5-10 Years Cross-cutting Priorities on the Topic of Nuclear Data Covariances and Uncertainty Quantification for Users

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The Nuclear Data Uncertainty Quantification Working Meeting Advisory Panel

The members of the advisory panel of the "Nuclear Data Uncertainty Quantification Working Meeting" (NDUQWM) are listed. The listed individuals provided presentations about the nuclear data uncertainty needs of their institutions or for their subject area, took part in discussions, and drafted this document.

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Short Summary

A cross-cutting area of nuclear data user needs is that for nuclear data covariances and uncertainty quantification. These needs were identified at the virtual Nuclear Data Uncertainty Quantification Working Meeting (NDUQWM) from Oct. 11 to 13, 2022 by a group of thirty invited participants representing:

- Nuclear data producers: spanning from differential experiments, nuclear theory, evaluation, processing, validation, integral experiments,
- Nuclear data users: covering astrophysics, antineutrino physics, forensics, nuclear criticality safety, isotope production, neutron dosimetry, nuclear medicine, global security, reactor design, reactor operations and safety, safeguards, space applications, spent fuel inventory, stockpile stewardship, etc.

The Department of Energy (DOE) Office of Science asked that NDUQWM be convened because of the need for improved uncertainty quantification across many programs. In addition to the DOE Office of Science's advocacy for this meeting, ten other program managers were present for the first day to see the high-level needs presented by the participants in their advisory role.

The **goal** of this meeting was to draft a **whitepaper on prioritized nuclear data covariance and uncertainty quantification needs impacting users for the next 5 to 10 years**. These needs are described herein in an actionable context (i.e., a high-level plan is given to address them), and are feasible for the community to tackle the need (i.e., high-level idea of funding is provided). It should be noted that each of these proposed projects are ideal for training new nuclear data evaluators who are also integrated into application needs.

Five high-priority needs applying to many of the subject areas listed above

1. Medium-fidelity covariances are needed for several subject areas in the spirit of the low-fidelity covariance project undertaken in Ref. [1]. These covariance must be complete with respect to the chart of nuclides. For example, ENDF/B-VIII.0 does not contain covariance data for many existing nuclides at all or not for all relevant data for this nuclide. [2]. For many of those isotopes, no experimental data are available. Hence, a robust modeling effort— taking into account anchor experimental data—is the backbone of this large-scale project.

    - In a first phase, covariances tied to mean values for neutron-induced cross-sections, neutron multiplicities, and prompt fission neutron spectra (where applicable) from thermal energies up to 60 MeV should be provided,
    - followed by angular distributions in a second phase.
    - The third phase should cover charged-particle induced reactions from thermal energies up to 250 MeV.

    All three of the projects are *large (> 5 million dollars, several staff/ students/ Postdoc, >5 years duration), multi-year efforts.*

2. All users present at the meeting strongly emphasized the need for quality assurance of covariances in ENDF/B before their release via standardized V&V:

   - While recommendations exist on counter-checking covariances [3, 4], these have yet to be implemented in a small effort *(half an FTE,* <1 *million, 1–3 years)* in covariance testing codes. These codes should be publicly available.
   - Another need that was raised was for proper documentation that should clearly indicate, for users, whether covariances are a lower/ upper/ realistic bound of nuclear data uncertainties to aid them in a realistic assessment of what their application bounds represent. This could be addressed in another small project *(half an FTE,* <1 *million, 1–3 years).*

3. Nuclear data users highlighted needs related to differential experimental data:

   - They emphasized the need for a more complete and easier accessible EXFOR database [5] as well as a sister database that stores expert's judgments of experimenters and evaluators on those data in EXFOR. The reason producers highlighted that need was that a significant amount of routine work on experimental data could be reduced by having an easier accessible database. The sister database would reduce the need of evaluators to have to "re-invent the wheel" on re-analyzing past data for their evaluations. Aforementioned users supported this need as they benefit from these developments by (a) having a faster (i.e., cheaper) turn-around on evaluations, (b) more reliable evaluated nuclear data covariances due to streamlined and consistent uncertainty quantification of input experimental data, and (c) having improved reproducibility of evaluated nuclear data mean values and covariances. The very same needs are being highlighted by the Nuclear Energy Agency Working Party on International Nuclear Data Evaluation Co-operation Subgroup 50 [6], but a concerted *medium-scale project (3–5 years, 1–5 millions)* would be needed at the datacenters to implement these recommendations.
   - A more consistent and complete uncertainty quantification across several data sets could be achieved in a second medium-scale project *(3–5 years, 1–5 millions)* by applying templates of expected measurement uncertainties [7–10] to the EXFOR database to supplement missing uncertainties for a more complete and automatic assessment of uncertainties. New templates may need to be added.
   - Lastly, the need for having ready-to-use tools to assess unrecognized systematic uncertainties [11] in experimental databases was discussed *(small project; half an FTE,* <1 *million, 1–3 years).*

4. Many users requested expanded training on covariances, existing uncertainty quantification methods, and tools:

   - A small-scale project *(small project; half an FTE,* <1 *million, 1–3 years)* could develop a curriculum.
   - After that, a sustained *small-scale effort (half an FTE,* <1 *million, sustained for many years)* would be needed to carry this over many years to support and inform users on the best ways to incorporate the covariance data into their applications.

5. Both, nuclear data users and producers, highlighted the need for open-source adjustment tools; these tools should include pre-processed sensitivities, nuclear data mean values, and covariances for adjustment studies. This *medium-scale project (3–5 years, 1–5 millions)* could build upon experience gained through existing adjustment tools, for instance those of Ref. [12,13] funded by the Nuclear Criticality Safety Program (NCSP).

Other cross-cutting needs that may impact one program more than another In "()" we provide examples of what stakeholders/ programs would be interested in these covariances:

- Open-source tools are needed to compute sensitivities for various integral responses (those subject areas that are already performing adjustment such as general validation, nuclear criticality safety, reactor physics, neutron dosimetry, etc.). This need could be met in four phases:
  - Code comparison and review of existing tools,
  - Provide tools to compute sensitivities for reaction rates and spectra of critical assemblies as well as sub-critical assembly observables,
  - Provide tools to compute sensitivities for fixed source experiments, reactivity coefficients,
  - Make recommendations how other user communities can use existing tools.
- Evaluations of covariances where none are currently provided:
  - Thermal Scattering Law (NCSP, nonproliferation, space reactors, Nuclear Regulatory Commission (NRC), nuclear energy),
  - Fission Product Yields (anti-neutrinos, reactors, NRC, nonproliferation, safeguards, astrophysics),
  - Decay constants (isotope production, nuclear medicine, oonproliferation, astrophysics, safeguards),
  - Branching ratios (NRC, reactors, safeguards, isotope production, nonproliferation, astrophysics),
  - Stopping power (isotope production, space application shielding design, neutron dosimetry, nonproliferation, detector technologies),
  - Delayed neutrons (safeguards, astrophysics, nonproliferation).
- Sampling tools are needed that support applications where uncertainty propagation must address non-linear dependences based upon the underlying parameters and for uncertainty propagation to metrics that cannot be analyzed with other (perturbation theory-based) methods,
- Identify historic integral experiments for re-evaluations.

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