Microscopic Description of the Fission Process

Kyle Godbey and Witold Nazarewicz, Michigan State University

2023 Stewardship Science Academic Programs Symposium
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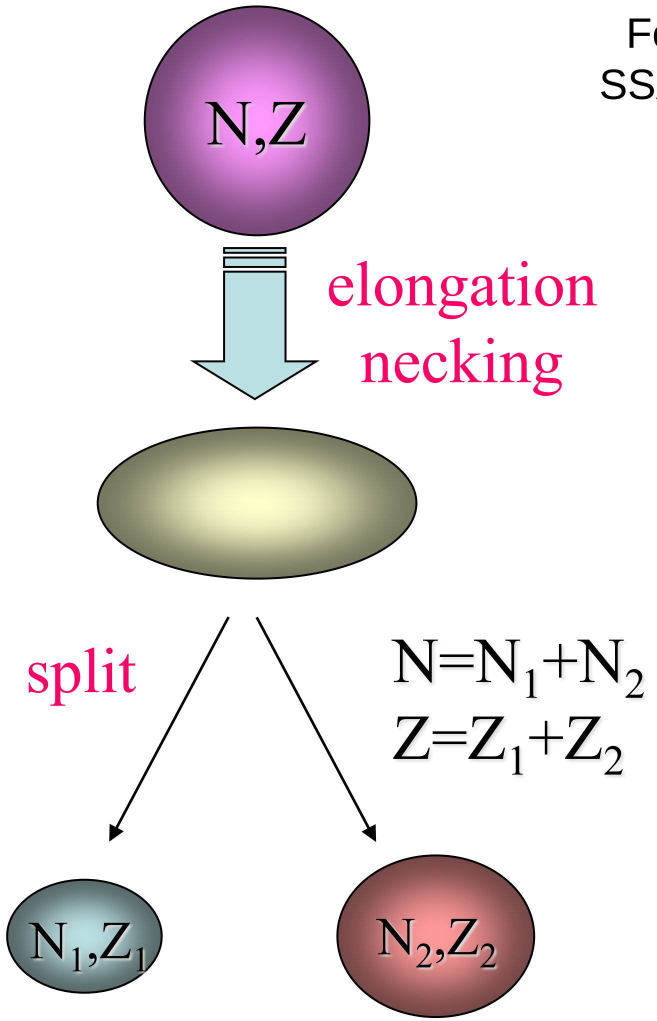
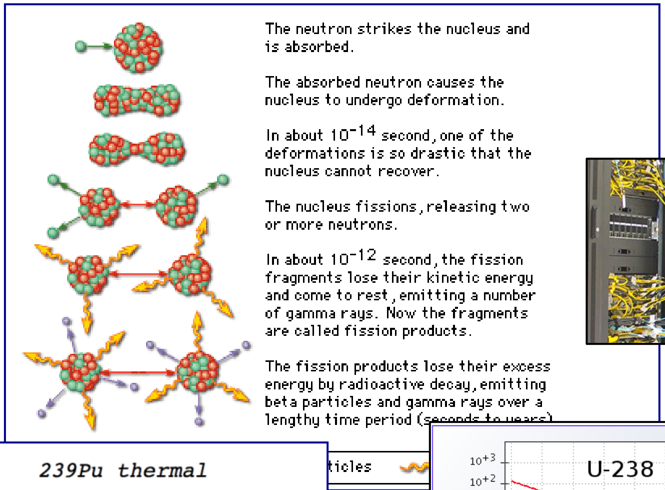
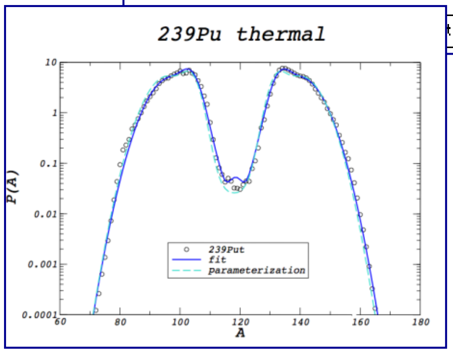
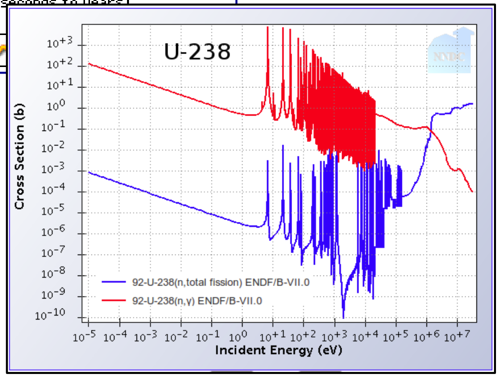
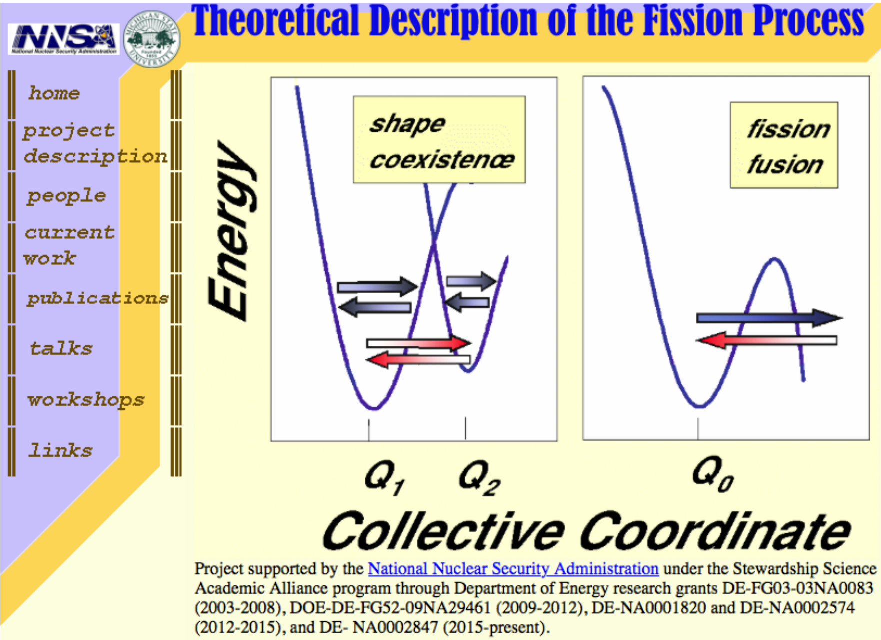
SSAA grant DE-NA0004074 (since 2003)











https://people.nscl.msu.edu/~witek/fission/fission.html

- Fission is a complex process involving the collective motion of all nucleons – One of the most difficult problems in nuclear physics
- Most practical applications have been based on simplified theories tuned to existing data
- We are developing a microscopic model that will be predictive

The Team

PI: Witold Nazarewicz

PhD students:

- Daniel Lay
- Eric Flynn

Post Docs:

- Sylvester Agbemava
- Kyle Godbey

+ Samuel Giuliani (Madrid)

+ Jhilam Sadhukhan (Kolkata)

+ NUCLEI (SciDAC-5)

+ BAND Framework

NUCLEI Nuclear Computational Low-Energy Initiative

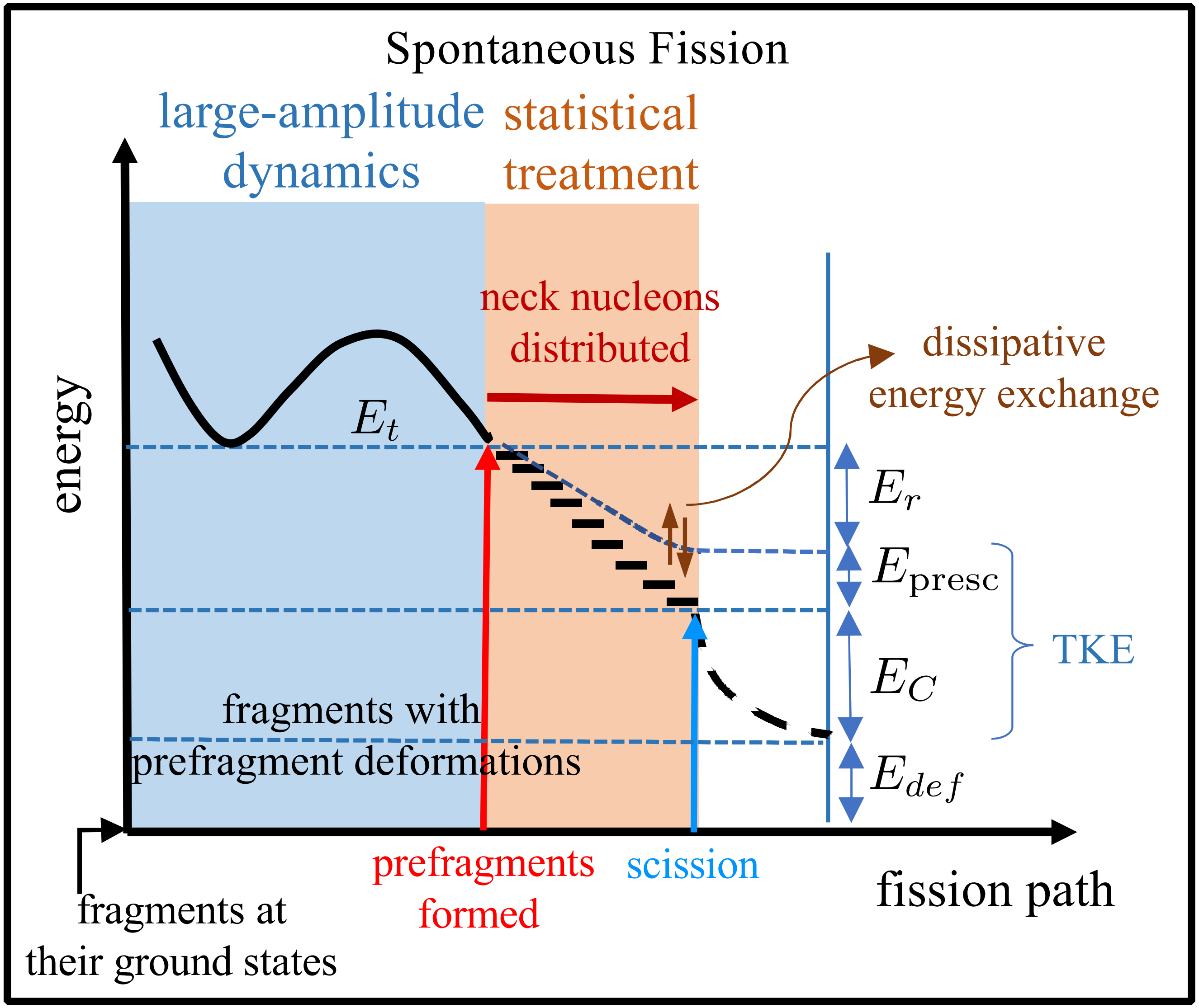
BAND Bayesian Analysis of Nuclear Dynamics

Five components of our program

I. Quantified input (optimized energy density functionals)
II. Microscopic model based on a quantified input
   - Density functional theory, including TDDFT
   - Stochastic Langevin framework
III. Confrontation with experiment
   - Fission
   - Heavy-ion fusion
IV. Systematic predictions
   - Superheavy elements
   - Astrophysical applications: r-process
V. Machine learning and uncertainty quantification
   - Linear regression
   - Bayesian machine learning
   - Dimensionality reduction

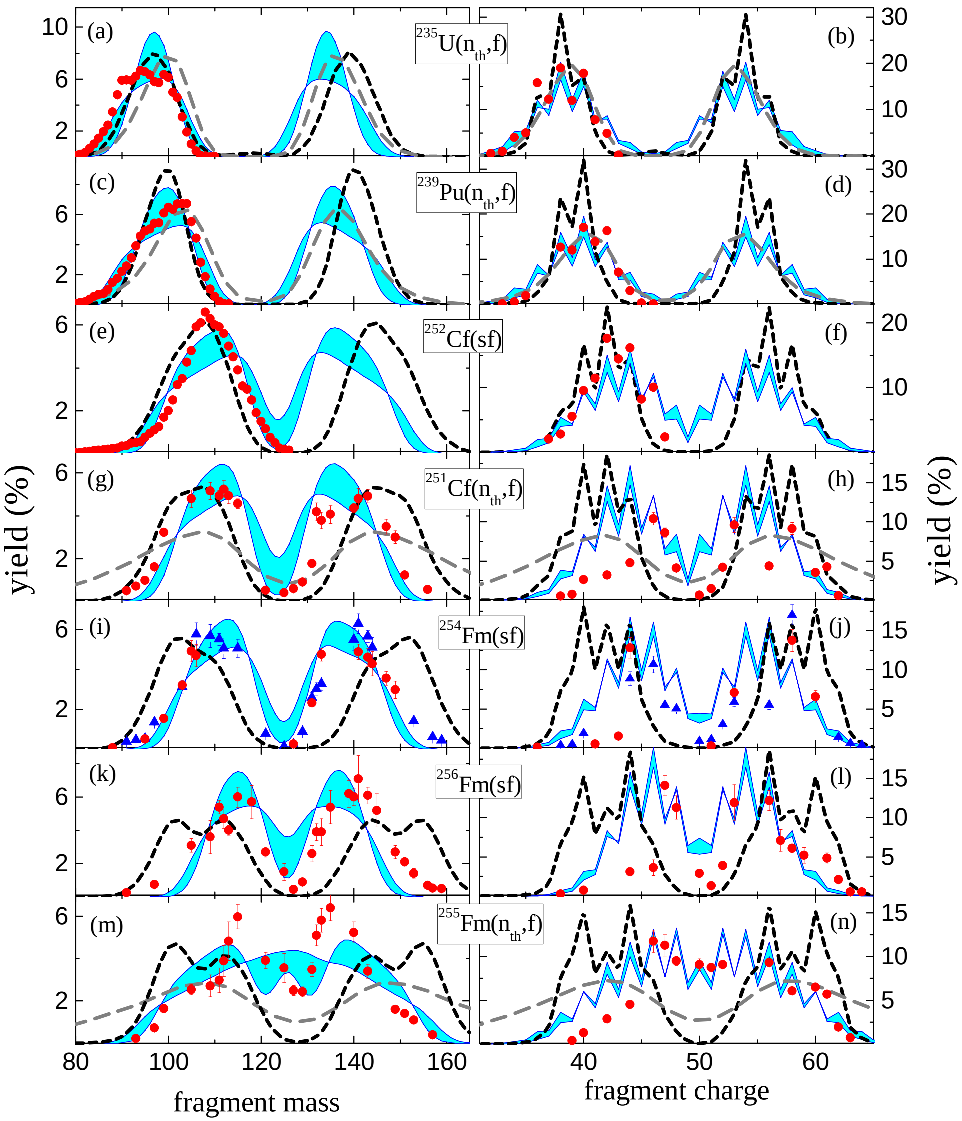
Efficient method for estimation of fission fragment yields

J. Sadhukhan, S.A. Giuliani, and WN, Phys. Rev. C 105, 014619 (2022)

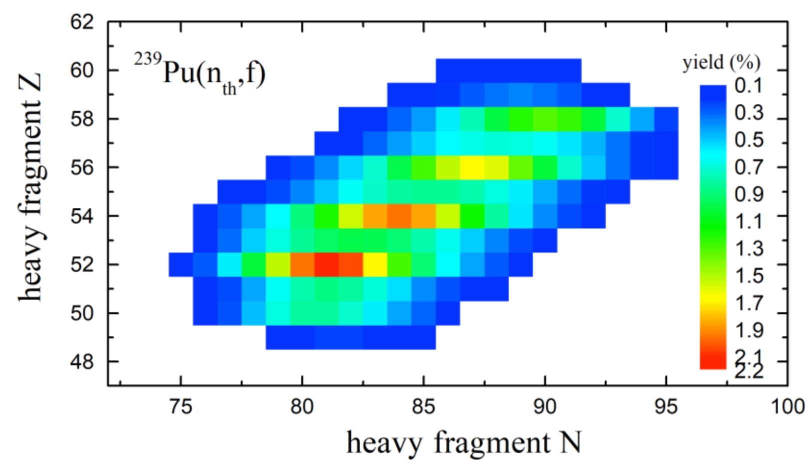


Microscopic description of the odd-even effect in fission yields

Phys. Rev. C 105, 014619 (2022)

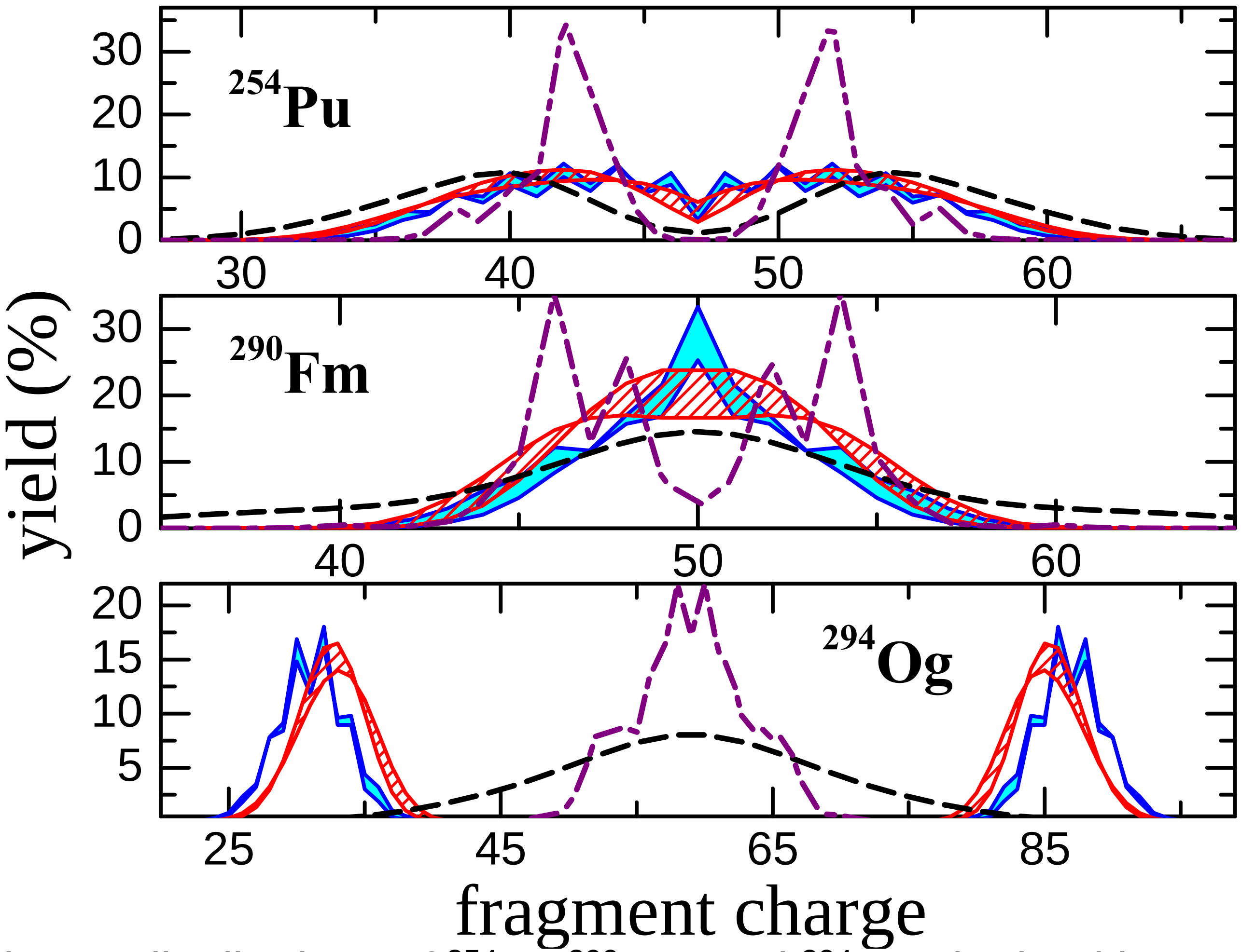


Calculated mass (left panels) and charge (right panels) fission fragment distributions using the model described in this study (blue bands), the Brownian shape-motion approach (BSM, gray dashed lines), and the scission-point model (SPM; black dashed lines). Red and blue symbols show experimental data.



Challenge: r-process and superheavy nuclei

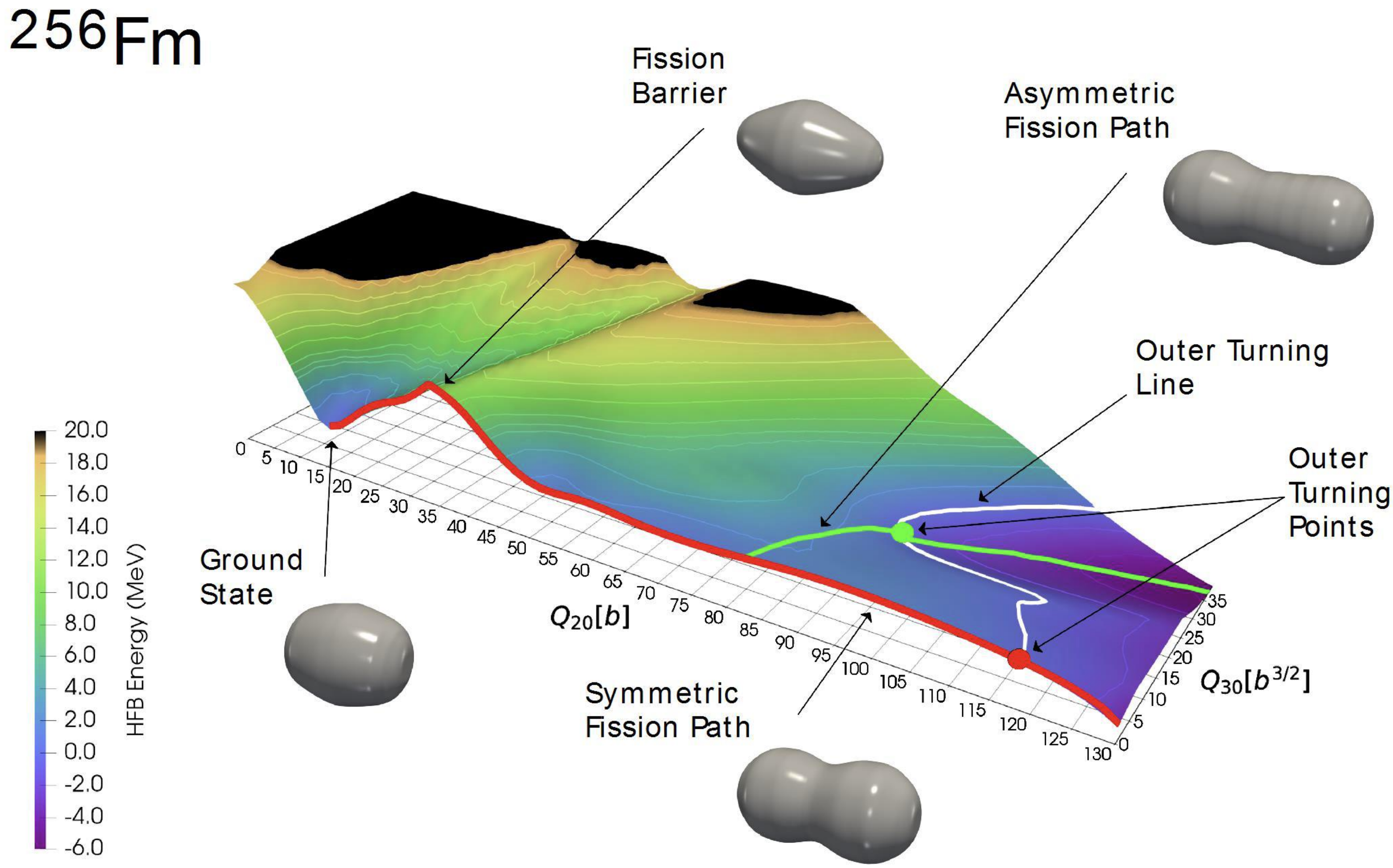
Phys. Rev. C 105, 014619 (2022)



Fragment charge distributions of ^{254}Pu,^{290}Fm, and ^{294}Og obtained in our work (blue bands) and predicted in previous work by neglecting odd-even staggering (red dashed bands). Predictions of BSM and SPM models are shown by dashed and dash-dotted lines, respectively.

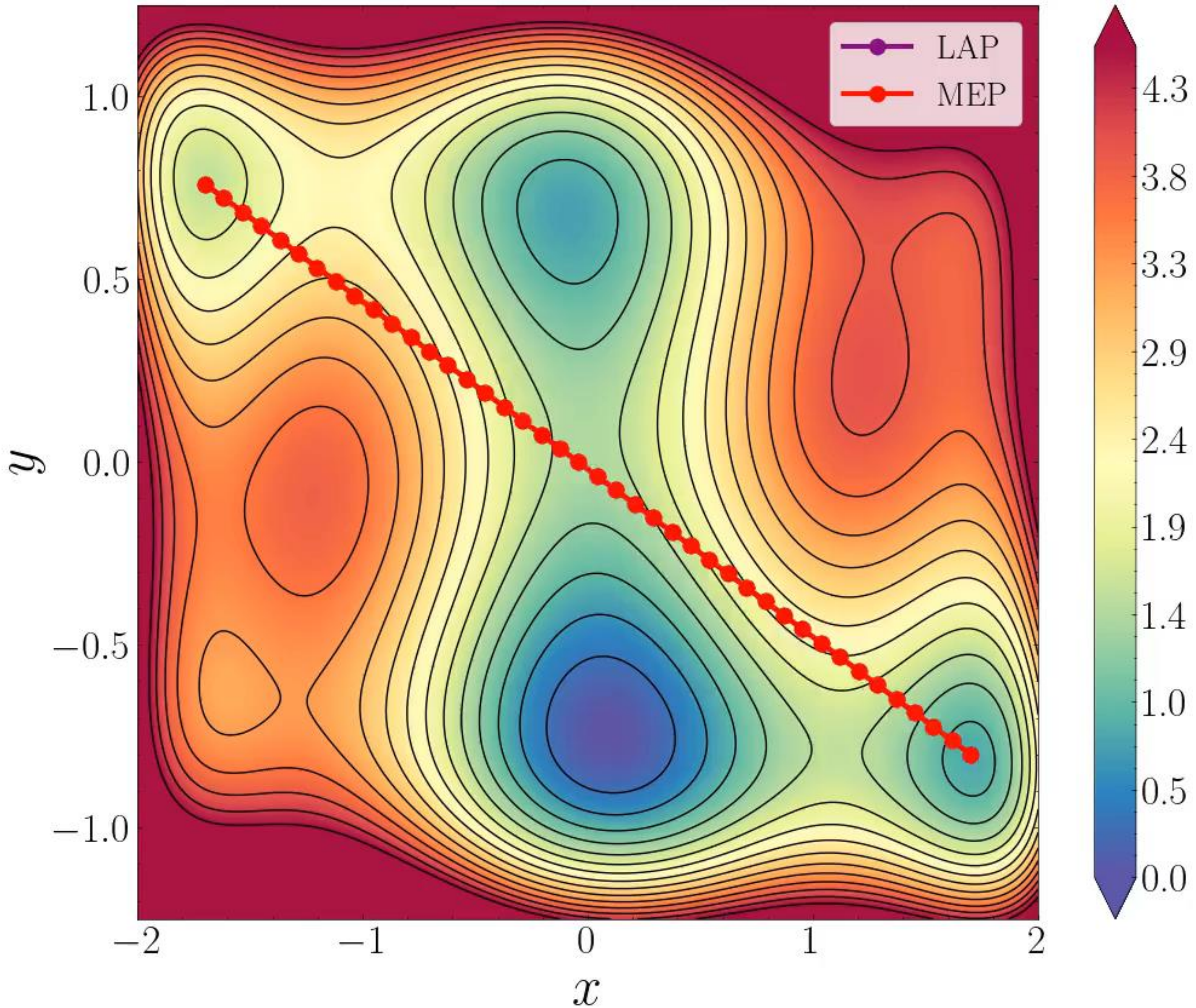
Nudged elastic band approach to nuclear fission pathways

E. Flynn, D. Lay, S. Agbemava, P. Giuliani, K. Godbey, W.N.,
Phys. Rev. C 105, 054302 (2022)

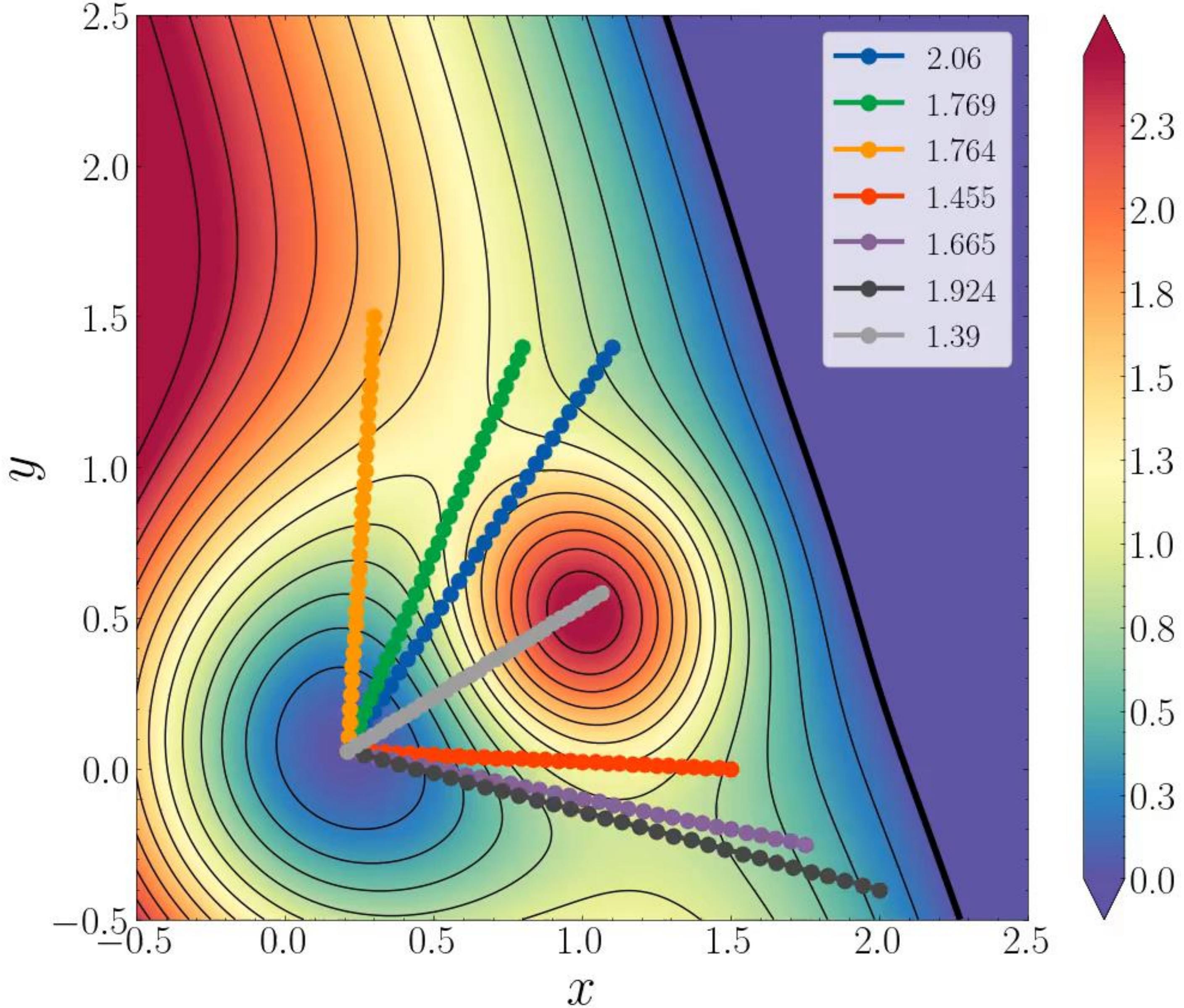


https://pyneb.dev

PyNEB in Action



PyNEB in Action



Fission half-lives

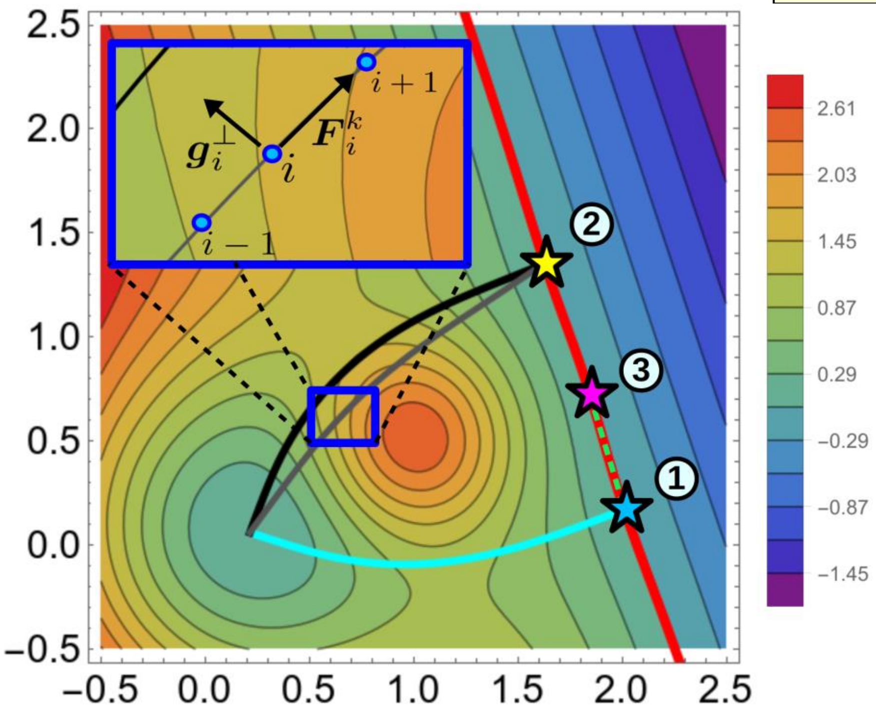
$$T_{1/2} = \ln 2/(nP) \qquad n = 10^{20.38}\mathrm{sec}^{-1} \qquad P = 1/(1+e^{2S})$$

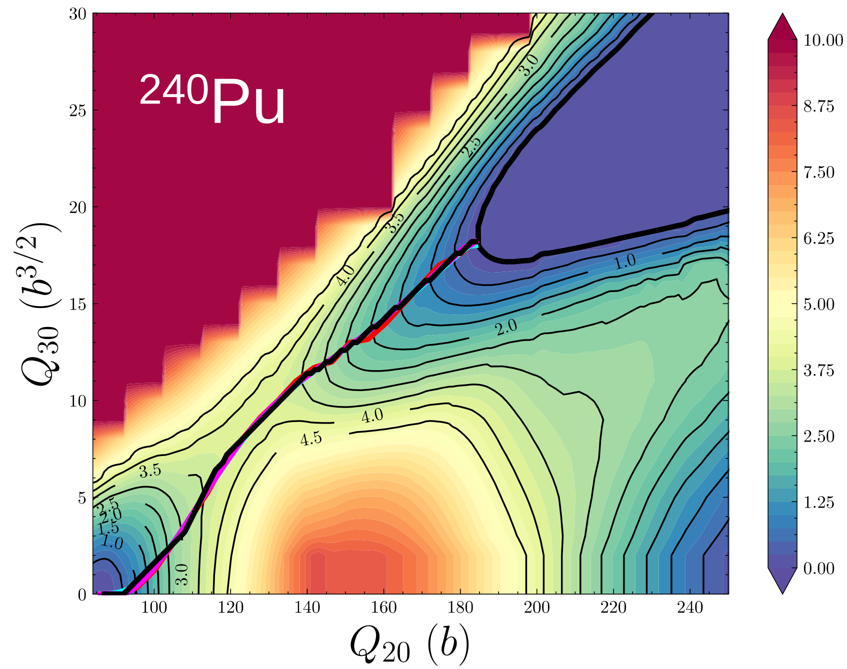
$$S = \int_{(s)} \left\{ 2\left[V(q) - E\right] \sum_{ij} B_{ij}(q) q'_i q'_j \right\}^{1/2} ds$$

collective inertia
(mass parameter)

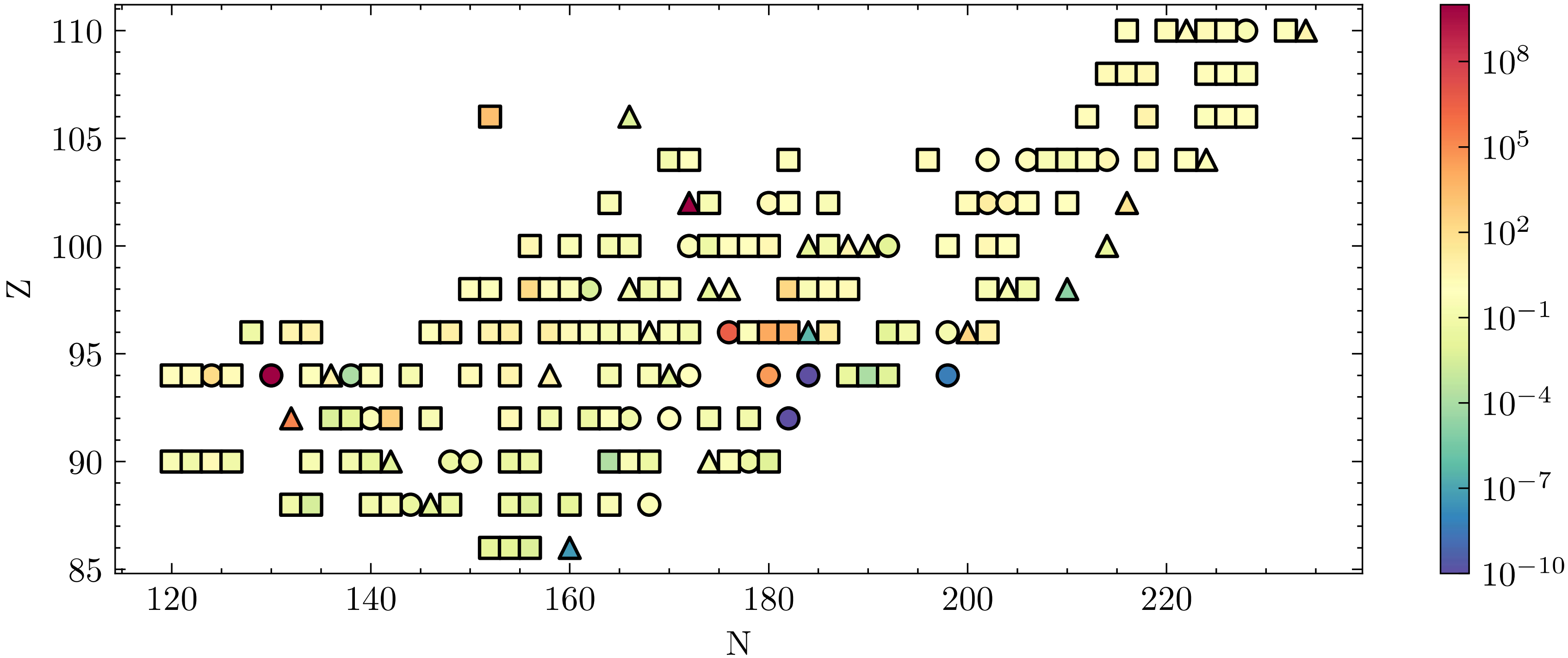
multidimensional space of
collective parameters

see the posters!

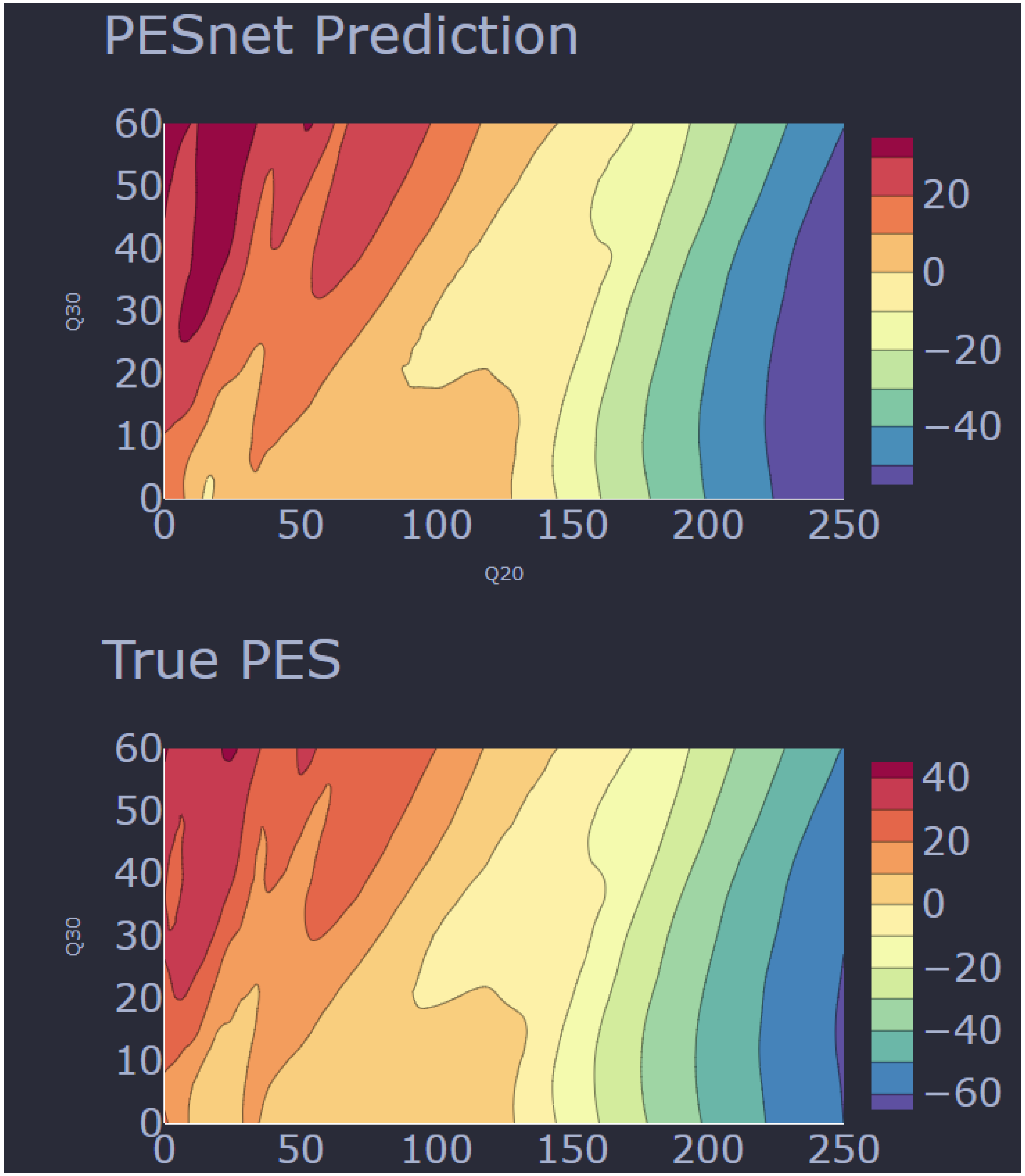




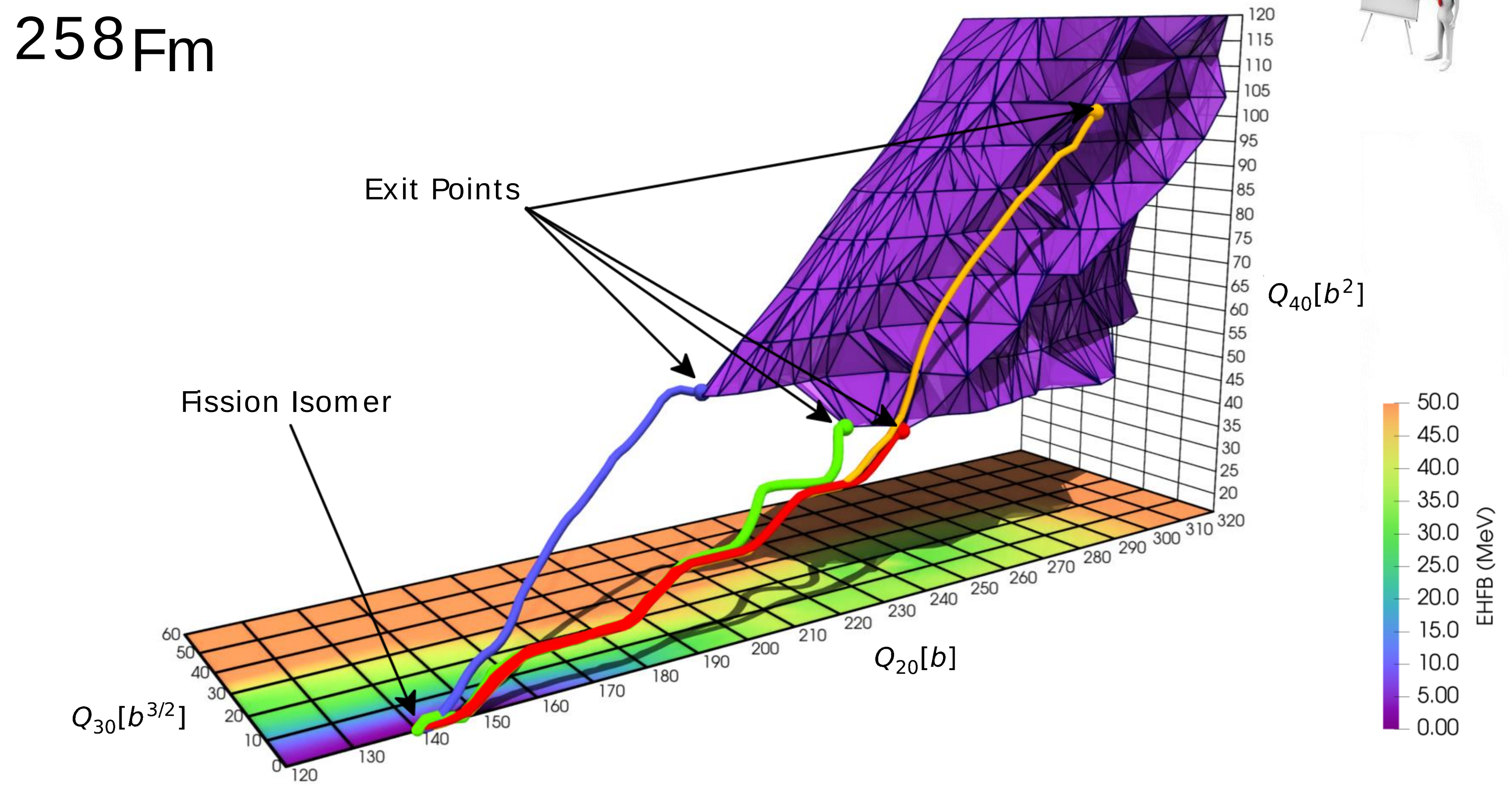
Potential Energy Surface emulation with neural networks and Impact on fission trajectories (poster by Daniel Lay)



The ratio of the lifetime predicted by the NN emulator to the lifetime predicted by the DFT PES. Lifetimes are computed using NEB on the surface. The lifetimes are typically within the same order of magnitude, indicating that the NN is able to accurately reproduce the parts of the PES relevant to (spontaneous) fission. Fission fragment yields (compared via the exit point values) tend to also agree well.


PESnet Prediction
Q30
Q20
True PES
60
50
40
30
20
10
0
0
50
100
150
200
250
20
0
−20
−40
40
−60

Multimodal fission (poster by Eric Flynn)

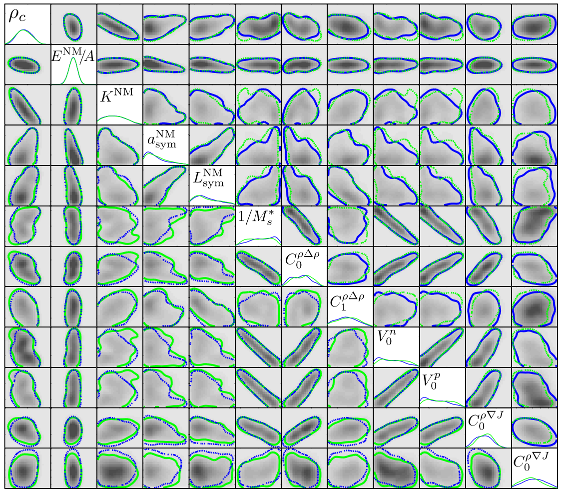


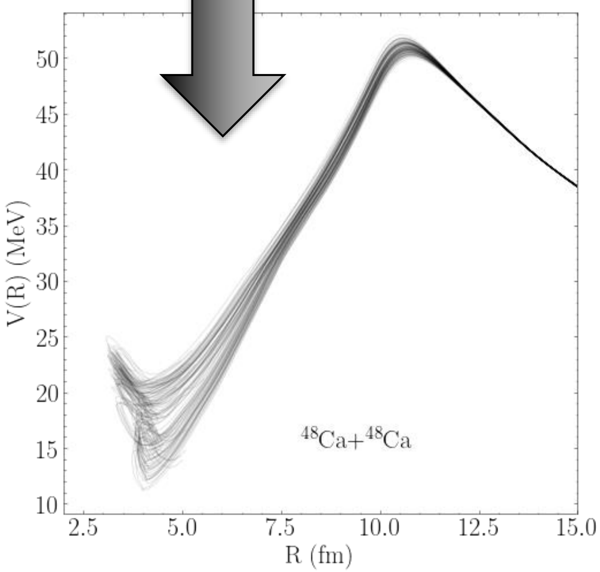
Multi-modal LAPs approaching the outer turning surface for 258-Fm using energy density functionals SkM* in 3 collective coordinates. Pathways are calculated for the constant inertia tensor M_{eff}.

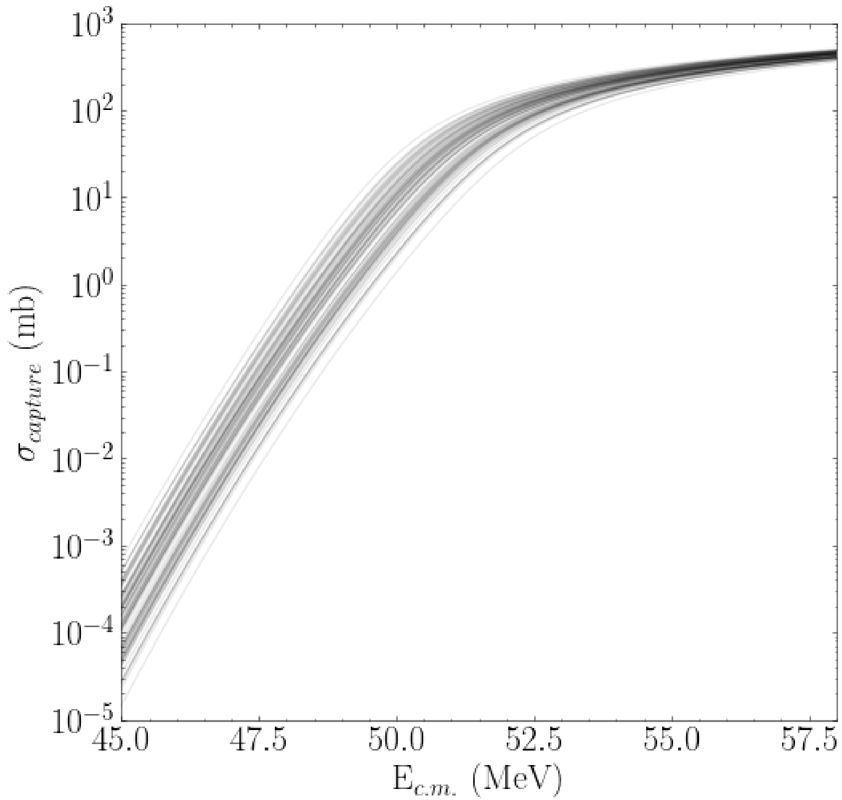
Theoretical uncertainty quantification for heavy-ion fusion

K. Godbey et al. Phys. Rev. C 106, L051602 (Editor's Suggestion)

PRL 114, 122501 (2015)







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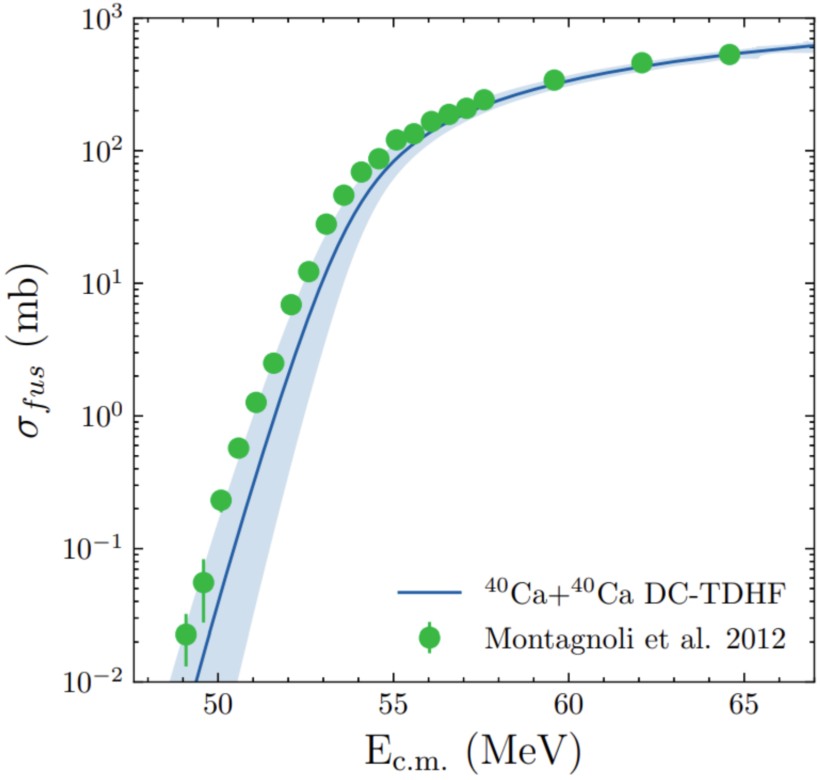
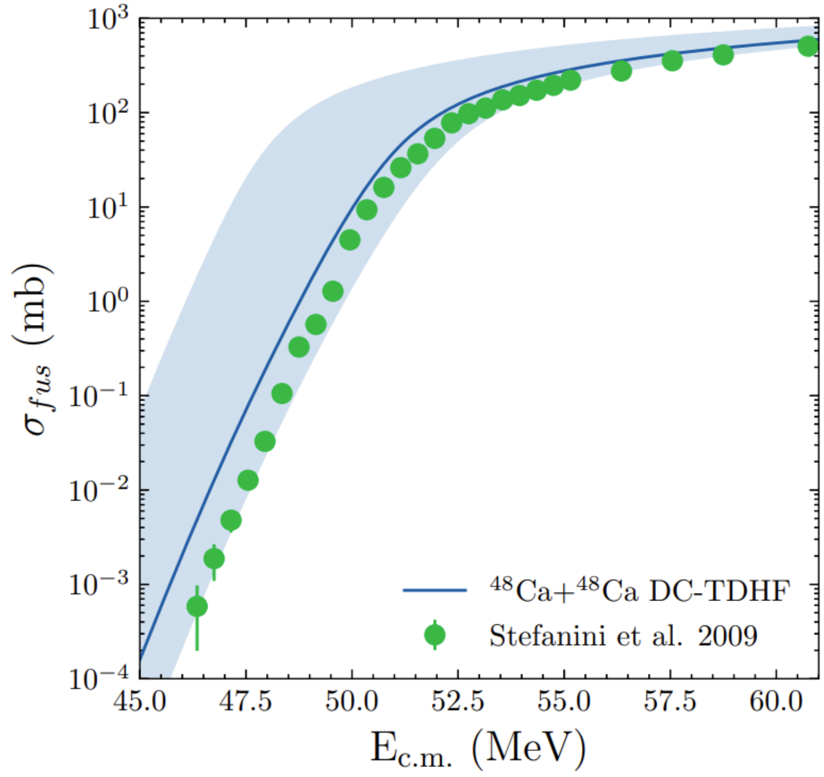
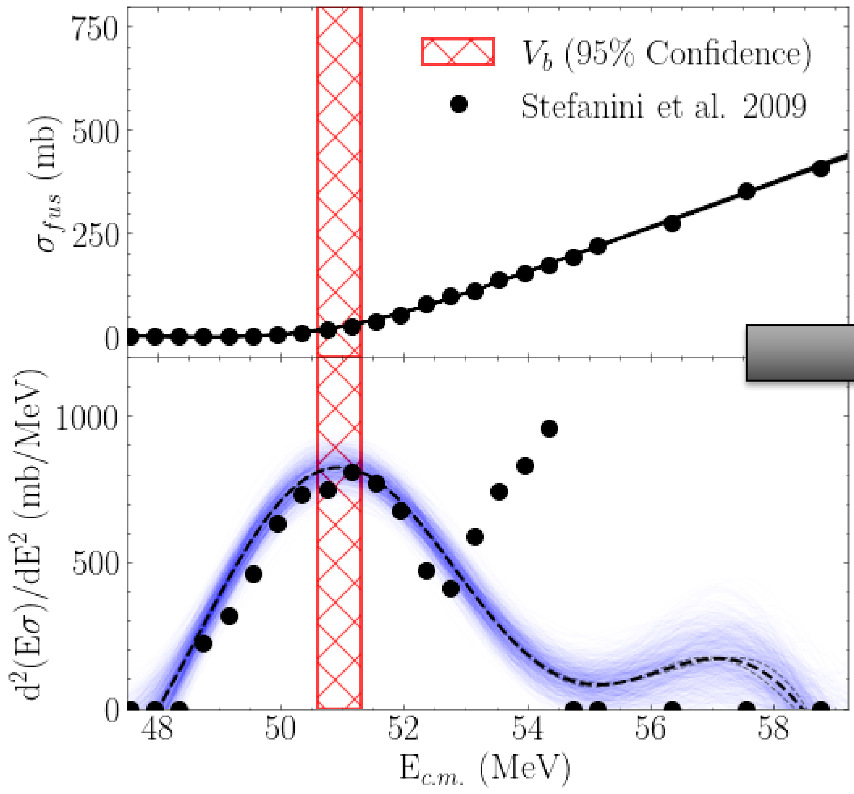
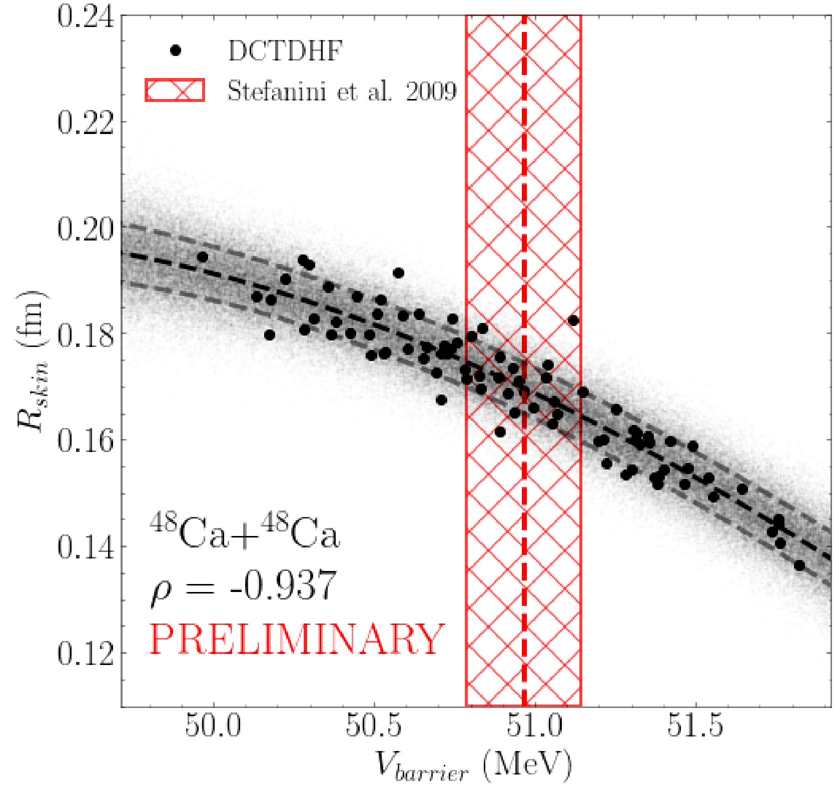




Barrier Correlations





First: Extract fusion barrier height from experimental data to provide prediction + regression uncertainty

Then: Plot model prediction correlations with experimental constraint on barrier height

Prospects

Current Status:

- Sophisticated calculations of spontaneous fission lifetimes: more collective degrees of freedom taken into account (currently 4D); the fission path determined by minimizing the collective action.
- Fission yield distributions explained by a statistical treatment with diffusive dynamics.
- Time dependent description of fission.
- Identification of pre-fragments through nucleon localizations.
- Identification of minimum-action path with nudged elastic band method.
- Ability to carry out reliable extrapolations in mass and isospin through Gaussian processes/neural networks and Bayesian model averaging.

Challenges:

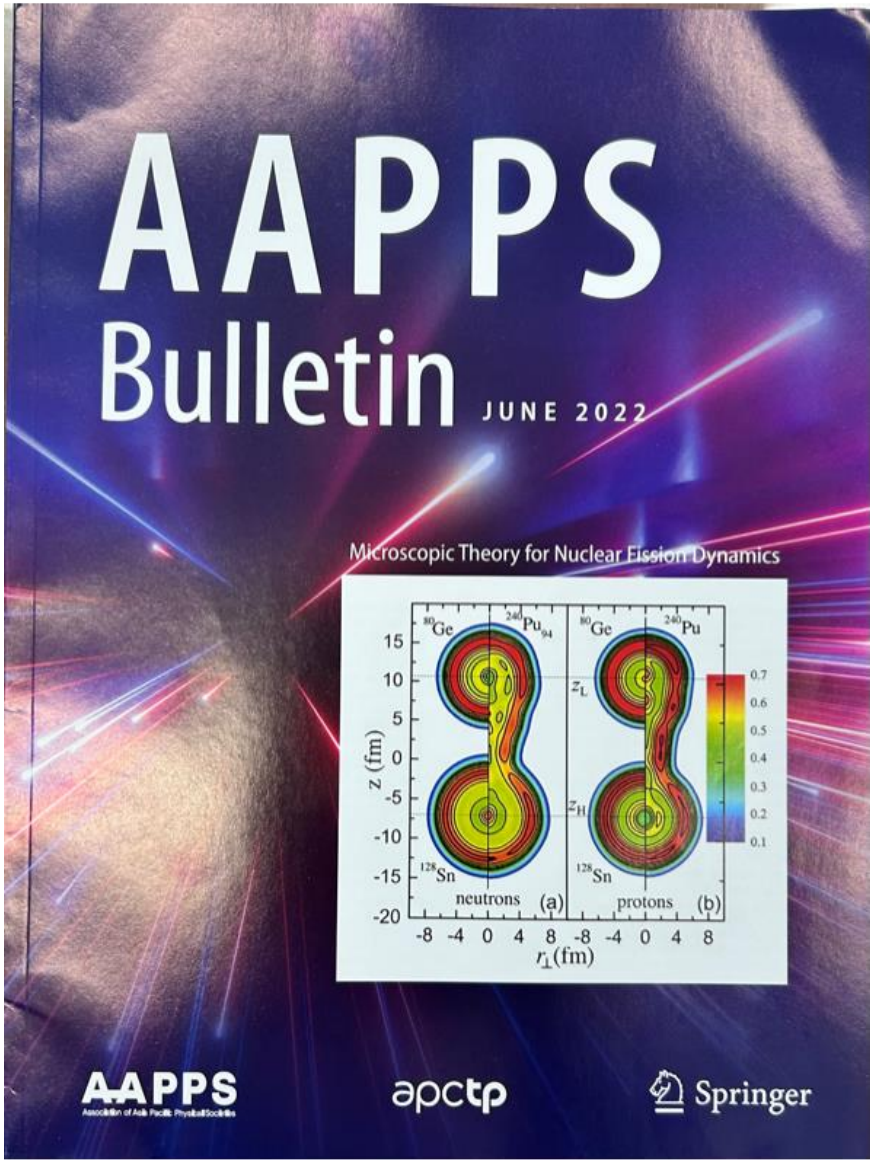
- Consistent description of various experimental fission data, including TKEs
- Global calculations of fission yields for r-process simulations.
- Quantification of uncertainties in fission observables using Bayesian Machine Learning techniques.

SUMMARY

- Deliverables since the last Symposium
  - 4 publications
  - 1 publication submitted
  - 7 presentations
  - 2 postdocs
  - 2 students

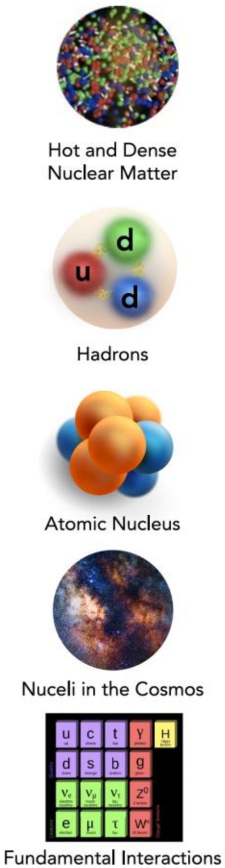
- Quantification of margins and uncertainties is important
- Fission and heavy-ion fusion are perfect problems for the extreme scale computing. Our project is well aligned with NUCLEI SciDAC-5 ASCR project and BAND NSF Framework.

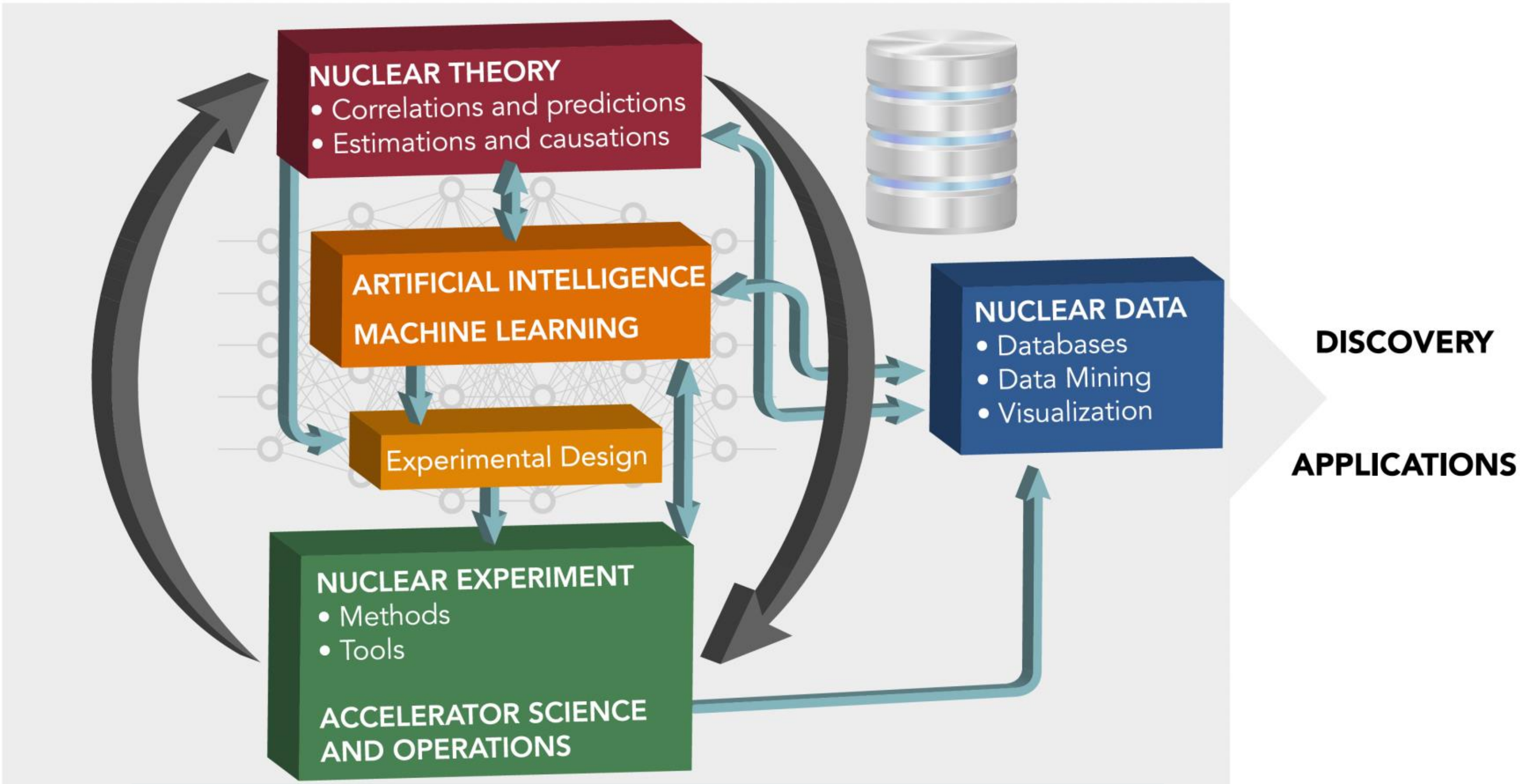
BACKUP



Microscopic theory for nuclear fission dynamics, J. Sadhukhan, 2022

Speeding-up the cycle of the scientific method with machine learning





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