# Consultancy Meeting on Information Exchange on Developments and Operations of Nuclear Data Dissemination Services

Report of Contributions

Contribution ID: 1 Type: not specified

### TALYSworld and connection to other GUI's

Monday, 15 January 2024 10:15 (45 minutes)

A short demonstration of TALYSworld was given, see https://nds.iaea.org/relnsd/talys/talys.html. This GUI is based on a concept sometimes called Computationa Steering, analogous to the Medical Isotope Browser at https://www-nds.iaea.org/relnsd/isotopia/isotopia.html

The idea is to change model parameters of TALYS on a webpage, and after clicking 'Run' TALYS will run in the background and after a few second plot curves on the screen in comparison with EXFOR data. With regards to the keywords and possibilities of TALYS, we consider that we are a bit more than halfway and in the near future the remaining TALYS parameters and other options will be added to the interface.

It was also shown that via parameter options in the URL, direct links to other interfaces like Livechart and the Reaction Data explorer can be provided.

**Primary author:** KONING, Arjan (IAEA)

Presenter: KONING, Arjan (IAEA)

Contribution ID: 2 Type: not specified

# Data dissemination: addressing users'feedback and needs for the livechart

Monday, 15 January 2024 11:00 (45 minutes)

Users'feedback has been the major driver for the development of dissemination tools at the IAEA Nuclear Data Section.

Some examples from the past, and future perspectives

Primary author: VERPELLI, Marco (IAEA)

**Presenter:** VERPELLI, Marco (IAEA)

Contribution ID: 3 Type: not specified

## 1. A tour of the BNL web system / 2. NSR

Monday, 15 January 2024 13:30 (1 hour)

- 1. A tour of the BNL web system
- 2. NSR

The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) has been gradually updating its web development process. It now uses software tools for each step –Gradle for compiling code, Git/GitLab for tracking changes, and Docker for deploying updates. The first presentation attached describes the general workflow for updating NNDC websites. The second presentation focuses on a website dedicated to the Nuclear Science References (NSR) database, and shows the steps taken for developing its new interface.

Primary author: SHU, Benjamin (BNL)

**Presenter:** SHU, Benjamin (BNL)

Contribution ID: 4

Type: not specified

# 1. Modernisation of the NDS website / 2. New and modernised databases (Stopping Powers and IDB)

Monday, 15 January 2024 14:30 (1 hour)

- 1. Modernisation of the NDS website
- 2. New and modernised databases (Stopping Powers and IDB)

This contribution presents an approach towards creating a repository for nuclear data collections and services that implements the FAIR (Findable, Accessible, Interoperable and Reusable) principles. The proposed platform provides an integrated environment for data collections, resources, and services to support the worldwide nuclear science and technology community. The repository is designed to organize different type of resources in a structured way and to provide a unified access point to all the heterogeneous collections that the Nuclear Data Section (NDS) hosts. The repository is implemented using a hybrid approach, where the core part of the system is based on the Invenio RDM framework. This part integrates with existing NDS and IAEA services, as well as with several newly built micro-services that implement specialized nuclear data retrieval and visualization products. In addition, the platform provides a secure and reliable environment to store and preserve nuclear resources. The presentation will provide a detail description of the underlying platform, Invenio RDM, for participants to see if this could be a good fit for some of their use cases.

The second presentation gives an overview of the current infrastructure powering the NDS website and services, security tools, version control and monitoring of availability. It will include a demo/walk-through of two new/modernized databases, implemented using the Django framework.

Primary author: MARIAN, Ludmila

Presenter: MARIAN, Ludmila

Contribution ID: 5 Type: **not specified** 

### **IAEA Nuclear Reaction Dataexplorer Developments**

Monday, 15 January 2024 15:30 (1 hour)

An efficient and easy data access to the nuclear reaction data are essential to enhance the understanding and explanation of the fundamentals of theory and experiments of nulear reaction physics. The Experimental Nuclear Reaction Database (EXFOR) has a potential for utilization of modern computational analysis techniques to find hidden patterns by using machine learning (ML) applications, which helps improve our knowledge of nuclear reactions and accelerates the developments in the field. To facilitate such a study, EXFOR structure and data parsing computer program, EXFOR Parser, was developed. The EXFOR Parser convers EXFOR format into the widely adopted JSON format, and extract physical quantities in tabulated (x, y, dx, dy) datatable and stores into SQL database.

The RESTful APIs and the data plotting interface were built using Python on Flask and Dash, respectively, for easy access and quick visualizations of these converted datasets.

Primary author: OKUMURA, Shin (IAEA)

**Presenter:** OKUMURA, Shin (IAEA)

Contribution ID: 6 Type: **not specified** 

# 1. What's in old Sigma / 2. The ENDF project / 3. GNDS

Tuesday, 16 January 2024 09:30 (1 hour)

#### 1. What's in old Sigma

Sigma is a web app designed and hosted by the National Nuclear Data Center (NNDC) for the visualization of ENDF reaction data. Sigma allows the user to browse the contents of ENDF files in a mostly easy to use manner and, at one point, allowed the comparisons of ENDF data with experimental data from EXFOR. Currently the site is not well maintained at the NNDC for a number of reasons. This presentation described the operation of the legacy system and provided recommendations for a "refreshed" web app using GNDS and EXFOR-JSON as a foundation.

### 1. The ENDF project

The Evaluated Nuclear Data File (ENDF) library is the most widely used nuclear reaction data library in the United States. In this presentation, a brief overview of the ENDF project history, management of the Cross Section Evaluation Working Group, and the next ENDF release were provided. Emphasis was placed on the open nature of CSEWG and ENDF, evident from the beginning of the project. Also presented was the current review process for ENDF files, the status of the current Beta3 library and the status of the drafting of the library summary paper.

#### 1. GNDS

The Generalized Nuclear Database Structure (GNDS) is the successor format to the legacy ENDF format. The legacy ENDF format was designed to work on obsolete computational hardware and uses an outdated data model. This data model was adapted over the succeeding 50 years and now does not clearly follow a data model consistent with the understanding of the main user base of the library. GNDS is a complete redesign of the format and data model. GNDS can store both evaluated and processed data in the same hierarchy. GNDS is much easier to learn and use than the legacy ENDF format. The data community is still in the process of adopting GNDS.

**Primary author:** BROWN, David (Brookhaven National Laboratory)

**Presenter:** BROWN, David (Brookhaven National Laboratory)

Contribution ID: 7 Type: not specified

# endf-parserpy: A Python package for working with ENDF-6 files

Tuesday, 16 January 2024 10:30 (1 hour)

The ENDF-6 file format is adopted by the major nuclear data libraries for storing and disseminating evaluated nuclear data. However, publicly available tools supporting scientists in the translation of their data into the ENDF-6 format are scarce, posing an obstacle to newcomers to the nuclear data field. This presentation elaborates on the design and functionality of the recently developed Python package endf-parserpy to improve this situation regarding nuclear data development. Its unique design feature is that it leverages a formal ENDF description to enable a bidirectional one-to-one translation between ENDF-6 formatted data and Python dictionaries. This functionality in combination with Python's powerful facilities for data handling greatly facilitates the creation and manipulation of ENDF-6 files as well as access to their data. Furthermore, this package provides rigorous format validation, semantically meaningful comparisons of ENDF-6 files and the loss-free translation from and to other container formats, such as JSON. The package is available on the Python Package Index (PyPi) and fully documented. Further details can be found at its GitHub repository https://github.com/iaea-nds/endf-parserpy

Primary author: SCHNABEL, Georg (IAEA)

Presenter: SCHNABEL, Georg (IAEA)

Contribution ID: 8 Type: **not specified** 

### **YANDF Format in TALYS**

Tuesday, 16 January 2024 11:30 (30 minutes)

A simple but sufficient data format YANDL (yet Another Nuclear Data Format) was introduced. TALYS-2.0 now produces all its output in YANDF format. This is a YAML-esque format aiming to provide complete metadata in each output file of TALYS. Moreover, the same format is used for EXFOR (in the incarnation of EXFORtables) and ENDF (as resulting from ENDFtables), allowing for consistent automated use of TALYS, EXFOR and ENDF data in further applications.

Primary author: KONING, Arjan (IAEA)

Presenter: KONING, Arjan (IAEA)

Contribution ID: 9 Type: not specified

# **EXFOR - An early overview and opinionated** assessment

Tuesday, 16 January 2024 14:15 (45 minutes)

Exfor is a library central to the nuclear sciences. In this presentation I give an overview on current practices for library maintenance, distribution and community involvement. I provide proposals to improve aspects of each of those three areas with respect to modern tools and workflows available. In the following discussion I hope to collect feedback on the presented proposals and gather alternative ideas for modernization efforts of the exfor ecosystem.

Primary author: SPRENGER, Julia (OECD/NEA)

**Presenter:** SPRENGER, Julia (OECD/NEA)

Contribution ID: 10 Type: not specified

### The NEA efforts to modernize JEFF and EXFOR

Tuesday, 16 January 2024 13:30 (45 minutes)

The main NEA Nuclear Data Projects, specifically JEFF and EXFOR, have undergone modernization efforts to align with FAIR principles. In the case of JEFF, the transition to using GitLab and SharePoint has made data more accessible to the community, allowing for immediate testing and feedback through automatic processing. The JEFF-Lab served as a training ground for users to adapt to the new tools. For EXFOR, the plan is to automate bibliography checks, TRANS checker, and text clarity, while JANIS checks, the most time-consuming part, will still require human intervention. GitLab is also used for EXFOR compilation, streamlining the review process through centralized comments and issue boards. The NEA aims for automation, transparency, reproducibility, and archiving of important information, minimizing reliance on email communication. The main challenge lies in overcoming resistance to change among users, suggesting a need for demonstrating the benefits of the new tools and implementing strategies for a smoother transition.

Primary author: FOLIGNO, Daniela (OECD/NEA)

Presenter: FOLIGNO, Daniela (OECD/NEA)

Contribution ID: 11 Type: not specified

### 1. DOI Pages & Status / 2. Nudat 3

Tuesday, 16 January 2024 15:20 (1 hour)

#### 1- DOI Pages & Status

The National Nuclear Data Center at Brookhaven National Laboratory has registered DOIs for ENSDF, XUNDL, and NSR. Each database has an associated persistent landing page which contains relevant metadata describing the deposit summary, dataset details, and publication details along with downloadable archives. This effort was motivated by the Department of Energy designating the NNDC as a Public Reusable Research (PuRe) Data steward.

The registration of DOIs goes through the BNL library which requests a DOI from OSTI through their E-Link API. The DOIs are then minted through DataCite. OSTI requires specific metadata which is relevant to DOE records such as DOE contract numbers. The NNDC plans on registering additional DOIs in accordance with the general requirements for data registration.

#### 2- Nudat 3

The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) overhauled one of our most frequently visited web applications, NuDat. Nudat 3 visualizes the data contained in the Evaluated Nuclear Structure Data File (ENSDF). NuDat features responsive visualizations that significantly improved on the performance of its predecessor by relying on client side rendering using D3.js. NuDat uses Google analytics for a broad overview of how users are interacting with the web application. NuDat has custom analytics as well which allow for possible physics insights based on what nuclides are being searched for.

The NNDC plans to add additional features to NuDat based on user requests and will modernize other web applications. NuDat has a 3D version in development as well.

**Primary author:** MASON, Donnie

Presenter: MASON, Donnie

Contribution ID: 12 Type: not specified

## 3. Open Science efforts update: DOIs and Licenses

Tuesday, 16 January 2024 16:20 (45 minutes)

The presentation will give a status update on the NDS efforts to mint DOIs for resources available on the NDS website and on the efforts to use open licenses (CC-BY-4.0 in case of data libraries and MIT in case of software) for the open resources available on the NDS website.

Primary author: MARIAN, Ludmila

Presenter: MARIAN, Ludmila

Consultancy M  $\,\cdots\,\,$  / Report of Contributions

Discussions

Contribution ID: 13 Type: not specified

## **Discussions**

Wednesday, 17 January 2024 10:00 (2 hours)

Consultancy M  $\,\cdots\,\,$  / Report of Contributions

Discussions

Contribution ID: 14 Type: not specified

## **Discussions**

Wednesday, 17 January 2024 13:30 (3h 30m)

Contribution ID: 15 Type: not specified

## Report and summary

Thursday, 18 January 2024 13:30 (3h 30m)