Beyond the ENDF format: A modern nuclear database structure

NEA/Nuclear Science Committee/WPEC

24-25 May 2012

Dennis P. McNabb

Lawrence Livermore National Laboratory

LLNL-PRES-XXXXXX

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

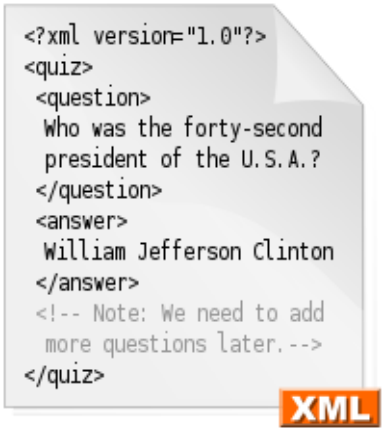
Circa 2000, LLNL realized its internal nuclear data infrastructure was limiting progress and was obsolete

- Back in 1960, LLNL developed ENDL (a precursor to ENDF)
- Problems arose in our simulation-heavy modern era with our database
  - Took up too much space -- only handles pointwise data
  - Only supports a fixed number of reactions
  - Other infrastructure also old and limiting
  - Couldn't share/compare -- Everybody else using ENDF
- Conclusion:
  - First step: Adopt ENDF and join the rest of the world
  - Second step: Design a new "structure" and infrastructure

LLNL saw important benefits to this transition:
- Develop expertise in a new generation of scientists and engineers
- Enhance simulation capabilities

We would like the international community to jointly develop a new nuclear data structure as an international standard

- Next generation is more comfortable with and interested in modern concepts
  - XML, HDF5, MySQL, Python, Java
- Leverage vast, well-tested infrastructure
  - Automated format controls
  - Routines for code access libraries automatically generated
  - Large user base from governments to industry
- Remove artificial limits imposed by legacy formats
  - Data precision essentially unlimited
  - Extensible without sacrificing backwards compatibility
  - Optimized I/O for large parallel simulations
- Link disparate databases to each other
  - Reactions, level structure, mass tables can all be cross referenced



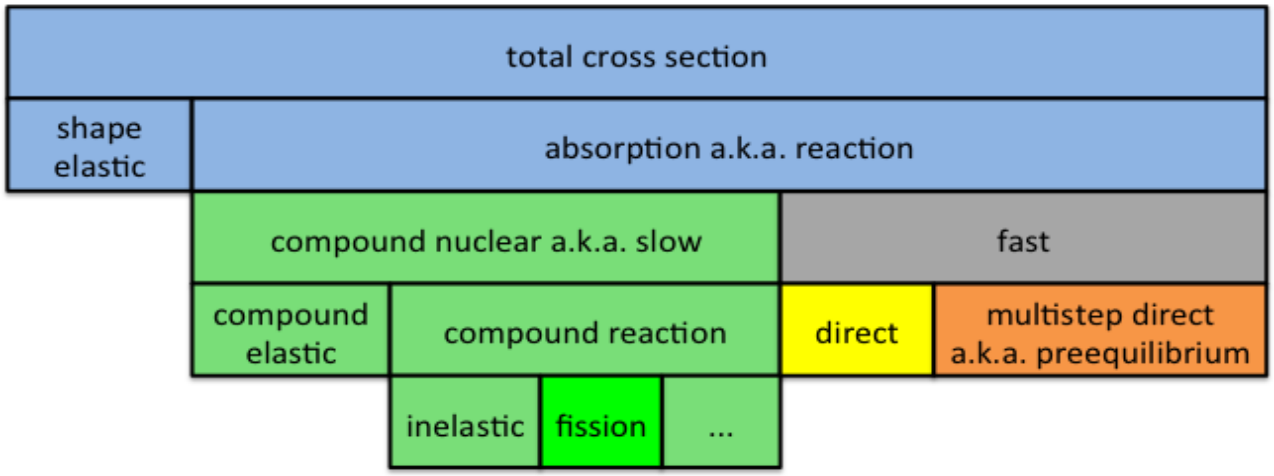
There is a cost to change,
but modern programming and database practices have real benefits

There are several key issues to be addressed by the proposed subgroup

- Define a common data model
  - How should the data be organized?
- Agree on a set of “best” practices and how to implement them
  - Engineered versus administrative controls
- Define a process to publish and update the standard
  - How do we agree things are ready?

Implement and test with current international data libraries

It seems clear that the data model should mirror our understanding of the physics of nuclear reactions



Hierarchy by time?

1. Two-bodies interact
2. Direct processes
3. Other fast processes
4. Compound nucleus
5. EM decay
6. Weak decay

Other likely requirements:

- Small set of general-purpose data containers
- Support for functional descriptions of data
- Support for multiple forms of the same data
  - Functional, Pointwise, Grouped, etc.
  - Evaluator enters the native data, other forms are derived

What are the best practices for evaluations?

- ‘Engineered’ controls can be enforced by design of GND:
  - Eliminate inconsistent data
    - Multiple particle masses in ENDF vs only one value in GND
  - Require certain channels or outgoing spectra
  - Require documentation
  - Require ‘nativeData’ to indicate form chosen by evaluator

- ‘Administrative’ controls enforced by quality assurance tools (i.e., checking codes):
  - Require same units throughout?
  - Require all quantities defined up to (at least) 20 MeV?

Achieving consensus on best practices will be challenging

Subgroup will also need to specify the process for approving new standard and future updates

- Agree on meta-language for exchanging data and specifying data model
  - Probably XML
- Develop quality assurance tests on standard
  - Convert from ENDF to GND back to ENDF
  - Supports data available in older formats
  - Plotting and validation tools exercised
- Propose a governance model

LLNL has made an initial attempt at a new format, which can be downloaded at https://ndclx4.bnl.gov/gf/project/gnd/

- Sub-group participants will
  - Develop a common data model for reaction data
  - Agree on best practices and how to “enforce” them
  - Test things out with their local ENDF-formatted databases
  - Propose a process for dissemination and future modifications
- LLNL and USNDP is committed to seeing this through
- Benefits are significant
  - Attract and retain next generation of scientists and engineers
  - Leverage significant infrastructure that will continue to evolve
  - Overcomes limitations of existing format in an extensible way
  - Positions community to link disparate data products to each other