

LA-UR-23-30519

Approved for public release; distribution is unlimited.

Title: What is nuclear data evaluation

Author(s): Neudecker, Denise

Intended for: MCNP® 2023 User Symposium, 2023-09-18/2023-09-21 (Los Alamos, New Mexico, United States)
Web

Issued: 2023-09-14



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

What is nuclear data evaluation

Denise Neudecker, XCP-5

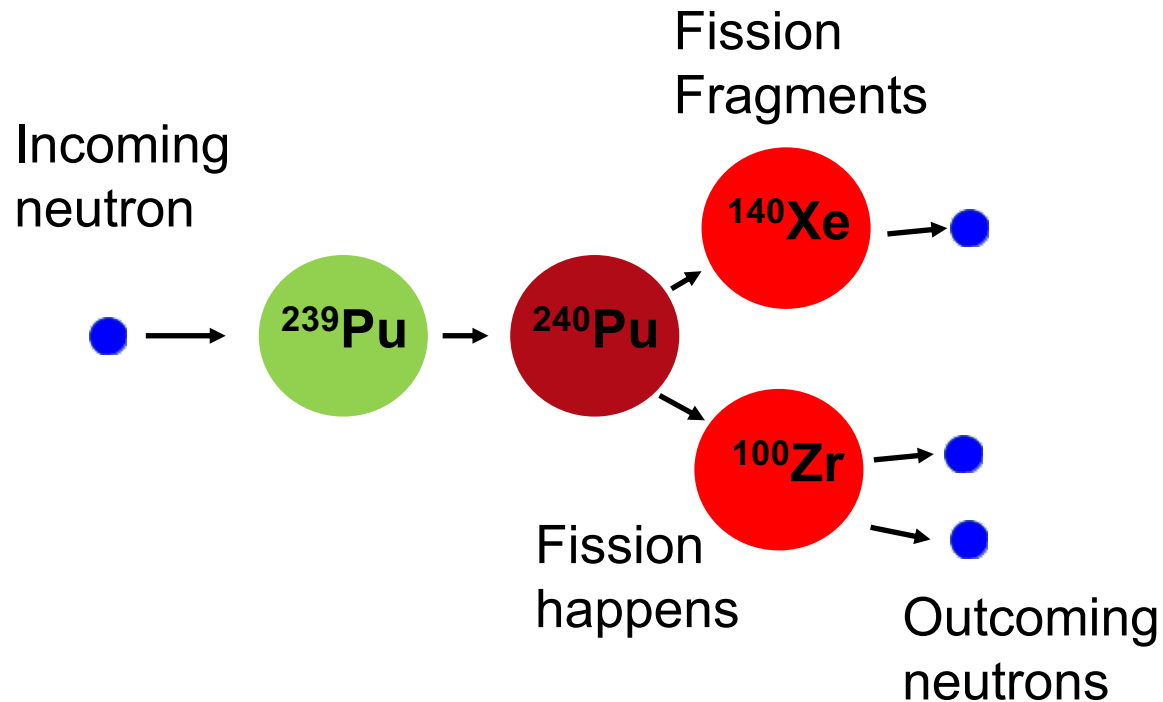
Questions/ Points addressed in the talk:

- **What are evaluated nuclear data?**
- **How are they obtained? What are they needed for? Who works on nuclear data evaluations at LANL, in the US and internationally?**
- **Evaluated nuclear data and their uncertainties evolve over time when we gain new insight through experimental data or nuclear models.**

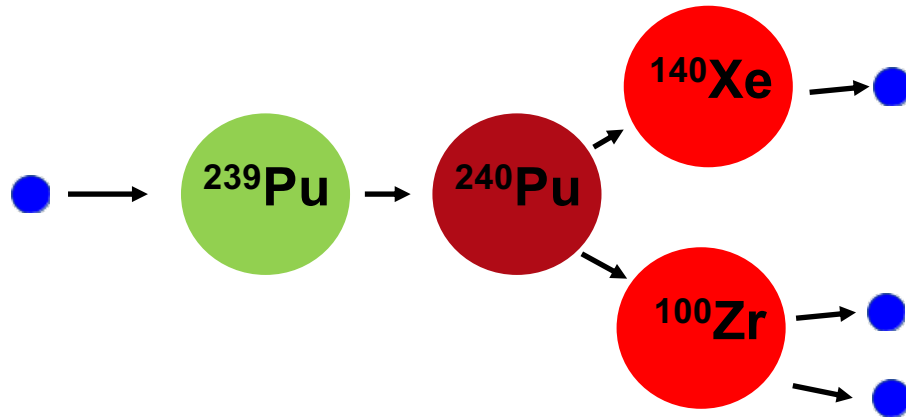
What are evaluated nuclear data?

Nuclear data tabulate physics reaction mechanisms of the nucleus for many isotopes/ materials.

Example: neutron-induced fission on ^{239}Pu



Examples of nuclear data:



Fission cross-section=probability that fission happens

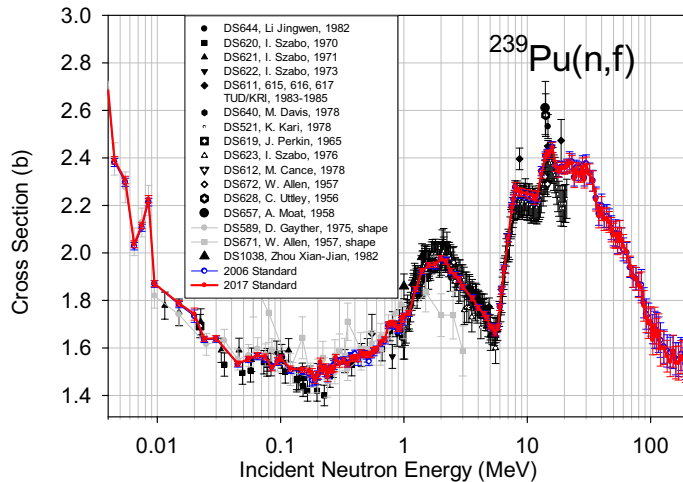
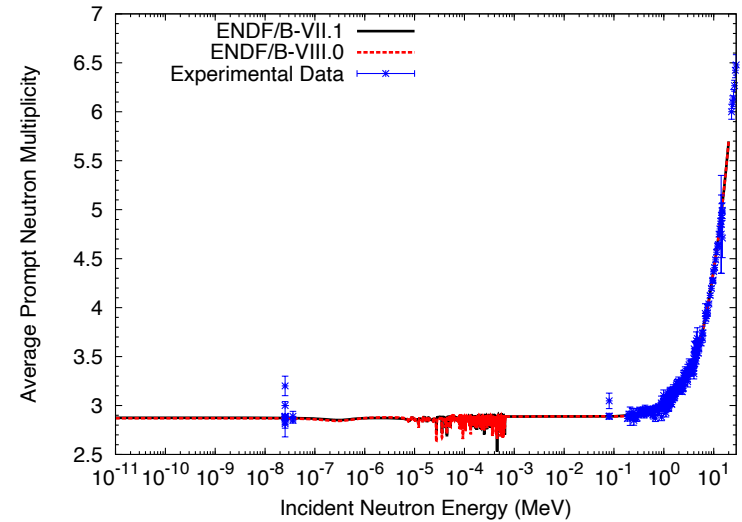
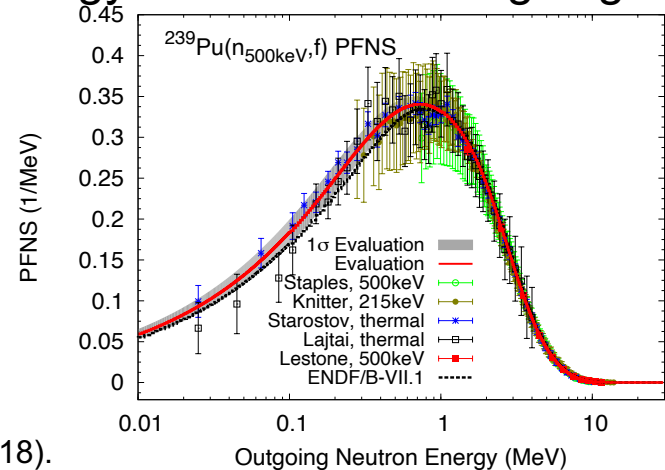


Fig. from Carlson et al., NDS 148, 143 (2018).

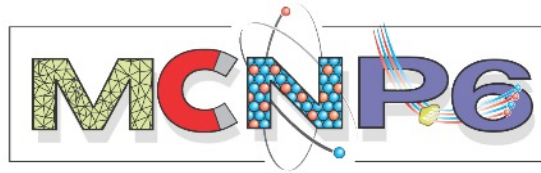
Average Prompt Neutron Multiplicity= Av. Number of outgoing neutrons



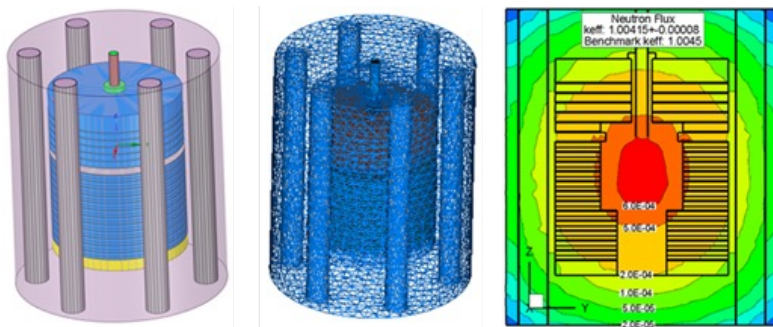
Prompt Fission Neutron Spectrum= Energy distribution of outgoing neutrons



Accurate ND are required for predictive simulations using MCNP or other transport codes.



- The accuracy of MCNP predictions is in part determined by the accuracy of its input nuclear data.
- A large international community works towards providing nuclear data.

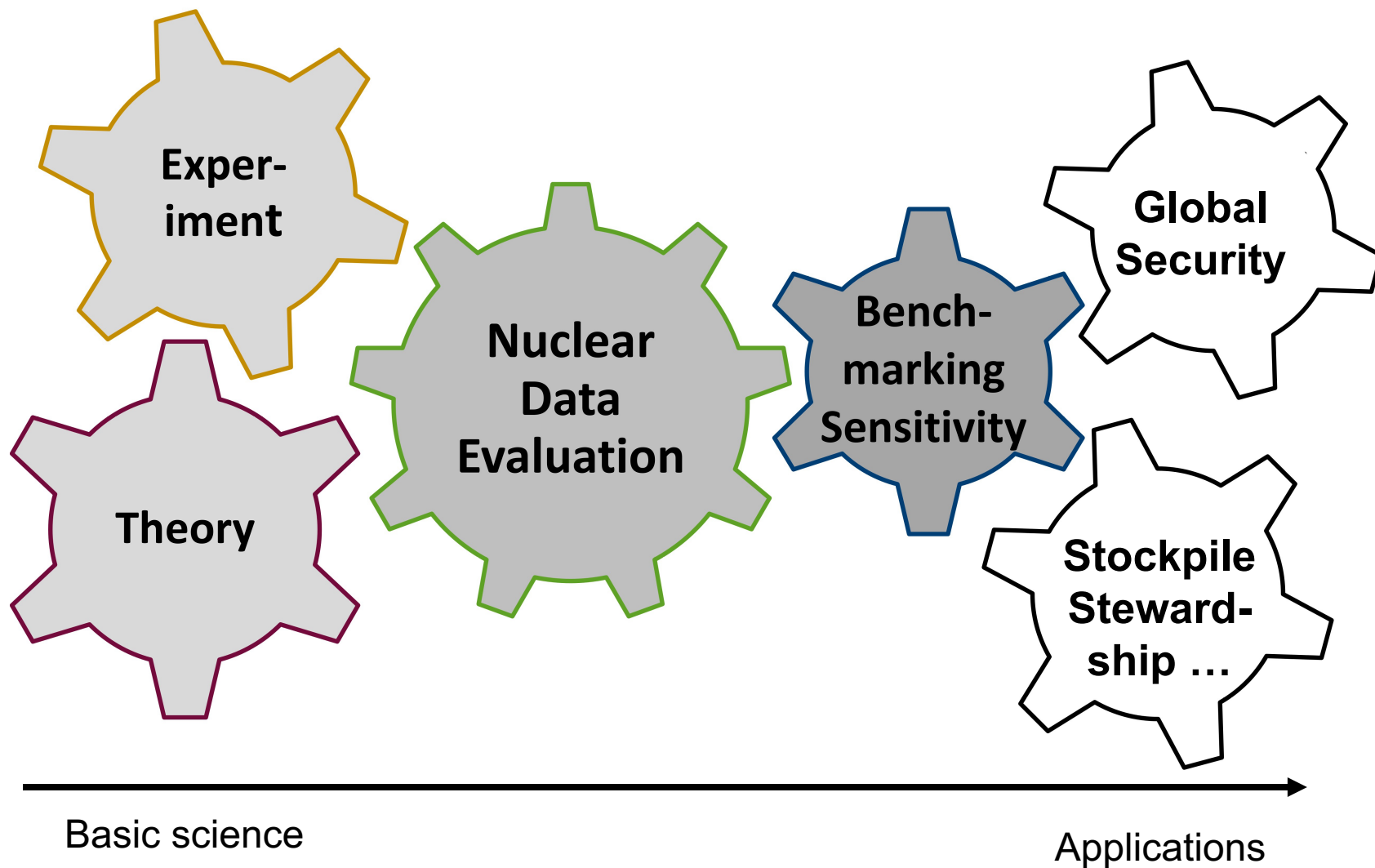


J. Spencer, J. Alwin, "Big Ten MCNP6 Unstructured Mesh Benchmark," LA-UR-19-25731 (2019).

The MCNP6[®] code makes use of nuclear data as key input for its predictive simulations used across a variety of application areas.

- Nuclear reactor physics
- Nuclear critical and subcritical experiments
- Criticality safety
- Nuclear diagnostics
- Survivability
- Intrinsic radiation
- Radiography
- Nuclear weapon effects and output
- Emergency response / nuclear threat assessments
- Nuclear safeguards and nonproliferation
- Radiation detection and analysis
- Medical and health physics

Evaluated nuclear data are produced in a complex pipeline from basic science to applications.



What are typical nuclear physics observables?

In our nuclear data libraries we store:

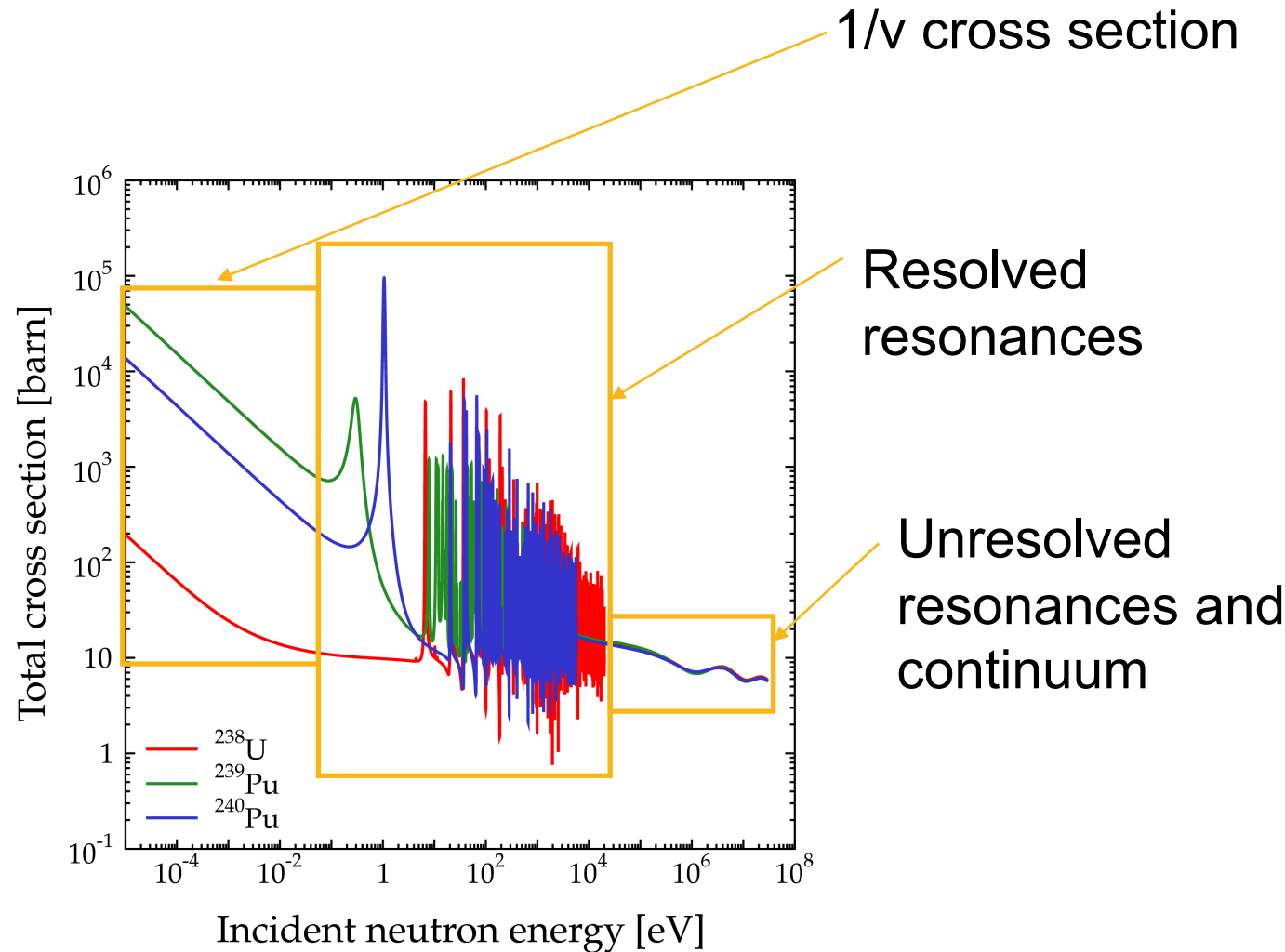
- Particle induced (mostly neutrons) cross-section
- Secondary particle angular distributions
- Secondary particle energy distributions
- Decay data
- Uncertainties (variances and covariances)
- ...

In ENDF-6 format that is processed into ACE format that can then be read by MCNP (see more about that in symposium talks by Wim Haeck, Bobbi Riedel and Noah Kleedtke).

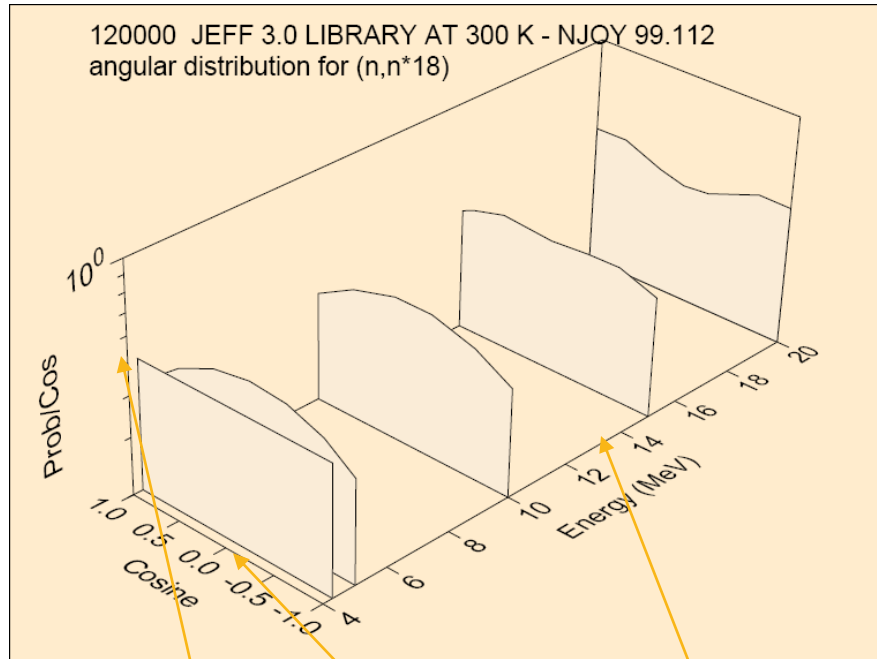
What are cross-sections? – A cross-sections gives the reaction probability

$^{238}\text{U}(n,\text{tot})$ means:
“ ^{238}U ” ... target nucleus is ^{238}U
“(n,” ... neutron in
“tot)” ... all particles out of the reaction

Parts from W. Haeck, LA-UR-18-22218.



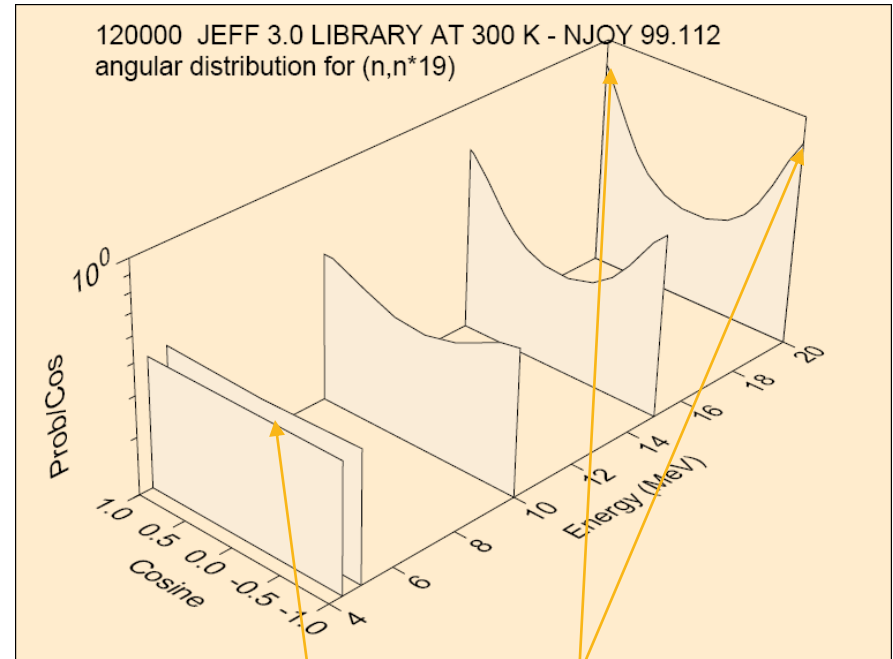
What are angular distributions? – Gives the probability for outgoing particle at specific angle



Probability

Incident energy

Outgoing cosine



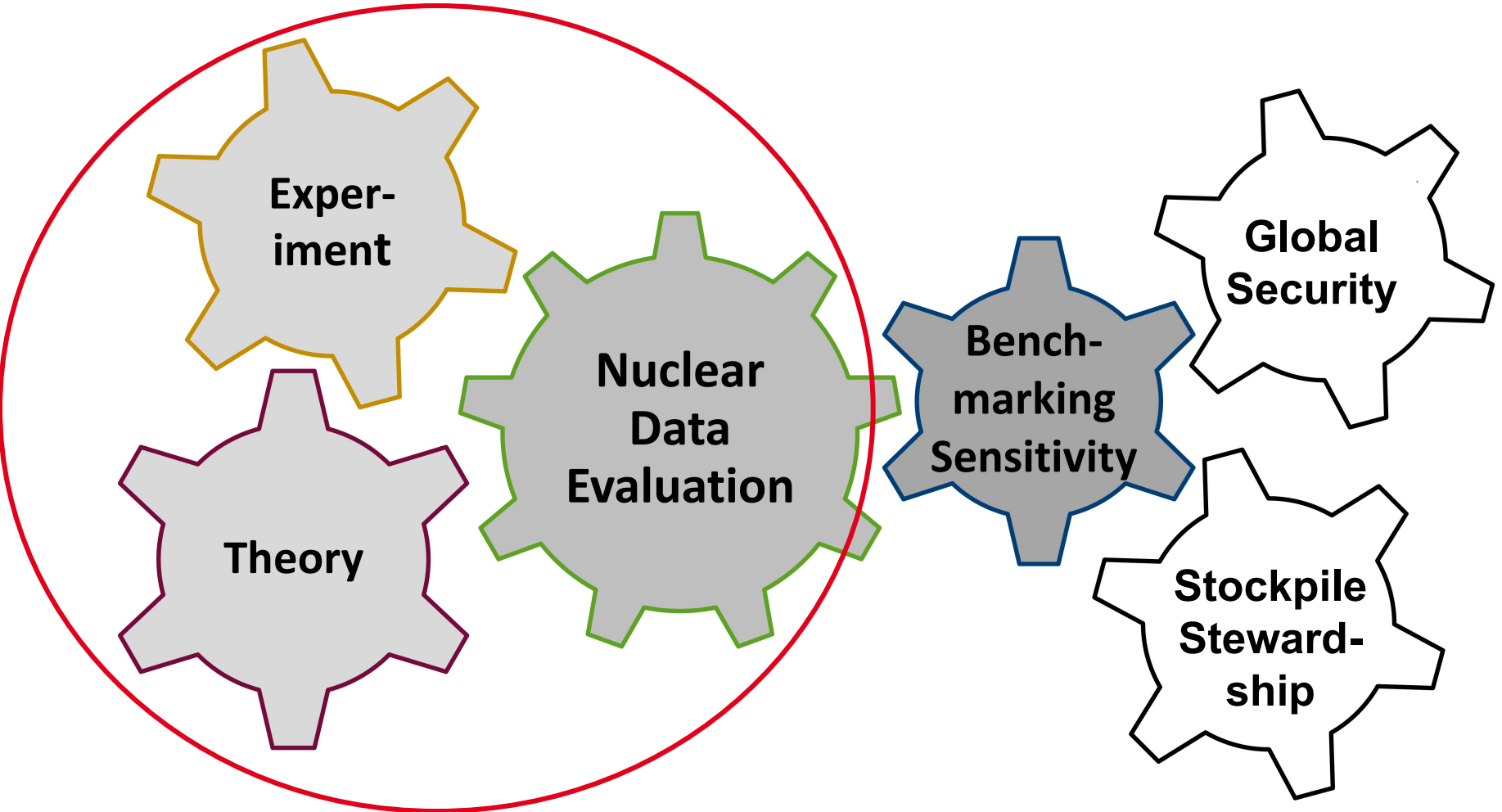
Isotropic

Strong forward and backward emission

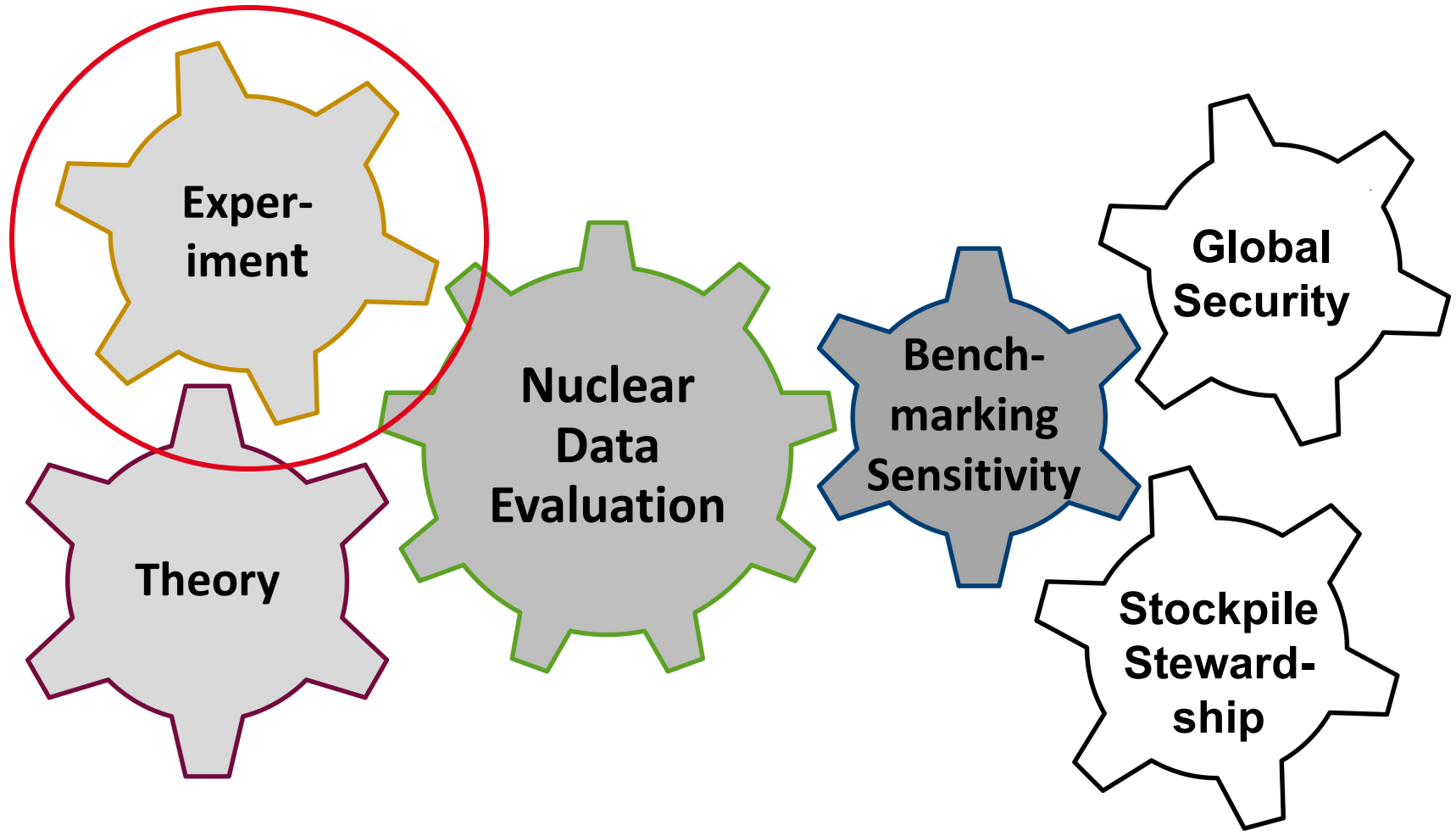
From W. Haeck, LA-UR-18-22218.

- **How are evaluated nuclear data obtained?**
- **What are they needed for?**
- **Who works on nuclear data evaluation at LANL/ US/ internationally?**

Complete data are obtained by statistically combining several experiments and/or models.



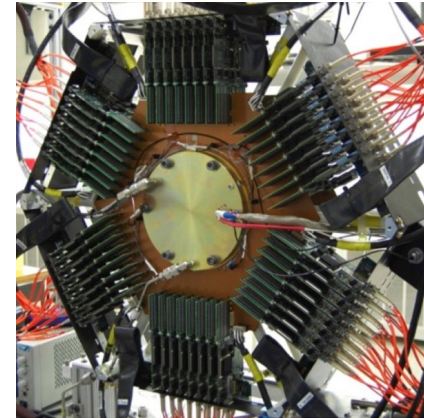
Differential experimental data:



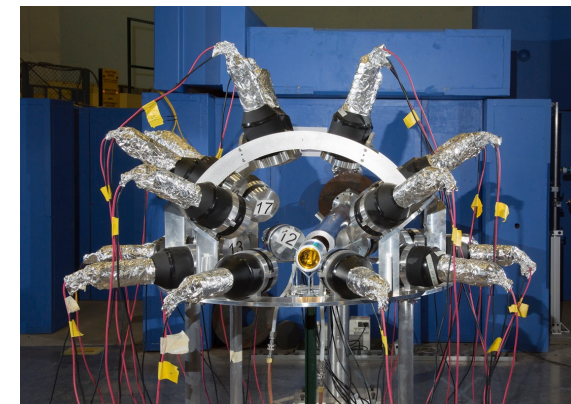
Differential experimental data are measured in dedicated nuclear physics experiments.

- We term experimental data “differential” if:
 - same observable is measured as evaluated,
 - Inform the model used for the evaluation.
- Data are measured at **LANL** by **P-Division and CNR experimentalists at LANSCE**, e.g., TPC, Chi-Nu or at ORNL, ANL, LLNL, RPI, CERN, etc.
- ***Evaluators pass judgment on the data, i.e., we update and change experimental uncertainties, truncate data and might even change mean values!***

NIFFTE TPC for (n,f)



Chi-Nu for PFNS



Data can be extracted from EXFOR: <https://www-nds.iaea.org/exfor/exfor.htm>



Experimental Nuclear Reaction Data (EXFOR) Database Version of 2023-08-16

Software Version of 2023-08-31

The EXFOR library contains an extensive compilation of experimental nuclear reaction data. Neutron reactions have been compiled systematically since the discovery of the neutron, while charged particle and photon reactions have been covered less extensively. [EXFOR Reference Paper: Nucl. Data Sheets 120\(2014\)272, \[arxiv\]](#). EXFOR Web database retrieval system provides: data search, output to various formats (incl.XML), plotting and comparison to ENDF, re-normalization old data to new standards, calculating data for inverse reactions and kinematics, constructing correlation matrices from partial uncertainties, etc. [EXFOR Web Database & Tools Paper: NIM A 888 \(2018\) 31, \[arxiv\]](#). The EXFOR database contains data from **24683** experiments (see [statistics](#) and recent database [updates](#)). Mirror-sites [+](#)

Search: [?](#)

Examples of requests: [1](#)[2](#)[3](#)[4](#)[5](#)[6](#)[7](#)...

Go to: [\[upload your data\]](#); [EE-View:CS,CS1,DA](#)

Request

Target	<input type="checkbox"/>	<input type="text"/>	?
Reaction	<input type="checkbox"/>	<input type="text"/>	?
Quantity	<input type="checkbox"/>	<input type="text"/>	?
Product	<input type="checkbox"/>	<input type="text"/>	?
Energy from	<input type="checkbox"/>	<input type="text"/>	to <input type="checkbox"/>
Author(s)	<input type="checkbox"/>	<input type="text"/>	?
Publication year	<input type="checkbox"/>	<input type="text"/>	?
Last modified	<input type="checkbox"/>	<input type="text"/>	?
Accession #	<input type="checkbox"/>	<input type="text"/>	?

- [Extended](#)
- [Keywords](#)
- [Expert](#)
- [Evaluator](#)

Submit in new Window

Options

<input checked="" type="checkbox"/>	Exclude superseded data
<input type="checkbox"/>	No reaction combinations (ratios,...)
<input checked="" type="checkbox"/>	Exclude evaluated/calculated data
<input checked="" type="checkbox"/>	Enhanced search of Products
<input type="checkbox"/>	Show evaluators flags //2021
<input type="checkbox"/>	Retrieve listing only
<input type="checkbox"/>	Disable Prompt-help
Sort by: <input checked="" type="radio"/> reaction <input type="radio"/> publication	
View: <input type="radio"/> basic <input checked="" type="radio"/> extended	

Ranges (Z,A)

Reaction Sub-Fields

Feedback and User's Input

Clone Request:

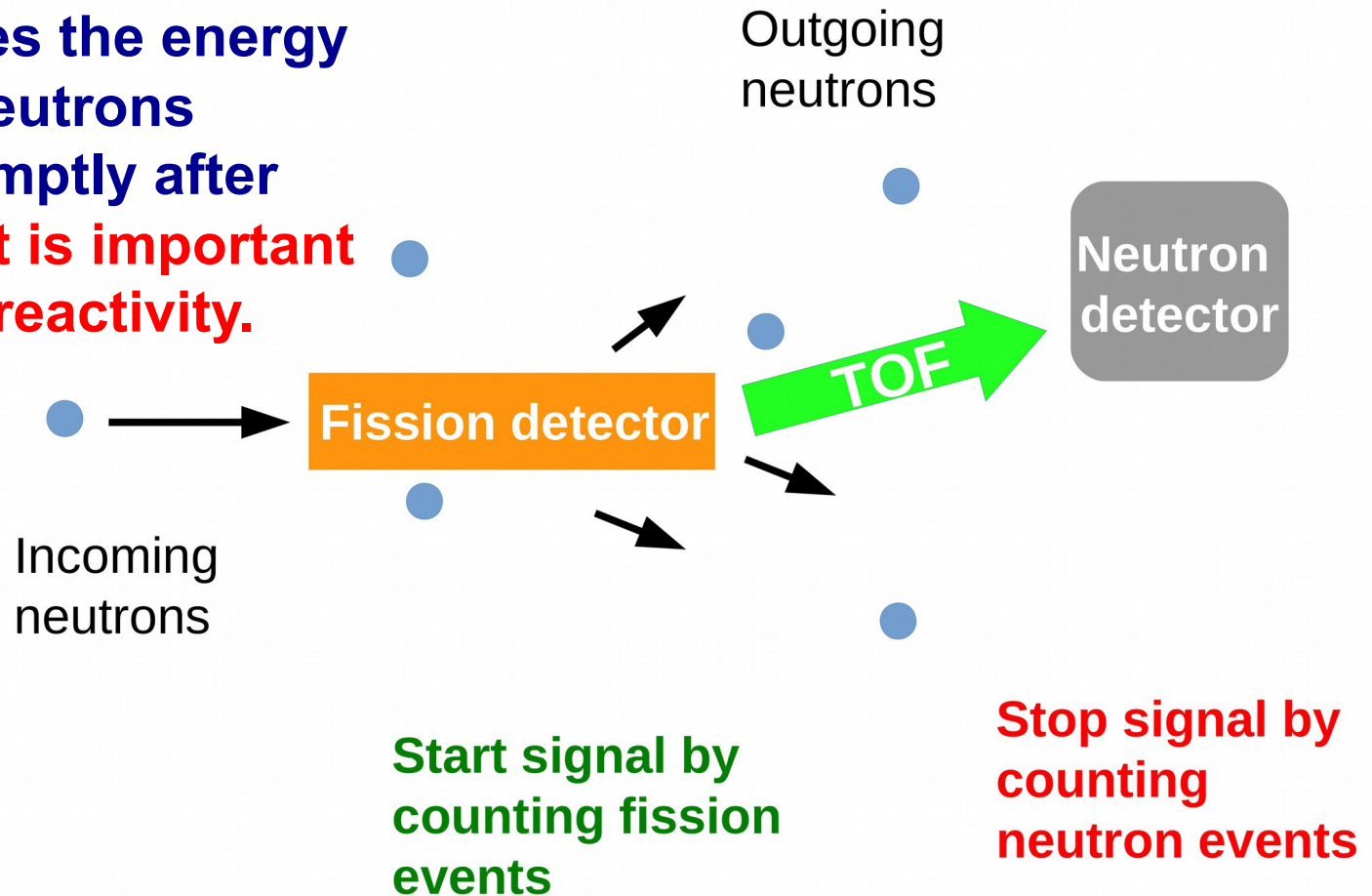
More Web Tools

[Plotting](#). See also: [\[video-guide\]](#)

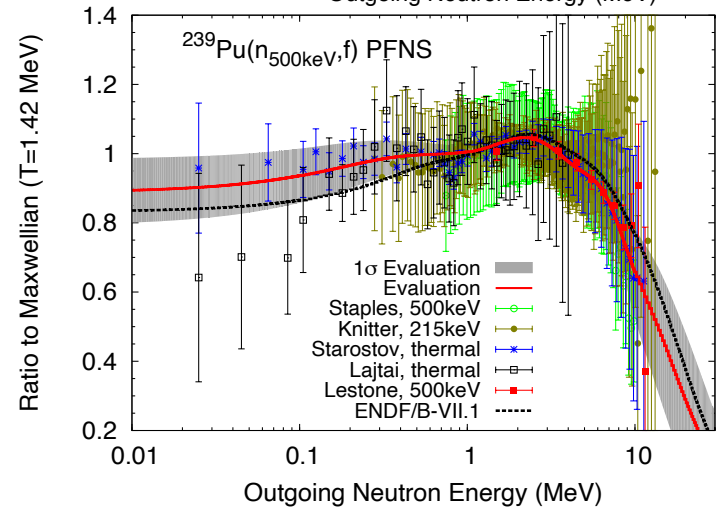
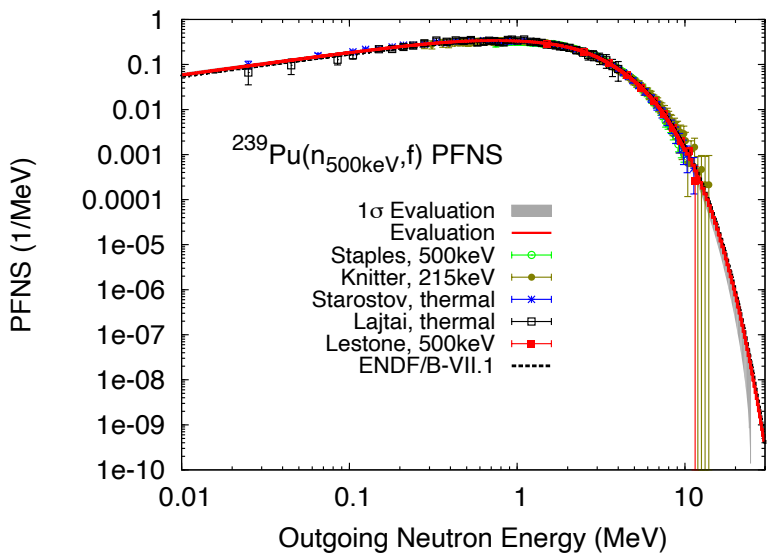
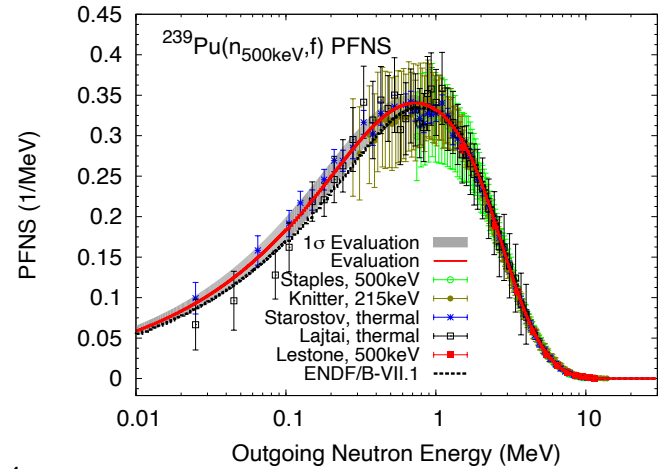
EXFOR is maintained by NRDC which includes NNDC/ BNL, IAEA, NEA, etc.

The observable used throughout this talk: the ^{239}Pu prompt fission neutron spectrum (PFNS)

A PFNS gives the energy distrib. of neutrons emitted promptly after fission [1]. **It is important to simulate reactivity.**

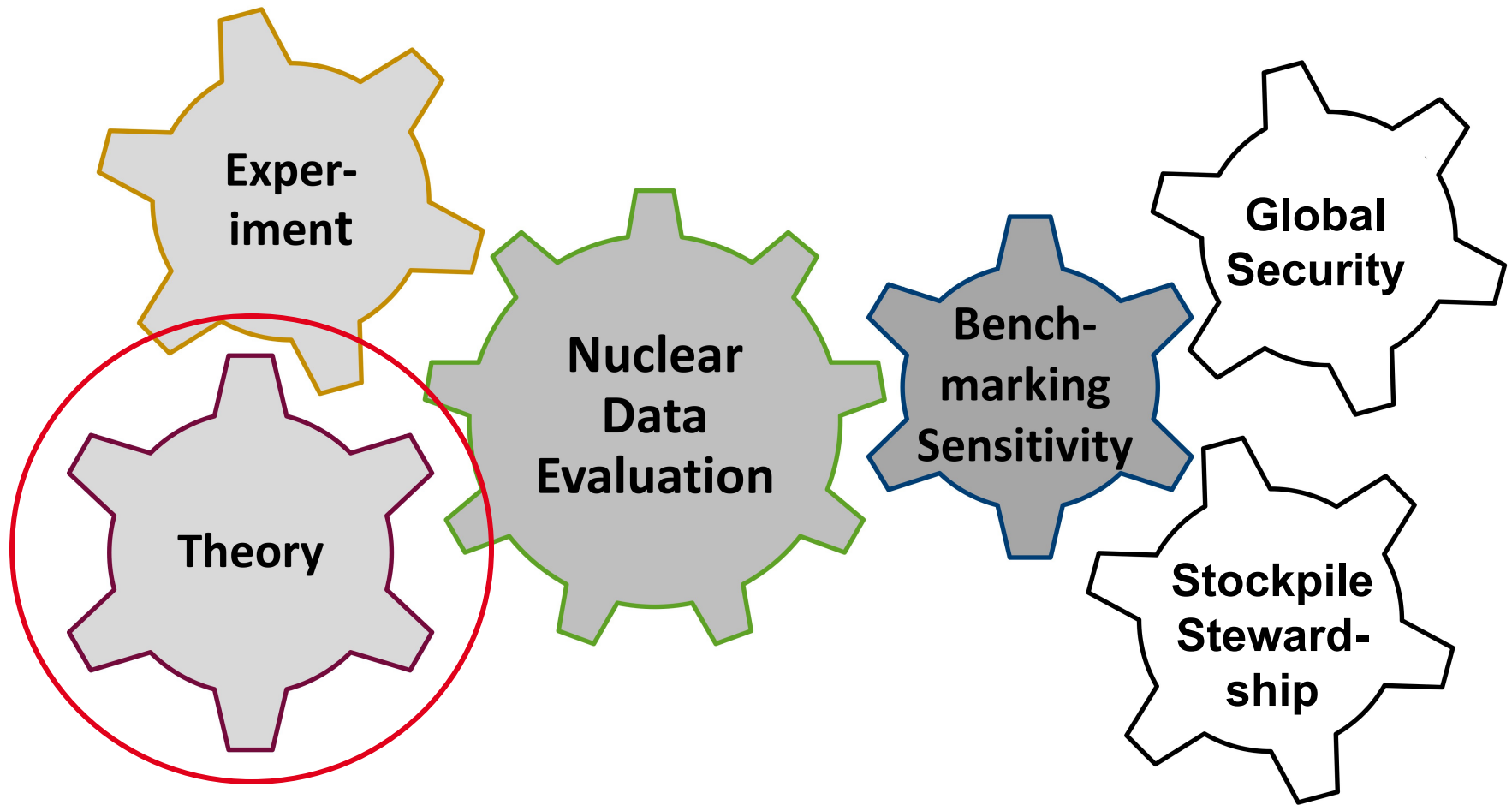


A PFNS covers many orders of magnitude.



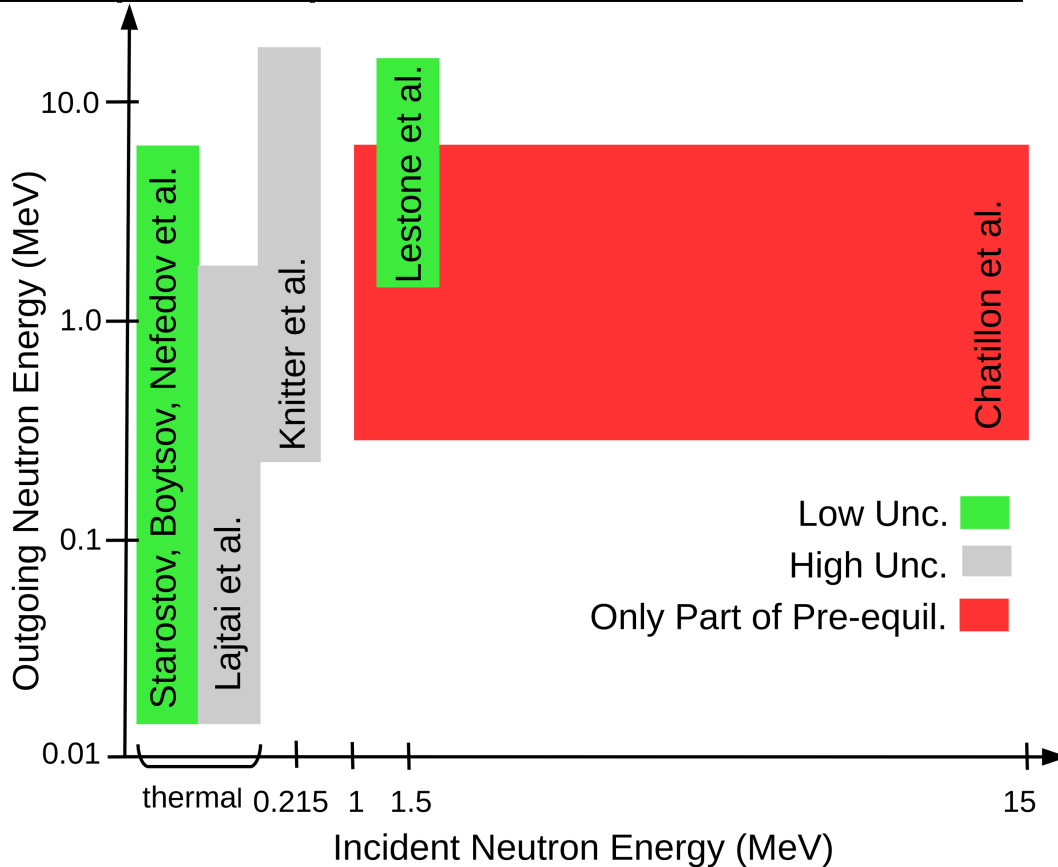
$$Maxw = C \sqrt{E} \exp(-E / T)$$

Models based on nuclear theory:



Nuclear theory models are essential in providing **COMPLETE** nuclear data.

Accepted exp. database for ^{239}Pu PFNS

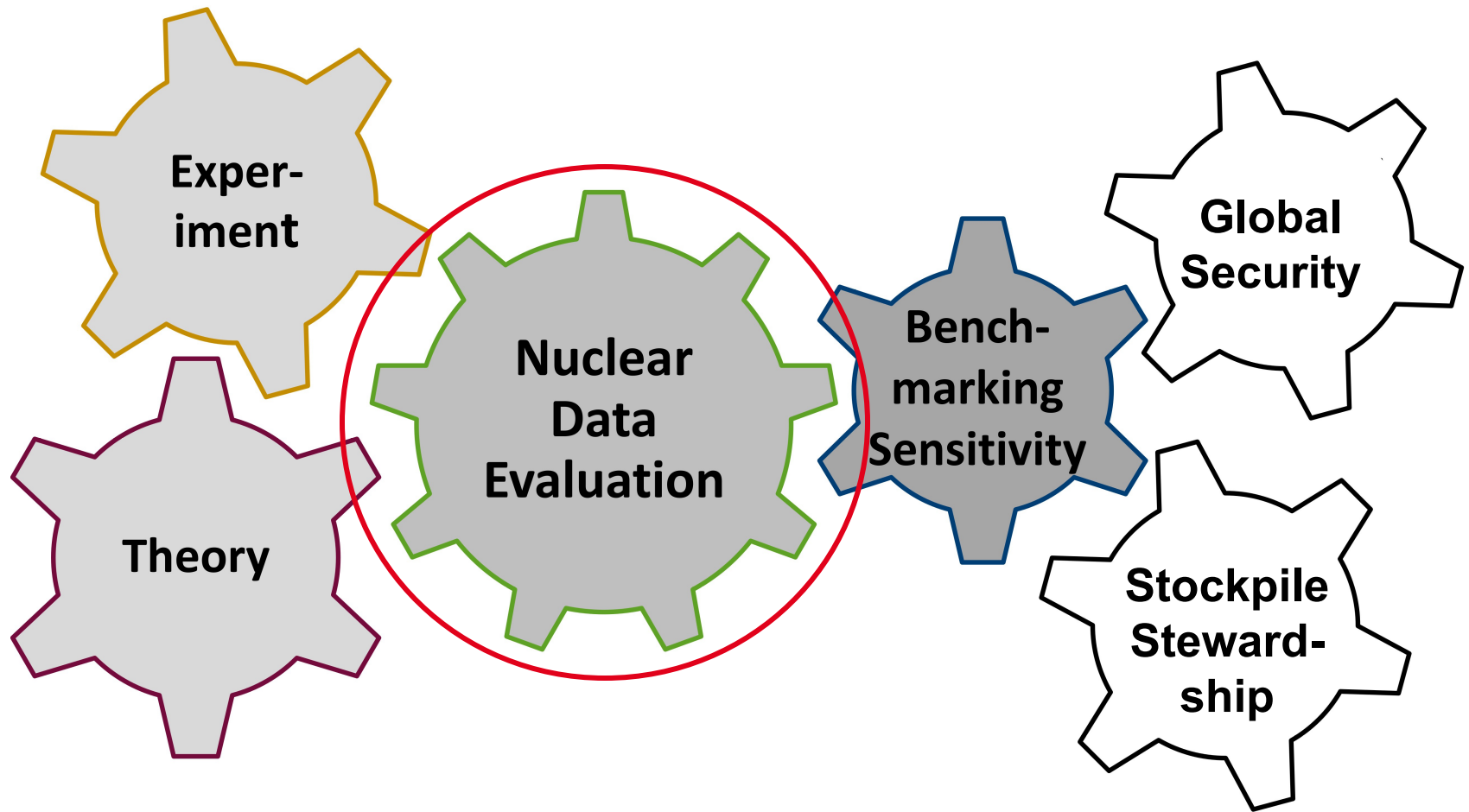


The present evaluation spans energies from thermal–30 MeV.

→ **Physics motivated evaluation only possible with model where experimental data are scarce.**

Nuclear theory and model development is undertaken at **LANL** mostly in **T-Division** but also **LLNL, IAEA, BNL, ORNL, etc.**

Nuclear data evaluation:



Generalized least squares is an algorithm often used for evaluations.

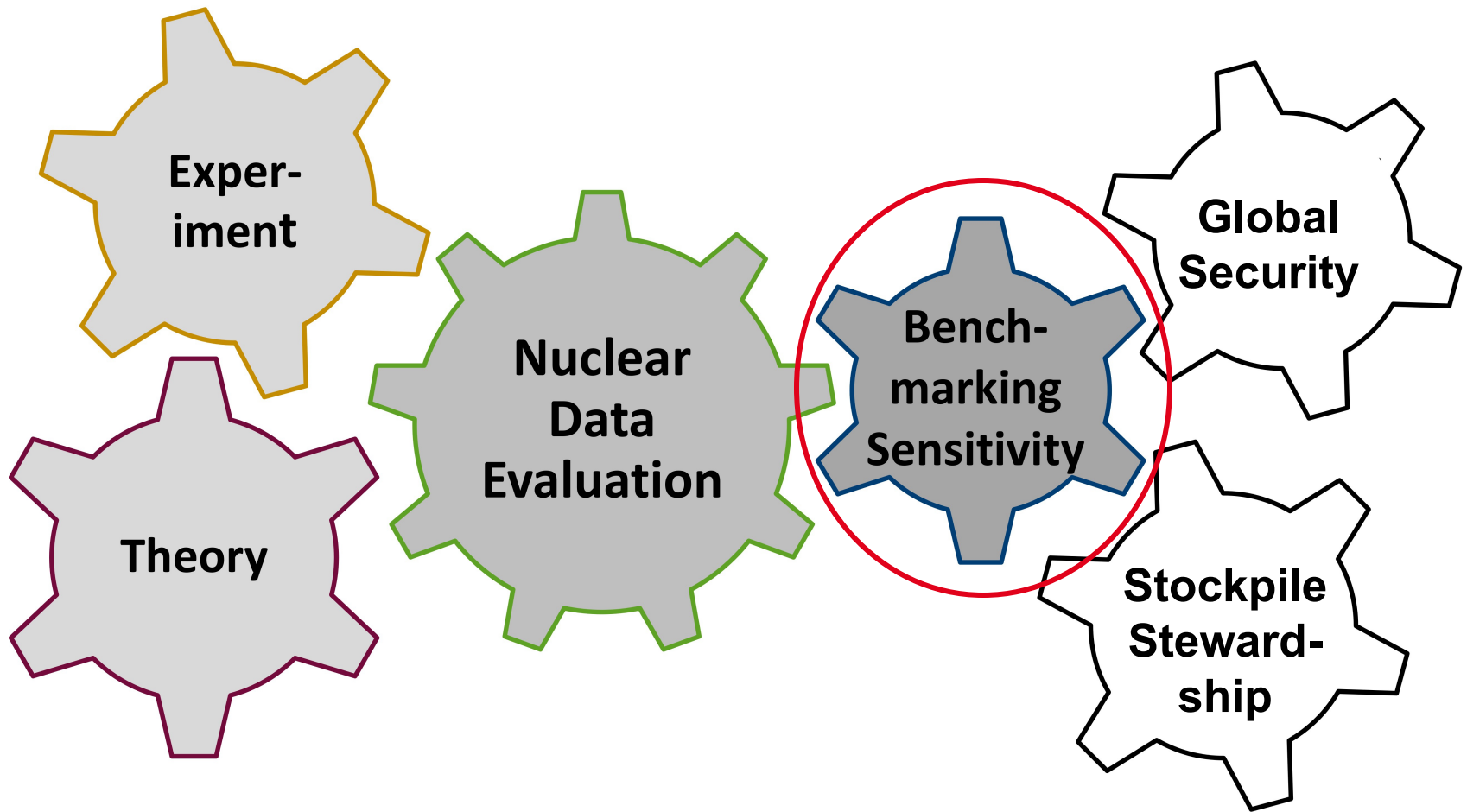
The **generalized least squares algorithm** combines **model (“M”)** and **experimental mean values (“x”)** and their associated covariances to evaluated mean values and covariances (“post”).

$$\underline{\phi}^{post} = \underline{\phi}^M + \mathbf{Cov}^{post} \mathbf{S}^+ (\mathbf{Cov}^x)^{-1} (\underline{\phi}^x - \mathbf{S} \underline{\phi}^M),$$
$$\mathbf{Cov}^{post} = \mathbf{Cov}^M - \mathbf{Cov}^M \mathbf{S}^+ (\mathbf{S} \mathbf{Cov}^M \mathbf{S}^+ + \mathbf{Cov}^x)^{-1} \mathbf{S} \mathbf{Cov}^M$$

S: design matrix that transforms from model parameter space to observable space or from energy of model to experimental one.

LANL evaluations are undertaken in **T-2** and **XCP-5**, algorithms are investigated there with support from **CCS**. BNL, ORNL, LLNL, RPI, LANL, IAEA, NNL, etc., contribute to US nuclear data libraries.

The data are validated & adjusted by simulating and comparing to *integral experiments*.



The *integral experiment* used throughout this talk: the Jezebel critical assembly

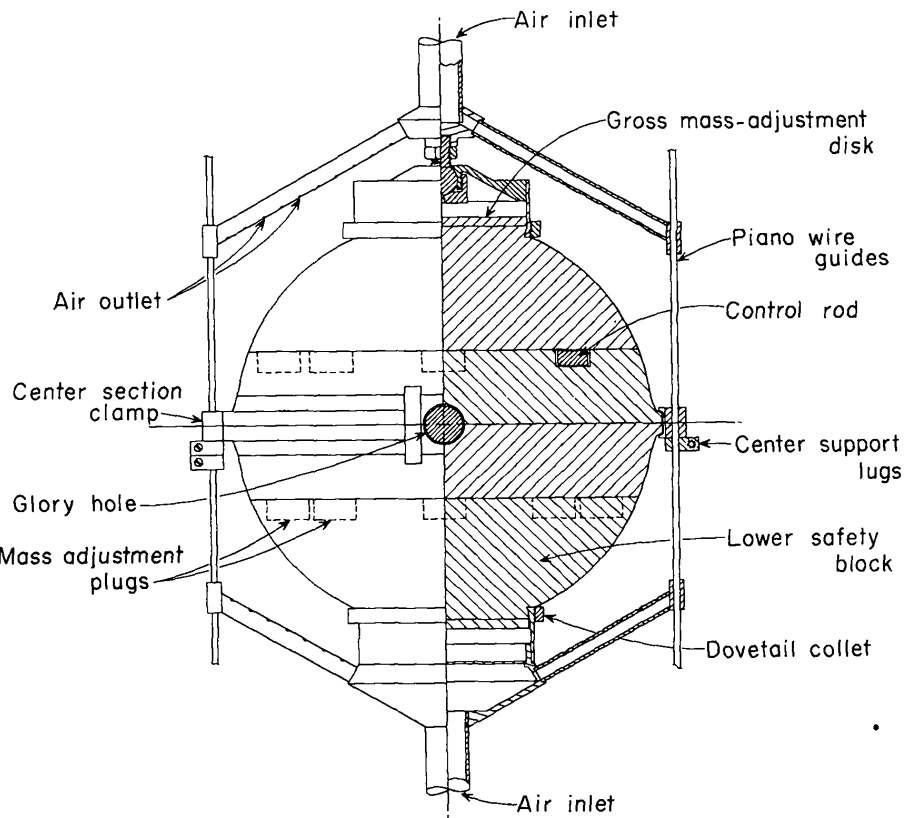


Figure taken from Hansen et al., LA-4208 (1969).

- Minimally reflected, nearly spherical Pu critical assembly.
- Effective multiplication factor $k_{\text{eff}} = 1$ \longrightarrow **as many neutrons are produced as are lost.**
- **PFNS, neutron multiplicity, (n,f) cross section, etc. enter neutron transport simulations of k_{eff}**
- **Simulated, e.g., with MCNP and PARTISN of XCP/CCS. Validated in T-2, XCP-5, XCP-3. XCP-7 at LANL, Exp. in NEN-2.**

210 pcm is the difference between a controlled & un-controlled nuclear reaction in a Pu-system

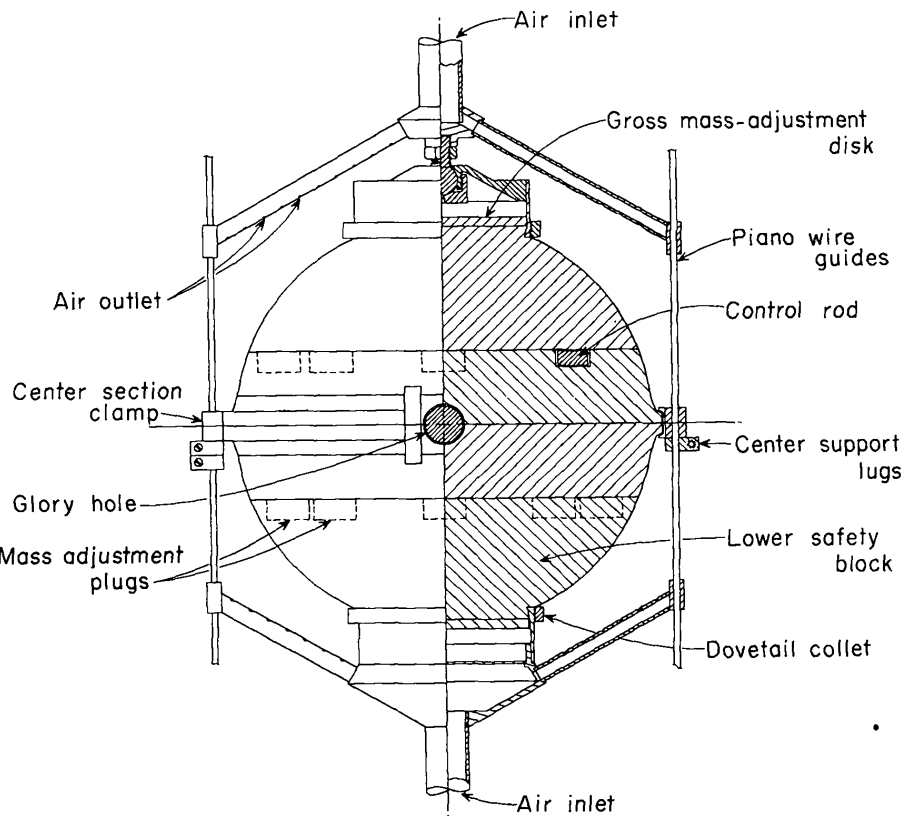
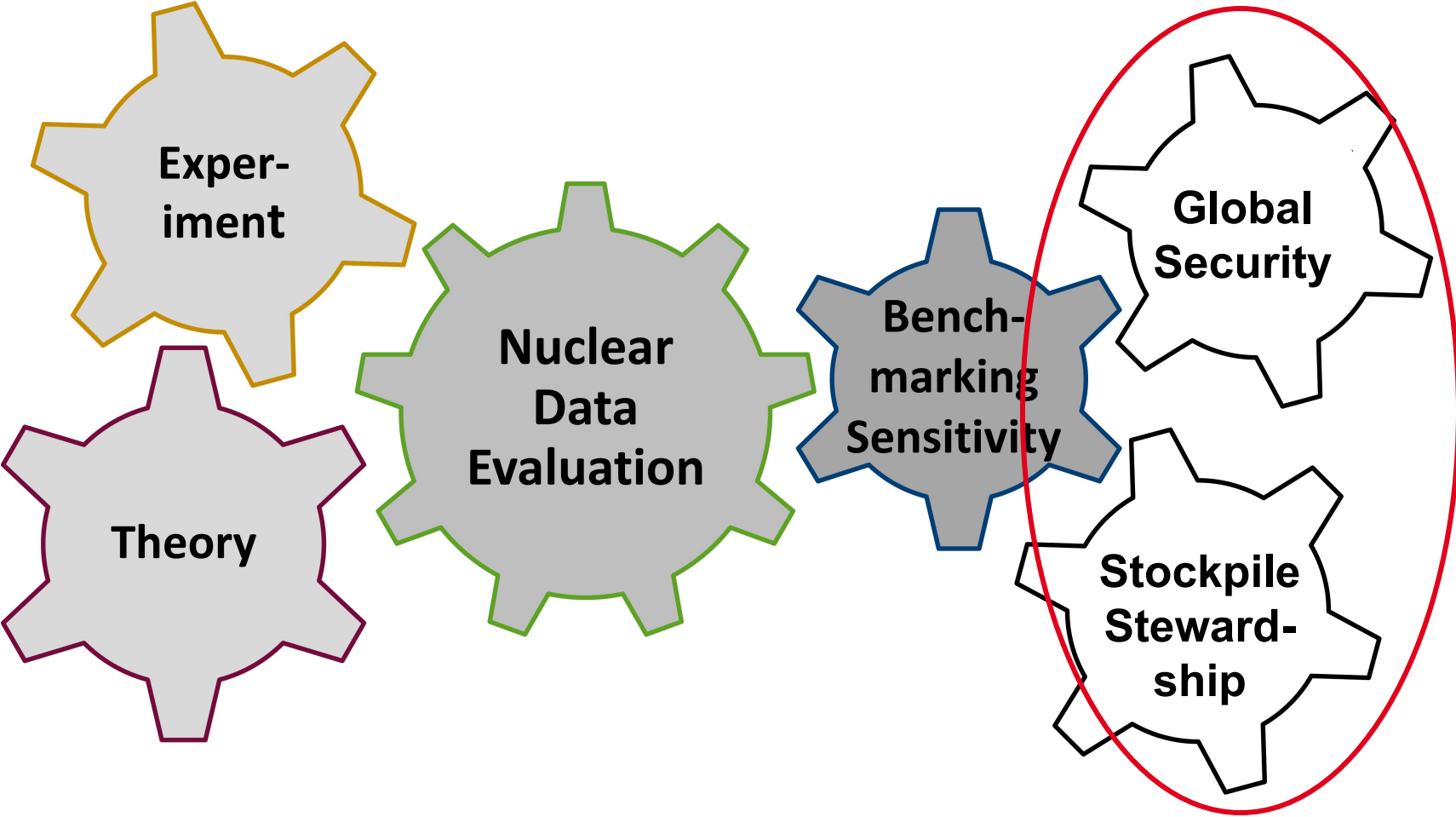


Figure taken from Hansen et al.,
LA-4208 (1969).

- Jezebel is a calibration point for **nuclear data libraries**. They **are adjusted to give 1.000 ± 0.0007**
- uncertainty $\sim 100\text{-}200$ pcm.
($1.0 + 100$ pcm = 1.001)
- **A change of 270 pcm could be the difference between a controlled and uncontrolled nuclear reaction.**
- Calculated $k_{\text{eff}} = 0.9976 \pm 75$ pcm for the example of this talk.

Nuclear data are used for nuclear application calculations.



After successful validation, data are stored in nuclear data libraries.

ENDF/B-VIII.1 coming soon (spring 2024)

Evaluated Nuclear Data File (ENDF) Database Version of 2023-08-25

Software Version of 2023-08-31



News & History

2023/08 Updated **JENDL-5** Japanese evaluated nuclear data library (2021) **Errata** including update-13, August 10, 2023 [page]
2023/08 New library: **INDEN-Aug2023** evaluations produced by International Nuclear Data Evaluators Network (coord. by the IAEA) [page]
2023/03 New software feature: plotting covariances of the average number of neutrons per fission MF31 [example]
2023/02 New software tool: **EE-View** - fast experimental-evaluated data viewer [about] → go to SIG:[eeview][eeview1]; DA:[eeview-da]
2022/10 New software feature: plotting covariances for angular distributions of secondary particles MF34 [example]

Core nuclear reaction database contain recommended, evaluated cross sections, spectra, angular distributions, fission product yields, photo-atomic and thermal scattering law data, with emphasis on neutron induced reactions. The data were analyzed by experienced nuclear physicists to produce recommended libraries for one of the national nuclear data projects (USA, Europe, Japan, Russia and China). All data are stored in the internationally-adopted ENDF-6 format maintained by CSEWG. See database summary [here].

Standard Request Examples: [1](#)[2](#)[3](#)[4](#)[5](#)[6](#)[7](#) Go to: [Advanced Request](#); [ENDF-Database Explorer](#); [EE-View:CS,CS1,DA](#)

Parameters:

Submit Reset

Target >>
Reaction >>
Quantity >>

[More Parameters...](#)

Submit

Libraries: All Selected [Check](#) [Reset](#)

[How to plot](#)

- Major Libraries
 - 1) ENDF/B-VIII.0 (USA,2018)
 - 2) JEFF-3.3 (Europe,2017)
 - 3) JENDL-5 (Japan,2021)
 - 4) CENDL-3.2 (China,2020)
 - 5) BROND-3.1 (Russia,2016)
 - 6) TENDL-2021 (TALYS, 2021)
 - IAEA Project Libraries
- Special Libraries
 - Archival
 - Derived

Current major nuclear data libraries.



CSEWG assembles, validates and distributes U.S. nuclear data libraries.

<https://www-nds.iaea.org/exfor/endl.htm>

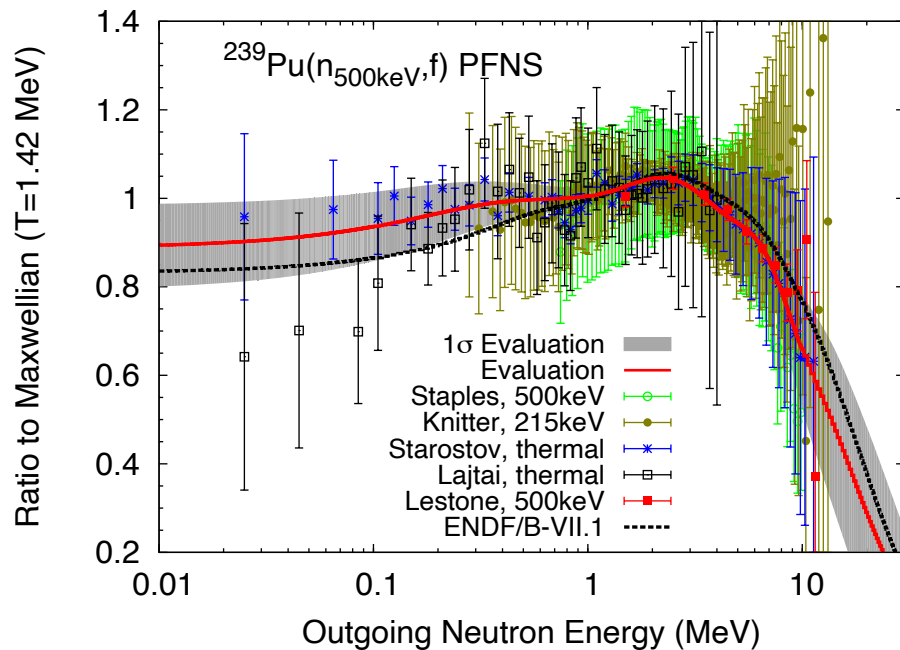
Nuclear data libraries are the pre-requisite for nuclear application calculations.

- The **general purpose libraries are often adjusted** to specific application areas **using benchmarks representing their needs.**
- **Typical application areas are:**
 - Stockpile stewardship
 - Non-proliferation, global and national security
 - Reactor physics, fusion physics and neutron dosimetry
 - Nuclear medicine, isotope production, ...
- At **LANL**, nuclear data libraries are used by **codes** such as **MCNP or PARTISN** to simulate, e.g., critical assemblies, experiments at LANSCE.

**Evaluated nuclear data and
their uncertainties evolve
over time when we gain
new physics insight!!**

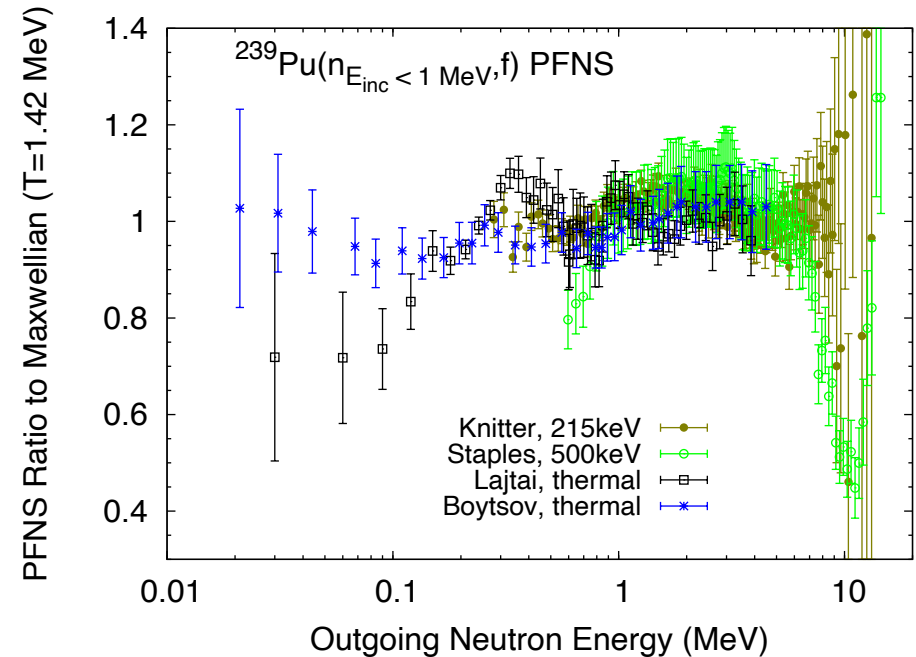
For instance: our understanding of past experiments evolves ...

Detailed uncertainty estimate



Detailed analysis of data and uncertainties for ENDF/B-VIII.0.

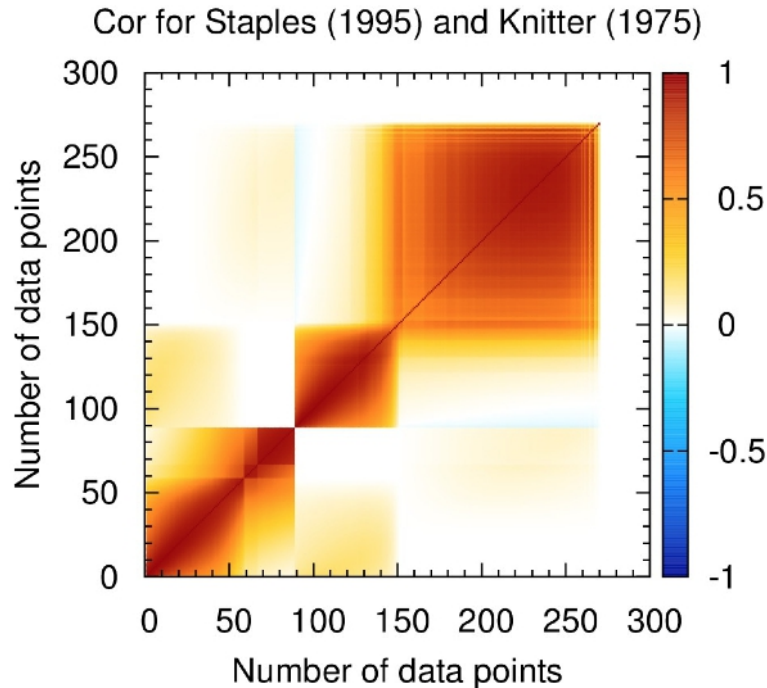
Simplified uncertainty estimate



Data and uncertainties taken as is from EXFOR for ENDF/B-VII.1!

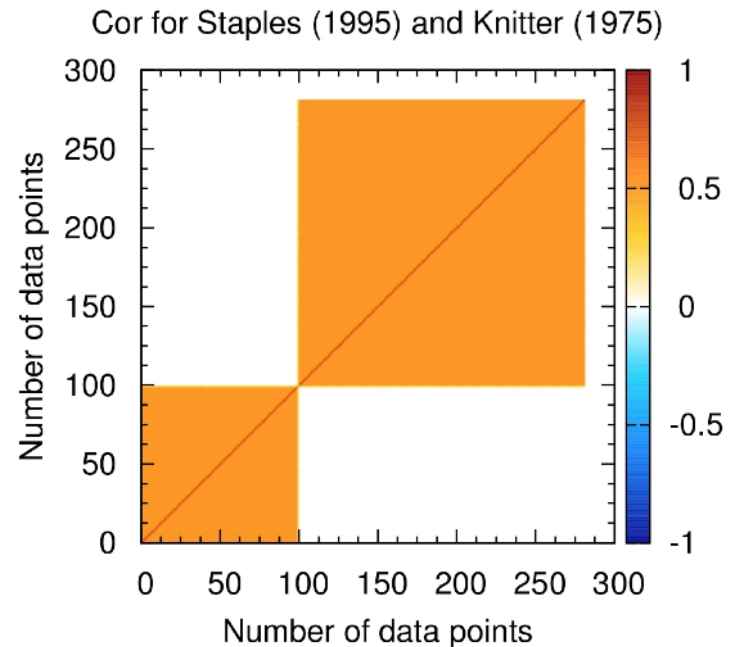
We also improve our uncertainty estimates over time ...

Detailed uncertainty estimate



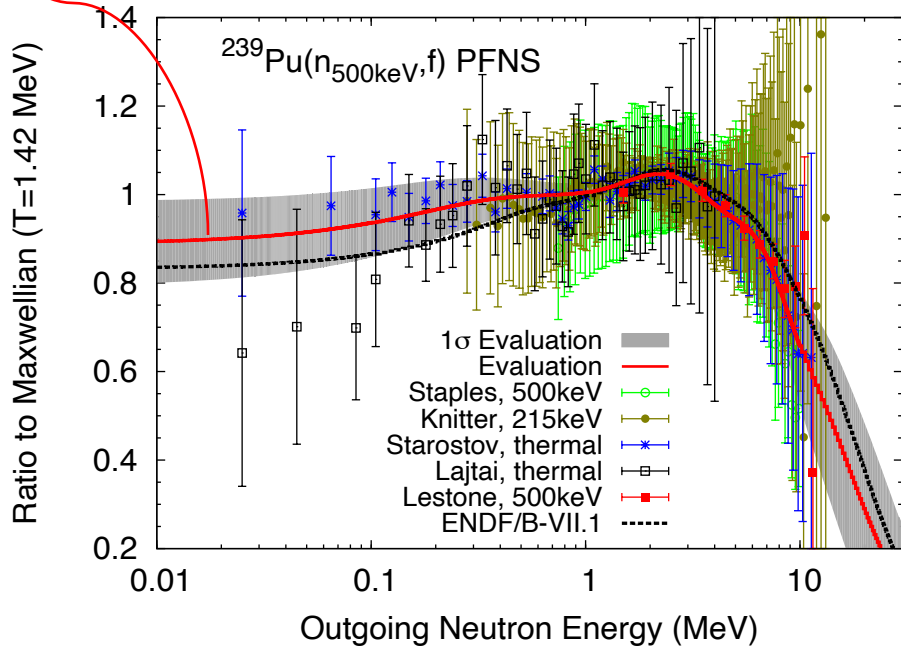
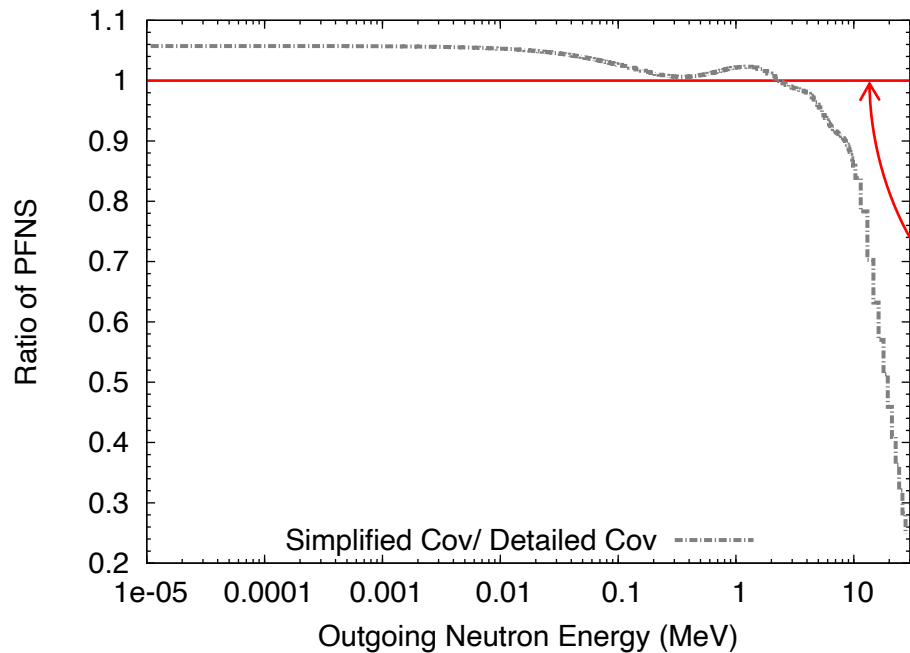
VII.0: Detailed uncertainty estimate.

Simplified uncertainty estimate

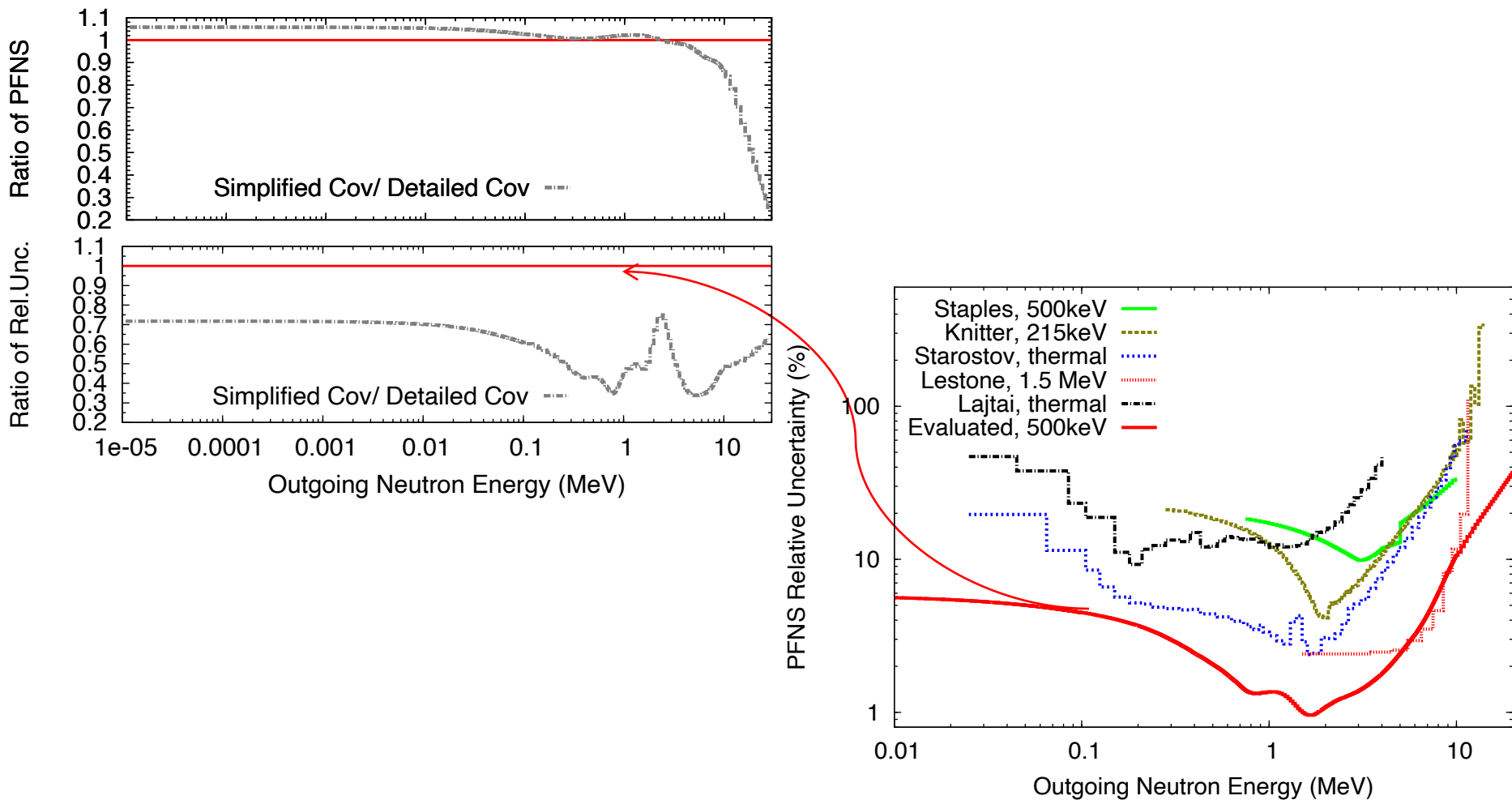


VII.1: Total uncertainties extracted from EXFOR and correlations of same exp. are 0.5, otherwise 0.

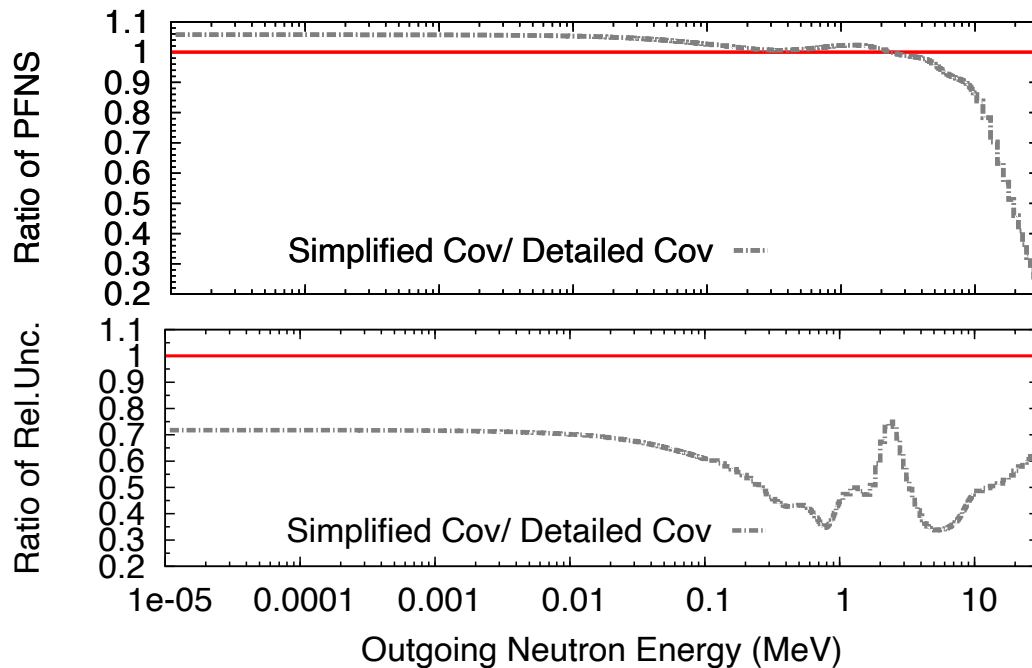
Simplified vs detailed uncertainty estimate leads to distinct change of evaluated PFNS.



Simplified versus detailed uncertainty leads to significantly underestimated evaluated unc.



Simplified versus detailed uncertainty estimate significantly impacts benchmark results.



**Change in Jezebel k_{eff} :
195 pcm !!!**

**Drop in Jezebel k_{eff}
unc. due to PFNS
uncertainty:
-69% !!!**

Questions/ Points addressed in the talk:

- **Evaluated nuclear data** are **recommended data sets of nuclear physics observables** needed for application calculations.
- Nuclear data are often **obtained by a statistical analysis of several experimental data sets and/ or nuclear physics models. Application areas** range from **global security to nuclear medicine**. Nuclear data are produced and used in many divisions at the lab.
- Evaluated nuclear data and their uncertainties **evolve over time** when we gain new insight through experimental data or nuclear models.

Further questions: nucldata@lanl.gov

Thank you for your attention!

Abstract

This talk provides an introduction to nuclear data which are key input for MCNP simulations. It discusses how nuclear data are obtained, what they are needed for and who works on producing them. Lastly, it discusses that evaluated nuclear data and their uncertainties evolve over time when we gain new insight through experimental data or nuclear models. The latter point is important to understand why MCNP results might differ if different nuclear data libraries are used as input.