Initial Conditions for the Deexcitation of Fission Fragments

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FIRE

NUCLEI
Nuclear Computational Low-Energy Initiative

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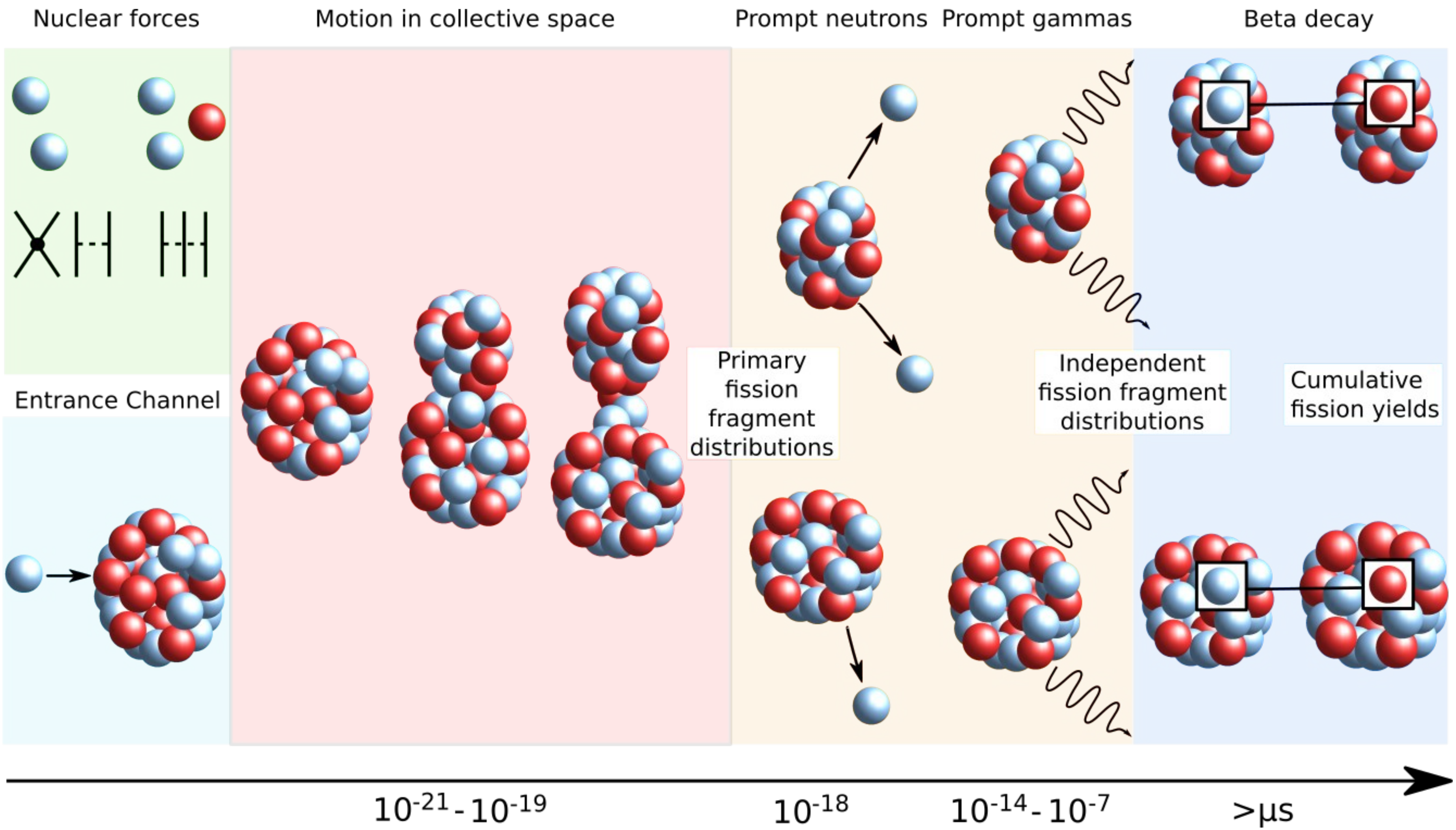
Nuclear Fission Process

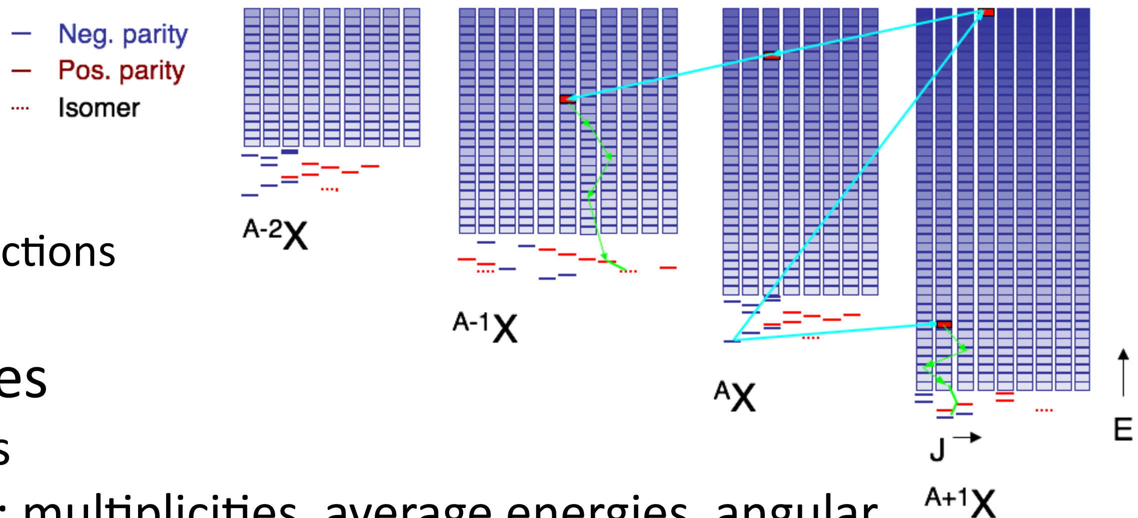
Experimental measurements of fission data is constrained by timescales of the various phases of the process



Deexcitation of Fission Fragments

Comparison with measurements require simulating the decay of the fission fragment from immediately after scission

- Statistical reaction theory code give fission properties
- Required inputs (as a function of excitation energy of compound nucleus)
  - Z, N, relative probabilities (=yields) Y(Z,N)
  - For given Z,N
    - Excitation energy E*
    - Spin distribution p(J)
    - Level density
    - Gamma strength functions
    - (Beta-decay rates)
- Measurable observables
  - Charge and mass yields
  - Neutrons and photons: multiplicities, average energies, angular correlations
  - Beta-decay: rates, branching ratios



Predictions versus Postdictions

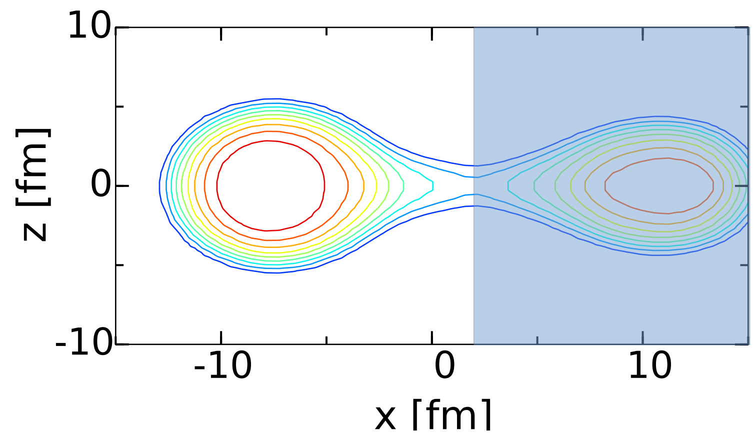
The large number of inputs and lack of experimental constraints require both predictive models and ML/AI techniques

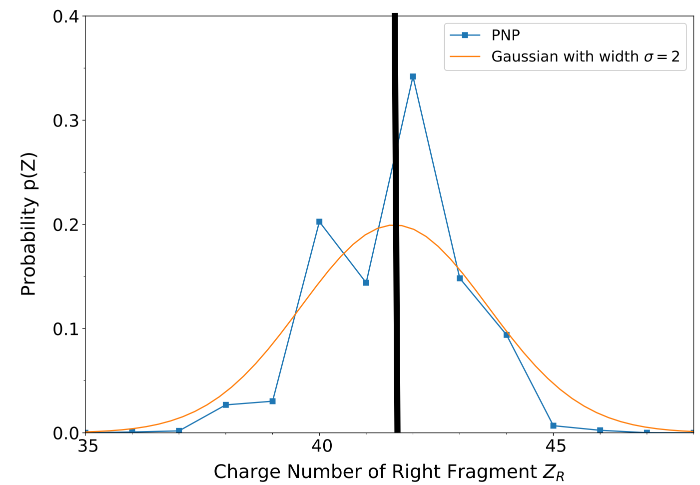
- Strategies:
  - Use inputs as adjustable parameters (possibly constrained by experimental measurements) to reproduce fission spectrum *ex post*
    - Provides leverage for very precise calibration of nuclear data
    - Number of parameters is large
    - Advanced statistical methods (ML/AI) help only so much
  - Use theoretical models (fission, decay, structure) to compute some of these quantities
    - Provides reliable trends where measurements are missing
    - Eliminates several empirical parameters and improves consistency
    - Precision is not good enough
- Recent progress in fundamental nuclear theory enabled by HPC
  - Particle number projection of Z,N in fragments: odd-even effect
  - Angular momentum projection techniques: spin distributions
  - Real-time evolution of fissioning nucleus: fragment excitation energy

Number of Particles in Fission Fragments

Particle number projection techniques are key to reproducing the odd-even effect of charge distributions

- All models of fission (statistical scission point model, semi-classical dynamics, quantum-mechanical approaches)
  - Describe fission as a deformation process
  - Obtain proton and neutron numbers by mapping them to a given deformed shape
- Mapping methods:
  - Standard approach
    - Numbers of particle = integrals of the density left and right of the neck
    - Non-integer values
  - Particle number projection
    - Use in nuclear structure theory to restore particle number in superfluid systems
    - Adapted in 2019 to quantify dispersion of particle number for scission configurations



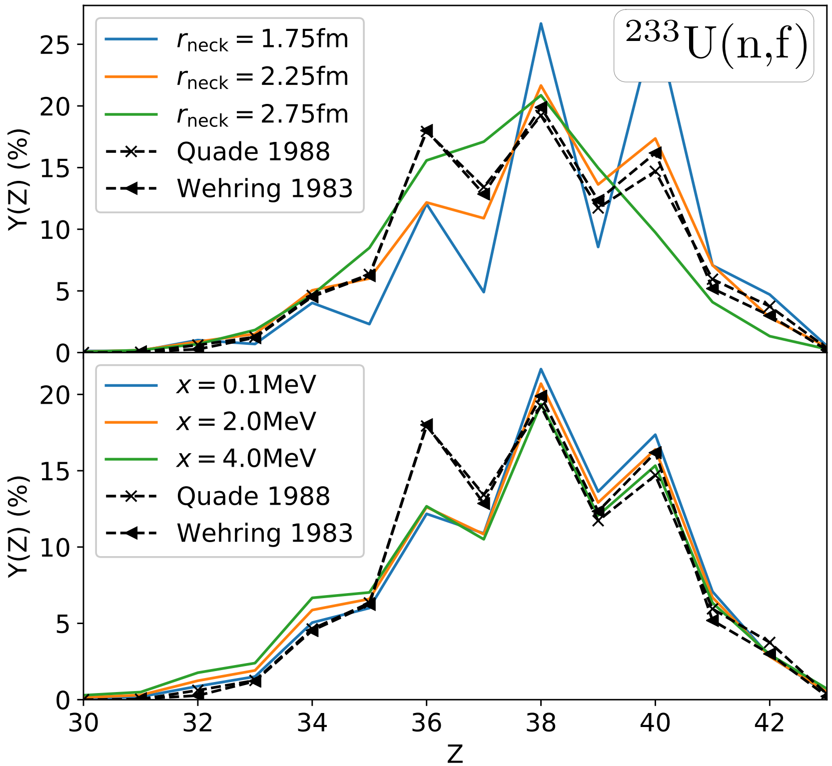


C. Simenel, PRL **105**, 192701 (2010); G. Scamps et al., PRC **87**, 014605 (2013); M. Verriere et al., PRC **100**, 024612(R) (2019)

Fission Fragment Distributions

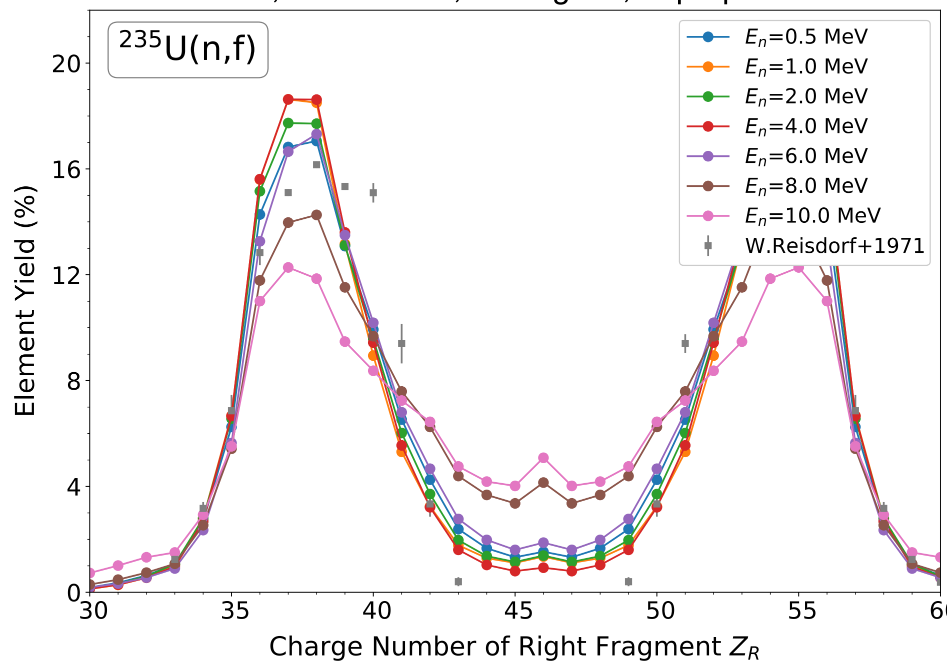
Particle number projection improve the fidelity of fission models to describe charge distributions

M. Verriere, M. Mumpower arXiv:2008.06639



- Semi-classical random walk on macro-micro PES

M. Verriere, N. Schunck, D. Regnier, In preparation



- Quantum-mechanical evolution with the time-dependent generator coordinate method

PNP can produce odd-even effects without the need of adjustable parameters

Spin Distributions

The prompt photon spectrum is extremely sensitive to the spin distribution of the fission fragments

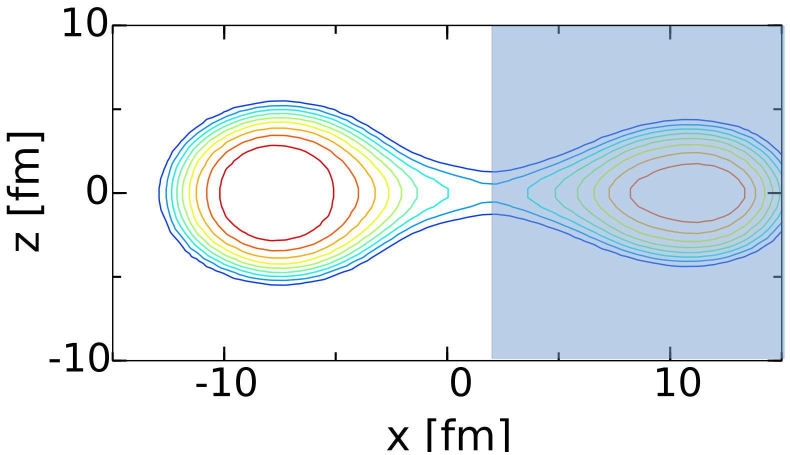
- Traditional approach is based on semi-empirical formula

$$p(J) \propto (2J+1)e^{-J(J+1)/\mathscr{I}}$$

  where $\mathscr{I}$ is the moment of inertia for the fragment (Z,N) at its excitation energy
  - Proper calculation of $\mathscr{I}$ requires advanced nuclear structure model
  - Alternative is to consider it as adjustable parameter

- Same projection techniques used for particle number can be extended to angular momentum
- Angular momentum for the fragment

$$\hat{J}_\mu \to \hat{J}_\mu^{(R)} = \hat{J}_\mu H(z - z_{\mathrm{N}})$$

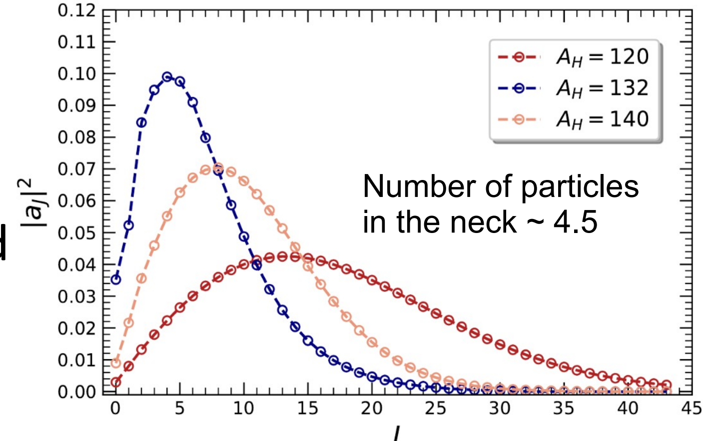


K. Sekizawa, PRC **96**, 014615 (2017)

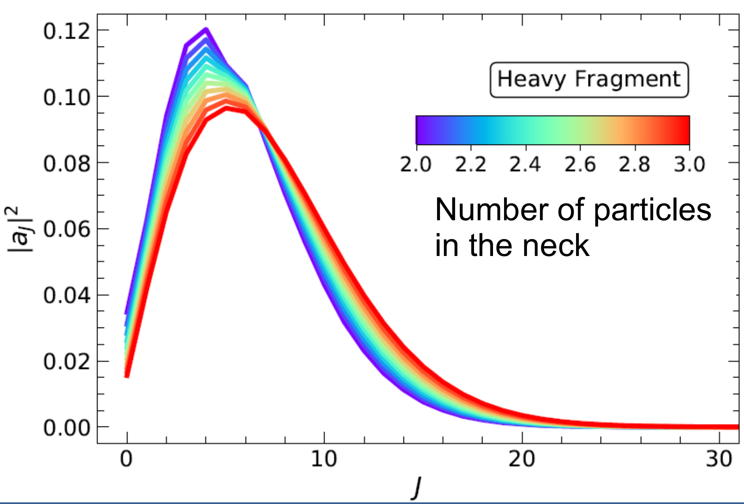
Microscropic Spin Distributions

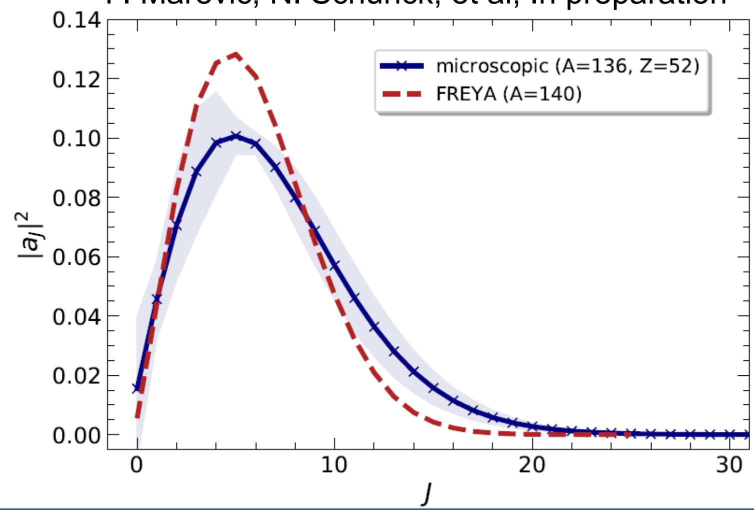
Angular momentum projection provides spin distributions consistent with fragment deformations

- Spin distribution is heavily correlated with fission fragment deformation
  - More deformed ⇒broader distribution
  - Parity distribution automatically determined
- Good agreement with FREYA results for neck sizes around 2-3



P. Marevic, N. Schunck, et al, In preparation



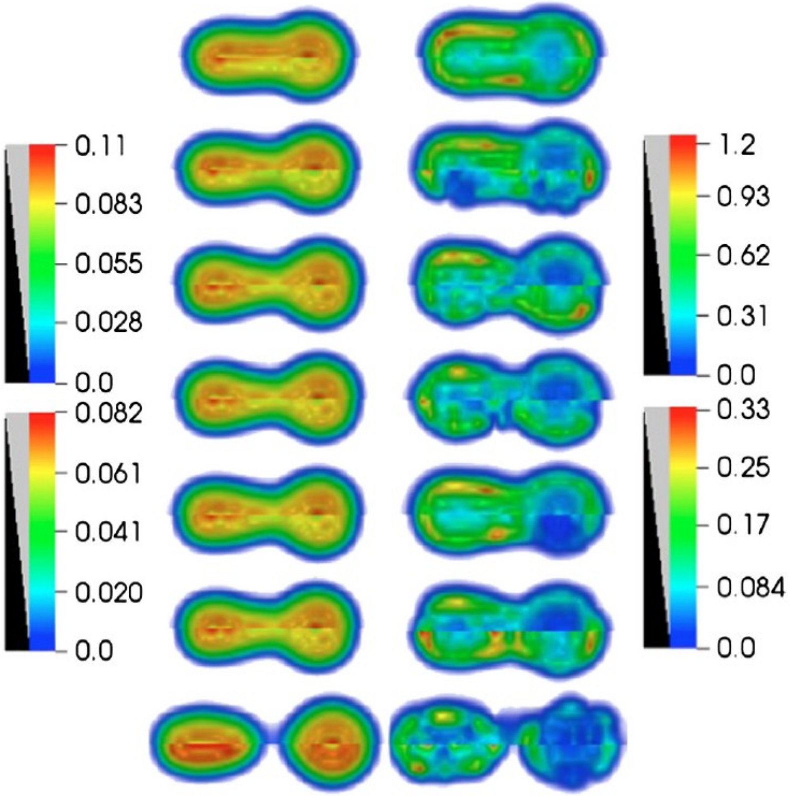


AMP results are sensitive to definition of scission configurations – like most other data

Excitation Energy

Time-dependent DFT provides rigorous framework to extract excitation energy of fission fragments

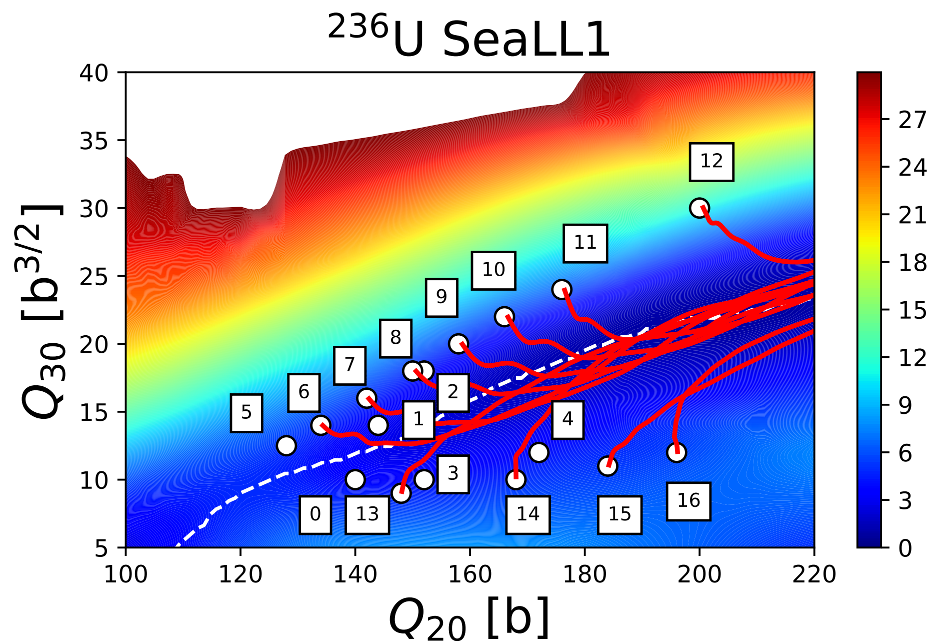
- "Adiabatic" methods based on precomputing a potential energy surfaces give only lowest energy at given deformation
  - "cold" fragments
  - Excitation energy has to be introduced by hand
- TDDFT is a real-time evolution of the nuclear shape
  - Initial condition near the saddle
  - Energy is conserved throughout
- Initial energy of compound nucleus becomes excitation energy and is distributed to fission fragments based on nuclear forces

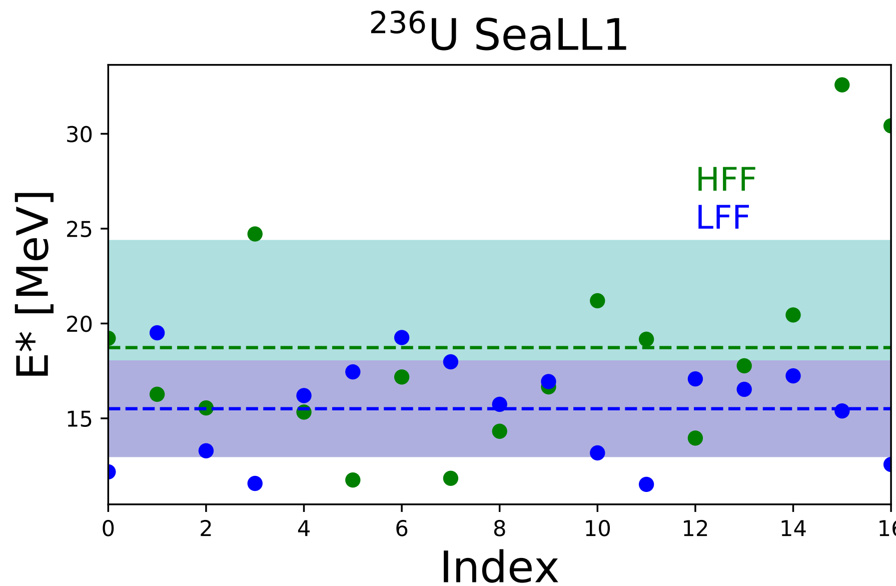


C. Simenel et al., PRC **89**, 031601(R), (2014)
G. Scamps et al, PRC **92**, 011602 (2015)
Y. Tanimura et al, PRC **92**, 034601 (2015)
A. Bulgac et al., PRL **116**, 122504 (2016)
A. Bulgac et al., PRC **100**, 034615 (2019)

Energy Sharing

Total excitation energy and energy balance replaced by explicit, parameter-free values of fragment excitation energy





- Direct access to excitation energy of each fragment
- No need to specify energy sharing mechanism: nuclear forces do it for you...

Challenge is to extend this technique to all scission configurations

Conclusions

- Fission spectrum depends on initial conditions of fission fragments just after scission
  - Inaccessible by direct experimental measurements for the most part
  - Come from theoretical models
- Microscopic methods are useful baselines upon which to build evaluations
  - Particle number projection leads naturally to odd-even effects
  - Angular momentum projection gives spin- and parity-distribution consistent with fragment deformation
  - Time-dependent density functional theory provides framework to extract excitation energy
- These tools can be combined with one another, and with empirical corrections

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