

Beyond the ENDF format: A modern nuclear database structure

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Recent developments indicate that there is a renewed international interest in using nuclear data to solve emerging problems

- Generalized Nuclear Data (or GND) structure
 - Prototyped at LLNL as a modern replacement for both the legacy ENDL format of LLNL and for ENDF-6
- New developments in nuclear data processing
 - De-facto standard NJOY
 - TRENDF, which is being developed at the CEA in France to support the Monte Carlo code TRIPOLI
 - Updated version of AMPX at Oak Ridge
 - Updated version of GRUCON at Kurchatov Institute
 - Livermore code Fudge to process nuclear data in multiple formats

As budgets continue to decrease, modernize to reduce long-term costs

Minimize effort to become proficient in utilizing nuclear data
Leverage mature tool sets already available

Developing a new nuclear data structure will transfer expertise to a new generation, provide new capabilities, enhance data sharing

- Ability to attract new talent who are more comfortable with and interested in modern concepts and who may be put off by existing set of nuclear data tools
- A nested, hierarchical structure will make data clearer and easier to understand
- Provides a clearer history of how processed data are derived from master representations
- Improved flexibility in the types of data that can be stored
- Leverage vast, well-tested infrastructure
- Remove artificial limits imposed by legacy formats
- Link disparate databases to each other
 - Reactions, level structure, mass tables can all be cross referenced

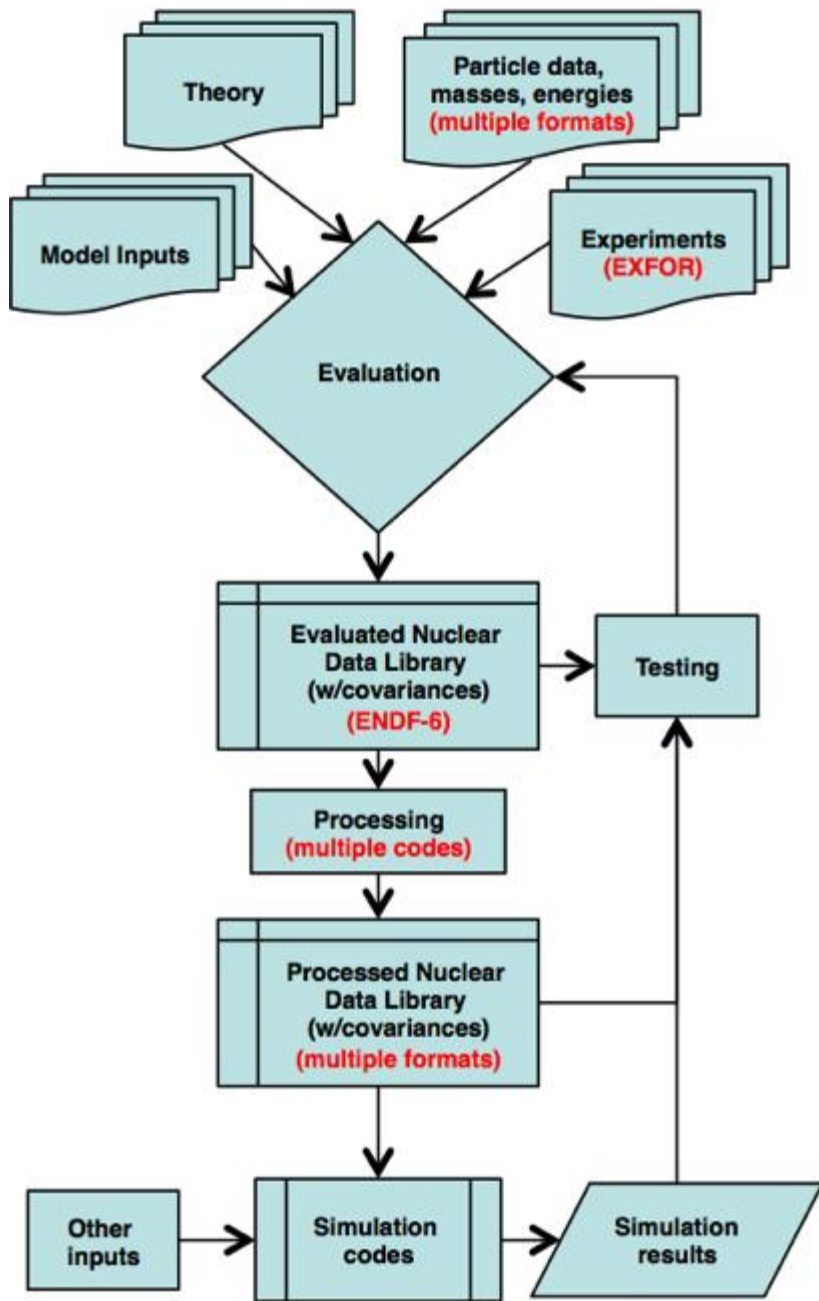
There is a cost to change,
but modern programming and database practices have real benefits

The first meeting of SG38 was held 29-30 Nov. 2012 here in Paris

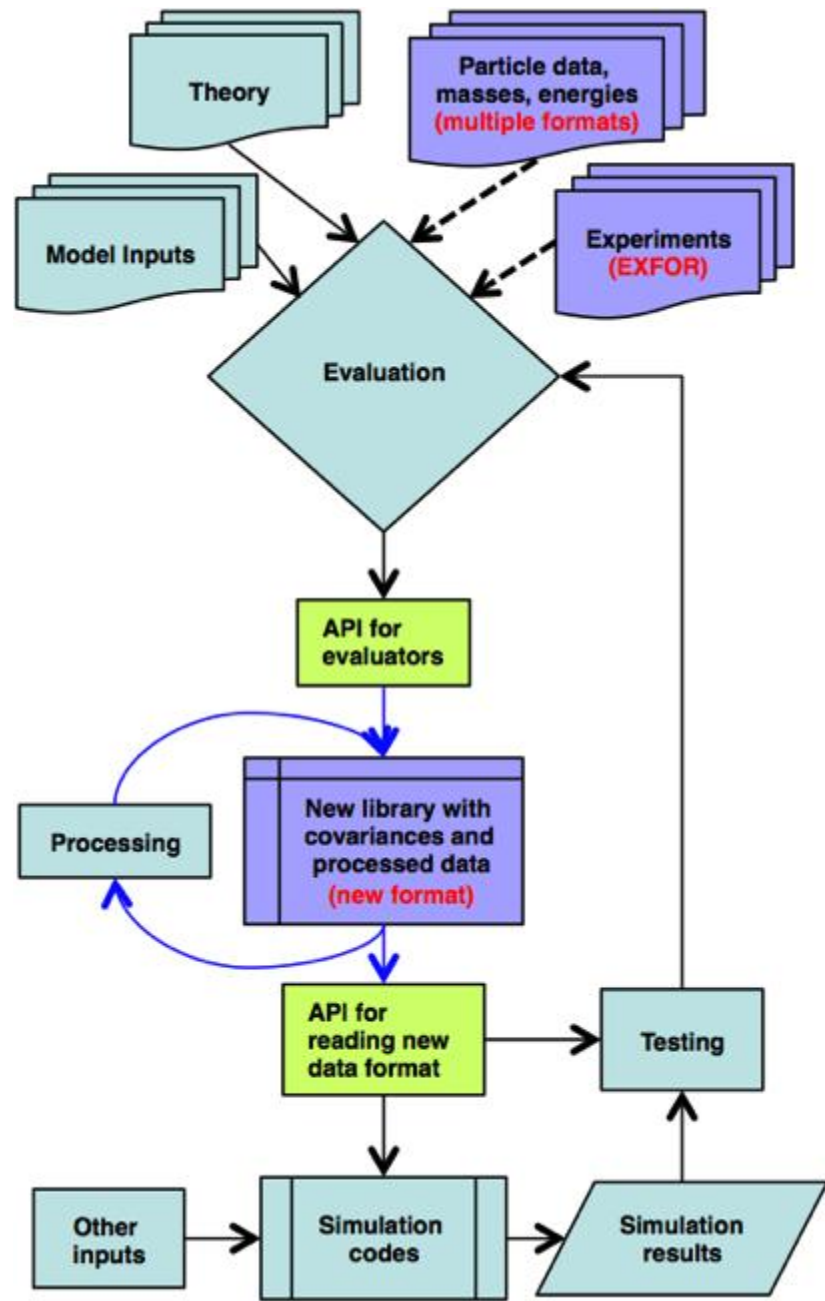
SG38 has >40 members -- Workshop had about 30 participants

- Session 0: Welcome and Introductions (E. Dupont, chair)
 - Welcome: Purpose and Goals for SG38 – D. McNabb Lessons from ENDF, EXFOR and Other Formats – V. Zerkin
 - Lessons from LLNL's First Attempt to Develop a Modern Format – C. Mattoon
- Session 1: Purpose of the new data structure (M. Chadwick, chair)
 - Perspective from A. Koning
 - Perspective from D. Brown
- Session 2: Nuclear Data System Overview
 - Perspective from L. Leal
 - Perspective from T. Fukahori
- Session 3: Benefits & requirements for data evaluation and processing (M. Coste-Delclaux, chair)
 - Perspective from J.C. Sublet
 - Perspective from R. Capote
- Session 4: Format perspective and Organization
 - Perspective from B. Beck
 - Perspective from I. Kodelli
- Session 5: Requirements for basic data structures (*J. Miss, chair*)
 - Perspective from W. Haeck
 - Perspective from R.W. Mills

Goal was to capture community viewpoints from a variety of perspectives



Current



Proposed

We developed a requirements document for a new format/data structure

- Introduction
- History
- Purpose of the new structure and expected benefits
- System Overview
- Benefits and requirements for data evaluation and processing
- Basic data containers
- Summary of requirements
 - Ten (10) high-level requirements for new format/data structure
 - Request that low-level data containers are common with EXFOR & RIPL
 - Two (2) broader recommendations to facilitate adoption

Based on initial feedback, we adopted some modifications on Tuesday
We are submitting this document to WPEC for approval

Requirements that apply to the structure for storing reaction data.

The new structure will...

- Be governed by a long-term WPEC sub-group that will define the structure and maintain the documentation.
- Use a hierarchy that reflects our understanding of nuclear reactions and decay, and that clearly specifies all data.
- Define APIs for reading and writing data in the structure. Open-source substantiations of these APIs will ideally be available for C, C++, Java and Fortran before adoption.
- Support storing multiple representations of the same quantity simultaneously (e.g. evaluated and processed forms).
 - A capability for evaluators to identify their preferred or recommended form will be provided and required.
- Support both inclusive and exclusive reaction data (i.e. discrete reaction channels as well as sums over them)
 - Requirements for consistency between inclusive and exclusive evaluated data is to be decided by the data projects

The new structure will...

- Contain provisions for evaluators and data processors to provide records of all the information needed to reproduce and extend their data. Information includes a bibliography, links to EXFOR data used including descriptions of the corrections applied, a description of codes and input parameters, and comments.
 - Additionally, the name and affiliation of evaluators and processors of new data or data modifications will be required
- Encourage the elimination of inconsistent nuclear masses, levels, and lifetimes by providing a way to link to an external particle database, specifically RIPL, to specify these quantities globally for each projectile-target combination. A capability to locally override these global values will also be provided.
- Support any particle and any combination of reaction products (and subsequent decay products).
- Require the evaluator or processor to specify the physical units and interpolation of the data. Also, the data structure should contain provisions for identifying the number of significant digits used by the evaluator and during processing.
- Support backwards-compatibility with ENDF-6 for as long as possible, although in the long term new features will likely be added that cannot be translated back to ENDF-6.

Some other recommendations were made to facilitate the adoption of new data structure

In addition to nuclear reactions, a hierarchical structure could also be used to organize nuclear structure data (as in ENSDF), experimental data (as in EXFOR), and reaction model parameters (as in RIPL). This leads to an additional goal:

- The structure should include reusable low-level data containers that are general enough to be shared between data products (e.g., EXFOR, RIPL and ENSDF)

In order to facilitate adoption it is recognized that supporting infrastructure is required to use the new data structure. This infrastructure should:

- Use open source codes to manipulate, search, plot, process, translate and check the data for quality. For better quality assurance and data checking, it is recognized that at least two independent sets of code infrastructure be available that can be compared.
- Be forgiving, meaning that access routines for the new structure must be able to recover gracefully and continue working if they encounter data containers that are not yet officially recognized as part of the structure.

Process to adopt the requirements document? Does it meet your needs in a new structure?

Important coordination issues have been resolved

- BNL will host a web site/wiki/repository for our project's work
- Identified representatives from data projects to be responsible for beta testing
 - First adopters
 - Ensure that new structure meets local requirements
 - Answer questions and needs of project communities
 - ENDF – David Brown/Advance
 - JENDL – Osamu Iwamoto
 - BROND – V. Sinitsa

Over the last two days we made good progress on how to execute the project

Organized the work into seven (7) work products/teams with team leads identified (and team members)

1. Low-level data containers – *Morgan White and Victor Zerkin*
2. Top-level hierarchy for storing nuclear reaction data – *Arjan Koning and David Brown*
3. Hierarchy for storing particles, level schemes and decays data – *Roberto Capote and Caleb Mattoon*
4. Infrastructure for data handling, processing, plotting, etc – *Bret Beck, Yannick Peneliau, Valentin Sinitsa*
5. API for reading and writing data in the new structure – *Bret Beck and Wim Haeck*
6. Defining the tests that will be needed to assure quality of data – *Michael Dunn and Jean-Christophe Sublet*
7. Documentation and governance – *Emmeric Dupont*

For each product, we fleshed out work to be done and who will do it
– but not written/finalized yet

Next steps for SG38

- Generate a SG38 Project Plan draft document
 - Iterate with product leads, then send out to SG38 (2 months?)
- Set up current GND website hosted by BNL to enable wiki functionality
- Each Product Team has tasks to complete before next meeting
- Draft charter for SG38 defining long-term subgroup, organization, and open source model for releasing structure and codes
- Work with Japanese to set dates for next workshop
 - Will aim for some parallel sessions so that folks can work at greater technical depth
 - Overview session for each product to report out progress and organizational discussions