# Combining the Statistical Model with Nuclear Structure Data for Nuclear Decay Property Studies

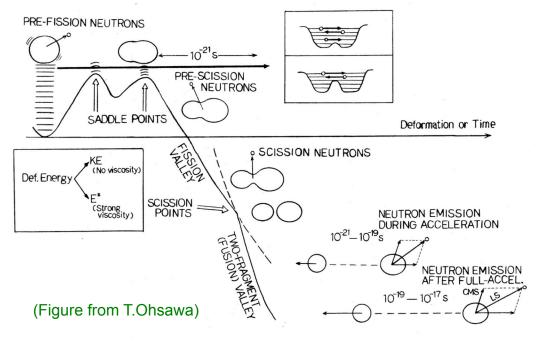
T. Kawano, S. Holloway, P. Talou, P. Möller Theoretical Division Los Alamos National Laboratory

Workshop on Gamma Strength and Level Density in Nuclear Physics and Nuclear Technology

Dresden-Rossendorf, August 31, 2010





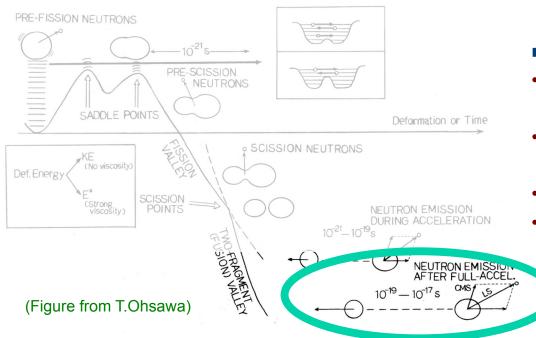


#### Several stages:

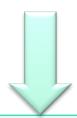
- Pre-scission (compound nucleus)
- Scission (neck break-up)
- During acceleration
- After full-acceleration







- Several stages:
- Pre-scission (compound nucleus)
- Scission (neck break-up)
- During acceleration
- After full-acceleration



Interested in these "later" time processes - "prompt" & "delayed" particle production





#### "prompt"

two fission fragments (FF) emit prompt n and  $\gamma$ -rays, de-excite to their ground state.

#### Probes of:

- nuclear configurations @ scission pt
- characteristics of the fission process - distribution of excitation energy, spin, etc.

#### "delayed"

~10% of energy released via  $\beta$ -decay

Complicated \( \beta \)-decay chain

Delayed neutrons produced when  $E_f > S_n$ .

Emitted n,  $\beta$ ,  $\gamma$  contribute to heating, reactor controls, etc. ( $\nu$ , non-reactive)

A detailed knowledge

- individual precursors
- fragment yields

needed to fully characterize the delayed particles.

Experimental data is incomplete.





#### "prompt"

two fission fragments (FF) emit prompt n and  $\gamma$ -rays, de-excite to their ground state.

#### Probes of:

- nuclear configurations @ scission pt
- characteristics of the fission process - distribution of excitation energy, spin, etc.

## "delayed"

~10% of energy released via  $\beta$ -decay

Complicated \( \beta \)-decay chain

Delayed neutrons produced when  $E_f > S_n$ .

Emitted n,  $\beta$ ,  $\gamma$  contribute to heating, reactor controls, etc. ( $\nu$ , non-reactive)

A detailed knowledge

- individual precursors
- fragment yields

needed to fully characterize the delayed particles.

Experimental data is incomplete.





## History - ENDF Decay Data Library

#### Evaluation for Delayed Neutron Spectra

- Brady M.C. & England evaluated 271 precursors (late 1980's)
- Delayed neutron energy spectra obtained for individual precursors
- BETA code employed to extend incomplete experimental data
- Modified evaporation model for unmeasured spectra
- 36 important precursors: Ga, As, Br, Rb, Y, In, Sb, Te, I, Xe and Cs





## History - ENDF Decay Data Library

### Evaluation for Delayed Neutron Spectra

- Brady M.C. & England evaluated 271 precursors (late 1980's)
- Delayed neutron energy spectra obtained for individual precursors
- BETA code employed to extend
- Modified evaporation model for 14.
- 36 important precursors: Ga, A 12

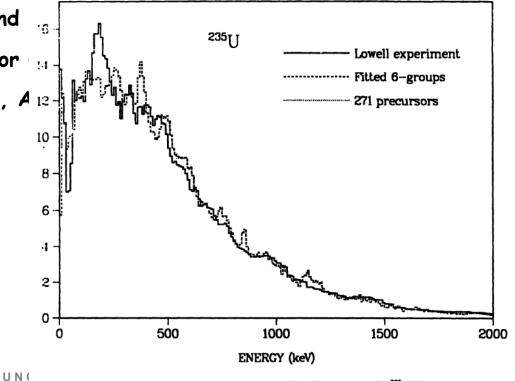
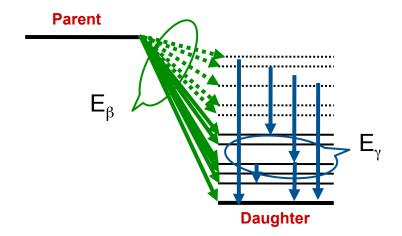




Fig. 1. Comparisons with Lowell equilibrium spectra for <sup>235</sup>U(T).

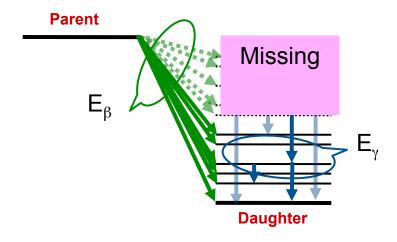
■ Early calculations utilizing standard nuclear data libraries, suffered from the "pandemonium" effect (Hardy et al., Phys. Lett. 71B, 307 (1977)).







Early calculations utilizing standard nuclear data libraries, suffered from the "pandemonium" effect (Hardy et al., Phys. Lett. 71B, 307 (1977)).



Limitations in Ge detectors Miss  $\beta$  transitions to higher levels

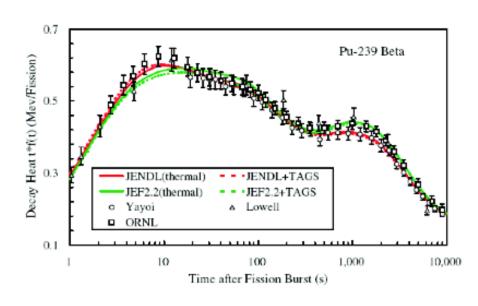
- $E_{\beta}$  overpredicted  $E_{\gamma}$  underpredicted

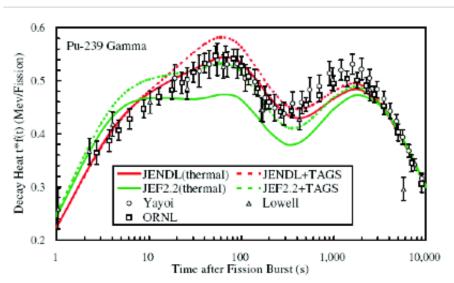




## Most data libraries supplement with Gross Theory of Beta-decay (K. Takahashi, M. Yamada, T. Kondoh, At. Data Nucl. Data Tables 12, 101 (1973))

#### Fairly good agreement with experiment.





N. Hagura, T. Yoshida, T. Tachibana J. Nucl. Sci. Tech. 43 (2006) pg. 497

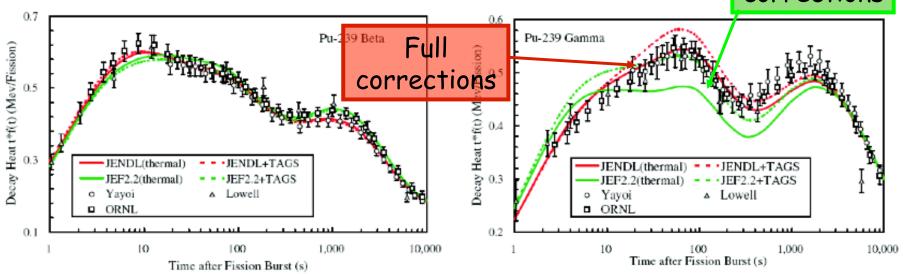




Most data libraries supplement with Gross Theory of Beta-decay (K. Takahashi, M. Yamada, T. Kondoh, At. Data Nucl. Data Tables 12, 101 (1973))

Fairly good agreement with experiment.

Minimal corrections

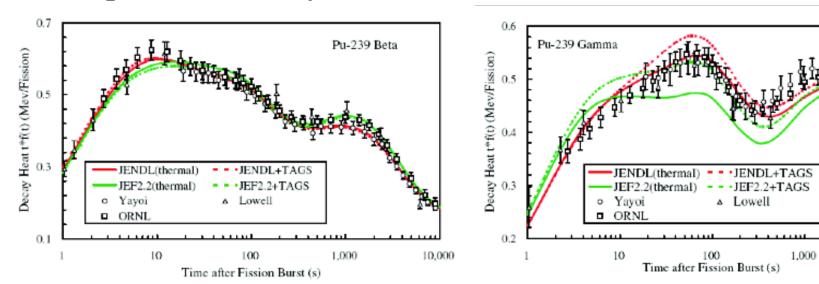


N. Hagura, T. Yoshida, T. Tachibana J. Nucl. Sci. Tech. 43 (2006) pg. 497





- Recent Total Absorption Gamma-ray Spectroscopy (TAGS) studies include transitions to higher levels eliminates "pandemonium"
- However, when individual nuclei are replaced with TAGS results, the agreement with experiment deteriorates.



N. Hagura, T. Yoshida, T. Tachibana J. Nucl. Sci. Tech. 43 (2006) pg. 497

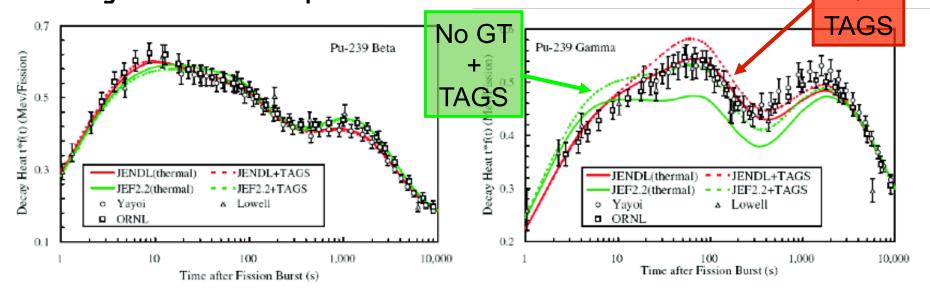




10,000

Recent Total Absorption Gamma-ray Spectroscopy (TAGS) studies include transitions to higher levels - eliminates "pandemonium"

However, when individual nuclei are replaced with TAGS results, Give agreement with experiment deteriorates.



N. Hagura, T. Yoshida, T. Tachibana J. Nucl. Sci. Tech. 43 (2006) pg. 497





## Objective

#### Develop a "more microscopic" approach to delayed particle production

#### Combine

Statistical Hauser-Feshbach Nuclear structure

#### Obtain (for each individual precursor)

Delayed-neutron yields
Delayed Particle Energy spectra

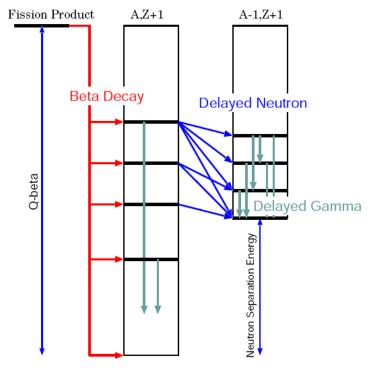
#### Benchmark

Summation Calculations
TAGS experiments





## Theory Developed



Nuclear Structure Model Nuclear Reaction Model

#### Nuclear Structure

- $\beta$ -decay rate
  - $\cdot$  Q<sub> $\beta$ </sub> from Möller mass model (FRDM)
  - QRPA Decay ME  $< f \mid \beta_{GT} \mid i >$  (Möller)
- Low-lying discrete state data from ENSDF

#### Nuclear De-excitation

- Neutron and  $\gamma$  emission rate
  - Statistical Hauser-Feshbach model
  - All possible transitions from (A,Z+1) to (A-1,Z+1) are included

We combine these two processes to calculate the energy distribution of emitted neutron T. Kawano, P. Möller, W.B. Wilson, PRC 78 0546-1 (2008)



## Microscopic Model for $\beta$ -decay

#### Solve Schrödinger Equation

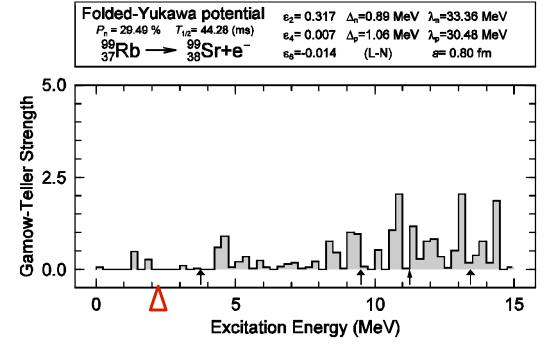
- 3D single-particle potential
- Residual interactions
   Pairing
   Gamow-Teller

#### Calculate

- Mass
- Ground state shape
- Q-values and wave functions

#### QRPA Decay rates

- calculate  $\langle f | \beta_{GT} | i \rangle$
- Obtain (E<sup>(k)</sup>, b<sup>(k)</sup>)
- If ENSDF β-decay data available, QRPA is replaced





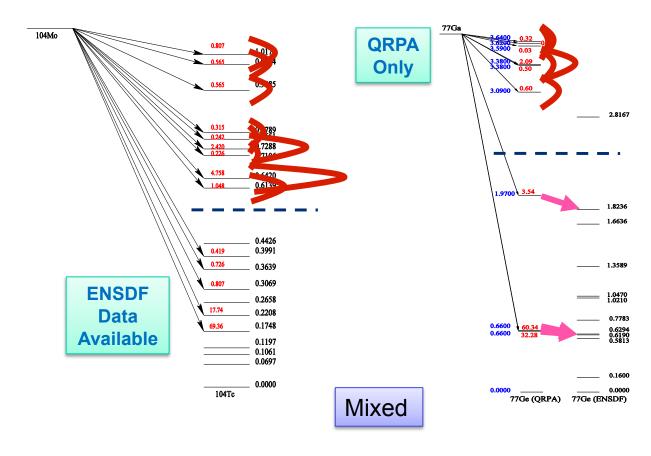
#### Transition Probabilities

#### Data Smoothing and Re-normalization

The QRPA calculation includes pairs  $(E_k,b_k)$ 

E<sub>k</sub> = excitation energy of the daughter nucleus b<sub>k</sub> = branching ratio to the state

Strength distribution is smoothed by a Gaussian with the width  $\Gamma$  of 30 keV or 100keV

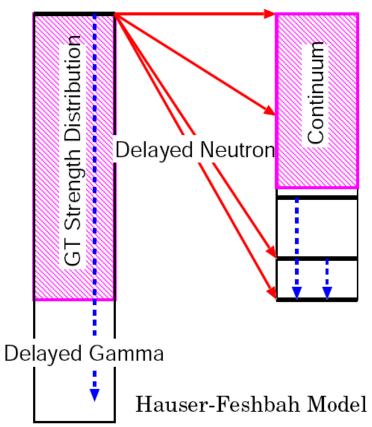






## Beta-Delayed Neutron Emission

#### Neutron emission from the daughter nucleus



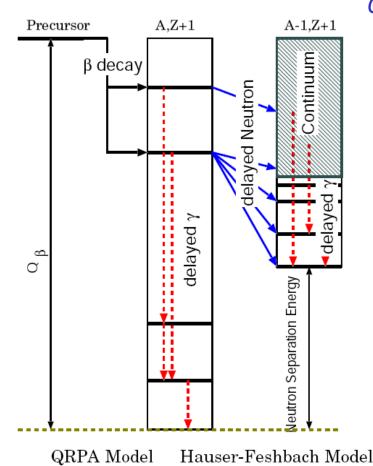
Assume excited state after  $\beta$ -decay is a compound state, having fixed J

$$|I-1| < J < I+1$$

- Neutron and  $\gamma$ -ray emissions calculated with the statistical Hauser-Feshbach theory (CGM code).
- The  $\gamma$ -ray emission competition is included.



## Beta-Delayed Gamma-Ray Emission



Gamma-ray emission multiplicity larger than unity

γ-ray emission takes place in both daughter and grand-daughter nuclei

To calculate delayed  $\gamma$  spectra, follow all  $\gamma$ -ray cascade

Individual low-lying transition is important

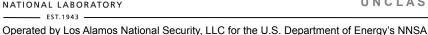
The evaluated structure data in ENSDF are incorporated

 $\beta$ -decay to discrete levels

γ-ray branching ratios

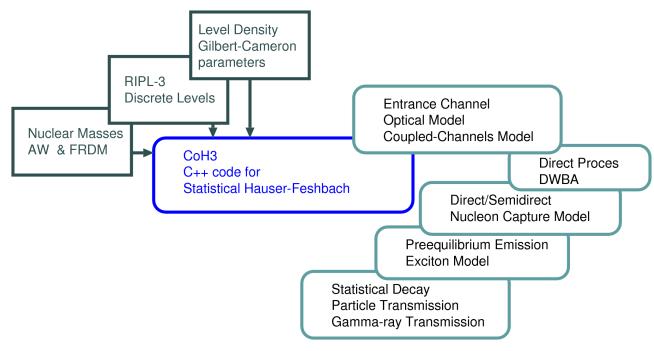
The whole decay process, including γn, is calculated with Hauser-Feshbach model.

os Alamos





### Statistical Hauser-Feshbach Code, CoH

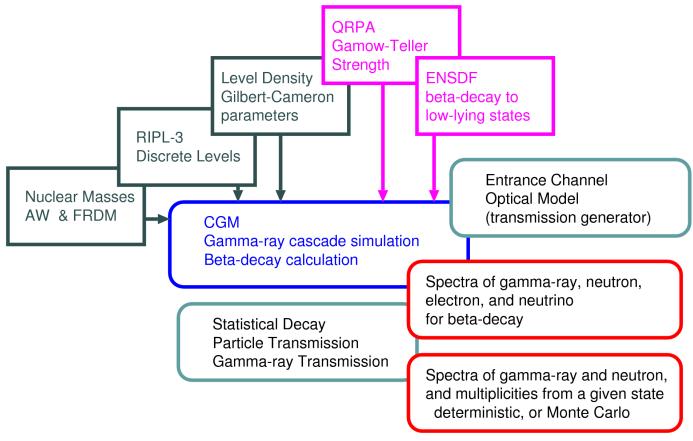


CoH calculates particle or  $\gamma$ -ray induced reactions on medium and heavy nuclei – reaction cross sections, particle and  $\gamma$ -ray energy spectra, isomer production in the MeV energy range.



Slide 20

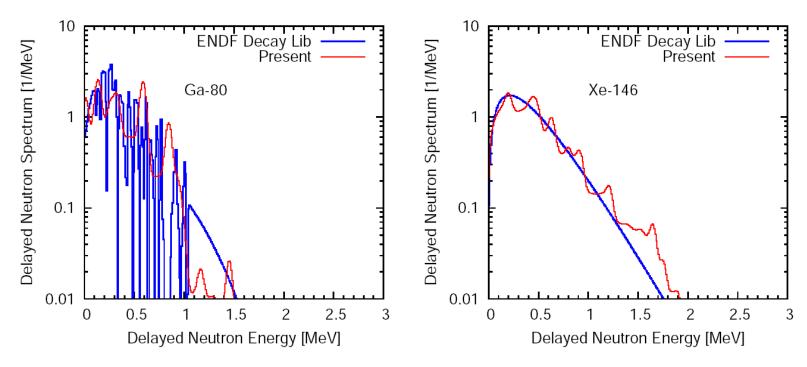
## Neutron and Gamma Decay Code, CGM





Slide 21

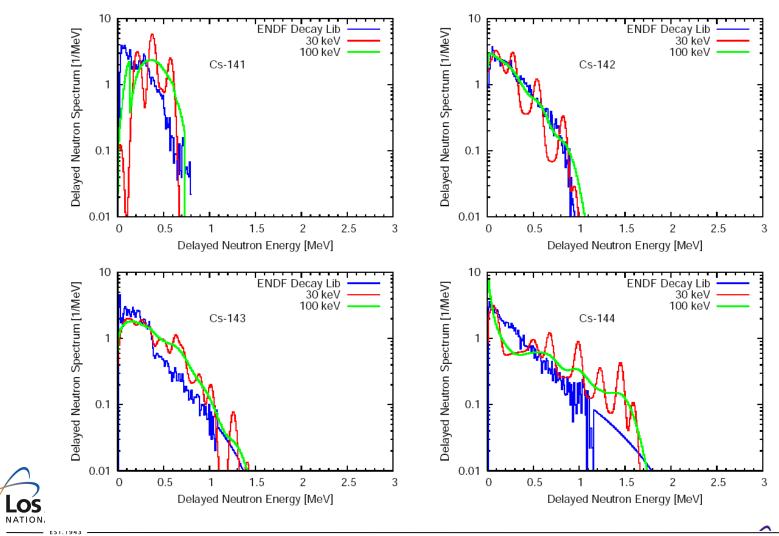
## Calculated Neutron Spectra



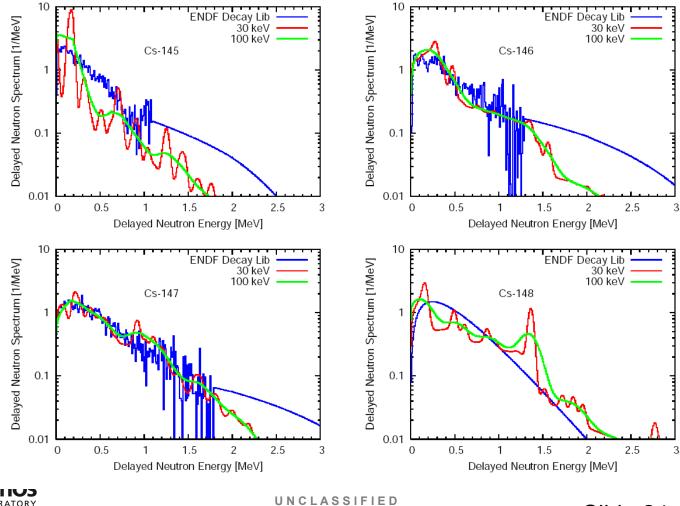
- ENDF decay library gives a simple evaporation spectrum
- 30 keV of energy resolution adopted
  - In our calculations, structures in the spectra persist



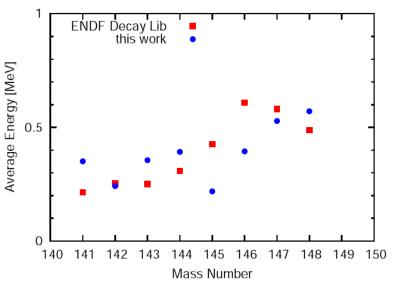
## Cs Isotopes, I

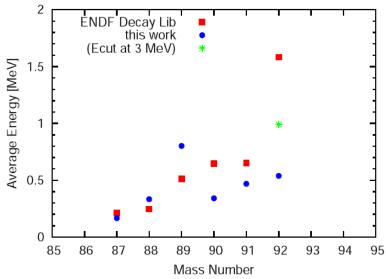


## Cs Isotopes, II



## Average Energy of the Spectra





The average energy varies smoothly with nuclear mass

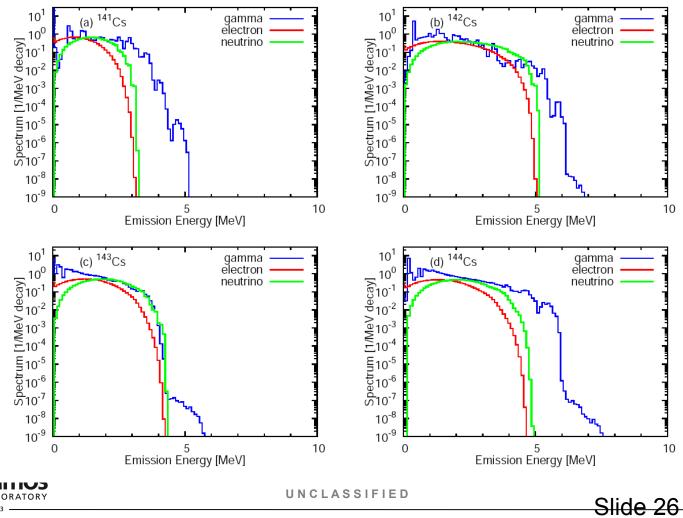
Maximum neutron energy  $E_{max} = Q_{\beta} - S_n$ 

Sudden jump seen in ENDF decay library, due to the extrapolation by using the evaporation spectrum

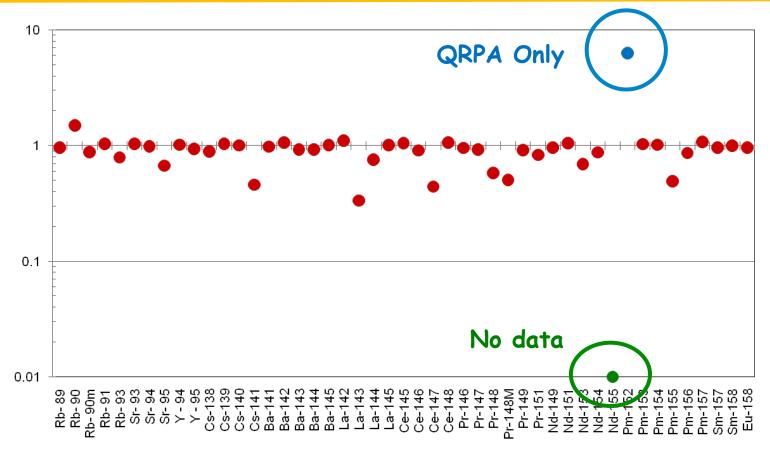




## Cs Isotopes



## Comparison with TAGS - Average E,

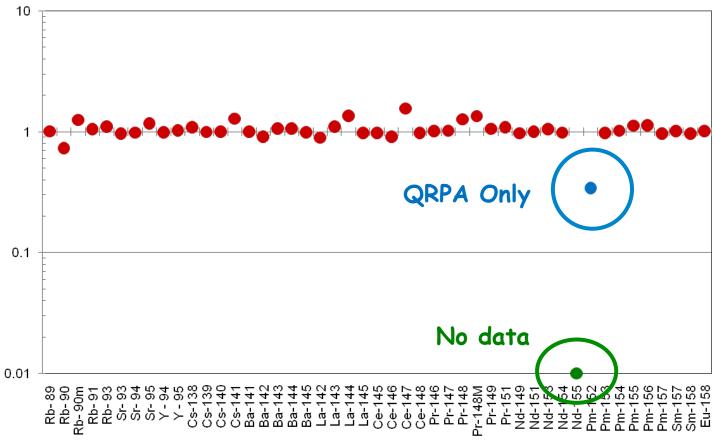




TAGS data: Greenwood et al.



## Comparison with TAGS - Average $E_{\beta}$





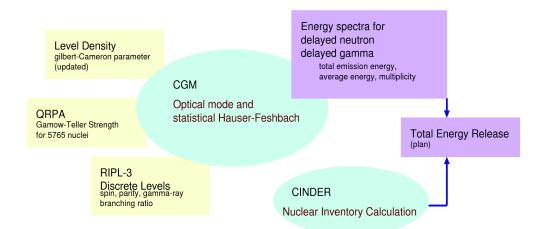
TAGS data: Greenwood et al.



## Decay Heat Calculations

#### Assembling microscopic data to compare with aggregated data

We perform the CGM calculation (average/total  $\gamma$  and  $\beta$  energies) for all fission products Nuclear inventory calculation, by CINDER, gives temporal abundance of each fission product.



#### We can obtain

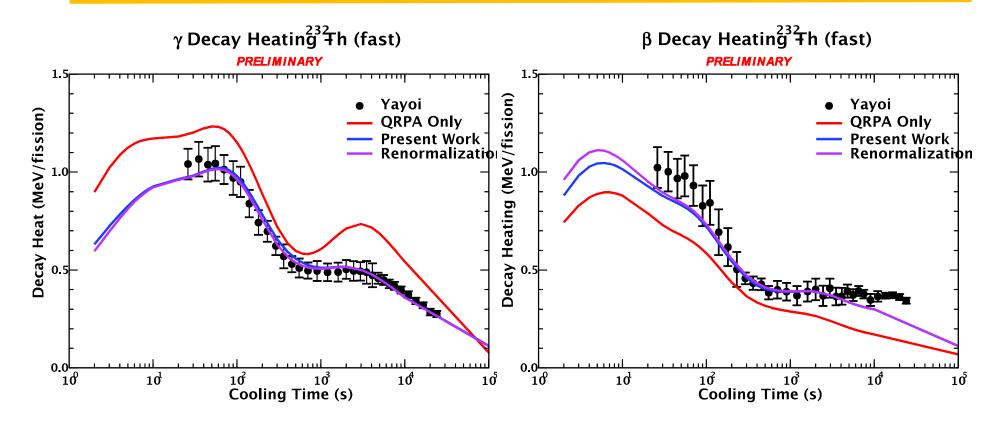
- $\cdot$   $\beta$  and  $\gamma$  heating after fission burst
- Dn spectra in a 6-group structure (reactor application)
- · delayed γ-energy spectra for fission







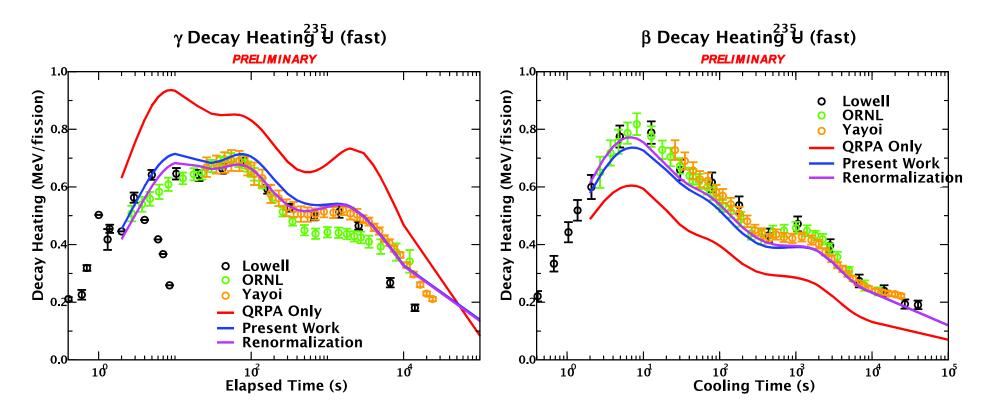
## Calculated decay heating 232Th



M. Akiyama & S. An, Proc. Nuclear Data for Sci. Tech., Antwerp (1982) p. 237



## Calculated decay heating 235U





M. Akiyama & S. An, ibid J.K. Dickens et al., Nucl. Sci. Eng. **74** 106 (1980) H. Nguyen et al., Nuclear Dat for Sci. Tech., Trieste (1997) p. 835.





#### "prompt"

two fission fragments (FF) emit prompt n and  $\gamma$ -rays, de-excite to their ground state.

#### Probes of:

- nuclear configurations @ scission pt
- characteristics of the fission process - distribution of excitation energy, spin, etc.

#### "delayed"

~10% of energy released via  $\beta$ -decay

Complicated \( \beta \)-decay chain

Delayed neutrons produced when  $E_f > S_n$ .

Emitted n,  $\beta$ ,  $\gamma$  contribute to heating, reactor controls, etc. ( $\nu$ , non-reactive)

A detailed knowledge

- individual precursors
- fragment yields

needed to fully characterize the delayed particles.

Experimental data is incomplete.





## Monte Carlo Simulation of Fission Fragment Evaporation - PFNS and more!

#### Madland-Nix or Los Alamos model:

Average over entire fission fragment distributions and neutron cascades

Several important assumptions regarding what happens near scission

Main advantage: very few tunable parameters!

Main disadvantage: computes averages only:

Average neutron multiplicity <n>

Average neutron spectra  $\langle \chi \rangle (E_{in}, E_{out})$ 

## From the prediction of a few average quantities $(\chi,n)$ to detailed exclusive quantities: P(n), $\chi_{(n=1,2,...)}$ , n-n correlations, ...

→ Monte Carlo simulation of the de-excitation of the primary fission fragments

#### Much more physics

→ to be used in advanced transport simulations

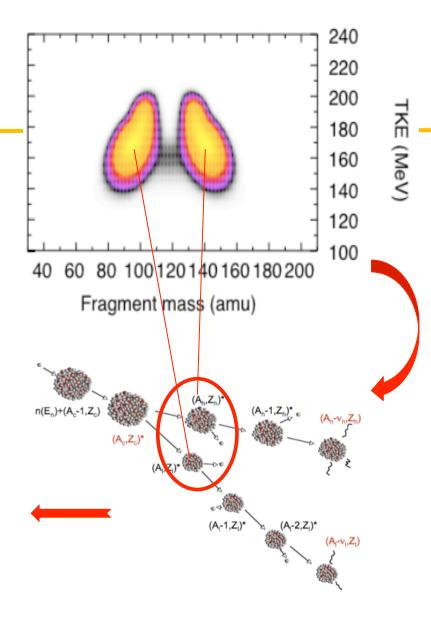




## Monte Carlo Hauser-Feshbach Simulations

- 1. Sample from Y(A,Z,TKE) distribution
- 2. Infer  $E^*_{tot}$  and  $J_{tot}$ , and partition between the two fragments
- 3. Infer temperatures  $T_1$  and  $T_h$  $\rightarrow R_T = T_1/T_h$
- 4. Apply Hauser-Feshbach equations

 $\langle \chi \rangle$ (E),  $\langle n \rangle$ , P(n),  $\chi$ (E)<sub>|n</sub>, n-n correlations, etc.

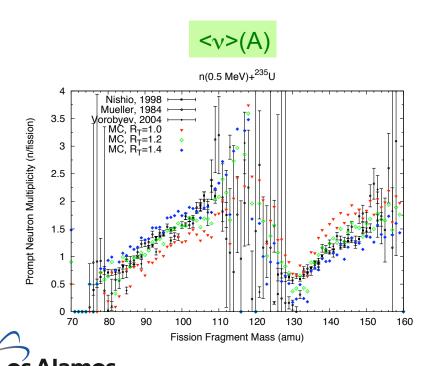


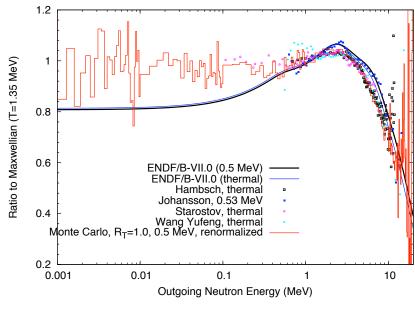


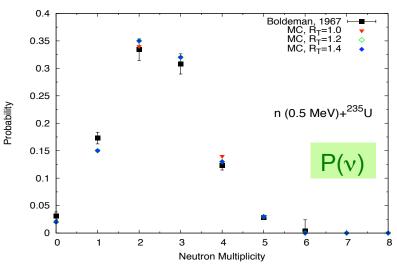
Slide 34

## Application to n+235U

## Using experimental primary fission fragment yields $Y_{exp}(A, KE)$ [F.-J.Hambsch, private communication]









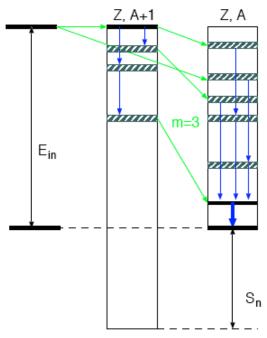


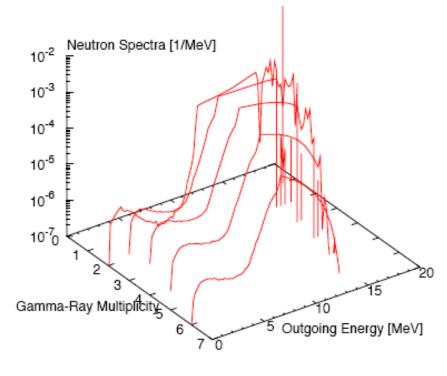
## Prompt Fission Gamma Rays... Monte Carlo Hauser-Feshbach Simulations

#### Towards a fully Monte Carlo Hauser-Feschbach solution

New code being developed in our group -> to be applied to this problem

Example: n(20 MeV)+56Fe gated on 0+-2+ E2 transition







## Concluding Remarks

- Microscopic Theory of  $\beta$ -delayed neutron and  $\gamma$  spectra
- We developed a new, more microscopic technique to calculate the delayed-neutron and  $\gamma$  energy spectra
- lacktriangle This technique obtains the eta-decay rates from
  - The FRDM and QRPA models, and
  - The neutron and  $\gamma$ -ray emission probabilities from the statistical Hauser-Feshbach model
- The calculated average energies for the spectra tend to be similar to those for the data in ENDF decay library.
- The aggregated  $\gamma$  and electron energy releases from fission products were compared with the decay heat measurements
- This method can be extended to include prompt fission spectra (in progress).
  - MC -> No longer limited to average quantities exclusive processes teach us more!





## Thank you!



