Lawrence Livermore National Laboratory

Obtaining the ^{239}Pu Fission Spectrum with FREYA

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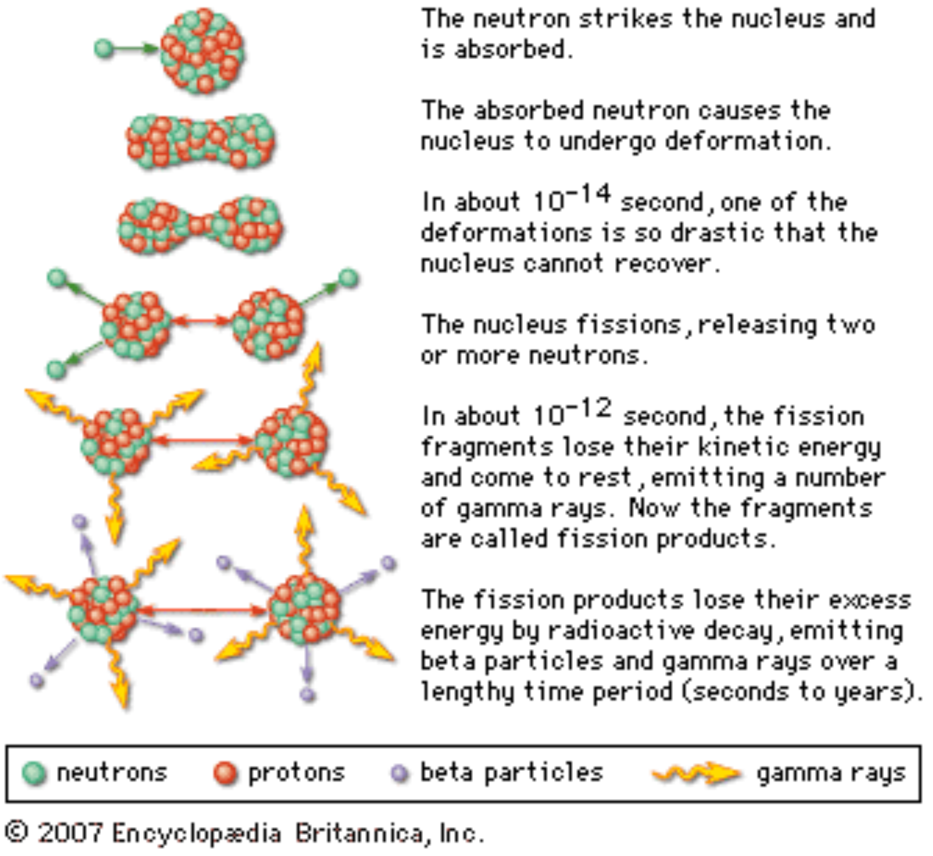
We have been modeling the ^{239}Pu fission spectra event-by-event

- Event-by-event modeling allows studies of correlations and more differential data



The neutron strikes the nucleus and is absorbed.

The absorbed neutron causes the nucleus to undergo deformation.

In about 10^{-14} second, one of the deformations is so drastic that the nucleus cannot recover.

The nucleus fissions, releasing two or more neutrons.

In about 10^{-12} second, the fission fragments lose their kinetic energy and come to rest, emitting a number of gamma rays. Now the fission fragments are called fission products.

The fission products lose their excess energy by radioactive decay, emitting beta particles and gamma rays over a lengthy time period (seconds to years).

FREYA (Fission Reaction Event Yield Algorithm) is used to do our spectral evaluation

- Collaborative theory and modeling effort at LLNL
  - E. Ormand, J. Pruet, R. Vogt and W. Younes
- LBNL Collaboration with J. Randrup on FREYA

How FREYA works

- For given incident neutron energy, E_n, and target nucleus, A_c, of charge Z_c assume binary fission
- Sample mass and charge of light, L, and heavy, H, fragments from fission fragment distributions conserving mass and charge
- Determine fission Q from light and heavy fragments, divide between kinetic and excitation energies of fragments
- Fix total kinetic (TKE) and excitation (TEE) energies of fragments by sampling either kinetic or excitation energy and fixing the other by energy conservation: TEE = Q - TKE
- Divide TEE between heavy and light fragments
- Evaporate neutrons from each fragment until its excitation energy is too low for further neutron emission
- After neutron emission ceases, gamma emission allowed albeit in preliminary form
- At higher energies, allow for multi-chance fission (to be implemented)

We identify which model parameters the spectra are most sensitive to

- We model fragment total kinetic energy with a Coulomb-type form

$$\begin{aligned} T_f^{\mathrm{tot}} &= \alpha\hbar c \frac{Z_H Z_L}{R_{A_H} + R_{A_L} + d} \\ R_A &= 1.2A^{1/3} \end{aligned}$$

  - The parameter *d* is the tip separation distance between the two fragments: larger *d* means lower TKE, higher TEE, more neutrons
- The asymptotic level density parameter, a_L, determines the temperature of the excited fragment

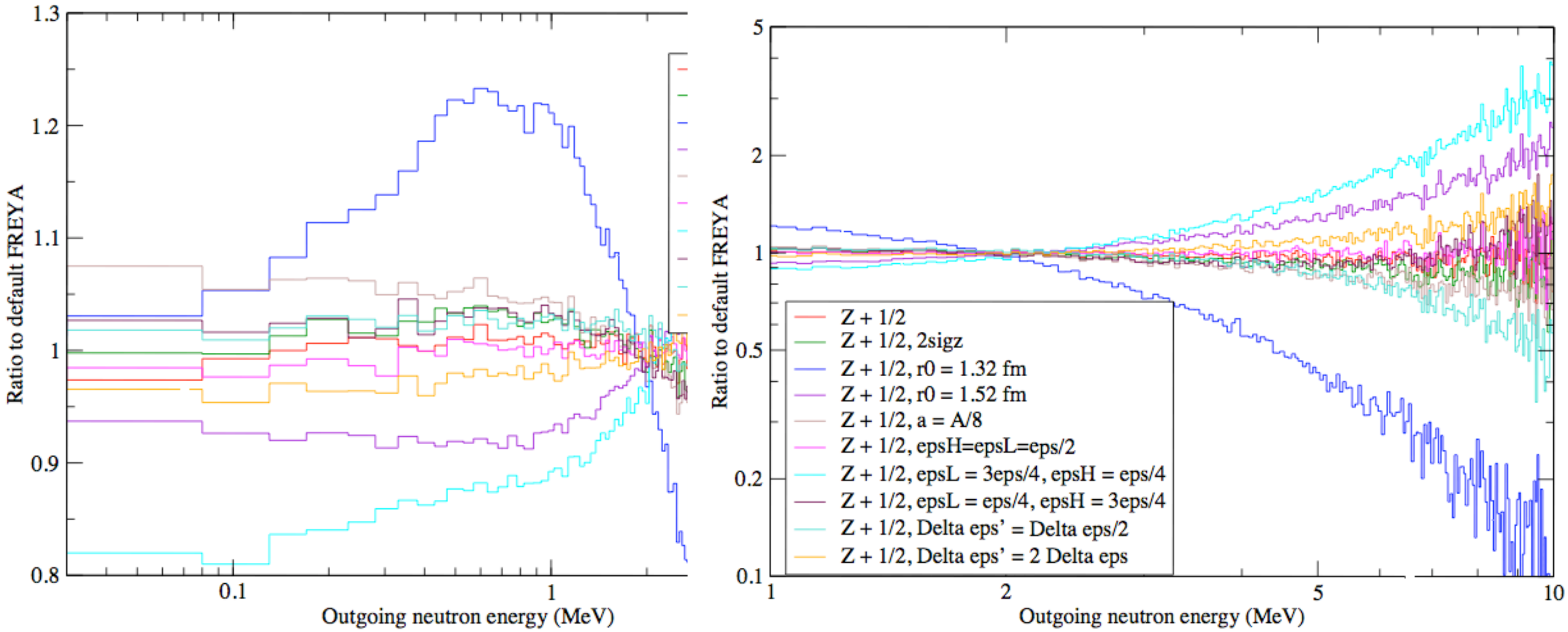
$$\begin{aligned} T_{\max} &= \left[\frac{Q_{\mathrm{evap}}}{a(A,Z,\epsilon)}\right]^{1/2} \\ Q_{\mathrm{evap}} &= E_{\mathrm{mother}} - E_{\mathrm{daughter}} - m_{\mathrm{ejectile}} \end{aligned}$$

- The balance between the light and heavy fragment excitation energies can be altered while conserving energy (no effect if $x = 1$)

$$\epsilon_L = x\epsilon_{\mathrm{tot}} \frac{A_L}{A} \quad \epsilon_H = \epsilon_{\mathrm{tot}} - \epsilon_L$$

- Effective *d* can be *A* dependent, $d(1-\varepsilon_d[A_L/A_H])$, default $\varepsilon_d = 0$
- Fit spectra with *d* and 3 other parameters: a_L, *x*, and ε_d with default values of $a_L = 7.25$ MeV^{-1}, $x = 1$ and $\varepsilon_d = 0$

Results of preliminary sensitivity studies with ^{235}U

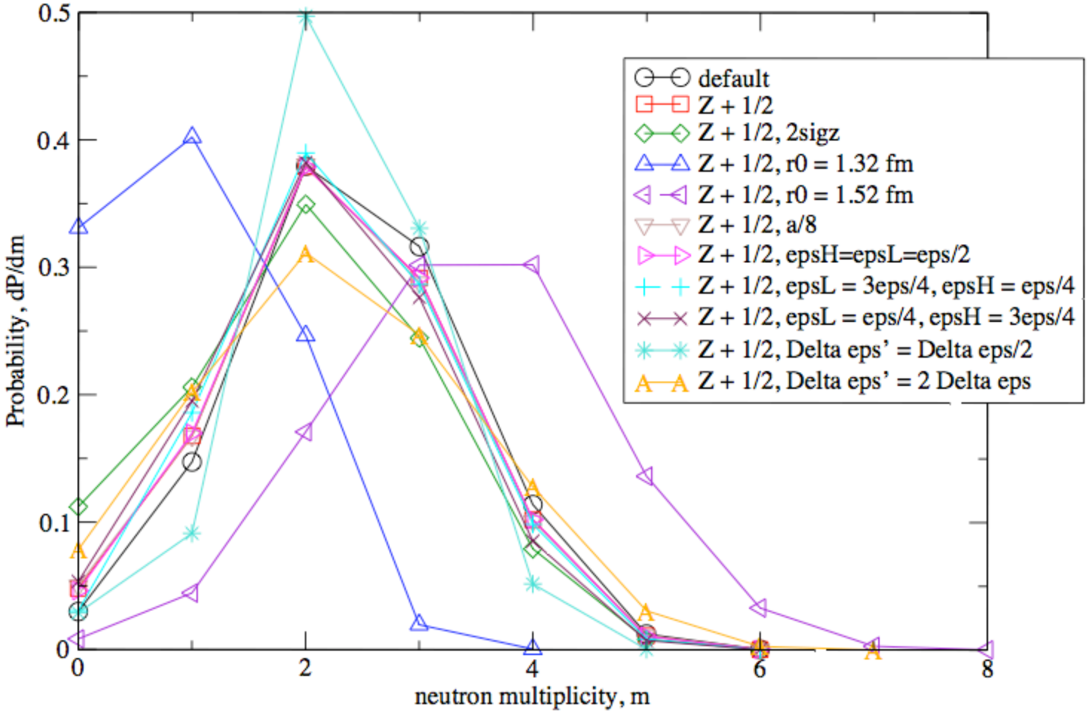


Large changes in these parameters (and others) necessary to change low end of spectrum, high energy end most strongly affected by changing *d* and relative excitation energy, *x*, can rather tightly constrain parameter range

Note crossover of all curves at outgoing neutron energy 2 MeV

Small changes in the spectra can have a large effect on average neutron multiplicity

- Neutron multiplicity (both average and $P(\nu)$) are more sensitive to parameter changes than spectra
- We use both the average multiplicity and the spectra to constrain our parameters

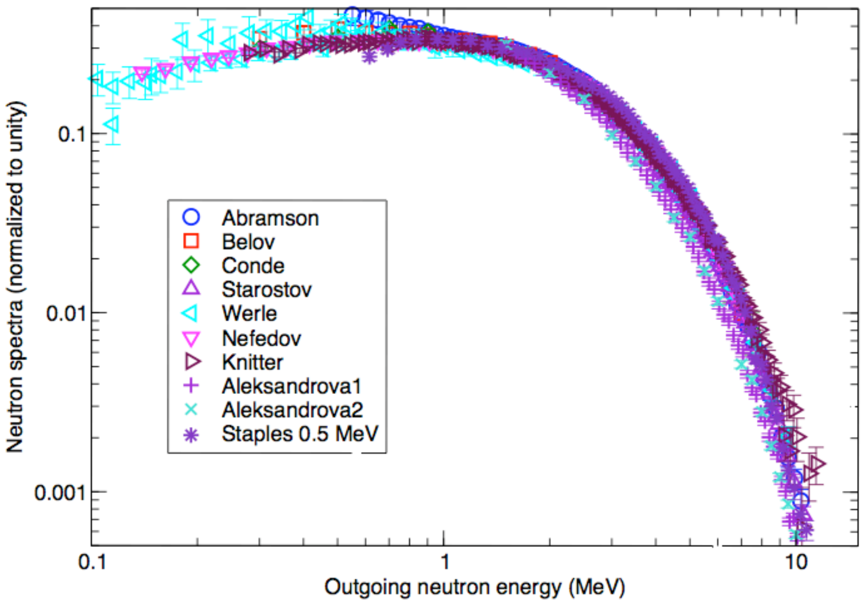


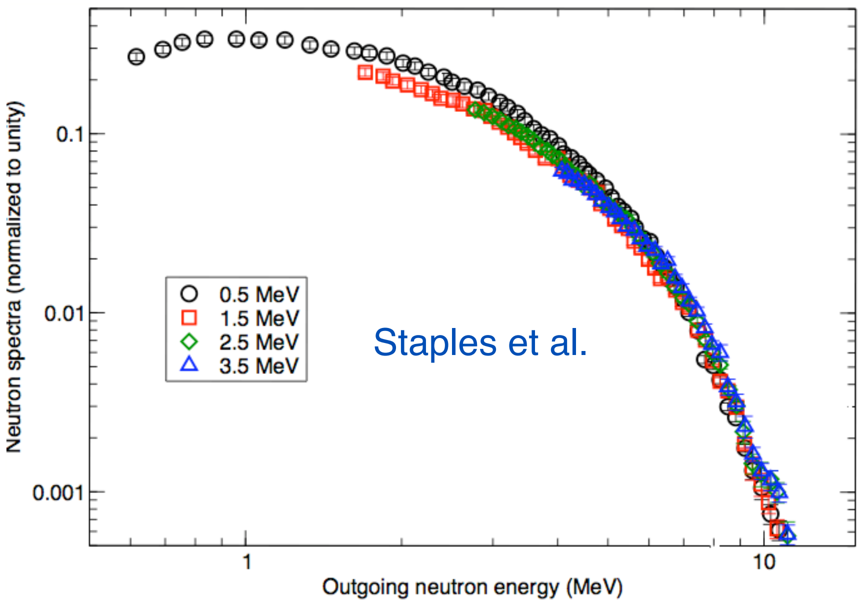
We fit FREYA parameters to ^{239}Pu spectra and $\langle\nu\rangle$

- Sparse spectral data on ^{239}Pu(n,f) above thermal energies, little more differential data
- Use spectral data with incident neutron energies of 0.5 MeV (Staples) and below for one fit (10 data sets); 1.5, 2.5 and 3.5 MeV data from Staples *et al* fit separately
- Not all data have errors included, add an error of 5% to data without errors -- probably an underestimate
- Average neutron multiplicities known for large energy range; At 0.5, 1.5, 2.5 and 3.5 MeV, take average multiplicities with 0.5% error on number
- Fit parameters to spectra and $\langle\nu\rangle$ for these four energies, both with free-floating normalization and with data fit to a Watt spectrum and normalized to unity

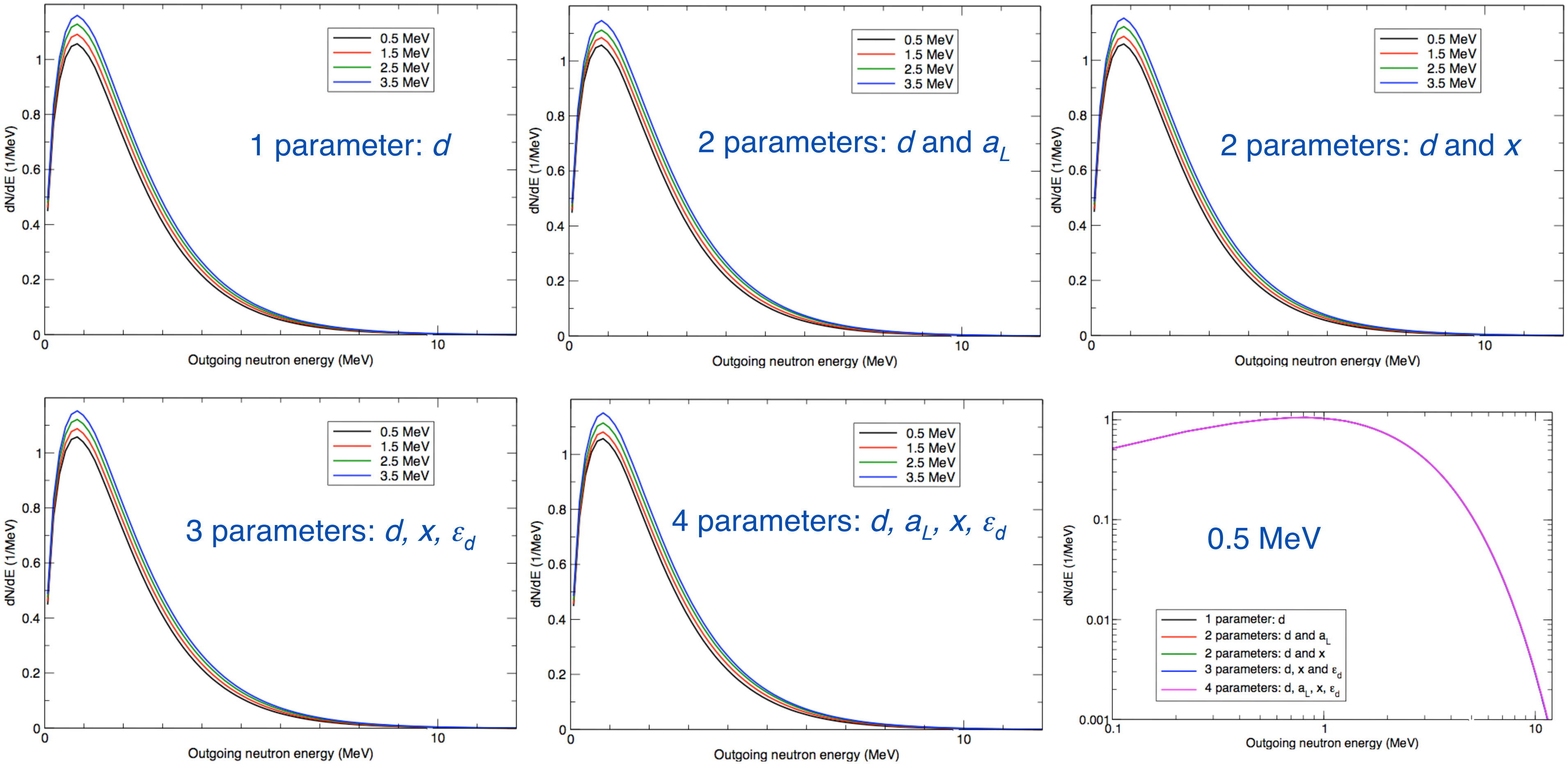
Sample of data used in spectral fits

- Staples spectra very hard at high neutron energy (not shown here)
- Higher energy data can’t tell us much about behavior of low energy neutron emission -- only lowest energy data sets provide insight in range $0.1 < E_n < 1$ MeV





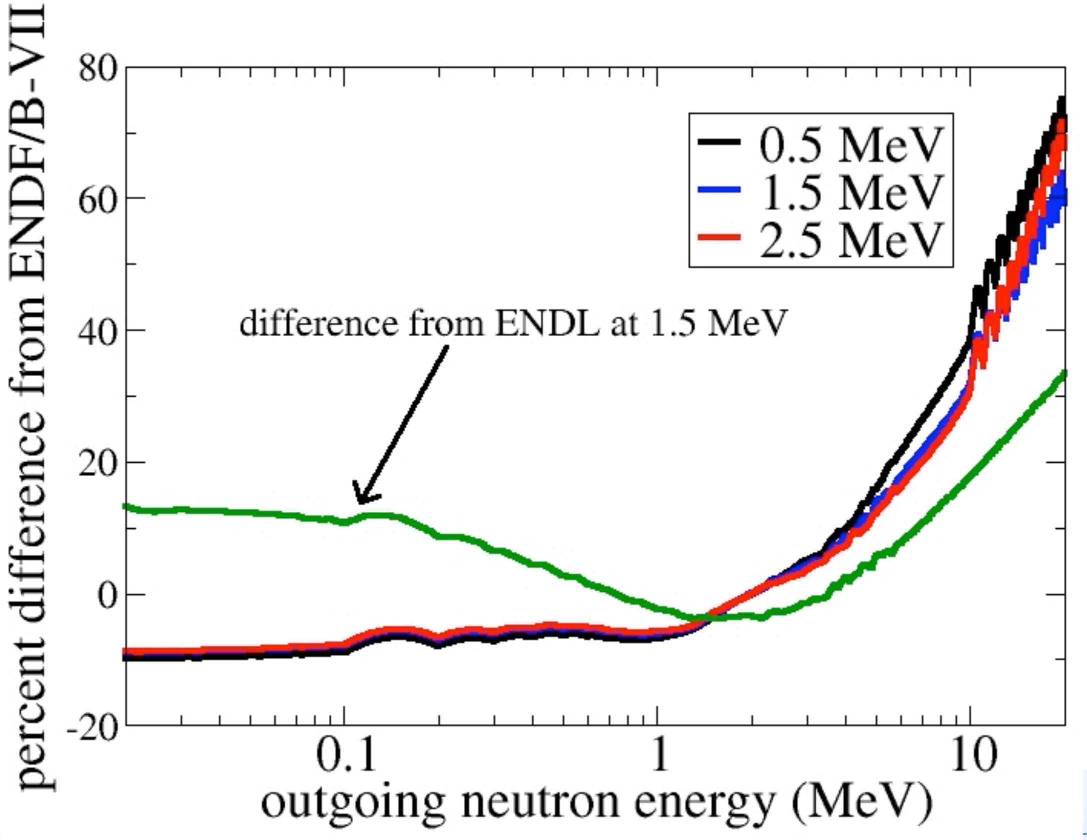
Relatively good FREYA fits can be obtained for all energies with 1-4 parameters (fits to Watt-normalized spectra shown here)



Correlations in the inputs plus correlations and covariances in the output spectra shown in covariance talk

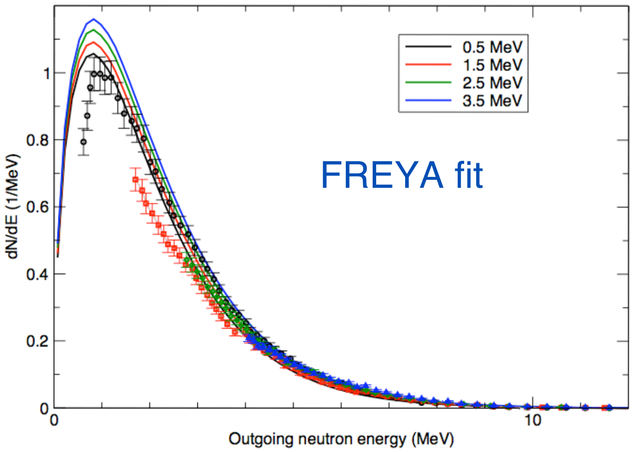
The evaluation so far can be compared to existing ENDL and ENDF evaluations

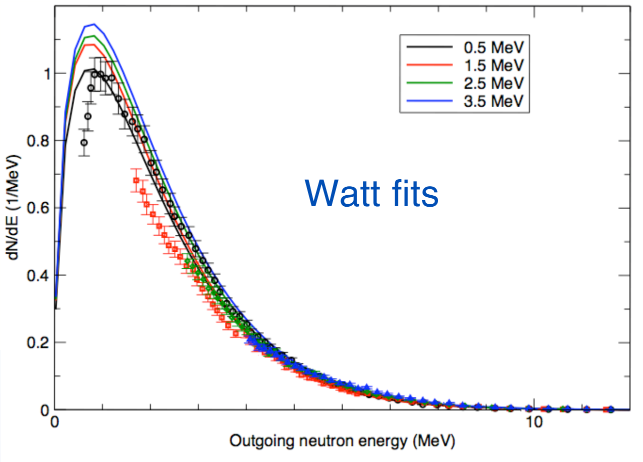
- Evaluation prepared with FREYA fits
  - Extrapolation to 10^{-11} MeV and up to 20 MeV done by fitting two different Watt spectra
- Differences in spectral shapes at both low and high energies
- Below 1 MeV, absolute difference between ENDL and ENDF are similar, sign is opposite

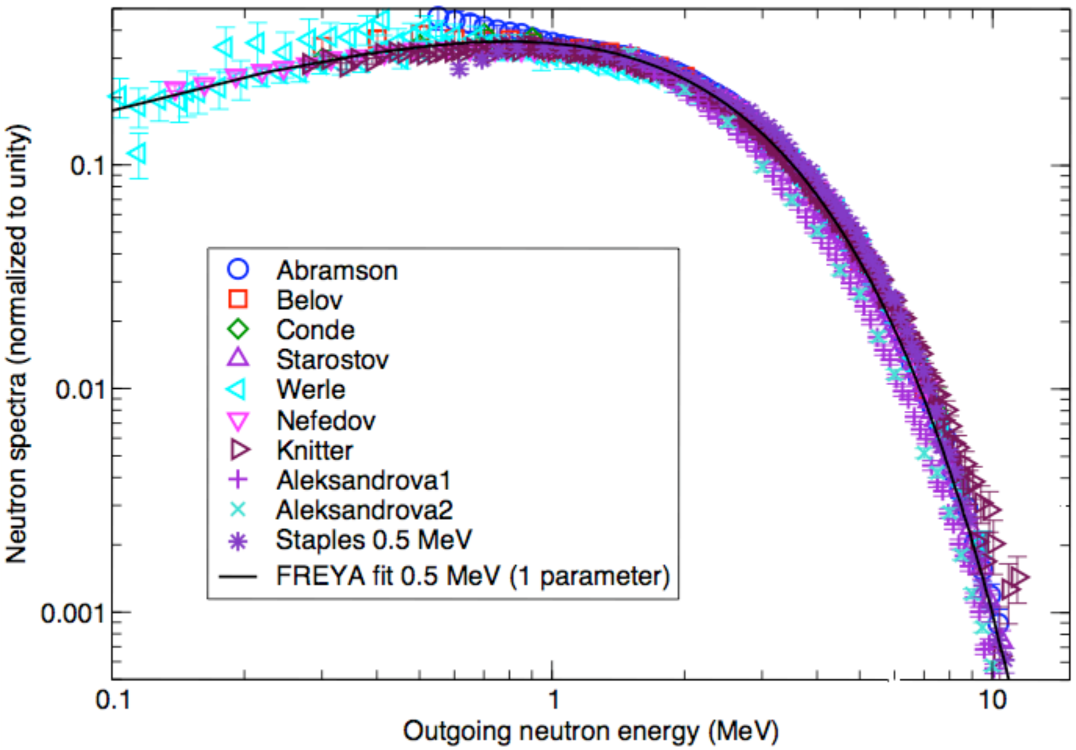


Comparison to Data

- Unable to achieve perfect fits of data to either FREYA or Watt, data do not necessarily agree with each other either (χ^2 of FREYA smaller than Watt)
- Not a good situation for making definitive evaluations







What’s Next? A To Do List

- For the spectra:
  - Extrapolation to higher energy? In a simple model, below the 2^{nd} chance fission threshold, the fewer parameters the better, e.g. letting *d* increase slowly with energy
  - Above thresholds, need a model for multichance fission
- In any case, although the parameters that fit the spectra and average multiplicity are fairly well constrained by the data that exist, it doesn’t mean that the model is right -- how to really tell?
  - Need to compare the fits with more differential data where available: $\nu(A)$, TKE*(A)*, etc.
  - Model inputs governing TKE, TEE can be replaced by theory when it becomes available