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Nuclear Data Portal Web Tools

Summary Report

IAEA Headquarters, Vienna, Austria

30 July – 1 August 2018

Prepared by

J. Shimwell and J.-C. Sublet

August 2018

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or to:

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

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Nuclear Data Portal Web Tools

Summary Report of the Consultant Meeting on Nuclear Data Portal Web Tools

IAEA Headquarters, Vienna, Austria

30 July – 1 August 2018

Prepared by

Jonathan Shimwell and Jean-Christophe Sublet

Abstract

The purpose of the Consultant Meeting on Nuclear Data Portal Web Tools was to firstly evaluate the existing tools and their capabilities; then to review the tools which are currently successfully deployed and thereby establish efficiency ratings, best practise and user satisfaction. The second phase will focus on proposing new web tools which will offer improved analytics, visualisation and imaging of nuclear data. The new tools will offer significantly greater capability in overcoming the challenges faced in the modelling, accessing and testing of nuclear data. They will be applicable to an extensive range of applications within the area of research. Throughout this process advice will be sought from professional scientific portal developers.

August 2018

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1. Introduction

The purpose of the Consultant Meeting on Nuclear Data Portal Web Tools is to firstly evaluate the existing tools and their capabilities; then to review the tools which are currently successfully deployed and thereby establish efficiency ratings, best practise and user satisfaction.

The second phase will focus on proposing new web tools which will offer improved analytics, visualisation and imaging of nuclear data. The new tools will offer significantly greater capability in overcoming the challenges faced in the modelling, accessing and testing of nuclear data. They will be applicable to an extensive range of applications within the area of research. Throughout this process advice will be sought from professional data analytics (Plot.ly) and scientific (CERN) portal developers.

2. Proceedings

“ShimPlotWell: an adventure in online nuclear data visualisation”, UKAEA, Jonathan Shimwell

This presentation covered the techniques used by www.cross-section-plotter.com to provide a web based cross section plotting experience. This project emerged from the perceived need to plot mixed reactions for different isotopes in an intuitive and interactive manner. The use of hosted functions in the form of URL based API's were discussed as a scalable solution to handling user requests. The scalability of cloud-based NoSQL databases was also explored. Three different versions of ShimPlotWell were examined, these versions illustrated the evolution in designs and uptake of new technologies. The latest (currently unreleased) version offers significantly greater user flexibility. Initial versions of this software facilitated easy access to pre-processed cross sections within databases. The latest version further expands user capabilities by facilitating the generation of nuclear data cross sections for materials (e.g. steel, concrete or H₂O). The cross sections are generated on the fly and result in a unified energy grid for all requested reaction channels. This operational versatility opens up further performance options, for example, enabling more complex operations such as the combination of MT numbers and the homogenising of multiple materials.

“The HPNSRL Website and the Baghdad Atlas”, UC Berkeley, Aaron Hurst

This presentation covers two nuclear data products that have been developed by the Nuclear Data Group at the University of California, Berkeley. The first part of the presentation describes the High Priority Nuclear Structure Request List website. This website was developed in response to “Action Item #28” from the recent 22nd *Technical Meeting of the Nuclear Structure and Decay Data Network* which was held at the Lawrence Berkeley National Laboratory, Berkeley, California, USA, May 22-26, 2017. At this meeting, the Experimental Activities Subcommittee were tasked with the creation of a website of high-priority nuclear structure and decay-data measurements for information and guidance. An overview of the website was given during the presentation, including examples illustrating its utility. The second part of the presentation concerned the development of a database of inelastic neutron-scattering gamma-ray data, commonly referred to as the “Baghdad Atlas”. This database is a compilation of energy-integrated fast-reactor neutron-scattering gamma-ray data that is disseminated through a set of CSV-style data files, together with the software required to build and utilise the SQLite

relational database. The complete data set comprises approximately 7000 gamma rays (energies and branching ratios) from 105 samples (76 natural and 29 isotopically-enriched targets) acquired from a consistent set of measurements which were performed under identical controlled conditions using a single Ge(Li) detector on a fast-neutron beam line at the IRT-5000 Reactor located at the Al-Tuwaitha Research Facility, Baghdad, Iraq. The application-oriented need motivating the dissemination of this database was also discussed.

“SWAN: Service for Web-based Analysis at CERN” CERN, Enric Tejedor Saavedra

This presentation covered SWAN, the Service for Web-based Analysis at CERN (<https://swan.web.cern.ch/>). SWAN allows users to perform interactive data analysis in the cloud, in a "software as a service" model. It is built upon the widely-used Jupyter notebooks, allowing users to write - and run - their data analysis using only a web browser. By connecting to SWAN, users have immediate access to storage (EOS, CERNBox), software (CVMFS, LCG releases) and computing resources that CERN provides and that they need to do their analyses. Besides providing a straightforward way of producing scientific code and results, SWAN is also a great tool to do collaborative analysis: notebooks and other files can be encapsulated in projects that are easily shareable among scientists, which favours reproducibility of results. In addition, SWAN can also be used as an entry point to exploit external computing resources (e.g. Spark clusters), which can be connected to a SWAN session so that users can submit computationally-intensive tasks to those resources and get the results back in their notebooks.

“Websites and tools in CNDC” CIAE, Xi Tao, Yongli JIN

The presentation introduced the websites and tools established by China Nuclear Data Center (CNDC). The Database of Nuclear Physics (<http://www.nuclear.csdb.cn/>) was built in China and is convenient for Chinese people to use. CNDC is devoted to the development of plotting software for nuclear data. The first Microsoft Windows plotting software named TT was released in 2002. To make it easier to use and add new functions, a new version was developed and named NDPlot. It can visualise: the cross sections, angular distributions, energy spectra, double differential spectra and fission yields. NDPlot could accept ENDF, EXFOR, PENDF, free format, NDPlot format data, and output graphs (jpeg, ps, pdf, etc.). Several new useful functions of NDPlot were shown in this presentation, Batch Plotting, Quick Choice, Ratios etc. GDgraph, GETZVD, GETTABLE and Autoplot were briefly introduced. The function of these tools is to provide researchers with both advice and inspiration. Tools established by CNDC were closely related to the tools provided by NDS. Thanks, were offered to NDS and IAEA.

“Web Knowledge Base on Low Energy Nuclear Physics” JINR, Andrey Denikin

The talk describes the principles of organization and operation of the NRV web knowledge base on low-energy nuclear physics (<http://nrw.jinr.ru/nrv/>). This integrates a large amount of digitized experimental data on the properties of nuclei (particularly, data provided by the services from the IAEA NDS portal). Additionally, the website includes nuclear reaction cross sections. Users of the website are able to interact with a wide range of computational programs

for the modelling of nuclear properties and various processes of nuclear dynamics. A feature of the NRV knowledge base are the illustrated interactive physics models, for example, elastic scattering reactions within the optical model.

“Web tools for structure and decay data”, IAEA, Marco Verpelli

The presentation summarises the status of the web-based applications for structure and decay data <https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html>. First, the goals and objectives underlying the design are described, then examples of the actual implementation are offered, followed by a summary of the technology. Information relating to the workflow of the design is given, together with the challenge of keeping alive the legacy applications and serving users with legacy technologies. New developments in terms of functionalities and technologies are presented, focussing on more user interactivity and on enabling users to perform some autonomous analysis on the data. A set of topics proposed for further discussion by the meeting’s participants concludes the talk.

“Web tools for reaction data” IAEA, Roberto Capote Noy

A brief interactive demonstration and overview of the current status of the IAEA/NDS web page <https://www-nds.iaea.org/exfor/endif.htm> and plotting capabilities was presented. An emphasis was made on different types of reaction data available and the possibilities of the current system that should be preserved.

“Web tools for atomic and molecular data”, IAEA, Christian Hill

The latest development status of the Atomic and Molecular Data (AMD) Unit’s website and principal databases was described. The current set of pages and search interfaces are more than 10 years old and lack some important functionality and usability <https://www-amdis.iaea.org/>. A new site, based on the Python Django Web Framework was demonstrated. Main features are:

- A Relational Database backend for important AMD Unit-related events, projects and meetings for a consistent and easy-to-navigate description of the Unit’s activities.
- An improved interface and database backend to the Unit’s main numerical database, ALADDIN, featuring interactive charting capabilities and improved search functionality.
- An explicit and searchable classification of atomic and molecular species and processes.

The software technologies deployed in this new site were briefly described: Python, Django, Bokeh, MySQL, HTML, CSS, JavaScript/JQuery. The local and broader security and privacy considerations surrounding this development were discussed.

“Plotly: The Web-based Data Visualization Platform for Engineering, Research and Data Science” Plotly Company, Rob Williams

Plotly creates leading open source tools for composing, editing, and sharing interactive data visualization via the Web. Plotly collaboration servers (available in cloud or on premises) allow data scientists to showcase their work, make graphs without coding, and collaborate with business analysts, designers, executives, and clients.

<https://f1000research.com/articles/6-1396/v1#f6>

<https://dash.plot.ly/gallery>

<https://plot.ly/python/webgl-vs-svg/>

<https://github.com/jupyterlab/jupyter-renderers/tree/master/packages/plotly-extension>

<https://github.com/plotly/dash-oil-and-gas-demo>

“Nuclear data analytics; a debut” IAEA, Jean-Christophe Sublet

Nuclear data analytics comprise many processes that need to be deployed on the basic data but also processed data forms. Different metrics are used in those processes: C refers to calculation or model, E to experiment and S to systematics.

C over E, C over S or even C over C are quantities of interest and when applied to: cross sections, effective cross section, resonance integral, Maxwellian average, fission over capture ratio, gamma lines or yields and properly visualized over the entire Mendeleev element and isotopic tables, helps our understanding of the physics and correlation at play.

<https://fispact.ukaea.uk/nuclear-data/fission-yields/>

<https://fispact.ukaea.uk/nuclear-data/high-energy-yields/>

<https://fispact.ukaea.uk/nuclear-data/>

<https://fispact.ukaea.uk/wp-content/uploads/2016/06/UKAEA-R1530.pdf>

3. Discussion and Conclusions

Representatives of the five institutions (CNDC, UKAEA, UC Berkeley, JINR, CERN) and a company (Plotly) had been invited to attend the meeting. All attendees gave presentations relating to the web portals which have been developed to serve their own specific needs. These web portals significantly extended the operational scope of the generic tools available from the IAEA-NDS web portal. Usage of the web portals varied from professional and expert analysis of nuclear data, educationalists and inquisitive amateurs.

The expert group advises the IAEA to carry out the following:

- Acquisition of user satisfaction for web tools to steer future development.
- Usage statistics for different areas of the IAEA NDS web portal (for example a heatmap).
- Addition of non-obtrusive, dynamic context related information to inform users of web tool functionality. Application examples, hover text.

- Reduce the use of multiple page submissions and clicks required for plotting data.
- Consultation with professional data centric web designers and GUI designers to create a cleaner interface.
- Provide the option to preserve user session data on the web server for future use, while avoiding the need for mandatory user registration.
- Allow access to the raw data:
 - Downloadable standalone data, in the form of a database, json, xml or other self-describing files.
 - Provision of a metadata schema (following [FAIR principles](#)).
 - Programmable access via software (e.g. via [python packages](#)).
 - Programmable access via URL based API (suitable for larger databases such as cross sections).
- Generation of report style information on individual isotopes which would include all available data on the isotopes (cross sections, decay data, mass, excitation states etc).
- Ability to compare differences between data forms (e.g. observed minus calculated residuals). This could appear as a subfigure below the existing data form.
- Deploy a prototype of a Jupyter-based server and expose it to the users, in order to gather their feedback regarding interactive computing interfaces for data analysis. A suggestion would be to use a version of SWAN that is easily installable on premises, called Science Box. The scripts to automatically install this version on a single server can be downloaded from <http://sciencebox.web.cern.ch/sciencebox/>.
- If the aforementioned prototype were successful, a more customized version could be deployed, in particular to provide the users with: (i) the software they need to do their analyses, which could be installed in an IAEA instance of CVMFS, and (ii) access to the nuclear data they need to analyze in their notebooks. For the latter, queries to SQL databases can be easily issued from notebooks, either using some wrapper libraries (e.g. in Python) or via SQL magic cells (<https://github.com/catherinedevlin/ipython-sql>).

The expert group recommends the IAEA NDS to keep current services available while exploring its modernisation. The expert group also recommends the IAEA to call upon the expert groups within 1 to 2 years to assess, evaluate the improvement, and progress made.

4. Work Plan Updates

CERN

The forthcoming SWAN developments are twofold. On the one hand, the new JupyterLab interface (<https://github.com/jupyterlab/jupyterlab>) will be investigated as a way to provide the user with a more desktop-like experience, combining notebooks, editors, file browsers, terminals and any other extensions in the same flexible environment. On the other hand, more external resources will be connected to the SWAN user sessions: there is an ongoing effort to support the submission and monitoring of batch jobs from SWAN, and future work includes the ability to plug in a GPU to a user session so that GPU-ready libraries (e.g. in the field of machine learning) can run their computations faster.

UKAEA

Development of cross section plotting web app for plotting macroscopic cross sections for materials, including the formation of a unified energy grid for the selected reactions. This will be accomplished via the use of OpenMC, Docker, Google Cloud and Plotly. Other aspects that are of particular interest to fusion energy include angular distributions and charged particle spectra.

JINR (Joint Institute for Nuclear Research)

Further development of the NRV project concerns including the conversion of Java to JavaScript technology in the data visualisation part (by using for example Plotly) including: new computational codes for modelling of the nuclear properties and reactions, preparation of new databases on the nuclear reactions with heavy ions (transfer, inelastic scattering, deep-inelastic scattering, etc.) in accordance with Flerov Laboratory of Nuclear Reactions JINR topics.

CNDC

NDPlot is still under development. More functions need to be improved, and more tests need to be carried out. We have already raised the funds and established a NDPlot server on the internet. NDPlot will be released in October 2018.

University of California, Berkeley

The inelastic neutron-scattering gamma-ray data contained in the “Baghdad Atlas” database is currently being evaluated to reconcile the decay schemes with the corresponding information in the Evaluated Nuclear Structure Data File (ENSDF) database. A future release of the atlas will comprise an enhanced schema, together with the updated data sets.

International Atomic Energy Agency

The IAEA-NDS will task, organize institutions with the aim of proposing new web tools which will offer improved analytics, visualisation and imaging capabilities for nuclear data. It will use its own internal resources to test and deploy the new web-tools.

List of participants

Elected Chairman: Aaron Hurst

Elected Rapporteur: Jonathan Shimwell

F4-CS-1703598**Consultancy Meeting on Nuclear Data Portal Web Tools****Vienna, Austria****30 July - 1 August 2018**

S. No.	Authority	Personal Details
1	Canada	Mr Rob Williams – <u>via Webex</u> Plotly Technologies 5555 Ave de Gaspe Montreal, Qc Canada Email: rob@plot.ly
2	China	Mr Xi Tao China Nuclear Data Center China Institute of Atomic Energy P.O. Box 275-41 Beijing China Email: taoxixishi@gmail.com
3	Russian Federation	Mr Andrey Denikin Joint Institute for Nuclear Research Flerov Laboratory of Nuclear Reactions Moscow Region Dubna Russian Federation Email: denikin@jinr.ru
4	Switzerland	Mr Enric Tejedor Saavedra CERN Physics Department 1211 Geneva 23 Switzerland Email: enric.tejedor.saavedra@cern.ch
5	United Kingdom	Mr Jonathan Shimwell Culham Centre for Fusion Energy Abingdon Oxfordshire United Kingdom Email: jonathan.shimwell@ukaea.uk

6	United States of America	Mr Aaron Hurst Department of Nuclear Engineering University of California, Berkeley Berkeley CA 94720 United States Of America Email: amhurst@berkeley.edu
7	IAEA	Mr Jean-Christophe Sublet – Scientific Secretary Nuclear Data Section Vienna International Centre 1400 VIENNA AUSTRIA Email: J.C.Sublet@iaea.org
8	IAEA	Mr Arjan Koning Email: A.Koning@iaea.org
9	IAEA	Mr Roberto Capote Noy Email: Roberto.CapoteNoy@iaea.org
10	IAEA	Mr Kalle Heinola Email: K.Heinola@iaea.org
11	IAEA	Mr Christian Hill Email: C.Hill@iaea.org
12	IAEA	Mr. Marco Verpelli Email: M.Verpelli@iaea.org
13	IAEA	Ms Aleksandra Peeva Email: A.Peeva@iaea.org



Consultancy Meeting on Nuclear Data Portal Web Tools

July 30th – August 1st, 2018, IAEA Headquarters, Vienna, Austria

Room M 0E69

Agenda

Monday July 30th, Room M0E69

- 08:30 Registration (IAEA Registration desk, Gate 1)
- 09:30 Welcoming address – Arjan Koning, SH-NDS
Introduction, Scope of the CM - J.-Ch. Sublet, UH-NDSU
Election of chairman and rapporteur
Adoption of agenda, administrative matters
- 10:00 “ShimPlotWell: an adventure in online nuclear data visualisation” UKAEA, Jonathan Shimwell
- 10:45 *Coffee Break*
- 11:00 “The HPNSRL website and the Baghdad atlas”, UC Berkeley, Aaron Hurst
- 11:45 NEA, Nicolas Soppera (Cancelled)
- 12:30 *Lunch*
- 14:00 “SWAN: Service for Web-based Analysis at CERN” CERN, Enric Tejedor Saavedra
- 14:45 “Websites and tools in CNDC” CIAE, Xi Tao, Yongli JIN
- 15:30 *Coffee Break*
- 15:45 “Web Knowledge Base on Low Energy Nuclear Physics” JINR, Andrey Denikin
- 17:30 End of Day One

Tuesday July 31st, Room M0E69

- 09:30 “Web tools for decay data, IAEA, Marco Verpelli
- 10:00 “Web tools for reaction data” IAEA, Roberto Capote Noy
- 10:30 *Coffee Break*
- 10:45 “Web tools for atomic and molecular” IAEA, Kalle Heinola

- 11:15 Discussion: *Best practices, User's need, Evaluations*
- 12:30 Lunch
- 14:00 Plotly: The Web-based Data Visualization Platform for Engineering, Research and Data Science” Plotly Company, Rob Williams (Remote)
- The Plotly Story
 - An Overview of the Plotly Platform and Ecosystem
 - Plotly.JS - D3/WebGL visualizations
 - The Plotly Feed - Sharing and collaboration
 - Chart Studio - Building interactive visualizations from different environments
 - Dash - The Pythonic Web Application Framework
 - Dash - Interactive Report Generation and Archiving
 - Plotly Enterprise Server
 - Q&A
- 15:00 “Nuclear data analytics; a debut” IAEA, Jean-Christophe Sublet
- 15:30 *Coffee Break*
- 15:45 Discussion: *Data analytics*
- 17:00 End of Day two
- 19:00 Evening Meal

Wednesday August 1st, Room M0E69

- 09:30 Discussion: *new tools*
- 10:30 *Coffee Break*
- 10:45 Discussion: *databases*
- 12:30 Lunch
- 14:00 Final remarks and review
- 15:00 Close of meeting

Presentations

All presentation materials are available on the web page for this meeting:

<https://www-nds.iaea.org/index-meeting-crp/WebToolsCM/>

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: <http://nds.iaea.org>
