Prediction of the Initial Conditions of Fission Fragments from Microscopic Theory

Possible Consequences for Evaluations

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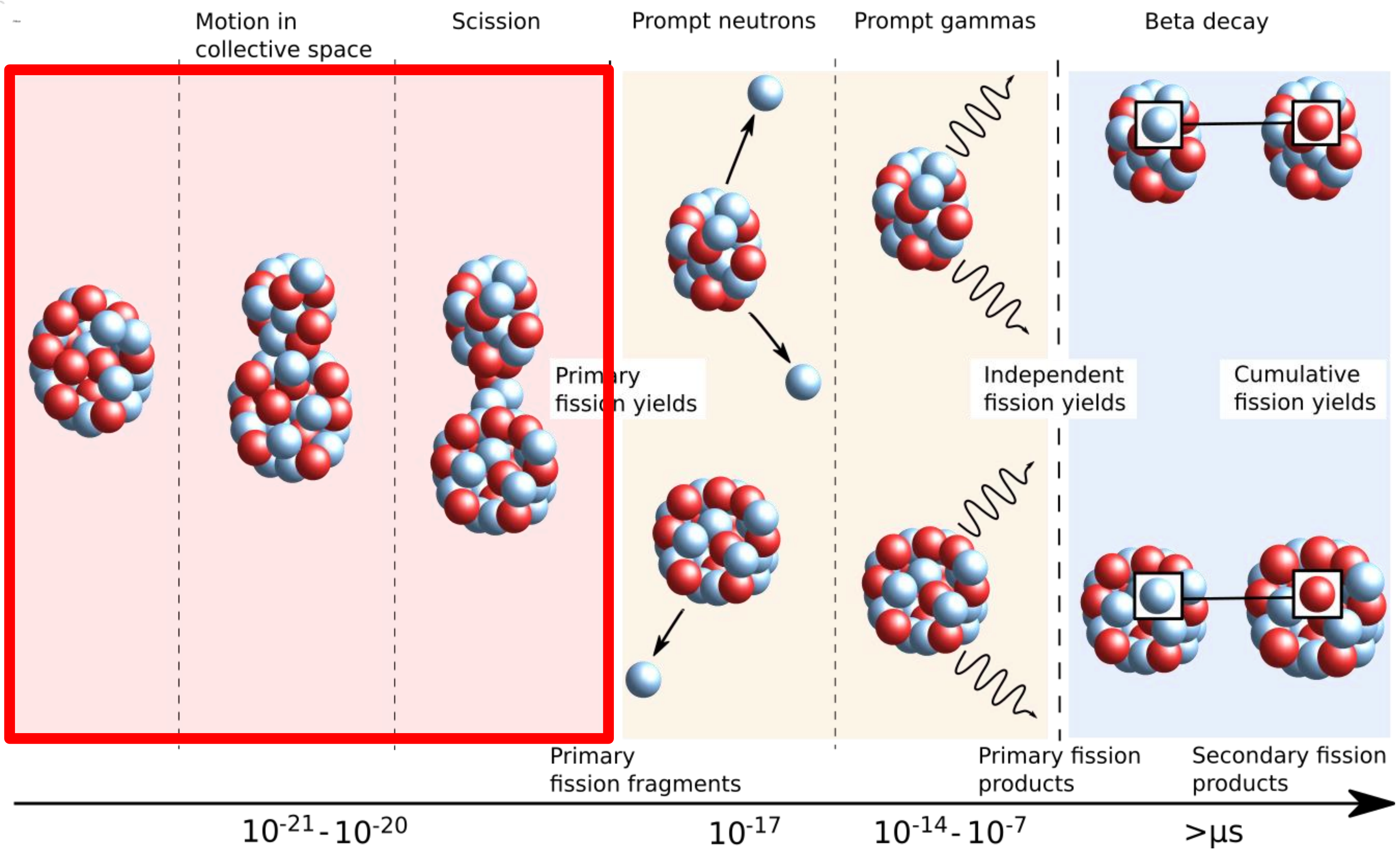
From Scission to Cumulative Fission Product Yields

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

- Cumulative fission product yields are the result of a complex chain of events
- Knowledge of initial conditions at scission is key to simulate decays
- No experimental measurements possible at scission: rely on theoretical models



Theoretical Framework

LLNL uses a fundamental approach to fission theory based on nuclear density functional theory to provide initial conditions for fission fragments – and an event generator (FREYA) to validate them

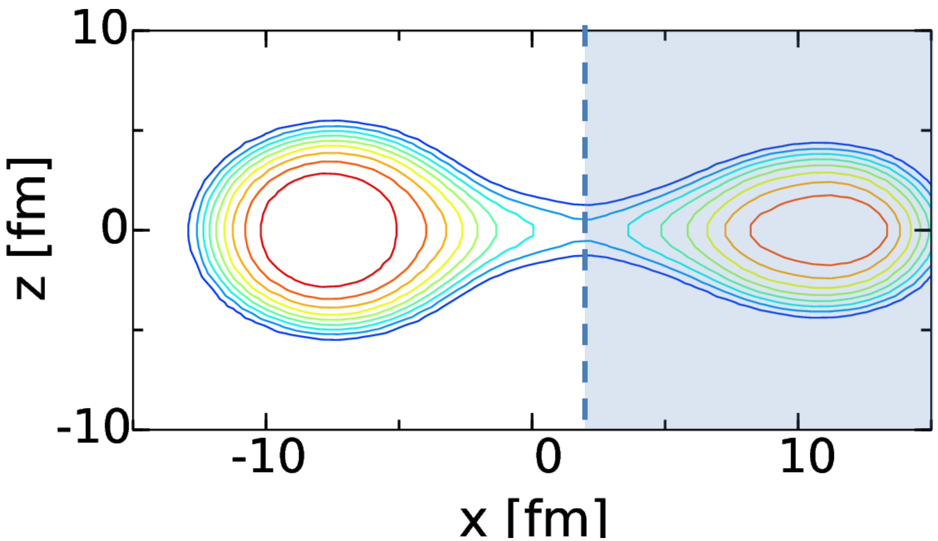
- Initial fission fragments: Nuclear density functional theory
  - Hierarchy of approximations:
    - Hartree-Fock-Bogoliubov (HFB): deformation properties and potential energy surfaces
    - Projection techniques (PNP and AMP): quantum numbers of CN or fission fragments
    - Time-dependent generator coordinate method (TDGCM): fission fragment distributions
  - Inputs: model of nuclear forces + quantum many-body methods
  - Outputs: distributions $Y(Z,A;E_n)$, spin distribution $p(I,\pi)$, excitation energy E^*, level density $\rho(U)$, etc.
- Independent yields and fission spectrum:
  - Fast Monte-Carlo event-by-event code that gives samples of complete fission events (full kinematic information of all final particles)
  - Inputs: distributions $Y(Z,A;E_n)$, spin distribution $p(I,\pi)$, excitation energy E^*, level density $\rho(U)$, etc.
  - Outputs: independent or cumulative yields $Y(Z,A,E_n)$, $\bar{\nu}$, N_γ, angular correlations, etc.

1. Number of Particles in Fission Fragments

For each scission configuration, particle number projection gives access to integer values for the proton and neutron number of the fission fragments and eliminates an empirical parameter

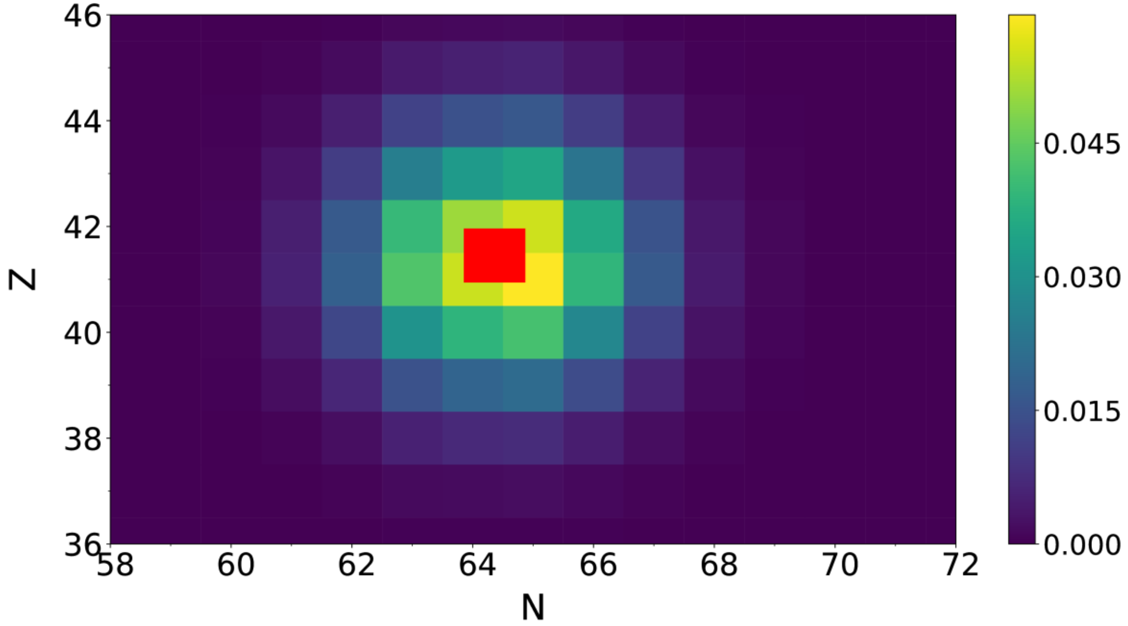
Before

- Identify position of the neck z_N between the prefragments
- Integrate density left and right of the neck to get $\langle Z \rangle$ and $\langle N \rangle$ at scission
- Introduce arbitrary Gaussian folding to account for dispersion around $\langle Z \rangle$ and $\langle N \rangle$ mean values



After

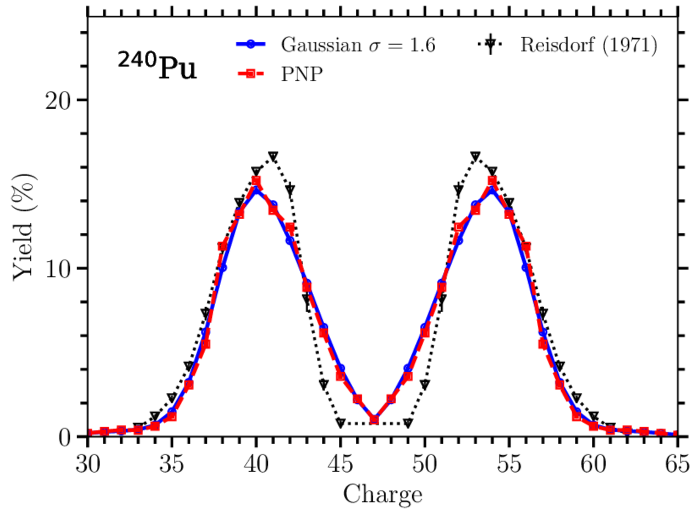
- Identify position of the neck z_N between the prefragments
- Use PNP to extract probability that left (right) fragment has exactly $N_f \in \mathbb{N}$ particles

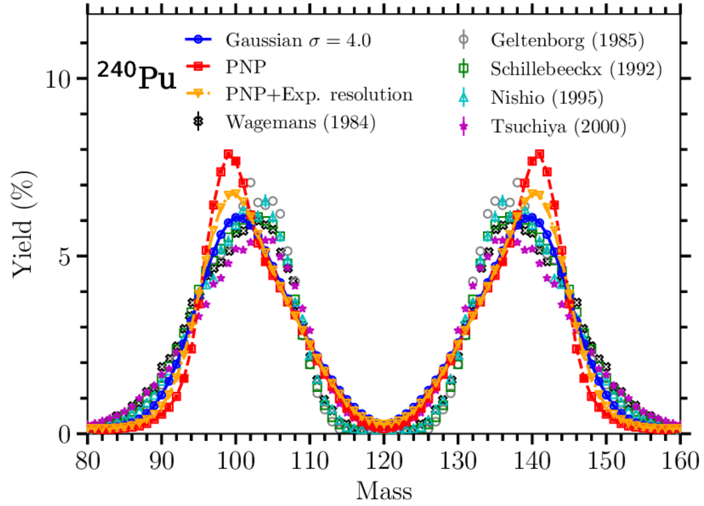


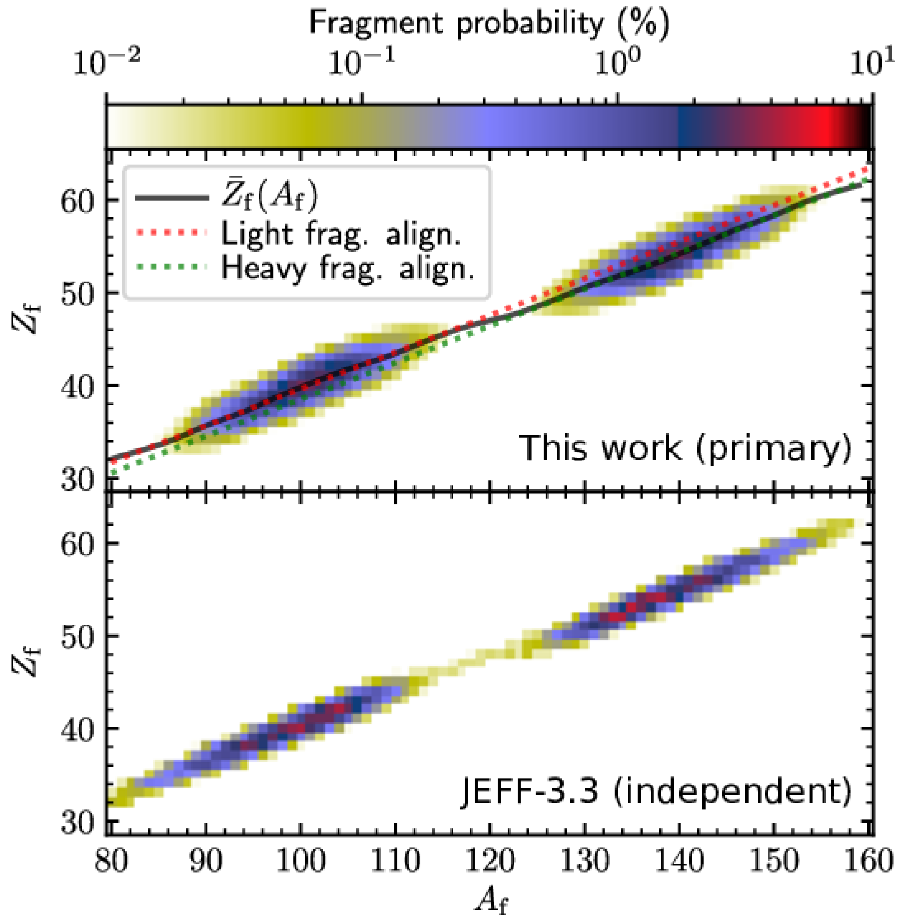
Primary Fission Yields

Fission fragment distributions are obtained by populating scission configurations and folding the probability of population with the dispersion in particle number at each configuration

- Fission yields are related to probability to populate scission configurations
- For each scission configuration
  - PNP gives dispersion in Z and N
  - TDGCM gives probability of being populated
- Example: charge Y(Z) and mass Y(A) yields for ^{239}Pu(n,f)
- Advantage of PNP: better estimate of isotopic yields Y(Z,A)

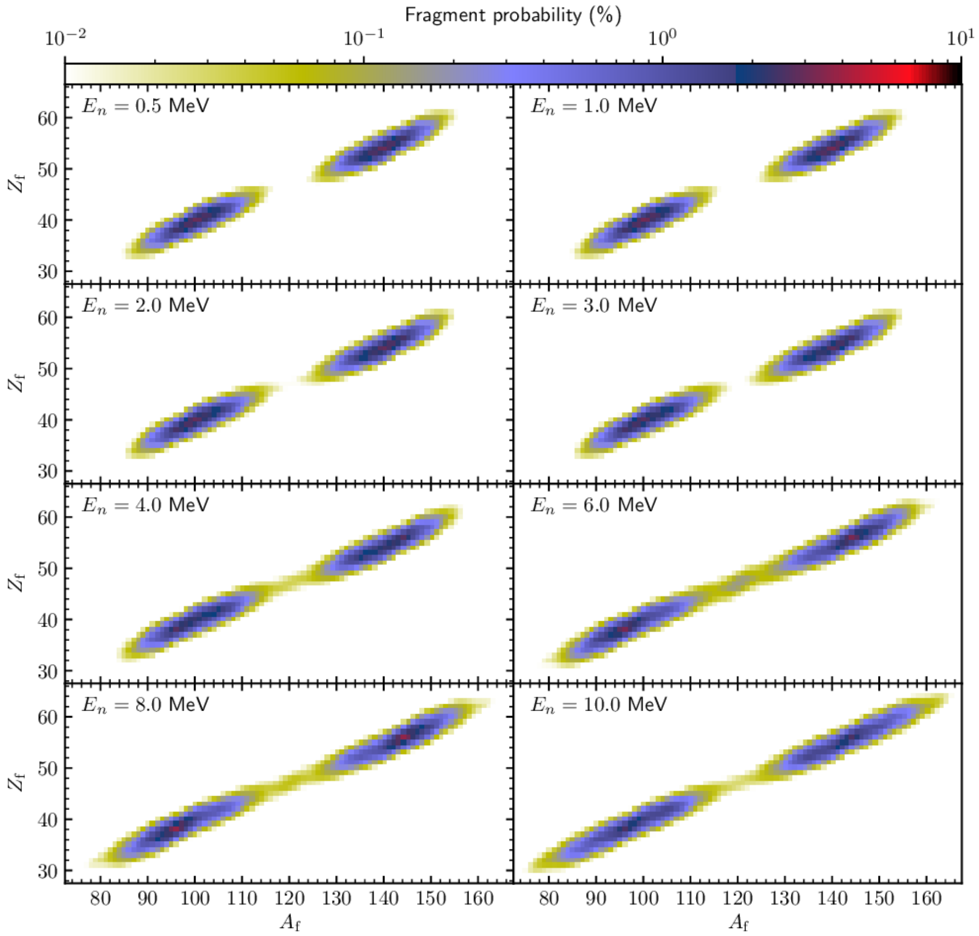




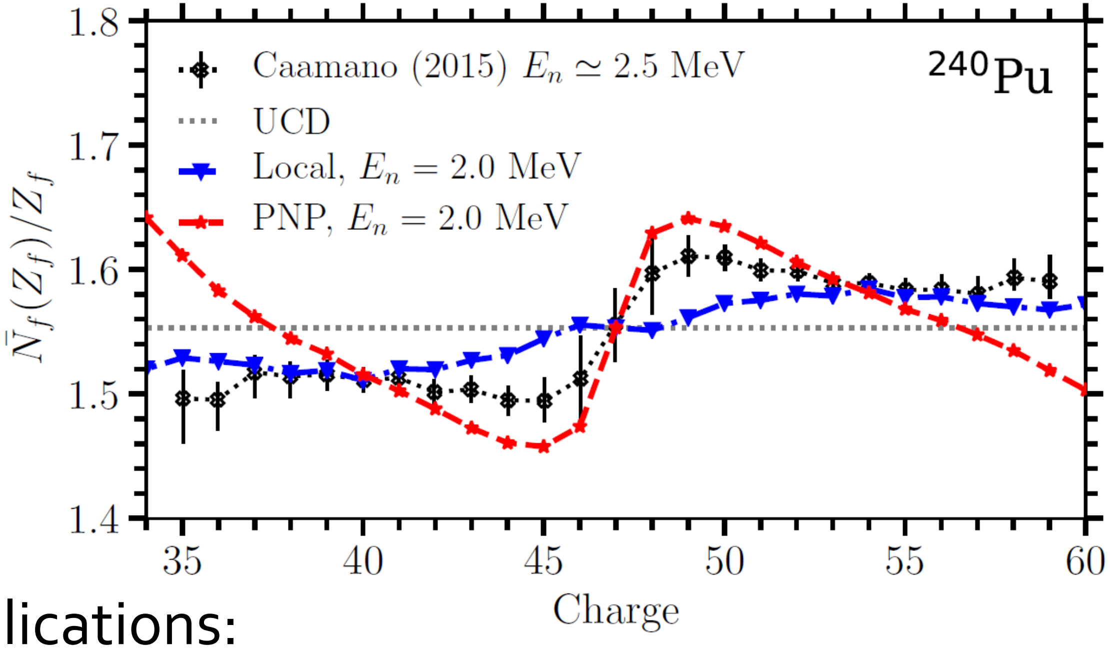


Guide for Evaluations

Trends from predictions of microscopic theories such as evolution of yields as a function of E_n or validity of UCD approximation can be used in evaluations



M. Verriere et al., Phys. Rev. C **103**, 054602 (2021)



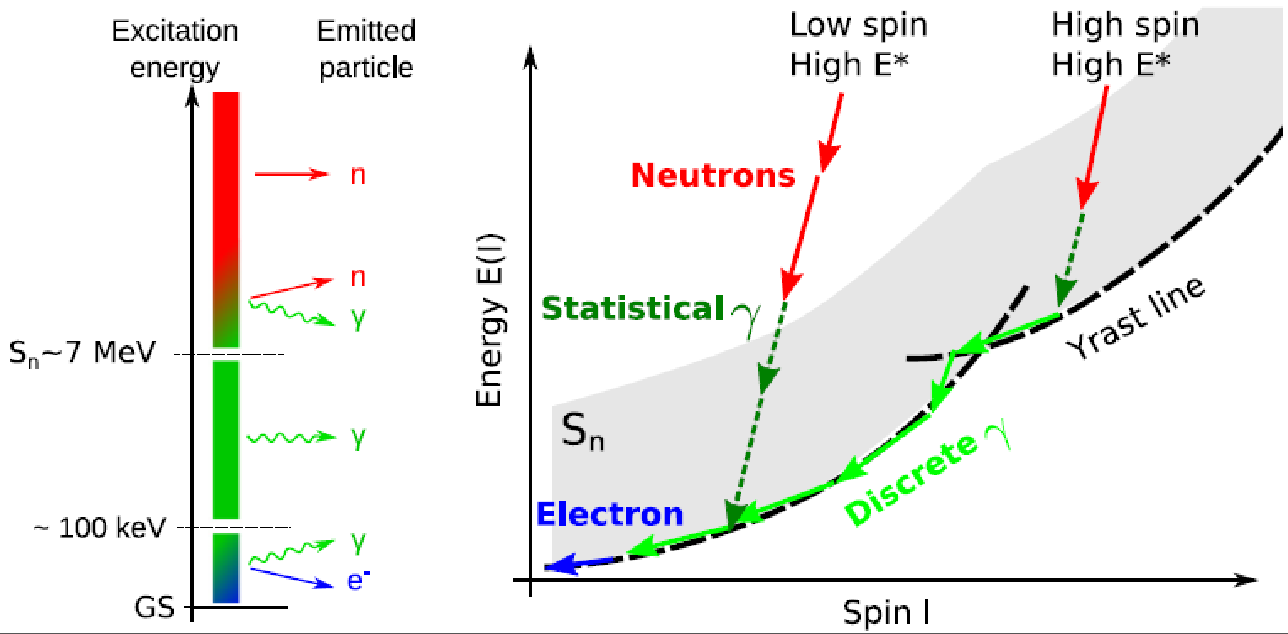
- Applications:
  - Trend of Y(Z,A) as a function of incident neutron energy
  - Validity of the UCD approximation, $\frac{\overline{N_f}}{Z_f} = \frac{N}{Z}$

Takeaway 1: The UCD approximation is not valid

2. Spin Distributions

Spin distribution of excited fission fragments affect prompt γ emission and anisotropy of neutron emission

- Characteristics of fission fragments at scission
  - High excitation energy ~10 – 30 MeV
  - Deformation possibly very different from the g.s.
  - Distribution of spin around mean value $\langle J \rangle$
- Competition between these effects



- Spin distribution very well fitted by

$$|a_J|^2 \propto (2J+1)e^{-J(J+1)/2\sigma^2}$$

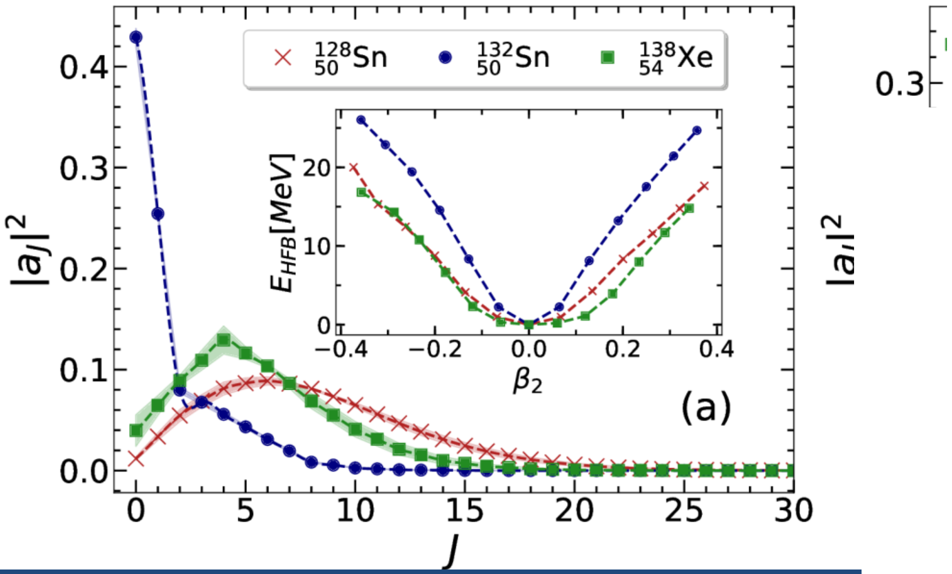
with $\sigma^2 = \mathcal{J}$ the spin cut-off parameter $\propto$ moment of inertia

- Problems
  - $\mathcal{J}$ is nuclear moment of inertia **at scission**
  - Analytical formulas are rough approximations of the real moment of inertia
  - Decay codes (FREYA, CGMF, etc.) often neglect the deformation dependency of $\mathcal{J}$

Angular Momentum Projection

We provided the first-ever microscopic prediction of spin distributions across a broad range of fragmentations and simulated γ emission with FREYA – good agreement with experimental measurements

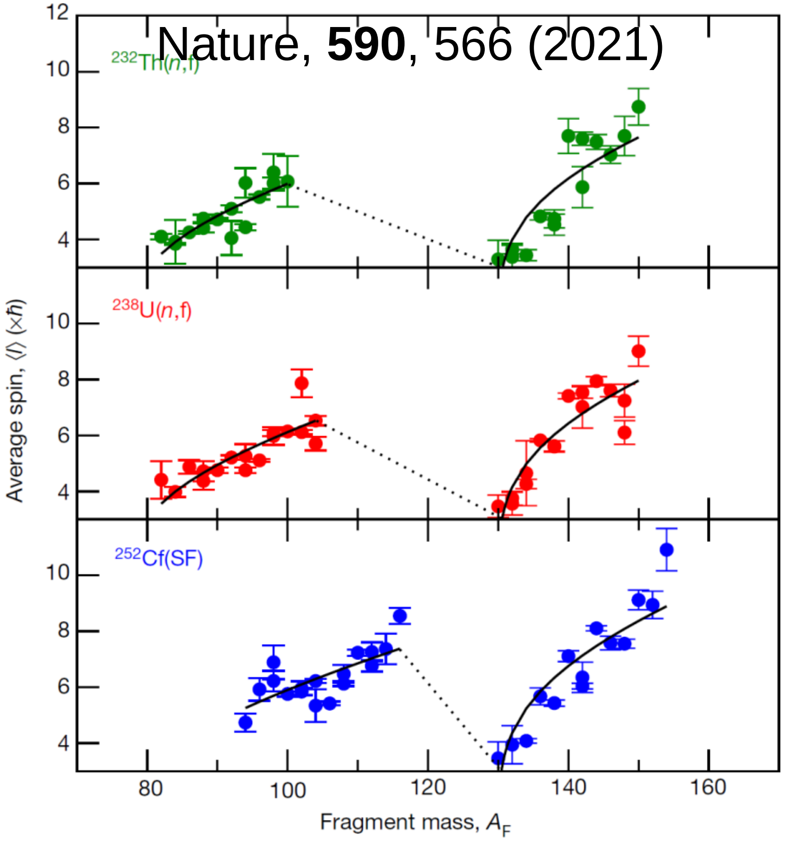
- Directly extract spin distribution of FFs by angular momentum projection (AMP)
- Spin distributions depend critically on deformations of fragments **at scission**



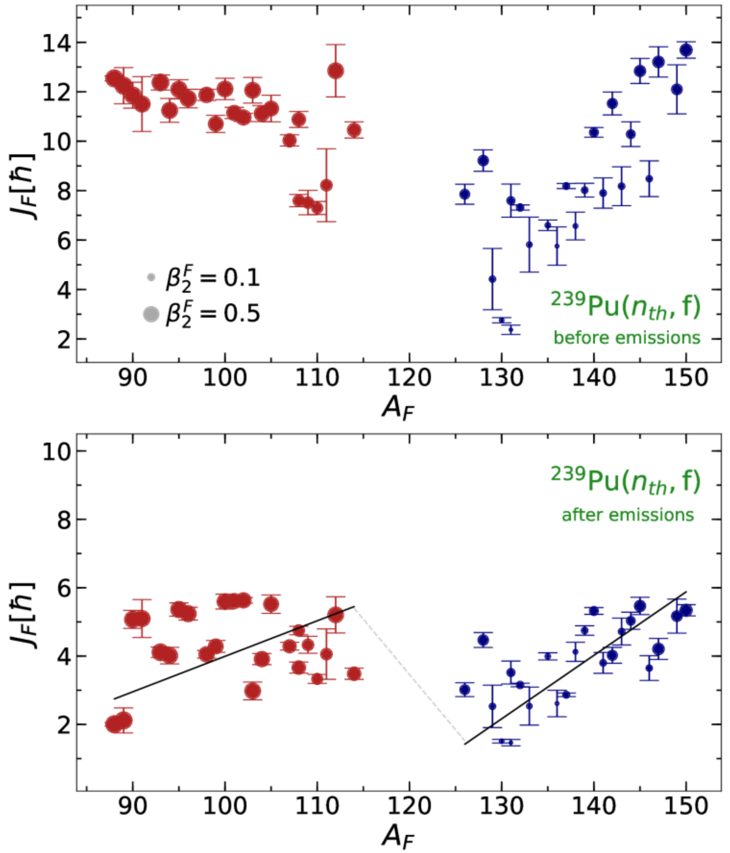
P. Marevic et al., Phys. Rev. C **104**, L021601 (2021)

Measurements

Nature, **590**, 566 (2021)



Calculations



Takeaway 2: The spin cut-off parameter depends on fragment deformation at scission

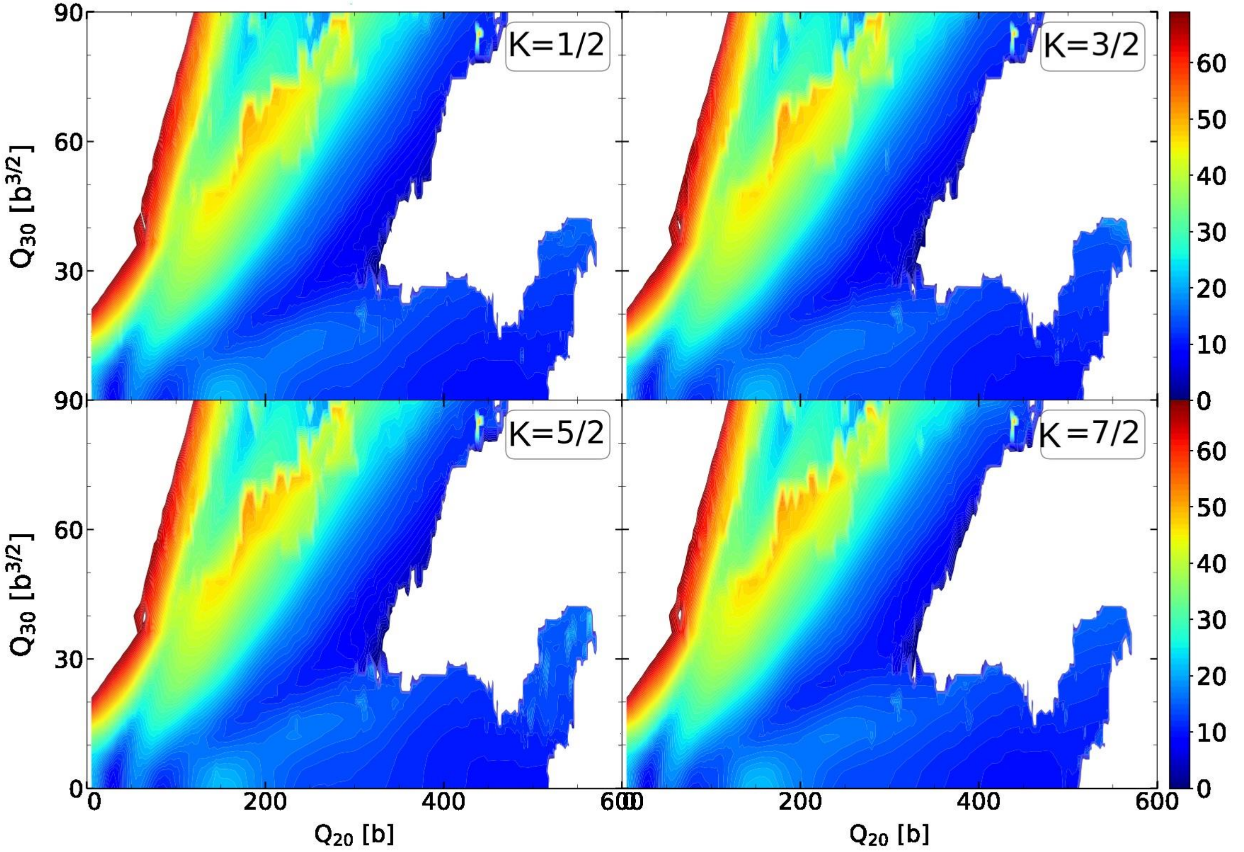
Prepared by LLNL under Contract DE-AC52-07NA27344.

3. Fission of Odd-Mass Nuclei

In an odd-mass nucleus, potential energy surfaces depend on the spin of the single particle (proton or neutron)

- Nuclei with odd number of particles:
  - All particles but one ("blocked") are paired
  - Many blocking configurations are possible
  - The spin of the blocked configuration fixes the spin of the compound nucleus
- Each blocking configuration gives a different potential energy surface

Spin projection K	1/2	3/2	5/2	7/2
Fission isomer E* [MeV]	2.72	1.79	2.89	3.23
Saddle (barrier) [MeV]	9.08	7.87	10.01	9.11



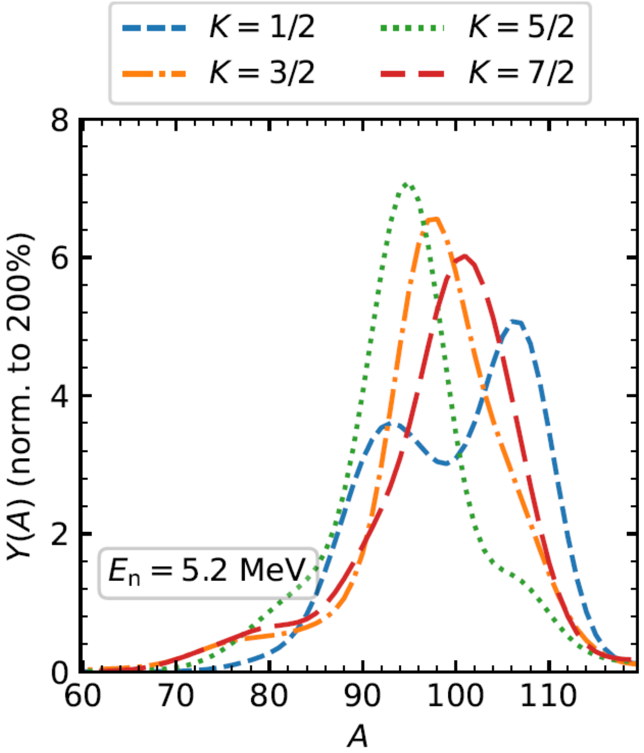
Takeaway 3: In odd-mass nuclei, fission barriers are spin-dependent

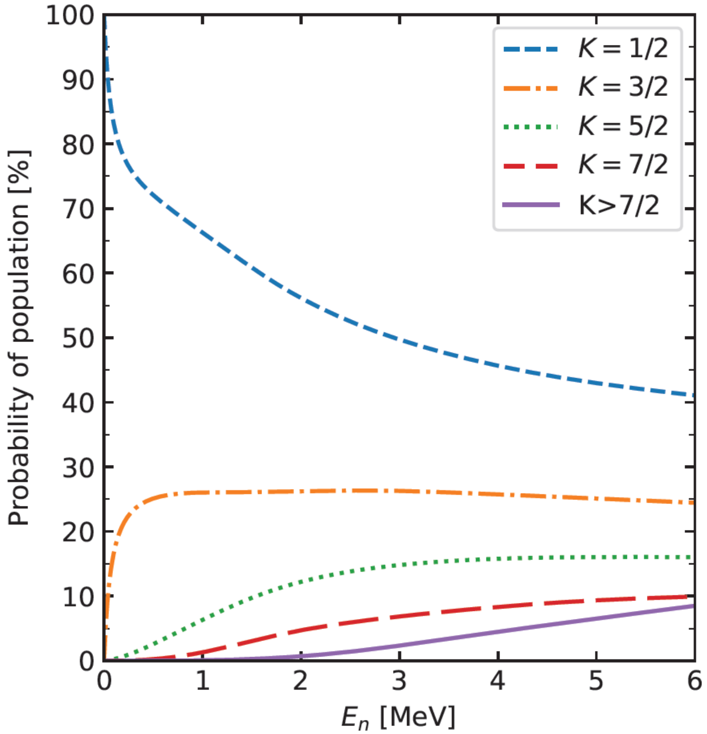
Primary yields of $^{238}U(n,f)$

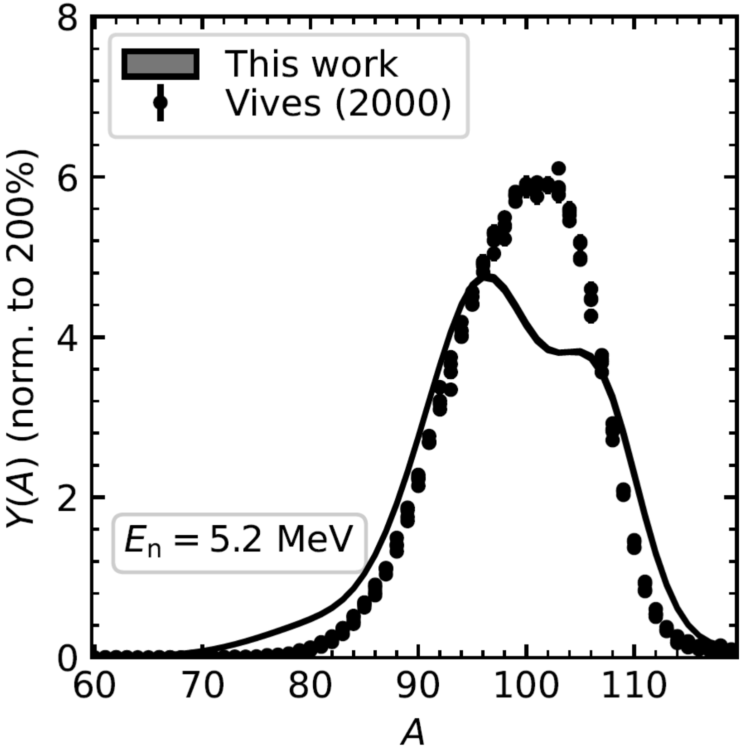
We computed the primary (=pre-neutron emission) charge and mass distributions of the $^{238}U(n,f)$ reaction for each K-channel and used reaction theory to estimate the total, weighted distributions

- Primary yields extracted from TDGCM for each K value
- Spin distributions computed from coupled channel

$$Y(A) \propto \sum p_K Y_K(A)$$







Takeaway 4: Primary yields of odd-mass compound nuclei depend on entrance channel

Conclusions

LLNL effort is focused on providing guidance for the evaluation of FPY by developing and applying microscopic models for the initial conditions of fission fragments

- Microscopic models of fission provide insights into fundamental mechanisms of fission
- Lessons learned:
  - **Number of particles in fission fragment** – UCD approximation is not valid
  - **Spin distributions of fission fragments** – Spin cut-off parameter must depend on the mass of the fragment and also on its deformation at scission
  - **Role of entrance channel in odd-mass nucleus** – Fission barriers are spin-dependent and primary yields depend on spin of compound nucleus
- Moving forward
  - (semi)Microscopic calculations in additional systems may provide enough data to fit
    - The function N(Z) for fission fragments
    - A systematics of deformation properties and/or moments of inertia
  - Role of spin in compound nucleus
    - Introduce spin-dependent fission barriers in cross sections calculations of odd-mass nuclei
    - Is there a spin dependency in even-even ones?

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