SG50 Data-format Requirement Document for an Automatically Readable, Comprehensive and Curated Experimental Reaction Database

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Abstract

In this report, we define for the automatically readable, comprehensive and curated experimental reaction database:

- metadata containers.
- data containers,
- correction and objective-testing containers,
- expert-judgment identifiers,
- codes used to transfer from EXFOR to our database,
- databases (mongoDB, etc.) used for storage of the data.

This database can serve as more automatically readable input for future evaluations, ML codes and preserves expert judgment of many man-years.

We apply the codes to a few selected files of different observables to showcase how these newly formatted data look like.

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Chapter 1

Introduction

- The aim of this work is establishing an automatically readable, comprehensive and curated experimental reaction database starting from EXFOR, and codes that translate from EXFOR into the database.
- The benefit of this database is:
  - easier automatized readability for evaluation input, ML, data comparisons, etc.,
  - preserving expert knowledge that cost a lot of man-hours.
- In order to reach this aim, we need to:
  - develop a format to store all of the information in an easily retrievable and unambiguously readable manner, Chapters 2–5,
  - develop codes for translation 6,
  - decide on a database structure 6.
- We give example database files for each observable covered here in Chapter 7.

1.1 The Different Layers of the Database

- Layer 1: translation of EXFOR-formatted files into new format, no changes to data. See Chapters 3 and 2.
- Layer 2: objective corrections (standards, decay data) and objective testing requirements (p-values, missing corrections), etc., see Chapter 4,
- Layer 3: subjective corrections: template corrections, expert judgment containers, see Chapter 5.

1.2 How to use these Requirements

1.3 Organization of this Document

1.4 Notation and Definitions

1.5 What is Similar to and What Goes Beyond EXFOR

Chapter 2

Metadata Storage Container for Layer 1

2.1 Bibliographic Information

- Authors,
- Institutes,
- Main reference including title,
- EXFOR entry numbers.

2.2 General Metadata Describing the Data

- Observable: (n,f) cs, PFNS, etc.
- Absolute: yes, no,
- Method: activation, ratio, etc.,
- Known issues: ...,
- Status,
- History,
- Analysis.

2.3 Neutron Flux

- Type: mono-energetic, white,
- Flux normalization,
- Neutron-flux monitoring reaction,
- Neutron-flux monitor type,
- Neutron source,
- Neutron-producing reaction,

- Neutron-producing facility,
- Secondary-neutron groups,
- Neutron flux monitored: yes, no, unknown,
- Secondary neutrons corrected: yes, no, unknown,
- Method to measure neutron flux: ASSOP, Mn baths, etc.,
- Beam-size diameter,
- Beam uniform: yes, no, unknown, not measured,
- Flight-path length.

2.4 Background

- Different types of background,
- Was background type corrected: yes, no, unknown, partial,
- methods for correcting background: fit, black-resonance filter, simulation, etc.

2.5 Detector efficiency

Here, we might need to distinguish for main detector and monitor detector.

- Detector type(s),
- Number of detectors,
- Dimensions of detector,
- Detector gas,
- Detector pressure,
- Detector material,
- Detector-efficiency value,
- Detector-efficiency-determination method,
- corrected for efficiency: yes, no, unknown, partial,
- Angular acceptance/ coverage (if more than one detector),
- Corrected for stopping power, forward-boost, angular distortion: yes, know, unknown, partial,

2.6 Sample

- Sample material,
- Impurities/ enrichment,
- Sample type: gas, powder, metal,
- Sample production: rolled, electroplated, electro-sprayed, vapor-deposited, painted,
- Dimensions of sample (thickness, mass, radius),
- Sample uniformity corrected: yes, no, unknown, partial,
- Backing material,
- Backing size,
- Sample roughness corrected: yes, no, unknown, negligible,
- Number of samples,
- Displacement of the sample corrected: yes, no, unknown, partial,
- Number of atoms in the sample determination technique: alpha-counting, micro-scales, etc.
- Sample configuration: PPAC, one sample, back-to-back,
- Number of atoms in the sample assessed: yes, no, unknown, partial,
- impurities corrected: yes, no, unknown, partial,
- Beam-sample overlap corrected: yes, no, unknown, partial,

2.7 Multiple Scattering, Neutron Leakage and Attenuation

- Corrected: yes, no, unknown, partial,
- Method for correction: simulation, measurement, etc.,
- Code for neutron-transport correction: MCNP, etc.,
- Nuclear data used for correction.

2.8 Resolution Functions

Somebody who is more an expert should fill that out.

2.9 Deadtime

- Deadtime corrected: yes, no, unknown, negligible.

2.10 Maxwellian Temperature

- Maxwellian temperature or Watt parameters per Einc.

2.11 Energy

- Energy-determination technique: TOF, mono-energetic,
- Energy spread,
- Energy spread corrected: yes, no, unknown,
- trsl,
- TOF length.

2.12 Monitor

- Monitor reaction,
- Monitor value,
- Monitor reference.

2.13 Decay Data

- Decay-data reaction,
- Decay-data value,
- Decay-data reference.

2.14 PFNS

for nu-bar measurements, can be similar to decay data or monitor, might need to take reference to Maxwellian temperature.

- PFNS reaction,
- PFNS value,
- PFNS reference.

2.15 Yield Extraction

- Somebody who knows that better than me should fill that out.

2.16 Correlation to Other Dataset

- EXFOR number,
- Correlating factors: same sample, same method for specific aspect of the measurement, etc.

2.17 Times

- Irradiation time, cooling time, counting time (activation),
- time gate open (nu-bar).

Chapter 3

Data Storage Container for Layer 1

3.1 Energy and Angle

3.2 Experimental Mean Values

3.3 Experimental Uncertainties

Different types, namely:

- counting statistics,
- background (should we distinguish types?),
- multiple scattering,
- attenuation,
- detector efficiency,
- angular distortion,
- deadtime,
- nuclear data (unc. of nuclear data used in simulations),
- TOF length,
- time resolution/ spread (in ns),
- Energy,
- impurity,
- neutron-flux monitoring,
- isotopic enrichment,
- sample uniformity,
- geometric effects,
- ability to extract yield from spectra,
- delayed γs,

- false fissions,
- PFNS,
- neutron leakage,
- displacement of sample,
- sample thickness,
- H/S content versus Mn,
- French effect,
- Number of atoms in sample or baths/ target-number density,
- resonance capture in Mn,
- flux normalization/ neutron flux,
- inscattering,
- resolution function,
- AMS reproducibility,
- beam overlap,
- stopping power,
- Decay constants,
- internal conversion.

but same format for all.

Questions: should we distinguish even further?

Also, we might need to allow for uncertainties we did not think of.

3.4 Covariance Data

- define format for covariances themselves,
- define unique nomenclature to trace it back to a specific uncertainty source as listed in section 3.3.

3.5 Corrections Undertaken by Experimentalists

Different types, namely:

- background (should we distinguish types?),
- multiple scattering,
- attenuation,
- detector efficiency,
- angular distortion,

- deadtime,
- nuclear data (unc. of nuclear data used in simulations),
- TOF length,
- time resolution/ spread (in ns),
- Energy,
- impurity,
- neutron-flux monitoring,
- isotopic enrichment,
- sample uniformity,
- geometric effects,
- ability to extract yield from spectra,
- delayed γs,
- false fissions,
- PFNS,
- neutron leakage,
- displacement of sample,
- sample thickness,
- H/S content versus Mn,
- French effect,
- Number of atoms in sample or baths/ target-number density,
- resonance capture in Mn,
- flux normalization/ neutron flux,
- inscattering,
- resolution function,
- AMS reproducibility,
- beam overlap,
- stopping power,
- Decay constants,
- internal conversion.

but same format for all.

Questions: should we distinguish even further?

Comment: Also, we might need to allow for corrections we did not think of. We need to allow for scalars and arrays.

Chapter 4

Correction and Objective Testing Containers for Layer 2

4.1 Corrections Undertaken

Corrected for:

- Monitors,
- Decay data.

4.2 Objective Data Testing

Objective data testing for:

- Listing of missing corrections,
- Listing of missing uncertainties according to templates,
- P-value of data to classify as outliers,
- SVR to classify as outliers.

4.3 Format for Corrections

Comment: I would re-use as much of the format for above as possible. E.g., missing uncertainties/ corrections could simply be listed under the key “Detector-efficiency correction”: unknown/ missing.

Additional format containers:

- “P-value” and value
- “Classified as outlier by SVR”: yes/ no
- “Monitor updated”: yes/ no, reference to monitor value (e.g., standard 2018) or monitor value
- “Decay data updated”: yes/ no, reference to monitor value (e.g., ENSDF version) or monitor value

Chapter 5

Expert Judgment Identifiers for Layer 3

Needs to be discussed.

Chapter 6

Code and Database Descriptions

Code:

- Which codes were already available,
- reasoning why we chose to start a new/ or from an existing code,
- input decks for each example given in Chapter 7.

Database:

- Which databases were considered,
- reasoning why we chose a specific database type,
- link to examples given in Chapter 7.

Chapter 7

Examples for Various Data Types Covered in the Database

Here, we could give a converted EXFOR files for each observables. This step should guarantee that we have all necessary metadata and data container to describe each observable we tackle.

7.1 Total Cross Section

- RRR,
- URR,
- fast.

7.2 Capture Cross section

- RRR,
- URR,
- fast.

7.3 Fission Cross Section

- RRR,
- URR,
- fast.

7.4 Charged-particle Cross Section

- ratio activation,
- ratio activation with assop or fission chamber,
- direct.

7.5 Scattering Cross Section

- RRR,
- URR,
- fast.

7.6 Angular Distributions

Someone more knowledgeable than me should fill that out.

7.7 Prompt-fission Neutron Spectrum

- Shape,
- Clean Ratio,
- Ratio Calibration.

7.8 Prompt- and Total-fission Neutron Multiplicity

- Absolute liquid scintillators,
- Ratio liquid scintillators,
- Mn baths,
- from PFNS measurements.

7.9 Fission Yields

- Activation,
- irradiation,
- chemical separation,
- assay,
- 2E-2v.

Table I: ...

...	...	....	...	...	...

Chapter 8

Summary

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Bibliography

[1] Experimental Nuclear Reaction Data Library (EXFOR), IAEA Nuclear Data Section. See https://www-nds.iaea.org/exfor (accessed on 8/11/2016), or for the NNDC at Brookhaven National Laboratory, the mirror site is http://www.nndc.bnl.gov/exfor (accessed on 8/11/2016); N. Otuka, E. Dupont, V. Semkova *et al.*, "Towards a More Complete and Accurate Experimental Nuclear Reaction Data Library (EXFOR): International Collaboration Between Nuclear Reaction Data Centres (NRDC)," Nucl. Data Sheets **120**, 272–276 (2014); V.V. Zerkin and B. Pritychenko, "The experimental nuclear reaction data (EXFOR): Extended computer database and Web retrieval system," Nucl. Instrum. Meth. in Phys. Res. Sec. A **888**, 31–43 (2018).

[2] D. Neudecker, D.L. Smith, F. Tovesson *et al.*, "Applying a Template of Expected Uncertainties to Updating ^{239}Pu(n,f) Cross-section Covariances in the Neutron Data Standards Database, " Nucl. Data Sheets , in press (2020).

[3] P. Schillebeeckx, B. Becker, Y. Danon *et al.*, "Determination of Resonance Parameters and their Covariances from Neutron Induced Reaction Cross Section Data," Nucl. Data Sheets 113, 3054–3100 (2012); F. Gunsing, P. Schillebeeckx and V. Semkova, IAEA Report INDC(NDS)-0647 (2013).

[4] P. Helgesson, H. Sjöstrand and D. Rochman, "Uncertainty-driven Nuclear Data Evaluation Including Thermal (n,α) Applied to ^{59}Ni," Nuclear Data Sheets, **145**, 1–24 (2017).

[5] A.D. Carlson, V.G. Pronyaev, R. Capote *et al.*, "Evaluation of the Neutron Data Standards," Nucl. Data Sheets **148**, 143–188 (2018).

[6] J. Bess (editor), "International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP)," Organization for Economic Co-operation and Development-Nuclear Energy Agency Report NEA/NSC/DOC(95)03 (2019).

[7] C.J. Werner (editor), "MCNP Users Manual - Code Version 6.2," Los Alamos National Laboratory Report LA-UR-17-29981 (2017).

[8] D.A. Brown, M.B. Chadwick, R. Capote *et al.*, "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," Nucl. Data Sheets **148**, 1–142 (2018).