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Title: What is nuclear data evaluation

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Web

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What is nuclear data evaluation

Denise Neudecker, XCP-5

Questions/ Points addressed in the talk:

- **What are evaluated nuclear data?**

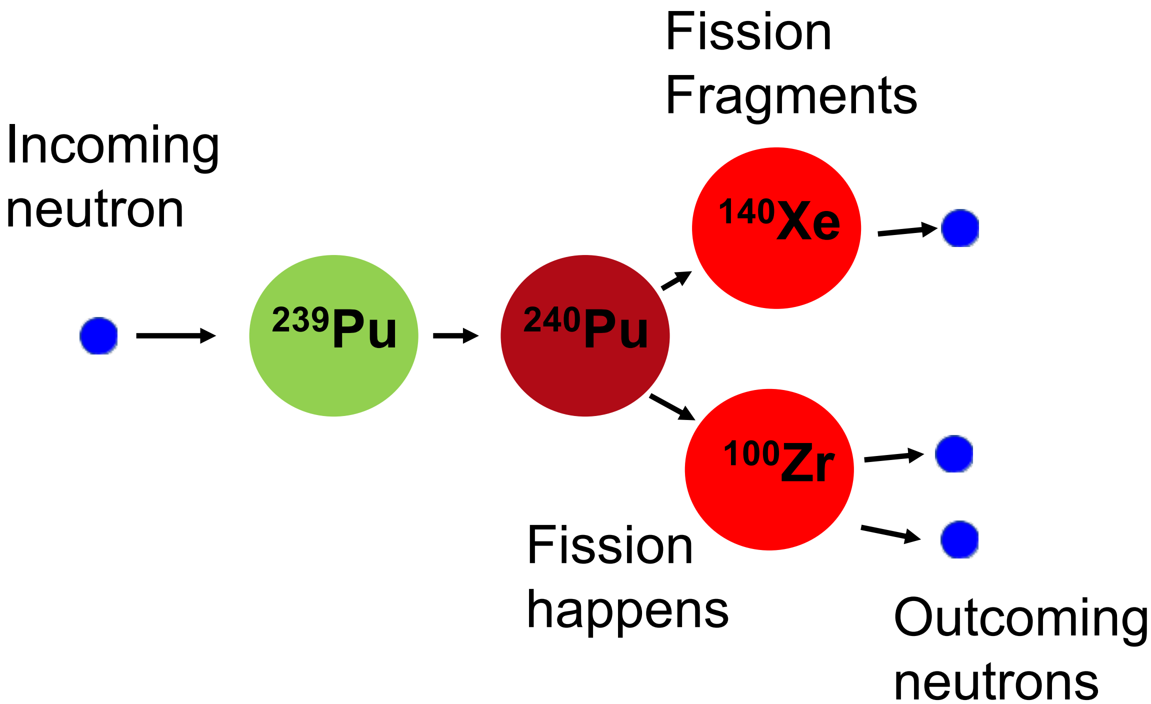
- **How are they obtained? What are they needed for? Who works on nuclear data evaluations at LANL, in the US and internationally?**

- **Evaluated nuclear data and their uncertainties evolve over time when we gain new insight through experimental data or nuclear models.**

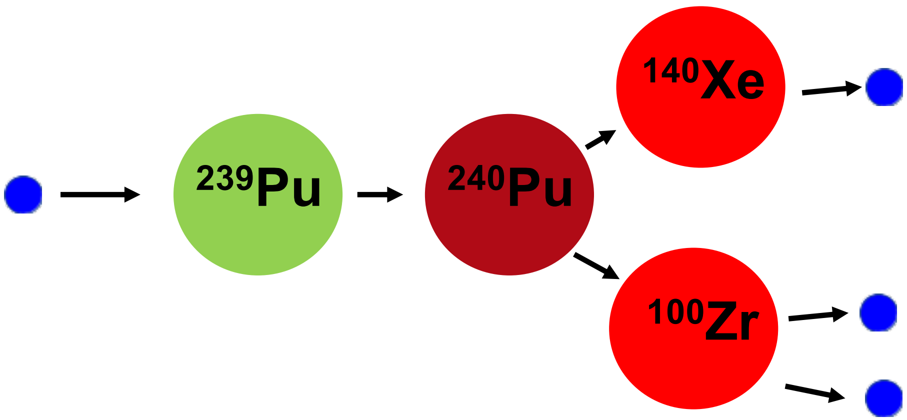
What are evaluated nuclear data?

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

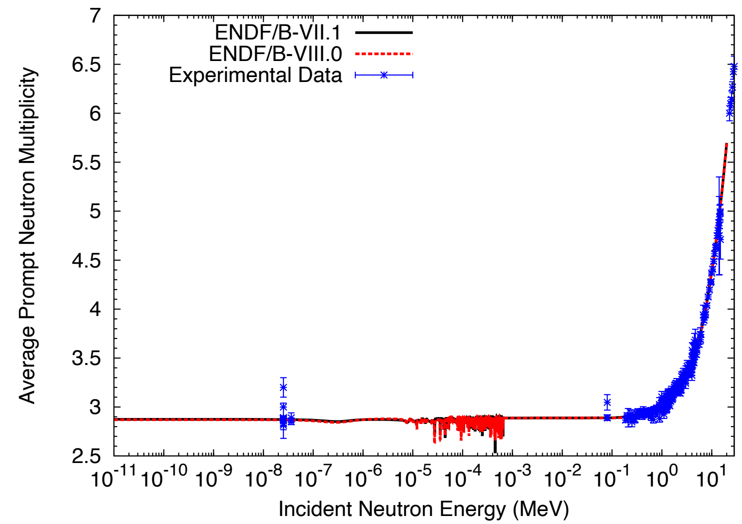
Example: neutron-induced fission on ^{239}Pu



Examples of nuclear data:



Average Prompt Neutron Multiplicity=
Av. Number of outgoing neutrons



Fission cross-section=probability that fission happens

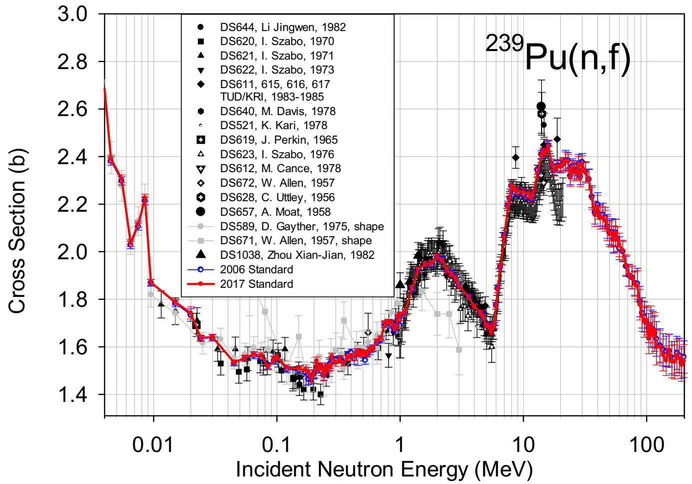
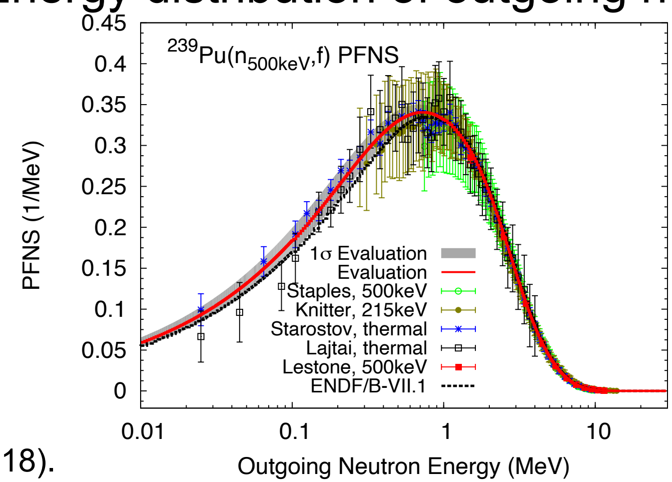


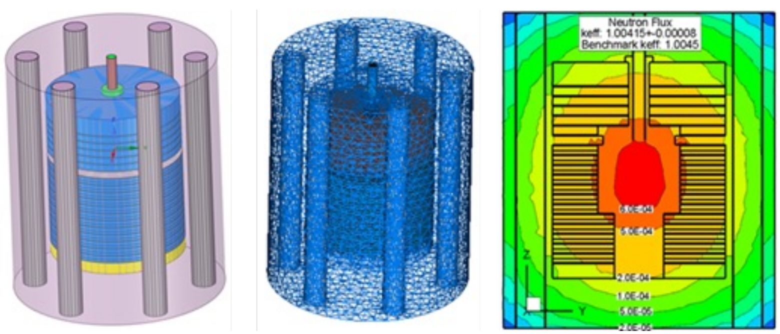
Fig. from Carlson et al., NDS 148, 143 (2018).

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.

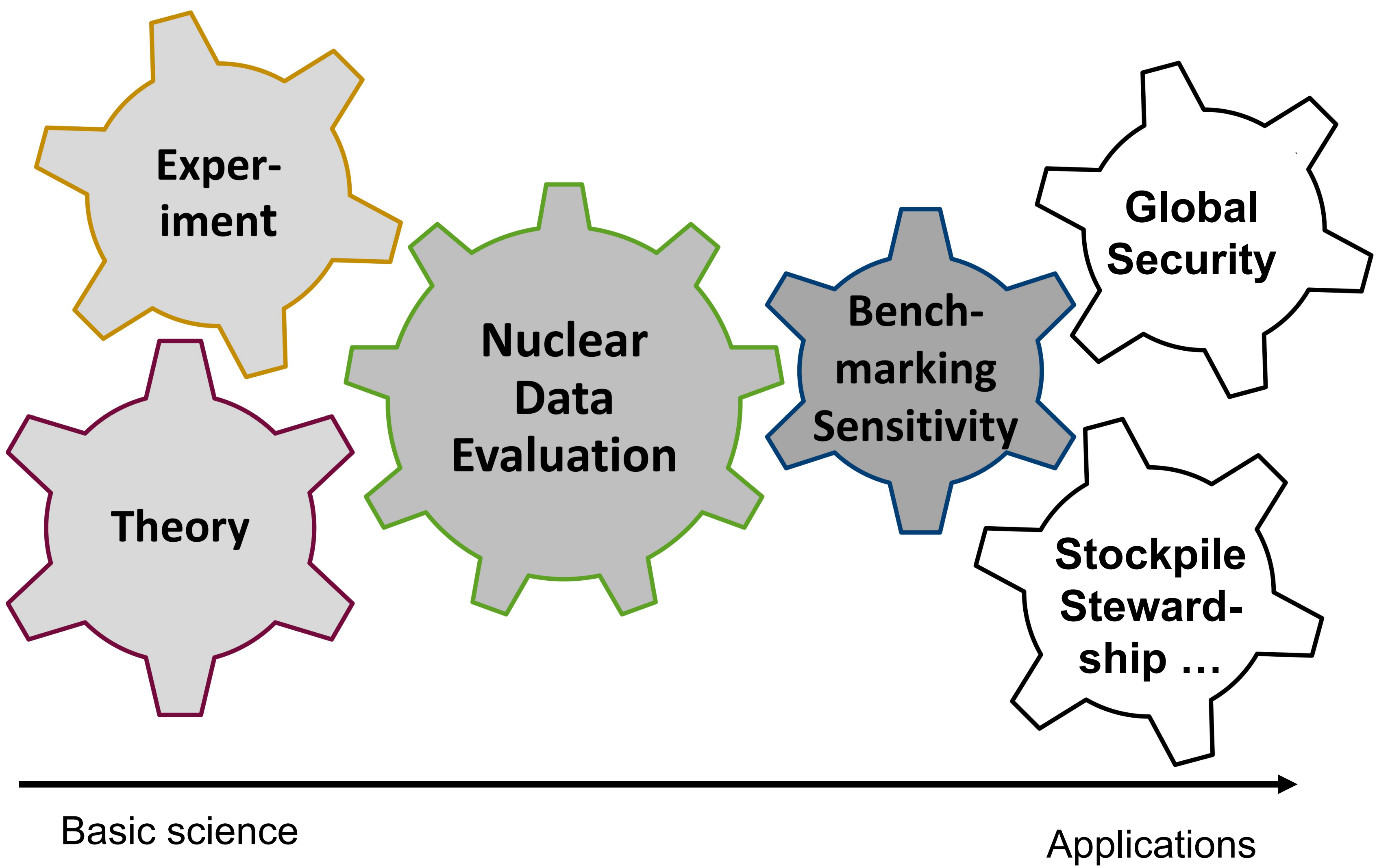


J. Spencer, J. Alwin, “Big Ten MCNP6 Unstructured Mesh Benchmark,” LA-UR-19-25731 (2019).

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:

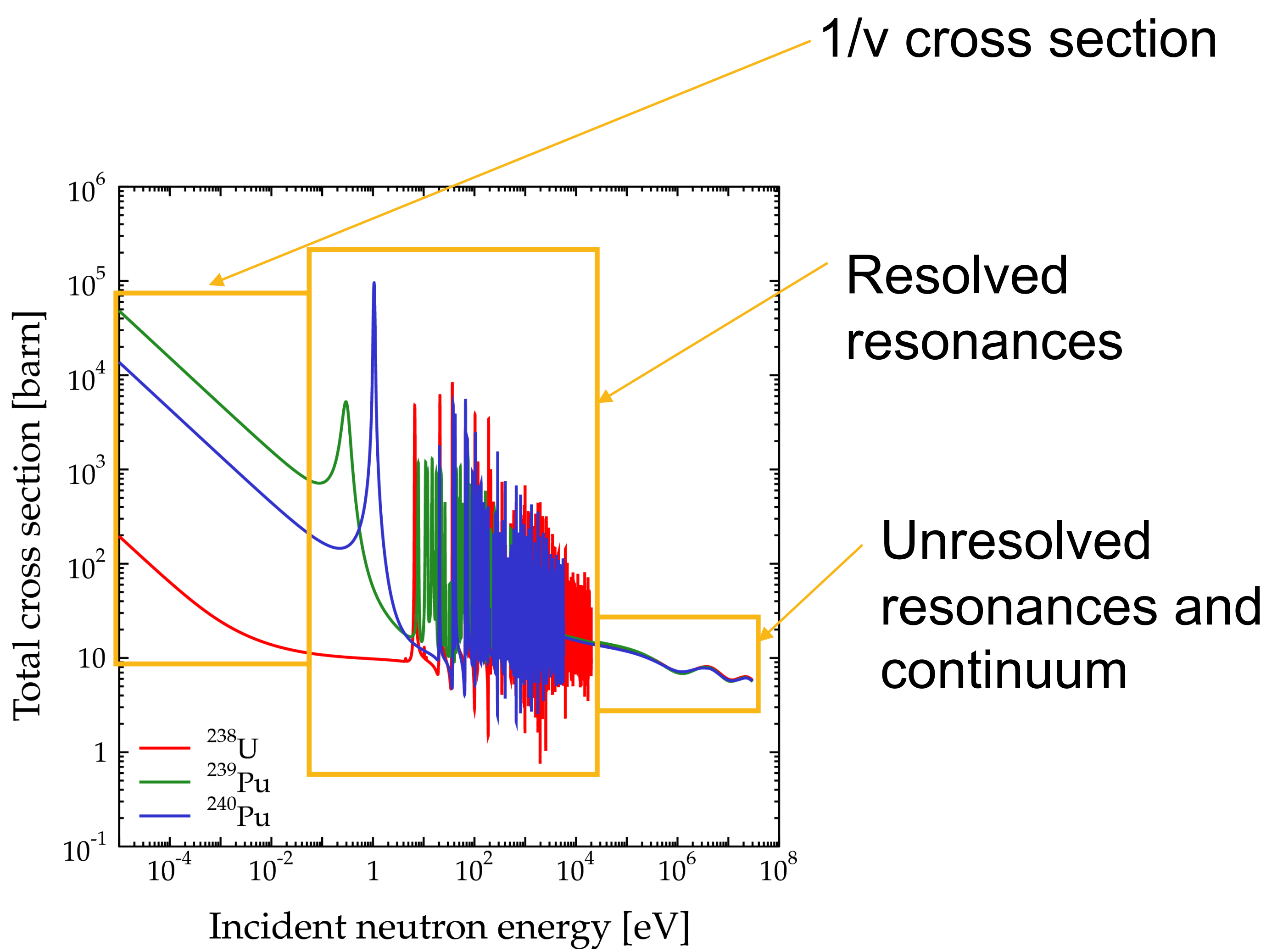
- Particle induced (mostly neutrons) cross-section
- Secondary particle angular distributions
- Secondary particle energy distributions
- Decay data
- Uncertainties (variances and covariances)
- …

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).

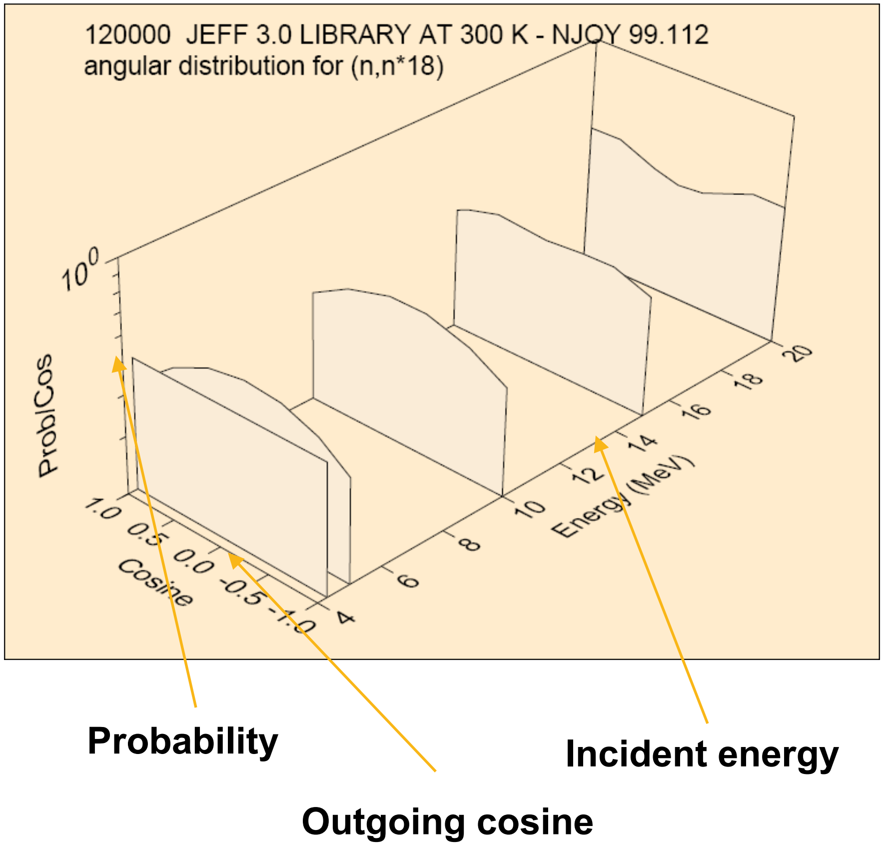
What are cross-sections? – A cross-sections gives the reaction probability

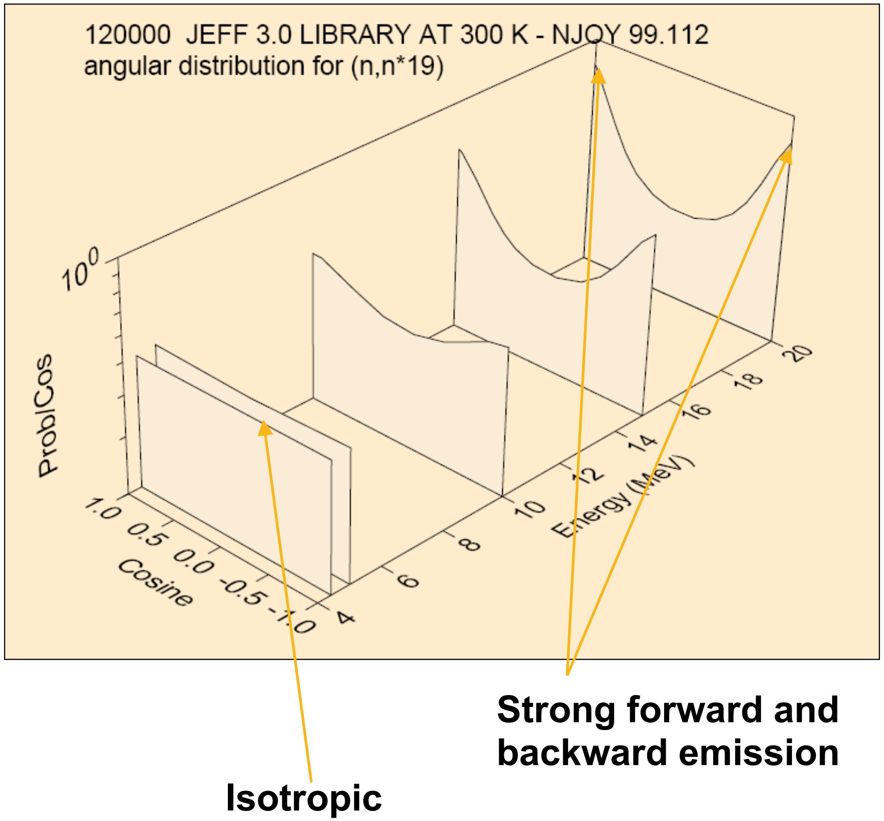
^{238}U(n,tot) means:
"^{238}U" … target nucleus is ^{238}U
"(n," … neutron in
"tot)" … all particles out of the reaction

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



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

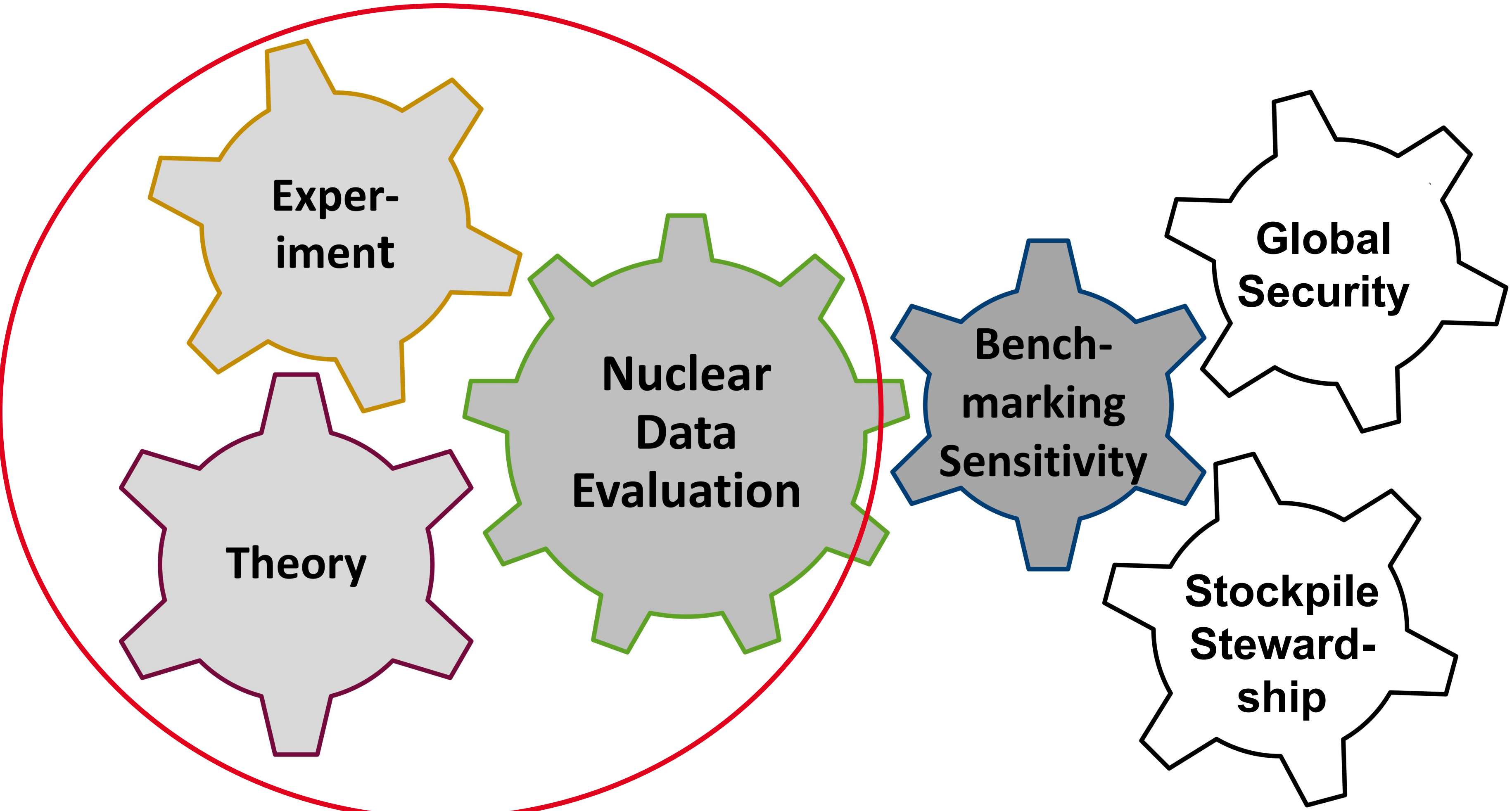




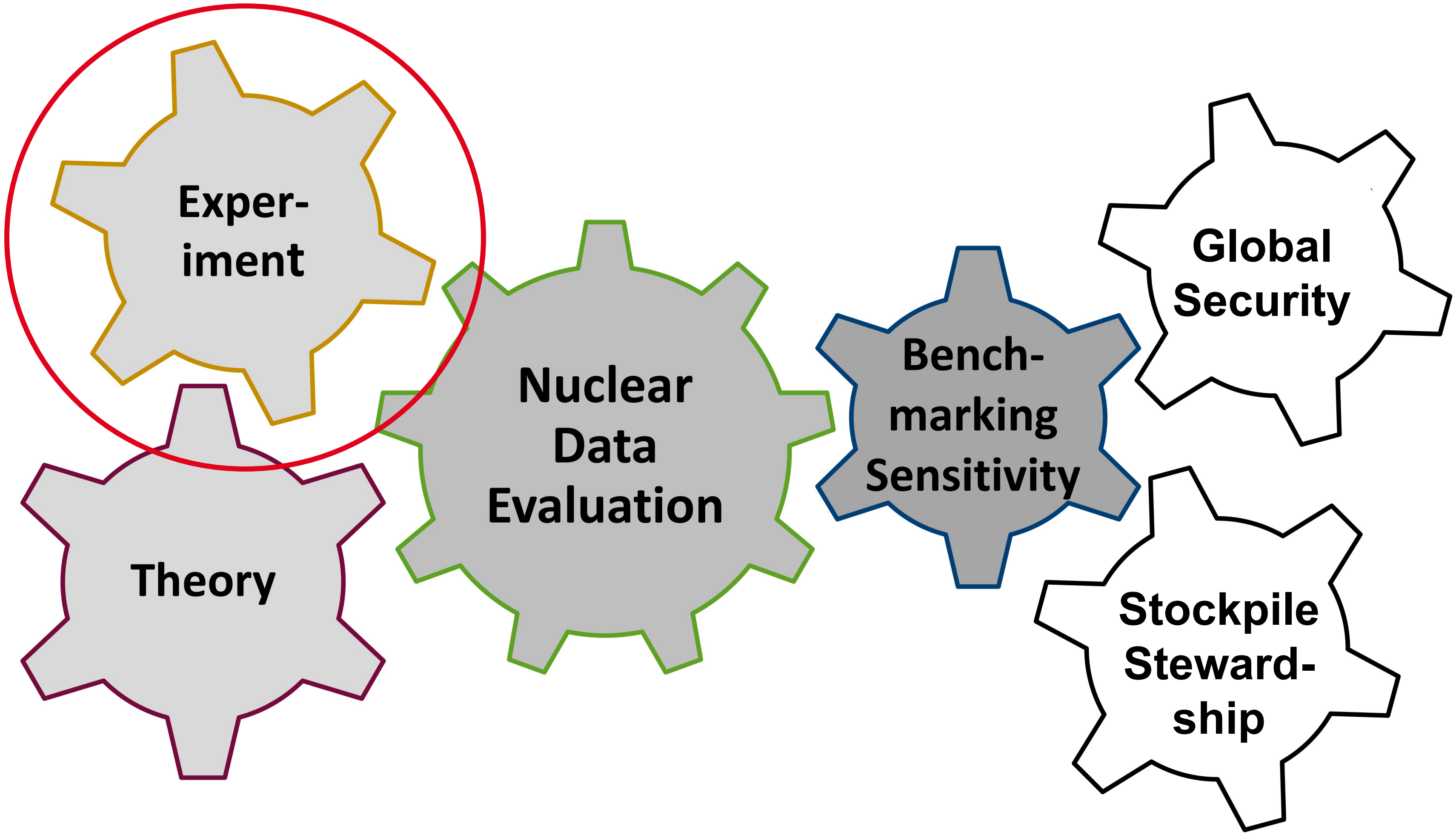
From W. Haeck, LA-UR-18-22218.

- **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:



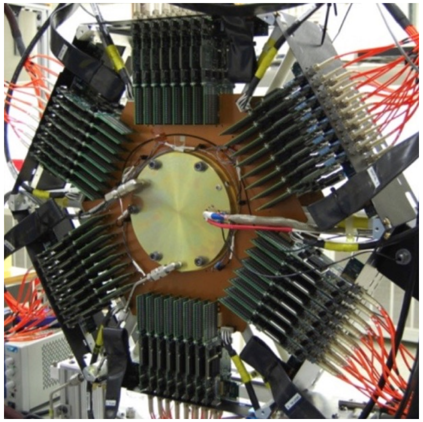
Differential experimental data are measured in dedicated nuclear physics experiments.

- We [**term experimental data "differential**](#)" if:
- same observable is measured as evaluated,
- Inform the model used for the evaluation.

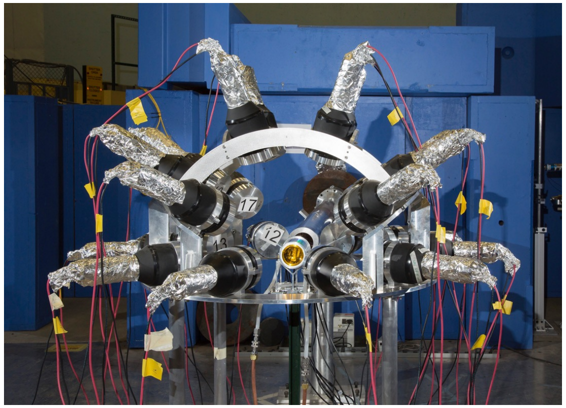
- Data are measured at **LANL** by **P-Division and CNR experimentalists at LANSCE,** e.g., TPC, Chi-Nu or at ORNL, ANL, LLNL, RPI, CERN, etc.

- ***Evaluators pass judgment on the data, i.e., we update and change experimental uncertainties, truncate data and might even change mean values!***

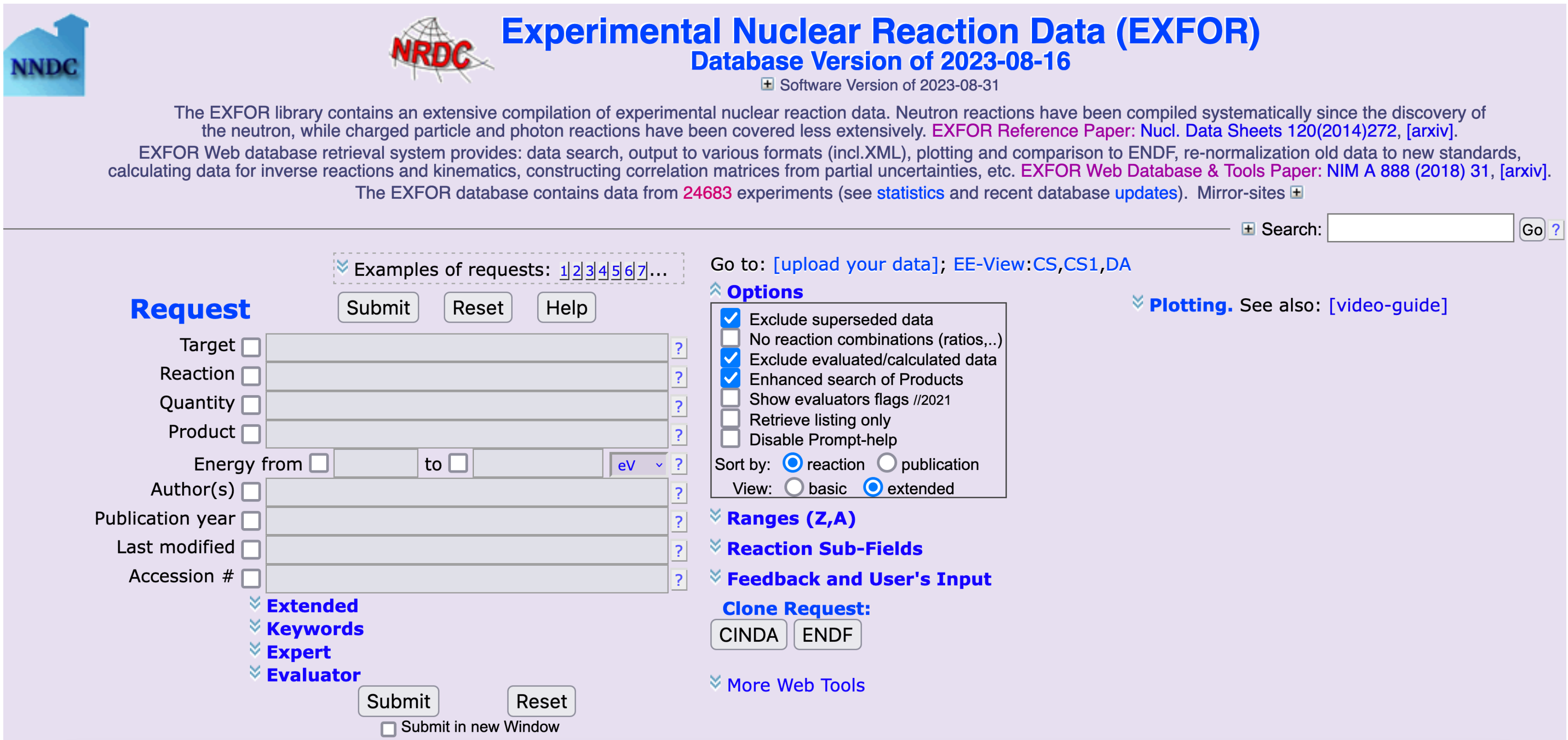
NIFFTE TPC for (n,f)



Chi-Nu for PFNS



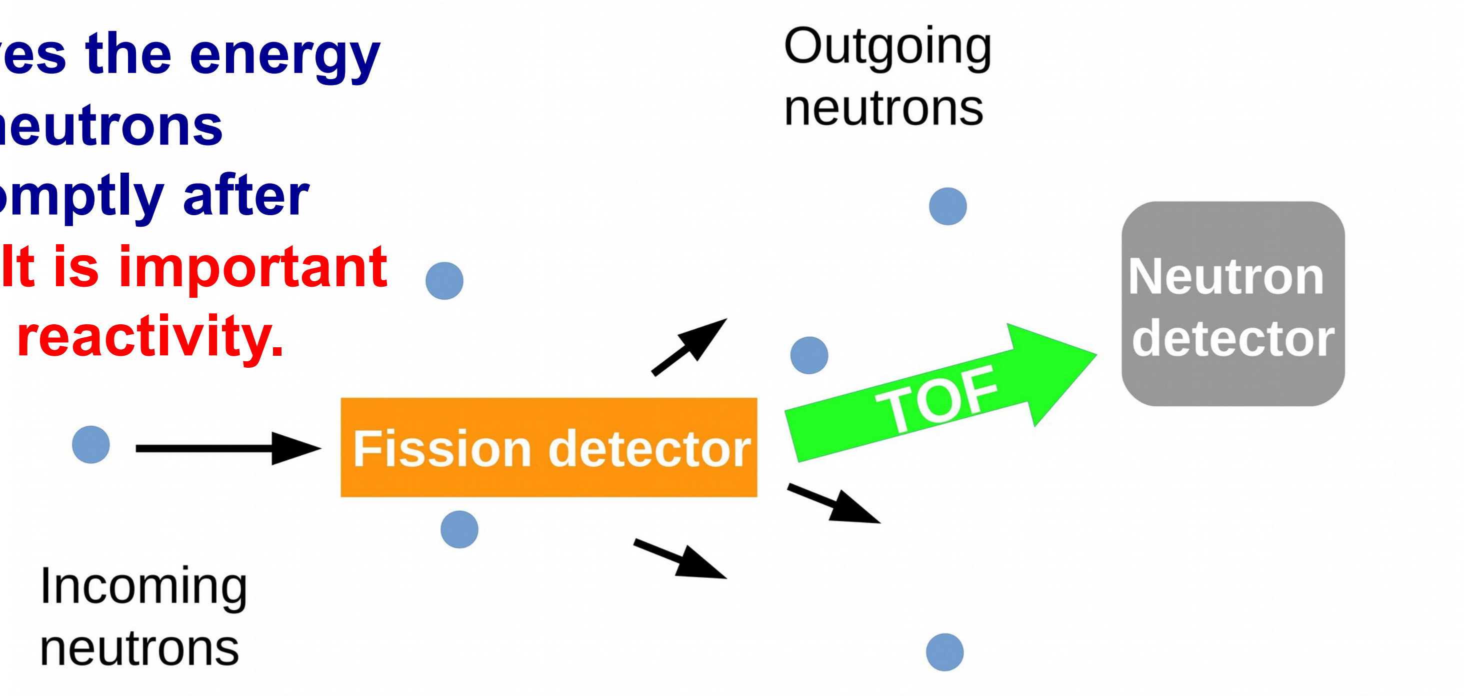
Data can be extracted from EXFOR: https://www-nds.iaea.org/exfor/exfor.htm



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)

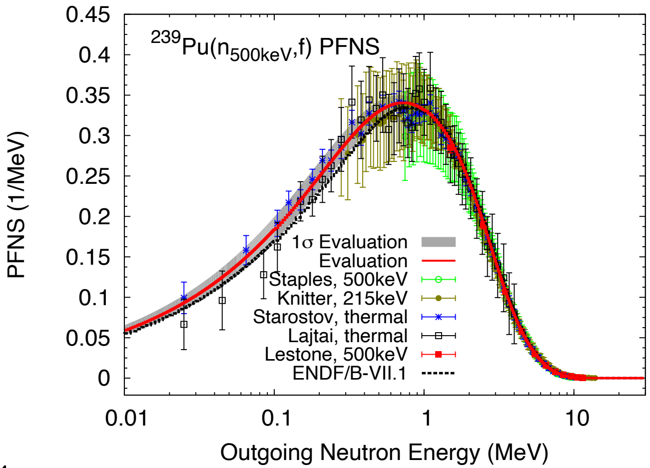
A PFNS gives the energy distrib. of neutrons emitted promptly after fission [1]. It is important to simulate reactivity.

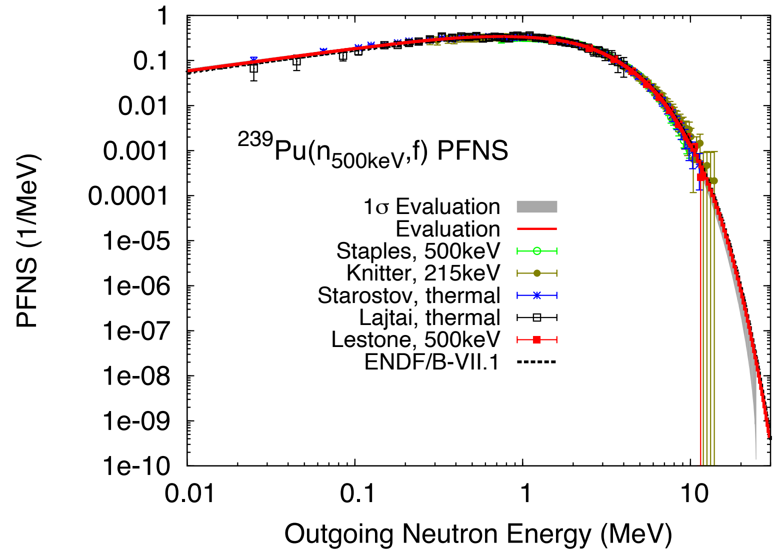


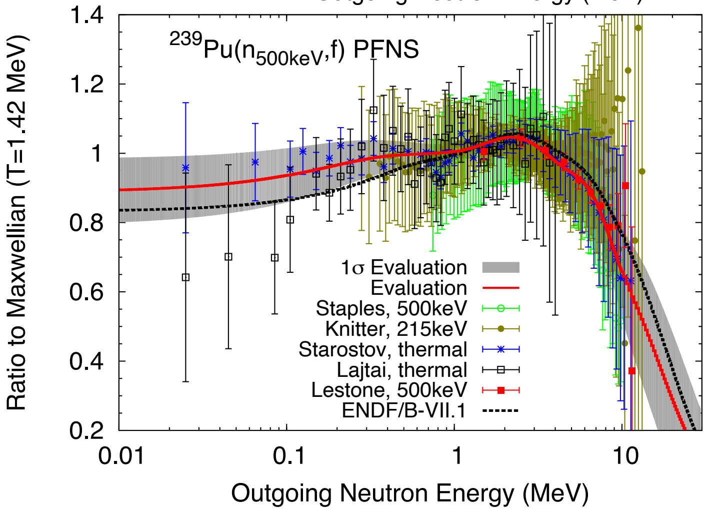
Start signal by counting fission events

Stop signal by counting neutron events

A PFNS covers many orders of magnitude.

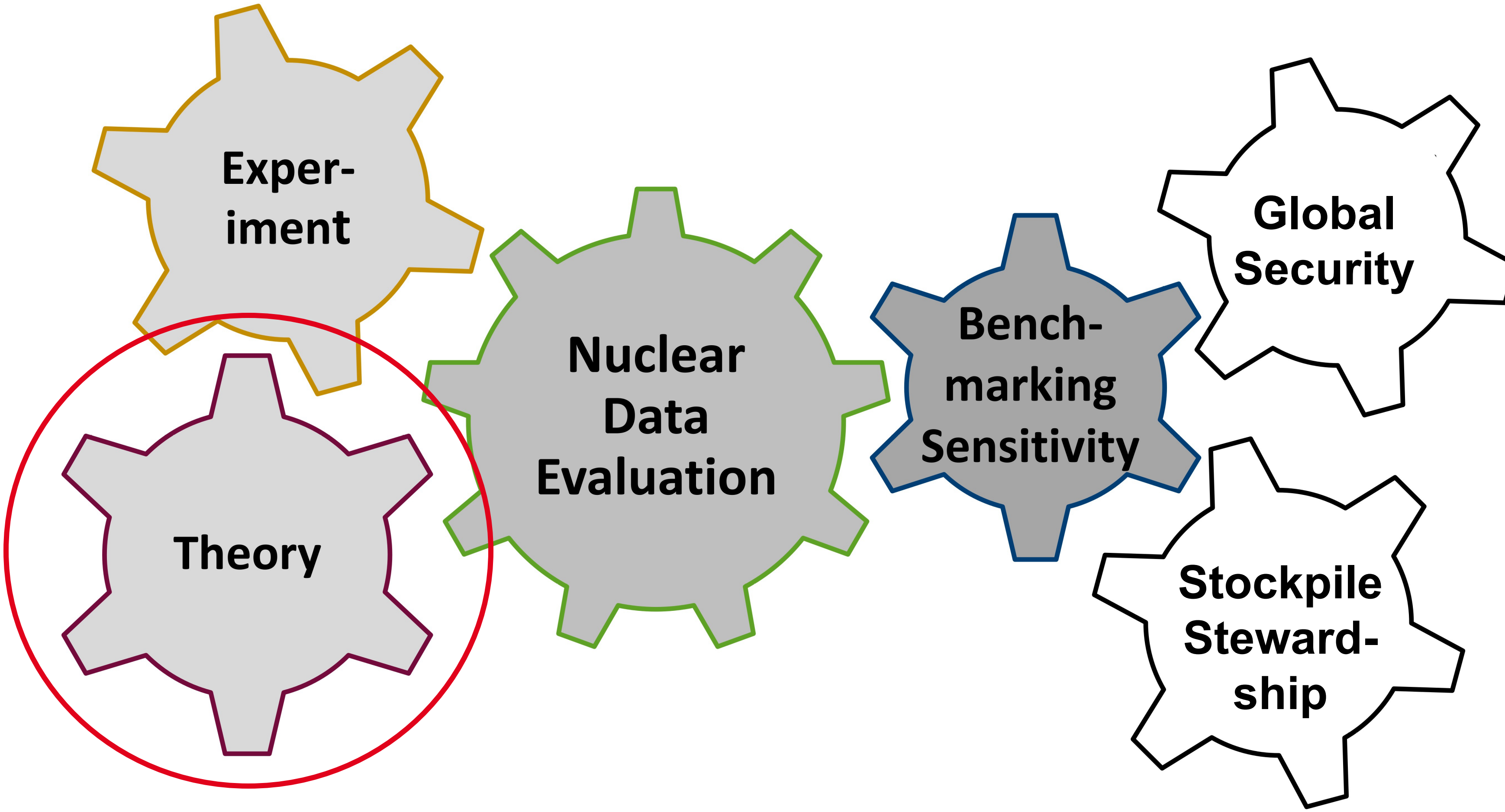






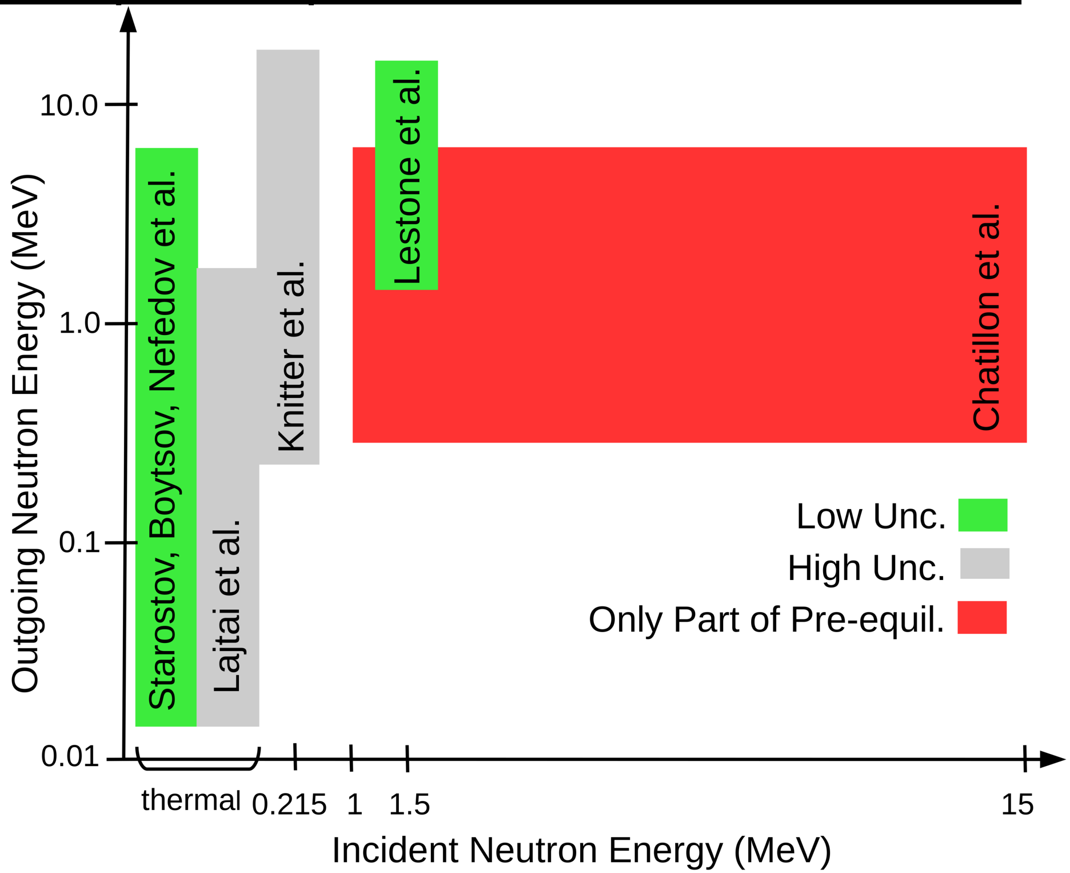
$$Maxw = C\sqrt{E}\exp(-E/T)$$

Models based on nuclear theory:



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

<u>Accepted exp. database for ^{239}Pu PFNS</u>

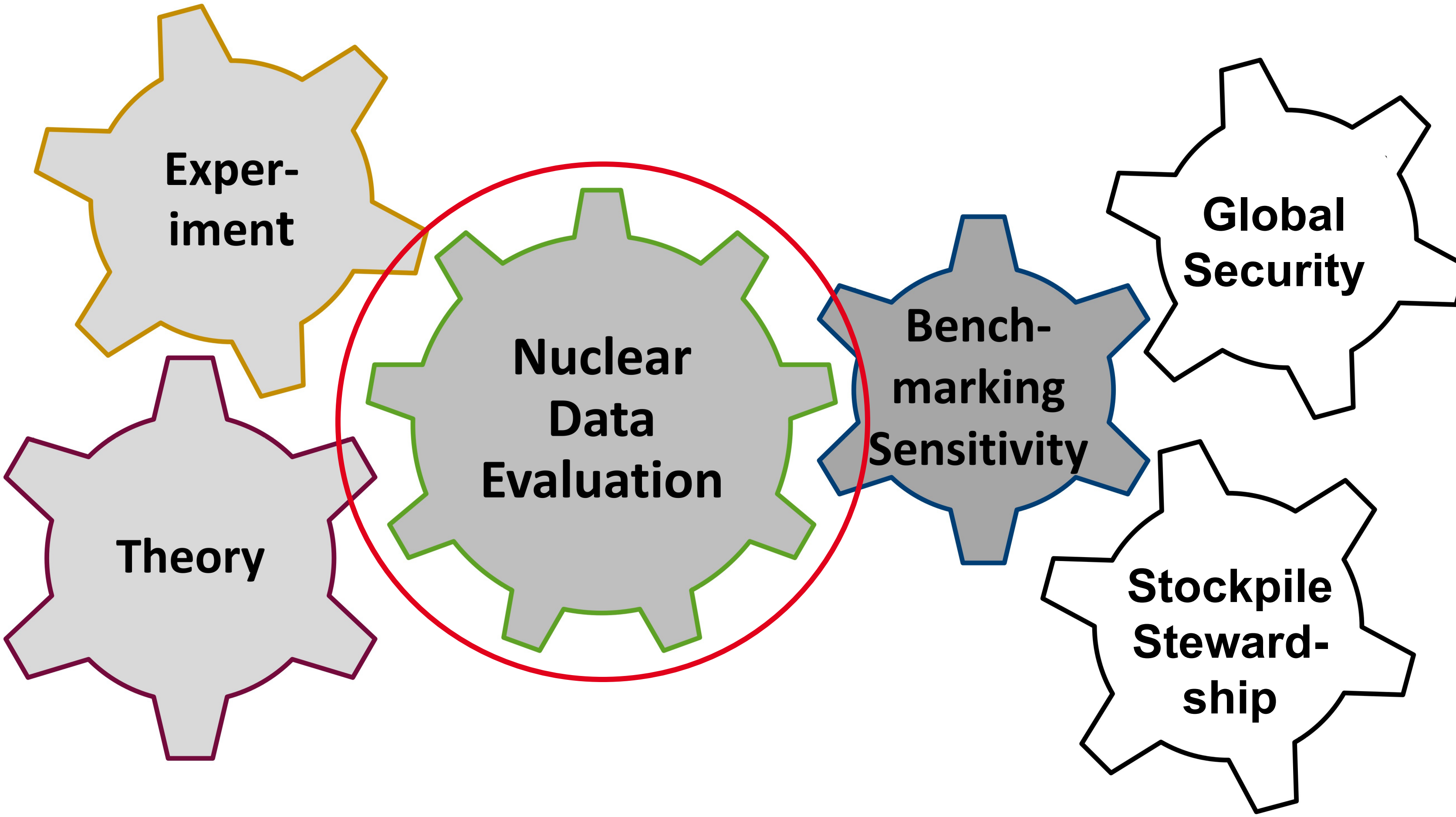


The present evaluation spans energies from thermal–30 MeV.

➔ **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").

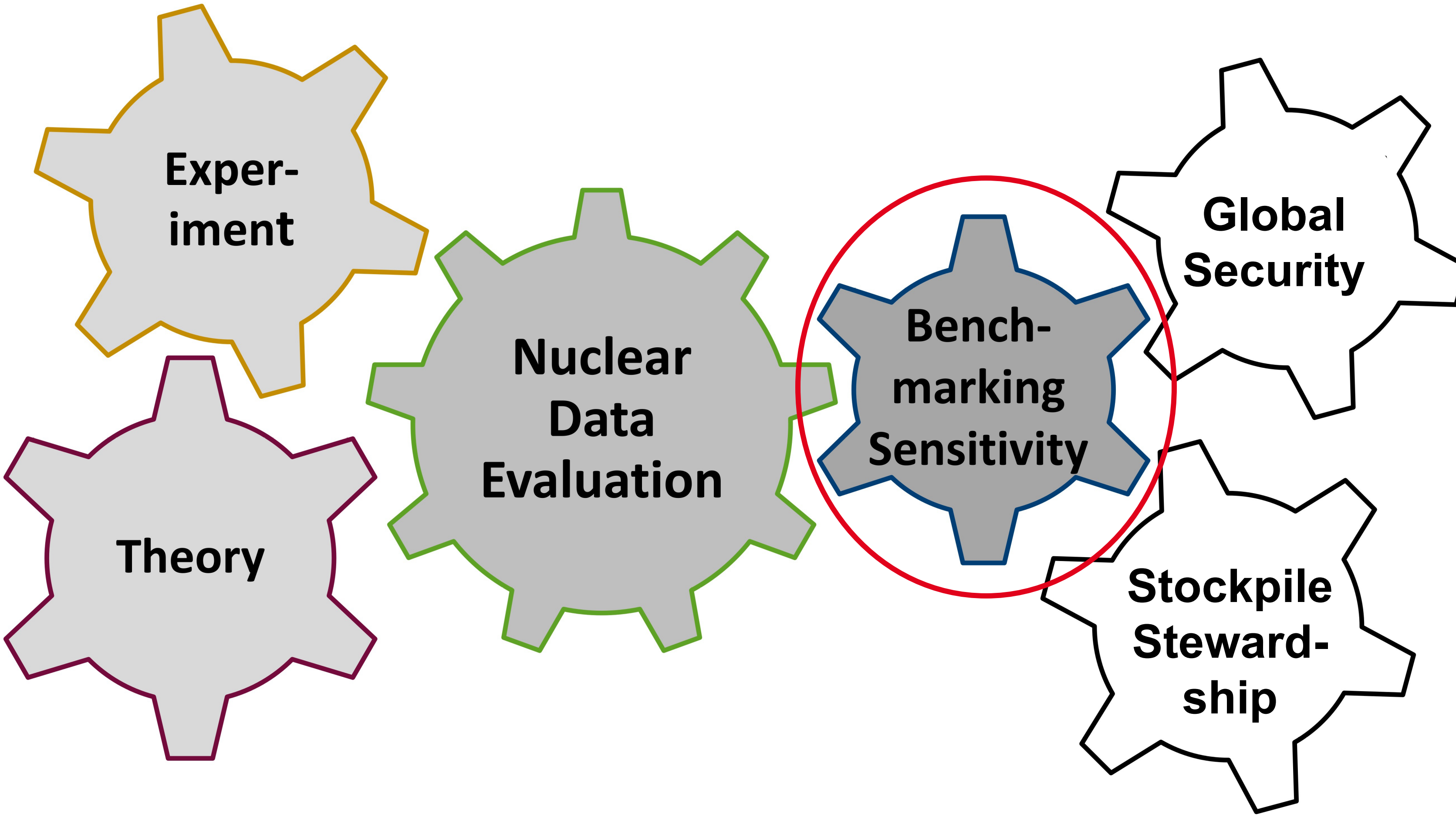
$$\underline{\phi}^{post} = \underline{\phi}^{M} + \mathbf{Cov}^{post}\mathbf{S}^{+}(\mathbf{Cov}^{x})^{-1}\left(\underline{\phi}^{x} - \mathbf{S}\underline{\phi}^{M}\right),$$

$$\mathbf{Cov}^{post} = \mathbf{Cov}^{M} - \mathbf{Cov}^{M}\mathbf{S}^{+}\left(\mathbf{S}\mathbf{Cov}^{M}\mathbf{S}^{+} + \mathbf{Cov}^{x}\right)^{-1}\mathbf{S}\mathbf{Cov}^{M}$$

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

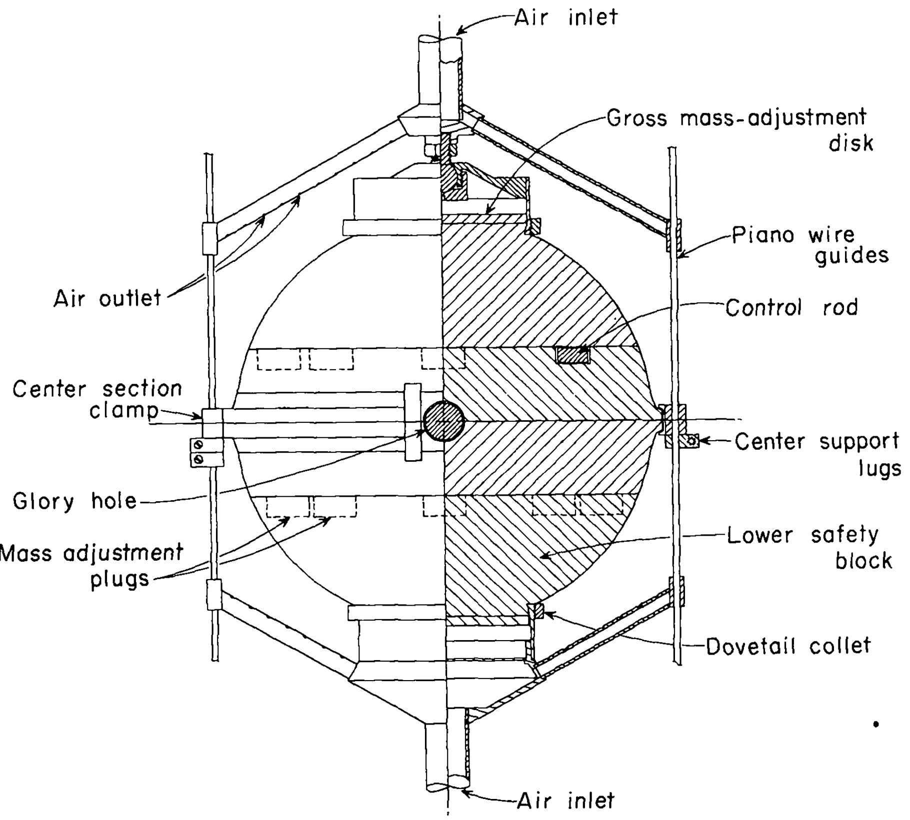


Figure taken from Hansen et al., LA-4208 (1969).

- Minimally reflected, nearly spherical Pu critical assembly.
- Effective multiplication factor $k_{eff} = 1 \longrightarrow$ **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.**

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

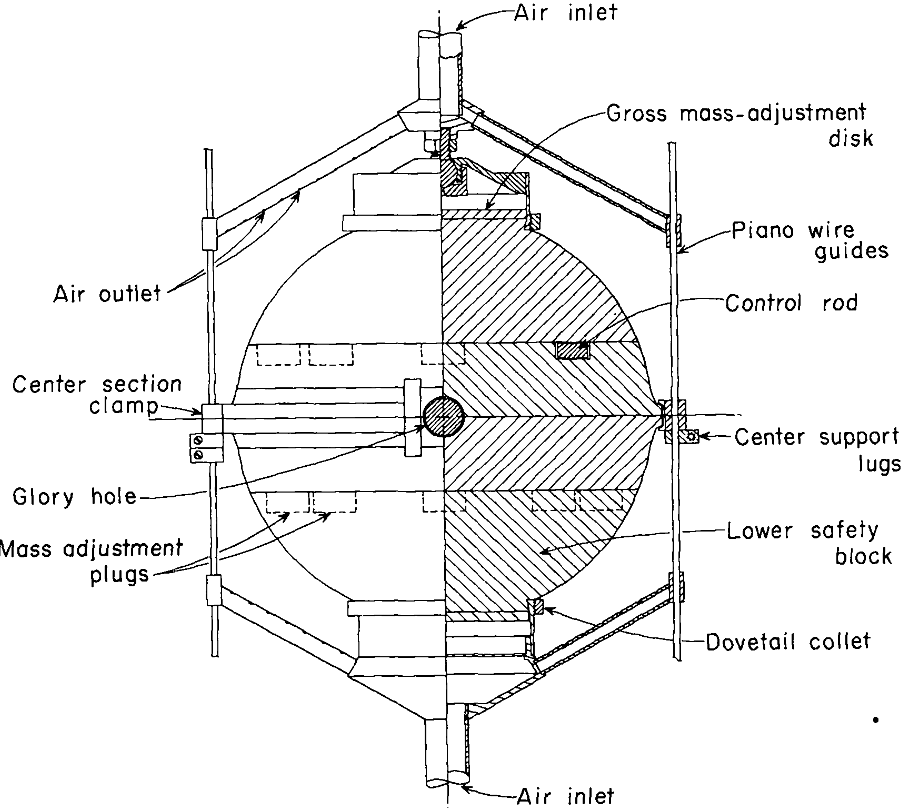
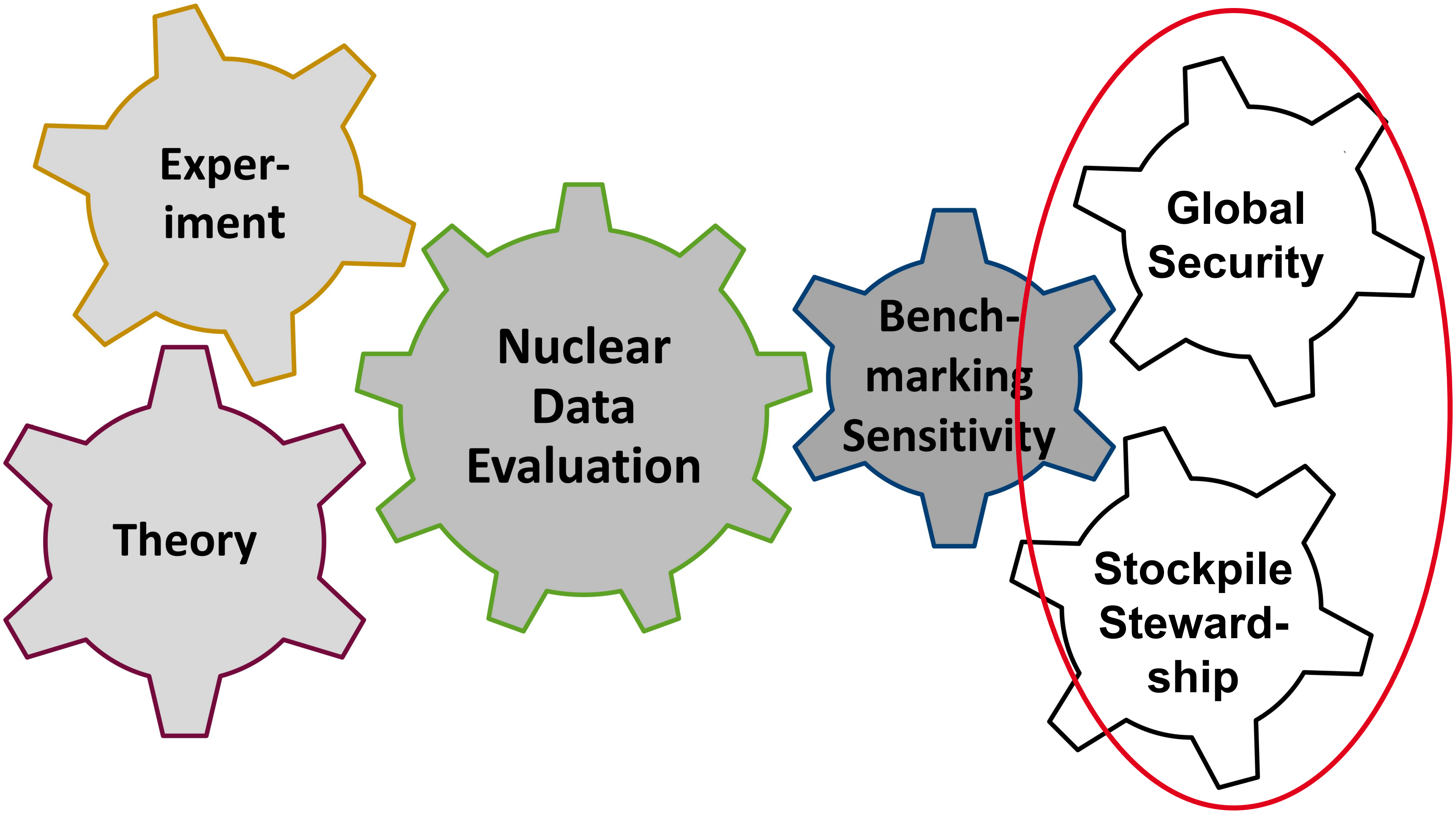


Figure taken from Hansen et al., LA-4208 (1969).

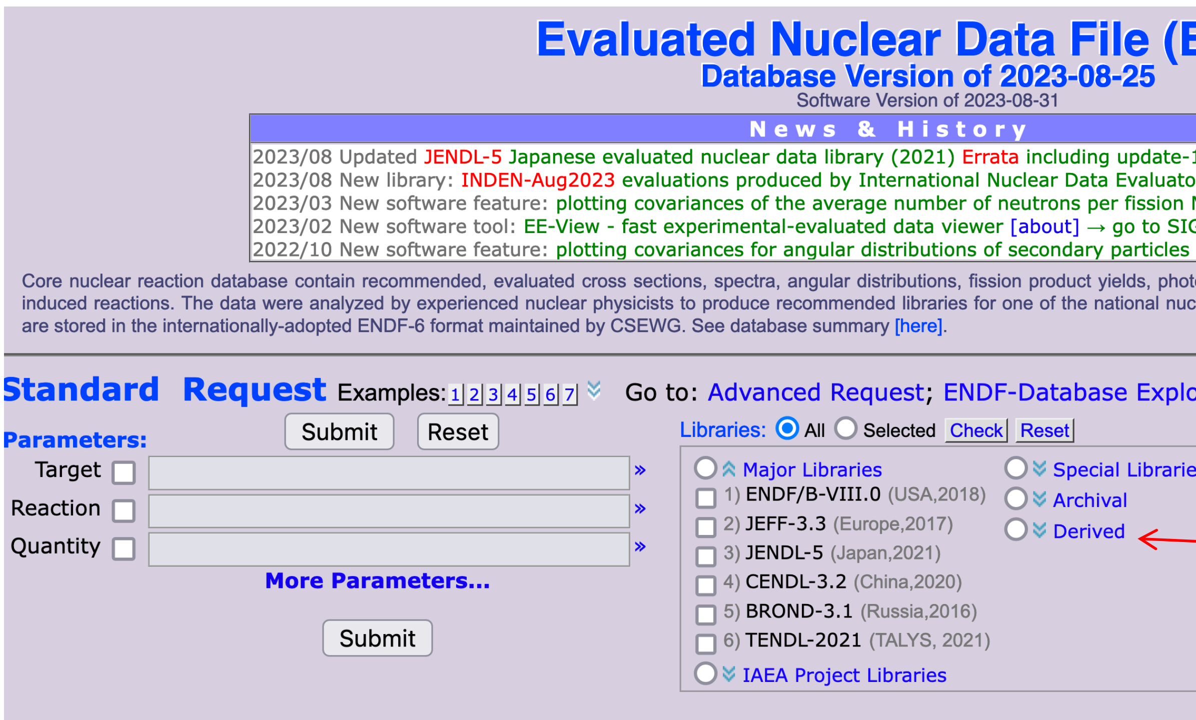
- Jezebel is a calibration point for **nuclear data libraries**. They **are adjusted to give 1.000 +/- 0.0007**
- uncertainty ~100-200 pcm. (1.0 +100 pcm = 1.001)
- **A change of 270 pcm could be the difference between a controlled and uncontrolled nuclear reaction.**
- Calculated k_{eff} = 0.9976±75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



Current major nuclear data libraries.

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

https://www-nds.iaea.org/exfor/endf.htm

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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.**

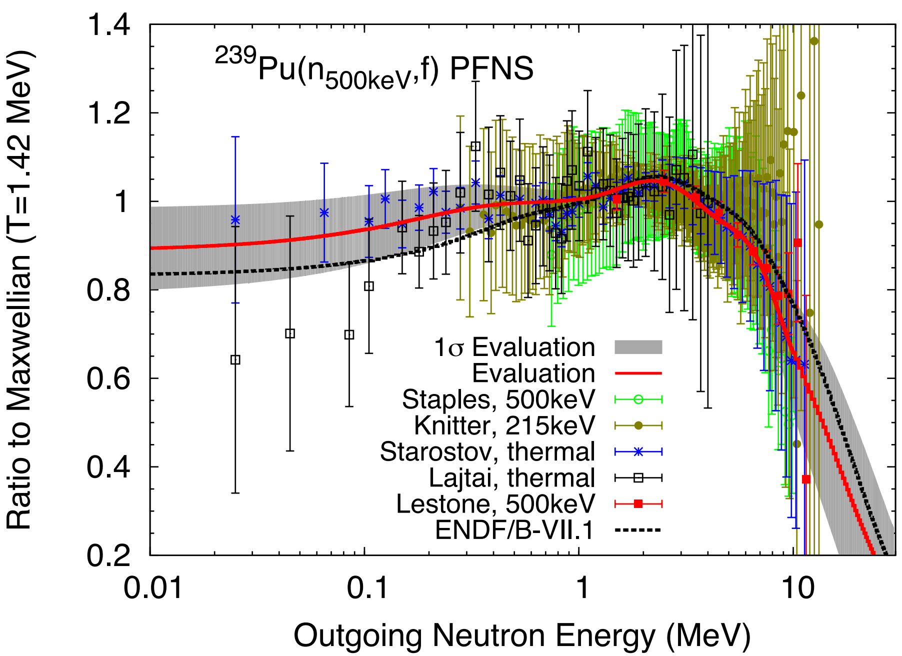
- **Typical application areas are:**
- Stockpile stewardship
- Non-proliferation, global and national security
- Reactor physics, fusion physics and neutron dosimetry
- Nuclear medicine, isotope production, …

- 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!!

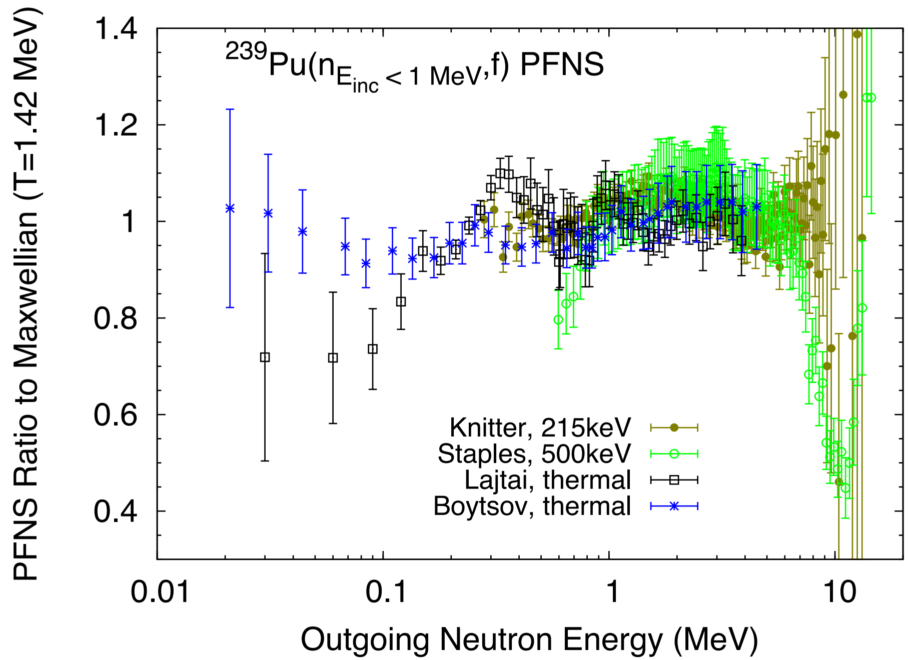
For instance: our understanding of past experiments evolves …

Detailed uncertainty estimate



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

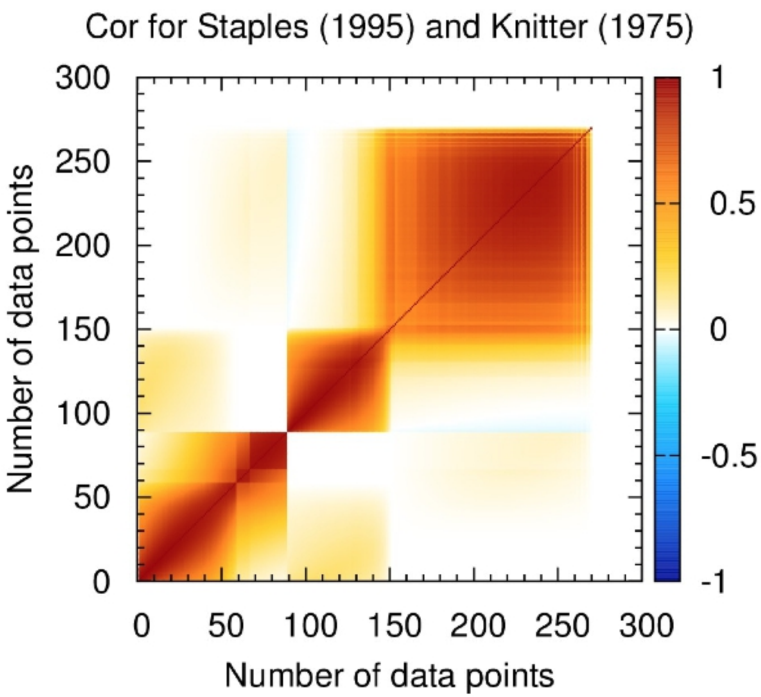
Simplified uncertainty estimate



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

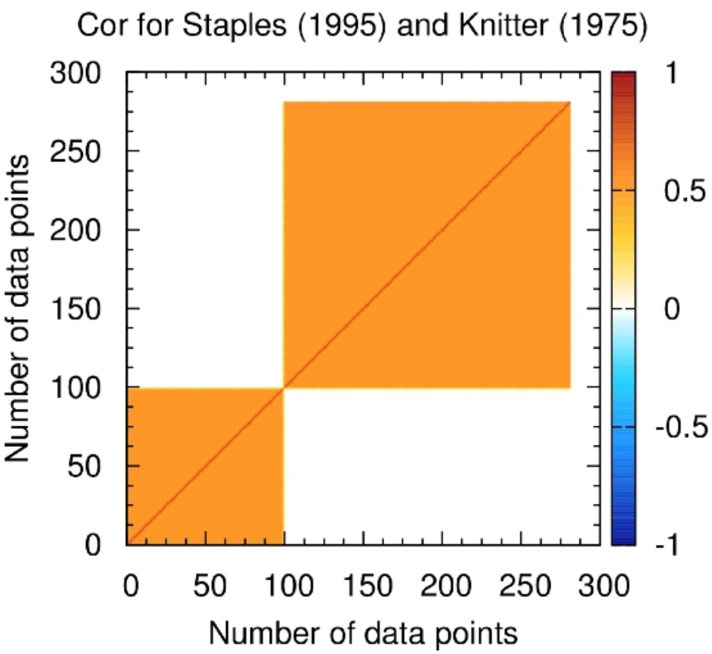
We also improve our uncertainty estimates over time …

Detailed uncertainty estimate



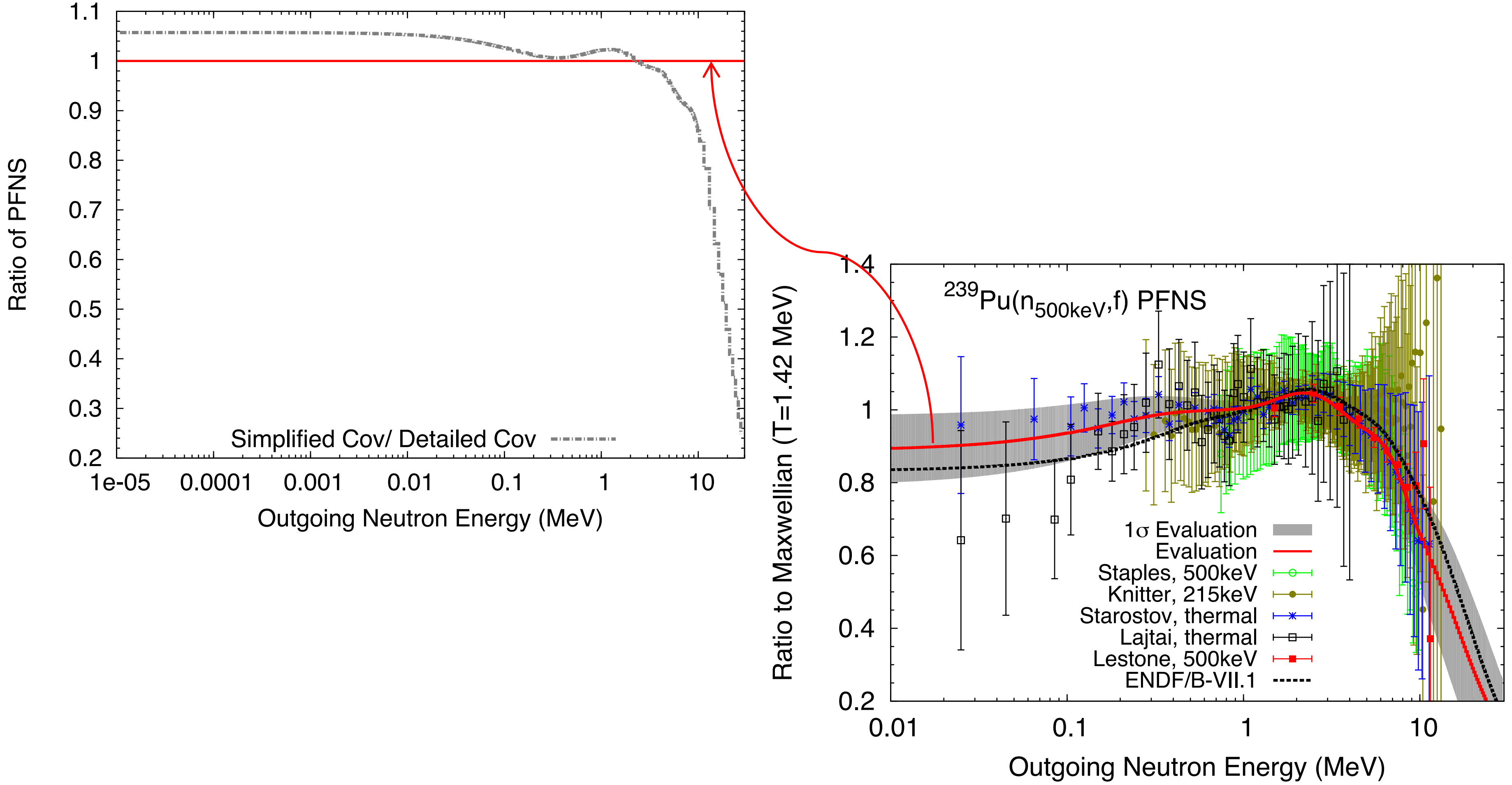
VII.0: Detailed uncertainty estimate.

Simplified uncertainty estimate

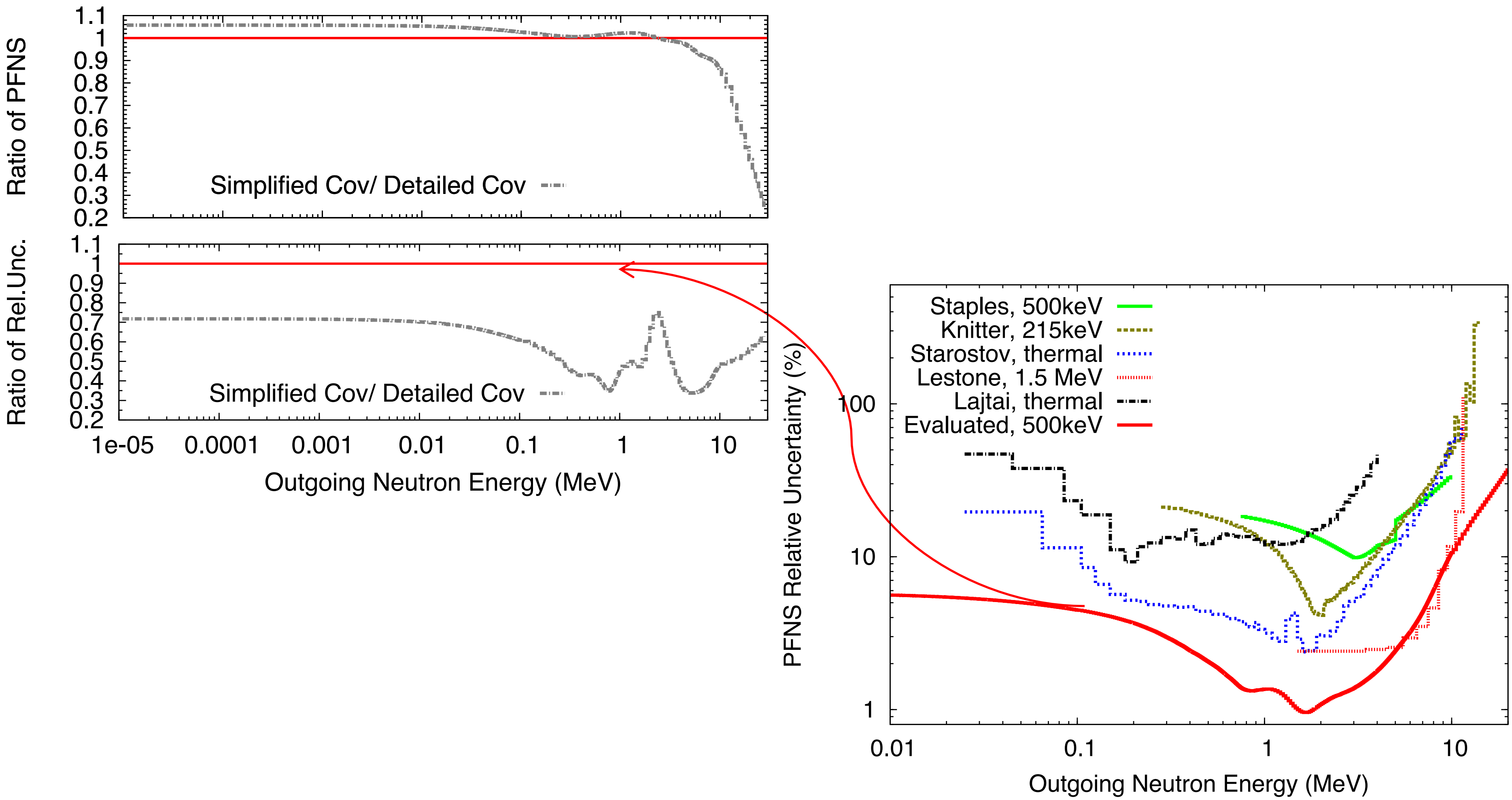


VII.1: Total uncertainties extracted from EXFOR and correlations of same exp. are 0.5, otherwise 0.

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



Simplified versus detailed uncertainty leads to significantly underestimated evaluated unc.



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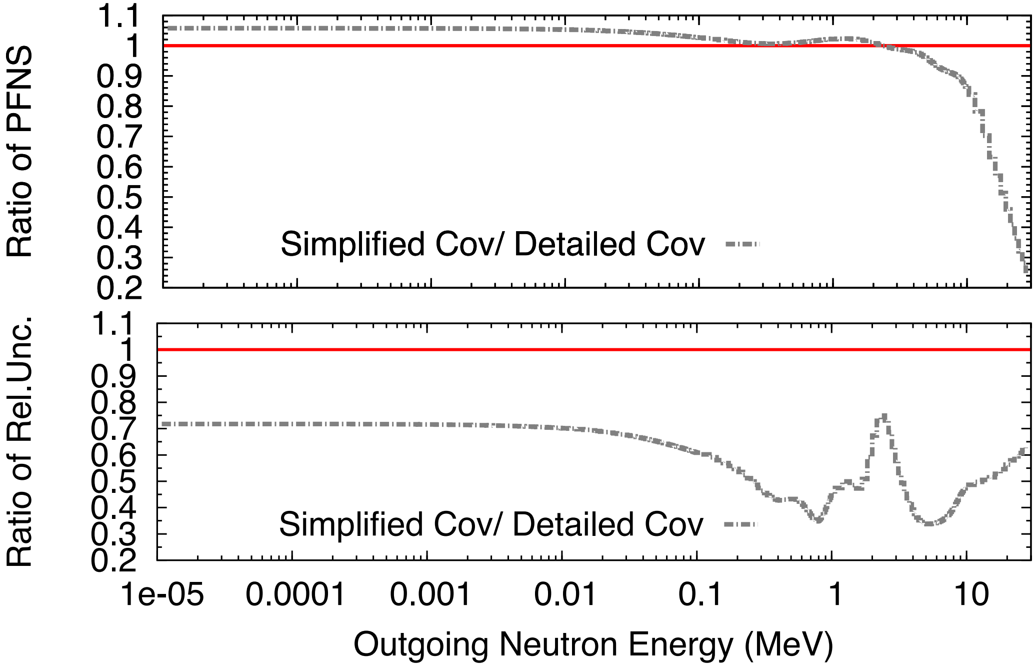
Simplified versus detailed uncertainty estimate significantly impacts benchmark results.



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

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

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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.