

Responses to the Charge and the 2020 NDAC Recommendations

NDAC Meeting
September 13th & 14th, 2023

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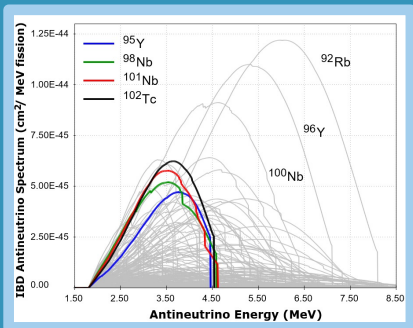
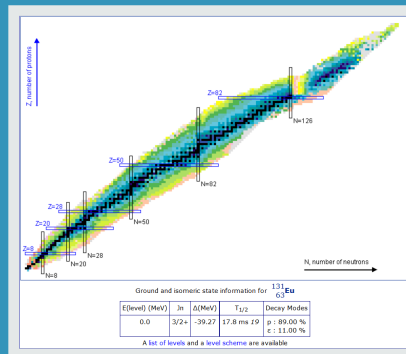
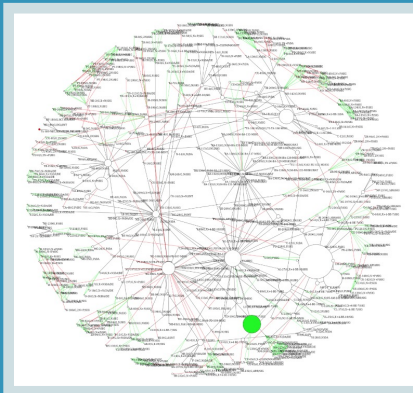
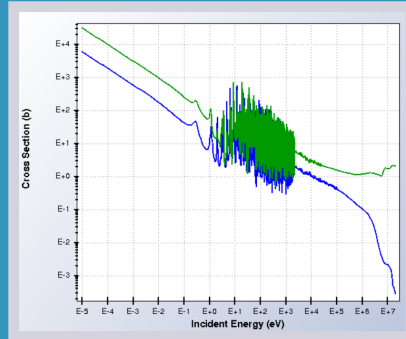
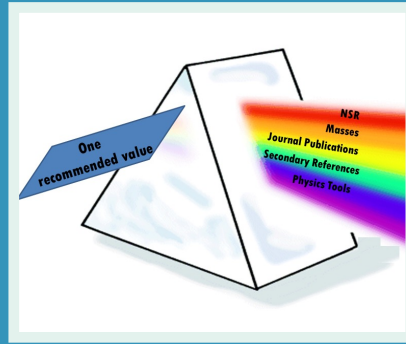
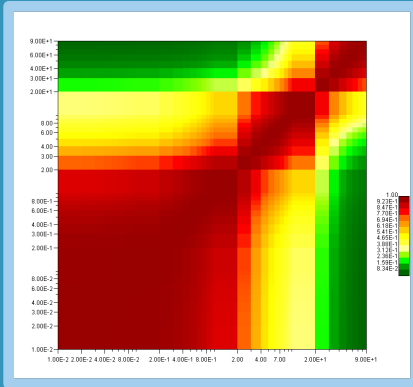
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Responses to the 2023 Charge Letter

- 1) Has USNDP adequately addressed recommendations from previous NDAC reviews? Is additional action required? If a recommendation has not been addressed, is there sufficient reasoning to not do so?

See responses below.

- 2) To what extent does the USNDP meet its established goals and priorities?

We will expand on this topic during the meeting. We believe the members of the USNDP have met their established goals and priorities, despite resource limitations. We do not believe anything has “fallen through the cracks”, but there is always a danger. Modernization efforts have eased the workload in some cases, and we hope that advances in the application of AI/ML techniques can continue this progress.

The USNDP resource limitations also impacts the USNDP’s ability to address emerging challenges and needs. This is discussed in the NSAC charge report(s) and will be discussed during the committee meeting.

3) What challenges are the USNDP encountering in carrying out their program? How might these be addressed? Are there compelling opportunities for program improvement or enhancements?

- *We will talk about this in the meeting but summarize here. Our biggest challenge is that our base funding has not kept pace with costs. This forces us to expend base effort to search for new opportunities/sponsors, eroding our productivity in the process. Nevertheless, we have successfully captured external funding and expanded our funding base. We will discuss other efforts in this direction on Thursday.*

- 4) To what extent does the USNDP function like a collaboration? What challenges exist to improving collaboration among USNDP sites?

We will expand on this topic during the meeting. Collaborators share resources and information, plan future projects together, launch new joint projects, are mutually supportive, seek out new members with similar goals, share responsibilities and credit. Here is a collection of projects that demonstrate our collaborative spirit:

Collaboration-wide on-going library development: ENSDF/XUNDL, NSR, ENDF

Selection of jointly developed/funded projects:

- 1. GRIN [2022-2024] (BNL, LLNL, LBNL),*
- 2. Two GRIN-testing projects [2024-2027] (JHAPL, LBNL, BNL; RPI, BNL)*
- 3. ENSDF Modernization [2020-2023] (BNL, ANL, LLNL)*
- 4. GENESIS [2019-2022] (LBNL, LANL, BNL)*
- 5. FIRE [2018-2022] (LANL, LLNL, BNL, NCSU and U. NotreDame)*
- 6. Fission Product Yields [2019-2025] (BNL, LANL, LLNL)*
- 7. Evaluation of gamma-ray Production [2022-2024] (LANL, LLNL)*

- 5) Assess the quality and effectiveness of any Codes of Conduct and/or DEIA initiatives within the USNDP. Other closely related efforts, such as the Cross Section Evaluation Working Group (CSEWG), where USNDP has a leading role, can be assessed as well.

We will discuss this during the meeting. Briefly, the USNDP has a long track record of recruiting and educating students (and junior staff) into the nuclear data community. The USNDP also endeavors to create a welcoming environment for these new members and all staff both in the USNDP itself and in broader collaborations in which USNDP is part (such as CSEWG, NRDC and NSDD).

- 6) Assess the NNDC's continued designation as a DOE PuRe Data Resource. The NNDC was designated by DOE Office of Science as a PuRe Data Resource (<https://science.osti.gov/Initiatives/PuRe-Data>) in FY21, signifying its importance to the nuclear science and applications community. Part of the designation includes the requirement of regular assessment of the resource's access procedures (user access, data access, etc.), technical metrics (data stored, new data added, number of users, etc.), scientific impact, and community engagement.

We will discuss this during the meeting. Additionally, a summary document will be shared with the committee.

Responses to the 2020 NDAC Recommendations

1) The major priority for ENSDF should be the effective management of the ENSDF evaluation effort and related file maintenance.

a) The ENSDF project needs to be proactively managed and funding reallocated to enhance overall productivity. Given the amount of nuclear structure data that will be produced at FRIB, ATLAS/CARIBU, and other such facilities over the next decade, we recommend that funding is re-allocated from the least productive current efforts in order to expand such data evaluation efforts at MSU and ANL. Both institutions have proposed to cost share new scientific staff positions between the experiment and data program, and the committee is highly supportive of this suggestion.

This recommendation appears to be geared to the USNDP program manager and not the USNDP PI's. Nevertheless, we disagree with the central premise of this recommendation. We do not think funding should be re-allocated as this assumes a sort of zero-sum game in which USNDP funding is constant. This would force the USNDP or the USNDP program manager into a "robbing Peter to pay Paul" situation where one institution's effort is gutted to fund another. This might help to marginally increase productivity in the short run but will destroy morale in the rest of the USNDP centers.

A more robust solution would be to expand the USNDP funding to cover the expected flux of new data from MSU, ANL and elsewhere. Such "mini-proposals" have been presented to the DOE at our annual budget briefings.

1. cont.

b) The NDAC supports the idea of establishing the position of an ENSDF project manager with the main responsibility of managing the workflow process related to the entire ENSDF effort. Our primary expectation would be that mass-chain and/or individual nuclide evaluations within the project are prioritized and completed in a more timely manner.

The international nature of the USNDP makes establishing an “ENSDF project manager” as described by the committee challenging. Currently, the ENSDF evaluation effort is under the auspices the Nuclear Structure and Decay Data Network, led by the IAEA. The network has its own policies and procedures for assigning work and defining priorities. In addition, an ENSDF project manager would not realistically be able to manage non-DOE funded ENSDF evaluation effort. Nevertheless, we are in agreement with the committee that there are specific areas which the US component of NSDD can improve on ENSDF effort and workflow

1b) cont.

(i) attracting new evaluators nationally and internationally;

New evaluators C. Morse, S. Ota and J. Wu are currently being trained to be full time ENSDF evaluators at the NNDC. Additionally, E. Gass and G. Gurdal have been brought under contract by the NNDC to perform single nuclide evaluations focusing on timely incorporation of new results from radioactive beam facilities.

In addition to our actions, there is a possibility that DOE might fund additional evaluator training, outside of USNDP base funding. This is a good start, but it has the nature of a one-time fix rather than a programmatic directive like an increase in the base would be. Since we will not get an increase in the base for doing the same work, that is where the new opportunities (space, fusion, pre-publication vetting, preserving experimental data...) are critical.

(ii) modernization of ENSDF (database format, codes, interfaces);

Summary of ENSDF modernization format, codes and interfaces will be presented during the committee meeting.

1b) cont.

(iii) provision of new tools to enhance evaluation efficiency and quality.

Tool development was an integral part of the ENSDF modernization project and will be presented during the committee meeting. Additionally, through the efforts of the MSU center, nearly all ENSDF codes have been modernized and equipped with new features which aim to increase the evaluation quality and productivity. Transitioning to a modern format will further enable the use of the AI and ML, which is planned for future ENSDF developments. Similarly, the reaction evaluation community has been aggressively pursuing improved and automated workflows, with goal of completely automatic (& reproduceable) generation a new ENDF when any single evaluation is updated. A key step in the reaction workflow is ensuring the correct metadata is available in an EXFOR-like experimental compilation.

1b) cont.

The role and responsibility of the ENSDF project manager needs to be well defined and should be developed and agreed upon by USNDP management and the ENSDF working group in close consultation with DOE management.

Defining the role of an ENSDF project manager (if this is the route that both DOE and the USNDP choose) is essential.

1c)

c) An agreed ENSDF business plan should also be finalized by the ENSDF project manager which defines required resources and expected deliverables in detail for different funding scenarios. Such a plan can be used by both the ENSDF project manager and USNDP to assess overall productivity of ENSDF evaluations on a year- to- year basis and should allow for action plans to be initiated in a timely manner if productivity issues arise.

While we disagree with the term “business plan”, the idea of a long-range nuclear data plan is appealing. Creating such a plan is daunting since the USNDP is only part of the broader nuclear data ecosystem. In particular, the ENSDF project is coordinated under the auspices of the IAEA by the Nuclear Structure and Decay Data (NSDD) network. As noted above, the competing priorities and capabilities of the NSDD hinder rapid changes.

Outside of the USNDP and the NSDD, planning is also driven by the Nuclear Data Interagency Working Group, the broader Office of Science long range planning, and the specific plans of additional sponsors.

*Finally, the DOE-NP and National Science Foundation have an additional community planning body, the Nuclear Science Advisory Committee. This committee released a pair of reports outlining potential work for the USNDP. These NSAC-ND reports are terrific at listing capabilities, identifying gaps, and suggesting priority needs. It is **not**, however, a funding proposal. DOE NP is not allowed to make a plan for the USNDP to fill the data gaps and capitalize on new opportunities; they can only respond to proposals that the community submits. It is up to the USNDP to write and submit proposals for funding enhancements that address the priorities listed by the experts in the NSAC-ND reports. This could be done one priority or topic at a time, or it could be done as a larger package and given to DOE NP, using the NSAC-ND report as justification as to why this work is important and needed.*

1d)

d) We recommend that the ENSDF community provide annual interim reports to DOE and NDAC on their progress and accomplishments against the metrics they have laid out. Since the deliverables from individual evaluators are expressed on a yearly basis, we suggest a report by the end of October each year summarizing the previous fiscal year accomplishments.

We believe this recommendation is met with the annual USNDP Workplan.

2)

2) Distribution of evaluation work merits improvement. USNDP management should articulate whether the employment of new evaluators can be supported by the base program, and how this base program might be restructured to do so.

We do not think restructuring the USNDP program is the best solution here. This assumes a no-growth scenario, the ready availability of the appropriate ENSDF/ENDF evaluators and a continuation of our current work processes. As an example of an alternative solution would be a strategic and limited investment in workflow improvements that would lead to enhanced evaluator productivity. Such improvements can leverage ongoing modernization projects and AI/ML expertise from across the USNDP and their host institutions. This will be discussed during the meeting, particularly on Thursday. However, the idea of expanding the USNDP base to hire more evaluators is something we are open to!

3a)

3) Identify and consider new approaches to increase community engagement in XUNDL and ENSDF, particularly internationally.

a) Compelling arguments need to be developed that will generate the interest and involvement of international communities. One possibility is to solicit in-kind contributions from non-US laboratories, especially in the area of XUNDL. The NDAC recommends that this matter be discussed at the next IUPAP C12/ WG9 meeting in June 2021. An “urgent request” should be formulated about the importance of nuclear data evaluation and send to C12 and WG9 for distribution. We suggest that the USNDP Chair and C12 and NDAC committee member Dillmann work together on this topic and report back to the committee after the C12/WG9 meeting.

E. McCutchan presented an urgent need for contributions to XUNDL and ENSDF at the June 2021 IUPAP meeting. E. McCutchan again emphasized this urgent need for international involvement in XUNDL and ENSDF in an invited talk at the IUPAP June 2023 meeting.

3b)

b) We encourage use of new mechanisms to prioritize individual and group evaluations based on their relative importance to user communities.

ENSDF evaluators are members of the Nuclear Structure and Decay Data Network, an organization coordinated by the IAEA. In this network, each center is assigned a region of the chart (in mass chain units) for which they are responsible for performing ENSDF evaluations. This organizational structure can make it challenging to quickly adjust the evaluation effort, as different centers can have different priorities or some centers might not have the resources to shift their evaluation effort. Prioritizing evaluations based on community input remains a challenge for the network and was recently highlighted, with a focus on decay data evaluations, in the latest NSAC report. A proposal was written to the 2023 NDIAWG funding call to create a pipeline for targeted decay data evaluations feeding in input from a number of user communities. Additionally, ENSDF evaluators have been participating in workshops where evaluations needs are discussed, for example the recent Microcalorimetry and Nuclear Data (MiND) workshop and an IAEA CRP on Nuclear Data for Isotope Production.

3c)

c) We strongly support nuclear data workshop at the Low Energy Community Meeting to form a community approach targeted around user facilities (FRIB, ATLAS, ARUNA, etc.).

There is a Nuclear Data Working Group, currently convened by Jun Chen and John Kelley. At each Low Energy Community Meeting, this Working Group has held sessions soliciting input from the community. In addition, this Working Group convened a session at the Low Energy Community Long Range Planning Town Hall meeting.

4)

4) Modernization is creating opportunities for new capabilities in the formulation of data products. More specifically, machine learning tools have high potential in data science. The expectation is that external funding opportunities in AI/ML will increase, and therefore we encourage the ENSDF community to compete aggressively for such new funds.

We agree with this recommendation. We are aggressively pursuing funds and/or collaborative efforts to modernize our toolsets. Some of the more prominent projects undertaken by USNDP members are:

- *ENSDF modernization - NDWG FOA funding*
- *ENDF-6 to GNDS transition - partly funded by the NCSP, significant input from Defense Programs and international collaboration*
- *Atlas of Neutron resonances modernization – partly funded by the NCSP*
- *Resonance spin group classification – funded by the NCSP*
- *Natural Language Processing for Nuclear Science References – currently funded by the USNDP base funding with a small amount of university support.*
- *The PyEGAF and PyENSDF tools developed by Aaron Hurst started with DTRA funding and has been continued using NA-22 and USNDP support includes a proper treatment of gamma-Xray as well as gamma-gamma coincidences.*

We note that a longer-term plan would be very useful to provide a vision to improving the workflow of our efforts, rather than focusing on just one or two aspects. For example, the most complex portion of the nuclear data pipeline – the bottleneck – is evaluations, yet there have been no efforts to revamp evaluations with AI/ML.

5)

5) NDAC endorses the proposal that evaluators devote ~20% of their programmatic nuclear data efforts to other nuclear physics research. Such a proposal needs to be clearly defined and equally applied to all evaluators.

We wholeheartedly agree with this concept. We hope the DOE can continue to support this concept as this allows our staff to continue involvement in basic science.

6)

6) Implement ways to improve diversity and inclusion. For instance: (i) work closely with the laboratory HR department to ensure that any advertised job postings are widely disseminated in order to reach as diverse an applicant pool as possible; (ii) liaise with APS Women and Minorities in Physics; (iii) organize sessions on nuclear data at undergraduate conferences.

We agree with these recommendations and will discuss our DEIA efforts during the meeting.

7)

7) Nuclear science references (NSR) compiles a database of articles related to nuclear physics research both in experiment and theory. Plans for enhancing NSR are under consideration around extending and improving how keywords are generated for each article. These plans appear reasonable and are supported by NDAC.

We will discuss our NSR modernization project(s) during the meeting with a specific talk on a Natural Language Processing effort (NucScholar) currently under development.

Mini-proposals addressing topic 1a)

Adding ENDF Evaluators

- Since David Brown has taken over Alejandro's administrative responsibilities and Gustavo Nobre's became ENDF library manager, we would like to hire an additional ENDF evaluator.
- The NNDC plays a valuable role in CSEWG: we cover materials other programs cannot or will not, such as Fe, Cr or Zr, all essential for new reactor concepts.
- Position could partly address EXFOR & NSR & Atlas succession planning
- Position was openly advertised,
 - 14 excellent candidates
 - 8 short-listed
 - Verbal offers to 2, but reduced to 1 after getting spreadsheet

New ENSDF evaluators at MSU and ANL



FRIB & ATLAS are the two DOS/SC/NP LE National User Facilities

- producers and users of vast amount of ENSDF-related Nuclear Data
- the two facilities and their users are one of the main USNDP stakeholders

Nuclear Data Needs and Capabilities for Basic Science, University of Notre Dame, August 2016

- urgent need for proper and timely inclusion of all new data into **XUNDL&ENSDF databases**

Nuclear Data Advisory Committee meeting report , November 2020

- **Executive summary:** “without significant changes to the way ENSDF conducts this vital mission, the community will fail to keep pace with the increase in the amount of data being produced worldwide”
- **Recommendation:** “ ... we recommend that funding be re-allocated ... in order to expand data evaluation efforts at MSU and ANL”

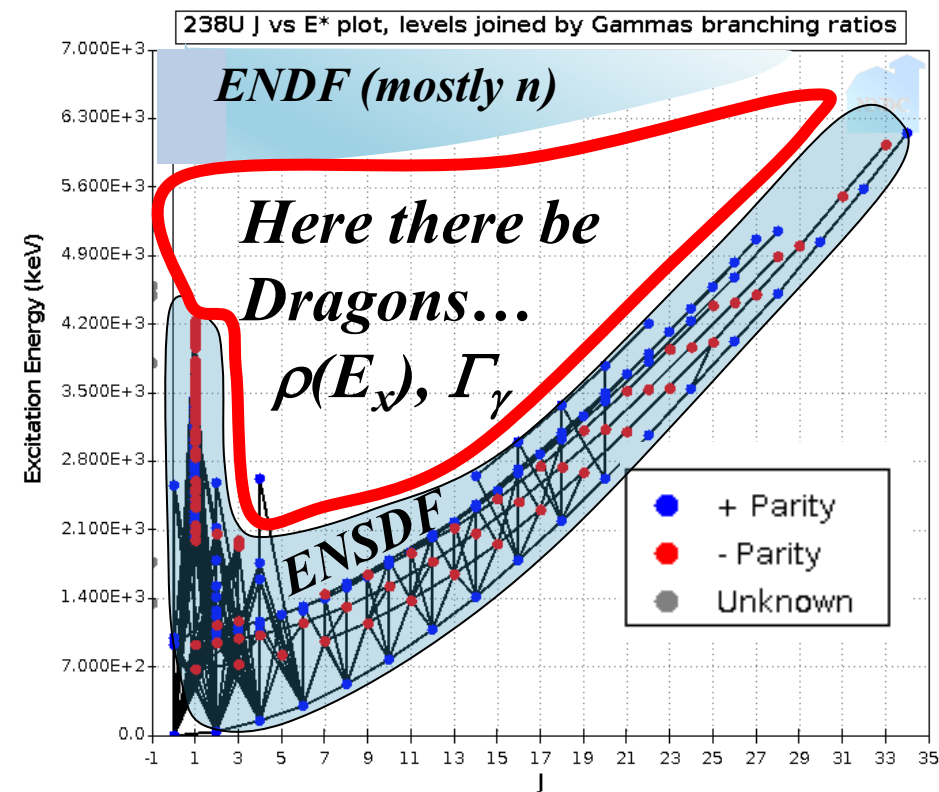
USNDP vision

- open two new full-time ENSDF evaluator positions – one at FRIB and one at ATLAS
- ✓ highly leveraged - half of the funding will be provided by MSU & ANL – two for the price of one



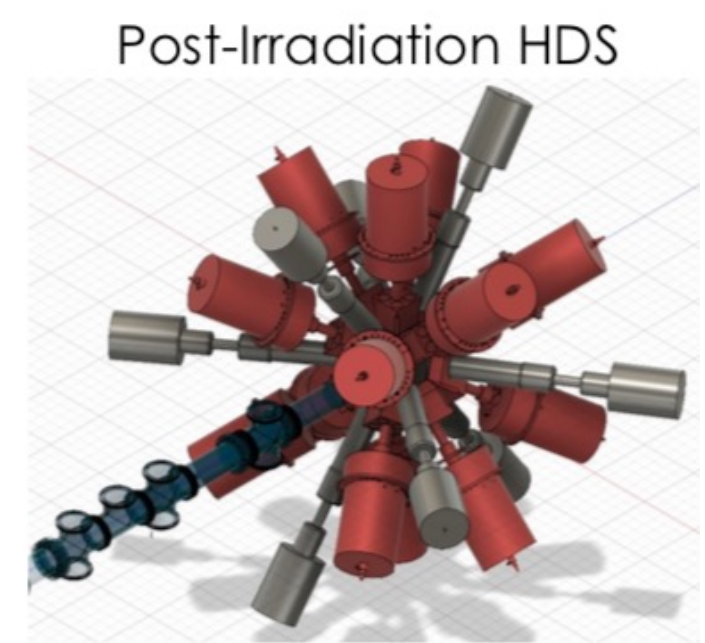
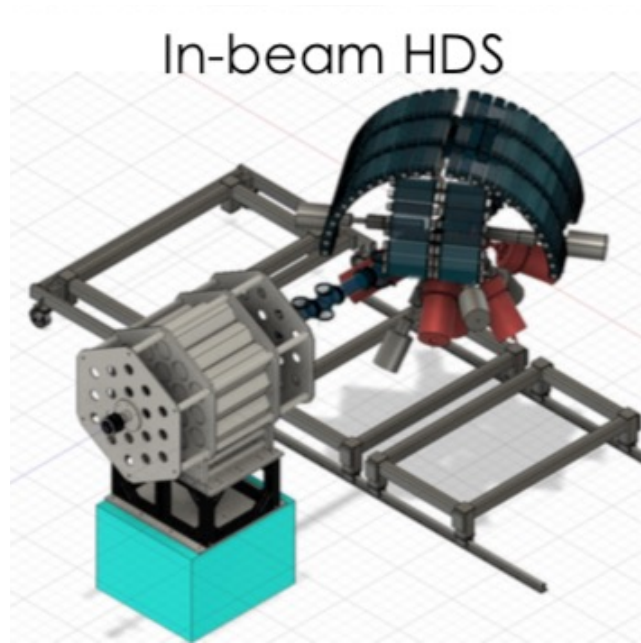
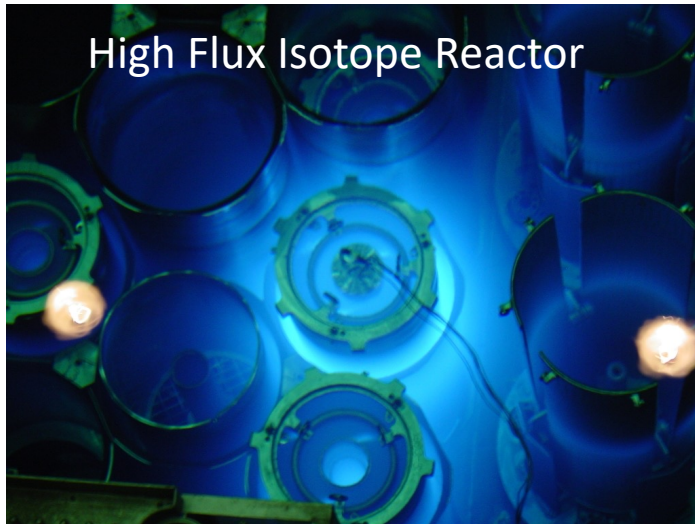
Adding Nuclear Level Density & Photon Strength Evaluator at LBNL

- There is a huge “evaluation gap” between ENSDF & ENDF – the statistical region.
- The data in this region (level density and radiative strength) are key to modeling photonuclear and capture cross sections for:
 - Stellar nucleosynthesis;
 - Reaction Evaluation, and
 - Isotope Production.
- FRIB will create a large body of this sort of data (b-Oslo method).
 - We are coupled to this through the NSSC (Spyrou, Liddick) and our long-standing collaboration with the University of Oslo.
- ***A new staff hire is planned***



We are in final negotiations with a strong candidate we can support on the existing base budget for the rest of FY23 and FY24 years

Nuclear Structure Data at ORNL



- Future Opportunity for junior scientist – **split position** for **measurements & evaluations** of level properties of nuclei formed with neutrons from HFIR
 - ORNL High Flux Isotope Reactor HFIR is a unique national resource for creating heavy neutron-rich nuclides
 - Two state-of-the-art monitoring / diagnostics end stations are proposed for HFIR for surveying rad isotopes & materials
 - Overlaps with neutron scattering, materials for advanced reactors, advanced fuel cycle and reactor design, security and forensics applications, isotopes/nuclear medicine, non-proliferation, accelerator-driven transmutation of waste
- ***Request for 0.5 FTE evaluator support from DOE NP Nuclear Data (start ~FY26)***

Proposal to hire a new evaluator in FY2023

Texas A&M University Cyclotron Institute Data Center - N. Nica

□ *Present Status*

- *USNDP senior mass chain evaluator, 1FTE*
- *Started evaluation in 2005 under contract with NNDC, 0.66 FTE for data evaluation and 0,33 FTE for experimental research at CI with John Hardy*
- *Mentored by Thomas Burrows, one of the ever-best evaluators*
- *Since 2018 we became an autonomous evaluation center financed by DOE-NP Office of Nuclear Physics, Office of Science of the U.S. Department of Energy under Contract No. DE-FG02-93ER40773.*
- *TAMU ENSDF Responsibility: 11 Rare Earth mass chains which are systematically of the highest size and complexity of Nuclear Chart*
- *Published 19 major full mass chain evaluations in Nuclear Data Sheets*
- *Published 18 publications on a series of 10 benchmark precise internal coefficient measurements with direct relevance for the USNDP ICC BrIcc code*
- *All 11 mass chains of TAMU center are less than 10 years since last full evaluation*

□ *Hiring 1.0 FTE new evaluator*

- *As an experienced senior USNDP evaluator, we need at TAMU center to hire an extra junior evaluator for 0.66 FTE and provide the mentoring in order to double ENSDF evaluation productivity, extend XUNDL compilation, and ensure the center will develop after our retirement*
- *As a novelty, for the remaining 0.33 FTE we want to imply the new evaluator in a **Data-based Physics Research**, i.e. using data repositories as the primary research resource for extra properties and possible new correlations left undisclosed in the data.*
- *Hands-on very intense training is necessary in order to build strong evaluation skills.*
- *Only the very hard-working and long-term committed candidates who can meet these demands should be selected for the job.*
- *I advocate that nonstandard candidates (other than experimentalists in low energy nuclear physics) be selected for our specific needs and to bring more dynamism to a field that is still considered clerical.*
- *Hiring a new such evaluator would be the way to give new strength to the USNDP effort.*

Nuclear Astrophysics Data Evaluation at MSU/FRIB (0.5 + 0.5 FTE)

- Focus on reaction rate data evaluation combining structure data, reaction data, theory data and theory tools
- Build on and expand JINA-CEE Reaclib infrastructure for dissemination and link to ORNL tools as well as other evaluation efforts
- Now is the time to start: JINA-CEE can help jumpstart the effort
 - Facilitate community engagement (including workshops, working groups etc)
 - Facilitate close collaboration with other evaluation efforts
 - Provide leverage
- Connection to USNDP and proposed Structure/Theory data efforts
 - Provides continuity and consistency
 - Enables to take advantage of synergies:
 - More comprehensive and faster use of nuclear structure, nuclear reaction, and theory data for astrophysics.
 - Provides a natural connection of structure and reaction efforts
 - Enhances impact of USNDP



A New Theoretical Database (0.5 + 0.5 FTE)

- Initially, content primarily produced by large-scale simulations
 - Large-scale surveys of nuclear observables produced by SciDAC programs
 - Data needed for further uncertainty quantification (covariance matrices, posterior distributions of parameters) also stored
- Examples
 - Ground-state properties of even-even nuclei: <https://massexplorer.frib.msu.edu>
 - Spectroscopic overlaps: <https://www.phy.anl.gov/theory/research/overlap/>
- The long-term perspective is to interface theoretical database with ENDSF to be able to directly compare theory with experiment
- In short: provide a theoretical counterpart to ENDSF, fully integrated with NNDC.

