FREYA and fission yields

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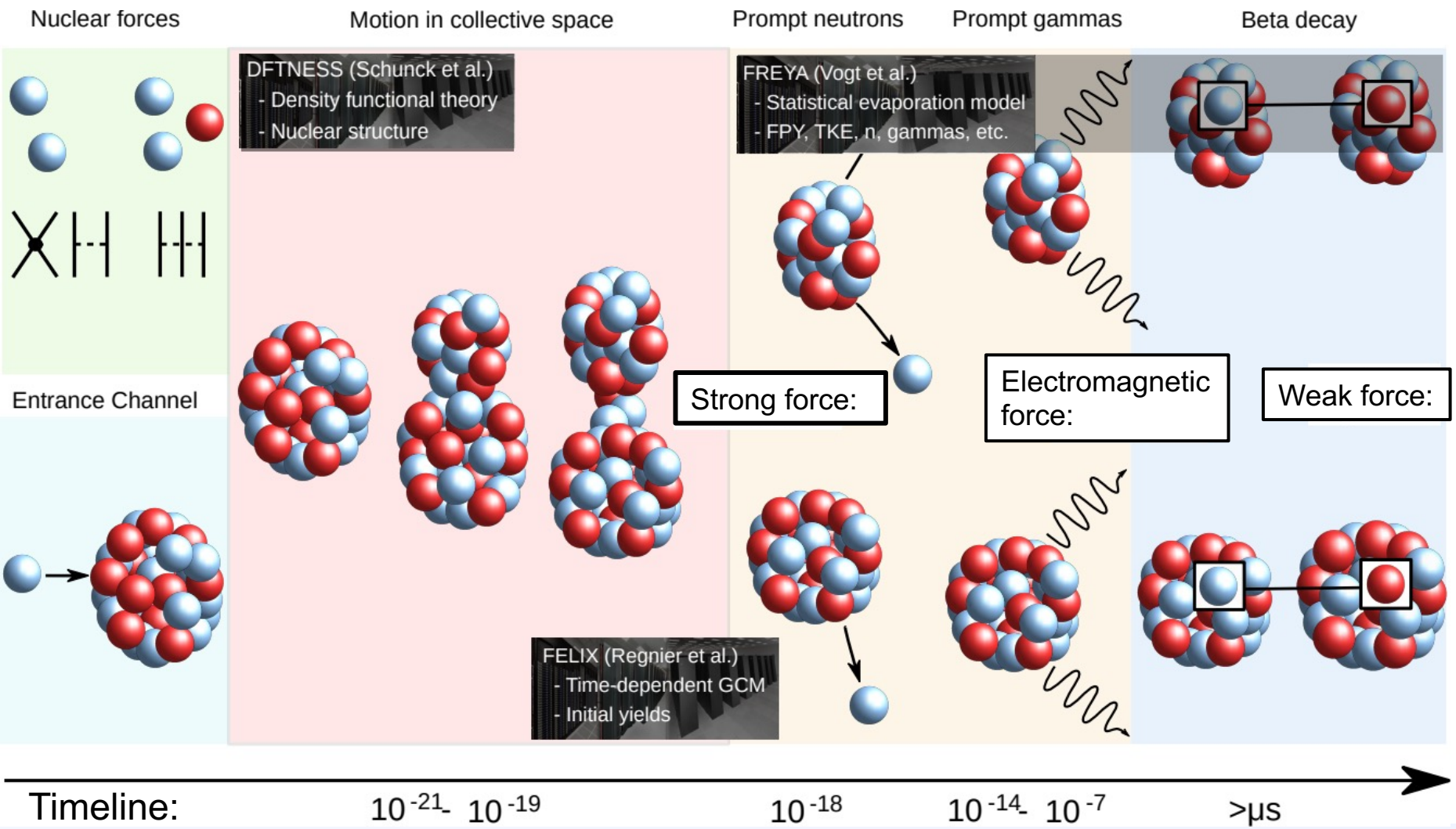
FREYA capability covers from fission process from compound nucleus through beta decay



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

Event-by-event (Monte Carlo) modeling has been used in high energy nuclear and particle physics when there are multiple outcomes – useful for studying detector response and predicting outcomes of experiment

Calculational framework easily adoptable 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: $\{ \boldsymbol{p}_n \}$, $n = 1,\ldots,\nu$

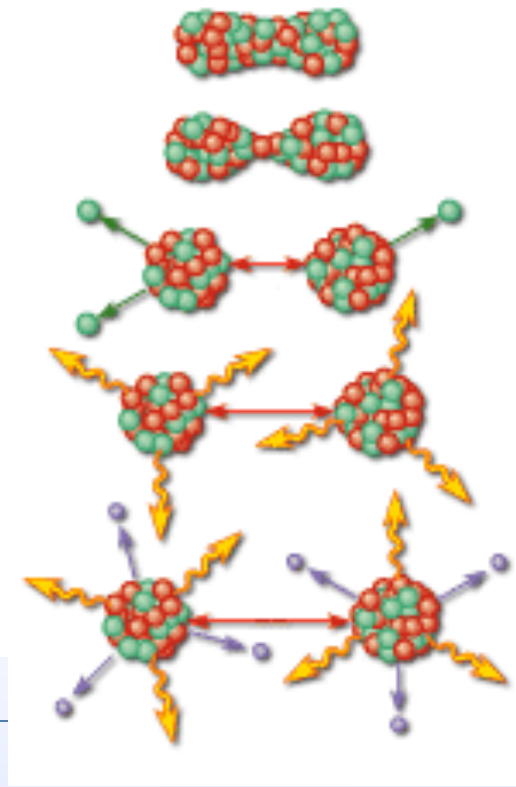
N_γ photons: $\{ \boldsymbol{p}_m \}$, $m = 1,\ldots,N_\gamma$

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



Brief summary of how FREYA works

- For a given Z, A and energy ($E_n = 0$ for spontaneous fission), **FREYA** selects mass and charge of fragment from either data or a model (5 gaussian) parameterization, working on making a transition to yields based on potential energy surfaces a la Randrup & Moller
- Second fragment mass and charge obtained assuming binary fission, mass and charge conservation
- From fragment identities, fission Q value is obtained using current nuclear mass tables
- TKE(A_H) sampled from distribution (generally data); TXE obtained by energy conservation
- 'Spin temperature' sets level of rotational energy, remaining TXE given to intrinsic excitation
- Intrinsic excitation divided between fragments, based on level densities, then thermal fluctuations introduced to obtain final excitation energy sharing
- Thermal fluctuations remove energy from TKE to maintain energy conservation, equivalent to width of TKE distribution
- Spin fluctuations (conserving angular momentum), introduced for wriggling and bending modes, tilting and twisting modes currently ignored
- Pre-equilibrium emission and n-th chance fission included for $E_n \leq 20$ MeV
- After scission, fragments are de-excited first by emitting neutrons (Weisskopf-Ewing spectra) until the remaining energy is less than the neutron separation energy
- Photon emission follows until fragment no longer excited (statistical, then discrete emission)

FREYA has few physics-based parameters

- The five parameters here, most accessible to user, depend on input modeling, particularly of excitation energy sharing, and directly affect certain observables, as outlined below, tuned by comparison with data and performing optimization
- The fissioning nucleus, with A_0 nucleons, has an initial excitation energy E_{sc} including statistical and rotational excitation of the fragments, E_{stat} and E_{rot} respectively
- The level density parameter, $a \sim A_0/e_0$, relates the temperature to the excitation energy, as in $E_{sc} = (A_0/e_0)\ T^2_{sc} - e_0$ is the first parameter
- The fragment 'spin temperature' fluctuates around the scission temperature T_{sc} according to second parameter c_s, $T_s \sim c_s\ T_{sc}$, affecting E_{rot} and photon observables
- Total excitation energy, $E_{sc} = E_{rot} + E_{stat}$, E_{stat} is dissipated through neutron emission
- Statistical energy is partitioned between light and heavy fragments according to level density parameters, $E_{stat} = E^*_L + E^*_H$
- The light fragment energy is enhanced by third parameter, $x > 1$, by $E'^*_L = x\ E^*_L$ so that $E'^*_H = E_{stat} - E'^*_L$, affecting neutron multiplicity vs fragment mass
- Fragments get thermal variance, fourth parameter, c, controlling maximum available excitation and affecting neutron multiplicity distribution and moments
- Fifth parameter dTKE adjusts average TKE to fix average neutron multiplicity
- All parameters affect neutron spectrum

FREYA also has “experimental” parameters

- g_{min} is the minimum photon energy accessible to a detector
- t_{max} is the time over which prompt photons are detected
- t_{delay} is the at which late (non-prompt) decays are measured
  - Several cases considered
    - No late decays, prompt emission only
    - “Infinite time”, where emission should continue to the ground state
    - Intermediate time corresponding to time of measurement
- There are other more “hidden” parameters involved also (similar for all complete model codes):
  - Branching ratios
  - Half lives
  - β decay information (endpoint is determined from Q value of decay)
  - Nuclear masses

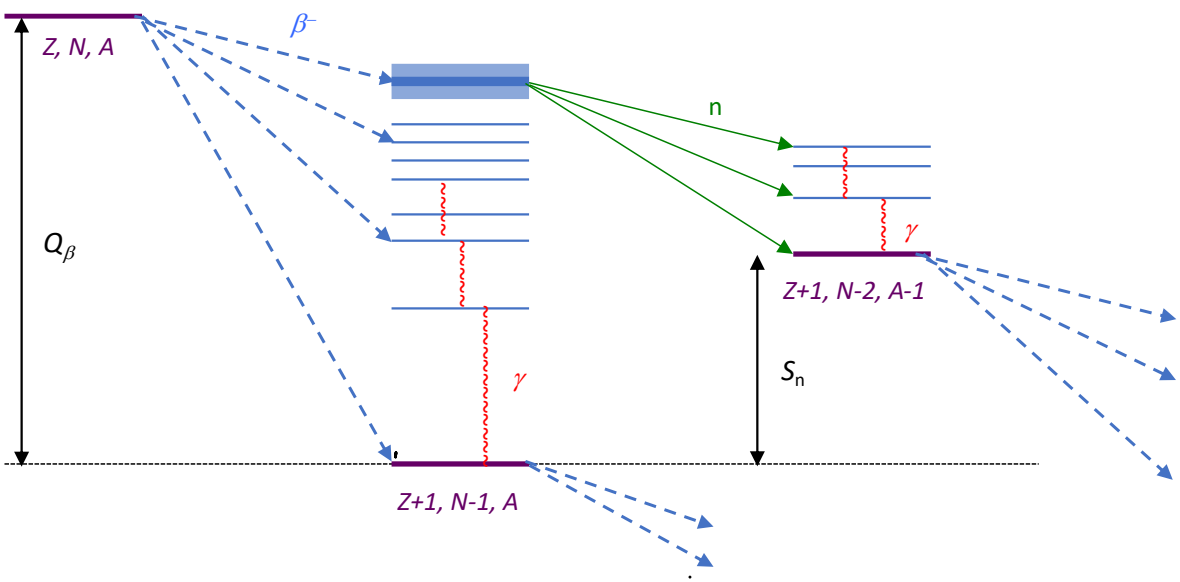
β-delayed emission has been included in FREYA

Before, FREYA included only prompt emission, allowing us to calculate only independent fission product yields

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

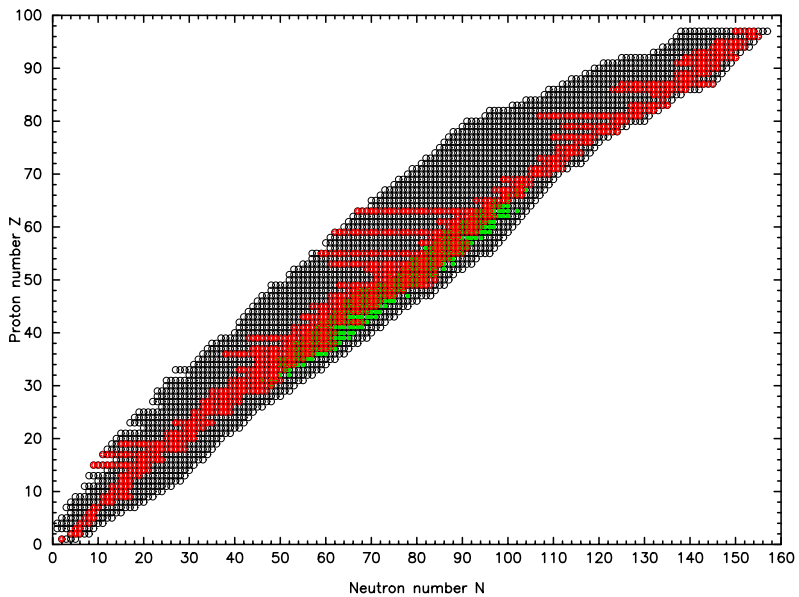
Studies of delayed emission kinematics are also possible

Main data included from: E. Matthews et al., NIMA 891, 111 (2018)
half lives and branching ratios for most of the nuclear chart;
β-decay endpoints and intensities available for subset of known nuclei

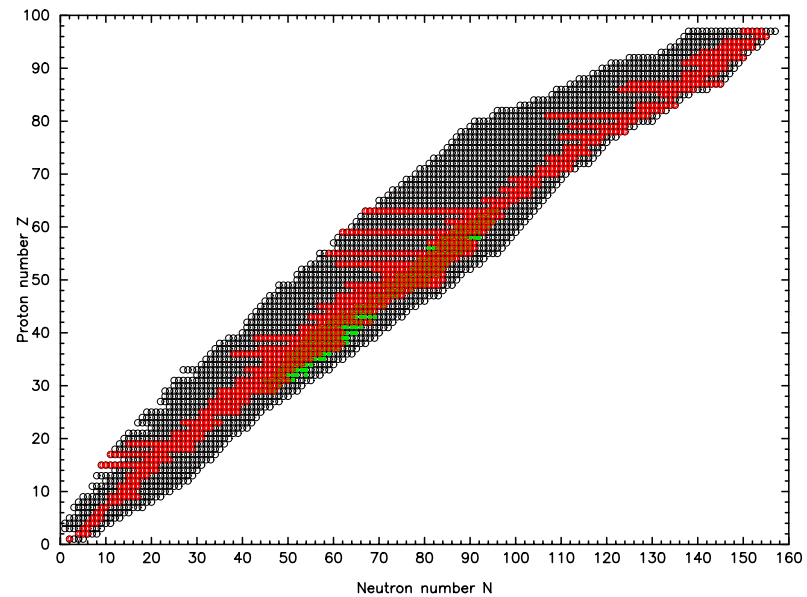


LBNL FIER package contains known delayed data

- 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)



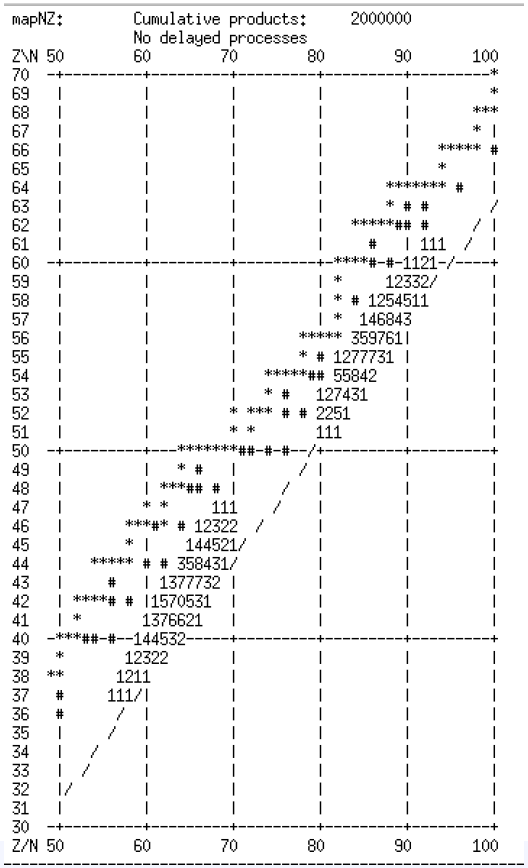
^{252}Cf(sf)

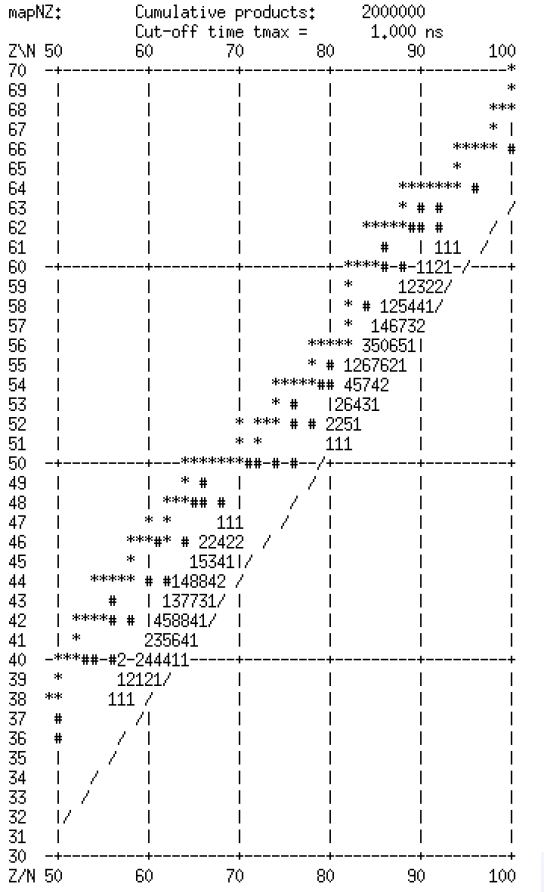
FIER: E. Matthews et al., NIMA 891, 111 (2018)

Fragments and Prompt Products

- == most stable isobar;
- # == endpoint of single beta decays (not double beta decay);
- / == Z/A

Prompt fragments



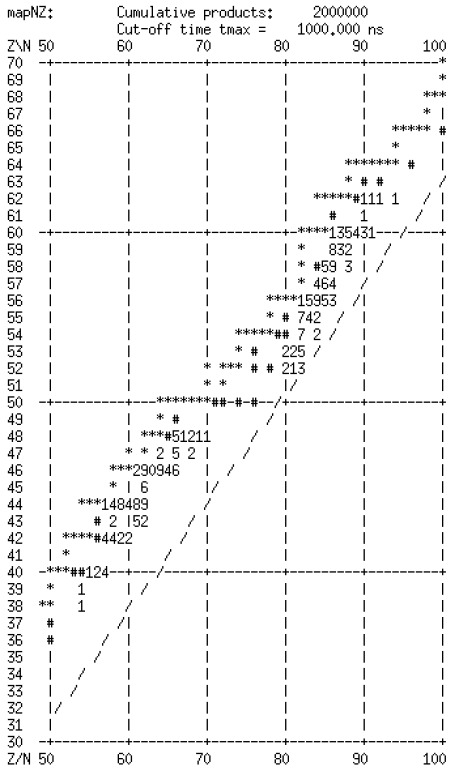


Prompt products (after neutron and prompt photon emission)

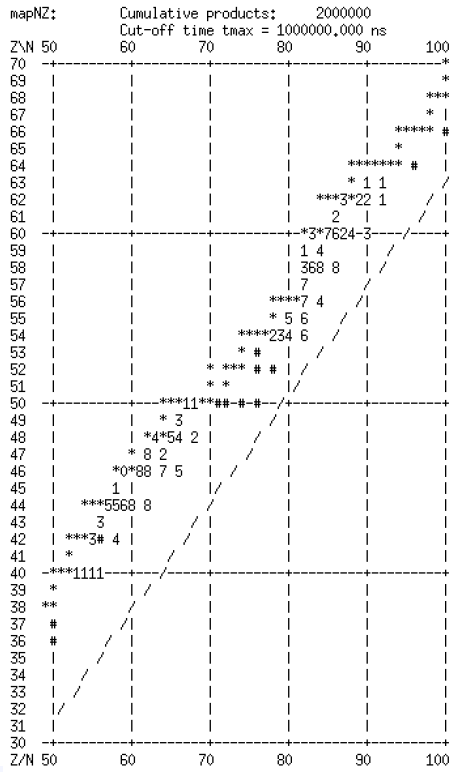
Cumulative Yields at different times

- == most stable isobar;
- # == endpoint of single beta decays (not double beta decay);
- / == Z/A

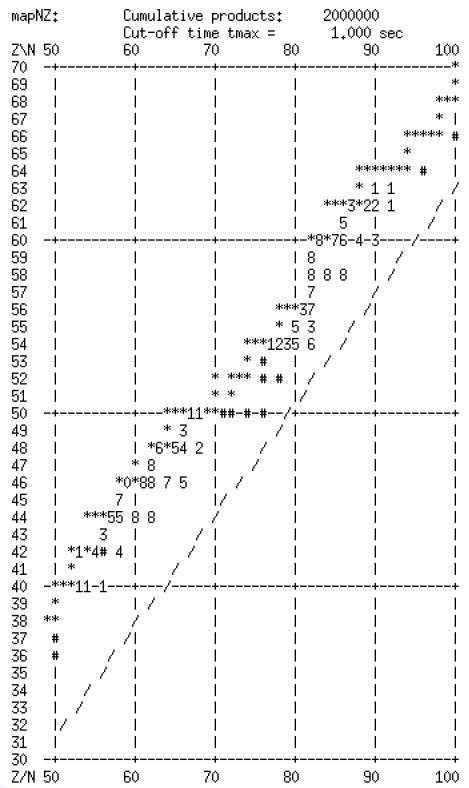
1 μs



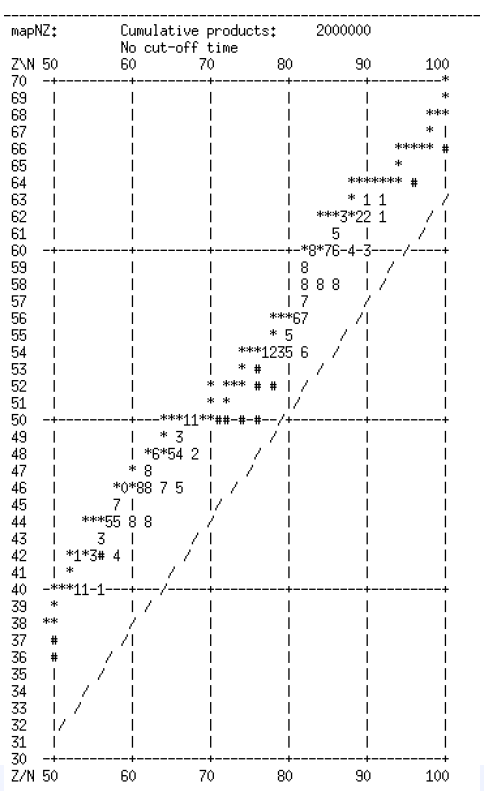
1 ms



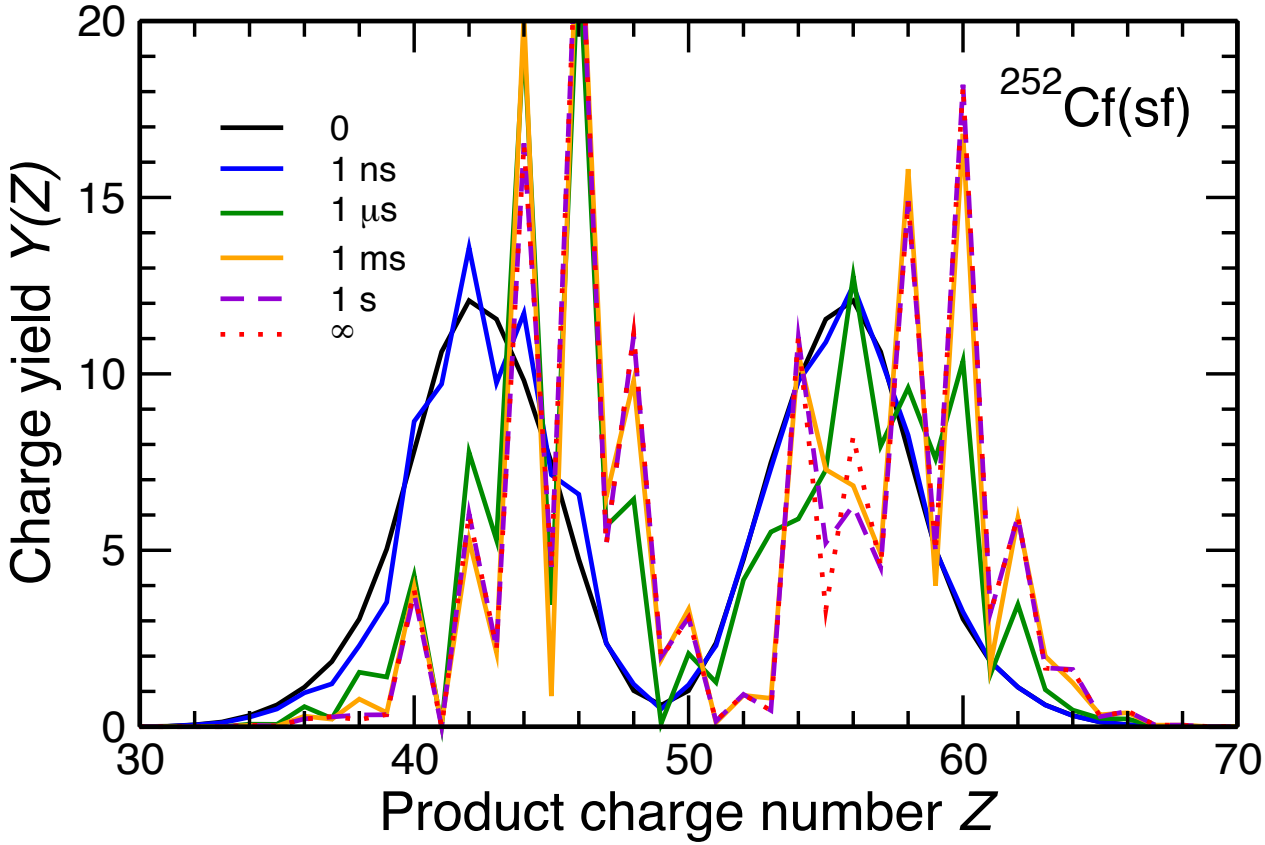
1 s



No cutoff



Biggest Changes in Y(Z) are at ~1μs, few afterward



FREYA and fission yields

- Unlike, say GEF, FREYA does not calculate the fission fragment yields, instead it uses fragment yield data or model calculations as input
- FREYA can be adapted to take a variety of yields
  - It was used in r-process nucleosynthesis calculations by taking the Y(A) and TKE(A) from GEF as input to study nuclear abundance patterns and photon emission as a fission signature from neutron star mergers
  - It can take model calculations of Y(A), together with TKE(A) from data – where available – or a parameterization
  - It can take Y(Z,A,TKE) – we studied the sensitivity of average neutron multiplicity to changes in TKE(A) with 10K realizations of Y(Z,A,TKE)
- FREYA is also very adept at studying the sensitivity of observables to changing yields and input parameters on
  - Neutron emission
  - Photon emission
  - Neutron-photon correlations
  - Spin-related effects and correlations

(Some) FREYA references – not comprehensive or entirely up to date

- **FREYA** developed in collaboration with J. Randrup (LBNL); neutron-transport code integration by J. Verbeke (LLNL)
- **FREYA** journal publications: Phys. Rev. C **80** (2009) 024601, 044611; **84** (2011) 044621; **85** (2012) 024608; **87** (2013) 044602; **89** (2014) 044601; **90** (2014) 064623; **96** (2017) 064620; version 1.0 in Comp. Phys. Comm. **191** (2015) 178; version 2.0.2 in Comp. Phys. Comm. **222** (2018) 263.
- Invited book chapter, R. Vogt and J. Randrup, "Nuclear Fission", Chapter 5 of '100 Years of Subatomic Physics', World Scientific, 2013
- Review (EPJ A **54** (2018) 9); Book "Nuclear Fission" (2023), edited with P. Talou
- Contributed to (and coauthored) papers on neutron polarization in photofission, Mueller *et al,* Phys. Rev. C **89** (2014) 034615; neutron-gamma correlations, Wang *et al*, Phys. Rev. C **93** (2016) 014606, Marcath *et al*, Phys. Rev. C **97** (2018) 044622, Marin et al, (3 papers), Giha et al (in press); neutron-neutron correlations, , Schuster et al, Phys. Rev. C **100** (2019) 014605; Verbeke *et al*, Phys. Rev. C **97** (2018) 044601; Pozzi *et al,* Nucl. Sci. Eng. **178** (2014) 250.
- Isotopes currently included: spontaneous fission of ^{252}Cf, ^{244}Cm, ^{238,240,242}Pu, ^{238}U and neutron-induced fission of ^{233,235,238}U(n,f), ^{239,241}Pu(n,f) for $E_n \leq 20$ MeV