WPEC Subgroup Proposal

Title

CIELO: Computational methods for integration of integral and differential nuclear data insights & covariance advances, for improved international evaluated cross section databases

Justification for a Subgroup

The CIELO pilot project, WPEC subgroup 40, was recently completed. It represented a large international nuclear science community effort, and led to 2 main evaluation options (in ENDF and JEFF), with advances in JENDL too, for evaluated cross sections and covariances on isotopes of H, O, Fe, U, Pu. Major peer reviewed publications on this work were released in a 2018 Nuclear Data Sheets issue. The products created already represent major advances in our understanding, and provide substantially-improved capabilities for our users.

The leaders of CIELO have discussed best mechanisms to continue the progress on CIELO, with leaders from the NEA and the IAEA. The conclusion is that an international collaboration on the continued improvement of the underlying cross sections and covariances will be coordinated by the IAEA (the INDEN project); while integral performance of criticality and transport, data sensitivity studies, and covariance impact on integral criticality assessments, will be coordinated by a NEA WPEC subgroup. This latter effort is the focus of this new WPEC proposal.

Despite the advances made for CIELO, the previous subgroup 40 collaboration identified a variety of gaps and deficiencies that need further attention. The following topics will be the focus of the next WPEC subgroup:

- **Use of modern computational tools**
- **Machine learning (ML) techniques**
- **Use of fundamental data**
- **Use of integral information**
- **Use of neutron transmission data**
- **Covariances and calibration**
- **Feedback to HPRL**
- **Processes for continuous improvement**

This set of topics for WPEC CIELO focus would be advanced in concert with close collaboration with the future IAEA/INDEN coordinated CIELO collaboration. Feedback on the performance of the CIELO evaluations - both those existing today and those that get produced by the IAEA collaboration- will be fed back to the IAEA international INDEN evaluators.

The value of having a new WPEC subgroup that is separate to the important new work in Subgroups 44, 45, 46, 47 is that this subgroup will focus on the integration of all these advances to improve the CIELO product. Thus, as well as exploring CIELO-related issues, and new computational method opportunities including machine learning, it will closely coordinate with Subgroups 44, 45, 46, 47.

Subgroup Monitor

TBD: possibilities include Plompen, Bauge, Cabellos

Subgroup Coordinator

M.B. Chadwick, Co-leader TBD (possibilities include Talou, Herman, others)

Subgroup Participants

Draft proposal – the data projects will identify appropriate participants from their respective communities.

Project Definition and Proposed Activities

This WPEC subgroup proposal is a continuation of the CIELO project. The anticipated end-product after 3 years will be: (a) development of new evaluation methods, including machine-learning approaches, that addresses how best to integrate differential and integral data, with covariances, into a suite of evaluated data files that jointly perform well; (b) integration of insights from Subgroups 44 (covariances), 45 (validation), 46 (efficient & effective use of integral experiments), and 47-planned (shielding) to advance the CIELO product; and (c) improved and refined CIELO cross section evaluation options (informed by the IAEA/INDEN project) that can be considered as input to the major evaluation efforts (ENDF, JEFF, JENDL, CENDL, etc.) of the future. The following topics will be the focus of the next WPEC subgroup:

- **Computational tools**. These will be advanced for CIELO library applications involving covariance/uncertainty quantification (UQ), sensitivity studies, and optimization methods. These will build upon tools developed by the NEA, IAEA, INL, LANL, LLNL, BNL, ORNL, CEA, JAEA and other labs. These tools will help expedite the identification of best nuclear data solutions - in a complex multidimensional space - that optimally represent fundamental data, integral measurements, and insights from theory. We will explore new machine learning methods that are being developed at many laboratories (a growth area at LANL) and universities, as described next.
- **Machine learning (ML).** This requires identifying a large enough suite of benchmarks specifically sensitive to the CIELO isotopes and reactions; developing the metadata

infrastructure needed to apply ML algorithms; using the sensitivity tools already mentioned; and applying some ML techniques already well-established such as decision trees and adaptive boosting.

- **Fundamental data.** CIELO will continue to endeavor to use the best information coming from fundamental cross section experiments and assessments from the Standards group. As the Standards are updated - for example to use new fission cross section data becoming available - the CIELO databases will be updated.
- **Integral information**. Integral criticality studies using CIELO files, with sensitivity and criticality computational tools (NDaST, MCNP/WHISPER, SENSMG *etc*), will help us understand the impact of uncertainties, and sensitivities, of different reaction channels. This analysis will benefit from close collaboration with Subgroup 46 and will help prioritize future work that is needed. Subgroup 46 will also provide valuable feedback from the user community.
- **Neutron transmission.** Neutron transmission and gamma-ray production integral data will be studied, versus simulations of mean values and uncertainties, to identify deficiencies in the current CIELO files, and point to future work that is needed. This will be supported by an evolving WPEC focus (Subgroup 47-planned) in neutron transmission/shielding benchmarks.
- **Covariances.** Covariances in CIELO for various channels often differ significantly by different subject matter experts (ENDF and JEFF), that need to be understood and resolved. Sometimes the covariances differ by factors of as much as 5-10. This was documented in the recent NDS2018 CIELO paper. We also need to better understand covariance correlations (between low-energy and higher energy parts of the library; between fission phenomena described by a consistent fission theory; and through use of integral data). This represents an area of study that will involve both the NEA (Subgroup 44) and IAEA collaborations; integration of advances made here will improve the CIELO product, our goal being the development of more reasonable/credible covariances.
- **Covariances and calibration**. It is understood that forward-propagation of CIELO covariances (uncertainties) leads to integral criticality uncertainties much larger than observed in the integral k values. This is because the mean values of CIELO data were tuned, or calibrated to the integral criticality results. This topic will be further investigated to define future methodologies, taking advantage of insights from Subgroup 44. Furthermore, benchmarks used in a calibration process should be explicitly known by users, for avoiding duplication when adjustment processes are used.
- **HPRL.** Feedback will be given on future priority experiments to the High Priority Request List (HPRL) WPEC coordinator.
- **Continuous improvement.** CIELO collaborators will survey feedback from the previous WPEC CIELO Pilot project, together with feedback from the user community, and develop and document ways in which the evaluation process can be improved within the context of technical rigor, thoroughness in documentation, robustness, and timeliness.

Relevance to Evaluated Data Files

This will be a continuation of the high-impact work of the CIELO project, which has resulted, and is expected to result in, the production of the evaluated nuclear data files for essential isotopes.

Time Schedule and Deliverables

It is anticipated that the experts of this SG should complete and document the activities (mandate) listed above within 3 years.

Date Deliverables

May-June 2018: TBD

May-June 2019: TBD

May-June 2020: TBD