Nuclear Data Pipeline, Part II

From ENDF to Application

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Nuclear Data Pipeline

The Nuclear Data Pipeline is a representation of the different steps that are required to get nuclear data all the way from being measured to where it will be used by scientists and engineers in application codes. The different steps are shown here and graphically in Figure 1.

1. Measurement
2. Theory
3. Evaluation
4. *Processing*
5. *Verification and Validation*
6. *Applications*

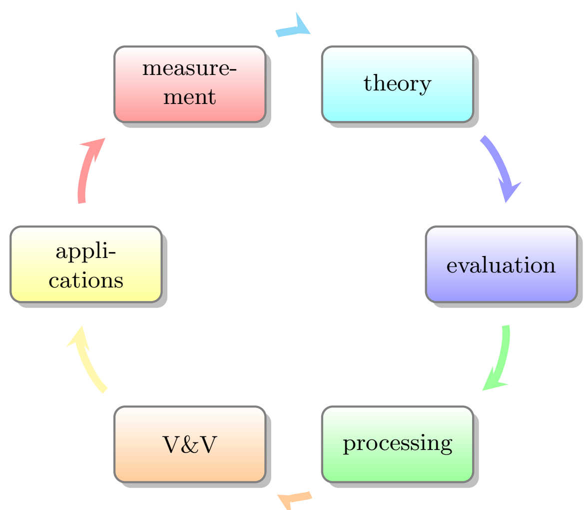


Figure 1: Nuclear Data Pipeline (in a non-pipeline graphic!).

Dave Brown spoke about the first half of the Nuclear Data Pipeline; I will complete the discussion by talking about what happens to nuclear data after it is part of a nuclear data library.

While the pieces of the pipeline are shown sequentially, there is a lot of feedback between each step that informs and improves the nuclear data for the next iteration.

Forms of Nuclear Data

There are several different forms of nuclear data. They are worth mentioning by name so that there is less confusion later on.

Evaluated Data

Data as produced by an evaluator Evaluated Data is data that is produced by an evaluator from theory and measurement. It nearly comes as ENDF-formatted data, but could also come as GNDS-formatted data. (GNDS is the proposed modern replacement for ENDF.)

- ENDF
- GNDS

Processed Data

Some (or all) processing is complete Processed Data is where some processing steps have been completed. We'll talk about some of the processing steps and physics calculations in a bit.

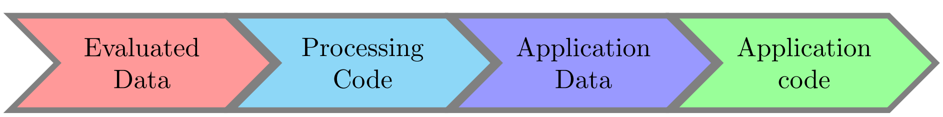
Application Data

Processed data in a form application codes can use Application Data is in a form that application codes can use. The form of the data is dependent on whether the transport code is a Monte Carlo or deterministic code and is often problem dependent.

- ACE—Monte Carlo
- NDI—deterministic

1 Processing of Nuclear Data

Nuclear Data Processing



Processing code:

- *Read evaluated data* Evaluated data must be generic in temperature so as to be applicable to many.
- *Perform physics calculations* Evaluated data becomes application and/or problem specific. The processing steps make the generic evaluated data applicable for more specific problems (e.g., at a certain temperature or assuming a particular flux profile).
- *Generate code-specific application data* Finally the processing code will write the data in a form that the application code can use.

It is important to note that without the processing step, *there will be no data that describes for the physics for the application code.*

Physics Calculations in Processing Codes

There are many different physics calculations that are done by a processing code in order to prepare the data for use by an application code. Please note that this is not a complete list.

- Resonance reconstruction Evaluated data contains resonance data in parameters. A major task in processing this data is taking those resonance parameters and converting them to cross section values. This must be done before other processing is completed.
- Doppler Broadening Doppler broadening will broaden the (previously) reconstructed resonances so that the data accurately represents the physics at a particular temperature.
- Secondary particle generation The production of secondary particles , e.g., the α-particle from the (n, α) reaction.
- Calculate energy deposition (KERMA) and radiation damage cross section If KERMA calculations will be performed, the heat production must be calculated from the available data in the evaluation file.
- Produce probability tables from unresolved resonance range
- Produce self-shielded cross sections in unresolved resonance range If there is an unresolved range, proper treatment requires processing this range and producing probability tables for Monte Carlo application codes.
- Calculate multi-group cross sections If processing data for deterministic transport codes, the data must be averaged over energy groups.

Other Processing Tasks

There are other tasks that processing codes can do.

- Generation of covariance matrices Processing codes can also process the uncertainty data in the evaluation files to produce covariance matrices.

  This is a good time to mention that uncertainty information must be considered at every step of the Nuclear Data Pipeline. Without uncertainty information, we don't know how good the mean values are and could be overly optimistic in the results of our calculations.
- Plotting data Since a processing code can read and understand the various data formats (e.g., ENDF, GNDS, ACE, NDI, etc.), then it should be able to plot the data. These plots can be used to identify issues with the data as well as for publishing in journal articles.
  - Cross sections
  - Secondary angle and energy distributions
  - Covariance matrices
  - etc.
- Formatting data for application codes The final step of a processing code is formatting the processed data so it can be consumed by the application codes. Unfortunately, each code has different requirements for its data and so there are a variety of formats that must be produced.
  - Monte Carlo
  - Deterministic

US Nuclear Data Processing Codes

There are three major processing codes being used in the United States:

Los Alamos
NJOY

Oak Ridge
AMPX

Livermore
FUDGE

All codes are undergoing major modernization efforts

- Adapting for the use of GNDS and ENDF Much of the motivation is driven by the anticipation of modern nuclear data formats—such as GNDS—to replace the venerable ENDF format.
- Simplifying and automating the generation of application data from evaluated data There is also a need to simplify the process by which application data is created. Not to remove the necessary physics, but to make it easier for the consumer to generate the needed data for her application.

ENDF Releases

You can see from Figure 2 that the volume of data is increasing with each release of the ENDF library. This poses certain problems.

- Number of evaluations is increasing
- Quantity of data is increasing

- *We can't continue to process/consume data as we once did.* There was a time when one could generate a library by hand. That time has long past.
  Many individuals and institutions have implemented some scripting (usually with Python) to facilitate processing a large number of files. This works, but has limitations. We need to update our processing code capabilities to be able to intrinsically process an entire library for a specific application. If done right, this could be done on the fly where we know the exact simulation characteristics (e.g., flux, temperature, etc.).
  On the application side, the mechanism for including many different isotopes is cumbersome. We need to rethink how to accomplish this to have the greatest fidelity available from the nuclear data.

2 Verification and Validation of Processed Nuclear Data

Verification and Validation of Processed Data

Once the processing has been completed, the data must be verified and validated

- Verify that data fits appropriate format
- Validate that data accurately describes Mother Nature
- Indirectly check that the application codes are using data correctly

Imperfections

- Evaluated data
- Processing codes
- Application codes

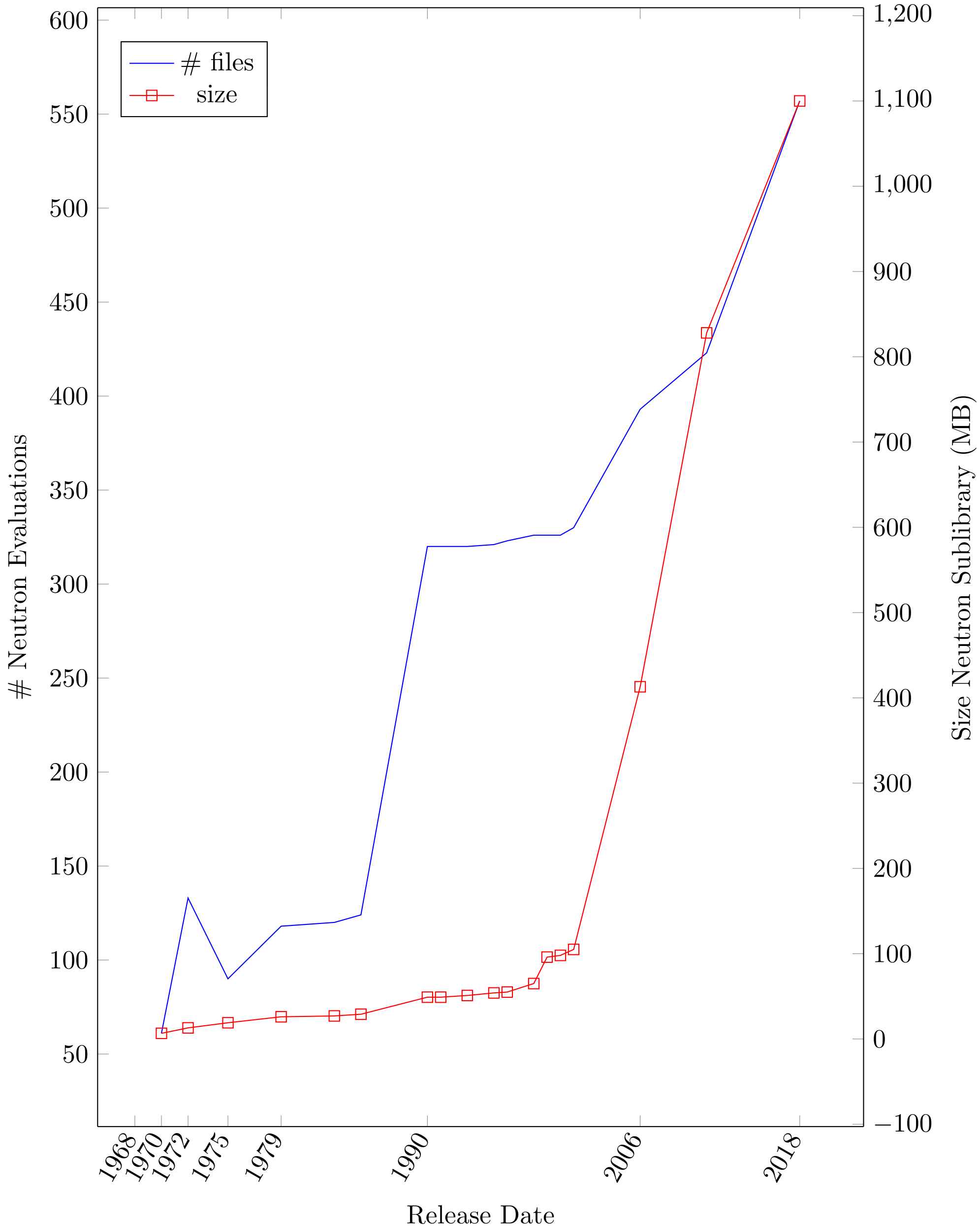


Figure 2: Growth of number of neutron evaluation files and the total size of the neutron sublibrary across the ENDF releases

Verification and Validation of Processed Nuclear Data

Verification:

- Are cross section values positive?
- Do partial cross sections sum to total?
- Are PDFs positive and normalized?
- $P_0 >= 0$
- $|P_n| < P_0, n = 1, \cdots, n_{\mathsf{max}}$
- etc.

Validation of data against experimental benchmarks

- 1000+ MCNP models of critical assemblies
- Compare calculated k_{eff} to experimental k_{eff}
- Plot change in results with changing input parameters
  - e.g., leakage vs. reflector thickness
- LLNL pulsed spheres

3 Use of Nuclear Data in Applications

US Application Codes

There are a variety of application codes used in the United States. Here is a list of just some of the transport codes used and developed at different laboratories in the US.

Los Alamos

- MCNP
- Partisn

Oak Ridge

- SCALE

Livermore

- Mercury
- ARDRA

New Data from Evaluations

When new data becomes available in an evaluation file several things must happen.

- $P(\nu)$ data introduced in ENDF/B-VIII.0 for $^{235}\mathsf{U}$, $^{238}\mathsf{U}$, $^{239}\mathsf{Pu}$.
  - Funded in part from NA-22, ASC-PEM, and NCSP

- Processing codes must be updated
- Application formats must be updated
- Application codes must be updated

- New data is (slowly) moving through the pipeline as capabilities are improved and updated It has been estimated that it takes about 10 year for data to move completely through the pipeline

Conclusion

- The quality and quantity of nuclear data is improving. Our understanding of Mother Nature grows with each revision of our nuclear data libraries.
- In order to take advantage of this increase in knowledge and understanding, we need to make sure that all pieces of the Nuclear Data Pipeline are working together.

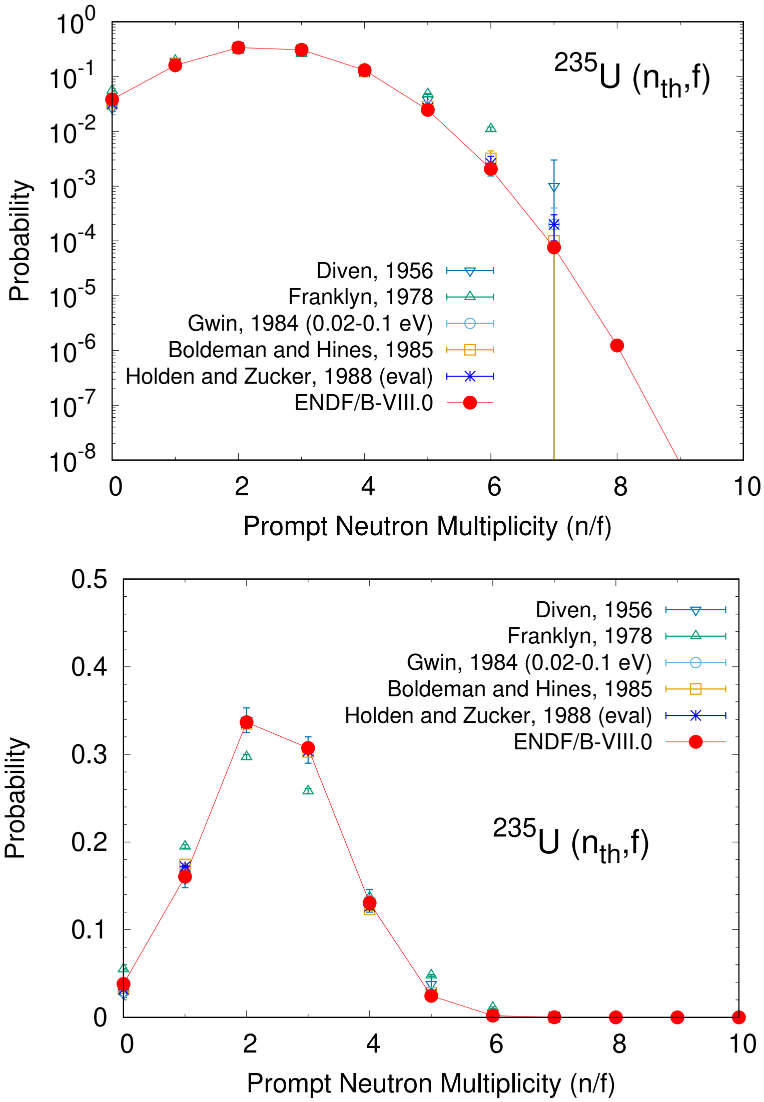


Figure 3: New prompt neutron multiplicity data included in ENDF/B-VIII.0.

- Adding new capabilities to our processing and application codes will help us to better utilize the nuclear data available to us. If we can utilize on-the-fly processing (e.g., Doppler broadening), then we can utilize better physics in our applications and calculate better answers with greater confidence.

Bottom Line

Improving the efficiency of the entire Nuclear Data Pipeline

We have three days of discussion about this Nuclear Data Pipeline in all of its gory details. A major, overarching, goal should be not only to maintain the core competence that are required for each section of the Nuclear Data Pipeline, but to develop tools and methods to optimize the efficiency of the pipeline.

I encourage you to think about improving the efficiency of the pipeline in our discussions this week.