Propagation of nuclear model uncertainties in science applications

Trevor Sprouse
Theoretical Division
Los Alamos National Laboratory

WANDA2021

LA-UR-21-20577

Background

Grand Challenge:

- *What is the astrophysical source of the heaviest elements in the universe?*

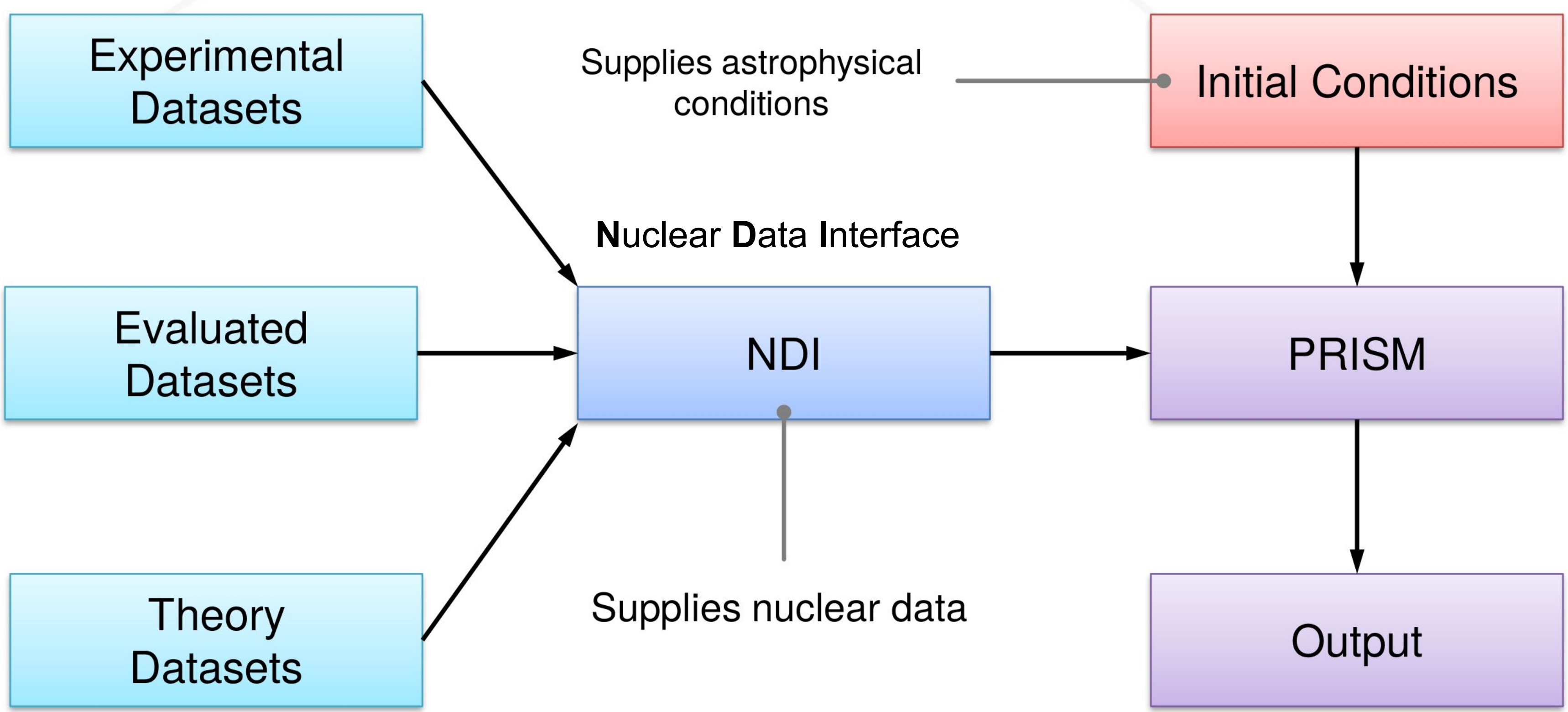
What are you doing?

- *Modeling astrophysical nucleosynthesis with robust propagation of nuclear model uncertainties.*

Why does it matter for nuclear data?

- *Nuclear reaction network calculations rely on a number of nuclear properties (half-lives, binding energies, cross sections, fission yields, etc.) for thousands of nuclei. These inputs come from nuclear data evaluations, experiments, and theory.*
- *Sensitive test for extrapolation of nuclear modeling*
- *Mirrors efforts in nuclear reactor applications*

Nuclear Data Pipeline for Nucleosynthesis



Computational Techniques

What techniques have you used?

- *Implement standard techniques for probing model parameter spaces.*
- *Based on Bayesian analysis.*

What algorithms and software?

- *All software is custom-designed.*
- *Our reaction network (PRISM) is currently open source.*

Hardware architecture that may be useful to your problem (CPU, GPU)?

- *Currently all calculations are performed with CPUs, generally compatible with highly parallelized workflows.*
- *Nucleosynthesis calculations would likely benefit from GPU support, but this support is not currently implemented in PRISM.*

Our Computations and Future Needs

Generate numerous complete datasets of nuclear model predictions subject to changes in model parameters:

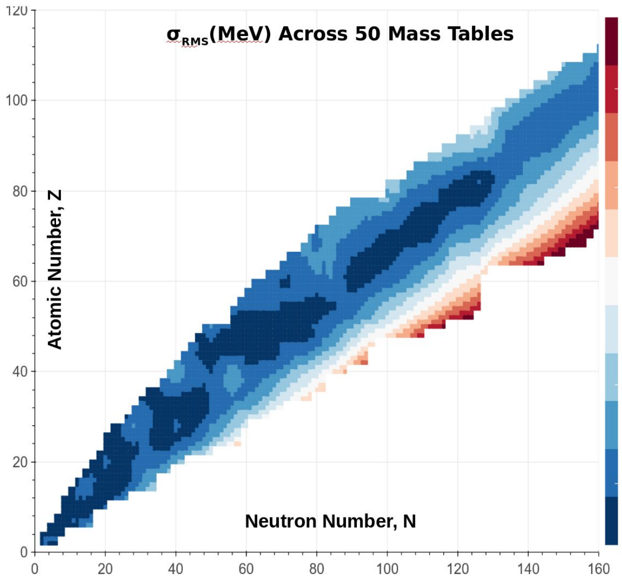
- *Propagate changes of state-of-the-art atomic masses to other nuclear properties using advanced HF cross section and de-excitation codes.*
- *Propagate these into nucleosynthesis calculations via the unique capabilities of our nuclear data (NDI+PRISM) workflow.*

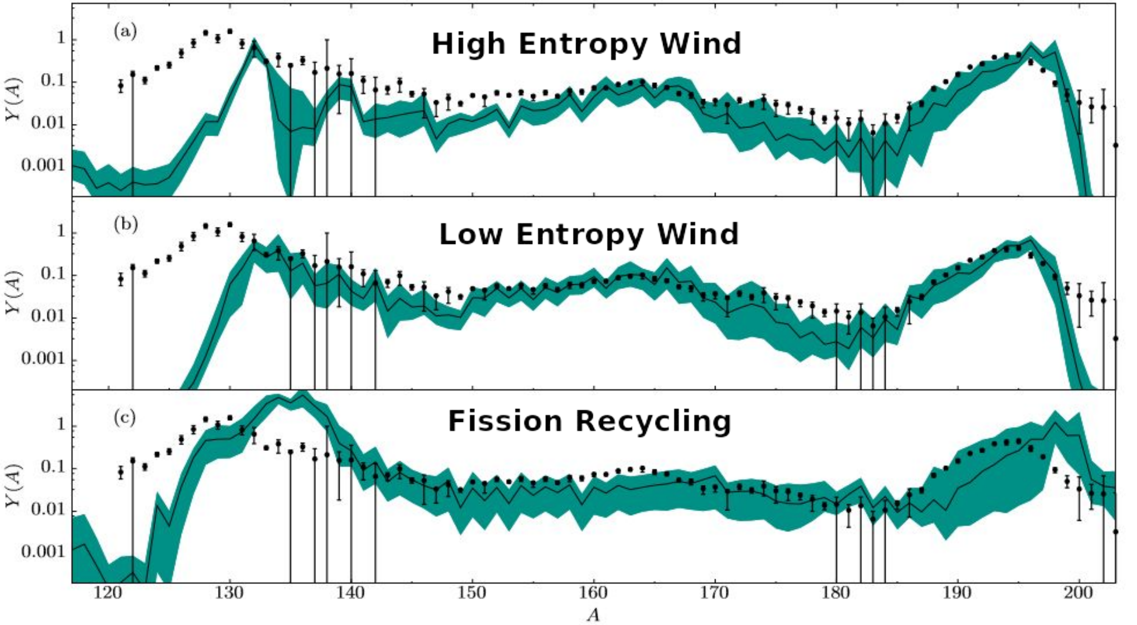
Opportunities for improvement:

- *AI/ML to emulate resource-intensive aspects of nuclear modeling -> greater number of parameter space samples for a given allocation of computational resources, improving statistics overall.*
- *Rapid incorporation of nuclear data is key driver of scientific discovery.*

Results

Sprouse *et al.* PRC 101 055803 (2020)

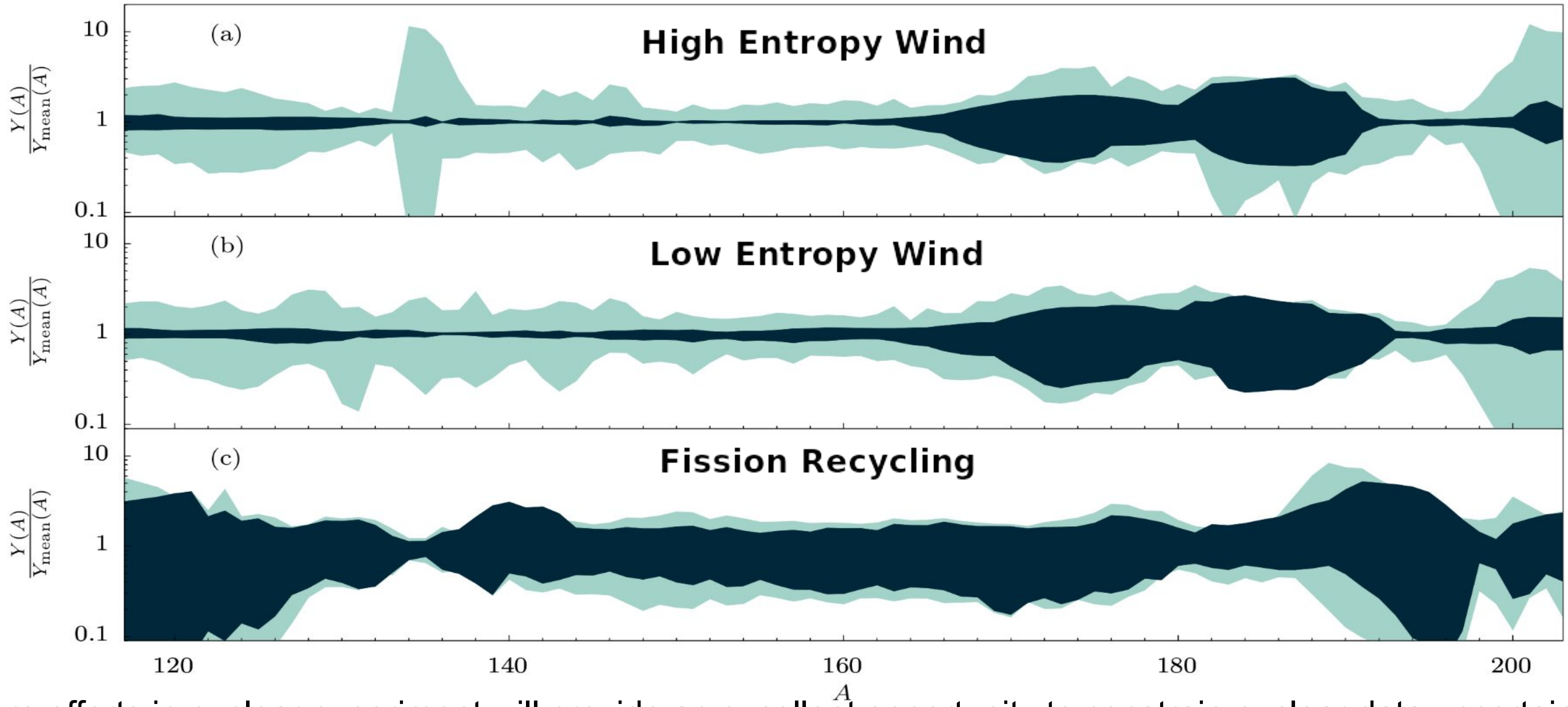




Starting with complete sets of atomic masses (left), we perform calculations to predict nucleosynthesis-relevant nuclear properties that integrate directly into the NDI+PRISM workflow to provide updated reaction rates. We may then quantify the propagated uncertainties in simulated nuclear abundances (right).

Results

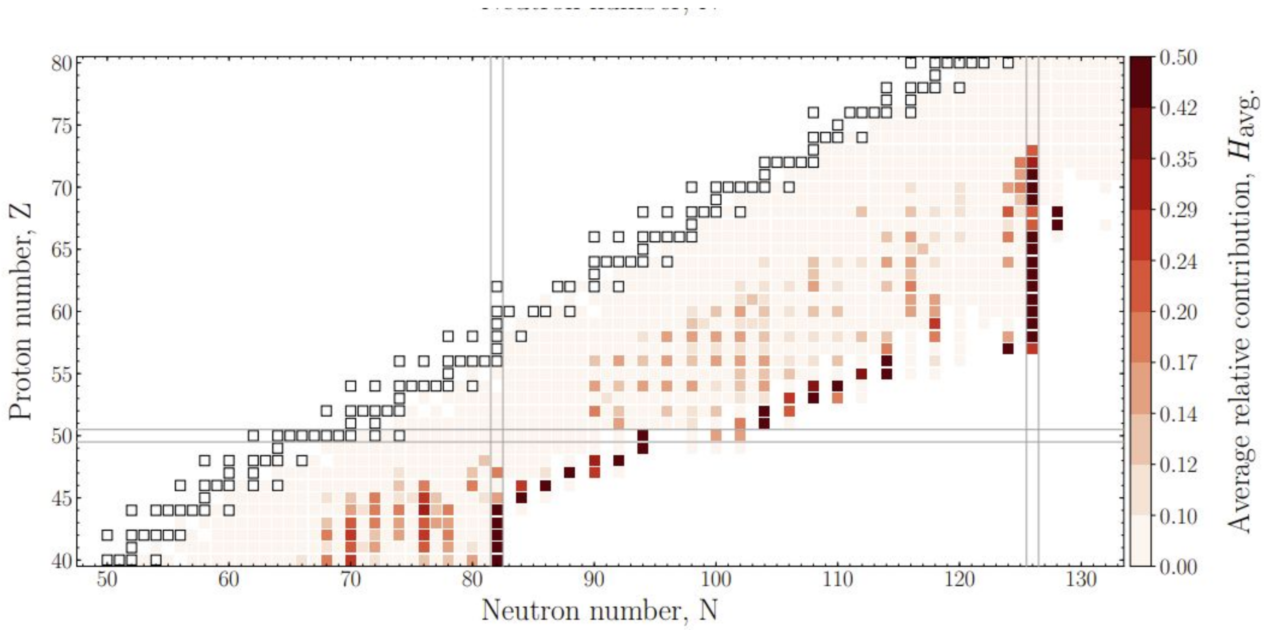
Sprouse *et al.* PRC 101 055803 (2020)



Near-future efforts in nuclear experiment will provide an excellent opportunity to constrain nuclear data uncertainties, with potentially dramatic improvements to studies in astrophysical nucleosynthesis. Here, simulated nuclear abundance uncertainties are estimated to improve from light green band (current) to dark green band (near-future).

Results

Sprouse *et al.* PRC (submitted) arXiv: 2008.06075



Our newly-developed *tracing framework* can be employed to identify key nuclear properties relevant to specific applications (here, we use it to identify important beta-decay rates for nucleosynthesis studies)

Results and Future Outlook

Open challenges going forward:

- *How can we rapidly and seamlessly integrate the latest nuclear data in science applications?*
- *The NDI+PRISM is a first step towards this effort for nucleosynthesis/astrophysics studies.*
- *There is a need for a computational nuclear data platform to centralize this effort and generalize it for a broad range of applications.*
- *AI/ML tools can assist with computational expensive aspects and offer more robust uncertainty quantification.*