企画セッション | 部会・連絡会セッション：計算科学技術部会

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[2J_PL] 国際的な計算コード・データベースの活用に関する枠組みと今後の展開

座長:鈴木 喜雄(JAEA)

[2J_PL01] OECD/NEAデータバンクの活動

*須山 賢也[1] (1. OECD/NEA)

[2J_PL02] IAEA核データサービスの活動

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2020年秋の大会

Computational Science and Engineering Division Session

International Framework for Utilization of Computer Codes and Databases and its Future Evolution

(1) Activity of the OECD NEA Data Bank

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1. Introduction [1]

The Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA) Data Bank offers a framework for collecting, testing, and distributing computer codes and exchanging nuclear data among its participating countries (NB: as of July 2020, the Data Bank has 27 participating countries). Since its foundation in 1978, it has provided services for over 40 years. The three main activities of the Data Bank are Computer Program Services (CPS), Nuclear Data Services (NDS) and Knowledge Preservation and Management (KPM) in the field of nuclear engineering in order to support, as well as collaborate with, other Standing Technical Committees of the NEA. This presentation focuses on the CPS which contributes to overall KPM as part of the international framework to share computer codes and databases.

2. Computer Program Services [1]

The Data Bank CPS maintains and updates a catalogue of over 1,500 computer codes, which code developers from the Data Bank participating countries have donated since the 1960s. Furthermore, thanks to arrangements with the International Atomic Energy Agency in Vienna and the Radiation Safety Information Computational Centre (RSICC) at Oak Ridge National Laboratory in the United States, CPS exchanges computer codes with non-OECD countries and with Canada and the United States (NB: the latter countries are not Data Bank participating countries). The CPS also helps fulfil the needs for information and knowledge preservation and management at the NEA. Indeed, the CPS preserves and controls the distribution of data taken by the joint projects of the NEA Division for Nuclear Safety Technology and Regulation and of integral experiments co-ordinated by the NEA Division for Nuclear Science. The CPS plays a role of “hub” for exchanging computer codes and experimental data in the nuclear community. In 2019, the CPS distributed approximately 1,000 code copies and 2,500 integral experimental data through 650 unique requests to end users.

The CPS also organises training courses on the most popular computer codes including MCNP® (Monte Carlo N-Particle Transport Code) and SCALE (A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design). This is an important activity of the Data Bank to support the community of users and authors of computer codes. In 2019, 11 training courses on six popular computer programs were organised, gathering over 150 participants.

3. Evolution of Computer Program Services [1,2]

Computational environment and infrastructure evolve continuously and dramatically. The intellectual property management and the export control measures have also significantly changed. To respond to these new demands and environment, the Data Bank has launched new initiatives in 2018, including: i) the revision of the licensing terms applying to the dispatched computer codes; ii) the re-organisation of the code catalogue categorisation; iii) the inclusion of open-sourced programs in its collection; and iv) the organisation of training courses away from NEA offices (located near Paris, France).

3-1. Revision of Licensing

For several decades, the CPS has distributed computer codes under the Single-Site Licence (SSL). It allows all staff members of an organisation (i.e. with the same affiliation and settled in the same geographic location) to share the same copy of an individual code. The CPS would dispatch only one copy of the code to a given establishment. It was an efficient and effective way of distributing codes when computers were a rare resource, as was the case when a centralised mainframe computer was being used by several people, as was the case in the 1970s. However, the current environment requires a more precise treatment of the end user information, and many newly developed computer codes require a "Single-User Licence." Following the decision of the Management Board for the Development, Application and Validation of Nuclear Data and Codes (MBDAV, the Data Bank Management Committee), the newly designed IT system for this Single-User Licence scheme is now ready to be deployed in 2020. It was decided to postpone the official launch of the new system until the restrictions due to the COVID-19 pandemic are lifted.

3-2. Re-organisation of code categorisation

The CPS has 25 categories of computer codes in its catalogue. This is an index for searching the computer codes and it has been set up during the 60 years of operation. However, it does not fit the needs of current computer codes users. Since 2018, the CPS has started re-organising the code categorisation, leading to a reduced number of categories (i.e. 12 instead of 25). This re-organisation aims to provide users with clearer guidelines for searching computer programs. The initial scope of work included 650 computer program packages which have been dispatched over the last 5 years (2014-2018). All these computer packages were reviewed and classified in accordance with the 12 new categories. The implementation of the new categorisation system will be done during the NEA website update project in 2020.

3-3. Treatment of Open-Source Programs

The use and development of open-source computer programs is now widely adopted in many research fields, including the nuclear science and technology sectors. Since 2019, the CPS has been developing a strategy for open-source codes. Some open-source codes are already included in its catalogue, and this trend is now more actively encouraged as seen with the inclusion in the CPS catalogue of FRENDY, a Nuclear Data Processing System for Evaluated Nuclear Data File (NEA-1907) developed in the Japan Atomic Energy Agency. To improve its services for open-source codes, the CPS is also working on its infrastructure to implement a platform to host a catalogue of open-source codes, which users could directly download.

3-4. Organisation of Training Courses outside of European Countries

Originally, the Data Bank training courses were organised at the NEA premises, in the Paris region. Because course participants must pay for their travel expenses, participants from neighbouring countries enjoyed a more affordable access to these events. To offer equal opportunities for all Data Bank participating countries and to provide code developers with frequent communication channels with the end users in many countries, the Data Bank has decided to organise training courses in Data Bank participating countries instead of Paris. In 2019, two training courses were organised outside of France: one on PENELOPE (the Code System for Monte-Carlo Simulation of Electron and Photon Transport) in Barcelona, Spain; and one on MCNP® in Bariloche, Argentina. The CPS also plans to organise a training course on MCNP in Japan in November 2020, provided that the covid-19 restrictions are lifted.

4. Conclusion

These examples show that the Data Bank and the CPS adapted their services in order to maximise the

benefit for the end users. In addition to these examples, the Data Bank and the CPS have also started organising “end-user meetings” to encourage and facilitate direct communication with end users of its services, with the aim to obtain feedback on its activities and to exchange opinions and ideas with its end users. This presentation is one of the end user meetings.

This presentation provides a summary of the Data Bank and CPS services and their evolution for providing better service to the end users. It emphasises the future of the computer code collection and dissemination, and explains the current status of our services. We will be pleased to answer your questions and welcome your feedback.

References

[1] Kenya Suyama, Franco Michel-Sendis, Alice Dufresne and Maria-Eleni Ragoussi, “Status of the Nuclear Energy Agency Data Bank – Services for Nuclear Data and Computer Programs,” Proceedings of the 2019 Symposium on Nuclear Data; November 28-30, 2019, Kyushu University, Chikushi Campus, Fukuoka, Japan.

[2] Alice DUFRESNE, “A new licensing scheme for the codes distributed by the NEA Data Bank Computer Program Services,” pp.16-18, Vol.37.2, Nuclear News (2020).

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International Framework for Utilization of Computer Codes and Databases and its Future Evolution

(2) Nuclear Data Activities of the IAEA Nuclear Data Section

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1. Introduction

The IAEA assists its Member States in using nuclear science and technology for peaceful purposes and facilitates the transfer of such technology and knowledge in a sustainable manner to Member States. The Nuclear Data Section (NDS) in the International Atomic Energy Agency (IAEA) is responsible for providing accurate and reliable nuclear data for nuclear energy and related application fields. The IAEA-NDS assembles, evaluates and recommends specific nuclear data, and also maintains nuclear structure, decay, and reaction databases, associated computer codes and infrastructures with collaborating actively with scientists from Member States. In this presentation, we describe recent activities in IAEA-NDS.

2. Nuclear Data/Database/Web Service

2-1. Medical Isotope Browser

The IAEA-NDS launch a new web application product, Medical Isotope Browser, for the prediction of medical isotope production yield of any diagnostic, therapeutic or theranostic isotope with accelerators. The Medical Isotope Browser gives a first guess to users who aim to find a new production route, an optimal incident energy, and so on. The isotope production yield can be calculated for any isotope production route for many targets, natural or enriched, reacting with incident protons, deuterons, tritons, helions or alpha particles. The Medical Isotope Browser can be reached via IAEA-NDS web site (https://nds.iaea.org/mib).

2-2. Experimental Nuclear Reaction Database

The experimental nuclear reaction data played crucial role in nuclear physics research and application development. The Experimental Nuclear Reaction Database (EXFOR database) is the publicly available large collection of experimental data which was established in 1967. Standardizing these experimental data formats promises to enable scientists to use for nuclear data evaluations, model predictions, or comparison of the experimental results across labs. The EXchange FORmat (EXFOR) is the exchange format for the transmission of data. These data have been compiled by a worldwide cooperation of 13 nuclear data centres, Nuclear Reaction Data Centres (NRDC) [1], under the auspices of the IAEA and been disseminated through the web-based user interface and an application programming interface [2]. The EXFOR database contains the nuclear reaction data of various nuclides with neutron-, proton-, photon-, and charged particles-induced reactions with low to high energies. The physical quantities are diverse, *e.g.* cross section, differential data with respect to angle, double differential cross section, resonance parameters, thick target yields, and fission observables such as fission product yields. The EXFOR database presently contains data from 23,577 experimental works.

2-3. Machine Learning Approaches to EXFOR Compilation Process

In order to reduce the amount of compilation work and to make it automated as possible in the future, IAEA-NDS took a first step to exemplify how advanced machine learning algorithms can be adopted to EXFOR data compilation process using open resources. The EXFOR compilation usually starts with identifying the relevant experimental work from publication web sites such as Physical Review C of American Physical Society

(https://journals.aps.org/prc/). The publication title is the principal information to identify a potential candidate of EXFOR relevant article. First, we tried a new approach to find potential EXFOR relevant articles with their titles only. Generally, such predictions rely on data mining, and the process of discovering patterns in large data sets using statistical methods is crucial. Fortunately, the EXFOR database contains all titles of original publications in their entries, so we put these titles as positive training examples by breaking the title into words. The algorithm generates the score based on the words constituting the titles of new publications.

3. Development of Nuclear Data

Nuclear data requirements are constantly monitored and identified through the International Nuclear Data Committee (INDC). A Coordinated Research Project (CRP) or Consultancy Meeting (CM) can be dedicated to the development and assembly of specific nuclear data files or database. Each CRP involves typically a period of 3-4 years with 5-15 scientists/groups from different countries working together to discuss the progress to deliver the products such as evaluated or recommended nuclear data library, decay data library, Reference Input Parameter Library (RIPL), and *etc*.

3-1. IAEA Photonuclear Data Library 2019

The first version of IAEA Evaluated Photonuclear Data Library was a product of a Coordinated Research Project (CRP) under the title "Compilation and Evaluation of Photonuclear Data for Applications" between 1996 and 1999 [3]. The new CRP was endorsed by the INDC meeting in 2014 and was initiated by the IAEA under the title "Updating the Photonuclear Data Library" [4]. All the 164 isotopes in the previous library were revised and re-evaluated and new evaluations were performed for another 37 isotopes for which experimental data are available, as well as for the 9 isotopes identified as relevant for medical applications. In IAEA Photonuclear data library 2019 (IAEA/PD-2019), 219 isotopes in total were evaluated and energies were extended up to 200 MeV [5]. Information is available on (https://nds.iaea.org/photonuclear/) and ENDF-6 format library data files can be retrieve from Github repository (https://github.com/IAEA-NDS/IAEA-PD2019).

3-2. New CRP on Fission Product Yield

Fission product yields (FPY) are important for both basic nuclear sciences and application fields. In basic sciences, FPY give fundamental aspects of the probability of fragment formation and therefore play an important role in our understanding of the nuclear fission process. FPY are also directly related to the understanding of the abundances of elements through the nucleosynthesis. In reactor design and operation, FPY are used in criticality and reactivity calculations performed for fuel and reactor core management, for reactor safety and for determining the limits of safe operation in new plants and for materials transport. The IAEA-NDS intends to start a new CRP on “Fission Yields of Actinides” in 2020. The experimental data are always been the foundation of the FPY data evaluations, where a complete set of the experimental FPY data are important as a common basis of new evaluation. Due to some reasons, many experimental FPY data have known to be missing in EXFOR. One of the reasons is because some FPY measurements have been classified and unclassified in recent years. Therefore, we conducted the completeness assessment of FPY data in EXFOR by comparison with the dataset used for ENDF-B/VI [6] and UKFY3.0 [7] evaluations. It was found that approximately 194 references are relevant to new compilation of EXFOR entry, and about 54 references must be checked with the existing EXFOR entries to ensure that the all experimental FPY data are properly compiled.

4. Conclusion

This presentation provides a summary of selected recent activities of IAEA-NDS. The IAEA-NDS assembles, develops, evaluates and recommends nuclear data, and maintains and disseminates the data libraries and

databases. The IAEA-NDS launch Medical Isotope Browser which calculates and visualizes isotope production yield. The IAEA-NDS has maintained EXFOR database with Nuclear Reaction Data Centres (NRDC) under the auspices of the IAEA. The IAEA-NDS took a first step to test the machine learning algorithms using EXFOR data as the feasibility study. The IAEA Photonuclear Data Library 2019 has been released as a result of CRP. New CRP on fission product yield will be launch in 2020.

References

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