WPEC sub-group proposal

Title

Reproducibility in Nuclear Data Evaluation

Justification for a Subgroup

Based on the experience acquired during the production of the main world nuclear libraries, a large part of the process involved in evaluations has not been recorded in a way that can be reasonably retrieved (e.g. selection of experimental data, adjustment factors, considered models and parameters, particular versions of codes). As a consequence, without the experts and tools that produced a given evaluation, it may be impractical or infeasible to reproduce the work. The number of nuclear data experts worldwide is generally decreasing, also representing a serious challenge for the maintenance of capacity to perform new and sound nuclear data evaluations. It is of crucial interest for the nuclear data community to take advantages of the advancement of computer hardware and software technologies, for instance, the opportunity to rigorously version control and automatically verify some, most or all aspects of nuclear data evaluation process. These may then be saved as the reference information behind the evaluations so that the evaluation is transparent and reproducible. It will also greatly assist future evaluation activities which may build upon the previous progress made by evaluators.

Subgroup Monitors

David Brown (BNL, USA) - ENDF
Arjan Koning (IAEA) - TENDL
Osamu Iwamoto (JAEA, Japan) - JENDL

Subgroup Coordinators

Dimitri Rochman (PSI, Switzerland) - JEFF
Michal Herman (LANL, USA) - ENDF

Subgroup Participants[1]

Ian Thompson (LLNL, USA) - ENDF
Marco Pigni (ORNL, USA) - ENDF
Roberto Capote (IAEA)
Andrej Trkov (IAEA)
Toshihiko Kawano (LANL, USA) - ENDF

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[1] Tentative list based on confirmed interest in advance of the WPEC-31 meeting

Cyrille de Saint Jean (CEA, France) - JEFF

Definition of the project and proposed activities

This subgroup is proposing to bring together experts to develop repositories to contain all of the required information that is used to produce a nuclear data evaluation, including codes and their inputs, experimental data sets and scripts or codes used to alter model calculation results and ultimately assemble formatted nuclear data files. These will be stored in version controlled systems and integrated with a continuous integration framework to verify the contents of the repositories. The contents of an evaluation for a given isotope will then be completely tracible and may be referenced in evaluated files.

Relevance to Evaluated Data Files

This subgroup will create recommendations and prototypes for the implementation of a system to store evaluation information and design a platform for reproducible, collaborative evaluation. The recommendations will be re-enforced in the various nuclear data projects, therefore creating links and common best practices between them. These repositories and the systems that interact with them (e.g. continuous integration frameworks) will be available to all participants enabling them to develop similar regional projects and/or utilise the system for international collaborative projects. Such improvements will answer existing and future expectations from nuclear data users, concerning the traceability of the nuclear data evaluation process, library production and validation.

Time-Schedule and Deliverables:

- Establish repositories in the NEA GitLab to support model codes and their inputs, using continuous integration systems and containerisation to demonstrate automatic and reproducible execution of calculations
- Develop repositories to contain input files and datasets that interact with code containers to allow version controlled model calculation results
- Develop repositories to support post-model-calculation modification of outputs and generate nuclear data files as outputs
- Report on the systems developed, lessons learned and recommendations for future version controlled and reproducible evaluation systems used by evaluation projects