Parameter Optimization of FREYA

Ramona Vogt (LLNL and UC Davis)

Alex Tuckey, David Breitenmoser, Shaun Clarke and Sara Pozzi (U Michigan)

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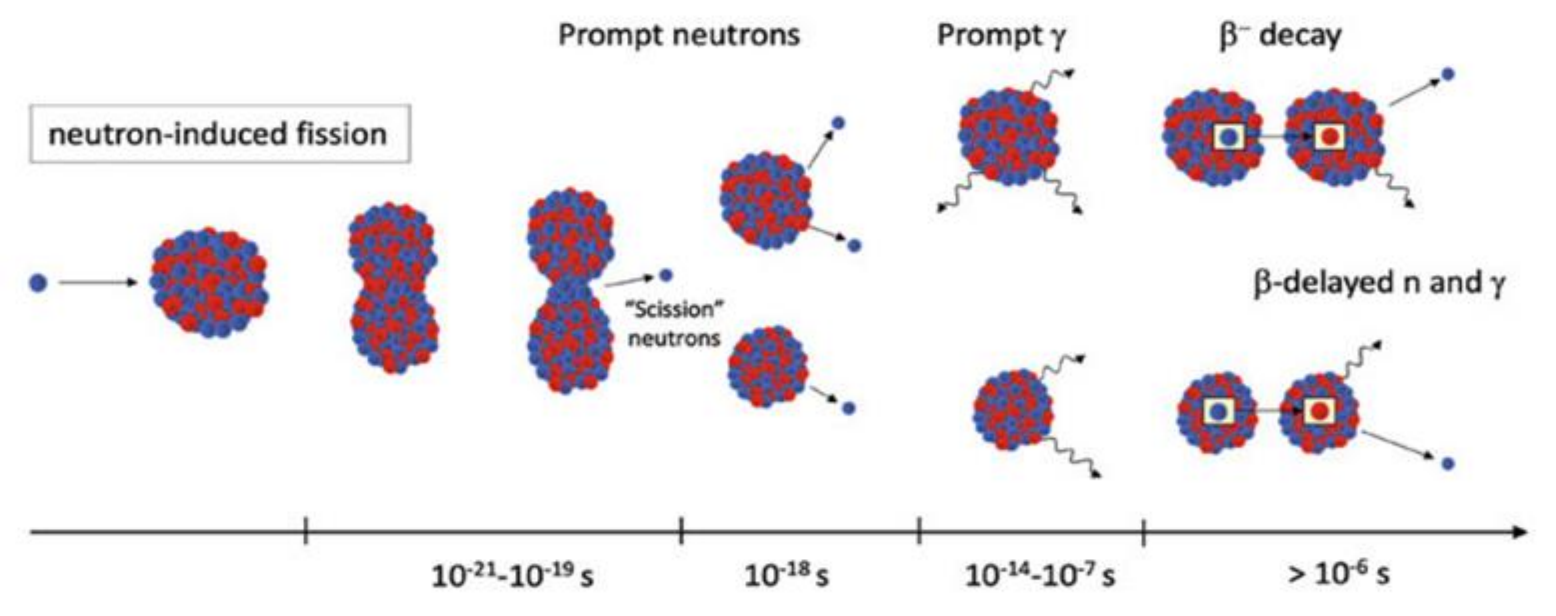
Motivation

- We first optimized parameters in FREYA beyond “best guess” values in 2019
- New data plus a desire to challenge and go beyond the parameters obtained in an analysis dominated by the neutron number distributions, particularly for the spontaneous fission of Pu isotopes, led us to make a new optimization
- We first check $^{252}Cf(sf)$ as a test of the optimization and then examine other isotopes



FREYA has 5 physics-based parameters

1) e_0: level density parameter, $a \sim A_0/e_0$, relates the temperature to the excitation energy, as in $E_{sc} = (A_0/e_0)$; Ignatuyk parameterization of a used

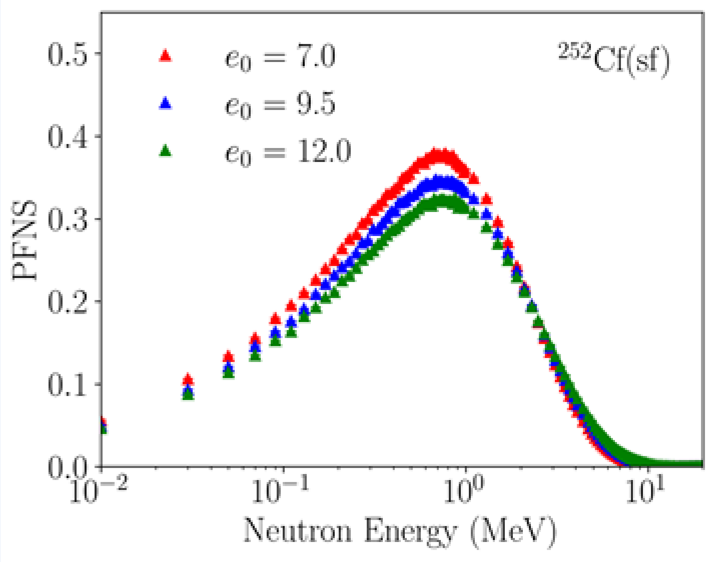
2) c_S: the fragment 'spin temperature', fluctuates around the scission temperature $T_s \sim c_s T_{sc}$, affecting rotational energy E_{rot} and photon observables

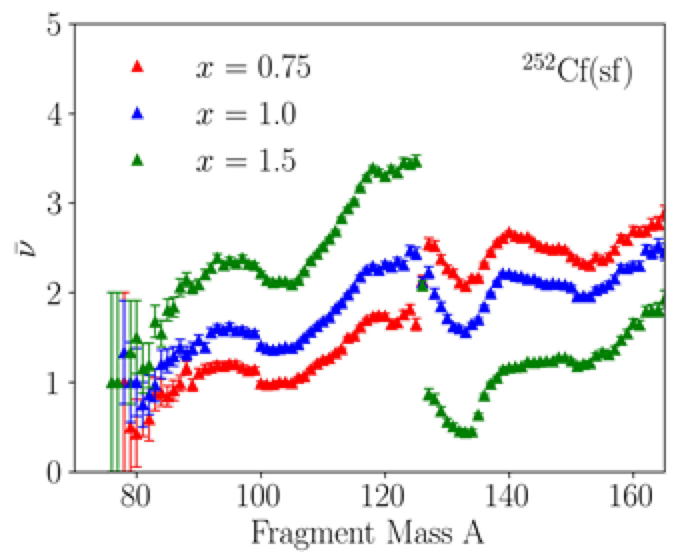
3) x: enhancement of light fragment excitation energy
   - Total excitation energy, $E_{sc} = E_{rot} + E_{stat}$, E_{stat} is dissipated through neutron emission
   - Statistical energy is partitioned between light and heavy fragments according to level density parameters, $E_{stat} = E^*_L + E^*_H$
   - Tthe light fragment energy is enhanced by $x > 1$, thus $E'^*_L = x E^*_L$ so that $E'^*_H = E_{stat} - E'^*_L$, affecting neutron multiplicity vs fragment mass

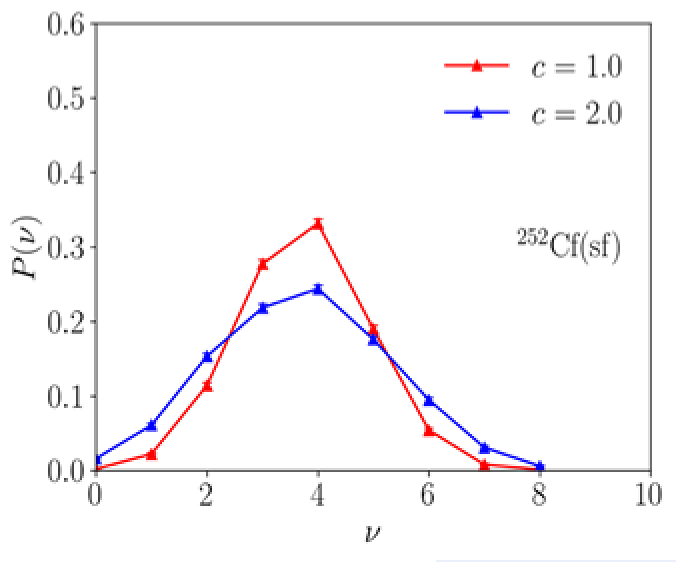
4) c: fragments given thermal variance, c, that controls maximum available excitation and affecting neutron multiplicity distribution and moments

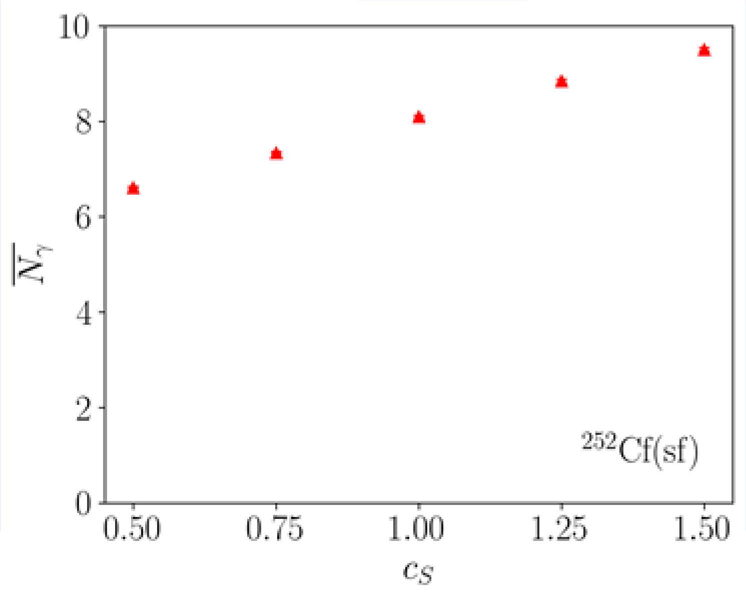
5) dTKE: adjusts average TKE to fix average neutron multiplicity

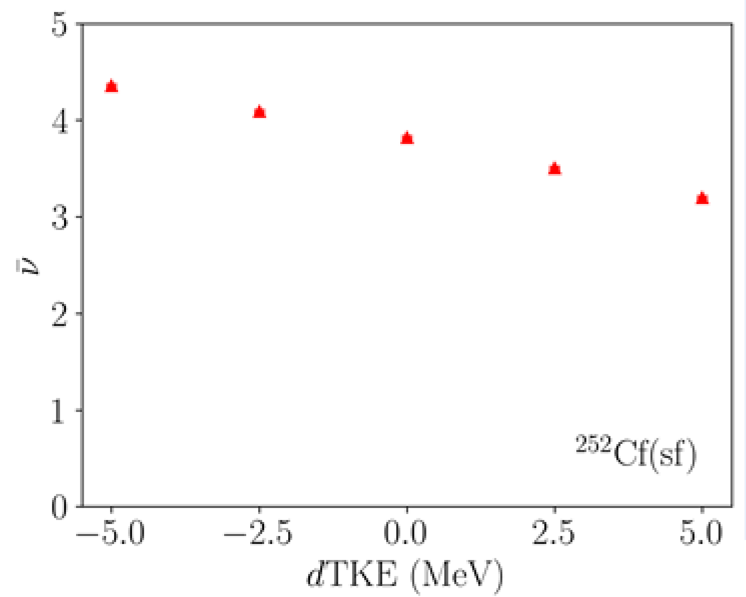
FREYA parameters directly affect fission observables











FREYA parameters first optimized in 2019

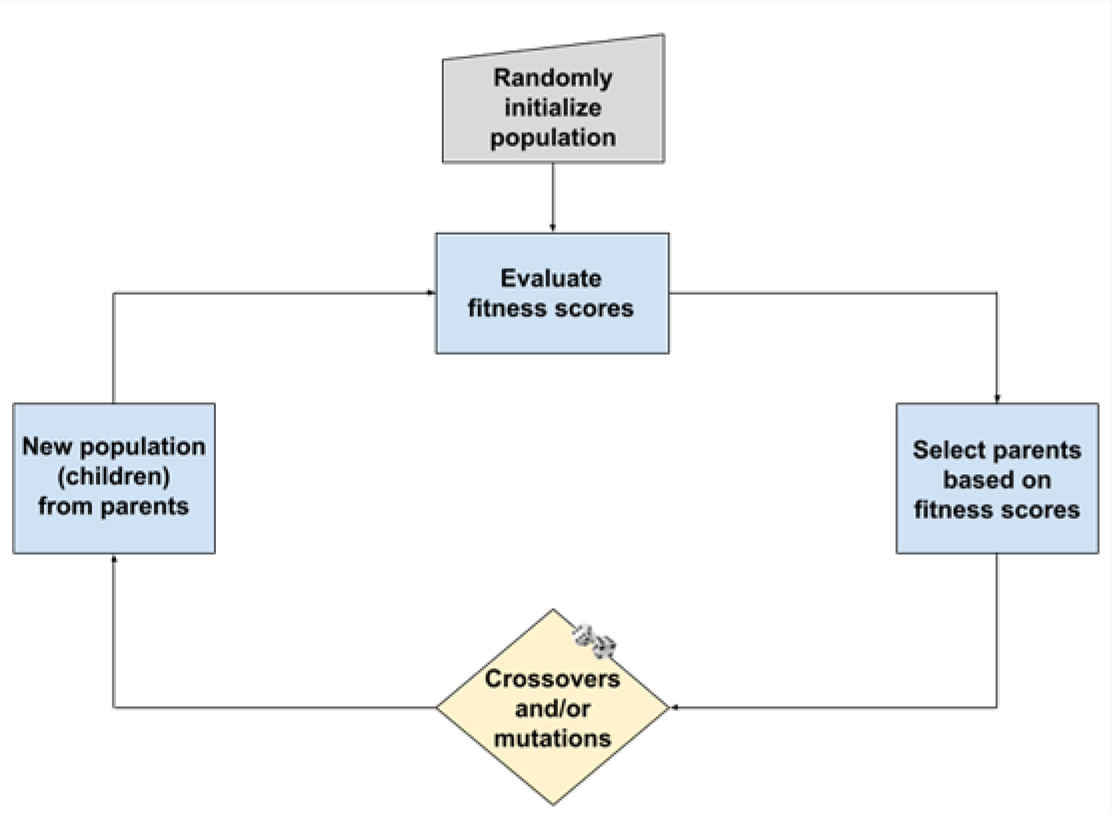
- FREYA parameters were first optimized for all spontaneously fissioning isotopes by vanDyke, Bernstein,& RV NIM A **922** (2019) 36

- Simulated annealing employed for optimization:
    - User specified initial guess
    - Generates random guess and calculates uncertainty
    - A new solution nearby is randomly generated and its uncertainty is calculated
    - New solution is accepted if it has a lower uncertainty
    - New solution may not be accepted If the uncertainty is higher
    - Over time, the algorithm is less willing to go to regions of higher uncertainty, allowing it to avoid local minima
- More data are used now for ^{240,242}Pu

Isotope	# Data Sets + Evaluations	Key Observables
^{252}Cf	6 (6)	PFNS, $P(\nu)$, $\langle\nu\rangle$, $\nu(A)$, $\langle N_\gamma \rangle$
^{238}Pu	2 (2)	$P(\nu)$, $\langle\nu\rangle$
^{240}Pu	4 (2)	PFNS, $P(\nu)$, $\langle\nu\rangle$, *n-n*, $\langle N_\gamma \rangle$
^{242}Pu	3 (2)	PFNS, $P(\nu)$, $\langle\nu\rangle$, $\langle N_\gamma \rangle$

We now use a genetic algorithm to improve optimization

- Similar to evolution in nature, a genetic algorithm employs crossovers (exchanging material between parents) and mutations
- It is independent of the initial guess (randomly generated initial population) and parallelizable



Crossover

parent1 = 0011
parent2 = 1100

0011 1100

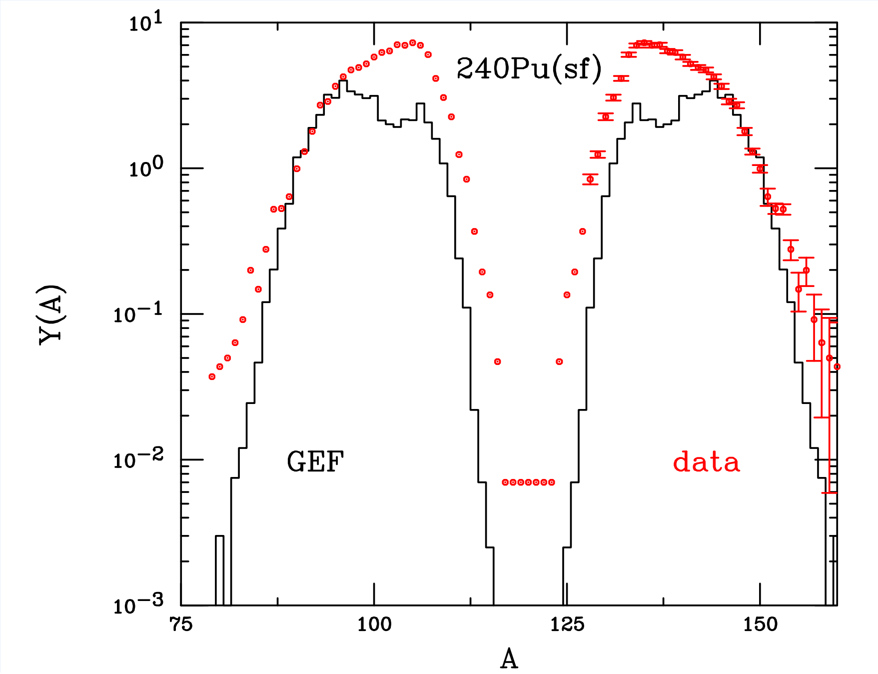
child1 = 0000
child2 = 1111

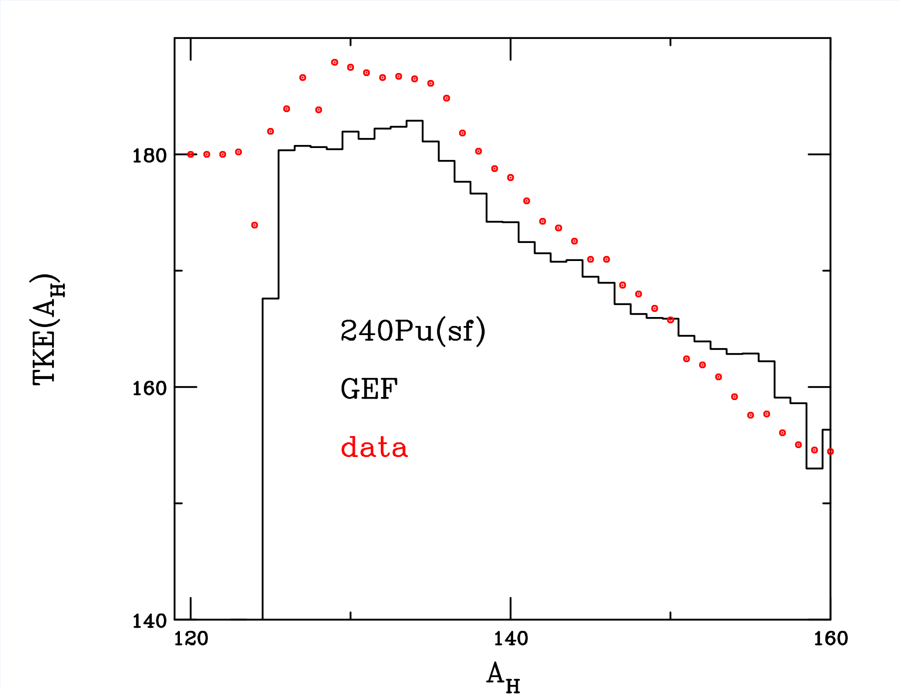
Mutation

0011 → 0001

We explored the choice of initial yields for Pu(sf)

- We checked the Schilibeeckx yields (NPA **545**, (1992) 623) used in FREYA against the GEF yields and decided to stick with the data-based yields already in FREYA
- GEF Y(A) was much narrower than data; TKE missing at symmetry & different slope than data

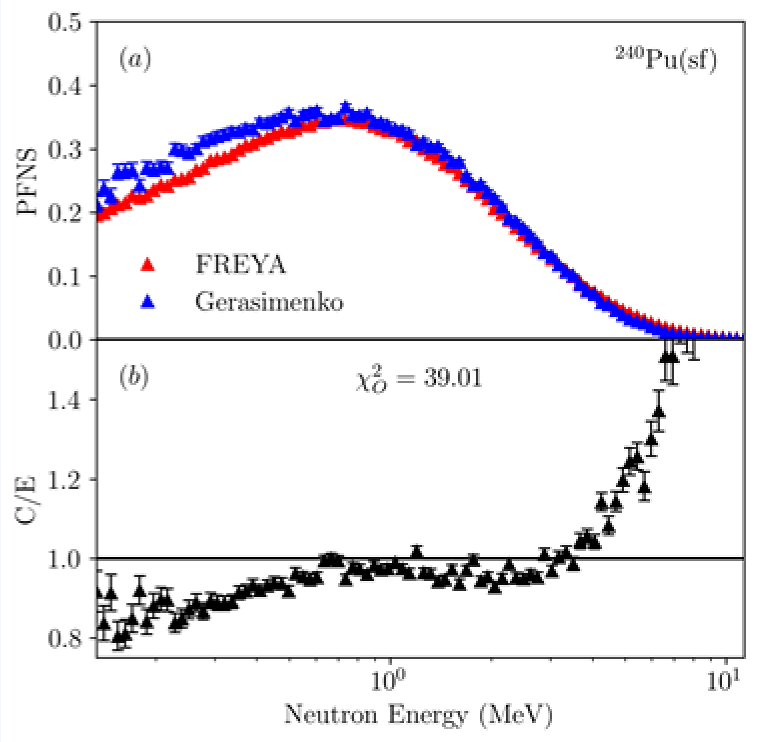


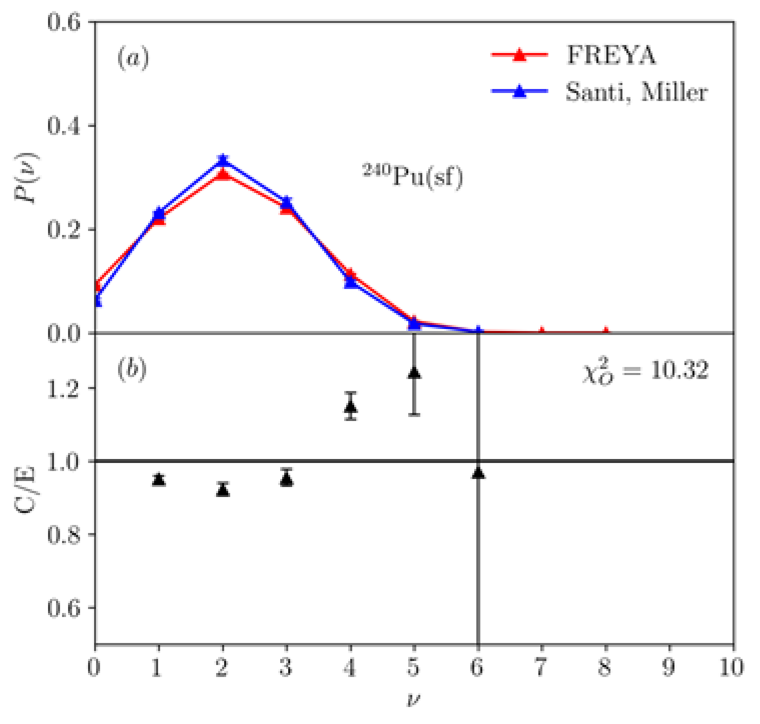


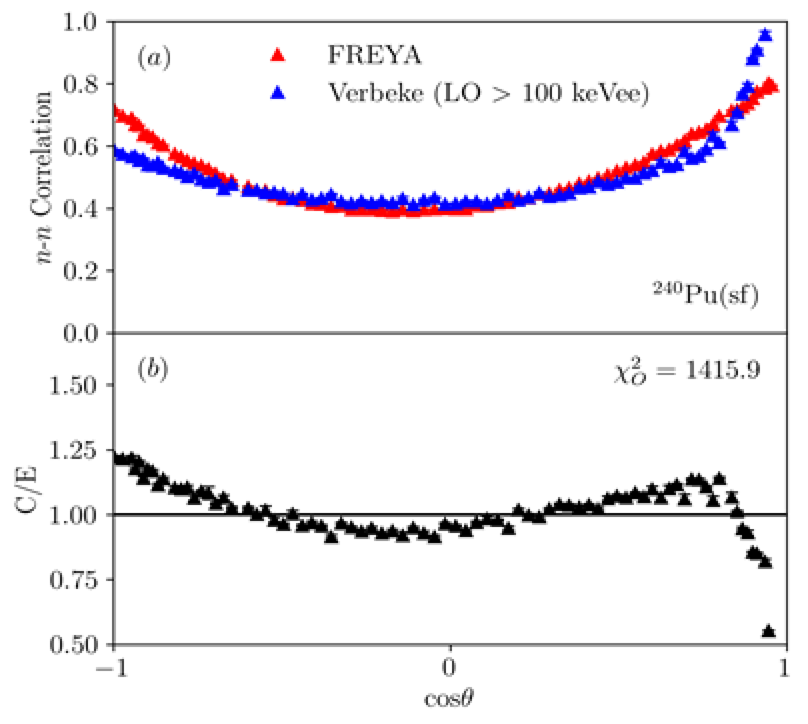
Improved χ^2 compared to VanDyke et al.

	e_0 (1/MeV)	x	c	c_S	dTKE (MeV)	χ^2
^{238}U(sf)						
this work	9.675 ± 0.384	1.338 ± 0.063	1.011 ± 0.007	1.029 ± 0.055	-1.512 ± 0.102	0.729
Ref. [1]	10.391 ± 0.352	1.220 ± 0.071	0.929 ± 0.283	0.899 ± 0.280	-1.375 ± 0.727	1.248
^{238}Pu(sf)						
this work	7.318 ± 0.492	1.000 ± 0.029	1.922 ± 0.028	1.198 ± 0.082	-1.462 ± 0.122	0.321
Ref. [1]	10.521 ± 0.581	1.232 ± 0.221	1.968 ± 0.071	0.893 ± 0.071	-1.408 ± 3.424	1.001
^{240}Pu(sf)						
this work	11.892 ± 0.022	1.410 ± 0.004	2.635 ± 0.048	1.393 ± 0.037	-3.898 ± 0.083	3222.886
Ref. [1]	10.750 ± 0.138	1.307 ± 0.071	3.176 ± 0.355	0.908 ± 0.023	-3.219 ± 0.112	4706.974
^{242}Pu(sf)						
this work	7.092 ± 0.573	1.499 ± 0.041	2.093 ± 0.044	0.974 ± 0.019	-1.557 ± 0.109	64.551
Ref. [1]	10.018 ± 1.768	1.144 ± 0.152	3.422 ± 0.341	0.911 ± 0.257	-1.662 ± 0.118	149.775
^{244}Cm(sf)						
this work	8.362 ± 0.389	1.478 ± 0.012	1.292 ± 0.038	0.714 ± 0.079	-3.954 ± 0.121	68.221
Ref. [1]	10.488 ± 1.519	1.239 ± 0.148	1.291 ± 0.582	0.906 ± 0.322	-4.494 ± 0.167	152.740
^{252}Cf(sf)						
this work	10.430 ± 0.496	1.260 ± 0.006	1.185 ± 0.021	0.890 ± 0.064	0.508 ± 0.293	288.708
Ref. [1]	10.429 ± 1.090	1.274 ± 0.187	1.191 ± 0.362	0.875 ± 0.020	0.525 ± 0.078	299.686

^{240}Pu(sf) fit results with n-n correlations included

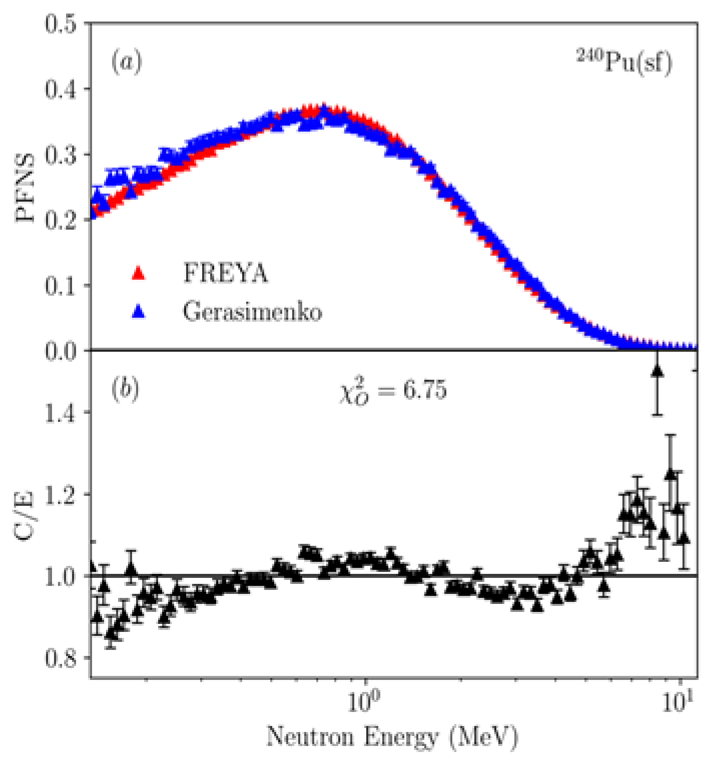


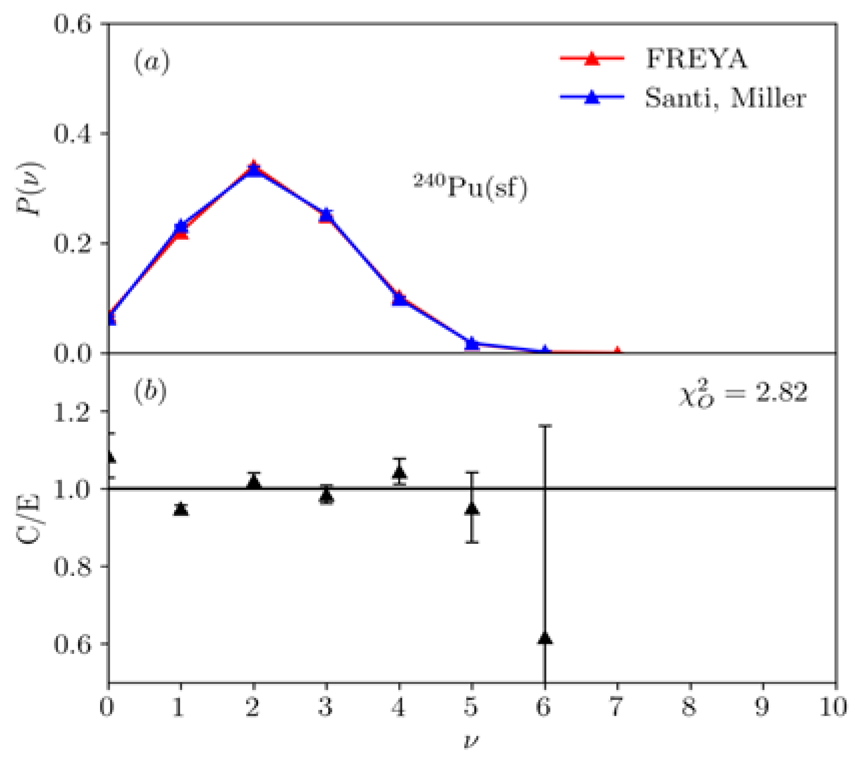


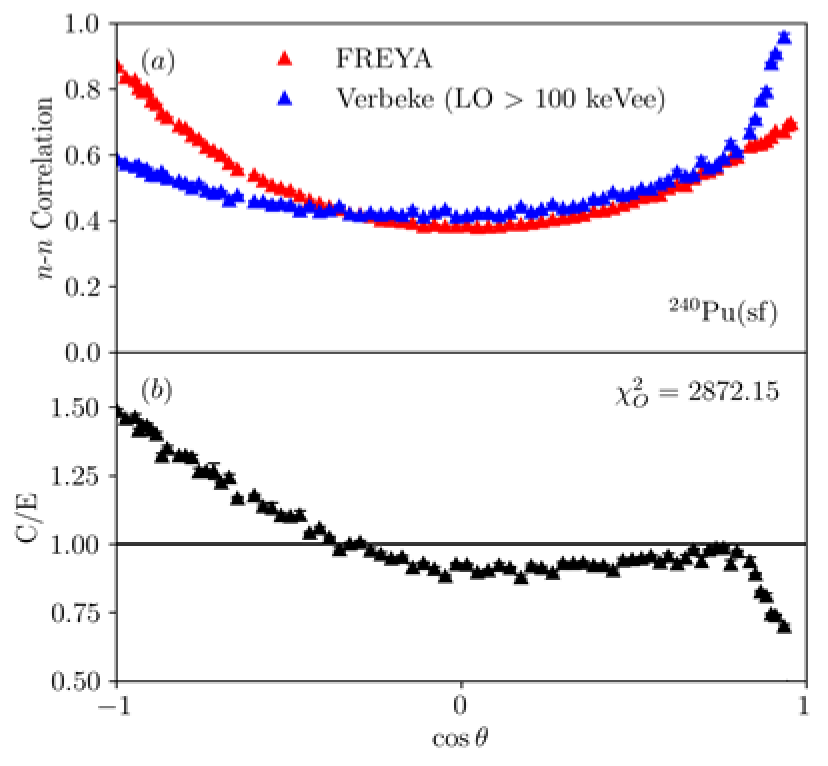


^{240}Pu(sf) fit results without n-n correlations included

^{240}Pu(sf)	e_0 (1/MeV)	x	c	c_S	dTKE (MeV)	χ^2
this work	11.304 ±1.208	1.267 ±0.139	1.708 ±0.136	1.469 ±0.136	-3.833 ±0.401	15.380
Van Dyke et al.	10.750 ± 0.138	1.307 ± 0.071	3.176 ± 0.355	0.908 ± 0.023	-3.219 ± 0.112	616.988







Summary

- We have improved the FREYA optimization by using a genetic algorithm
- We are checking the effect of including n-n correlations on the ^{252}Cf(sf) fit where we also have $\nu(A)$ data to see if it biases the fits
- We are finalizing a paper on the spontaneous fission results, along with fits to thermal neutron-induced fission
- Looking ahead, we want to optimize the parameters in neutron-induced fission as a function of incident neutron energy