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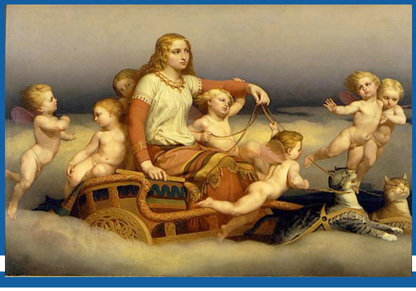
^{239}Pu Spectral Evaluation: Fun with FREYA



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How FREYA works

- Assume binary fission of compound nucleus with mass A_c and charge Z_c formed by incident neutrons with energy E_n on actinide with mass $A_c - 1$
- Sample mass and charge of light, L, and heavy, H, fragments from fission fragment distributions, conserving mass and charge
- Determine fission Q from fragments, divide Q value between fragment kinetic and excitation energies
- Fix total kinetic energy, TKE, by sampling kinetic energy due to mutual Coulomb repulsion, obtain total excitation energy by conservation, $\mathrm{TEE} = Q - \mathrm{TKE}$
- Divide TEE between light and heavy fragments
- Allow for temperature fluctuations in small systems; adjust TKE accordingly to retain total energy conservation
- Evaporate neutrons from each fragment until excitation energy is too low for further neutron emission
- Prompt gamma emission follows after prompt neutron emission ceases
- Still to be implemented: multi-chance fission for E_n greater than a few MeV

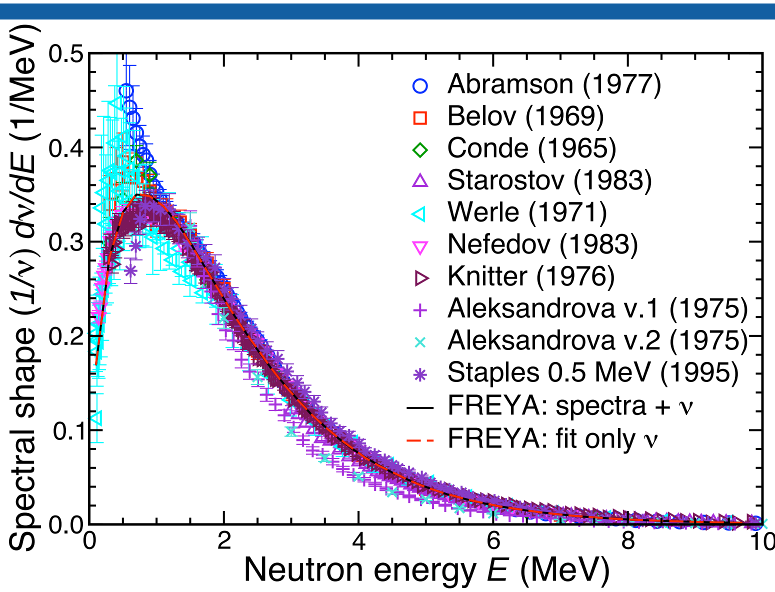
Fitting to data isn't all it's cracked up to be

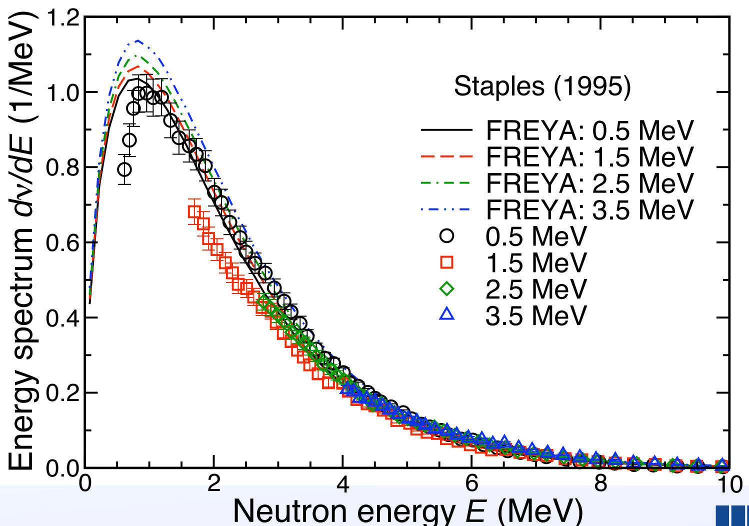
An improved spectral evaluation involves understanding more than just the spectra

- There are big uncertainties in our overall understanding of fission. To reduce these uncertainties, we need to look at the 'big picture', not just spectra since other physics processes feed into the spectra.
- Both the average neutron multiplicity, $\overline{\nu}$, and the spectra, $d\overline{\nu}/dE$, depend on the physics of the fission process. The two are intimately linked and can't really be treated separately, N.B. $\int dE(d\overline{\nu}/dE) = \overline{\nu}$.
- Improvements in the spectral evaluation will come with improved modeling of fission.

Data are often insufficient for comprehensive understanding of fission process

- Spectral data for thermal neutrons are inconsistent with each other and have large uncertainties in important regions, much larger than the constraints on $\overline{\nu}$ itself
- Published spectral data do not extend into the low energy region, only extend to incident neutron energies of a few MeV
- Measurements of other quantities such as total fragment kinetic energy and neutron multiplicity as a function of fragment mass only exist for low incident energies
- Modeling of complete fission events helps fill the gaps in data





Statistical methods used to match FREYA simulations to data

Three `FREYA` parameters 'tuned' to both spectral data and average neutron multiplicity, $\overline{\nu}$, or to the more accurate measurements of $\overline{\nu}$ alone:

- the scale factor s of the average distance between fragment tips, obtained from $\mathrm{TKE}(A_H)$;
- the asymptotic level density parameter, e_0, which sets the fragment 'temperature' for neutron evaporation;
- the relative excitation of the light and heavy fragments, x where $x = 1$ is the equal temperature situation with the same number of neutrons emitted from both fragments while $x > 1$ gives more neutrons evaporated from the light fragment than the heavy fragment.

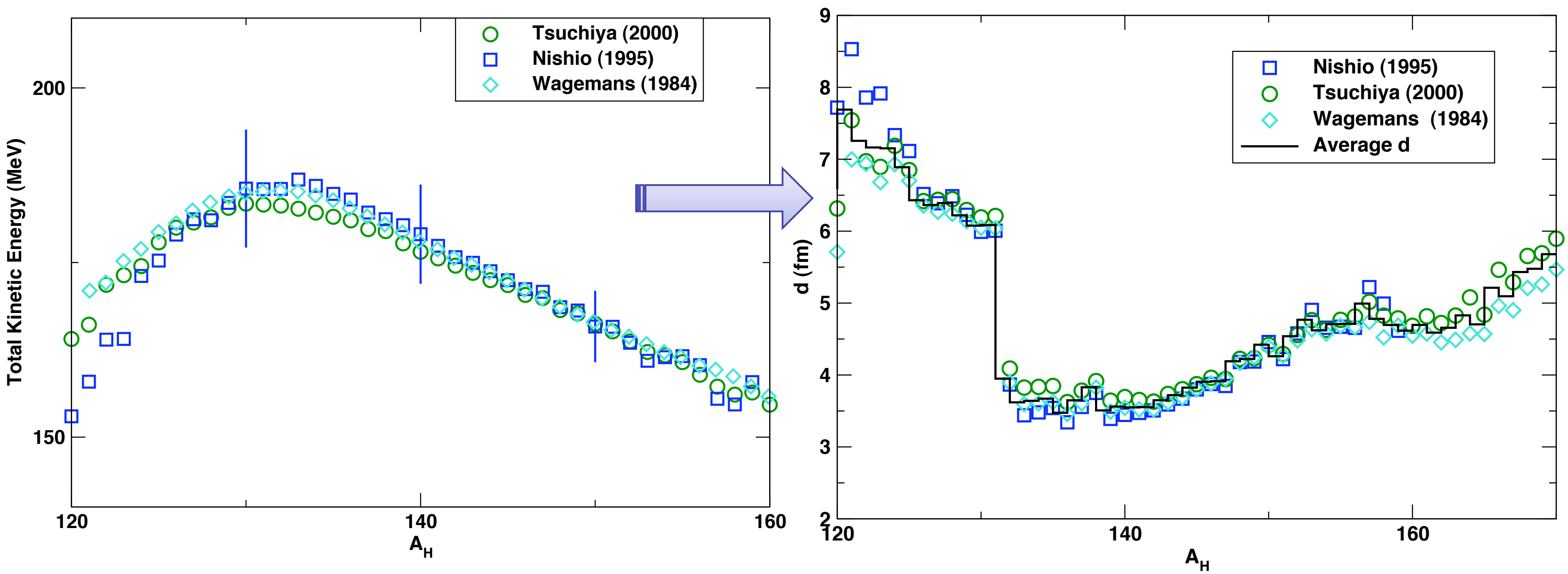
Randomized set of parameters s, e_0 and x chosen over a reasonable range to obtain spectra and $\overline{\nu}$ for each set of parameters, χ^2 minimized to obtain optimal parameter set

$$\mathrm{TKE} = e^2 \frac{Z_L Z_H}{c_L + c_H + s(E_n) \underline{d}_{LH}(A_H, E_{\mathrm{thermal}})}$$

$$\begin{aligned} E_i^* &= a_i T_{LH}^2 \\ a_i &\propto \frac{A_i}{e_0} \end{aligned}$$

$$\begin{aligned} E_L^* &= x \frac{a_L \mathrm{TEE}}{a_L + a_H} \\ E_H^* &= \mathrm{TEE} - E_L^* \end{aligned}$$

Tip separation distance fixed from low energy TKE data



Dip in distance at A_H = 132 due to doubly magic closed shell at Z_H = 50, N_H = 82, resistant to deformation

Approximating the TKE by fixing the distance as a function of A_H leads to correct behavior of $\nu(A)$ which can fix multiplicity without needing to rely on more uncertain spectral data

Obtaining the most likely set of fit parameters

- Assume our model parameters $\{\alpha_k\} = \{s, e_0, x\}$ are uniformly distributed in parameter space
- For each specified set of parameters, $\{\alpha_k^{(m)}\}$, generate a large set of fission events with `FREYA` (about 1M for each m) and extract observables $\{\mathcal{C}_i\}$ which are compared to experimental values, $\{\mathcal{E}_i\}$
- We then calculate the χ^2 deviation of the observables from their measured values,

$$\chi^2_m \;\equiv\; \chi^2\{\alpha_k^{(m)}\} \;\equiv\; \sum_i \frac{(\mathcal{C}_i\{\alpha_k^{(m)}\} - \mathcal{E}_i)^2}{\sigma_i^2}$$

and obtain relative weights that give likelihood for calculations with the given set of parameters to give the "correct" result,

$$w_m \;\equiv\; w\{\alpha_k^{(m)}\} \propto \; \mathrm{e}^{-\frac{1}{2}\chi^2\{\alpha_k^{(m)}\}}$$

- Obtain probability density in model parameter space, $P\{\alpha_k\} \equiv w\{\alpha_k\}/W$, where $W \equiv \sum_m w_m$, used to obtain best estimate for the model parameter values, the likelihood-weighted average

$$\tilde{\alpha}_k \;\equiv \prec \alpha_k \succ \equiv\; \frac{1}{W}\sum_m w_m \alpha_k^{(m)} \;\approx\; \alpha_k^0$$

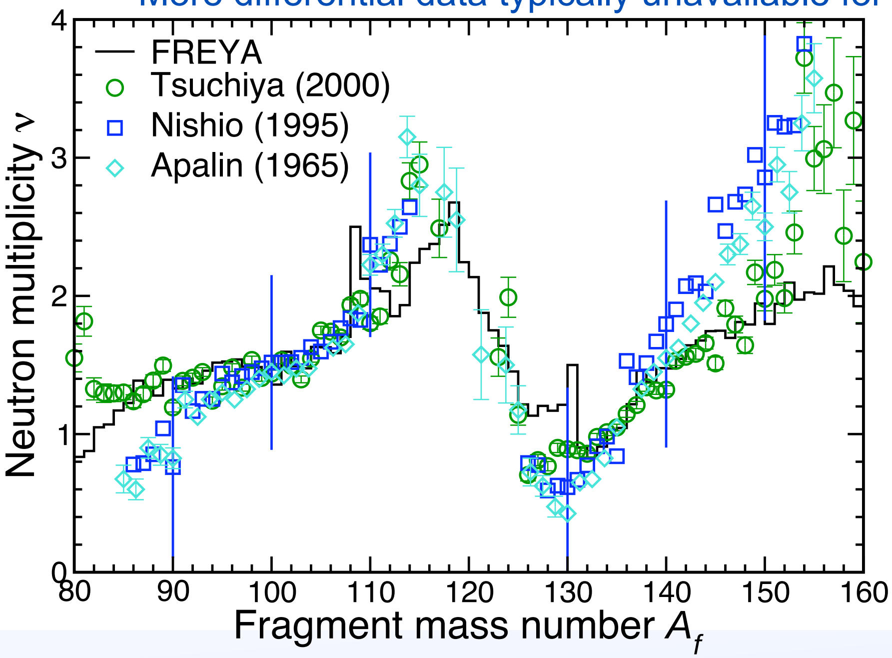
where the best estimate is that with the largest likelihood

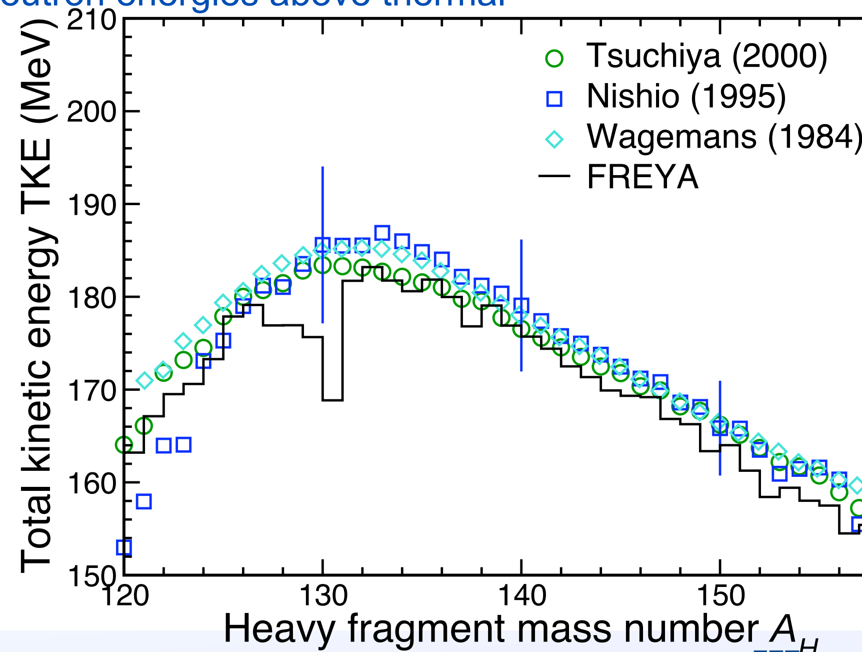
FREYA parameters ultimately fit to multiplicity alone up to 5.5 MeV, 2nd chance threshold

Best fit parameters as a function of incident neutron energy, resulting multiplicity and χ^2

E_n (MeV)	s^0	e_0^0	x^0	$\overline{\nu}$	$\chi^2_{\overline{\nu}}$
0.5	1.05449 ± 0.00567	8.01571 ± 0.57905	1.10264 ± 0.05909	2.948 ± 0.015	4.26×10^{-3}
1.5	1.05887 ± 0.00585	8.03595 ± 0.56938	1.10178 ± 0.05736	3.090 ± 0.015	8.46×10^{-4}
2.5	1.06590 ± 0.00858	7.99259 ± 0.57795	1.09969 ± 0.11359	3.242 ± 0.016	1.88×10^{-2}
3.5	1.06886 ± 0.00902	8.00688 ± 0.57295	1.09987 ± 0.11745	3.373 ± 0.017	3.78×10^{-2}
4.5	1.07598 ± 0.00699	7.99282 ± 0.57734	1.09889 ± 0.05829	3.527 ± 0.017	2.55×10^{-2}
5.5	1.08418 ± 0.00752	8.00467 ± 0.58166	1.09892 ± 0.05758	3.681 ± 0.019	1.50×10^{-2}

More differential data typically unavailable for neutron energies above thermal





Covariances/correlations in input parameters

Covariances between parameter values are,

$$\tilde{\sigma}_{kk'} \equiv \prec (\alpha_k - \tilde{\alpha}_k)(\alpha_{k'} - \tilde{\alpha}_{k'}) \succ$$

On the diagonal, $\tilde{\sigma}_{kk} = \tilde{\sigma}_k^2$, are variances where $\tilde{\sigma}_k$ are standard deviations of the parameter values; the squares of the uncertainties on the values of the individual model parameter α_k. The off-diagonal elements give the covariances between two model parameters.

Associated correlation coefficients,

$$C_{kk'} \equiv \frac{\tilde{\sigma}_{kk'}}{\tilde{\sigma}_k \tilde{\sigma}_{k'}} \ ,$$

are positive if α_k and $\alpha_{k'}$ increase together and negative if α_k increases while $\alpha_{k'}$ decreases. There is no correlation if $C_{kk'} = 0$.

E_n (MeV)	$C_{s\,e_0}$	$C_{s\,x}$	$C_{e_0\,x}$
0.5	0.608	-0.569	0.0156
1.5	0.611	-0.561	0.0042
2.5	0.465	-0.776	0.0212
3.5	0.464	-0.766	0.0441
4.5	0.757	-0.569	-0.0053
5.5	0.693	-0.480	-0.0130

Covariances/correlations between observables

Covariance matrix between spectral strengths at different outgoing neutron energies

$$\tilde{\sigma}_{kk'} \equiv \prec (E_k - \tilde{E}_k)(E_{k'} - \tilde{E}_{k'}) \succ$$

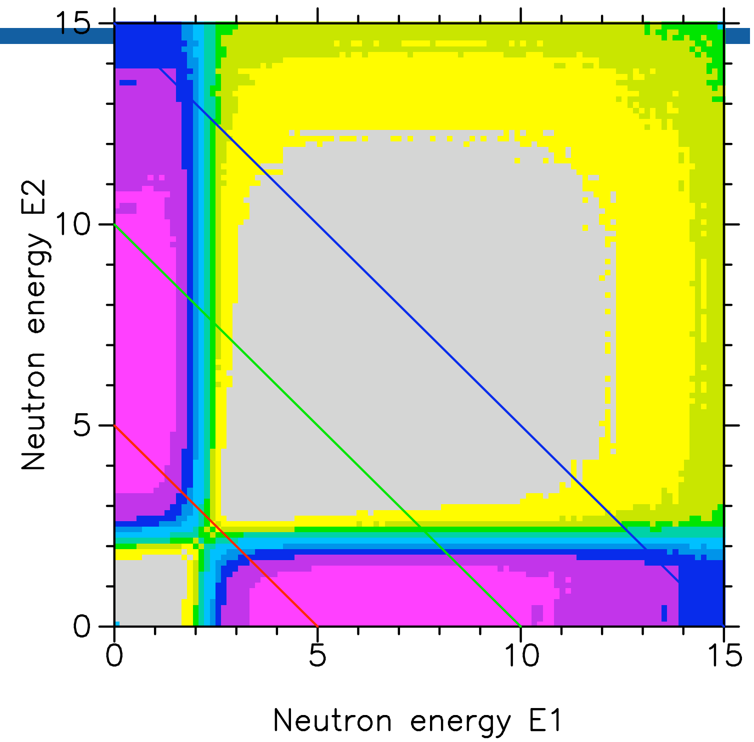
For continuous observables, such as spectra, there is a singularity along the diagonal,

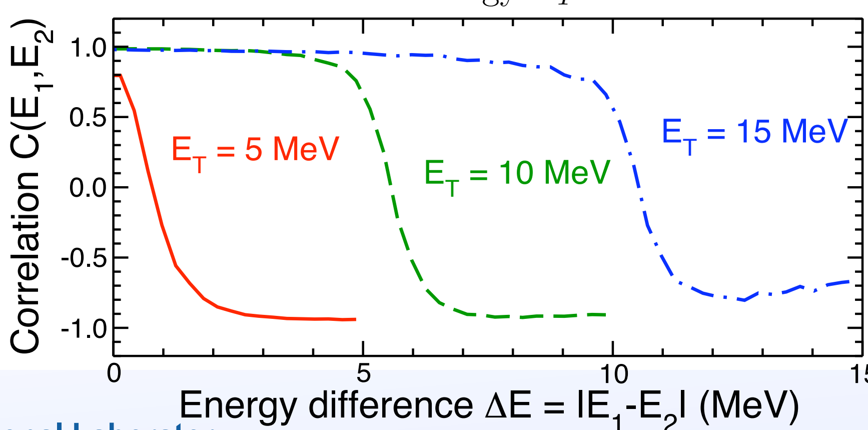
$$\tilde{\sigma}(E_k, E_{k'}) = \tilde{\sigma}^2_{E_k}\, \delta(E_k - E_{k'}) + \tilde{\sigma}_{E_k E_{k'}}$$

where $\tilde{\sigma}^2_{E_k}$ is the variance in the differential yieldat E_k while $\tilde{\sigma}_{E_k E_{k'}}$, is the correlation between yields at two different energies, E_k and $E_{k'}$. After the singular part has been removed, the correlation coefficient matrix is obtained:

$$C(E_k, E_{k'}) = \tilde{\sigma}_{E_k E_{k'}} / [\tilde{\sigma}_{E_k} \tilde{\sigma}_{E_{k'}}]$$

The behavior of $C(E_k, E_{k'})$ for constant total neutron energy $E_T = E_k + E_{k'}$ is also shown.



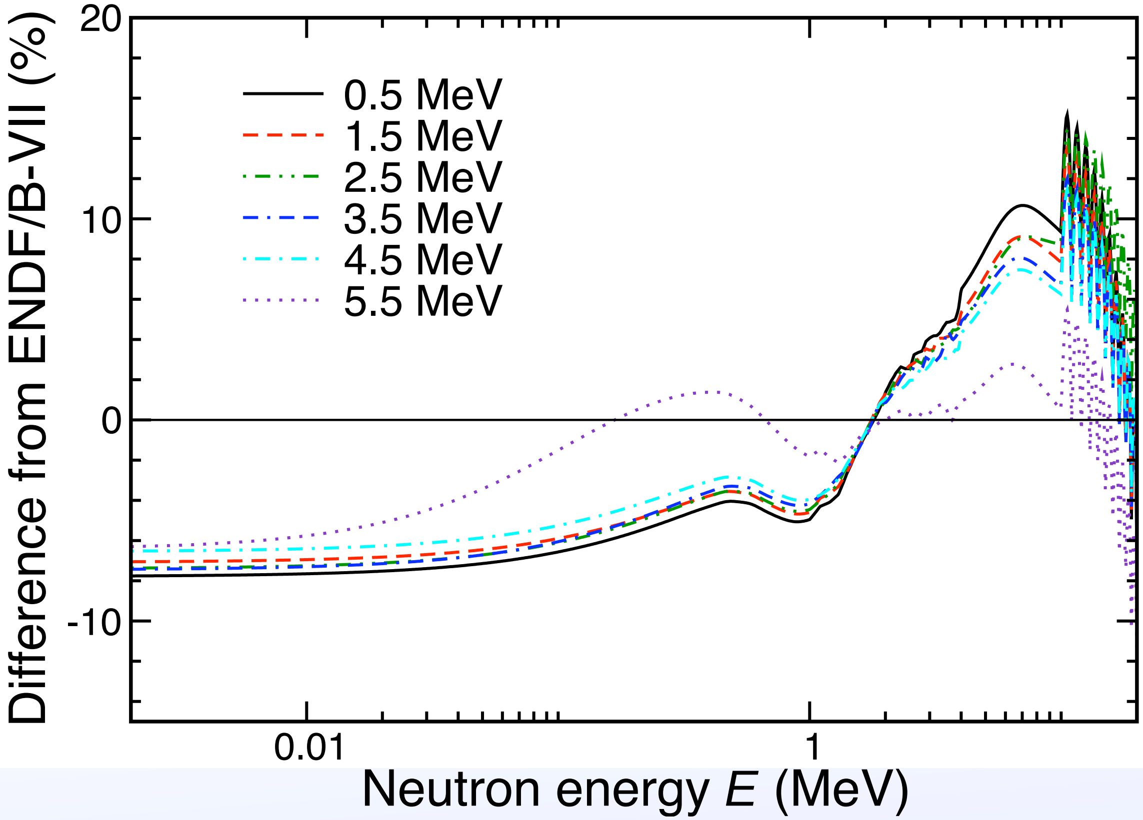


Results shown for 0.5 MeV,

similar for all incident energies

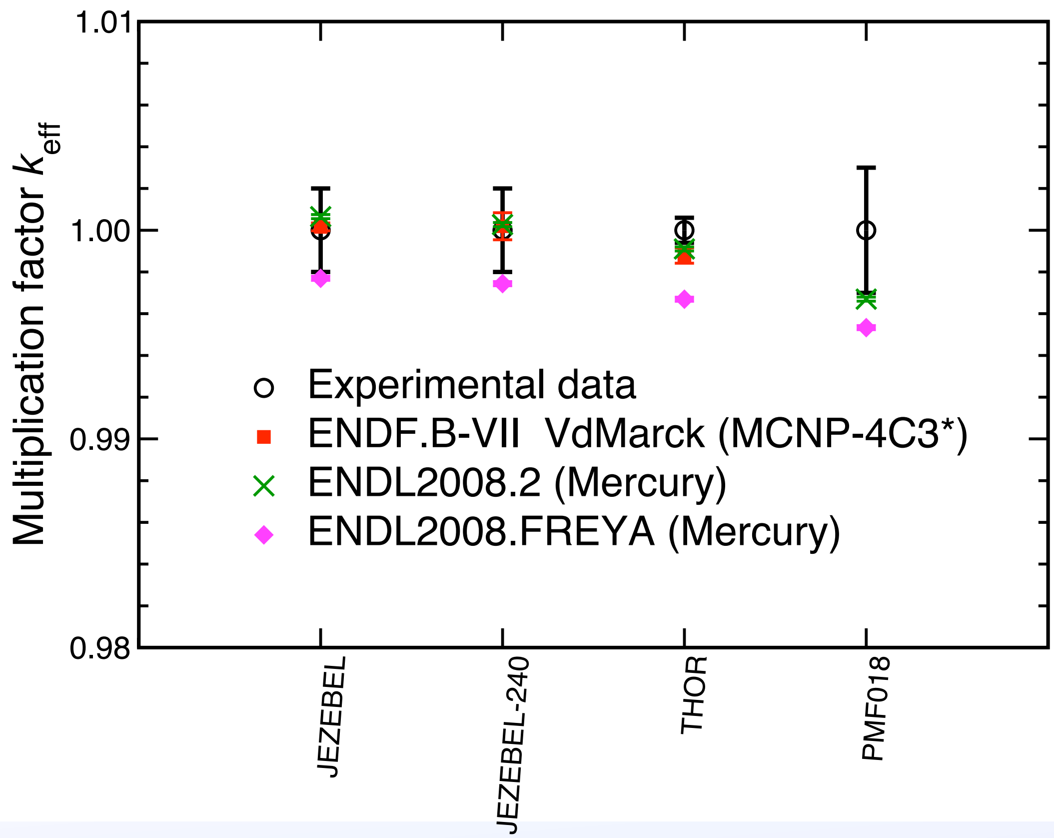
FREYA evaluation can be compared to existing ENDF evaluation

- Evaluation prepared with FREYA fits
  - Extrapolation to 10^{-5} MeV and up to 20 MeV done by fitting two different Watt spectra
- Differences in spectral shapes at both low and high energies



Preliminary critical assembly tests

Critical assembly test results shown here with Mercury Monte Carlo, results slightly better with deterministic Amtran code



What's Next?

Evaluated neutron spectra not strongly influenced by spectral data, $\overline{\nu}$ with its much smaller associated uncertainty is more important

Improvements in modeling will come from better knowledge of the complicated fission process through microscopic models and high statistics, less inclusive data

`FREYA` bridges models and data by addressing complete events with full energy-momentum conservation and correlations between observables

Next step, including multi-chance fission in `FREYA` to address higher incident energies