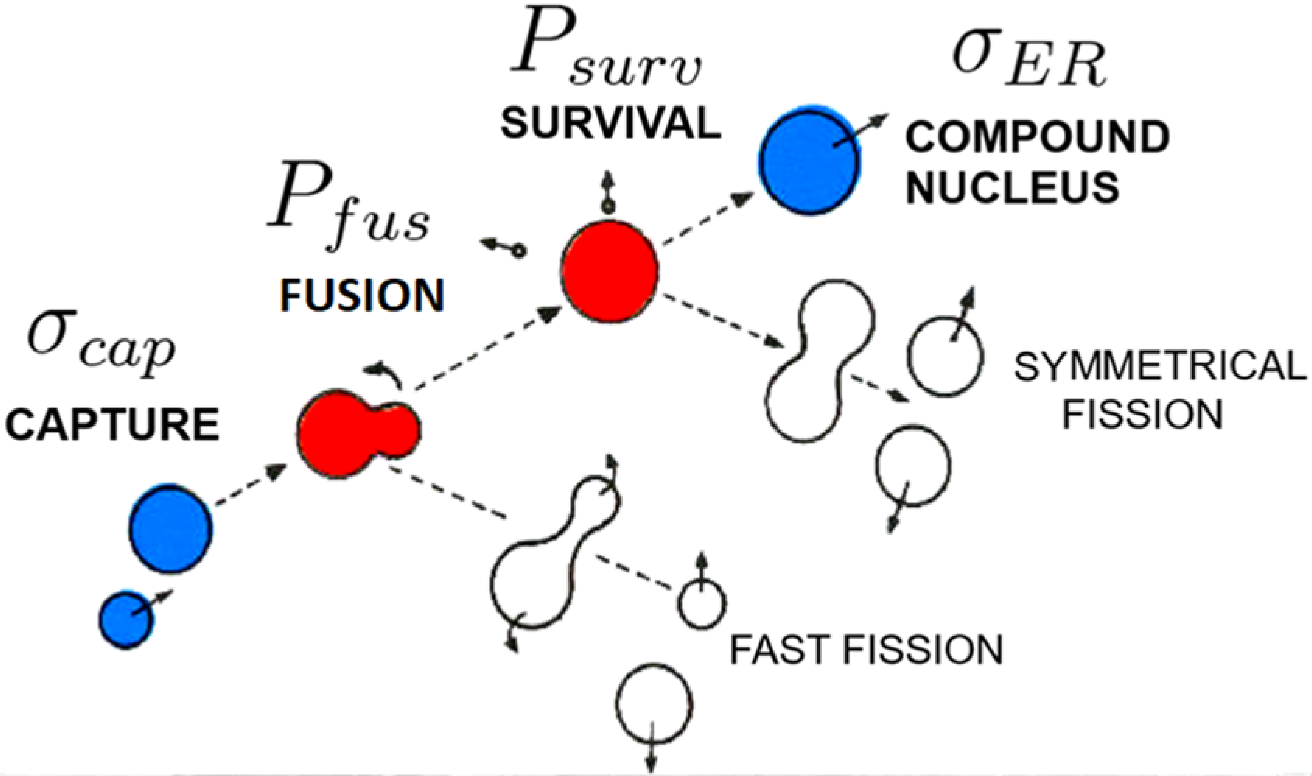




* A. Augustyn *et al.*, in progress

Summary

- The developed framework allows for the description of multiple steps of the fusion/fission process
- Gives access to multiple experimental observables (probability of fusion, ground state masses, barriers, mass fragment distributions, and potentially more)
- Future work might allow for the full description of the process within one model



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