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Title:	Upcoming Release of the US Nuclear Data Library ENDF/B-VIII.1
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Los Alamos NATIONAL LABORATORY

Upcoming Release of the US Nuclear Data Library ENDF/B-VIII.1

Denise Neudecker (for the CSEWG collaboration)

MCNP User Symposium August 19, 2024

LA-UR-24-xxxx

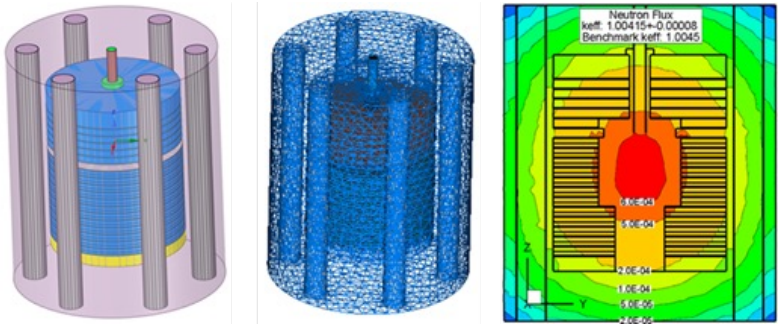
Questions/ Points addressed in the talk:

- **What are evaluated nuclear data?**
- **What is new in ENDF/B-VIII.1?**
- **Where can I get the data from?**

What are evaluated nuclear data?

Nuclear data are key input for MCNPs predictive simulations.

- 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.



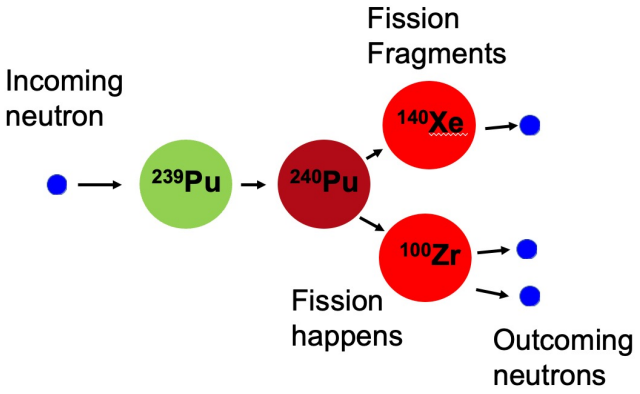
J. Spencer, J. Alwin, “Big Ten MCNP6 Unstructured Mesh Benchmark,” LA-UR-19-25731 (2019).

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

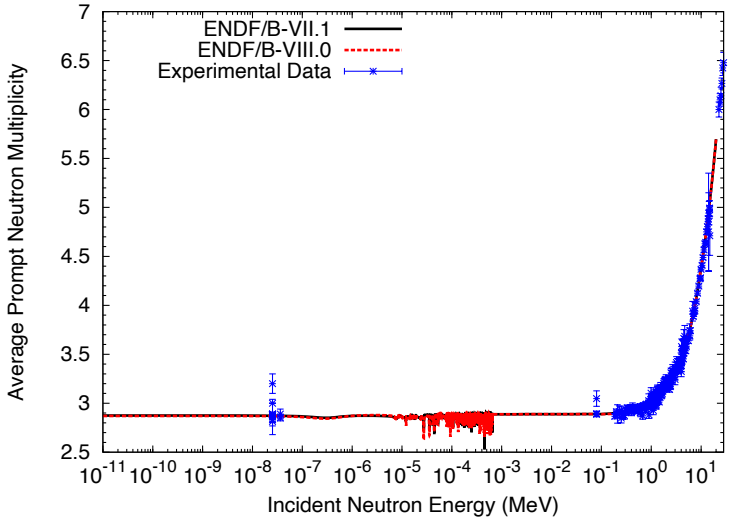
- Nuclear reactor physics
- Nuclear critical and subcritical experiments
- Criticality safety
- Nuclear diagnostics
- Survivability
- Intrinsic radiation
- Radiography
- Nuclear weapon effects and output
- Emergency response / nuclear threat assessments
- Nuclear safeguards and nonproliferation
- Radiation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

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

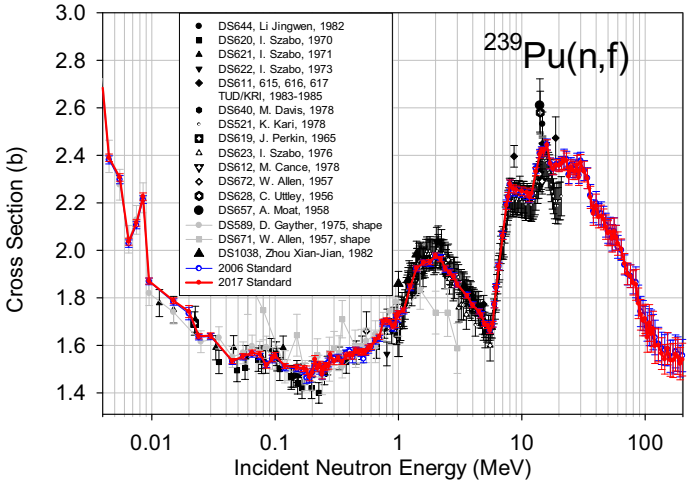
Example: neutron-induced fission on ^{239}Pu



Average Prompt Neutron Multiplicity= Av. Number of outgoing neutrons



Fission cross-section=probability that fission happens



Prompt Fission Neutron Spectrum= Energy distribution of outgoing neutrons

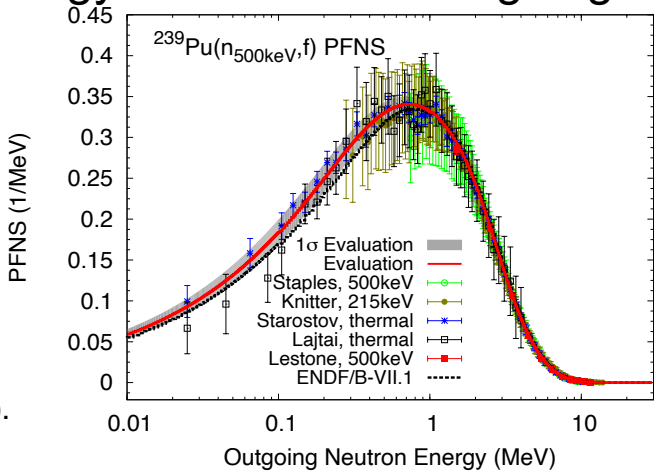
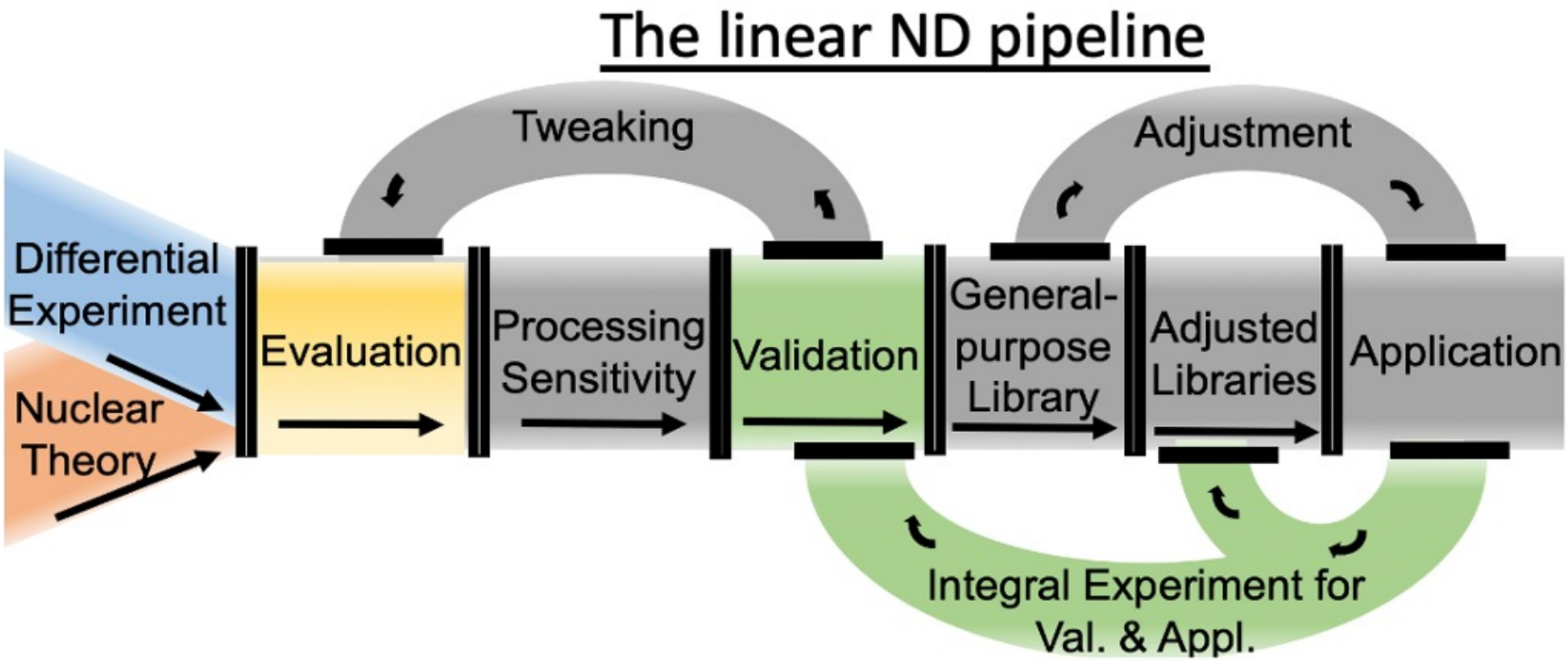
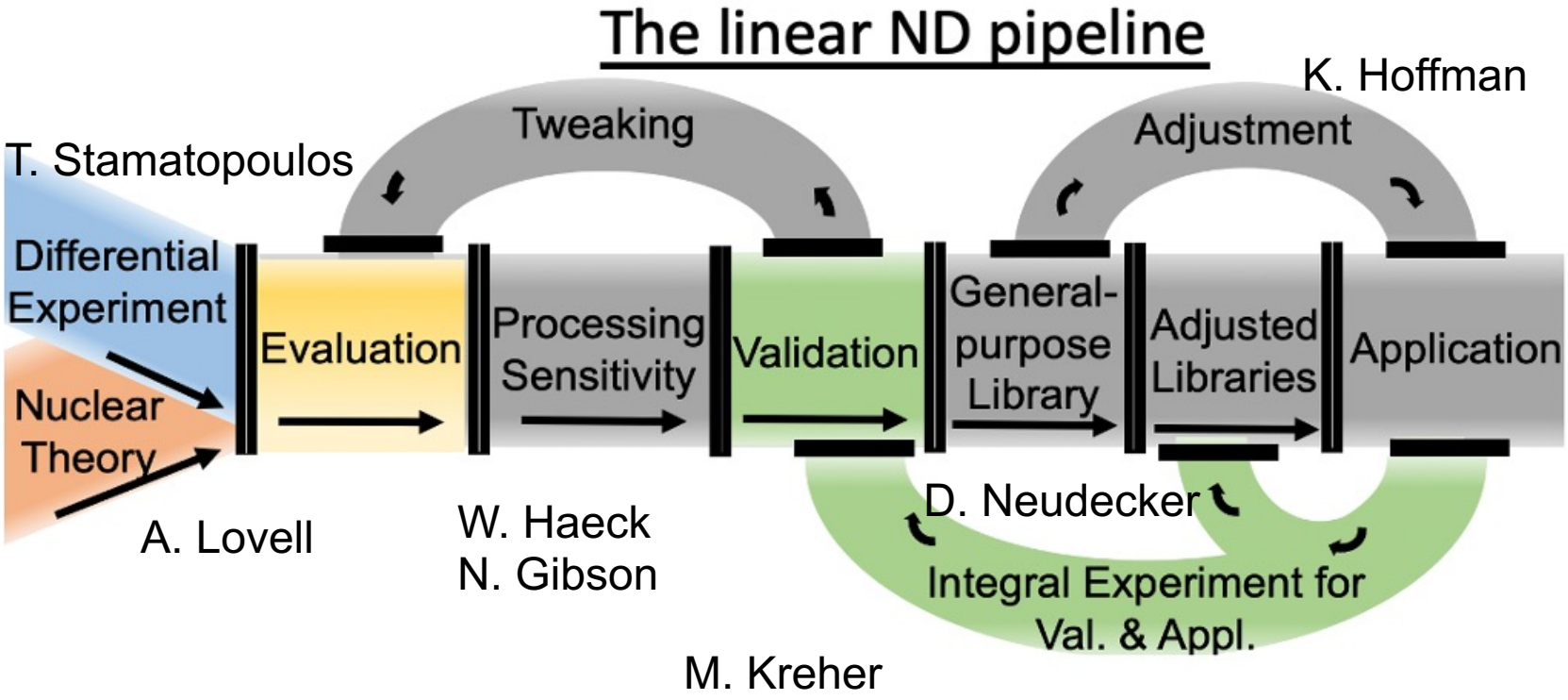


Fig. from Carlson et al., NDS 148, 143 (2018).

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



There are a couple of talks on the nuclear data pipeline from LANL here (just a subset) …



J. Hutchinson, A. Maldonado, G. Siemers, I. Michaud, N. Kleedtke, P. Brain

What is new in ENDF/B-VIII.1?

ENDF/B-VIII.1 is the upcoming U.S. nuclear data library assembled, V&Ved, released by CSEWG.

ENDF/B-VIII.1: Updated Nuclear Reaction Data Library for Science and Applications

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Contributions to ENDF/B-VIII.1 come from U.S. national laboratories, universities, industry, international working groups (e.g., INDEN by the IAEA), international collaborators and many more.

Several sub-libraries were updated as part of ENDF/B-VIII.1:

- Neutrons including light elements (^{3}He, ^{6}Li, ^{9}Be, …), structural materials ($^{50\text{-}54}$Cr, ^{54,56,57}Fe, …), and fuels (^{233,235,238}U, ^{239}Pu, …).
- Neutron reaction covariances.
- Thermal Neutron Scattering Law (TSL) data for moderators (light water, nuclear/ reactor graphite, …) and fuel (Plutonium dioxide, uranium carbide/ nitride, …).
- Photo-nuclear sub-library.
- Charged-particle reaction sub-libraries.
- Fission-yield sub-libraries.
- Atomic sub-libraries.

Substantial changes in neutron sub-library are coming, many INDEN evaluations were adopted.

Isotope	Change	Isotope	Change
^{16}O	Small	^{3}He	Substantial
^{18}O	Small	^{6}Li	Substantial
^{19}F	Substantial	^{9}Be	Small
^{28,29,30}Si	Substantial	^{51}V	Substantial
$^{50\text{-}54}$Cr	Substantial	^{88}Sr	Substantial
^{55}Mn	Small	^{103}Rh	Substantial
^{54,56,57}Fe	Substantial	^{140,142}Ce	Substantial
^{63,65}Cu	Substantial	$^{156,158,160\text{-}164}$Dy	Substantial
^{139}La	Substantial	^{181}Ta	Substantial
^{233}U	Substantial	$^{190\text{-}198}$Pt	Substantial
^{238}U	Substantial	$^{206\text{-}208}$Pb	Substantial
^{240,241}Pu	Substantial	^{234}U	Substantial
^{239}Pu	Substantial	^{236}U	Substantial

INDEN (International Nuclear Data Evaluation Network) managed by the IAEA (Co-ordinators: Capote, Dimitriou, Schnabel) is an international project with contributors from around the world.

Light-element example: ^{19}F changes improve simulations of integral experiments.

From A. Trkov/ IAEA.

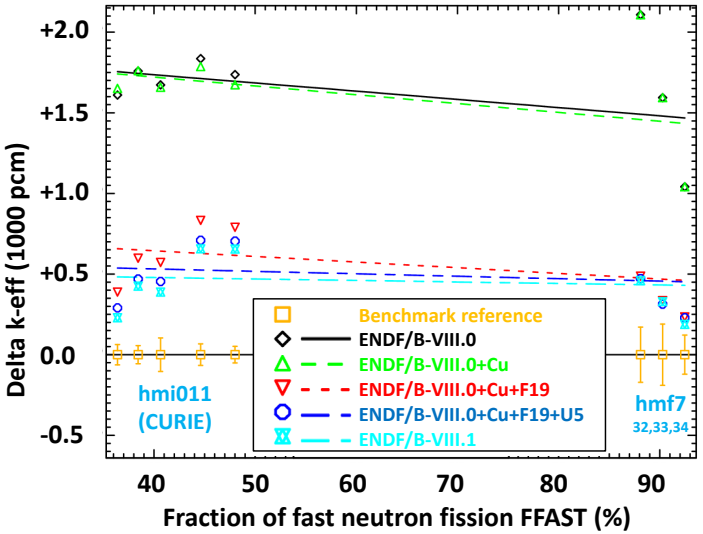
Updates:

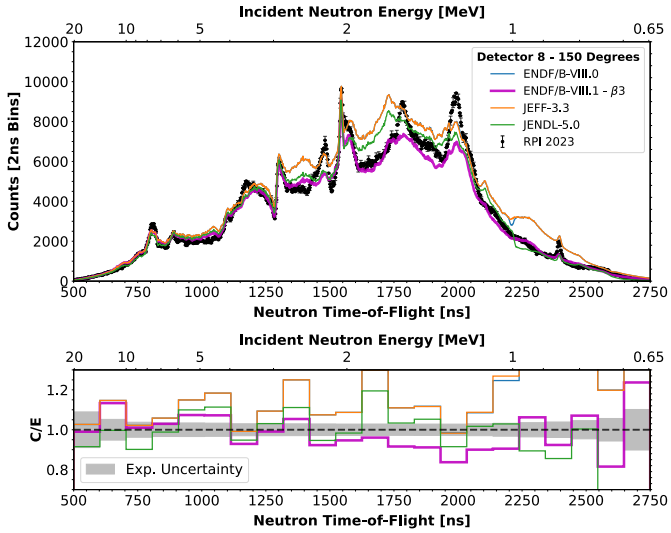
- New elastic angular distribution below 2 MeV, above carried over from JENDL-5.0.
- Total and capture cross sections adopted from JENDL-5.0.
- First two inelastic level cross sections were updated.
- (n,2n) cross sections adopted from IRDFF-II.

Leads to distinct improvements in simulating criticality and scattering experiments.

More work to do on inelastic cross sections.

Work by the INDEN collaboration (IAEA, RPI, etc.).



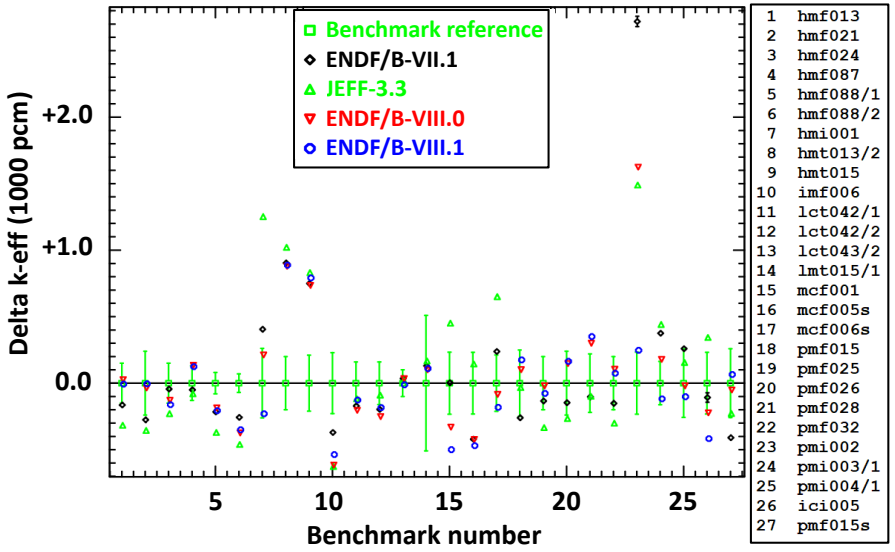


Neutron scattering measurement on Teflon by RPI.

Structural-material example: New $^{50\text{-}54}$Cr & ^{56}Fe improve simulations of crit k_{eff}.

Updates:

- $^{50\text{-}54}$Cr: model calculations extended to 65 MeV (for fusion applications), adopted selected capture resonance widths from BROND-3.1, model-extrapolation to unstable ^{51}Cr.
- ^{56}Fe: Changes to elastic, inelastic and capture cross sections, resonance parameters from Perey and Perey from V.0.
- Validation shows improvements.
- More work planned for IX.0 such as providing new evaluated $^{50\text{-}54}$Cr covariances.



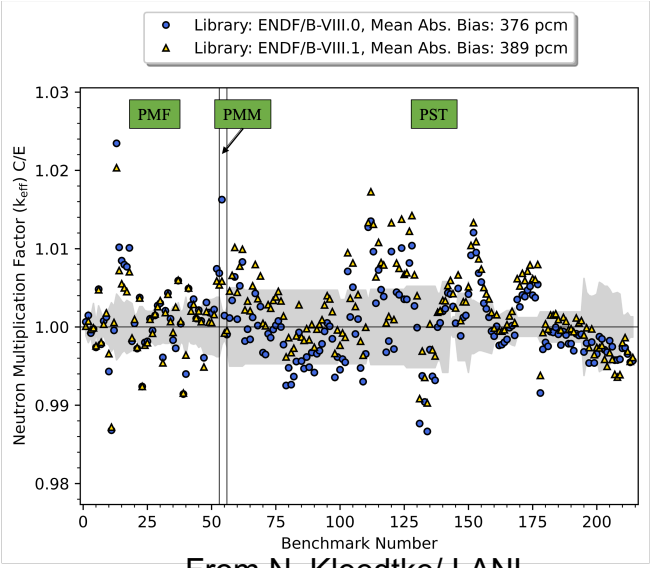
From A. Trkov/ IAEA.

Work by the INDEN collaboration (BNL, IAEA, etc.).

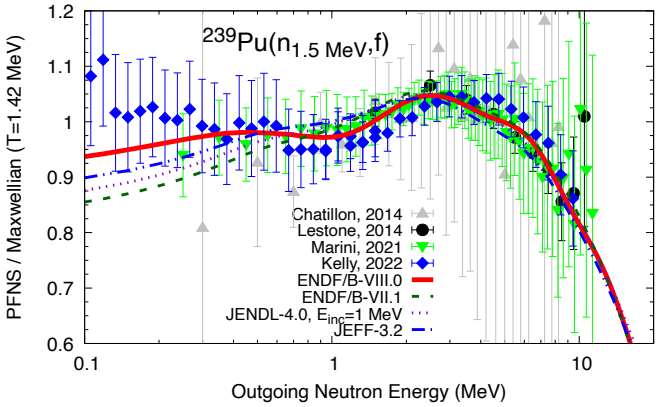
Fuel-isotope example: Substantial change to ^{239}Pu via (inter)national contributions.

Updates:

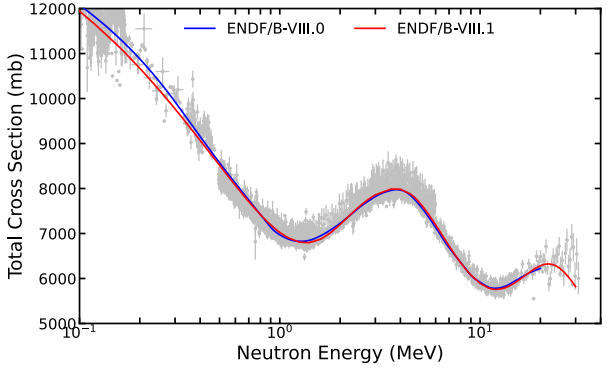
- New prompt neutron multiplicities (ORNL, INDEN, LANL)
- New cross sections in the RRR (ORNL).
- New cross sections in the fast (INDEN, LANL).
- New PFNS from thermal-30 MeV (INDEN, LANL).
- Despite substantial changes, good performance maintained in simulating critical assemblies.



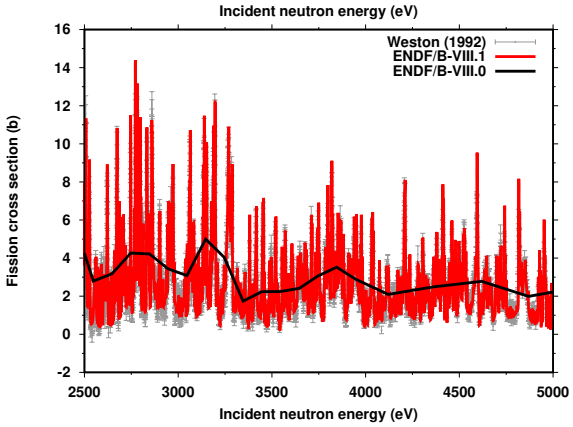
From N. Kleedtke/ LANL.



LANL eval. (D. Neudecker) Including LANL/ LLNL Chi-Nu and CEA PFNS data.



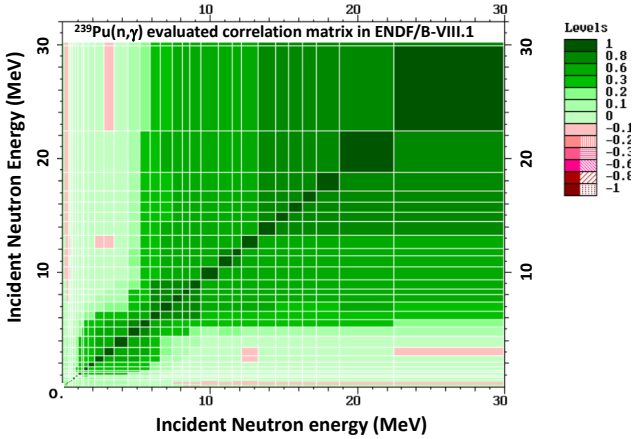
LANL eval. (M. Mumpower).



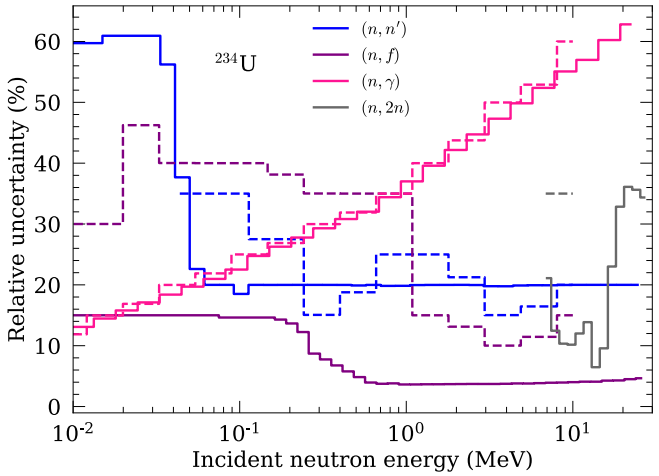
ORNL eval. (M. Pigni).

Work by INDEN, LANL, LLNL, ORNL.

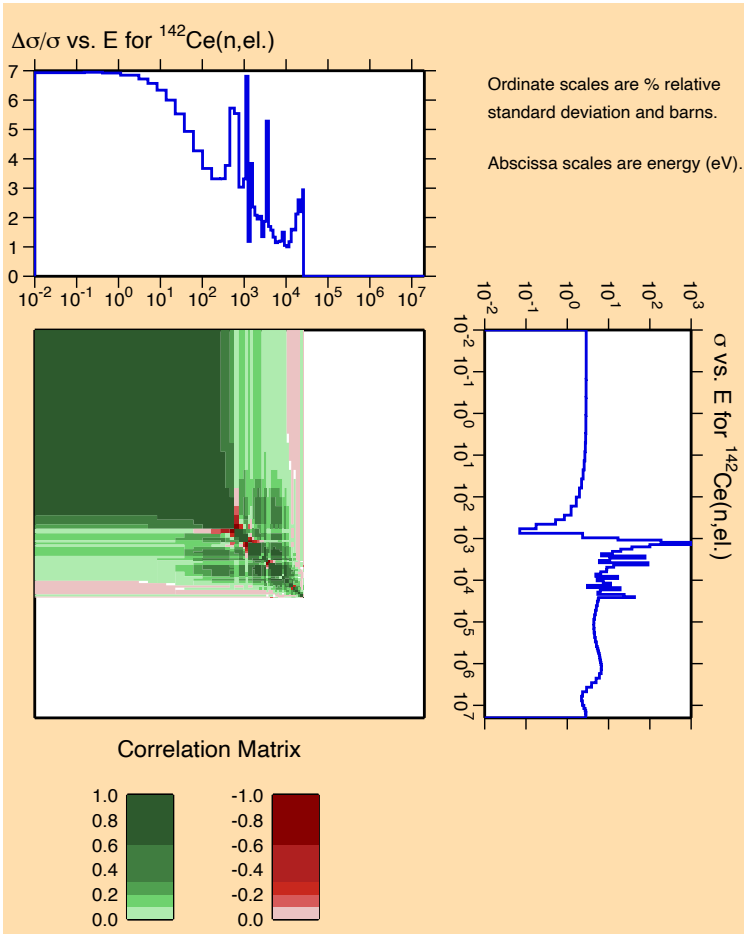
For Whisper users: New covariances provided among them for ^{239}Pu, $^{234\text{-}236}$U, Ce, Pb, Ta, etc.!



By INDEN collaboration (Capote).



By LANL (Lovell, Stetcu).



By ORNL (Pigni).

For Whisper users: CSEWG tested covariances for VIII.1 more stringently but work remains.

Testing included:

- See if covariance could be processed via LANL's NJOY and ORNL's AMPX processing codes (i.e., formats are correct),
- Mathematical properties (positive semi-definite, -1 <= cor <= +1, covariance constraints,
- Are uncertainties within reasonable limits given standards and templates of expected measurement uncertainties (see:)?
- Forward-propagating uncertainties through integral testing uncertainties.

To-Do:

- We still miss covariances for several isotopes and energy ranges,
- Discussion on uncertainties in RRR.
- Updates to newest standards.

Fissile material		**PU**			
Spectrum		FAST	INTER	MIXED	THERM
Number of Benchmarks		152	4	9	624
Experimental Uncertainty (pcm)		334	710	587	426
Total (pcm)	**ENDF/B-VIII.1b4**	**931**	**551**	**536**	**645**
	ENDF/B-VIII.0	**921**	1403	1055	1099
	ENDF/B-VII.1	436	565	459	625
Cross-sections (with correlations)	**ENDF/B-VIII.1b4**	**841**	**360**	**224**	**106**
	ENDF/B-VIII.0	**857**	1368	983	998
	ENDF/B-VII.1	409	546	356	500
P1-elastic	**ENDF/B-VIII.1b4**	66	-	-	-
	ENDF/B-VIII.0	66	-	-	-
	ENDF/B-VII.1	-	-	-	-
nubar	**ENDF/B-VIII.1b4**	**390**	**389**	**479**	**632**
	ENDF/B-VIII.0	300	271	275	308
	ENDF/B-VII.1	76	88	114	168
PFNS	**ENDF/B-VIII.1b4**	27	**25**	**53**	**59**
	ENDF/B-VIII.0	117	106	265	297
	ENDF/B-VII.1	118	106	265	297

Table from Oscar Cabellos/ UPM.

Many new TSL were released by ESF, North Carolina State University, ORNL, etc.

Moderator material	Moderator material
Light water (94 temperatures!)	Beryllium-metal
Beryllium metal with distinct effects	Beryllium oxide
Calcium Hydride	FLiBe Molten Salt
Nuclear/ Reactor Graphite (20%)	Crystalline Graphite
Anhydrous Hydrogen Fluoride	Heavy Paraffinic Oil
Silicon Carbide	Silicone Dioxide
Polystyrene	Lucite
Zirconium	Beryllium Carbide
Zirconium Hydride	Lithium-7 Hydride and Deuteride
Yttrium Hydride	

Fuels
Plutonium Dioxide
Uranium Carbide
Uranium Metal
Uranium Nitride
Uranium Dioxide
Uranium Hydride

Special Purpose
Liquid hydrogen and deuterium
Sapphire Single-Crystal Neutron Filter
Magnesium Oxide Neutron Filter
Magnesium Fluoride Neutron Filter
Beryllium Fluoride Neutron Filter

Part of IAEA2019 photonuclear data library used. (https://www-nds.iaea.org/photonuclear/)

220 isotopes included in the IAEA2019 Photonuclear Data Library that was part of an IAEA Co-ordinated Research Project (Co-Ordinator: V. Dimitriou).

Four categories:

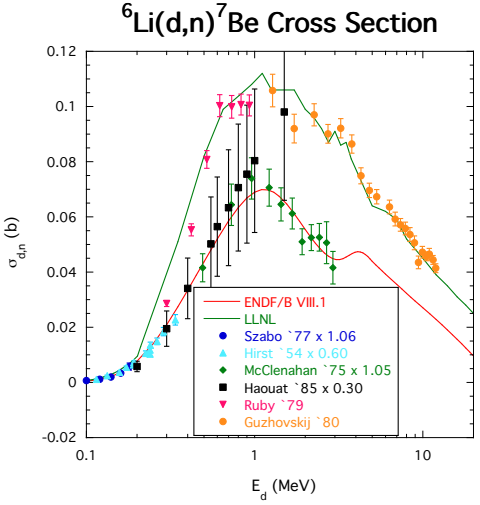
- Structural, shielding, and bremsstrahlung target materials: Be, Al, Si, Ti, V, Cr, Fe, Co, Ni, Cu, Zn, Zr, Mo, Sn, Ta, W, and Pb.
- Biological materials: C, N, O, Na, S, P, Cl, and Ca;
- Fissionable materials: Th, U, Np, and Pu;
- Other materials: H, K, Ge, Sr, Nb, Pd, Ag, Cd, Sb, Te, I, Cs, Sm, and Tb.
- Potential diagnostic and therapeutic radionuclides.

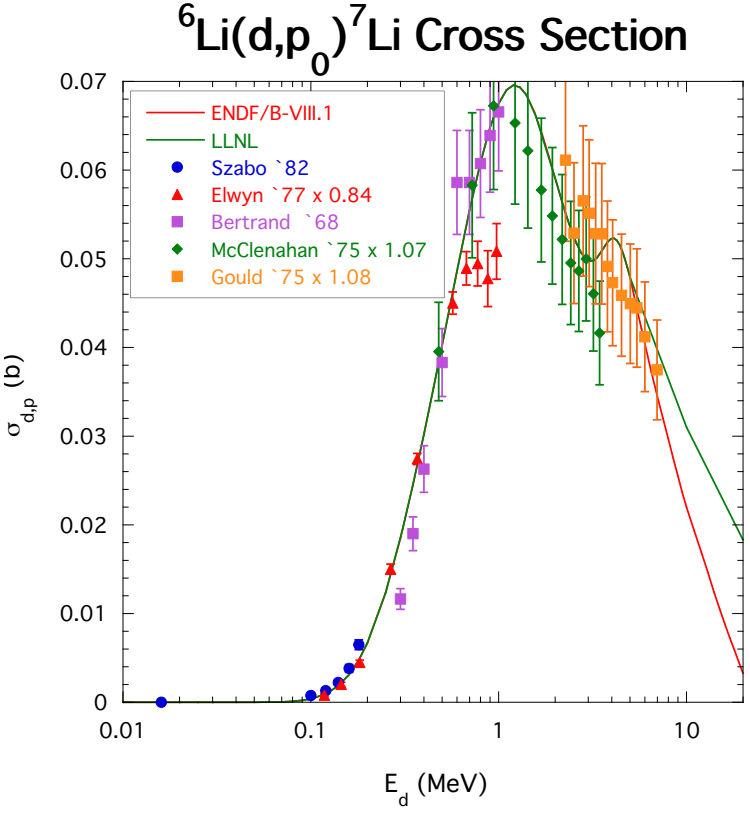
Most of these files were adopted for VIII.1.
Previous US evaluations were retained unless new experimental data have been taken that support IAEA2019 work over previous libraries.

Work ongoing at LANL to be able to process these files (See W. Haeck's talk).

Charged-particle libraries provided for incident alphas, deuterons, p, tritons by LANL/ LLNL.

Work is ongoing at LANL to process these files (see W. Haeck's talk).





Alphas	Deuterons	Protons	Triton
^{4}He	^{3}H	^{4}He	^{4}He
^{9}Be	^{3}He		
^{17}O	^{3}Li		
^{18}O			

LLNL work

Calculated with the LANL R-matrix code by G. Hale, M. Paris.

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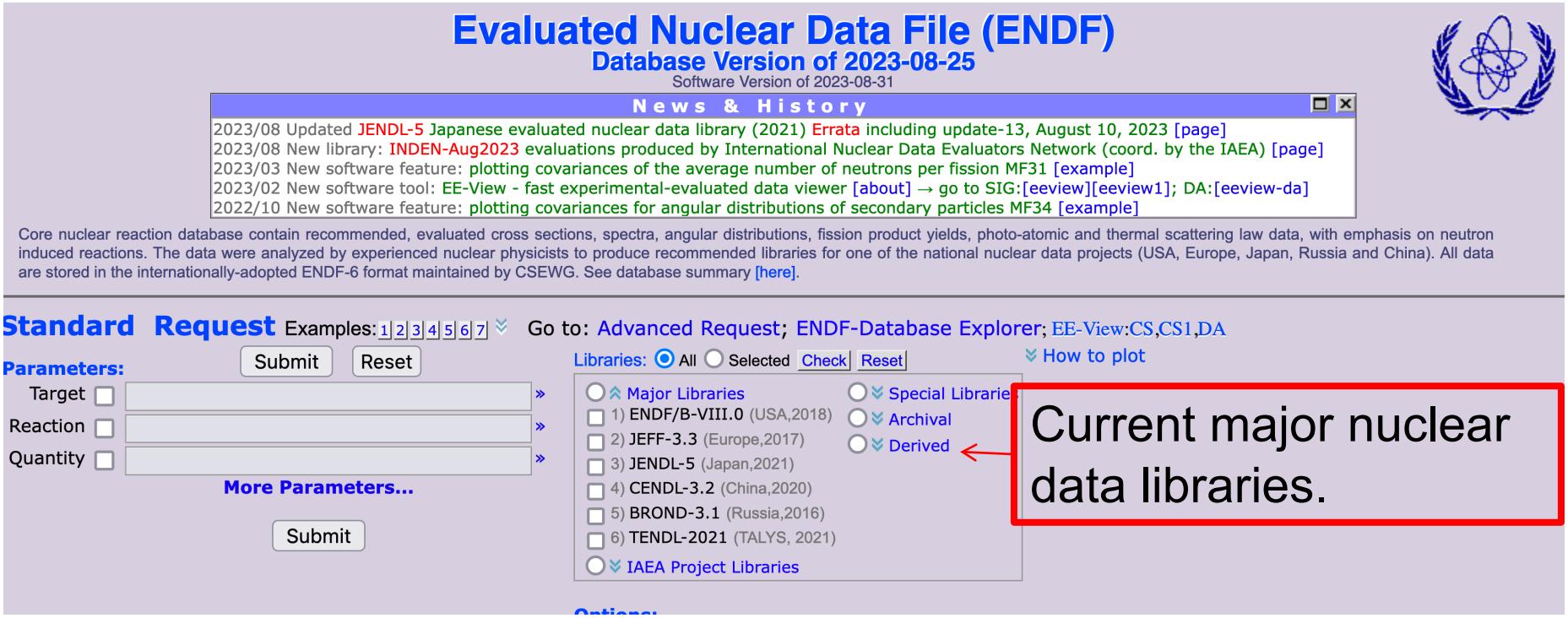
Where can I get the data from?

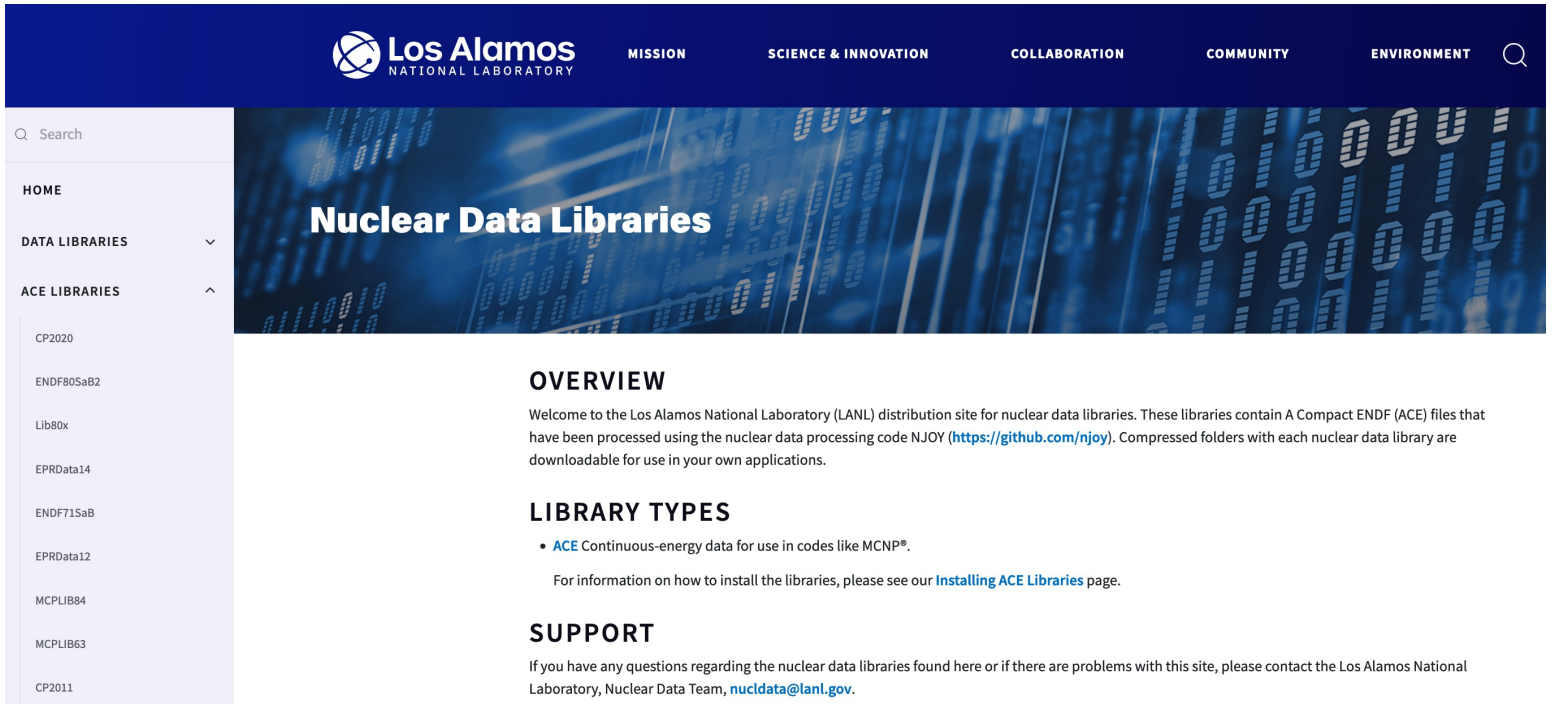
Where can I get the data: for plotting go to: https://www.nndc.bnl.gov/endf/

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



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

Where can I get the data in ACE format for MCNP. Go to: https://nucleardata.lanl.gov/



- Data will be processed with NJOY and tested with in-house capabilities as soon as released.
- Data in ACE format will be curated by XCP-5 LANL nuclear data team and then released on this homepage after testing.
- We will send a message to the MCNP forum.
- Questions? nucldata@lanl.gov or Q&A session on Wed.