EG-GNDS STATUS REPORT

DAVID BROWN (NNDC, BNL)

GOALS FOR EG-GNDS MEETING

- **GNDS-1.9 & other news**
  - Publication status
  - SG-43 news
- **Approve (and name) next GNDS release**
- **"Lessons learned" from preparing next GNDS**
- **Plan for future**
  - Format areas of focus (atomic, FPY, particle properties)
  - Mandate extension

AGENDA

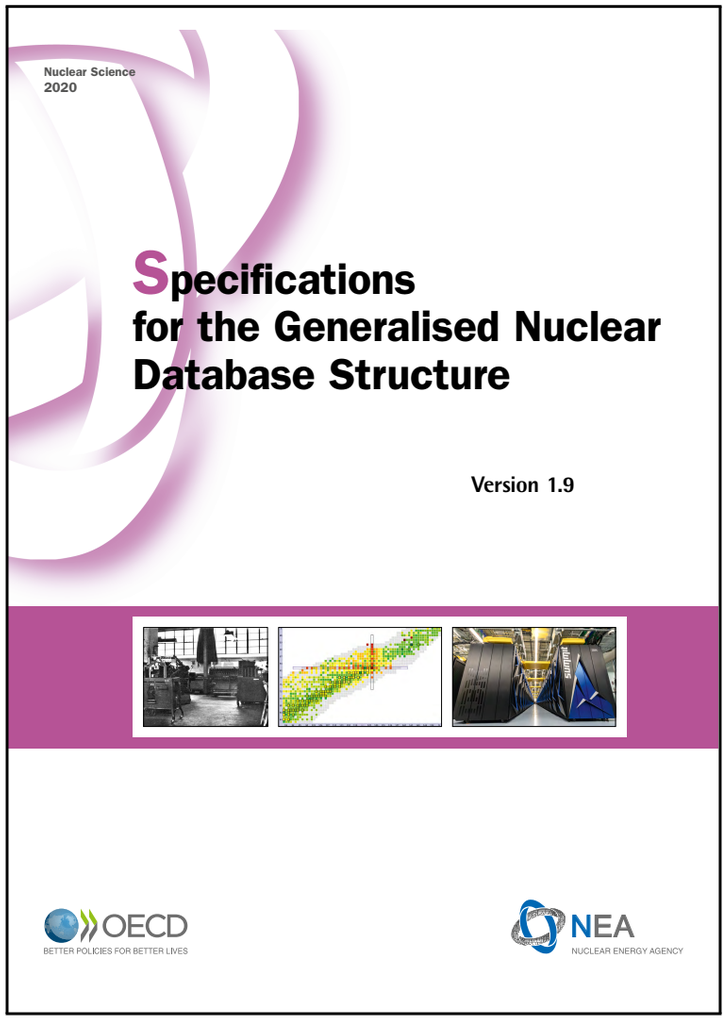
Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:10	03:00	**12:00**	19:00	Welcome	D. Brown
00:10	03:10	**12:10**	19:10	GNDS-1.9 publication	M. Fleming
00:15	03:20	**12:20**	19:20	API status / SG43	F. Malvagi
00:15	03:35	**12:35**	19:35	Specifications vs requirements / ENDF-6	D. Brown
00:15	03:50	**12:50**	19:50	Atomic data	M.G. Pia
00:15	04:05	**13:05**	20:05	Fission product yields	D. Brown
00:10	04:20	**13:20**	20:20	Discrete, excited and isomeric states	J-Ch. Sublet
00:10	04:30	**13:30**	20:30	Short break	
00:20	04:40	**13:40**	20:40	Status of proposals	D. Brown
00:20	05:00	**14:00**	21:00	Discussion on next release	All
00:10	05:20	**14:20**	21:20	Version numbers	C. Mattoon, J. Conlin
00:15	05:30	**14:30**	21:30	Review of the GNDS Schema Build System	G. Gert
00:15	05:45	**14:45**	21:45	Discussion on system	All
00:10	06:00	**15:00**	22:00	Requests for format improvements	All
00:20	06:10	**15:10**	22:10	Guidelines for format proposals	All
00:15	06:30	**15:30**	22:30	Mandate extension	D. Brown
	06:45	**15:45**	22:45	Close	

GNDS-1.9 &

OTHER NEWS

What is being published?

1. GNDS-1.9 specifications @ 342 pages
2. 'Policy Brief' for general/high-level audience @ 2 pages



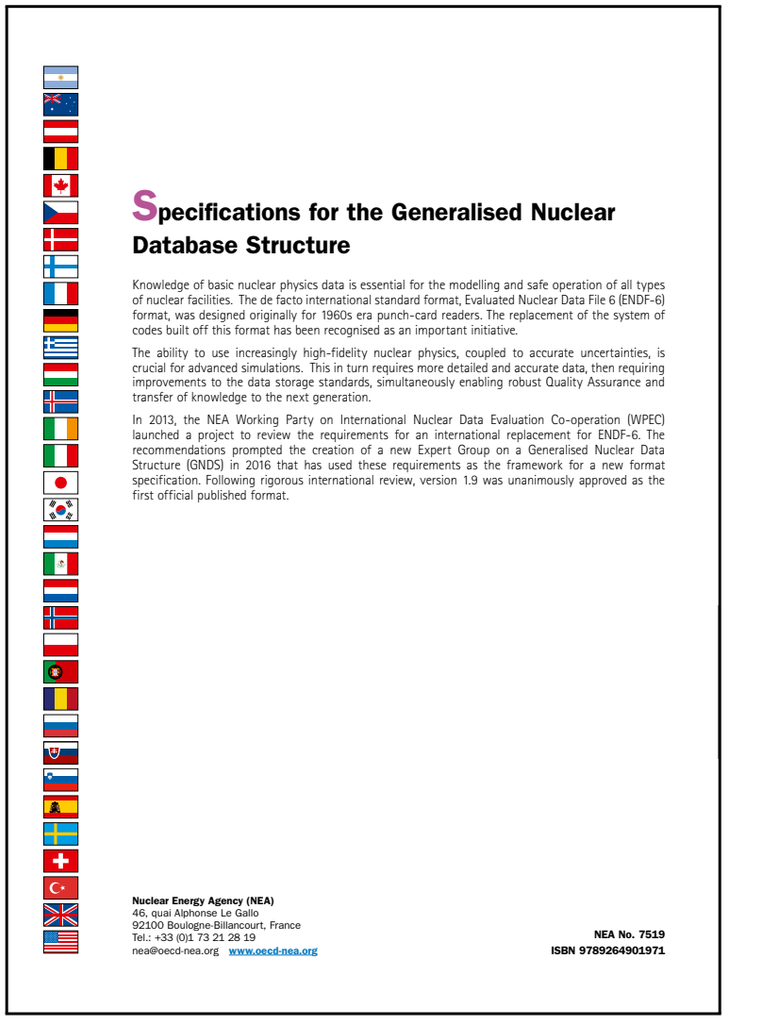
Nuclear Science
2020

Specifications for the Generalised Nuclear Database Structure

Version 1.9

OECD BETTER POLICIES FOR BETTER LIVES

NEA NUCLEAR ENERGY AGENCY



Specifications for the Generalised Nuclear Database Structure

Knowledge of basic nuclear physics data is essential for the modelling and safe operation of all types of nuclear facilities. The de facto international standard format, Evaluated Nuclear Data File 6 (ENDF-6) format, was designed originally for 1960s era punch-card readers. The replacement of the system of codes built off this format has been recognised as an important initiative.

The ability to use increasingly high-fidelity nuclear physics, coupled to accurate uncertainties, is crucial for advanced simulations. This in turn requires more detailed and accurate data, then requiring improvements to the data storage standards, simultaneously enabling robust Quality Assurance and transfer of knowledge to the next generation.

In 2013, the NEA Working Party on International Nuclear Data Evaluation Co-operation (WPEC) launched a project to review the requirements for an international replacement for ENDF-6. The recommendations prompted the creation of a new Expert Group on a Generalised Nuclear Data Structure (GNDS) in 2016 that has used these requirements as the framework for a new format specification. Following rigorous international review, version 1.9 was unanimously approved as the first official published format.

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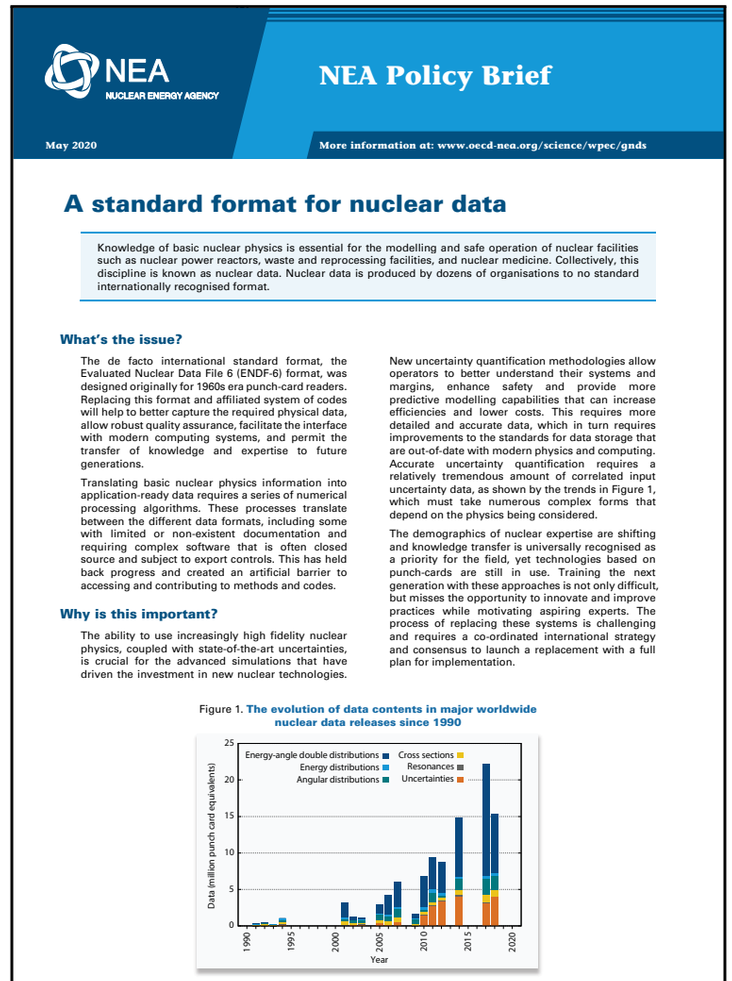


NEA NUCLEAR ENERGY AGENCY

NEA Policy Brief

May 2020

More information at: www.oecd-nea.org/science/wpec/gnds

A standard format for nuclear data

Knowledge of basic nuclear physics is essential for the modelling and safe operation of nuclear facilities such as nuclear power reactors, waste and reprocessing facilities, and nuclear medicine. Collectively, this discipline is known as nuclear data. Nuclear data is produced by dozens of organisations to no standard internationally recognised format.

What's the issue?

The de facto international standard format, the Evaluated Nuclear Data File 6 (ENDF-6) format, was designed originally for 1960s era punch-card readers. Replacing this format and affiliated system of codes will help to better capture the required physical data, allow robust quality assurance, facilitate the interface with modern computing systems, and permit the transfer of knowledge and expertise to future generations.

Translating basic nuclear physics information into application-ready data requires a series of numerical processing algorithms. These processes translate between the different data formats, including some with limited or non-existent documentation and requiring complex software that is often closed source and subject to export controls. This has held back progress and created an artificial barrier to accessing and contributing to methods and codes.

New uncertainty quantification methodologies allow operators to better understand their systems and margins, enhance safety and provide more predictive modelling capabilities that can increase efficiencies and lower costs. This requires more detailed and accurate data, which in turn requires improvements to the standards for data storage that are out-of-date with modern physics and computing. Accurate uncertainty quantification requires a relatively tremendous amount of correlated input uncertainty data, as shown by the trends in Figure 1, which must take numerous complex forms that depend on the physics being considered.

The demographics of nuclear expertise are shifting and knowledge transfer is universally recognised as a priority for the field, yet technologies based on punch-cards are still in use. Training the next generation with these approaches is not only difficult, but misses the opportunity to innovate and improve practices while motivating aspiring experts. The process of replacing these systems is challenging and requires a co-ordinated international strategy and consensus to launch a replacement with a full plan for implementation.

Why is this important?

The ability to use increasingly high fidelity nuclear physics, coupled with state-of-the-art uncertainties, is crucial for the advanced simulations that have driven the investment in new nuclear technologies.

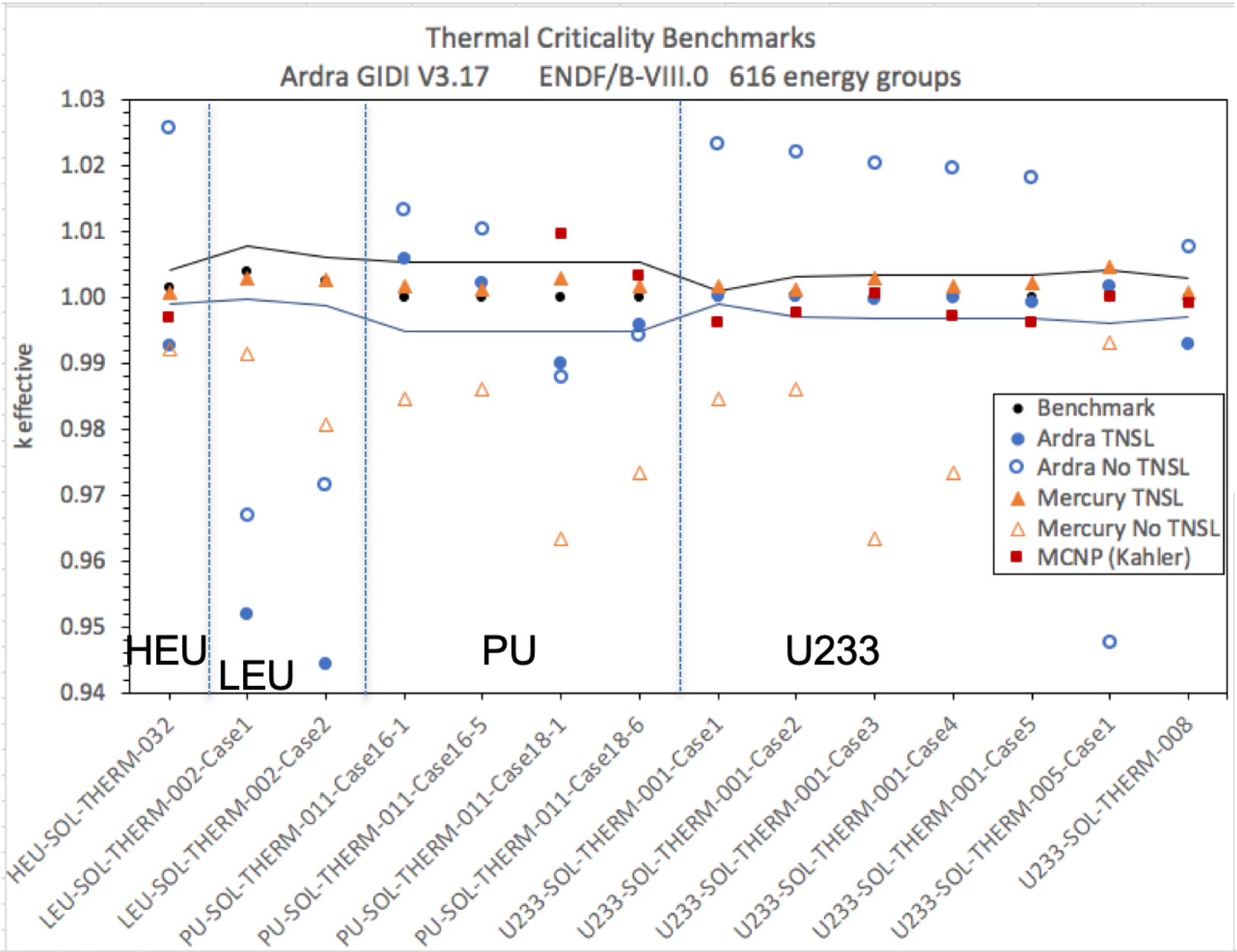
Figure 1. **The evolution of data contents in major worldwide nuclear data releases since 1990**

GNDS reading/writing implementations

Code Name	Institution	Status	Availability when / where
FUDGE	LLNL	Full Implementation	Now github
GIDI+	LLNL	Full Implementation	Now github
AMPX	ORNL	Partial Implementation (1D XS + Cov)	Soon ORNL site
NJOY	LANL	In progress	? ?
GALILEE	CEA	In progress	2021? NEA
FRENDY	JAEA	Planned	2023? NEA

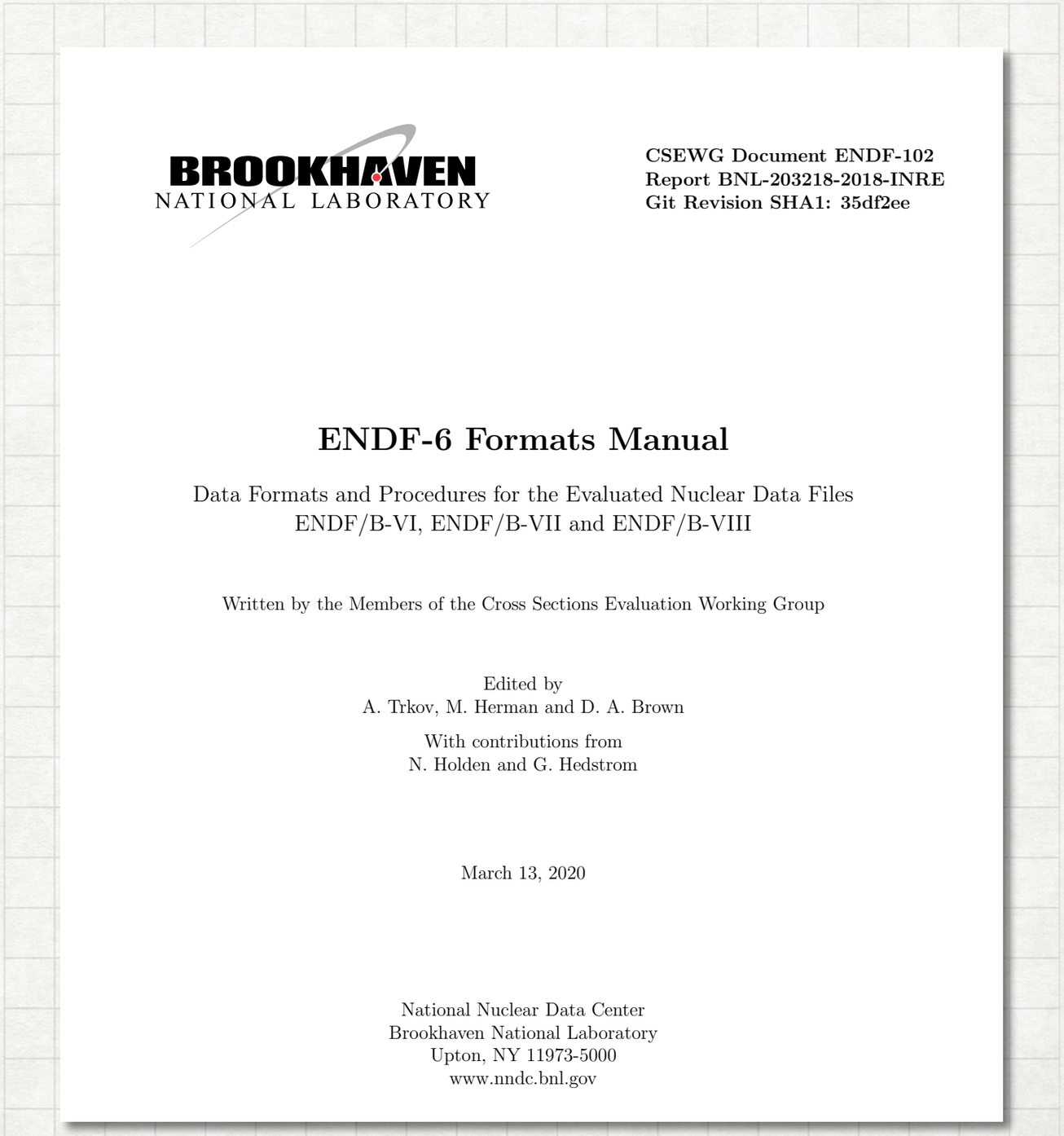
Demonstration of capability

- LLNL transport codes have been updated to run problems using GNDS data via GIDI API



GNDS VS. ENDF-6

- All MF/MT's in ENDF-6 manual have GNDS analogs
- All low level formats in ENDF-6 are either obsolete or have GNDS analogs
- Developed 4 page summary showing connection between ENDF-6 and GNDS.
  - **Suggest making it an appendix to specifications**
- **TO DO: detailed (LIP/LAW/ whatever level) comparison between formats**



BROOKHAVEN NATIONAL LABORATORY

CSEWG Document ENDF-102
Report BNL-203218-2018-INRE
Git Revision SHA1: 35df2ee

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown

With contributions from
N. Holden and G. Hedstrom

March 13, 2020

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GNDS VS. SG-38 REQUIREMENTS

- Approved map/library/xsdir/etc file markup
- Proper treatment of EOS in TNSL data
- Some elements of atomic data
- Improved FPY markup
- Processed data types
- Radiation damage
- dE/dx
- Resonance things: Brune transform, CP RRR
- **Improved TNSL markup (see proposal/TNSL)**
- **Improved documentation markup (see proposal/documentation)**
- **Support for the sandwich formula (see proposal/sandwichProduct)**
- **TO DO: detailed comparison between format and each requirement sub-bullet**

Generally unwise to force format discussion until we see what evaluators can provide & see what users need

APPROVE & NAME

NEXT GNDS RELEASE

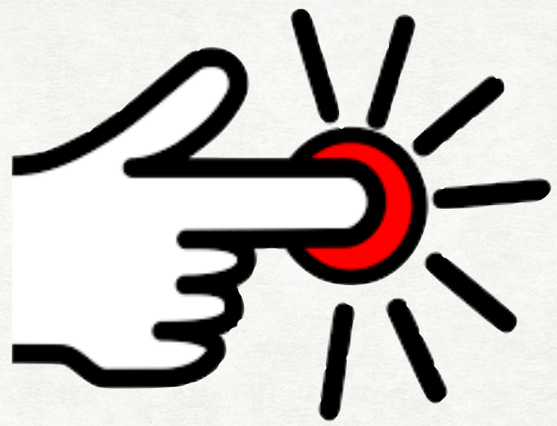
KEY: NEEDED FOR ENDF-6 DATA, SG-38 REQUIREMENT

✓ = APPROVED, 🚧 = UNDER CONSTRUCTION, 🤔 = WE'LL DISCUSS

Name	Description	Status
multiGroupStyleFix	improve multi group data style	✓
interaction	denote what kind of reactionSuite we're dealing with	✓
childFunctions	add functional container organization to low-level containers	✓
pids	resolve possible discrepancy between branchings & PoPs	✓
fissionFragmentData	consolidate & clean up fission data support	✓
TNSL	improved TNSL markup, per requirements document	✓
atomicConfigurations	support for electron sub shells, per ENDF-6 format	✓

Name	Description	Status
externalFiles	denote external resource that may need to be read before processing	✓
orphanProduct	fix inconsistency in orphan product organization	✓
sandwichProduct	support for "sandwich product" covariance, per requirements document	✓
documentation	improved documentation markup, per requirements document	🚧
outerDomainValue	rename 'value' attribute for clarity in multi-D containers	✓
res_v1	option #1 for resonance re-arrangement	🤔
res_v2	option #2 for resonance re-arrangement	🤔

WHAT NEXT?



- **“Push the button”**
  - Merge 12 approved formats into **development** branch
  - Deconflict & merge **development**, **master** & **NEA-publication** branches
- **Next version will be version 2.0;**
  there are too many important changes for anything less!
  - Figure out last 2+ proposals
  - Create and process a few more we feel are needed for 2.0
- **Will require a few extra meetings to push this through**

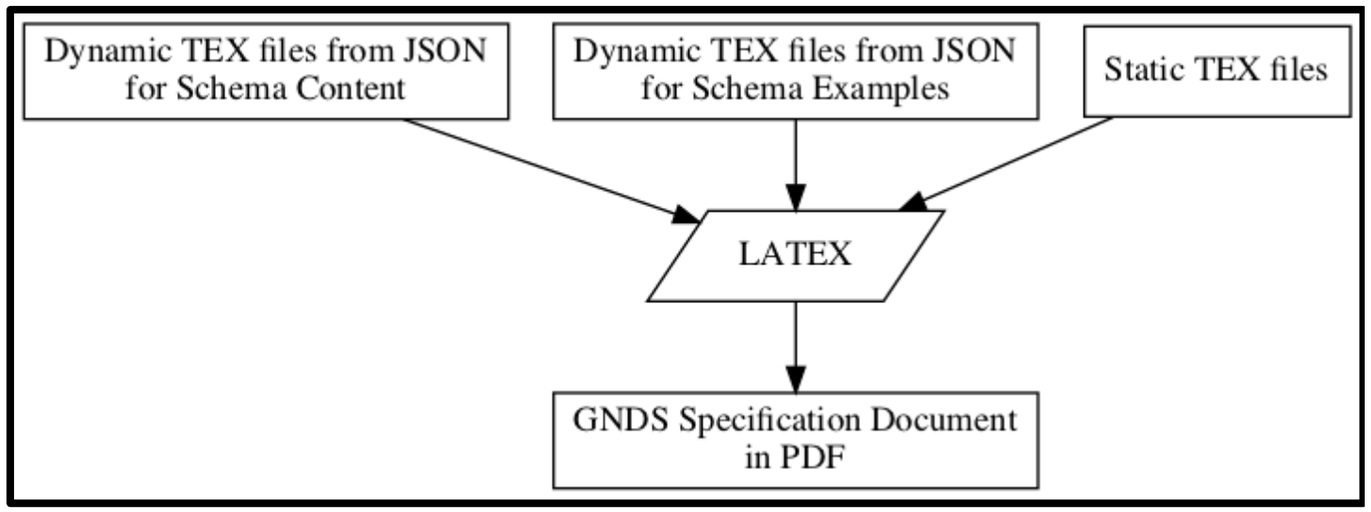
LESSONS LEARNED FROM THIS RELEASE PROCESS

Specification Build System

FOLDERS

- gndsFormat
  - Conventions
  - DataContainers
  - Documentation
  - grokGNDS
  - PoPs
  - Styles
  - TopLevel
  - bibliography.bib
  - bibliography.tex
  - GNDDesignPhilosophy.md
  - GNDXMLStyleGuide.md
  - index_style.ist
  - intro.tex
  - Makefile
  - preamble.tex
  - README.md
  - specifications.tex
  - TODO.txt

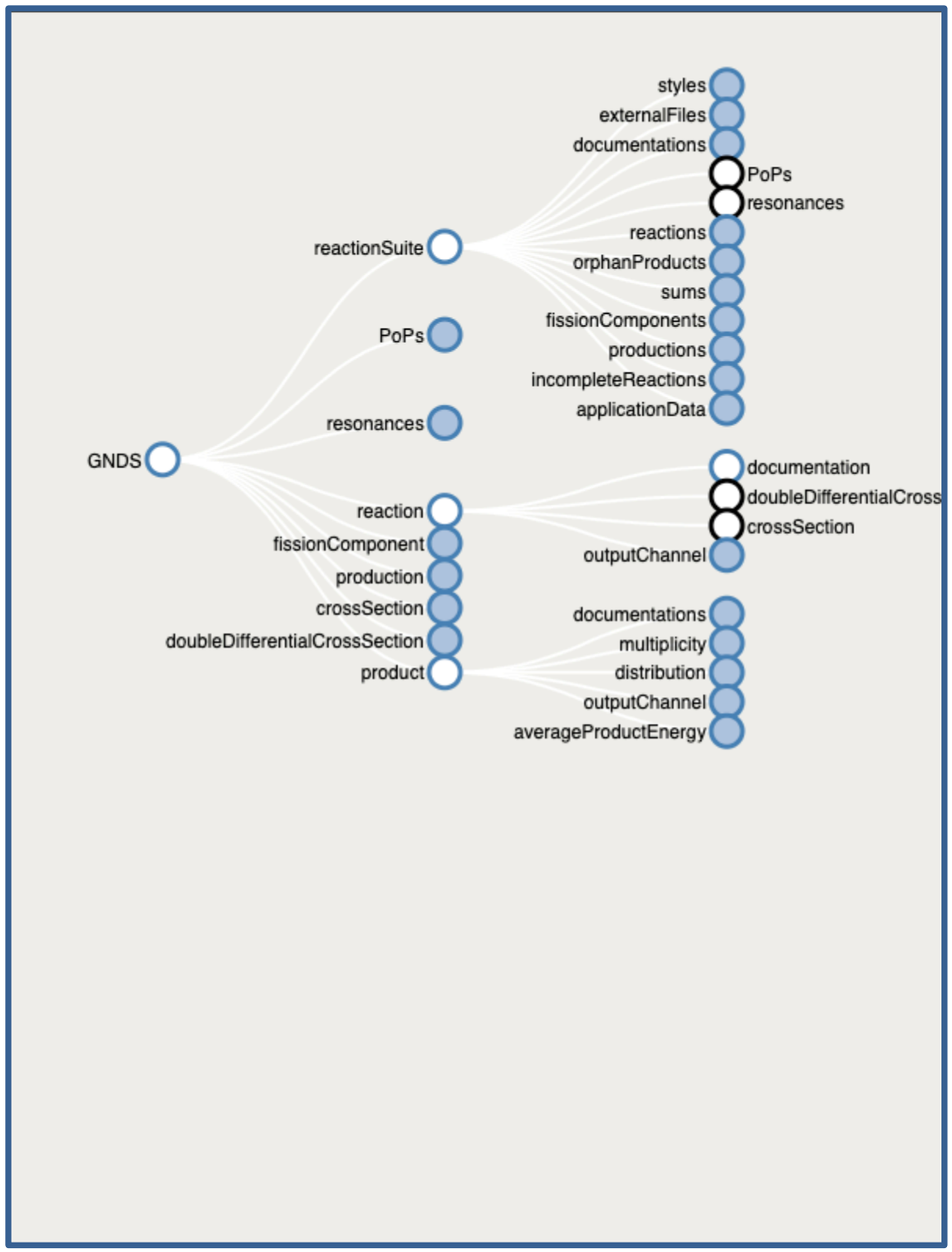
1. JSON specification
   - Originally from XSD and GNDS Examples
2. Convert JSON to TEX
   - Specification text
   - Examples
3. Convert TEX to PDF



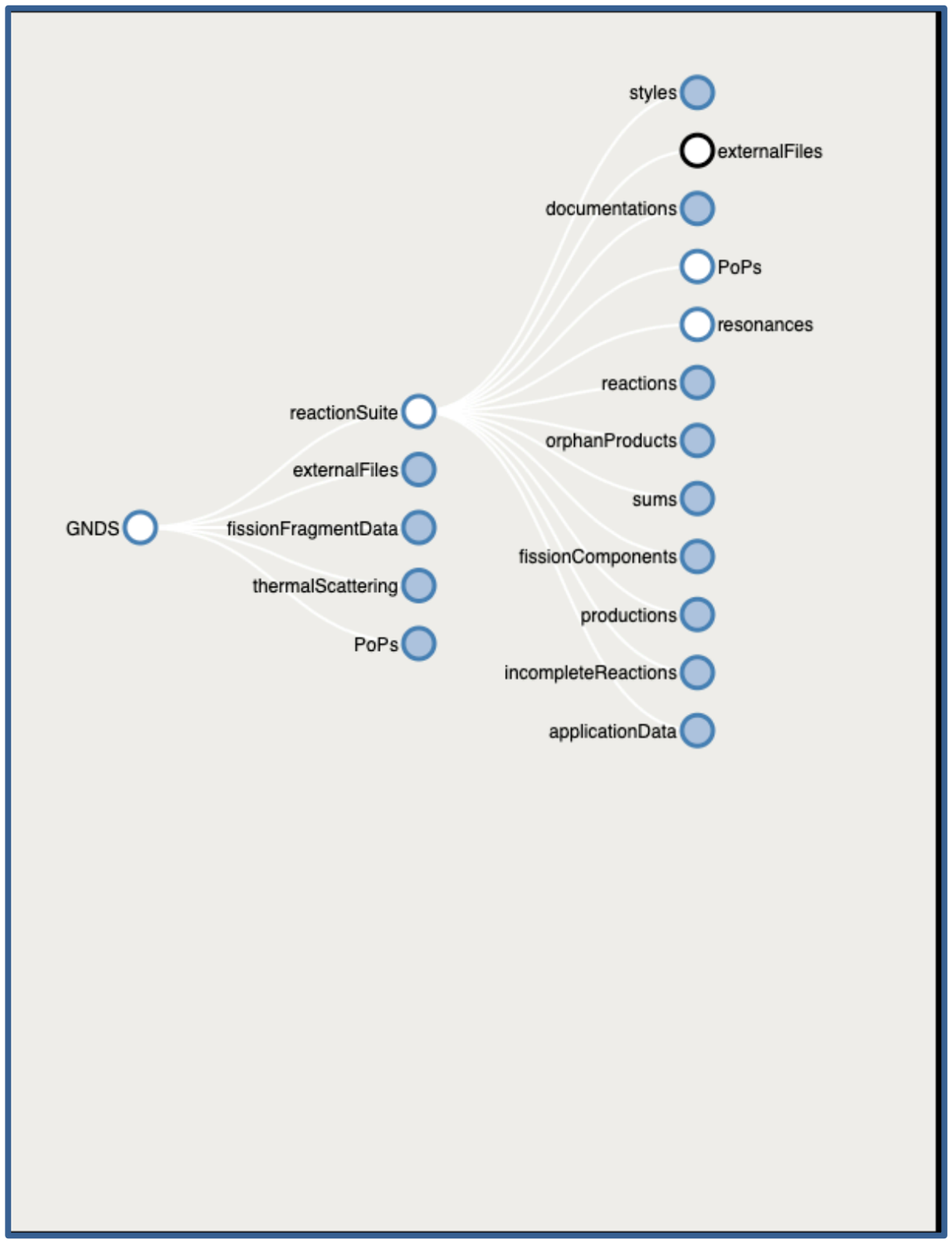
Proposed Improvements

- Visualization Tool
  - Complement to Schema Report
  - Sourced from either XSD or JSON
    - Compare XSD to JSON
    - Remove inconsistencies
    - Translate between XSD and JSON

- General Updates
  - Reduce Complexity
  - Compliment dynamic examples with static ones



From XSD



From JSON

General Updates

- Expand use of __namespace__
  - Resolve incorrect links:
    - reactionSuite/reactions/reaction/outputChannel/products/product
- Ordering of nodes
  - Should it be imposed?
- Static TEX files for examples in GNDS report
  - Complement existing dynamic examples from JSON
- Official JSON schema specification
  - Latest draft: September 2019
  - *https://json-schema.org*

PLANNING FOR THE FUTURE

IAEA

On unifying the definition of discrete, excited and isomeric states across the nuclear data model and form frames

J.-Ch. Sublet
UH-NDSU

International Atomic Energy Agency
Nuclear Data Section

"WalletCraft" - Object-oriented databasing for nuclear data

Adam Hayes, Benjamin Shu, Libby McCutchan,
Shaofei Zhu, Alejandro Sonzogni

National Nuclear Data Center
Brookhaven National Laboratory

WPEC EG-GNDS
12 May 2020

Meeting of the **WPEC Expert Group**
on the Recommended Definition of a
General Nuclear Database Structure (EG-GNDS)

Atomic Data

Sandra Parlati[1], **Maria Grazia Pia**[2], Elisabetta Ronchieri[3], Paolo Saracco[2]

[1]INFN Laboratori Nazionali del Gran Sasso, Assergi, Italy
[2]INFN Sezione di Genova, Italy
[3]INFN CNAF, Bologna, Italy



WebEx meeting
12 May 2020

Foreword
Due to limited time allocation, mainly an introduction to topics for discussion

FISSION PRODUCT YIELDS

D. Brown, A. Sonzogni, A. Mattera (NNDC, BNL)

NNDC

IAEA

On unifying the definition of
dis… …ric
sta… …ata

J.-Ch.
UH-NDS

International Atomic Energy Agency
Nuclear Data Section

NAMING CONVENTION & UNIFICATION OF BOUND & UNBOUND STATES IN GNDS

"Walle…
datab…

Adam Ha…
Shaofei Z…

National Nuclear Data Center
Brookhaven National Laboratory

WPEC EG-GNDS
12 May 2020

OOP DATABASE + OTHER TOOLS FOR GENERATING NUCLEAR WALLET CARDS (TECHNOLOGY TO STEAL!)

Meeting of the **WPEC Expert Group**
on the Recommended Definition of a
General Nuclear Database Structure (EG-GNDS)

Sandra P… …o Saracco[2]

…Assergi, Italy
…Genova, Italy
…Bologna, Italy

…eting
12 May 2020

Foreword
Due to limited time allocation, mainly an introduction to topics for discussion

ATOMIC DATA IS IN PRACTICE ORPHANED. INFN NEEDS SUPPORT TO HELP KEEP UP VALIDATION WORK + THERE ARE NEW FORMATS TO DEVELOP.

PRODUCT FIELDS

D. Brown, A. Sonzogni, A. Mattera (NNDC, BNL)

NNDC

FPY EVALUATIONS ARE HARD AND WE ONLY HAVE A PARTIAL PICTURE OF FORMAT NEEDS

BIG QUESTION: DO WE SUBSUME THE WORK OF SG-43 INTO EG-GNDS?

- SG-43 is wrapping up
- The work isn't done — it should be an ongoing task!
- The effort is tightly coupled with the format development itself
- This is a joint decision for SG-43 and EG-GNDS
- EG-GNDS is OK with it