Recent results with FREYA on the ^{239}Pu(n,f) Prompt Fission Neutron Spectrum

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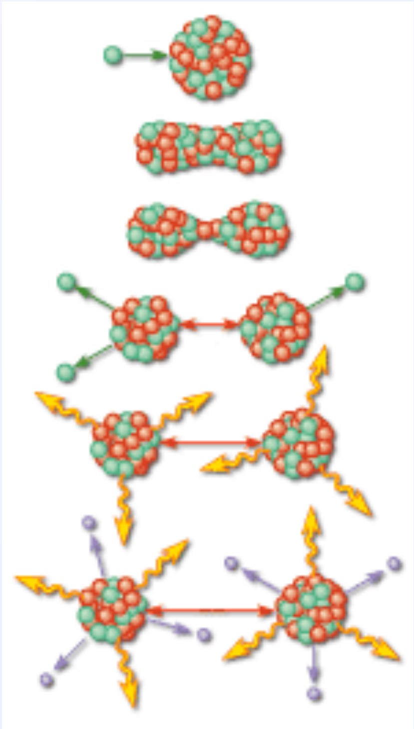
We have used FREYA to complete the ^{239}Pu(n,f) prompt fission neutron spectrum evaluation

- 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, TEE = Q − 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



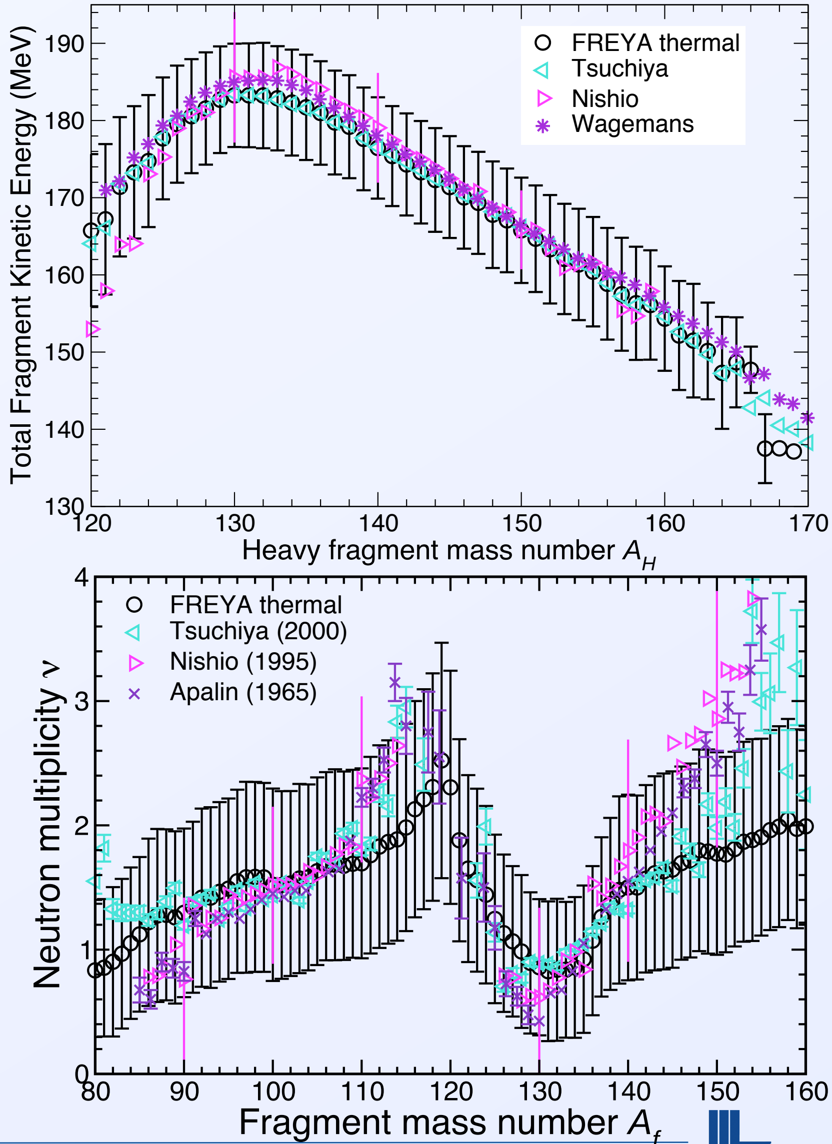
FREYA

Evaluation requires improved fission modeling at all energies, not just thermal

Spectra data alone are often insufficient for a comprehensive understanding of fission

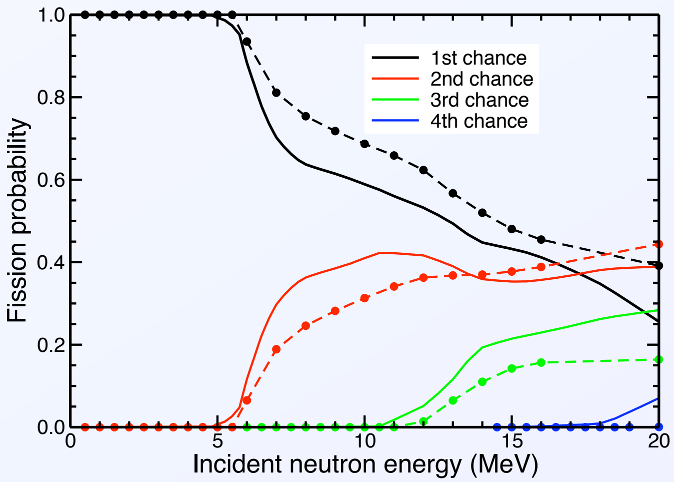
Poor quality of spectral data means we must rely on extrapolations and inclusive quantities such as average total multiplicity

Improved spectral evaluations require better modeling of all aspects of the physics of fission process and/or new data over entire energy range of evaluation similar to that shown here

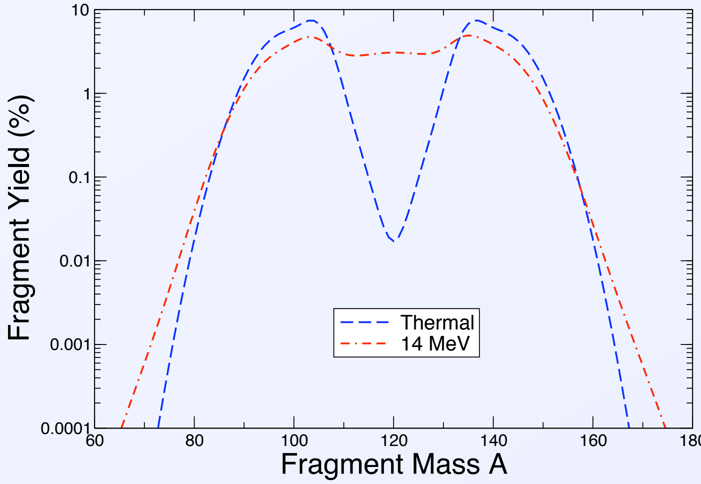


Three important contributions at high incident neutron energy

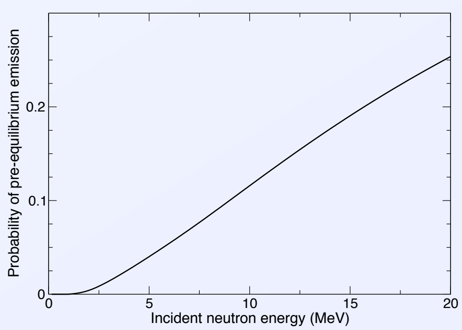
- **Multi-chance fission**, emission of one or more neutrons from excited compound nucleus pre-fission, turns on when incident neutron energy is above neutron separation energy for compound nucleus (^{240}Pu, 1st chance; ^{239}Pu, 2nd chance; ^{238}Pu, 3rd chance)
- Comparison to ENDF ^{239}Pu evaluation (**GNASH** calculation, not measured) with **FREYA** using same barrier heights but fitted level density parameter

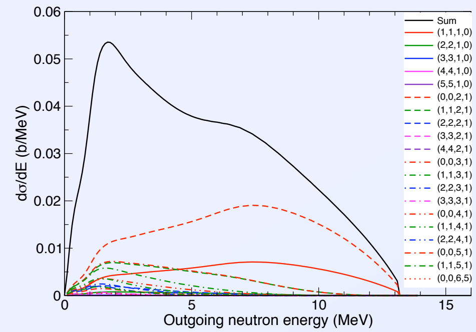


- **Transition from asymmetric to symmetric fission:** more symmetric with increasing incident neutron energy



- **Pre-equilibrium emission**: captured neutron fails to equilibrate and is re-emitted; biggest effect for smallest number of intermediate excited states (right) and high incident neutron energies (left)





- **Missing ingredients to improve analysis at all incident neutron energies:**
    - **more comparison data e.g. Y(A,TKE)**
    - **more differential data like $\nu(A_f)$**
    - **better modeling of yields, kinetic energies with 'hot' fission (dynamics)**

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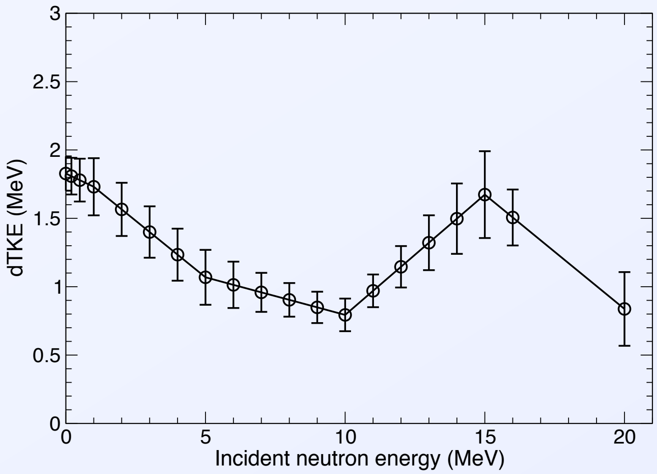
Statistical methods used to match average FREYA neutron multiplicity to the ENDF-B/VII evaluated result, including covariance

Three FREYA parameters 'tuned' to average neutron multiplicity, $\overline{\nu}$:

- shift of $\mathrm{TKE}(A_H)$, $d\mathrm{TKE}$, from average of data at thermal energies – the shape is assumed to remain the same as a function of energy, not necessarily the case if system is excited enough for shell effects to be negligible
- 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 $d\mathrm{TKE}$, 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. We assume that e_0 and x are independent of energy and that $d\mathrm{TKE}$ varies linearly between fixed points at incident energies of 10^{-11}, 1, 5, 10, 15 and 20 MeV to ensure a good fit with a reasonable number of realizations (1000 on a Latin Hypercube parameter grid).

Result for dTKE



Energy-independent parameters:
$e_0 = 8.542 \pm 0.5449$ MeV^{-1}
$x = 1.139 \pm 0.0616$

Correlations between input parameters reveals characteristics of fit

We can calculate the covariances among pairs of input parameters in the set α_k,

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

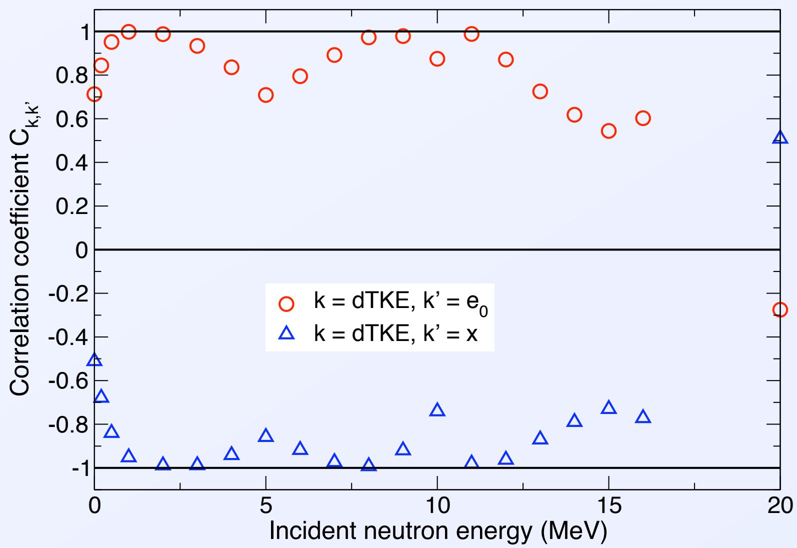
The diagonal elements, $\tilde{\sigma}_{kk} = \tilde{\sigma}_k^2$, are the variances and $\tilde{\sigma}_k$'s are the standard deviations of the parameter values (squares of the individual model parameter uncertainties). The off-diagonal elements give the covariances between two parameters.

We can also calculate the sometimes more transparent associated *correlation coefficients*,

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

If the parameters are uncorrelated, $C_{kk'} = 0$. Correlated parameters lead to nonzero correlation coefficients. If $C_{kk'} > 0$, α_k increases as $\alpha_{k'}$ increases. On the other hand, if $C_{kk'} < 0$, α_k increases as $\alpha_{k'}$ decreases.

Changes in correlation coefficient occur near fixed points of the fits



$C_{e0,x}$ = -0.946, both e_0 and x are energy independent

Correlations between outputs reveals physics features

Covariances between different observables, $\mathcal{C}_i$, are calculated as

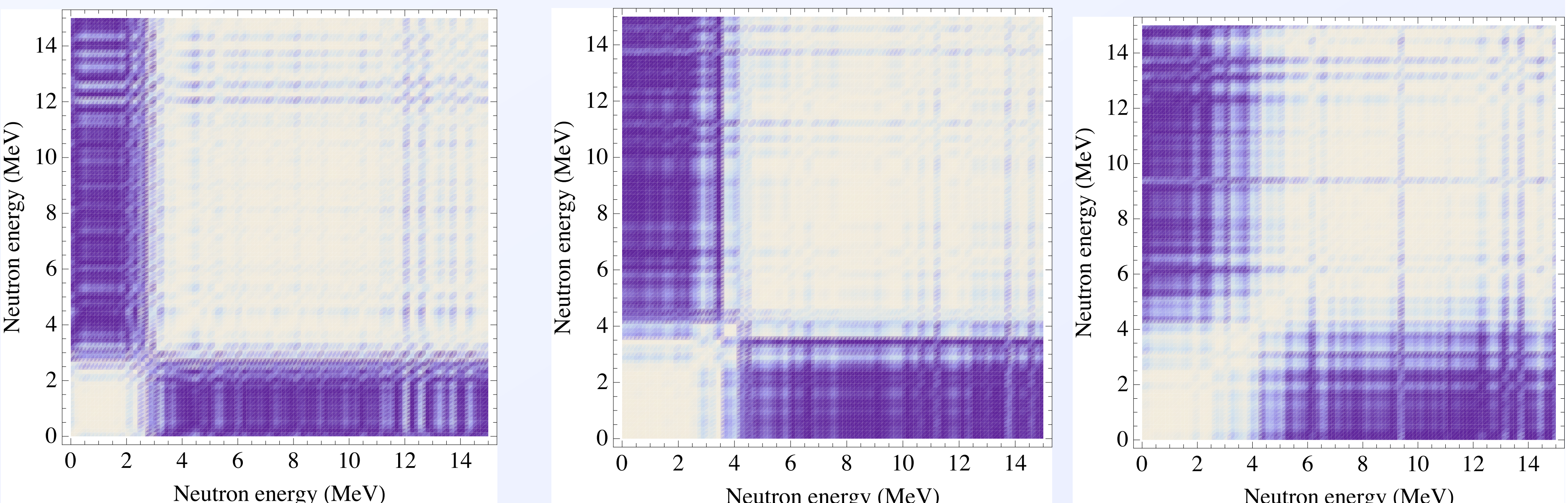
$$\tilde{\sigma}_{ij} \equiv \prec (\mathcal{C}_i - \tilde{\mathcal{C}}_i)(\mathcal{C}_j - \tilde{\mathcal{C}}_j) \succ \ .$$

The diagonal elements are the squares of the standard deviations, $\tilde{\sigma}_i$, of the calculated values $\mathcal{C}_i$ resulting from uncertainties in the model parameter values. Here the correlation coefficients between the observables $\mathcal{C}_i$ and $\mathcal{C}_j$ are

$$C_{ij} \equiv \frac{\tilde{\sigma}_{ij}}{\tilde{\sigma}_i \tilde{\sigma}_j} \ .$$

Spectral correlations between outgoing neutron energies

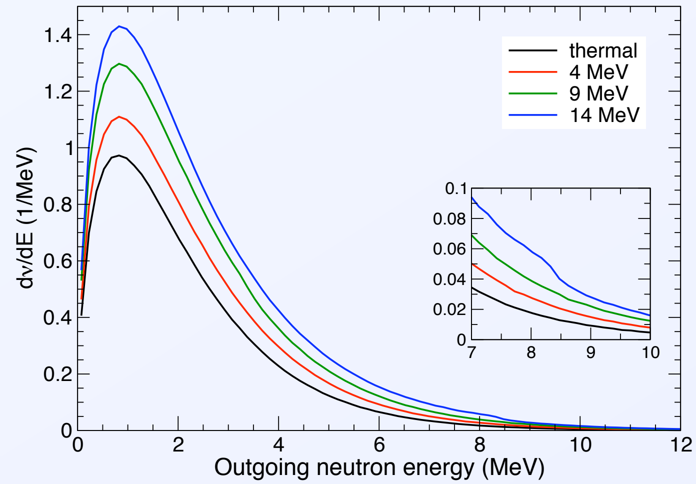
E_n = 0.5 MeV | E_n = 6 MeV | E_n = 14 MeV



FREYA result determined from energy-energy correlations in <ν> covariance

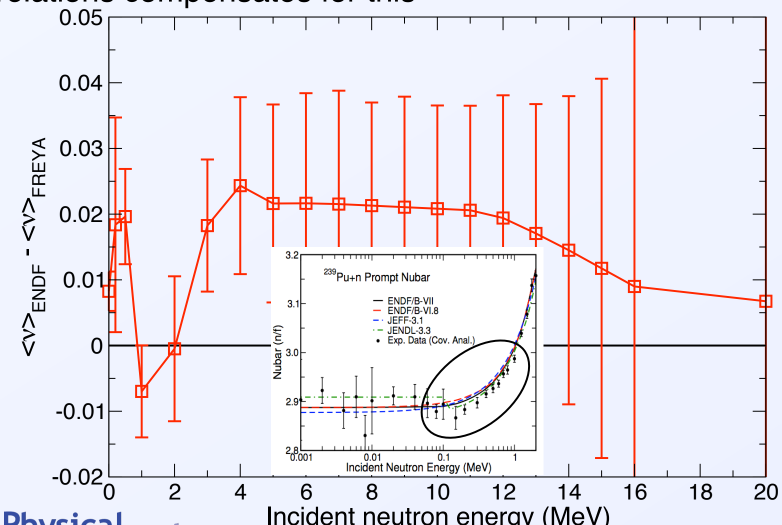
FREYA spectra shows physics effects absent in Los Alamos model/ENDF/B-VII which samples neutrons from same shape distribution, regardless of multiplicity and whether or not the neutron is due to pre-fission or pre-equilibrium emission

FREYA also implements correct fragment temperature profile

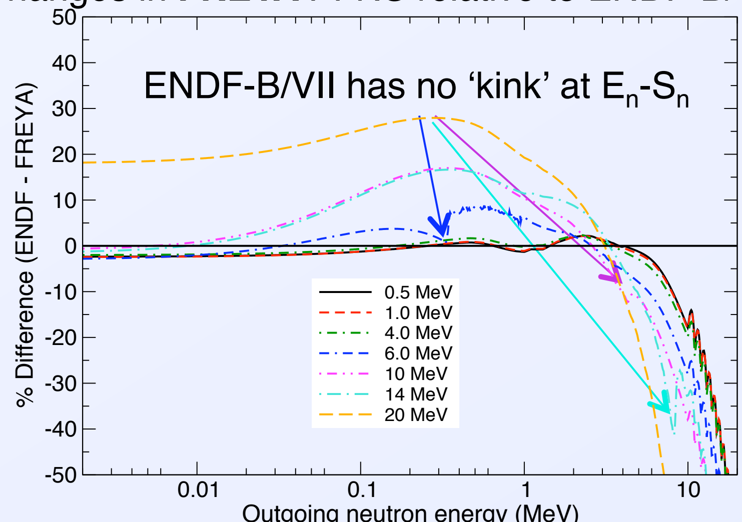


'kink' is at difference between E_n and neutron separation energy – it's real physics

Difference between ENDF-B/VII and **FREYA** (plot below) are largest in region where ENDF-B/VII <ν> overshoots evaluated data to obtain agreement with Jezebel assembly: **FREYA** fit from <ν> covariance with introduced energy-energy correlations compensates for this

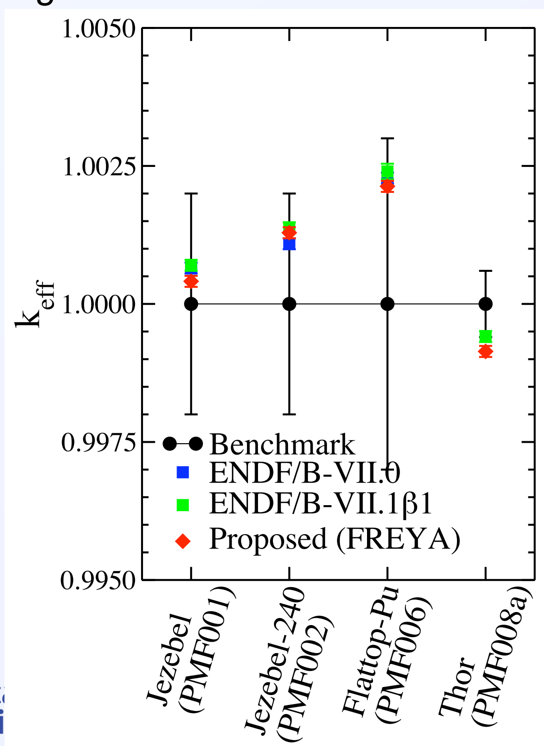


Changes in **FREYA** PFNS relative to ENDF-B/VII

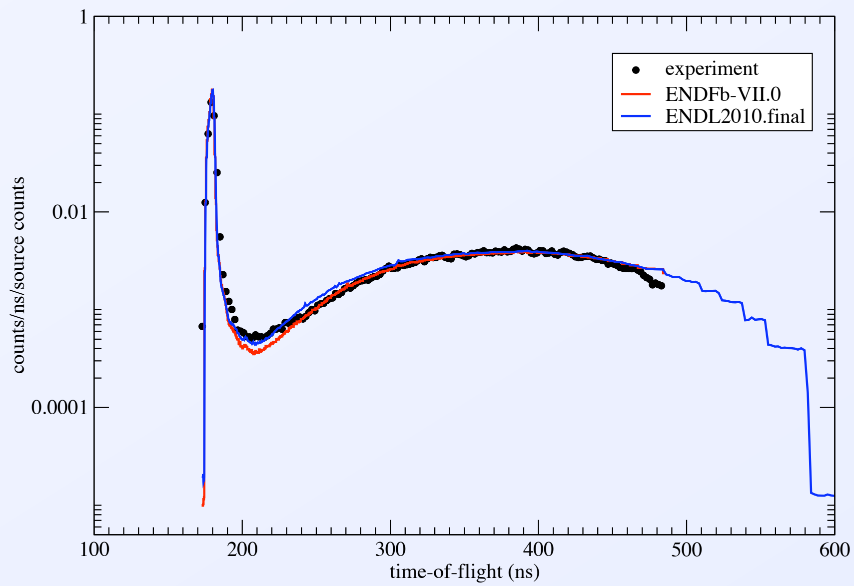


New evaluation passes key integral tests

Critical assemblies (k_{eff}) designed to determine critical mass
k_{eff} is eigenvalue of neutron transport equation, measures relative neutron gain and loss in material
Benchmark for PFNS evaluations, Jezebel is classic criticality test
FREYA agrees well with Pu assemblies



Pulsed spheres have 14 MeV neutron source at center of material to be tested
Description of neutron time of flight immediately after pulse tests PFNS in material
FREYA result improves pulsed sphere description in important region, ~ 200 ns
(Disagreement at late times due to imprecise modeling of objects in room outside sphere)



Future plans for FREYA

- Finalize ^{239}Pu results and submit paper to journal
- In FY11, we will apply our evaluation method to ^{235}U and ^{238}U
- FREYA funded by NA22 to study correlations for detection of SNM