LLNL FPY Modeling and Evaluation

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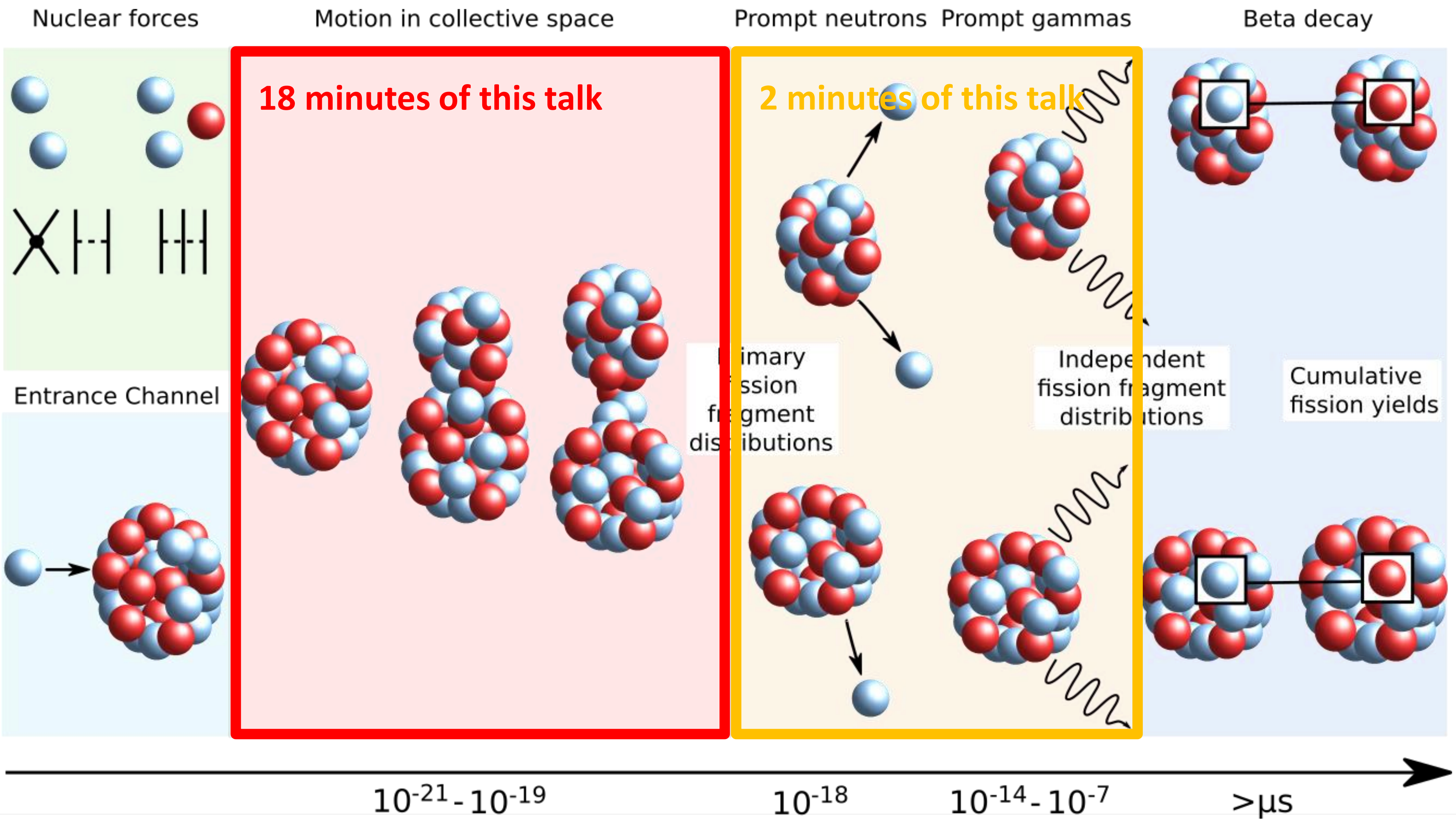
Outline

- Fission modeling: Predictions of fission fragments initial conditions
  - Mass distribution of fission fragments: Plutonium isotopes (2D simulations)
  - Number of particles in fragments: Collective fluctuations on particle number
  - (Spin distributions: Combined AMP+PNP)
  - Total kinetic energy: Projection + direct Coulomb
- New computational capabilities
  - FPY: FELIX-3D (ASC/PEM L2 milestone)
  - Real-time Fission events: TDHFB solver
  - Evaluation: FETA framework

Fission Science

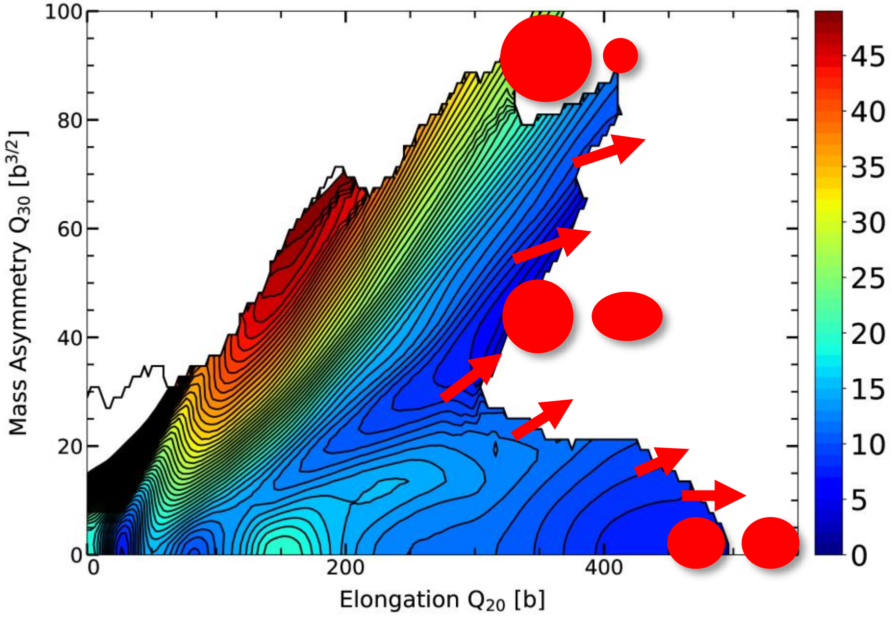
Two major research areas for fission theory: cross sections (~ probabilities that fission happens) and fission products (includes neutrons, gammas, fragments, etc.)

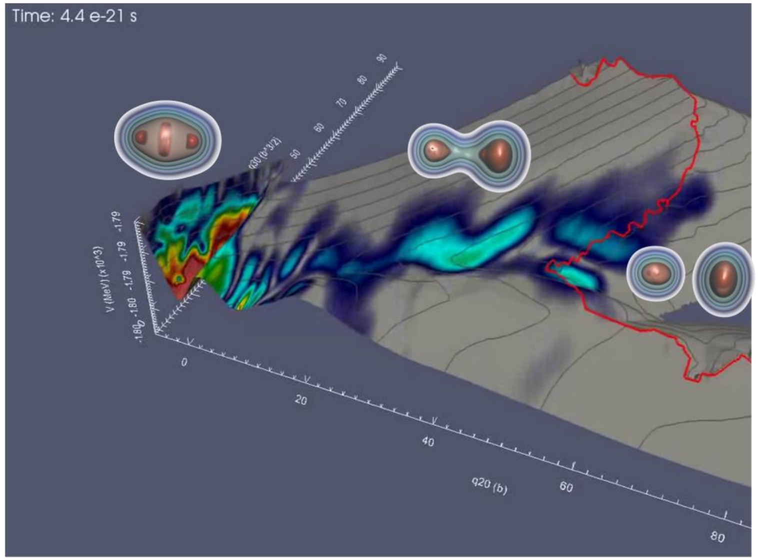


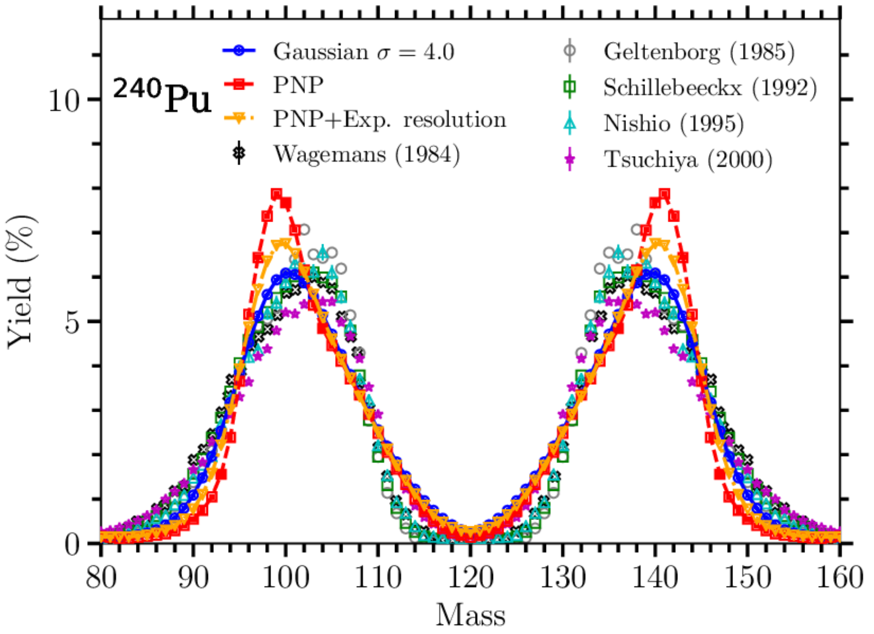
Fission Theory Pipeline

Physics-based fission models involve calculations of static nuclear properties (=nuclear structure) and time-dependent simulations (=large-amplitude collective motion)

Potential energy surface → Time-dependent dynamics → Actual observables







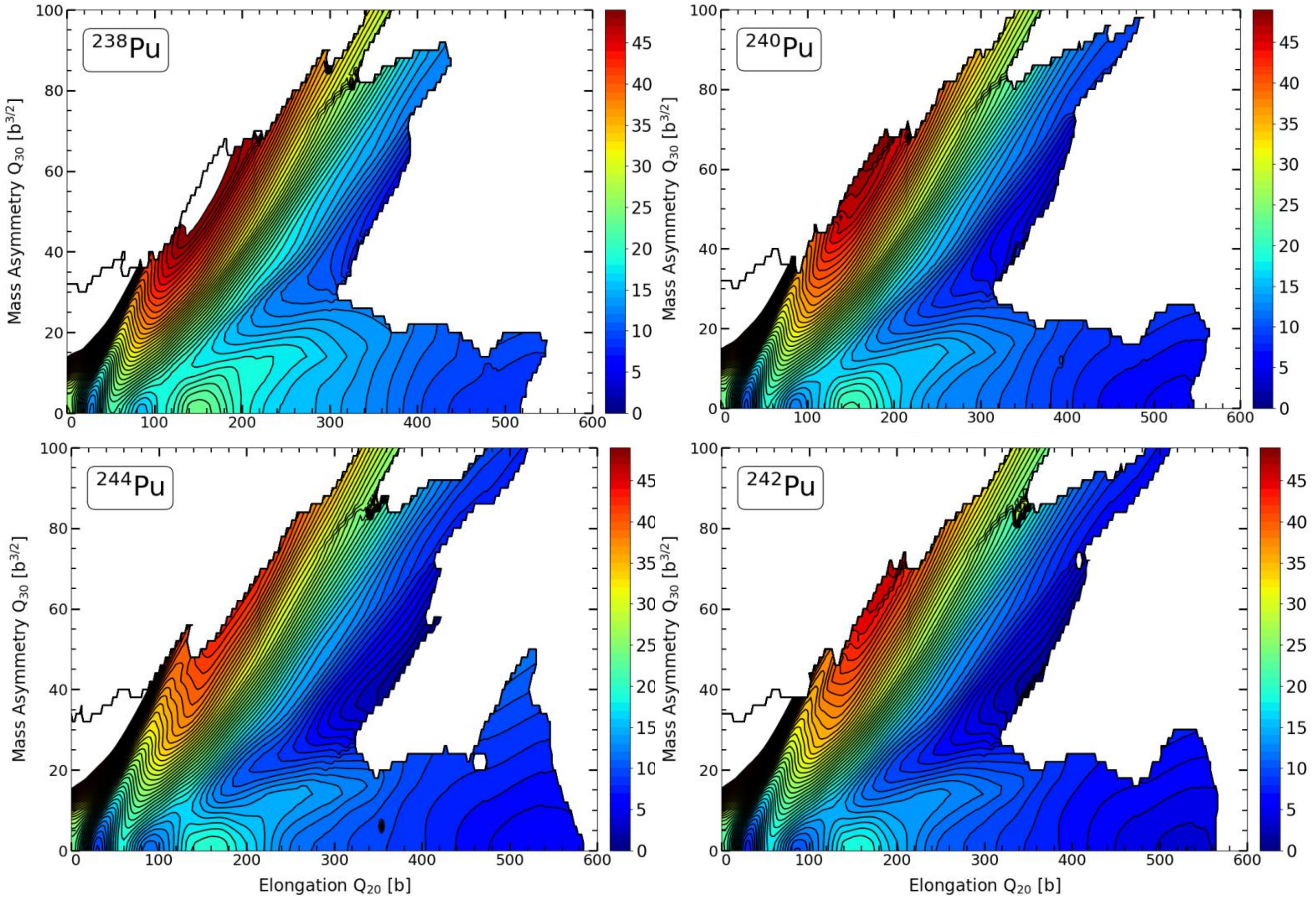
- Particle number (PNP)
- Spin distribution (AMP)
- Excitation energy (PNP, TDHFB)

- Fission fragment distributions (TDGCM)
- Real-time fission events (TDHFB)

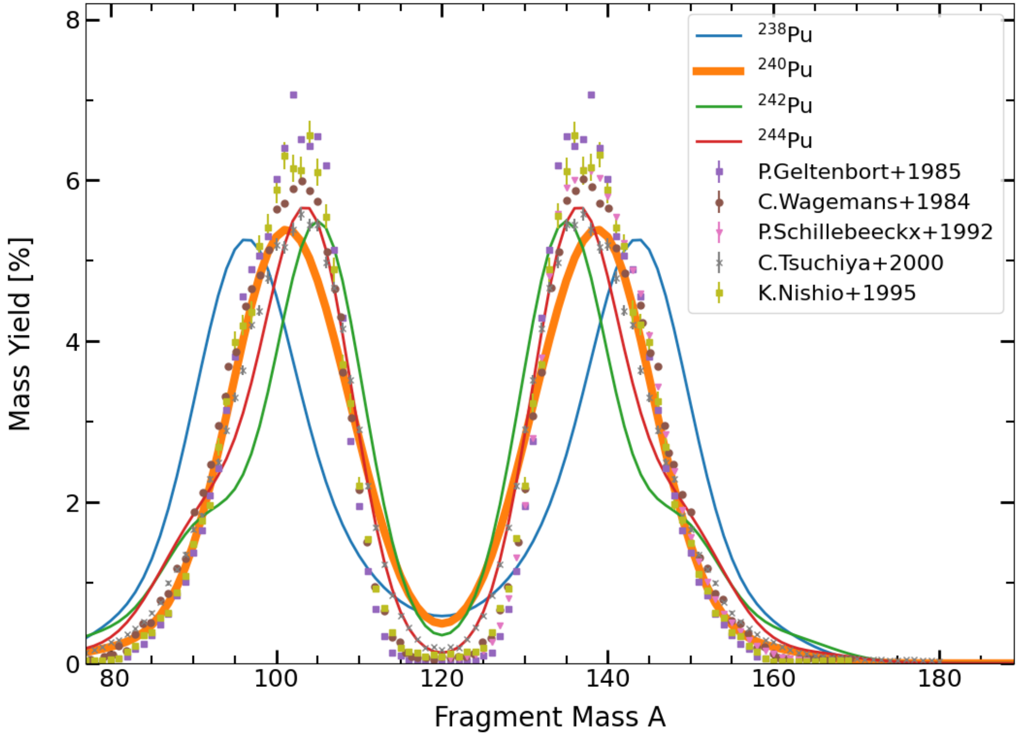
- Fission evaluation (FETA)

Modeling: Distribution of fission fragments

We computed the systematics of initial fission fragment distributions at $E_n \approx 1$ MeV for plutonium isotopes with our PESO framework

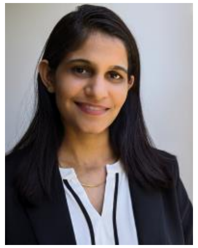


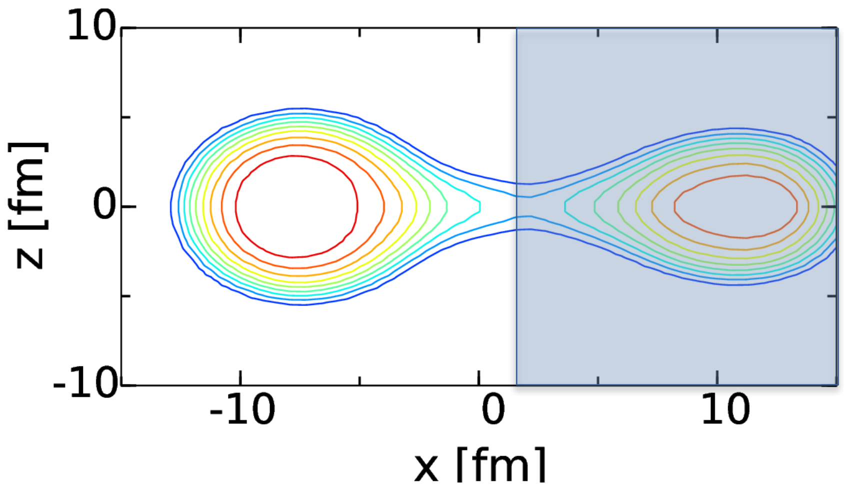
Initial mass distribution of fission fragments in even-even Plutonium isotopes (SkM*)

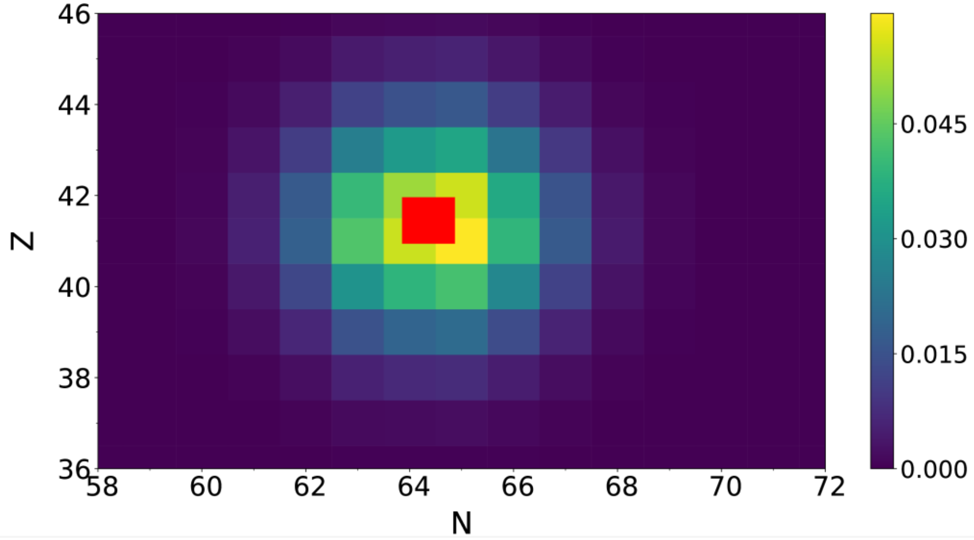


Modeling: Number of particles

Particle number projection techniques can be extended to estimate a distribution of particle number in fission fragments for each scission configuration







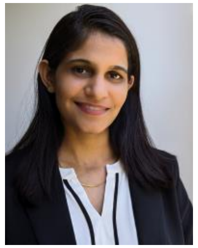
- Average number of particles in fission fragments obtained by integrating the density
- Better estimates with particle number projection:
  - Integer values…
  - Distribution of particle numbers at each scission point
- Collective dynamics in deformation space implies:

$$\langle \quad | \hat{P}_N \hat{P}_Z \hat{P}_{N_f} \hat{P}_{Z_f} | \quad \rangle \neq 0$$

What is the impact of collective correlations on particle number in fission fragments?

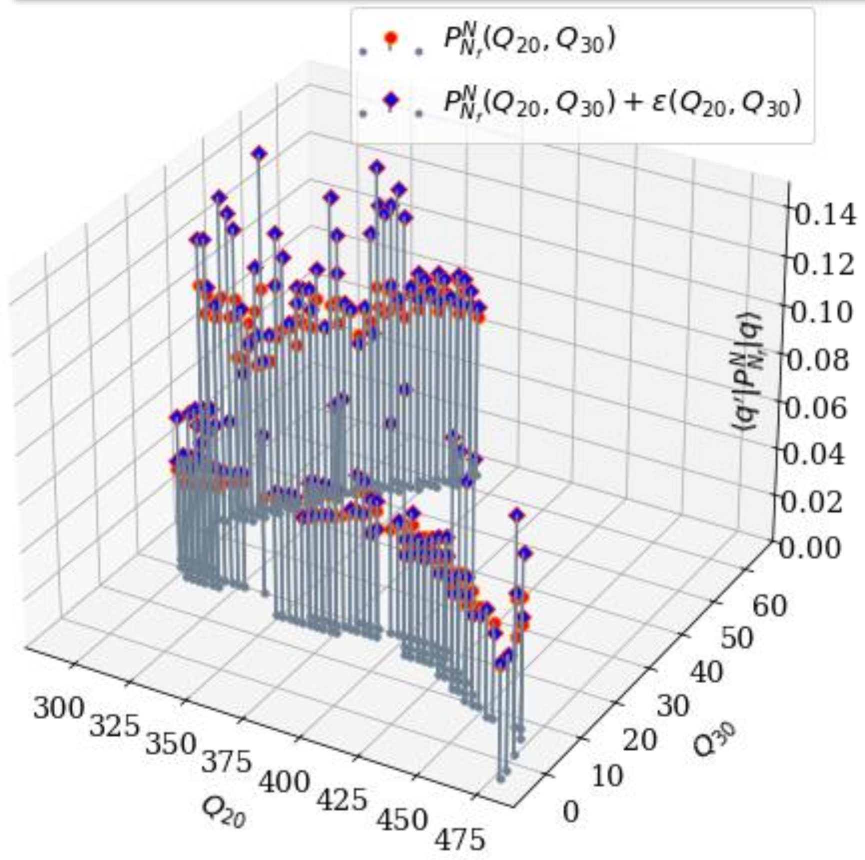
Modeling: Number of particles

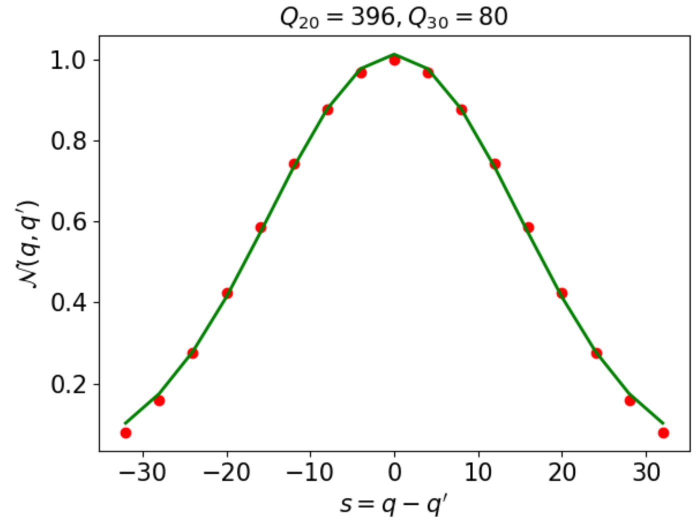
We are extending the generator coordinate method with Gaussian overlap approximation (GOA) to include quantum corrections in estimates of particle numbers in fission fragments

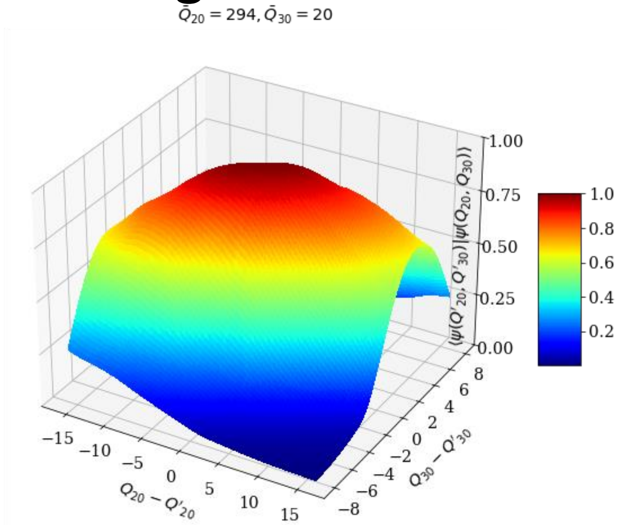


- Extend GCM+GOA to the projection operator on particle numbers in fission fragments
  - Equation of motion for change in particle number from deforma
  - Probability of (Z_f, N_f) modified by quantum correction term
- Validity of GOA determines validity of the calculation
- Technical challenges due to non-orthogonal bases

Probability of having N_f neutrons in scission configurations with average value $\langle N_f \rangle$

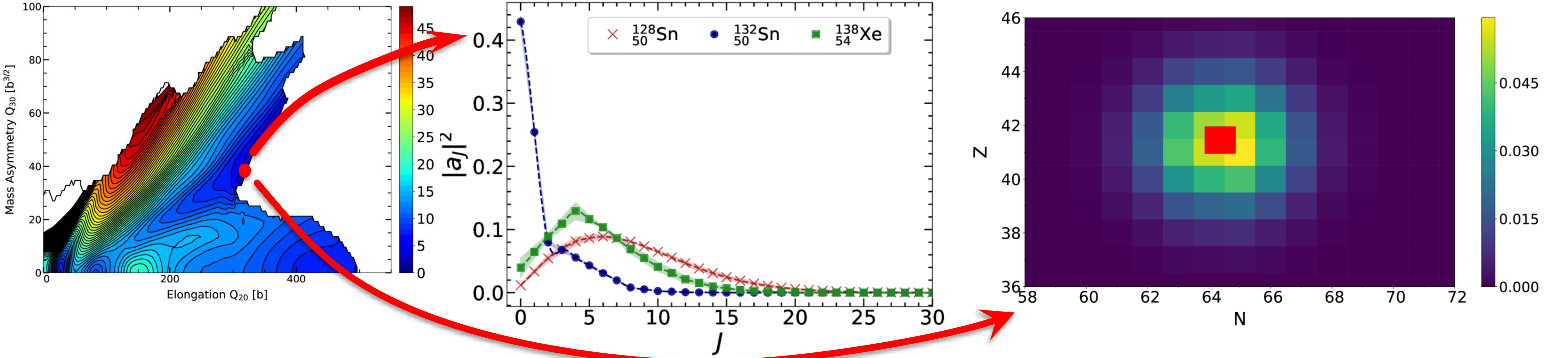






Modeling: Spin distributions of fission fragments

We combine angular momentum projection, particle number projection and large-amplitude collective dynamics to predict the spin distributions of fission fragments



- Angular momentum projection (AMP) gives spin distribution of in scission configuration ***q***
- Particle number projection gives particle content at each scission configuration q
- TDGCM gives probability of populating scission configuration q
- All of the above combined will give spin distribution of fission fragment with Z_f protons and N_f neutrons

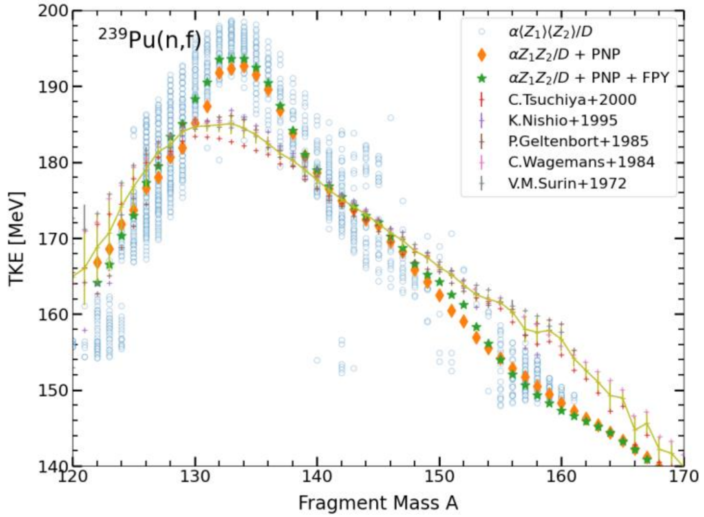
Modeling: Predicting TKE

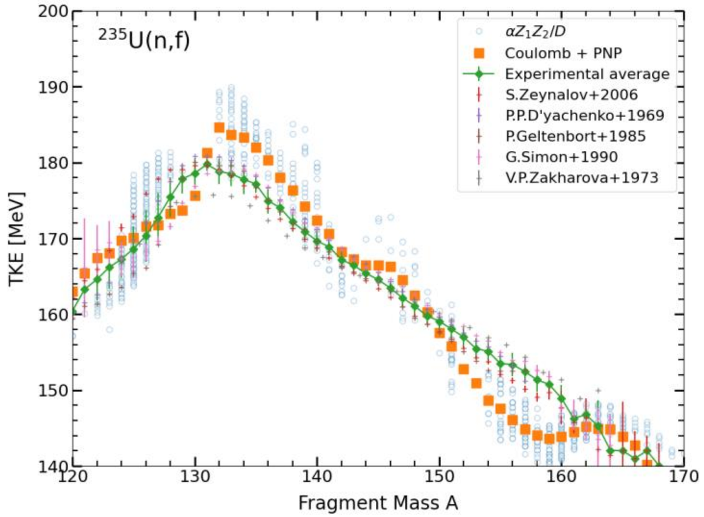
We are developing a model to predict TKE in fission by leveraging particle number projection techniques and estimates of the Coulomb repulsion between fragments

- TKE are used to determine total excitation energy (TXE) of fission reaction from energy conservation
  - Direct measurements of E* of each fragment not possible in < 10^{-15}s…
  - Calculations of E* among the most challenging
- TKE ≈ (Direct) classical Coulomb interaction energy between fragments ∝ $\alpha Z_L Z_H / D$

$$\mathrm{TKE}(A_f) \propto \sum_{\boldsymbol{q}} \mathbb{P}(\boldsymbol{q}) \times \sum_{Z_f+N_f=A_f} p(Z_f, N_f, \boldsymbol{q})\,\alpha \frac{Z_f(\boldsymbol{q})(Z - Z_f(\boldsymbol{q}))}{D(\boldsymbol{q})}$$

Quality of TKE very dependent on quality of potential energy surface and scission configurations

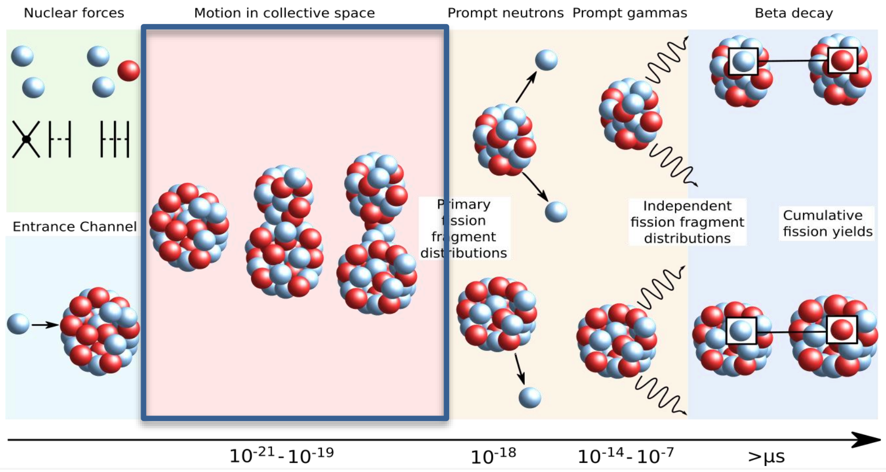




Capabilities: FELIX3D

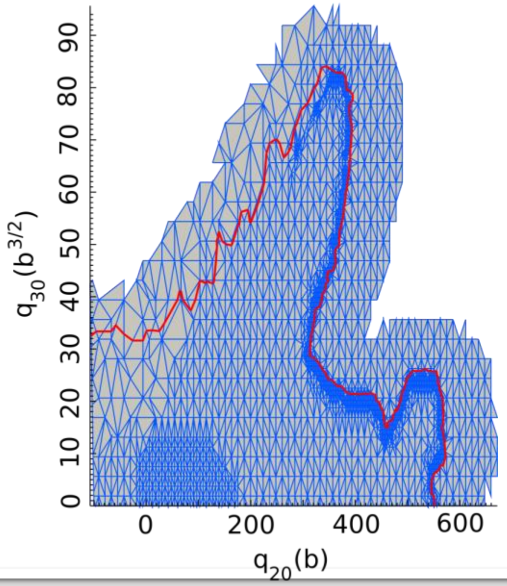
We have extended the capability of our TDGCM code to simulate fission dynamics in 3-dimensional deformation spaces

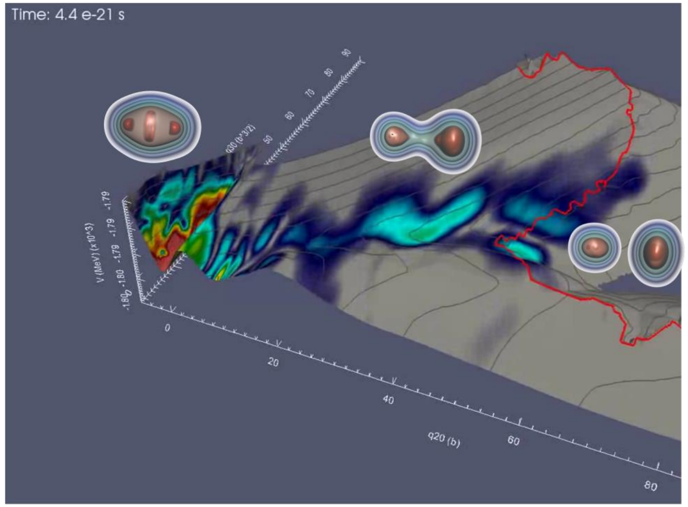
- DEFTNESS: Static properties of nuclei
  - HFBTHO: axial symmetry
  - HFODD: no symmetry
- **FELIX: Large-amplitude collective dynamics**
- TDHFB: Real-time nuclear dynamics
- FETA: Evaluation of fission data based on statistical reaction theory



- FELIX gives the probability for the fissionning nucleus to have a given shape ***q*** at time t
- Solution of a Schrödinger-like equation

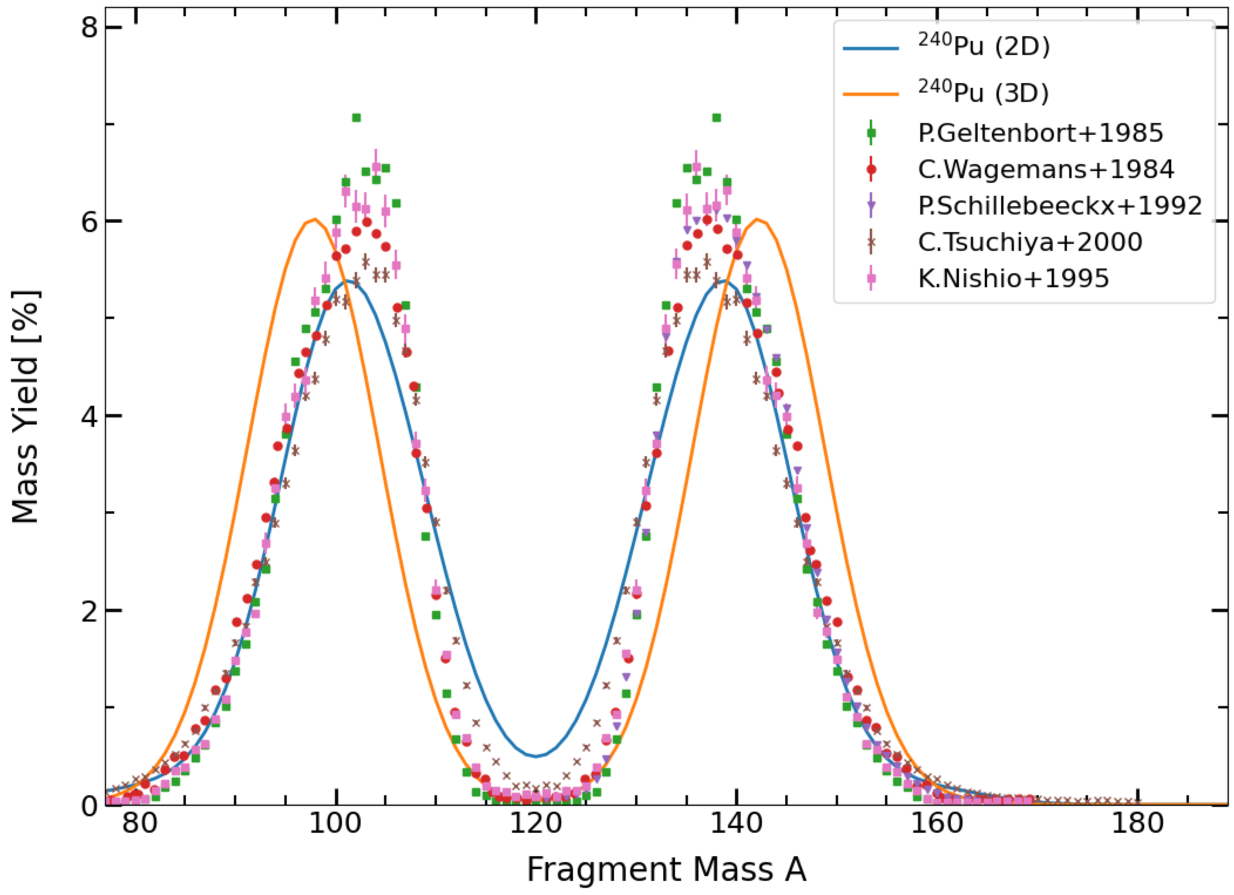
$$i\hbar \frac{\partial g(\boldsymbol{q},t)}{\partial t} = \left[-\frac{\hbar^2}{2} \gamma^{-\frac{1}{2}}(\boldsymbol{q}) \nabla \cdot \gamma^{\frac{1}{2}}(\boldsymbol{q}) B(\boldsymbol{q}) \nabla + V(\boldsymbol{q}) - iA(\boldsymbol{q}) \right] g(\boldsymbol{q},t)$$

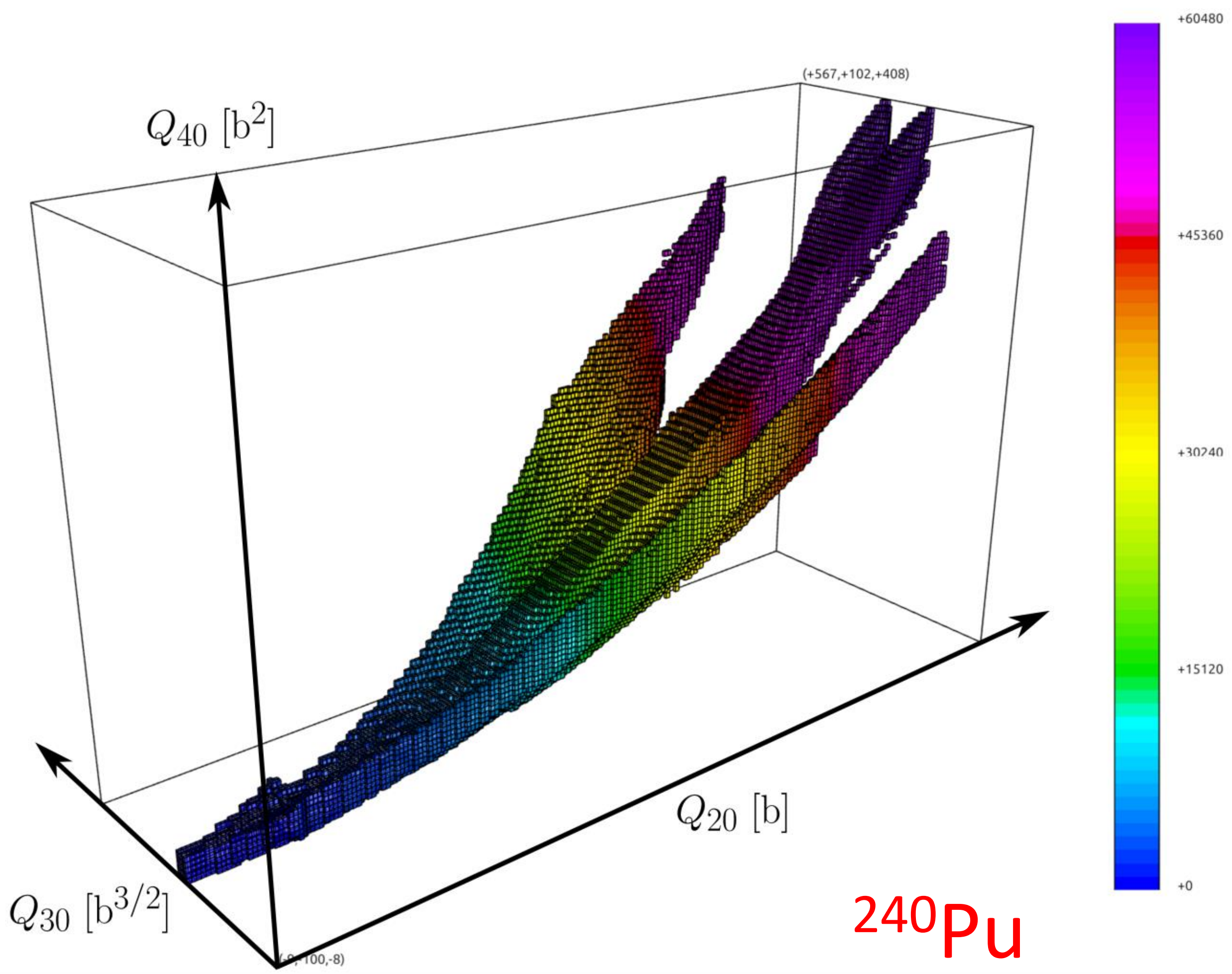




Capabilities: FELIX3D

Very preliminary results with a sub-par 3D potential energy surface give encouraging results: symmetric fission is (too much...) hindered compared to simulations in 2D collective spaces.

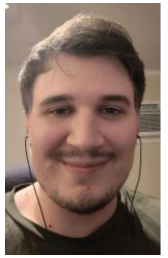




^{240}Pu

Capabilities: TDHFB Solver

We have developed a new code to solve the time-dependent Hartree-Fock-Bogoliubov (TDHFB) equation to simulate real-time fission events and extract the excitation energy of fission fragments



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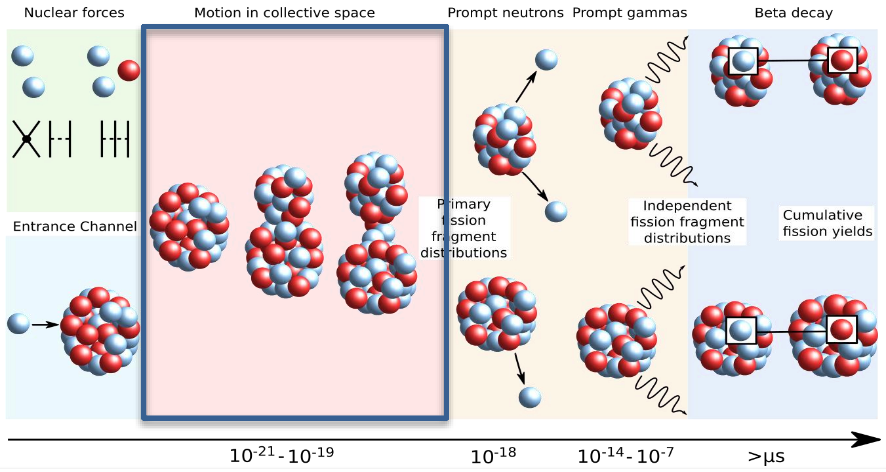
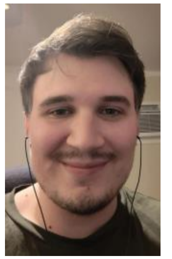
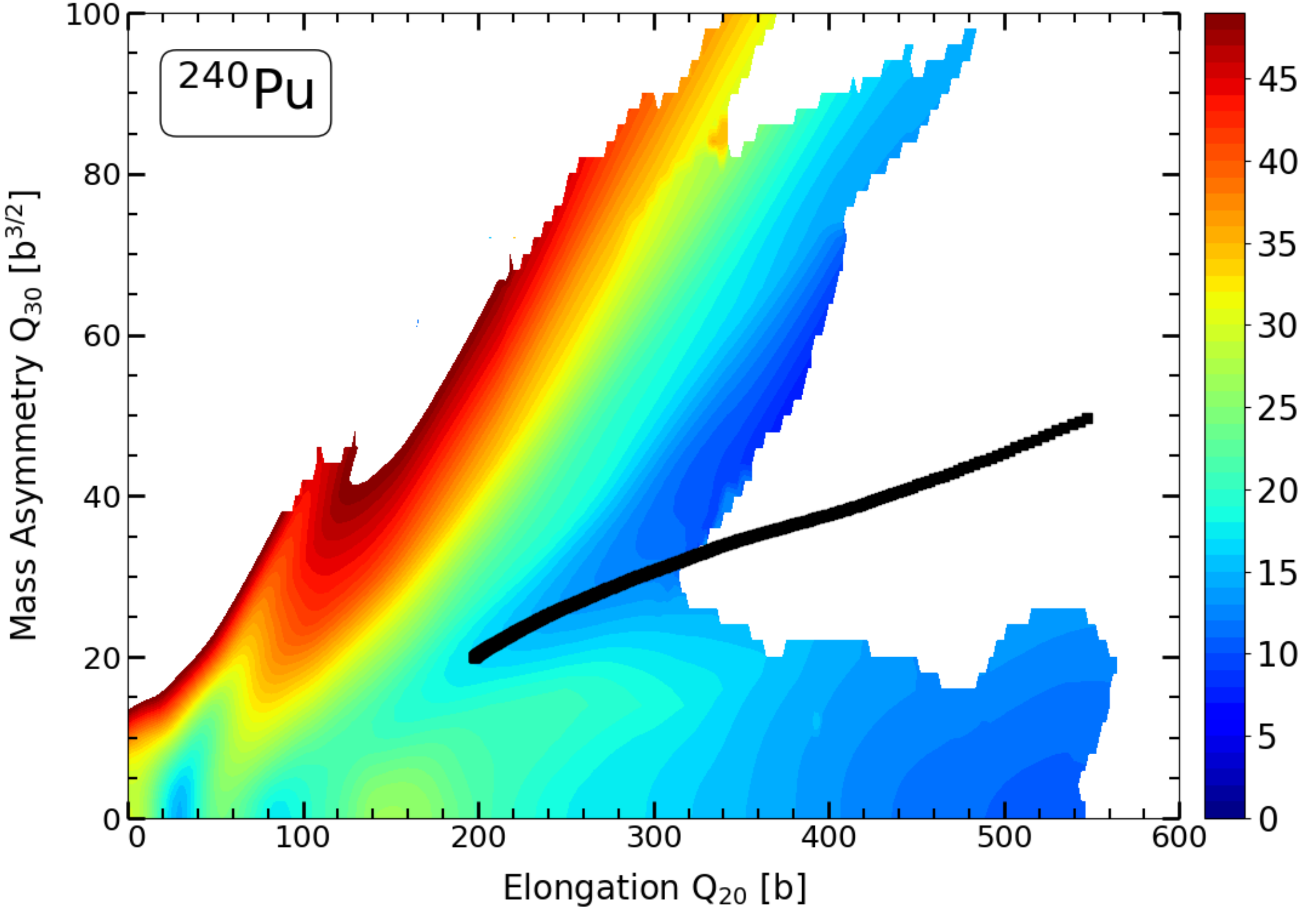


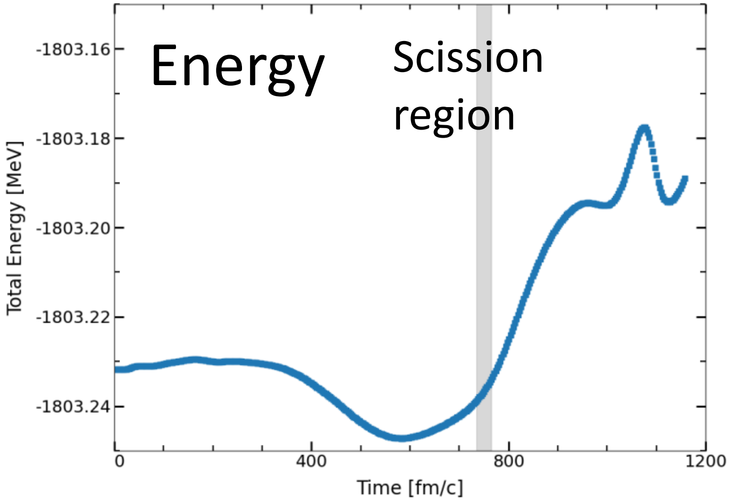
- Modular, template-based C++ code
  - Expansion of time-dependent HFB spinors in one-center harmonic oscillator basis
  - Fully interfaced with HFBTHO and with a newly-developed Skyrme HFB solver
  - OpenMP threading and placeholder for GPU accelerations through placeholders for performance portability layers (RAJA, KOKKOS, etc.)
- Version 1: proof of principle
  - ✓ Verify system can actually fission…
  - ✓ Quantify conservation of energy and particle number
  - ✓ Quantify drift in center of mass (0 if infinite basis)

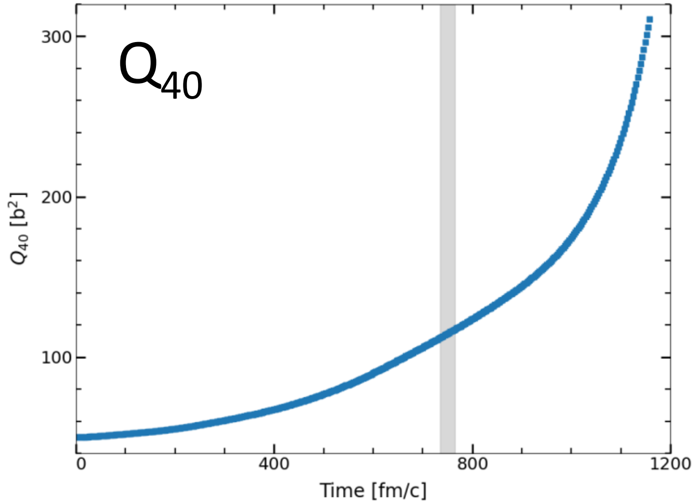
Capabilities: TDHFB Solver

We find that a heavy actinide nucleus such as ^{240}Pu can fission even when TDHFB implemented in the HO basis and that conservation laws are obeyed with excellent precision









Capabilities: Fission Evaluation Tools and Analytics (FETA)

We are developing a suite of tools to compute independent (and cumulative) fission yields as well as the prompt (and delayed) fission spectrum

- DEFTNESS: Static properties of nuclei
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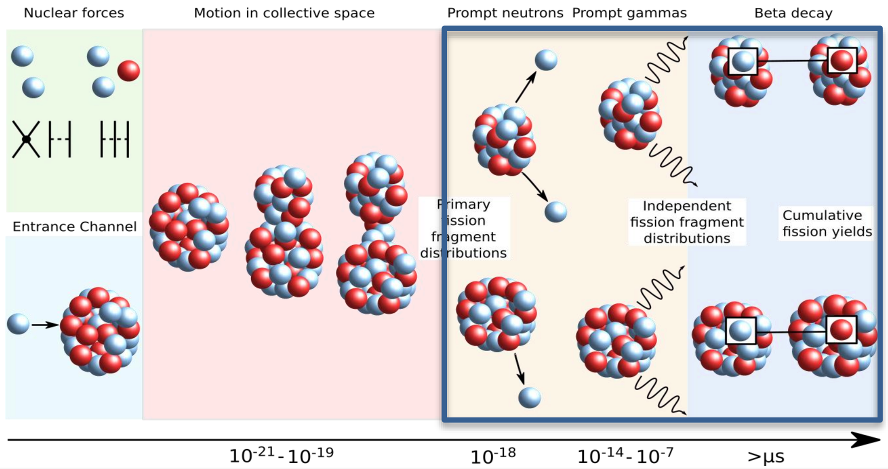


- Design principle: every physics input/model should be easily replaced by the user
- Modular Python-based framework
  - Characteristics of fission fragments at scission externally provided by user through tables, experimental data or preset inputs
  - Fission fragments decayed with YAHFC
  - Fission observables reconstructed from YAHFC outputs
- Version 1: observables
  - Independent fission yields
  - Prompt neutron and gamma spectrum

Capabilities: Fission Evaluation Tools and Analytics (FETA)

FETA is easy to use – it relies on a YAML configuration file and runs all fragment decay in parallel using MPI

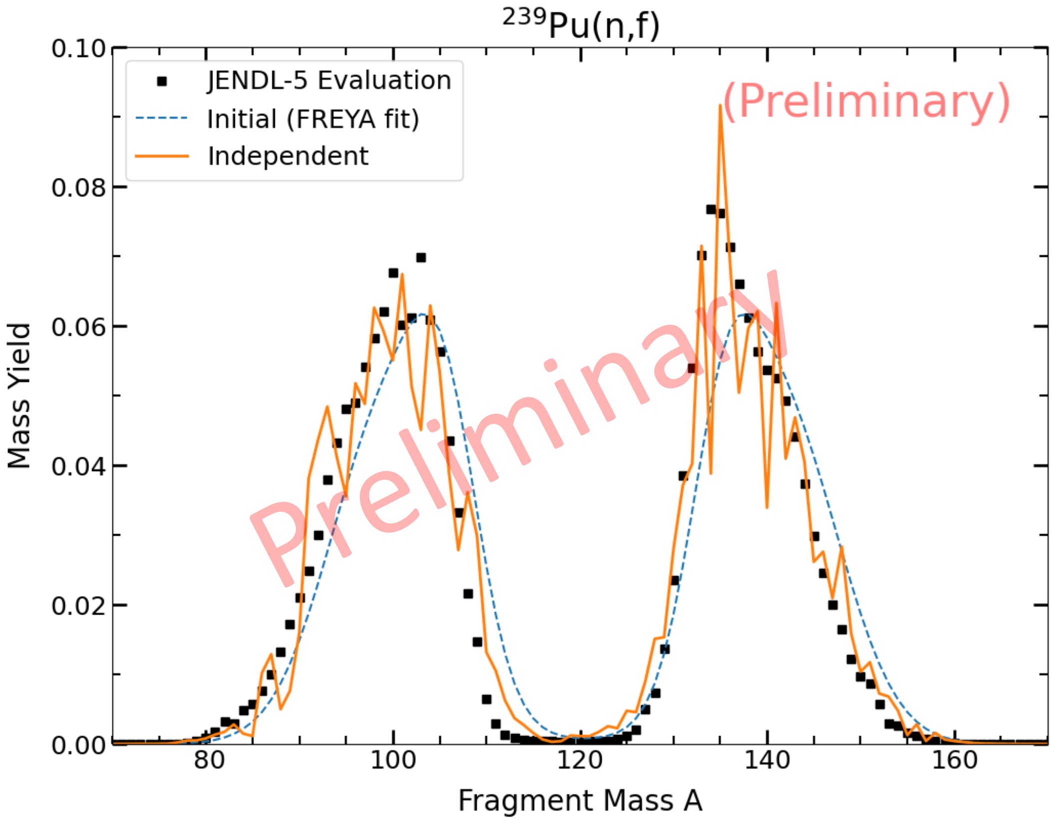
```
from fpy import config,yields,task_manager,io

# setup MPI environment
do_mpi = True
mpi_setup = task_manager.MPISetup(do_mpi)

# rank 0 reads configuration (only relevant if MPI is active)
conf_0 = None
if mpi_setup.rank == 0:
        conf_0 = config.Configuration('/home/toto/git/fpy/tests/fpy.yaml')
if do_mpi:
        conf = mpi_setup.comm.bcast(conf_0, root=0)
else:
        conf = conf_0

# define instance for independent yields and decay fission fragments
new_yields = yields.IndependentYields(conf, mpi_setup)
dico_decay = new_yields.run_decays()

# rank 0 computes yields and records the results
if mpi_setup.rank == 0:
        mat        = new_yields.set_transitions(dico_decay)
        all_Y_ind = new_yields.get_yields()
        output = io.IO(conf.conf_data['Files']['Yields']['Write'])
        output.write(dico_decay, new_yields)
```



Conclusions

LLNL effort is focused on developing and applying microscopic models to describe the initial conditions of fission fragments and provide guidance for evaluations

- We have focused our modeling efforts on
  - Efficiently generating FPY at scission with PESO framework and FELIX (2D)
  - Improving estimates of particle number in FFs with quantum corrections
  - Developing a semi-phenomenological model for TKE
- We have extended our FELIX capability by allowing simulations of FPY in 3D collective spaces
- We have developed two new capabilities
  - TDHFB solver in a basis to estimate excitation energy of fission fragments
  - FETA framework based on YAHFC (for now) to perform in-house FPY evaluations
- On-going work:
  - Finalizing study of quantum corrections on particle numbers in FFs
  - Predict spin distributions of fission fragments by combining AMP+PNP+FPY
  - The fun stuff: Physics studies with new FELIX-3D and TDHFB tools

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