NJOY2016 improvements for ENDF/B-VIII.0

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- **Making a new ENDF/B library …**
- **Overview of important updates**
  - – Changes to HEATR
  - – Changes to PURR
- **Other updates and fixes**

Making a new ENDF/B library …

We like to change formats and add new data previously not available in each ENDF/B generation

ENDF/B-VIII.0 is no exception to this

- Fission neutron and gamma probabilities in MF6/MT18
- Sub-actinide and non-neutron induced “fission” in MF10/MT18
- Tabulated fission energy release components in MF1/MT458

Update NJOY modules to use or ignore the new formats as required

- MODER so that we can safely toggle between ASCII and binary
- HEATR for the new fission energy release formats
- GROUPR for treating the new sub-actinide fission formats and ignore the fission neutron and gamma probabilities

But also fix for processing problems whenever they come up

Fission energy release data in ENDF-6

Fission energy release is a complex process

We define the basic fission energy components

- Q_k kinetic energy of the fission fragments
- $Q_{n,p}$ and $Q_{n,d}$ energy of prompt and delayed neutrons
- $Q_{\gamma,p}$ and $Q_{\gamma,d}$ energy of prompt and delayed γ-rays
- Q_β energy of the delayed β-rays
- Q_ν energy carried away by the neutrinos

We can also define some composite components

- $Q_f = Q_k + Q_{n,p} + Q_{n,d} + Q_{\gamma,p} + Q_{(\gamma,d)} + Q_\beta + Q_\nu$
- $Q_r = Q_f - Q_\nu = Q_k + Q_{n,p} + Q_{n,d} + Q_{\gamma,p} + Q_{\gamma,d} + Q_\beta$

These components are energy and time dependent …

Fission energy release data in ENDF-6

Option 1: thermal point evaluation

- The original format introduced in 1985 for ENDF/B-V
- Based on Sher-Beck systematics

$$Q_i(E) = Q_i(0) - \delta Q_i(E)$$

$$\delta Q_k(E) = 0$$
$$\delta Q_{n,p}(E) = -1.307E + 8070000\big(\nu_t(E) - \nu_t(0)\big)$$
$$\delta Q_{n,d}(E) = 0$$
$$\delta Q_{\gamma,p}(E) = 0$$
$$\delta Q_{\gamma,d}(E) = 0.075E$$
$$\delta Q_{\beta}(E) = 0.075E$$
$$\delta Q_{\nu}(E) = 0.100E$$

$$\delta Q_r(E) = -1.157E + 8070000\big(\nu_t(E) - \nu_t(0)\big)$$
$$\delta Q_f(E) = -1.057E + 8070000\big(\nu_t(E) - \nu_t(0)\big)$$

Fission energy release data in ENDF-6

Option 2: polynomial evaluation

- Introduced in 2010 for ENDF/B-VII
- Thermal point assumes that Q_k and $Q_{(\gamma,p)}$ is energy independent but this is not supported by experimental data and models

$$Q_i(E) = \sum_i c_{i,n} E^n$$

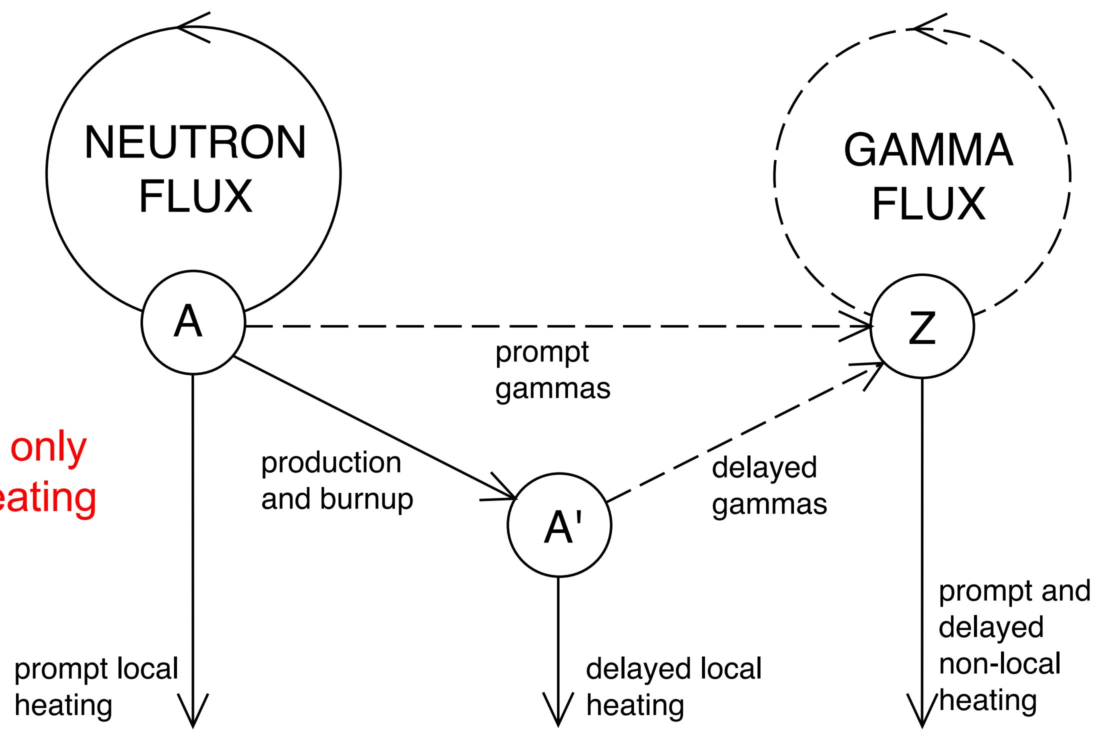
Option 3: arbitrary tabulated function

- Introduced in 2017 for ENDF/B-VIII
- Currently only used for 235U, 238U and 239Pu

Each can handle its predecessors but not the other way around

Total and partial KERMA in HEATR

HEATR produces pointwise heating production cross sections and radiation damage energy production



Important: HEATR only handles prompt heating

Total and partial KERMA in HEATR

Heating is described by Kinematic Energy Release in Materials or KERMA k_{ij}

$$H(E) = \sum_i \sum_j \rho_i k_{ij}(E)\phi(E)$$

KERMA can be calculated using an energy balance:

$$k_{ij}(E) = \left[E + Q_{ij} - \bar{E}_{ij}^{n} - \bar{E}_{ij}^{\gamma}\right]\sigma_{ij}(E)$$

- Total available energy in a reaction equal to $E + Q_{ij}$
- Energy taken away by neutron and photons equal to $\bar{E}_{ij}^{n} + \bar{E}_{ij}^{\gamma}$

HEATR separates neutron and photon heating

$$k_{ij}(E) = k_{ij}^{n}(E) - \bar{E}_{ij}^{\gamma}\sigma_{ij}(E)$$

Partial fission KERMA

Fission is a special case with respect to KERMA

- The fission Q value is energy dependent
- It contains both prompt and delayed components

Total prompt energy release from fission

$$Q_p = Q_r - Q_{n,d} - Q_{\gamma,d} - Q_\beta = Q_k + Q_{n,p} + Q_{\gamma,p}$$
$$Q(E) = Q_p(E) - E$$

Total energy removed by neutrons

$$\bar{E} = \bar{\nu}_f \bar{E}_f = Q_{n,p}$$

Important: Prior to NJOY 2016.21, thermal point evaluations used a different formula

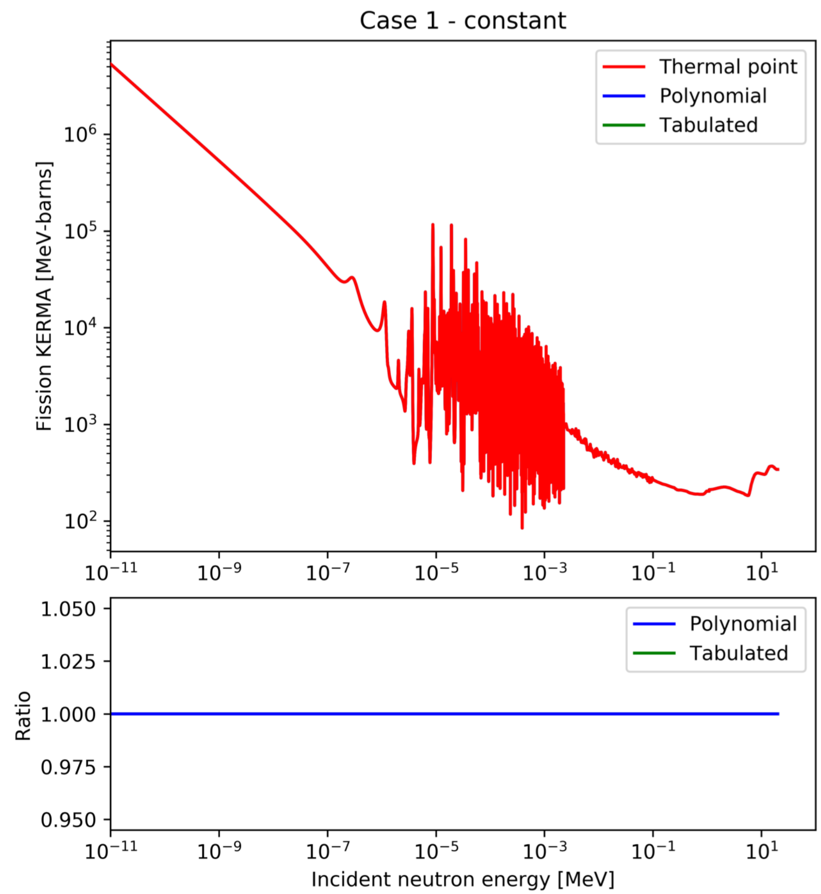
The partial fission KERMA is thus equal to

$$k_f^n(E) = [E + Q(E) - \bar{E}]\sigma_{ij}(E) = \left[Q_k(E) + Q_{\gamma,p}(E)\right]\sigma_{ij}(E)$$

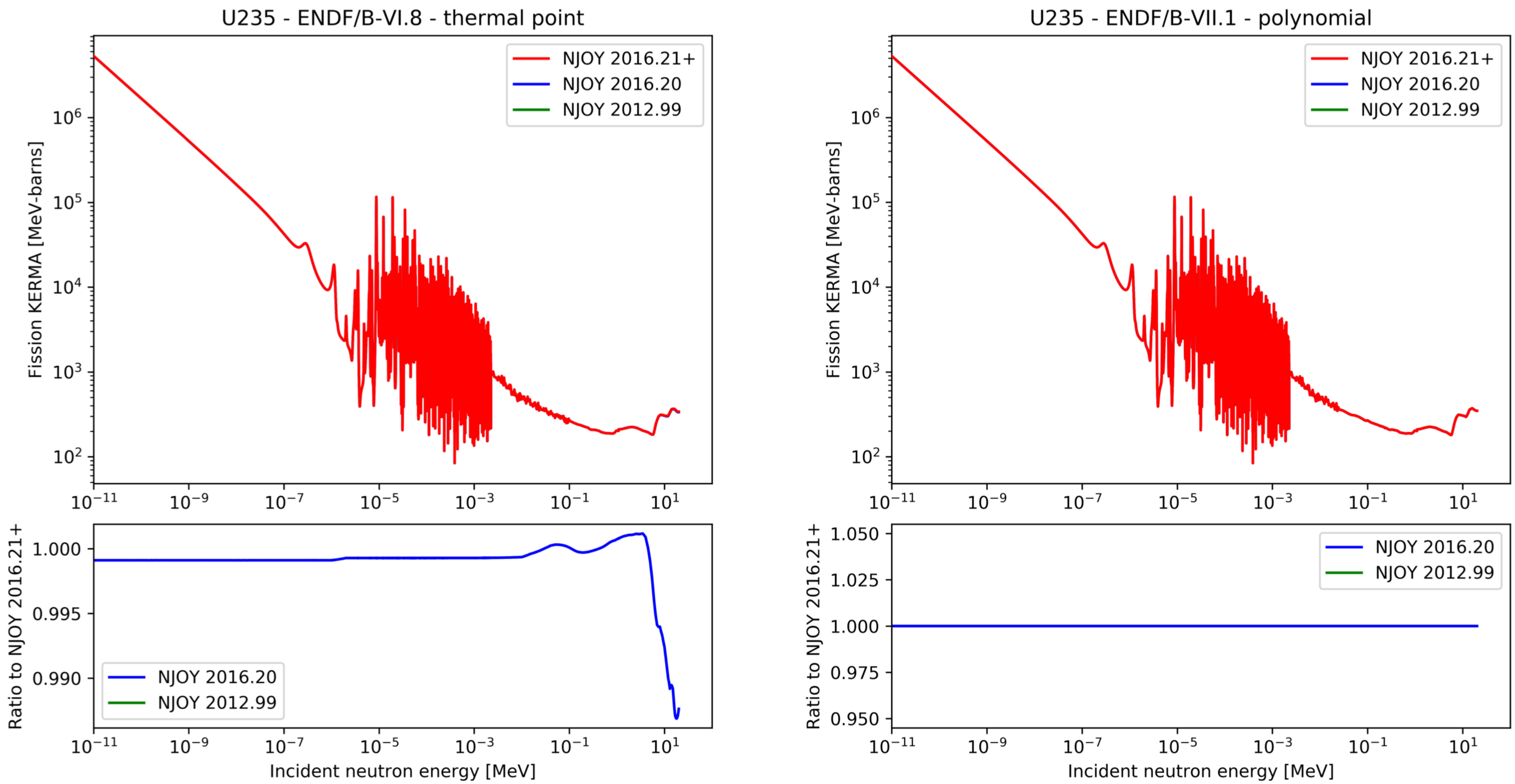
Verification and validation

Multiple tests

- Analytical data that can be represented in all formats and should give the same results
- Comparison with NJOY 2012.99 and NJOY 2016.20



Verification and validation



Unresolved resonance probability tables from PURR

Probability tables have a number of long outstanding issues and some of these have cropped up during ENDF/B-VIII.0 processing

- Some tables have bins with an associated probability of zero
- Some tables exhibit zero or negative cross section values

How does PURR generate these tables

- PURR determines an energy range using the lowest value of the average level spacing it can find in the evaluation
- 10000 cross section values are sampled in this energy range
- The cross section values are sorted and corrected by the background cross section
- The values are subdivided into bins with corresponding probability

Known cases from the past still in ENDF/B-VIII.0: ^{22}Na, ^{36}Ar, ^{106}Cd

Unresolved resonance probability tables from PURR

Zero probability bins: the case of ^{210}Po

The problem was traced back to the way PURR determines the lowest average level spacing

- PURR set the initial value of this variable to 500 eV before comparing to the evaluation
- For ^{210}Po, this is actually 30 keV so PURR leaves it at 500 eV because it is smaller
- This resulted in the generation of ~9500 cross section values that are exactly equal
- This then results in the generation of cross section bins with limits smaller than the previous bins so that no samples are accumulated, leading to a zero probability

NJOY changes – available in NJOY 2016.24 and above:

- The initial value for the average level spacing is now 100 keV
- PURR will signal cases where this value is still too small

Unresolved resonance probability tables from PURR

Negative cross section values: the case of ^{240}Pu with LSSF set to 1

- The unresolved resonance parameters are only to be used for self-shielding
- MF3 contains the actual infinite dilute cross sections to be used

The problem was traced back to the infinite dilute cross sections

- The total cross section was not equal to the sum of its components
  - For example: $\sigma_t = 14.19534$ and $\sigma_e = 15.271$ at 5.7 keV
  - Note: this happens in several ENDF/B-VIII.0 evaluations
- PURR computes a background cross section which may lead to negative values when the sampled cross section values are small enough

NJOY changes – available in NJOY 2016.35 and above:

- PURR now sets the background cross section to zero in the following cases:
  - σ_t is smaller than the sum of its components
  - σ_t is larger than the sum of its components below the competition threshold
- PURR indicates whenever this happens or when negative cross section are detected

NJOY issues and follow up

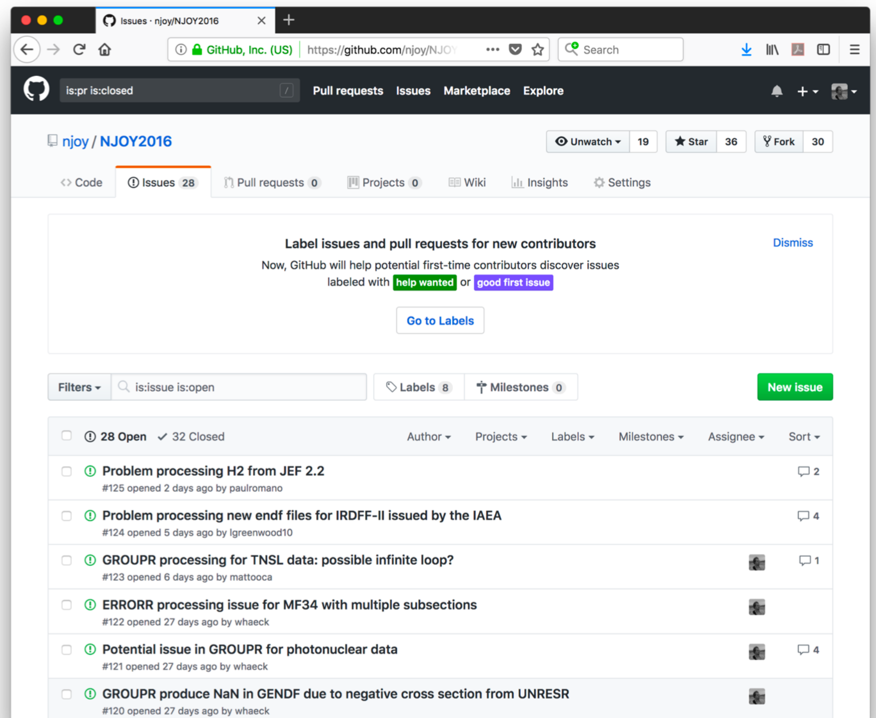
The NJOY Github page tracks all identified issues

- https://github.com/njoy/njoy2016/issues

Report an issue

- Open an issue on Github
- Send us an email at njoy@lanl.gov

If you see something, say something!



Conclusions

Changes were made in NJOY for new formats

- Fission neutron and gamma probabilities in MF6/MT18
- Sub-actinide and non-neutron induced "fission" in MF10/MT18
- Tabulated fission energy release components in MF1/MT458
- MODER, HEATR and ACER were updated

New libraries tend to push the limits leading to fixes and updates

- ACER, ERRORR, LEAPR, PURR and THERMR were updated

The NJOY2016 test suite continues to expand

- There were originally 21 tests in the test suite
- Today, there are 47 tests in total – if I haven't added any new ones, that is ;-)

Additional reading

Reports related to NJOY updates

- W. Haeck, “New fission heating capabilities in the NJOY2016 HEATR module”, Los Alamos National Laboratory Report LA-UR-18-22546
- W. Haeck, J. L. Conlin, A. P. McCartney, A. C. Kahler, “NJOY2016 updates for ENDF/B-VIII.0”, Los Alamos National Laboratory Report LA-UR-18-22676

Paper and presentation related to NJOY updates

- W. Haeck, “Updating NJOY’s HEATR module for ENDF/B-VIII.0”, ANS RPSD 2018 conference, August 26-31, 2018, Santa Fe, NM, USA

Issue tracking for NJOY2016

- https://github.com/njoy/njoy2016/issues