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Title: Informing Nuclear Data Evaluations by combining ML/AI and CoH Sampling, and Integrating the New Model into CGMF

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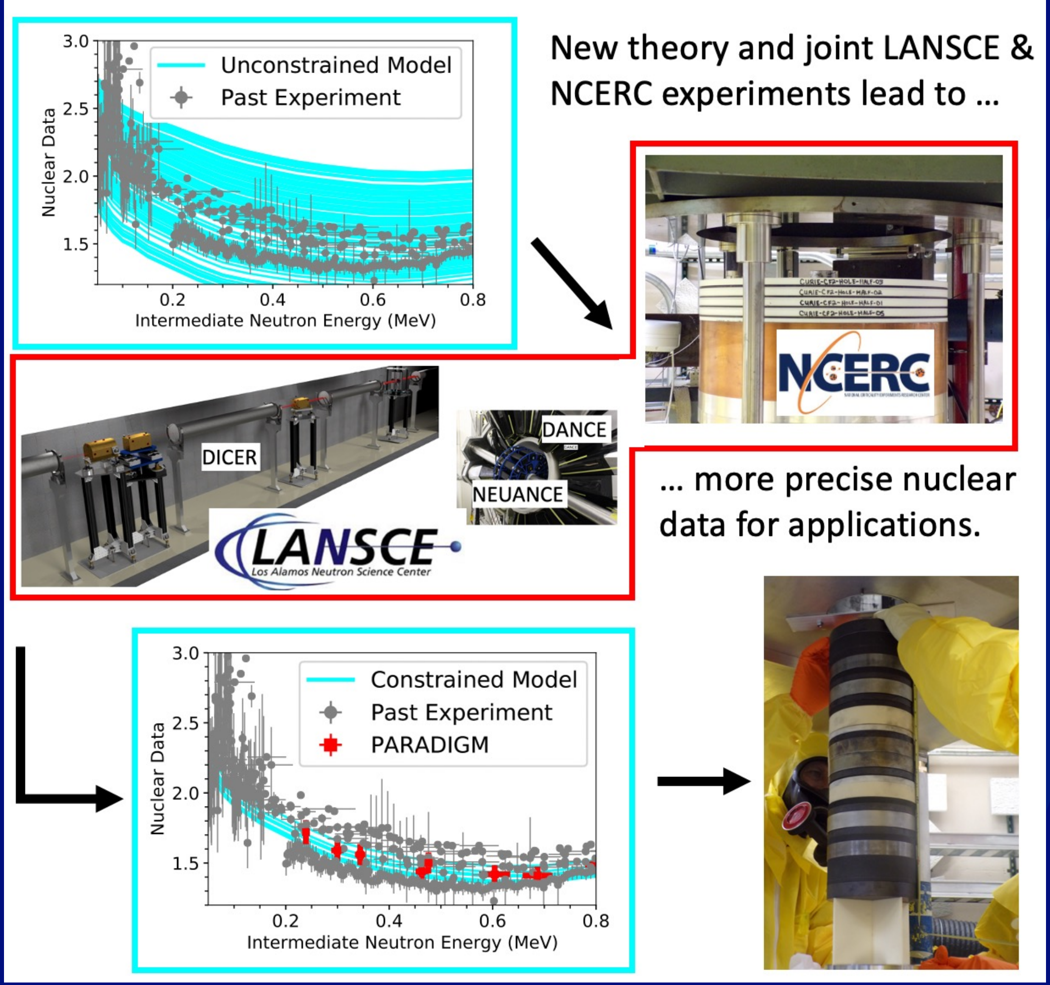


Los Alamos
NATIONAL LABORATORY

PARADIGM

PARallel Approach of Differential and InteGral Measurements

LDRD

NNSA

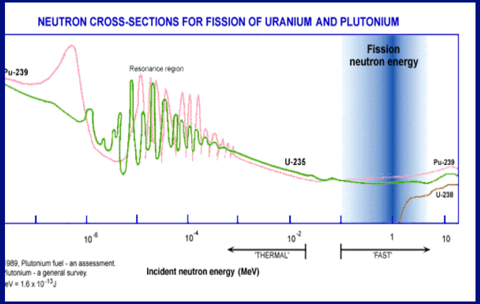
Informing Nuclear Data Evaluations by combining ML/AI and CoH Sampling, and Integrating the New Model into CGMF

Fanta Diaby [Presenter], Denise Neudecker, Amy Lovell, Michael Grosskopf, Noah Walton

CNR*24

Connecting Fission Cross-Section to CGMF

Purpose: Connecting various stages of the fission process – Fission Cross-Section to Prompt-Fission



Experimental Data

Experimental UQ Analysis → **Machine Learning** → **CoH** → (n,f)cs barriers → **CGMF**

- Use ML on experimental data to reduce data discrepancy
- Feature Biases and Experimental data vs Evaluated data

Theory: Hauser Feshbach Statistical Codes

- Fission fragment decay code
- Input: sampling parameters in fission cross section models CoH

- Improving Experimental Database by detailed uncertainty quantification
- Unrecognized sources of uncertainty related to measurement features

- LANL-developed Hauser-Feshbach statistical theory code, used for cross section modeling
- Sampling parameters

P. Talou et al. Fission fragment decay simulations with the CGMF code, Computer Physics Communications, Volume 269, (2021

Kawano, T. Unified description of the coupled-channels and statistical Hauser-Feshbach nuclear reaction theories for low energy neutron incident reactions. Eur. Phys. J. A 57, 16 (2021).

Experimental Data Uncertainty Quantification

ARIADNE Code

A tool developed for evaluators to estimate detailed uncertainties and covariances for experimental data consistently and efficiently

Experimental Features

Aspects related to the experiment:
Eg: Hardware Features
Method Features…

UQ Template

Can be used by evaluators for uncertainty quantification of a specific dataset when an uncertainty source is missing

Template of expected measurements uncertainties were used to estimate missing uncertainties of ^{235}U fission cross-section data of the Neutron Data Standards

Unc. Source	Absolute	Clean Ratio	Indirect Ratio
Sample Mass	> 1%	Both Samples	Both samples
Counting Statistics	Sample-dependent	Both, combined	Both samples
Attenuation	0.2-2%	0.02-0.2%	0.2-2%
Detector Efficiency	1-2%	0-0.3%	1-2%, 0.5-1%
FF Angular Distrib.	~0.1%	Less than for abs.	~0.1%
Background	0.2 - >10%	0.2 - >10%	0.2 - >10%
Energy Unc.	1%, 1-2 ns	Combined	Both detectors
Neutron Flux	>1%	Cancels or small	Cancels or small
Multiple Scattering	0.2-1%	Reduced for abs.	0.2-1%
Impurit. in Sample	Sample-dependent	Both samples	Both samples
Dead Time	>0.1%	Both, combined	Both detectors

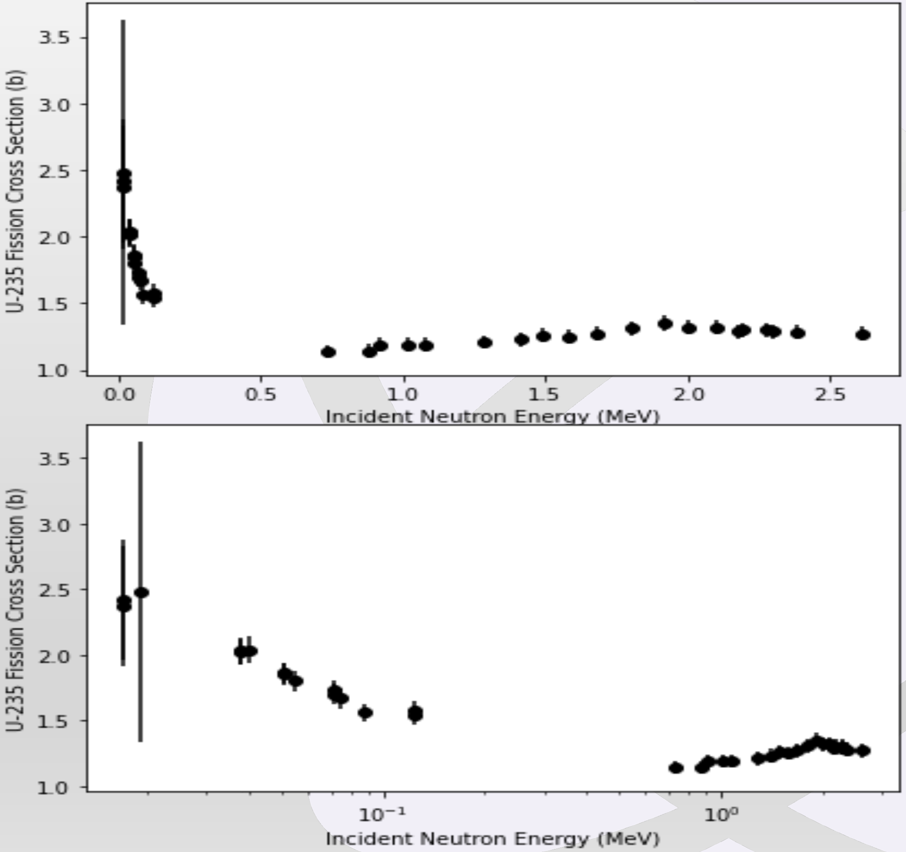
D. Neudecker et al. Applying a Template of Expected Uncertainties to Updating 239Pu(n,f) Cross-section Covariances in the Neutron Data Standards Database, Nuclear Data Sheets, Volume 163, (2020)

Denise Neudecker, ARIADNE – a program estimating covariances in detail for neutron experiments, EPJ Nuclear Sci. Technol. 4, 34, (2018)

A.D. Carlson et al. Evaluation of the Neutron Data Sandards, Nuclear Data Sheets, Volume 148 (2018)

Experimental uncertainties of $^{235}U(n,f)$ cross sections in the standards database were reviewed

GMA-number	Author and Year	Energy-min (MeV)	Energy-max (MeV)	Uncertainty-min (%)	Uncertainty-max (%)
643	Li Jingwen et al., 1982	14.7	14.7	2	2
645	Li Jingwen et al., 1986	14.2	14.2	1.7	1.7
564	M.C.Davis et al. 1978	0.14	0.964	2.1	2.3
567	R.K.Smith et al., 1956	2.22	20.5	5.2	7.4
570	O.A.Wasson et al., 1981	0.2445	1.196	2.2	2.6
523	A.D Carlson et al., 1984	0.3097	2.825	2	2.3
518	G.F.Knoll+W.P.Poenit, 1967	0.03	0.03	4.7	4.7
581	F.Kaeppeler, 1973	0.546	1.175	2.7	3
580	D.M.Barton et al., 1976	1	6	1	2.4
499	P.H.White, 1965	0.04	0.505	2.6	3.2
500	P.H.White, 1965	0.505	2.25	2.5	2.6
501	P.H.White, 1965	2.25	5.4	2.8	3.8
502	P.H.White, 1965	14.1	14.1	2	2
725	J.L.Perkin et al., 1965	0.0222	0.0222	2.9	2.9
503	I.Szabo et al., 1970	0.0175	1.01	3	3.2
504	I.Szabo et al., 1971	0.0115	0.199	3.1	3.3
505	I.Szabo et al., 1973	0.017	2.61	3.1	3.2
506	I.Szabo et al., 1976	2.35	5.53	3.4	4.1
596	M.Cance+G.Grenier, 1978	13.9	14.6	1.9	2
597	M.Cance+G.Grenier, 1983	2.5	4.45	1.6	2.1
598	M.Cance+G.Grenier, 1983	2.5	2.5	2.8	2.8
599	O.A.Wasson et al., 1982	14.1	14.1	1.4	1.4
522	N.N.Buleeva et al., 1988	0.624	0.785	3.3	3.4
591	Tud/Kri Collab., 1983	2.6	2.6	1.24	1.24
592	Tud/Kri Collab., 1983	8.46	8.46	2.2	2.2
593	Tud/Kri Collab., 1983	14.7	14.7	1.6	1.6
590	Tud/Kri Collab., 1984	4.45	4.45	2.2	2.2
554	W.P.Poenitz, 1977	0.193	4.449	2	2.9
555	W.P.Poenitz, 1977	4.396	8.275	2.1	3.6
557	W.P.Poenitz, 1974	0.8	0.8	2.5	2.5
558	W.P.Poenitz, 1974	3.5	3.5	2.4	2.4
560	W.P.Poenitz, 1974	0.498	0.498	3.9	3.9
561	W.P.Poenitz, 1974	0.448	0.664	3.6	3.8
528	K.Yoshida et al., 1983	13.49	15.01	5.3	5.4
738	Yan Wuguang et al., 1975	0.5	1	4.6	4.7
525	E.A.Schagrov et al., 1980	0.046	0.12	3.6	3.7
573	B.C.Diven, 1957	1.27	1.27	3.8	3.8
878	I.M.Kuks et al., 1973	2.5	2.5	4.2	4.2
526	C.A.Uttley+J.A.Phillips, 1956	14.1	14.1	3.5	3.5
584	A.Moat, 1958	14	14	4.4	4.4
1025	A.D.Carlson,R.G.Johnson et W,Carlson, 1991	1.1	5.99	1.9	2.9
1026	V.A.Kalinin et al., 1991	1.88	2.37	2.3	2.3
1027	T.Iwasaki et al., 1988	13.51	14.9	2.5	2.8
1036	R.Nolte, 2003	19	199.02	3.95	9.05
1031	V.I.Goldanskiy et al., 1955	120	380	3.1	3.1

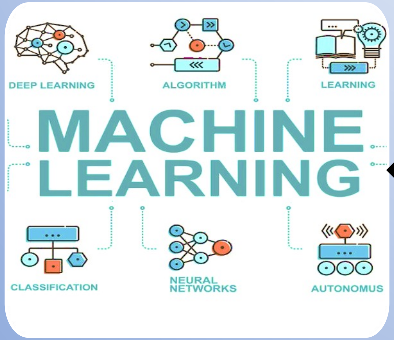


Output from ARIADNE

505 Szabo, 1973

Data Discrepancy in Machine Learning

- We used ^{239}Pu experimental data to see what measurement features drive bias
- At the moment, we are looking for a bug in our ML code
- If we can have realistic fission cross sections using ML, with reliable uncertainties, then we can sample parameters within the fission cross section model in CoH to encompass the uncertainty in this data. We then use this to connect to the prompt fission observables in CGMF



Improved Fission Cross Section Data

Theory:

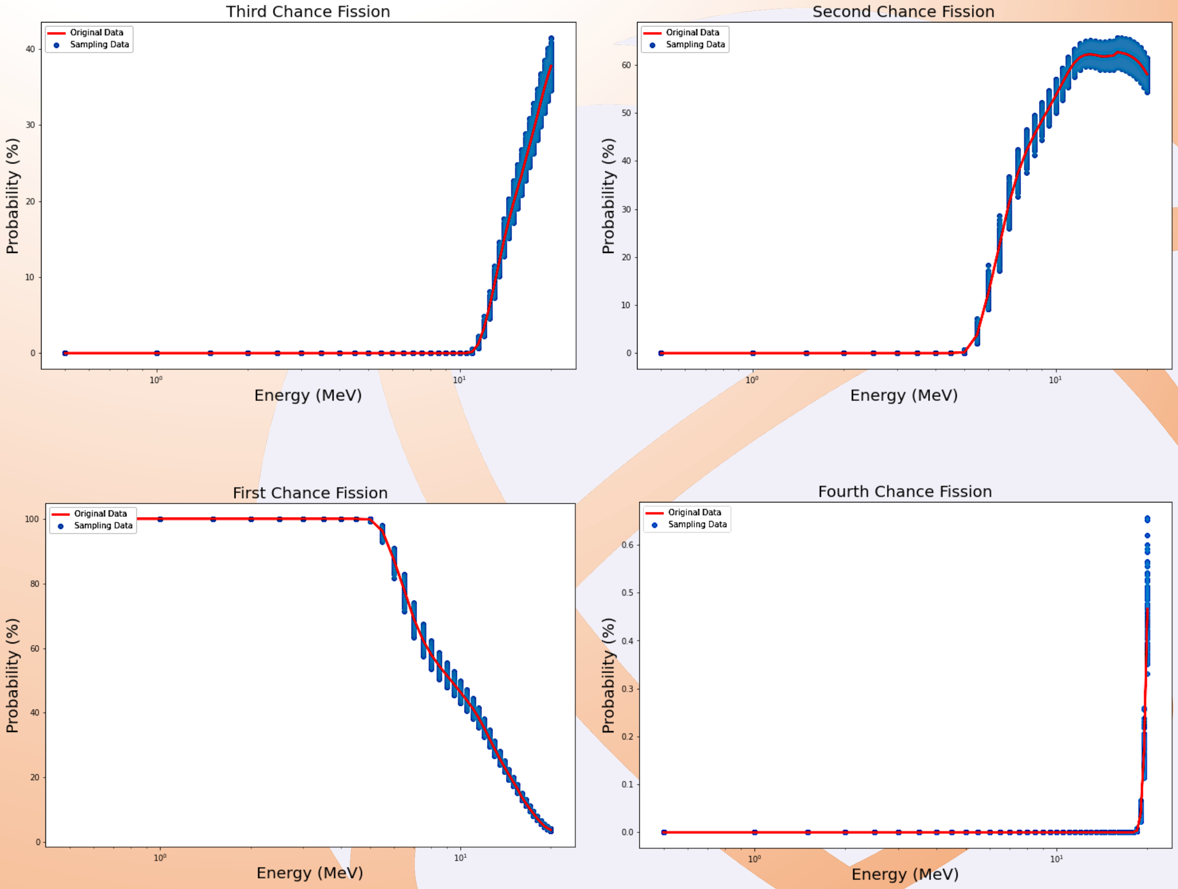
CoH

CGMF

Multi-chance fission probabilities from sampling the fission cross section parameters with CoH

Multi-chance fission probabilities from sampling the fission cross section parameters with CoH

- The barrier parameters were sampled uniformly +/- 2% for the Height and +/- 10% for the Curvature = spread in the probabilities
- Number of Samples: 100
- Energy Points: 0.5 to 20 MeV in steps of 0.5 (40 Energy Points)
- The Multi-chance fission probabilities are one of the inputs of CGMF from sampling the fission cross section parameters with CoH



CoH Sampling: Multi-chance fission probabilities

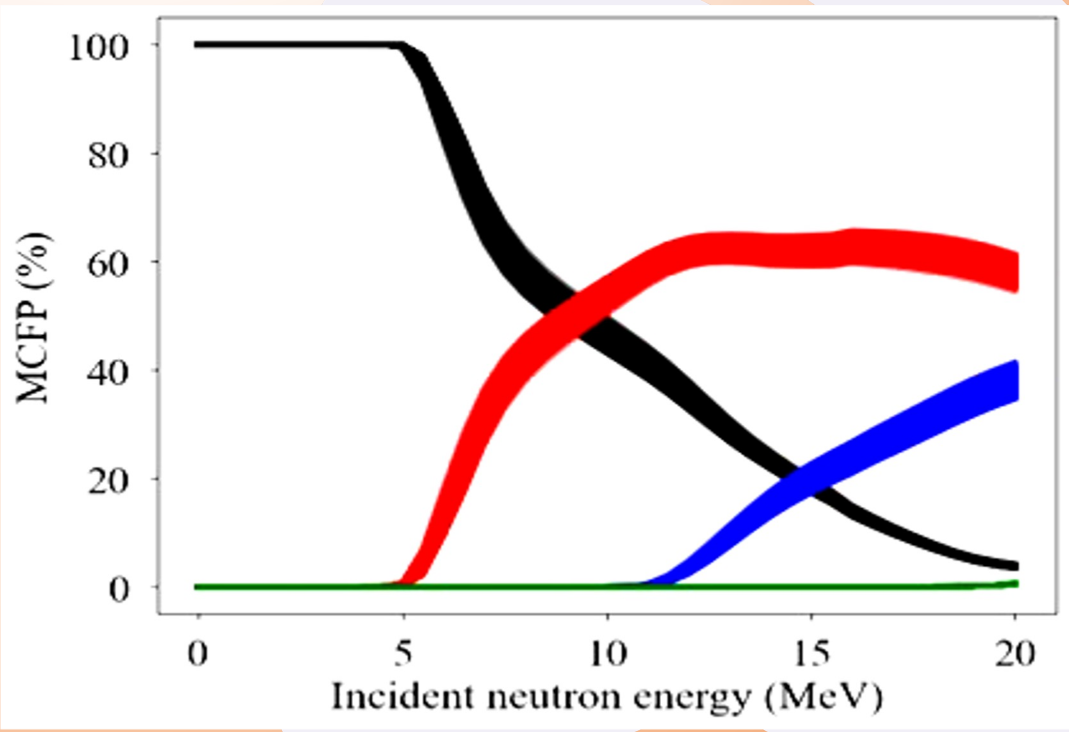
- Changes in the multi-chance fission probabilities ~ 20%

$$MCFP_{\%} = (\sigma_{max} - \sigma_{min}) / \sigma_{base}$$

σ_{max} = Maximum fission probability

σ_{min} = Minimum fission probability

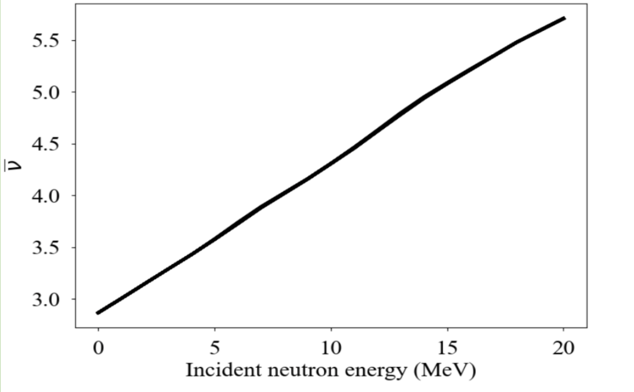
σ_{base} = Original fission probability

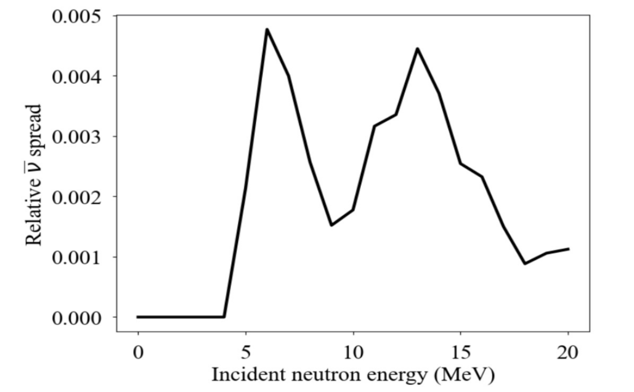


First Chance Fission Probability
Second Chance Fission Probability
Third Chance Fission Probability
Fourth Chance Fission Probability

Amy E. Lovell, MCFP Plot, LANL 2024

CGMF simulations with sampled fission probabilities lead to only small variations in nu-bar





- Small changes in nu-bar and relative nu-bar change plot shows changes of 0.5% near the start of the multi-chance fissions, which is small compared to spread in the multi-chance fission probabilities of 20%

Amy E. Lovell, CGMF Calculations and Figure, LANL 2024

Summary and Outlook

What we did:

- We investigated experimental uncertainties of ^{235}U and ^{239}Pu fission cross sections using templates of expected measurement uncertainties and starting from the Neutron Data Standards database
- We forward-propagated sampled fission cross sections via CoH to see spread in nu-bar using CGMF. The impact is small.

To Do:

+) We will work with the Neutron Data Standards community on updated ^{235}U fission cross section uncertainties

+) We will finalize applying ML to ^{235}U and ^{239}Pu fission cross section experimental data to see clues of what features could potentially drive measurement biases

Thank you for your attention

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