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Compilation of Nuclear Data Experiments for Radiation Characterization

Summary Report of a Technical Meeting

IAEA Headquarters, Vienna, Austria

10 – 14 October 2022

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March 2023

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Objectives

The purpose of the event is to transfer into technology the experimental integral radiation information to be used as part of the validation and verification processes of nuclear model and simulation code systems, to provide various schemas to perform validation and verification, and to deploy the numerical data streams to users through open application programming interface. <https://conferences.iaea.org/event/302/>

The meeting brings together the different savant societies and experts able to determine and support the necessary enhancements, processes and schemas, foreseen for the multiple energy, non-energy, earth and life sciences applications of data, and to support high-fidelity open-source Multiphysics simulation efforts.

Seventeen experts, from eight member states countries attended the meeting in person, with two participating online. The average age of the expert panel was forty-three.

Applications

Verification and Validation activities, processes on nuclear model and simulation codes deployed in support of nuclear energies: fission, fusion, accelerator alike. Those are established research and development fields were basic physical sciences data streams and practical engineering solutions need to work in unison to simulate often complex physical processes in specific nuclear environment and to compare their simulation results to observables. Long-standing reputation and a broad users' base are usually linked to extensive, wide-ranging verification and validation suites.

It was noted that synergies exists between parts of the IAEA driven CoNDERC project <https://www-nds.iaea.org/conderc/> and the OECD/NEA Sinbad project https://www.oecd-nea.org/jcms/pl_32139/sinbad-shielding-integral-benchmark-archive-and-database. Some of the underlying blocs, mainly the open access computational parts are similar in nature and usage. Those blocs refer in majority to reference simulation code input decks, numerical experimental information, and numerical outputs. In addition, open-source post processing tools (shell, python scripts, Jupiter notebook etc.) may be present. Both Project's contributor/developer and user communities have a strong interest, are benefitting from harmonising, co-ordinating those blocs.

Introduction

Fusion

Recently, a combined effort between NIER Ingegneria, University di Bologna and Fusion for Energy, private and public sectors, led to the development of JADE [\[1\]](#), a python-based open-source software for the Verification and Validation of nuclear data libraries. Nuclear data is fundamental for particle and radiation transport simulations which, in turn, are responsible for the evaluation of key quantities for fusion-related device design such as nuclear heating, displacement per atom, particles production and dose rates. The aim for the project is to offer standardization and automation to the V&V process of code schema and libraries to speed up their release cycles and, at the same time, improve the quality of the simulation. JADE takes advantage of MCNP6® [\[2\]](#) for the particles and radiation transport simulations and, even if it is potentially applicable to the whole nuclear industry, a particular focus on fusion applications and metrics is obtained through the selections of the relevant benchmarks that have been implemented.

- Motivation of JADE is to provide an automated and standardised methodology for nuclear data V&V. It is accessible, tested with pytest and driven from the command line.
- In addition to the experimental data on CoNDERC/SINBAD for C/E, the JADE team would also like to implement computational databases C/C to complement the V&V landscape.

Neutronics informs key engineering and design plant conceptual decisions, including shielding specifications, safe operating procedures, and dose limits. Neutronics workflows are typically validated by simulating selected prototypic experiments from which experimental data has been collected. This allows for the calculation of uncertainty estimates due to systematic and stochastic errors. Characterization of these uncertainties allows for evaluation of their relative importance to key modelling output and gives insight to engineers on design margins and trade-offs. Currently there are insufficient benchmarks in the Shielding Integral Benchmark Archive and Database (SINBAD) to comprehensively cover all aspects of neutronics in fusion devices. Moreover, some evaluations are lacking in detail. Several crucial areas of interest have been identified by both public and private enterprises who are in the process of designing fusion pilot plants.

- A two-fold campaign of benchmark experiments is proposed: first a series of computation benchmark experiments which would focus on the validation of neutronics workflows used to determine quantities of interests: coolant activation, analysis of very large models, sky-shine effect, variance reduction techniques, homogenization effects and shutdown dose rate calculations. Second a set of new experimental benchmark designs driven by the needs identified by the computational benchmarks
- Oak Ridge National Laboratory is planning to develop a fusion neutronics handbook to support US commercial fusion, welcome inputs and collaborations from the community

The FNS Duct experiment is a neutron streaming experiment performed in the JAERI Fusion Neutronics Source facility. It aims at studying the transport of neutrons in a complex labyrinth. A deuterium beam hits a titanium hydride target (enriched in tritium) and produces 14 MeV neutrons. A stainless-steel block with a dogleg inside is in front of the neutron source and suitable detectors measure activation rates and neutron flux spectra in the dogleg or behind the steel block. These

dogleg configurations are typical of ITER diagnostic configurations. Monte Carlo TRIPOLI-4® [3] simulation results are compared with experimental information using both FENDL-2.1 and FENDL-3.1d nuclear data libraries.

- Significant issues are encountered due to the size of the neutron source definition files for both TRIPOLI-4 and MCNP. Source definition from DT reaction is not available in all codes, and thus tabulated neutron angular and energy distribution are required.
- Variance Reduction technical are critical to such type of simulation.
- Special mention of the t4_geom_convert code which provides a conversion from MCNP inputs to TRIPOLI, now available in CoNDERC

Case study for neutron flux calculations in the EU fusion DEMO divertor region in the case of the Helium Cooled Pebble Bed (HCPB) concept used as a breeding blanket (BB) was made. MCNP6 simulations were performed supported by and ADVANTG (Automated VARIance reduction Generator) with FW-CADIS variance reduction parameters tool for the variance reduction implementation. Varying the nuclear data libraries from FENDL-2.1 to FENDL-3.1b lead to differences in total fluxes of up to +/- 25%.

- Notable C/C differences persist in fusion neutronics; stochastic, VR and/or data driven remain to be solved.

Work to create a fusion-relevant nuclear data benchmark suite based on a series of experimental campaigns performed at the ASP DT accelerator in the UK has begun. The experiments involved the irradiation of thin foils samples in a near mono-energetic 14 MeV neutron source. High-resolution gamma spectroscopy was then performed with time evolution to produce activity decay curves for each gamma signal (corresponding to different nuclear reactions) produced. To date, the analysis has only looked a few of the several 100 experiments performed in those campaigns, which could become a useful, scriptable, and rapid test suite for many key reactions that produce short-term gamma activation in materials. Key status of benchmark development:

- Description of the data acquired 2011-2015 using ASP 14 MeV DT accelerator – typical fluxes 10^9 n/cm²/s, range of irradiation times (up to 1 hour) and gamma spectrometry measurement times (up to 1 day). The full database contains ~330 experiments.
- Analysis of data acquired for W and Mo has been performed as a prototype to roll-out to the remainder of the dataset.

Fission

Several benchmark compilations have been developed in recent years that are utilized by nuclear data testers worldwide. These include Handbooks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [4], and the International Reactor Physics Evaluation Project (IRPhEP) [5], as well as the Shielding Integral Benchmark Archive Database (SINBAD) and the Spent Fuel Isotopic Composition Database (SFCOMPO) [6]. Preceding these was the Cross Section Evaluation Working Group's (CSEWG) Benchmark Book. First issued in the 1970s with updates in the

1980s and 1990s, it contains separate chapters for Fast and Thermal critical systems, the Coupled Fast Reactor Measurement Facility (CFRMF) Dosimetry Benchmark as well as a variety of Shielding Benchmarks. Beyond that there have been thousands of critical experiments performed over the decades, yielding a wealth of data unevenly suitable for cross section data testing. Some benchmark's experimental uncertainty is in the 500 pcm and above range. A review can be made of several long-standing approximations that exist in current Monte Carlo benchmark models. These approximations date from when the typical stochastic uncertainty in a Monte Carlo's k_{calc} calculation was several hundred pcm, as opposed to modern calculations that often produce single digit stochastic uncertainties. With the recent release of a new Japanese Evaluated Nuclear Data Library, JENDL-5 [7], as well as on-going nuclear data testing to support future nuclear data file releases (e.g., JEFF-4 and ENDF/B-VIII.1) now is an opportune time to review the applicability of these approximations and set of useful benchmarks.

- Other approximations: material, geometry (e.g. extruded 2D versus real 3D)
- Processing: emitted particle angular/spectral distribution forms, fixed energy grid for Thermal Scattering Law

With escalating costs of nuclear experiments, there has been a growing reliance on Monte Carlo simulations for the design of advanced reactors and the “validation” of high-fidelity deterministic transport codes, but validation is also needed for Monte Carlo codes. The current integral experimental database is composed of many simple critical experiments and small research reactors, but often lack the complexity and pitfalls of real nuclear systems. The BEAVRS benchmark was developed as a realistic test of high-fidelity methods and challenge some of the limitations of both the methods and benchmark. The benchmark has been used by many groups to test both deterministic and stochastic codes with great success, but the results also highlight some of the limitations of the benchmark from the difficulties in modelling the geometric complexity of a relatively “simple” reactor design to the limitations of the measurement acquisition systems. Additionally, while the design is meant to be symmetric, a large tilt is observed in the core detector measurements which is unexplained from the core description. Without accounting for this tilt through post-processing of the results, the comparison with high-fidelity codes is quite poor and the addition of corrections increases the uncertainties of the measurements.

The benchmark and the results gathered from the literature also present another interesting conclusion in that deterministic codes provide just as good results as the Monte Carlo results. While this is not entirely surprising since no-one publishes bad results, it also highlights the fidelity of multigroup self-shielding methods and the limitations of Monte Carlo codes in getting statistically significant results in many small regions and convergence issues on such large systems.

Recent validation effort for the energy domain has been made, analytical benchmark developed where the flux is resolved analytically in energy. Those benchmark definition relies on the pole representation of nuclear data and provides an analytical expression for the scalar flux. Additionally, the benchmark can be extended to also compute the adjoint flux, thus allowing for the validation of uncertainty quantification methods.

- Batch sizes are typically too small for real reactor calculations (35 million pellets in BEAVRS!)
- There is a lack of clean, reliable operating data, often because of proprietary issues.

- It is important to properly model the thermal expansion, particularly with respect to coolant flow and the fuel rod expansion, when calculations are performed at real operation temperature and power. These effects are not uniform in an operating plant with hundreds of assemblies (thousands of rods) but are necessarily symmetric in a current computer model. In practice the rod may wiggle within a grid plate unit cell; a feature that can only be approximated in a random fashion within the computer model and simulation processes.

An overview of the development and applications of Serpent [8] at VTT Technical Research Centre of Finland Ltd focusing on the nuclear and atomic data needs of Serpent as well as the validation of Serpent at VTT was given. Serpent transports neutrons and photons in a decoupled or coupled manner starting from a criticality source, a fixed source or a radioactive decay source. Serpent is often used for fuel burnup calculations.

Neutron interaction modelling in Serpent is based on ACE format data, with some application specific data either appended to the end of normal ACE-files (such as additional nonlocal/local energy deposition data) or read directly from ENDF files (dec, nfy, sfy data and energy dependent branching ratios). Photoatomic interactions are modelled based on data that is not as cohesively collected as the neutron interaction data is: At the moment ACE-format photoatomic cross sections are complemented with additional data from auxiliary files.

Neutron interaction data processing at VTT is conducted with NJOY2016. Serpent contains an automated stochastic testing routine for ACE libraries, based on reaction, energy and angular sampling for neutrons in randomly generated materials. This routine is utilized at VTT to identify inconsistencies in newly generated libraries. Serpent also executes several checks to the nuclide data included in a calculation to identify inconsistencies in the data such as stable nuclides with decay channels and issues a warning to the user.

The validation of Serpent at VTT has been application and target specific. The largest amount of preparation has gone to the criticality safety validation package, which contains several hundred Serpent inputs for critical experiments from the LEU-COMP-THERM section of the ICSBEP handbook. Intended for criticality safety validation of Serpent for wet storage geometries, this effort is mainly intended for determining the Upper Safety Limit for the k_{eff} for a specific application. A smaller amount of effort has been put to using SINBAD experiments for the validation of the photon transport in Serpent and to using SFCOMPO data for the validation of Serpent's burnup capabilities.

- Chebyshev Rational Approximation Method (CRAM) method is used for depletion calculations within Serpent, utilising 1-group reaction rates collapsed from pointwise ACE files and combined with fission yields and decay data.
- Having reached full maturity in the fission application the Serpent developers are gearing themselves to answer radiation shielding, characterisation, fusion applications

The OpenMC [9] community has relied extensively on benchmark models from the ICSBEP handbook for both cross-code comparisons and comparison to experiment. To date, about 400 different benchmark models from ICSBEP have been created with OpenMC. Along with this, a set of Python tools has been developed for automating the execution and analysis of benchmark simulations.

Separately, tools have been developed for cross-code comparison of simple broomstick and spherical shell models that have been invaluable for neutron and photon physics validation.

Recently, a set of OpenMC models based on ICSBEP benchmarks has been created for inclusion in the CoNDERC repository, taking advantage of the unique capabilities in OpenMC. These benchmarks go beyond simple evaluation of K_{eff} and include reaction rate tallies, spatial flux profiles, and other physical measures. These additions to CoNDERC lay the groundwork for future additions of OpenMC models focused on other areas (e.g., SINBAD benchmarks for shielding/fusion applications).

Two pathways for converting MCNP models to OpenMC models currently exist: the `csg2csg` converter, developed by Andy Davis and a more recent project called `openmc_mcnr_adapter`. These capabilities provide another useful resource for performing cross-code comparison.

- Different ways to define the same thing make code-to-code comparisons tricky
- Precision and accuracy are two different things
- Common Exchange Format for more consistent sharing of input files

The PATMOS app [\[10\]](#) is a prototype of a massively parallel Monte Carlo particle transport code, developed at CEA in order to conceive alternative algorithms for novel HPC architectures, in view of the forthcoming TRIPOLI-5[®] production code. Recently, the sampling laws for modeling neutron physics as provided in nuclear data libraries have been implemented into PATMOS, first within the so-called “free-gas” model and then by adding thermal neutron scattering treatments in order to include crystal or molecular bound-effects.

As a first step towards the validation and verification of this implementation, code-to-code comparisons have been performed between PATMOS and two other reference Monte Carlo transport codes, TRIPOLI-4[®] and OpenMC, over around 560 isotopes taken from the JEFF-3.3 nuclear data library. First, the energy or angle distributions have been compared between the three codes for each isotope and reaction, at various incident energies, by resorting to Kolmogorov-Smirnov statistical tests, thanks to dedicated sampling routines. Then, the evaluation of the microscopic cross sections (as well as the multiplicity) by each code has been verified, in order to detect possible discrepancies. Finally, more than 5000 configurations have been tested for a simple benchmark consisting in a sphere filled with a single isotope, irradiated by a single-energy and isotropic source located at the center of the sphere (ten representative incident energies have been considered). The results of the metric quantity (flux per unit of lethargy) obtained with PATMOS and with the other reference Monte Carlo codes have then been compared by using the Holm-Bonferroni statistical test.

The comparison between PATMOS and TRIPOLI-4[®] was found to be more involved because of the post-processing of nuclear data; indeed, TRIPOLI-4[®] relies on ENDF files, while PATMOS relies on ACE files, which leads to discrepancies in underlying nuclear data “seen” by the different codes. This work has allowed to:

- Validate the implementation of the free-gas model and of the thermal scattering laws in PATMOS, thanks to the perfect statistical agreement between PATMOS and OpenMC
- Highlight some inconsistencies in nuclear data interpretations
- Detect some implementation errors in the sampling routines

- Conclude that library evaluators need to incorporate more ‘basic’ consistency check, the actual tools are not potent enough nor actively maintained.

A work that follows MCNP - TRIPOLI-4 comparisons for criticality benchmarks using U5, U8, Pu9, for which comparisons were made between ENDF/B-VIII, JEFF-3.3, TENDL-17, TENDL-19 libraries, studying shielding benchmarks shows differences between the libraries results for different nuclei and indicates the importance of the scattering anisotropy. Three points that highlight differences in processing and simulation between NJOY/MCNP and GALILEE/TRIPOLI-4 have been addressed:

- The first one concerns the probability tables in URR. The competitive width allows the calculation of probability tables for inelastic scattering, for example in the case of U238. GALILEE/TRIPOLI-4 has the capability to compute this cross section as resonant or not. The difference is about 60 pcm in the case of the IMF-007-TZH configuration and helps explain the differences between MCNP and TRIPOLI-4 results.
- A second point address the reconstruction of TSL. GALILEE can refine the energy grid proposed by the user. This makes it possible to obtain a more precise incoherent inelastic cross section when needed.
- A third point concerns the use of photonuclear data. Slight modifications are necessary on the thresholds in the laboratory frame for a set of reactions/nuclei in evaluated files. Some threshold reactions start with non-zero cross sections, which leads to discrepancies between the total cross section and the sum of the partial cross sections.

The Nuclear Criticality Safety Division at Lawrence Livermore National Laboratory is developing an extended suite of validation benchmarks for its Monte Carlo code COG [11]. The benchmarks serve to validate nuclear data and to support COG's software quality assurance framework. The current database has 3,395 criticality benchmarks. However, particular focus has been given to including benchmarks that are not criticality experiments. These experiments include β_{eff} , shielding, photoneutron, spectral indices, neutron spectra, subcritical assemblies, Godiva thermo-mechanical behavior after a pulse, time of flight spectra, pulsed neutron die-away in moderators, and pulsed sphere experiments. Many of these benchmarks are reproductions of historical experiments, but some are new experiments that have been conducted at Lawrence Livermore National Laboratory and submitted to international benchmark databases. The benchmarks under investigation and results on the simulation bias with different computational methods and nuclear data libraries were presented. Three new beta-eff estimators are available in one run as prompt and delayed neutrons and gammas are treated as separate particles. SINAD benchmarks were expanded beyond OKTAVIAN.

Pulsed-Neutron Die-A (PNDA) experiments can be useful benchmarks to validate neutron Thermal Scattering Laws (TSLs). The experiment uses a neutron generator to impinge a short ($\sim 10^{-4}$ s), mono-energetic neutron pulse on a target sample. After the pulse, the neutron population within the sample moderates and reaches thermal equilibrium with a fundamental spatial mode and characteristic decay-time eigenvalue. The eigenvalue can be extracted from the experimental measurements of the neutron flux and used as an integral parameter in validation. For certain materials and geometric configurations, the eigenvalue is heavily influenced by thermal neutron scattering of only the target material. For that reason, a PNDA experiment can have a higher sensitivity to TSLs than is commonly available in critical experiments. Herein, we present results for a series of new PNDA experiments conducted at Lawrence Livermore National Laboratory with plastic

materials (high-density polyethylene and Lucite) and for light water. Experimental integral parameters were compared to simulated results and report trends in the biases.

- Novel benchmark types are foreseen for submission to ICSBEP
- Issue, lacune (i.e., missing data block) in nuclear data library need to be recorded and shared.

The determination of decay heat (DH) is a major safety issue for a reactor in operation but also for the transport of burnt fuel and nuclear waste management. The calculation of decay heat through the summation method relies on the combination of reactor simulations to estimate the fuel inventory and on nuclear data: decay properties of the fission products and actinides, fission yields and cross sections. Some fission products in the decay data libraries have decay schemes which are biased by the Pandemonium effect. The Pandemonium effect arises from the low efficiency at high energy of Germanium detectors. This effect has direct consequences on decay heat calculation with an overestimation of the β - contribution and an under-estimation of the γ contribution. To overcome this effect, the Total Absorption Gamma Spectroscopy (TAGS), based on the full detection of the deexcitation gamma cascade for each populated level is used. The impact of these new decay data measurements performed with the TAGS technique on decay heat calculations is important. The needs of extra DH pulse experiments were underlined but also some extra work on the identification of extra Pandemonium nuclei in the cooling range where the simulations underestimate the experimental data is needed.

- Include in CONDERC some decay heat experiments performed at CARIBU@LLNL
- Include in CONDERC the decay heat results of the MERCI experiment performed at OSIRIS@CEA
- Correct the DH pulse data for the capture effect: case of ^{237}Np

A Python package for radioactive decay calculations from the independent yields, $Y_i(Z,A,M)$, has been developed by keeping track of the inventory including isomeric states. It supports decay chains of radioactive nuclides, metastable states, and branching decays. By default, it reads ENDF-6 formatted decay data and converts it into simple text or JSON forms, and then create a decay chain from a particular fission product. The code solves the Bateman equation analytically. To undergo from $Y_i(Z,A,M)$ to the cumulative yields, $Y_c(Z,A,M)$, a time-independent calculation is performed. The package outputs are $Y_c(Z,A,M)$, decay heats from gamma and beta ray components, and delayed neutron yield. The code includes a plot method for showing decay chain diagrams. A web tools for the nuclear data visualizations, which is mostly for the cross sections, now also includes [fission product yields](#).

- it ensures consistencies among fission observables; it is important to calculate from the fission fragment to beta decay in one flow.
- it facilitate/modernize the access to the IAEA NDS livechart

Recommendations

A lack of coordination, harmonizing of validation suites exists, mostly due to the requirement of every independent national actor to develop extensive suite of validations benchmarks specific for their own, often then proprietary, simulation tools and needs. International cooperation on the development of validation suites starts to develop but is not yet as mature as the international cooperation related to the evaluation of the benchmark experiments themselves. The suites being developed serve to validate the data and simulation processes to support the specific software tool quality and assurance frameworks. Comparing different tools, using the benchmark suites, serves to assure the quality of the simulation process results in comparison to an observable reality. In CoNDERC particular focus is given to open access beyond legacy criticality experiments including but not limited to shielding, decay heat, photonics, spectral indices, neutron spectra, pulsed experiments and more, for which the benchmark experiments cover a broader set of metrics, timescales, physics but also geographical and experimental origins. Although publication networks improved those experiments' accessibility, significant efforts are always needed to properly mock-up, simulate and report them with any tools. Bias will exist toward specific needs prioritizing the suite QA. Knowledge, collection, classification, coordination and to ensure the continuation and accessibility of the numeric forms attached to any experiments is now a day paramount but require common effort. Essential for the reliability of the resulting data collections will be reliable quality assurance processes and version control.

Both the IAEA CoNDERC and OECD/NEA Sinbad projects rely on Git based version control with associated web services for cooperative development of the databases (GitLab, GitHub). A solution would need to be put in place for them to harmoniously benefit from one another. An important goal for both projects are the implementation of Continuous Integration/Continuous Delivery (CI/CD) workflows. The web service tools can also be used for recording and tracking user feedbacks.

Recent studies clearly demonstrate that large areas of the nuclear data landscapes are uncharted, too often relying on previous simulation results as if they had undergone V&V processes simply because they exist (agreement across a family of simulations with different tools does not guarantee correctness without validation against experimental reality). Advanced concepts, novel experiments relying on less known, curated, verified data streams and processes, are particularly sensitive to such lack of homogeneity and reliability. Recommendation is made to frame the V&V domains of the benchmarking activities adequately and honestly in terms of particles, energy ranges and result metrics. Room temperature fission reactors criticality benchmarking ICSBEP C/E results (< 2 MeV) when a single structural material is used as reflector says little to nothing to our ability to V&V neutron slowing down in the same structural material from the fusion source range (< 14 MeV) at operating reactor temperature. Primary heating has little to do with decay heating although both may occur simultaneously during operation.

Different styles of benchmark experiments and simulation processes are needed to validate our ability to properly simulate particle transport and interaction with matters for all multidisciplinary R&D activities that need them. Most are complementary to one another in many aspects, allowing us to better characterize source terms, processes, and observables. Diversity, independence,

openness, availability, and the ability to cross compare are important aspects of the V&V cycles across nations.

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