LLNL Efforts on FPY Evaluations

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LLNL work will ensure cross-validation and verification

Complementary approaches to FPY and their observable consequences:
- Density functional theory (DFTNESS & FELIX)
- Complete event Monte Carlo (FREYA)

Two main activities:
- Estimate the evolution of initial yields as a function of incident neutron energy
- Calculate the initial conditions of the fission fragments prior to de-excitation

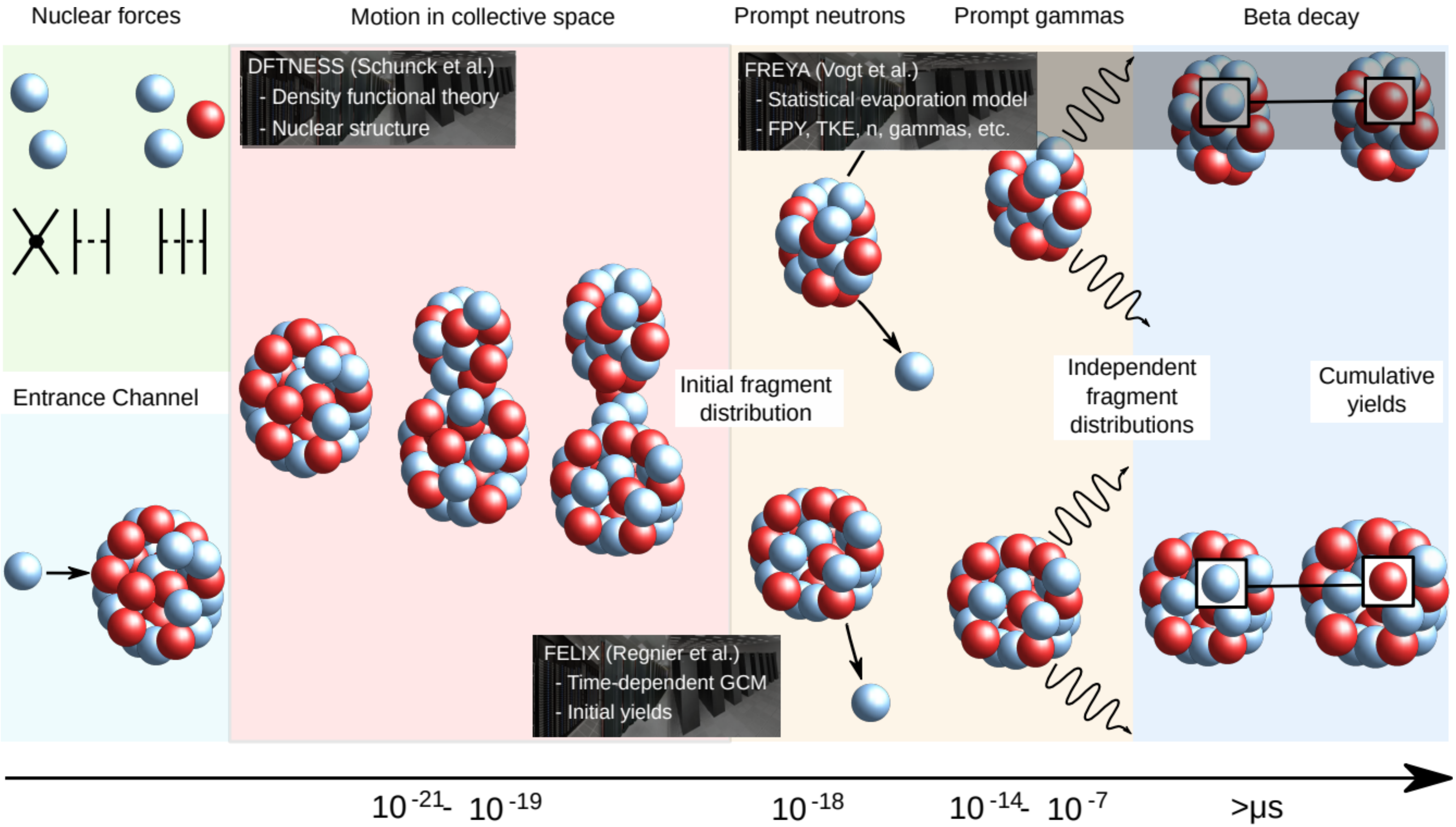
Microscopic calculations will provide insights into trends that can be encoded empirically and tested in FREYA

FREYA will be augmented by FIER data to be able to study both independent and cumulative FPYs for major and minor actinides

FREYA can also test empirical formulations of the fragment excitation energy calculated in the DFT approaches

The Physics Problem

Fission product yields are the end product of a complex process involving multiple phases described by different models



DFTNESS (Schunck et al.)
- Density functional theory
- Nuclear structure

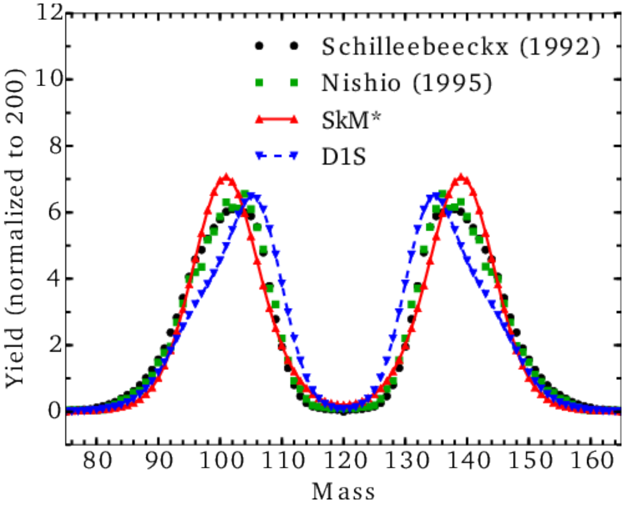
FREYA (Vogt et al.)
- Statistical evaporation model
- FPY, TKE, n, gammas, etc.

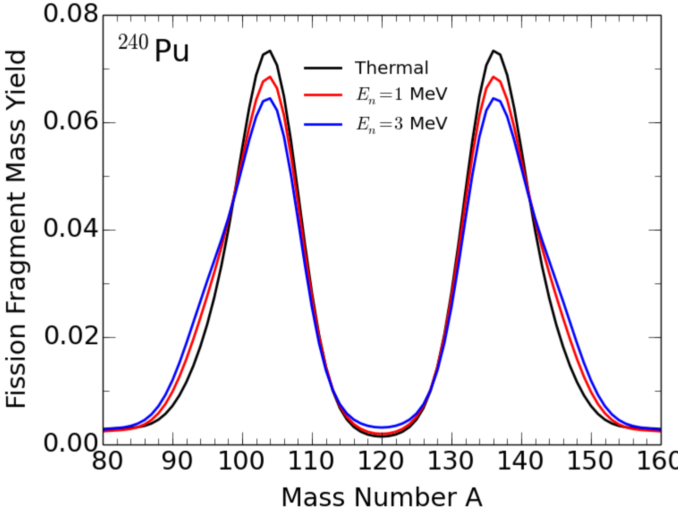
FELIX (Regnier et al.)
- Time-dependent GCM
- Initial yields

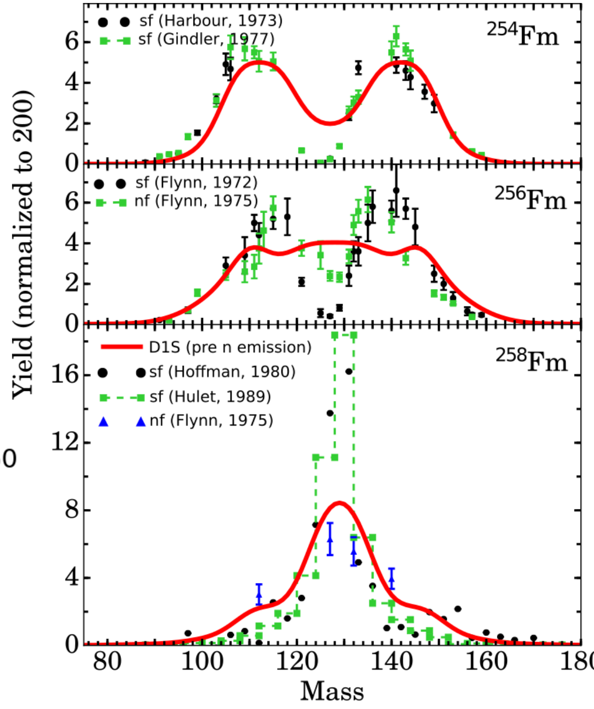
Fission Mass Distributions

Microscopic models have predictive power and can provide baseline or trends as a function of Z, N and neutron incident energy

D. Regnier, *et al.*, Comp. Phys. Comm. **200**, 350 (2016); D. Regnier, *et al*, Comp. Phys. Comm. **225**, 180 (2018); D. Regnier, *et al.*, Phys. Rev. C **93**, 054611 (2016), D. Regnier, *et al.*, Phys. Rev. C **99**, 024611 (2019)



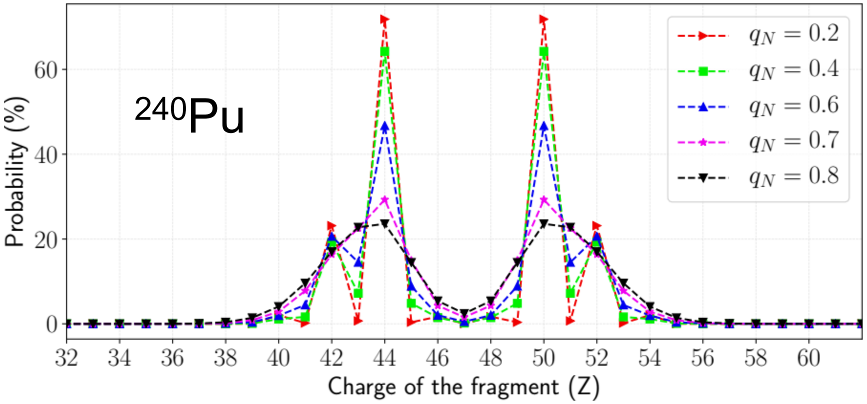




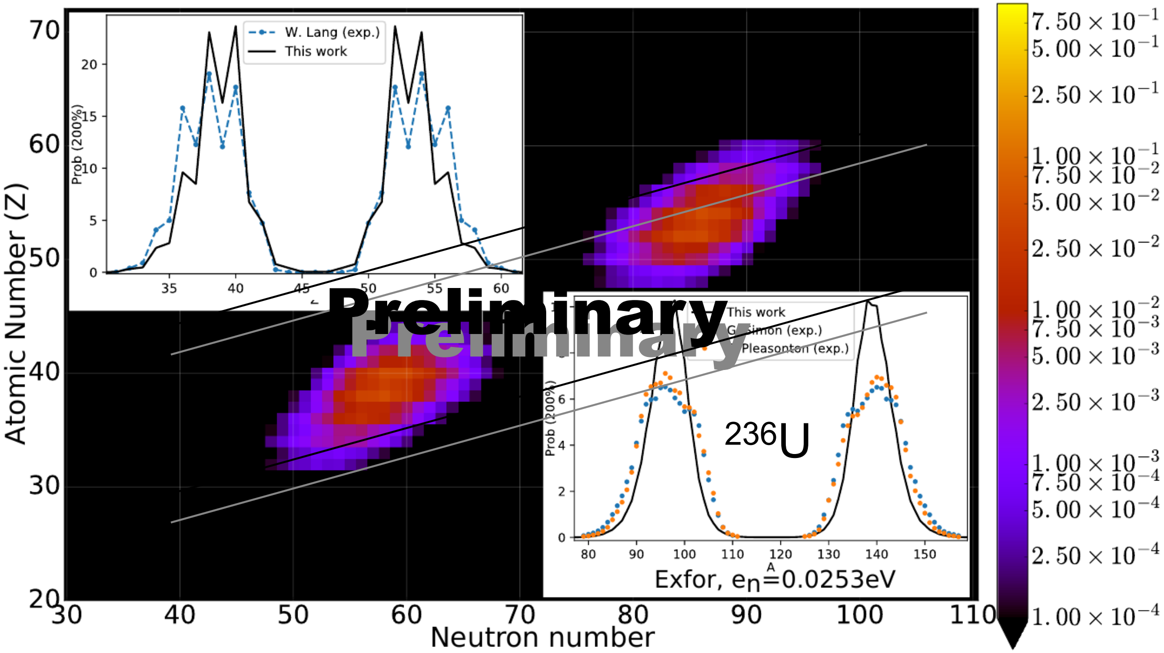
- Use density functional theory to compute primary fission yields as a function of neutron incident energy
- Calibrate predictions on experimental data when available
- Extract empirical formulas for evolution as a function of incident energy
- Apply formalism to odd-mass systems

Number of Particles in Fission Fragments

Particle number projection could be key to reproducing odd-even staggering effect of charge distributions



- Traditional models of fission do not give precise estimate of charge or mass
- Particle number projection techniques predict dispersion in particle number at scission

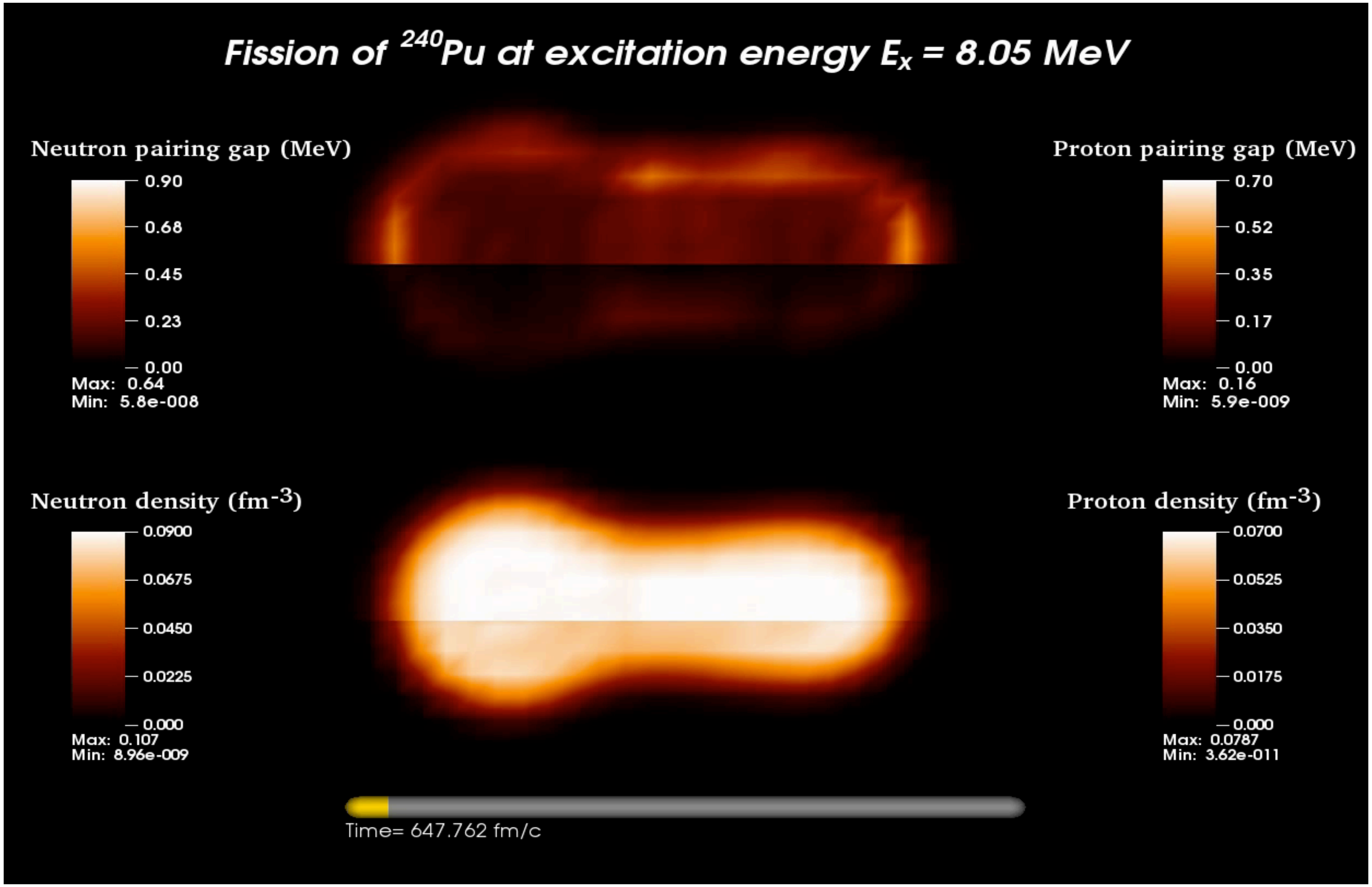


- Advantages
  - Generates odd-even staggering effect
  - Polarizability of fragment distributions
- Adapt work of M. Verriere under FIRE collaboration to FELIX solver

C. Simenel, Phys. Rev. Lett. **105**, 192701 (2010);
G. Scamps, *et al.*, Phys. Rev. C **87**, 014605 (2013);
M. Verriere, *et al.*, Phys. Rev. C **100,** 024612 (2019)

Time-Dependent Density Functional Theory

Real-time evolution of fissioning nucleus gives wealth of information on scission mechanism – including excited fragments



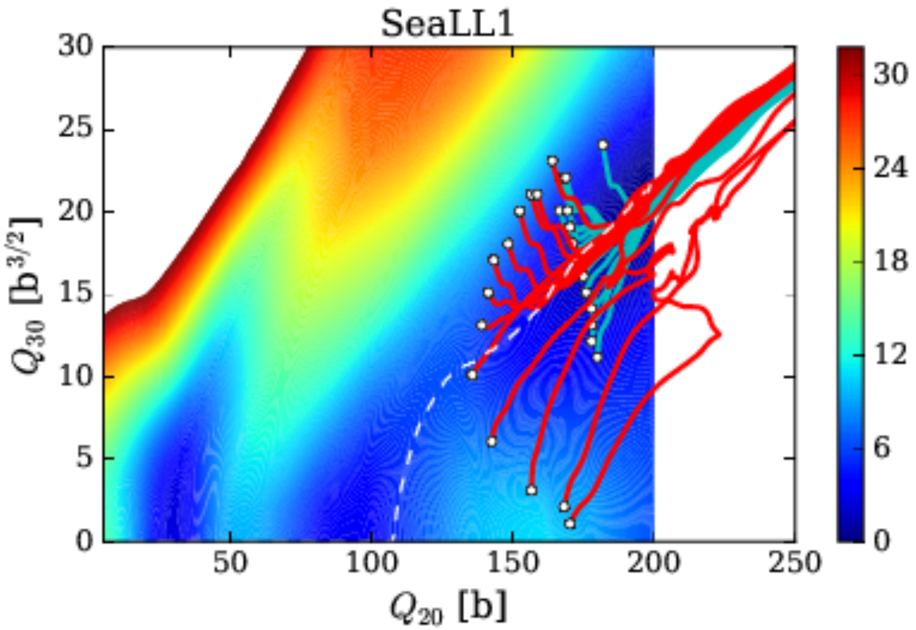
A. Bulgac, P. Magierksi, K. Roche, I. Stetcu, PRL **116** 122504 (2016)

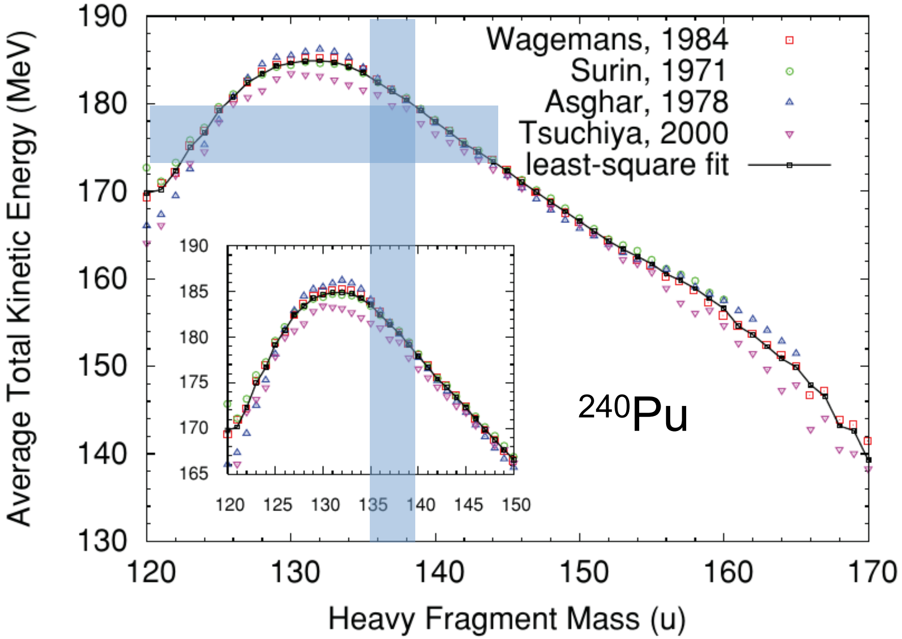
Excitation Energy Sharing

We will compute the excitation energy of fission fragments and extract empirical laws that can be easily implemented in FREYA/CGMF

Results for ^{240}Pu with different density functionals; excitation energy accessed directly at split

Label	E_{ini}	TKE	N_H	Z_H	N_L	Z_L	E^*_H	E^*_L	TXE	TKE+TXE
SeaLL1-1	-1808.0 ± 2.4	177.8 ± 2.8	83.5 ± 0.4	53.2 ± 0.4	62.8 ± 0.5	41.1 ± 0.4	17.0 ± 2.4	20.1 ± 2.0	37.1 ± 2.7	214.9 ± 2.4
SeaLL1-2	-1813.9 ± 1.1	178.0 ± 2.3	82.9 ± 0.4	52.9 ± 0.2	63.3 ± 0.5	41.5 ± 0.3	19.5 ± 3.8	14.0 ± 1.9	33.5 ± 5.1	211.5 ± 3.3
SkM*-a	-1780.5 ± 2.2	174.5 ± 2.5	84.1 ± 0.9	53.0 ± 0.5	61.8 ± 0.9	40.9 ± 0.5	16.6 ± 3.1	14.9 ± 2.3	31.5 ± 3.8	206.0 ± 2.4
SkM*-s	-1780.2	149.0	73.4	47.2	72.6	46.7	29.4	28.5	57.9	206.9





Event-by-event modeling in FREYA is efficient framework for studying fission

Goal(s): *Fast* generation of (large) samples of complete fission events

Complete fission event: Full kinematic information on all final particles

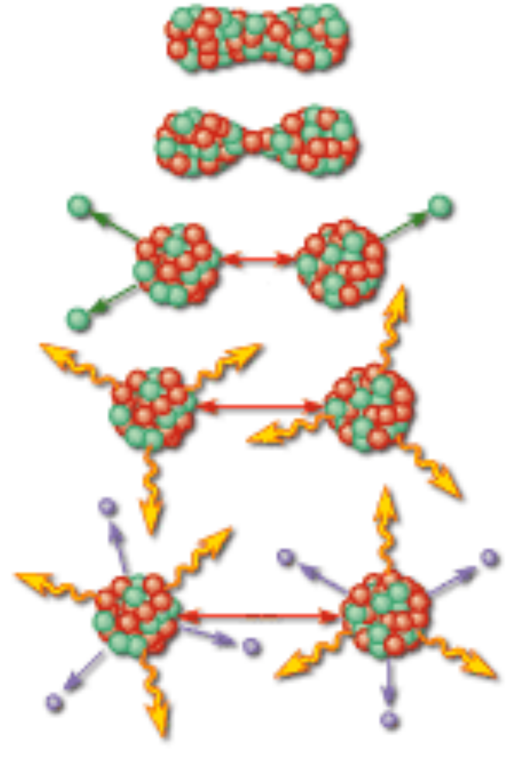
Two product nuclei: $Z_H, A_H, \boldsymbol{P}_H$ and $Z_L, A_L, \boldsymbol{P}_L$
ν neutrons: $\{ \boldsymbol{p}_n \}$, $n = 1,\ldots,\nu$
N_γ photons: $\{ \boldsymbol{p}_m \}$, $m = 1,\ldots,N_\gamma$

Advantage of having *samples* of complete events:

Straightforward to extract *any* observable,
including fluctuations and correlations,
and to take account of cuts & acceptances

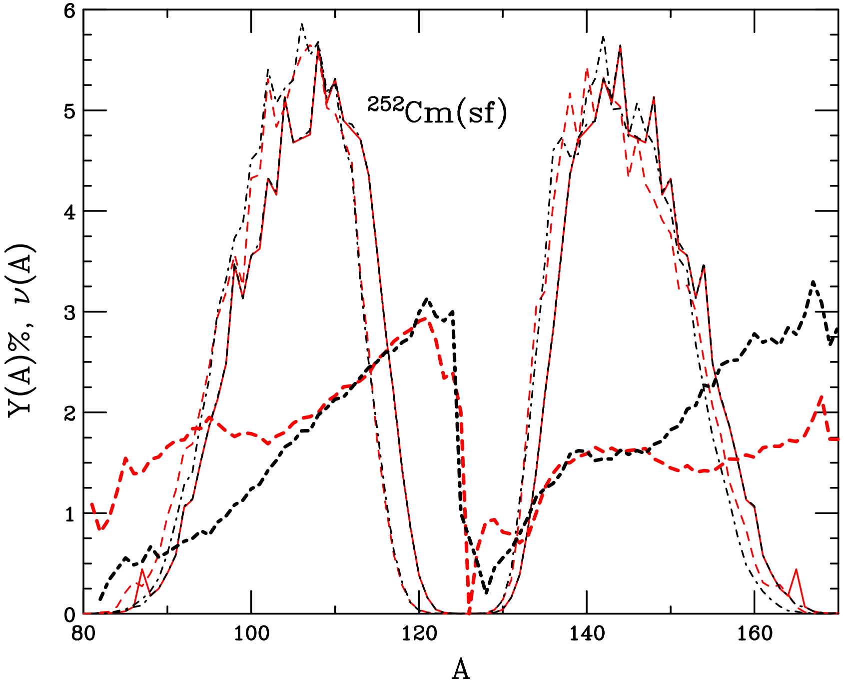
Advantage of *fast* event generation:

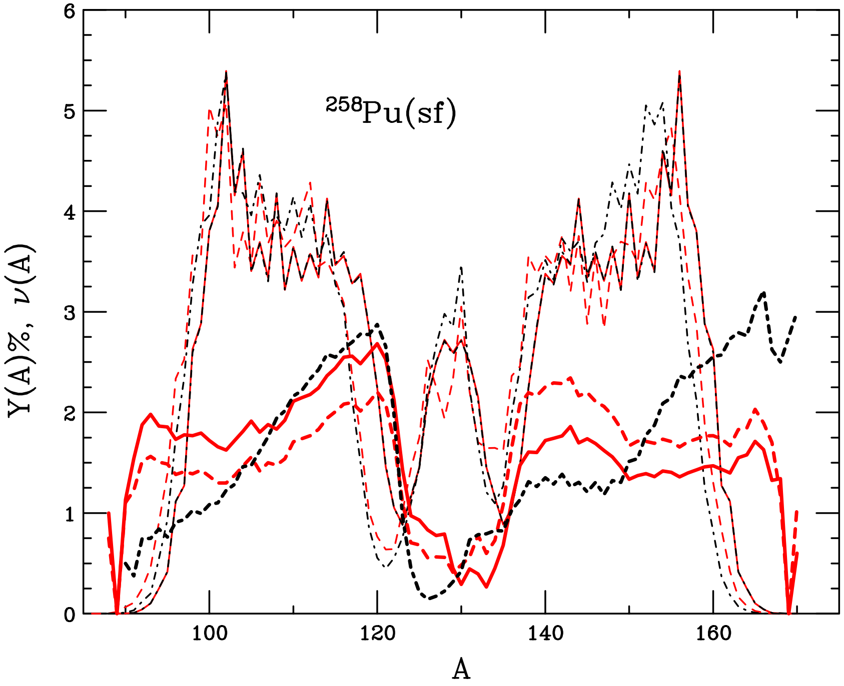
Can be incorporated into transport codes
Can easily be adapted to new model inputs &
provide a fast and efficient testing ground for models
of fission yields and excitation energies



^{252}Cm(sf), ^{258}Pu(sf) test cases: FPYs for r-process nucleosynthesis

- GEF fragment yields used as input to FREYA, tested effects of different de-excitation processes in the two codes on stellar abundances
- FREYA reproduces initial GEF yields precisely, some differences in FPYs due to handling of emission in two codes
- Differences are reflected in ν(A), as also shown



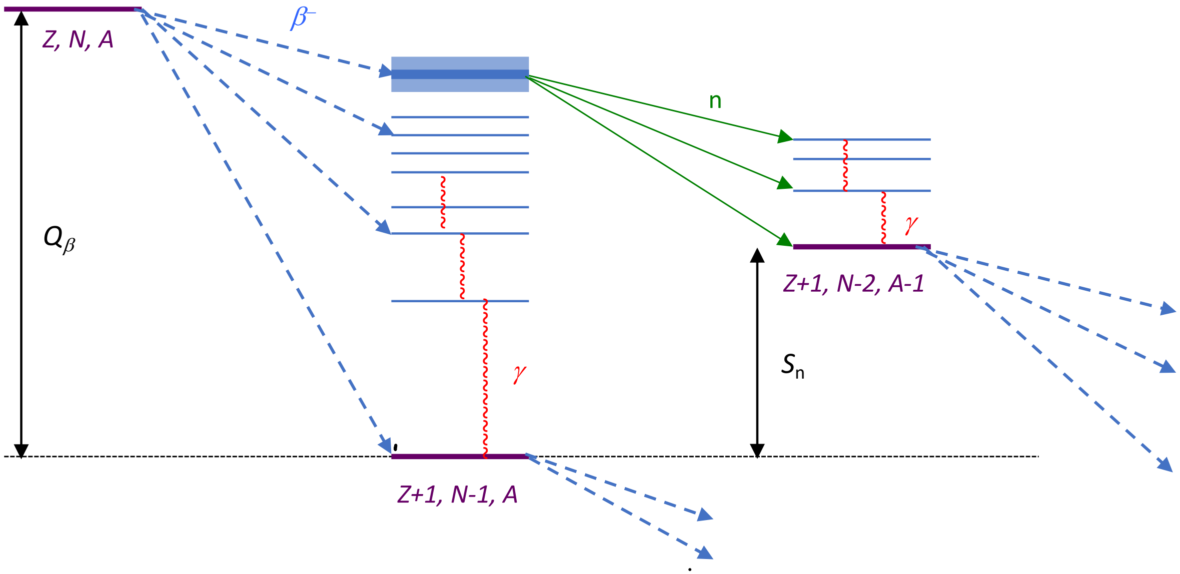


β-delayed emission needs to be included in FREYA for FPY evaluations

So far, FREYA includes only prompt emission, allowing us to calculate independent fission product yields only

To be fully effective for the study of cumulative yields, delayed emission must be added

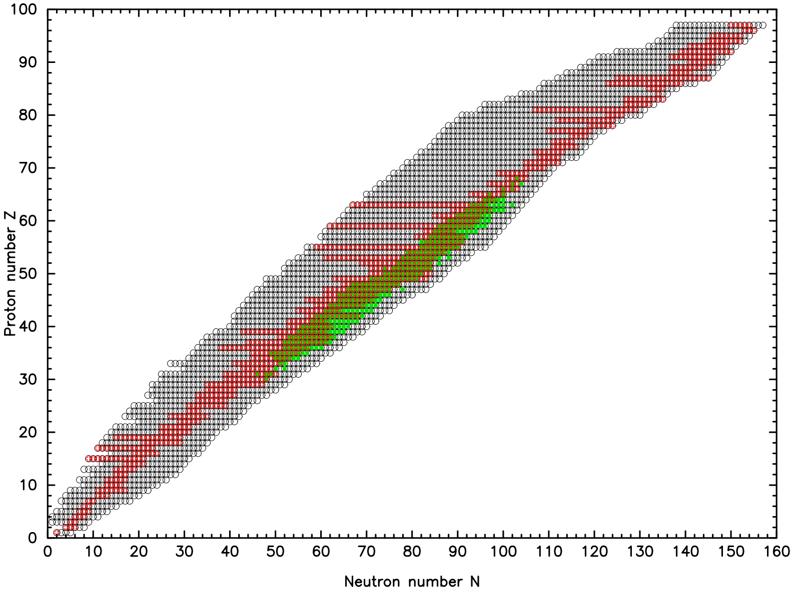
Studies of delayed emission kinematics would then also be possible



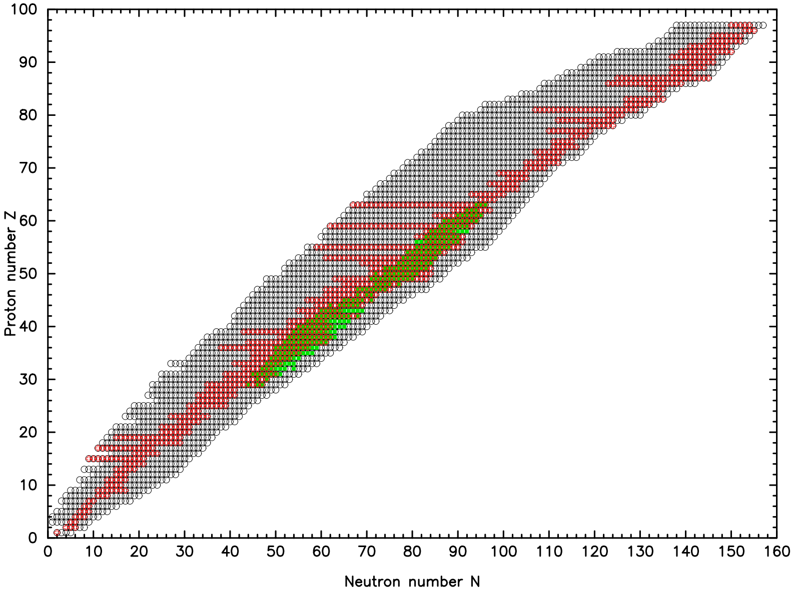
LBNL FIER package contains known delayed data

Can be incorporated in FREYA for cumulative yields

- Main data included in FIER:
  - half lives and branching ratios for most of the nuclear chart (black);
  - β-decay endpoints and intensities (red) available for subset of known nuclei;
- The overlap of the two includes most fission fragments (green)
- Modeling required to fill the gaps where β-decay data are missing



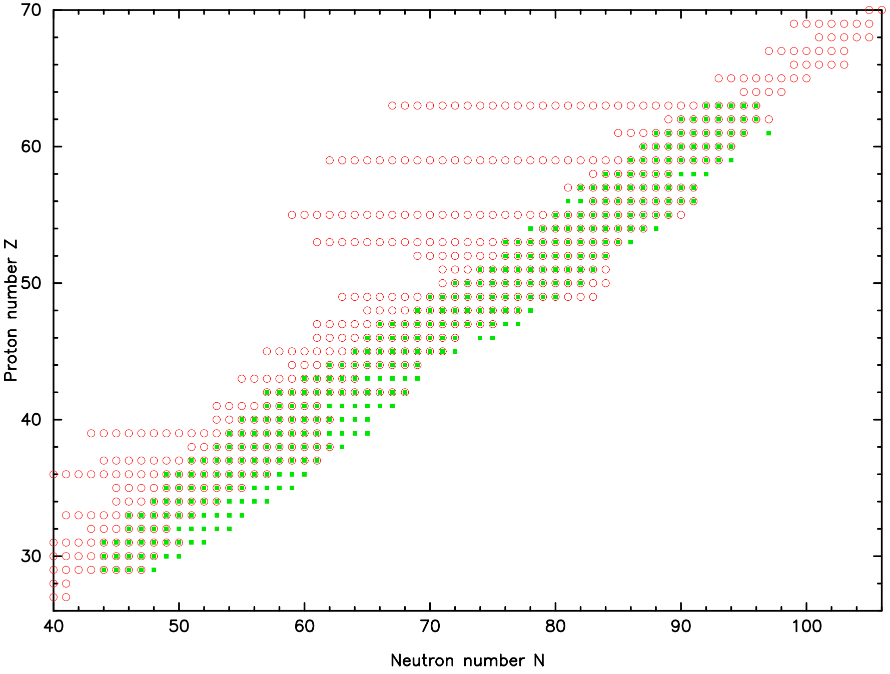
^{233}U(n,f)



^{252}Cf(sf)

FIER: E. Matthews et al., NIMA 891, 111 (2018)

Highlighting areas of β data and fission yield overlap



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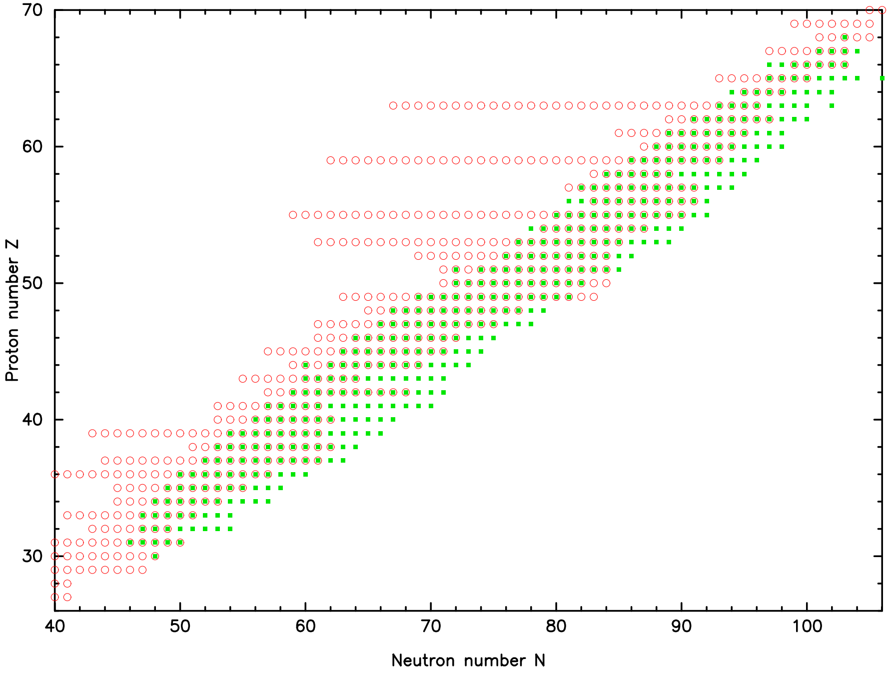

^{252}Cf(sf)

Timeline (I)

- FY20
  - Primary fission fragments for ^{239}Pu and ^{235}U as a function of E_n (DFTNESS+FELIX)
  - Fragment excitation energy E* from TDDFT runs for most likely fission in ^{239}Pu & ^{235}U
  - Effect of particle number projection in FELIX
  - Integrate FIER (β-decay and delayed photons) data into FREYA (prompt neutrons and photons)
- FY21
  - Finite-temperature calculations near scission for ^{239}Pu and ^{235}U (DFTNESS)
  - Evolution of fragment E* as a function of E_n for ^{239}Pu and ^{235}U on TDDFT runs
  - Empirical law for fragment E* as a function of E_n from TDDFT runs for ^{239}Pu and ^{235}U
  - Uncertainties of independent and cumulative yields from DFT inputs for ^{239}Pu and ^{235}U as a function of E_n (FREYA)

Timeline (II)

- FY22
  - Potential energy surfaces for odd-mass actinides ^{238}U and ^{232}Th (DFTNESS)
  - Initial fission yields for ^{238}U for thermal neutrons (FELIX)
  - Initial and independent yields for minor actinides (DFTNESS+FELIX, FREYA)
  - Independent and cumulative yields for ^{239}Pu and ^{235}U based on E* "law" extracted from TDDFT runs (FREYA)

- FY23
  - Initial yields for select minor actinides (DFTNESS+FELIX)
  - Independent and cumulative yields for minor actinides (FREYA)
  - FREYA under version control and code refactoring