Artificial Intelligence in Teaching, Research and Service: Pros and Cons
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Machine Learning Methods within the Nuclear Data Life Cycle

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The teacher

Oscar Cabellos
(UPM)

- I am Oscar Cabellos, full professor in nuclear engineering at the Polytechnic University of Madrid (UPM).
- I am coordinator of UPM courses on "Introduction on Nuclear Technology", "*Simulation of Nuclear Power* Plants", "Nuclear Energy for the Energy Transition" and "Design *and Simulation of PWRs*" which is one of the UPM coursed based on the CDIO (Conceive, Design, Implement and Operate) initiative.
- My background is **reactor physicist**, specifically in PWR simulations where I did my PhD in 1998. Since 2005 I have been involved in EU projects **working on nuclear data activities**: EUROTRANS (2005-2010), ANDES(2010-2013), CHANDA(2013-2018) and SANDA (2019-2023).
- In 2014-2017, I moved to NEA Data Bank as Nuclear Data Scientist working in the development of EXFOR and JEFF databases , and JANIS and NDaST web-tools. Currently, I am actively working in the JEFF project and WPEC activities of the OECD/NEA.
- Member of the JEFF-CG, WPEC (coordinator WPEC/SG46 and monitor of WPEC/SG47), WPNCS (monitor SG12 on Decay Heat). Member of the OECD/NEA - Nuclear Science Committee (NSC) and the Management Board for the Development, Application and Validation of Nuclear Data and Codes (MBDAV).
- Over 40 papers in international scientific journals with reviewers, more than 60 papers/presentations in proceedings of international conferences and more than 100 contributed talks in workshops.

Content: Machine Learning Methods within **the Nuclear Data Life Cycle**

1. Introduction: The role of nuclear data for nuclear applications

2. Activities associated with nuclear data: The nuclear data life cycle

   - EXFOR: “the mother of all libraries”

   - Nuclear reaction models and codes

3. The Evaluation of ND: The Bayesian’s Approach

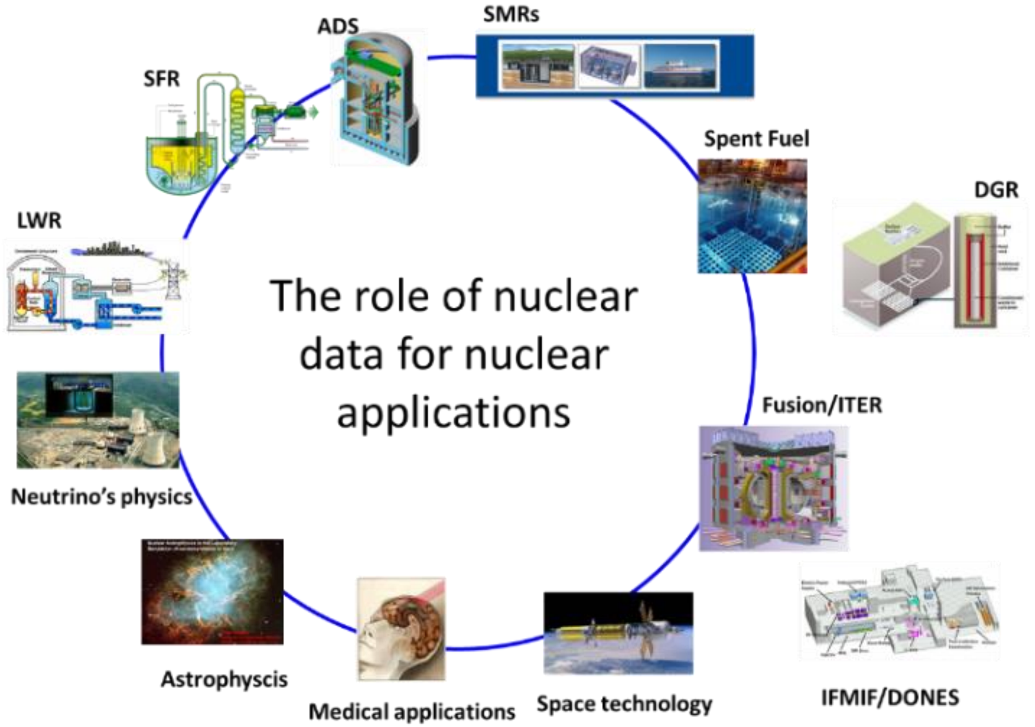
   - International efforts on evaluation of ND: The JEFF Project

4. Integral Databases for B&V: ICSBEP

An introduction to **DATA, DATABASES, MODELS, EVALUATIONS** … in the nuclear data field!!! where there is plenty of room for ML/AI algorithms!

1. Introduction: The role of nuclear data for nuclear applications

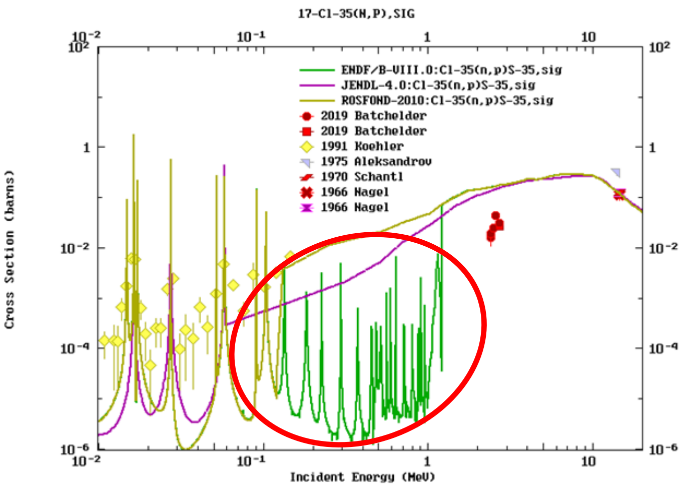
Figure 1. *Examples of nuclear applications where the nuclear data play an important role*



An example:

Nuclear data in Molten Salt Reactors

Figure 2. *The $^{35}Cl(n,p)$ cross-section: Experimental data versus evaluated data.*



1.1 Nuclear data for modelling nuclear systems

Figure 3. *Neutron transport Boltzmann equation*

$$\frac{1}{v}\frac{\partial \Psi}{\partial t} + \Omega \cdot \nabla\Psi + \Sigma_T \Psi = S + \int_E \int_\Omega \Psi(E', \Omega') \cdot \Sigma_s(E' \rightarrow E, \Omega' \rightarrow \Omega) dE' d\Omega'$$

$$S_{PF} = \sum_i N_i \int dE' \; \phi(E') \cdot \nu_i(\mathrm{E}') \cdot \sigma_{F,i}(E') \cdot \chi_{F,i}(E', E)$$

$$S_{dn} = \sum_k \lambda_k \cdot C_k(r, t) \cdot \chi_{d,k}(E)$$

Figure 4. *Bateman transmutation equation*

$$\frac{dN_i(t)}{dt} = -(\lambda_i + r_i) \cdot N_i(t) + \sum_{i \neq j} (\lambda_{j \rightarrow i} + r_{j \rightarrow i}) \cdot N_j(t) + PF_i$$

$$\mathrm{PF}_i = \sum_h N_h \cdot \int_0^\infty dE \cdot \phi(E) \cdot \gamma_{h \rightarrow i}(E) \cdot \sigma_{f,h}(E)$$

1.2 An Example: Nuclear data and Integral Experiments (e.g. keff)

A **set of nuclear data** are validated by **simulating** and comparing to **integral experiments**

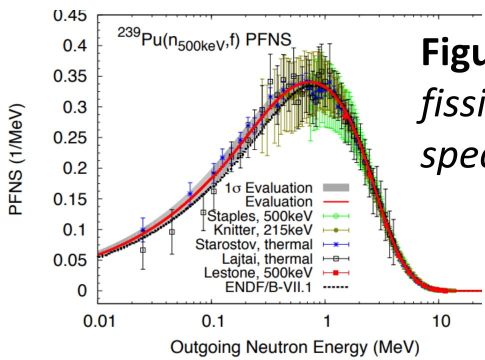


Figure 5. *Prompt fission neutron spectra*

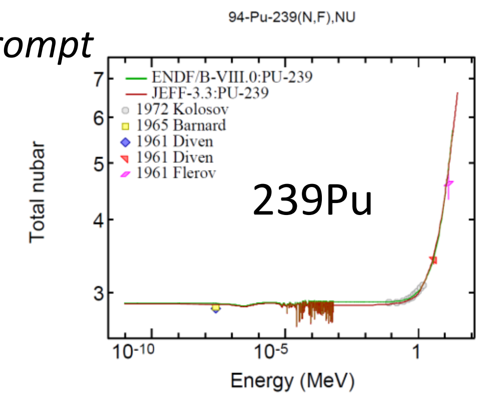


Figure 7. *Average prompt neutron multiplicity*

Figure 6. *Fission cross-section*

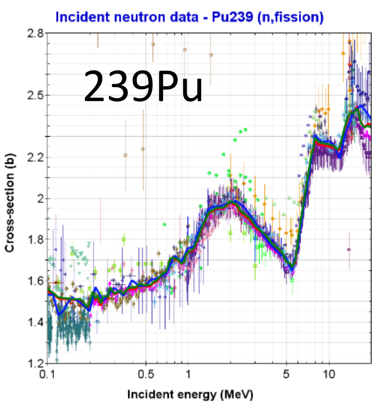
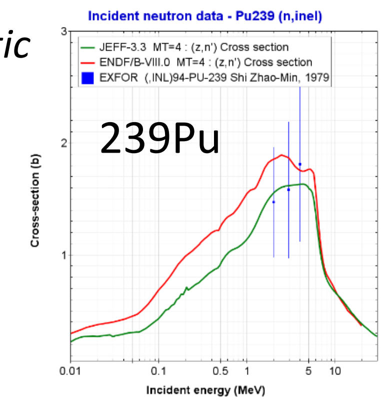


Figure 9. *The Jezebel 239Pu criticality assembly [1]*

Figure 8. *Inelastic cross-section*

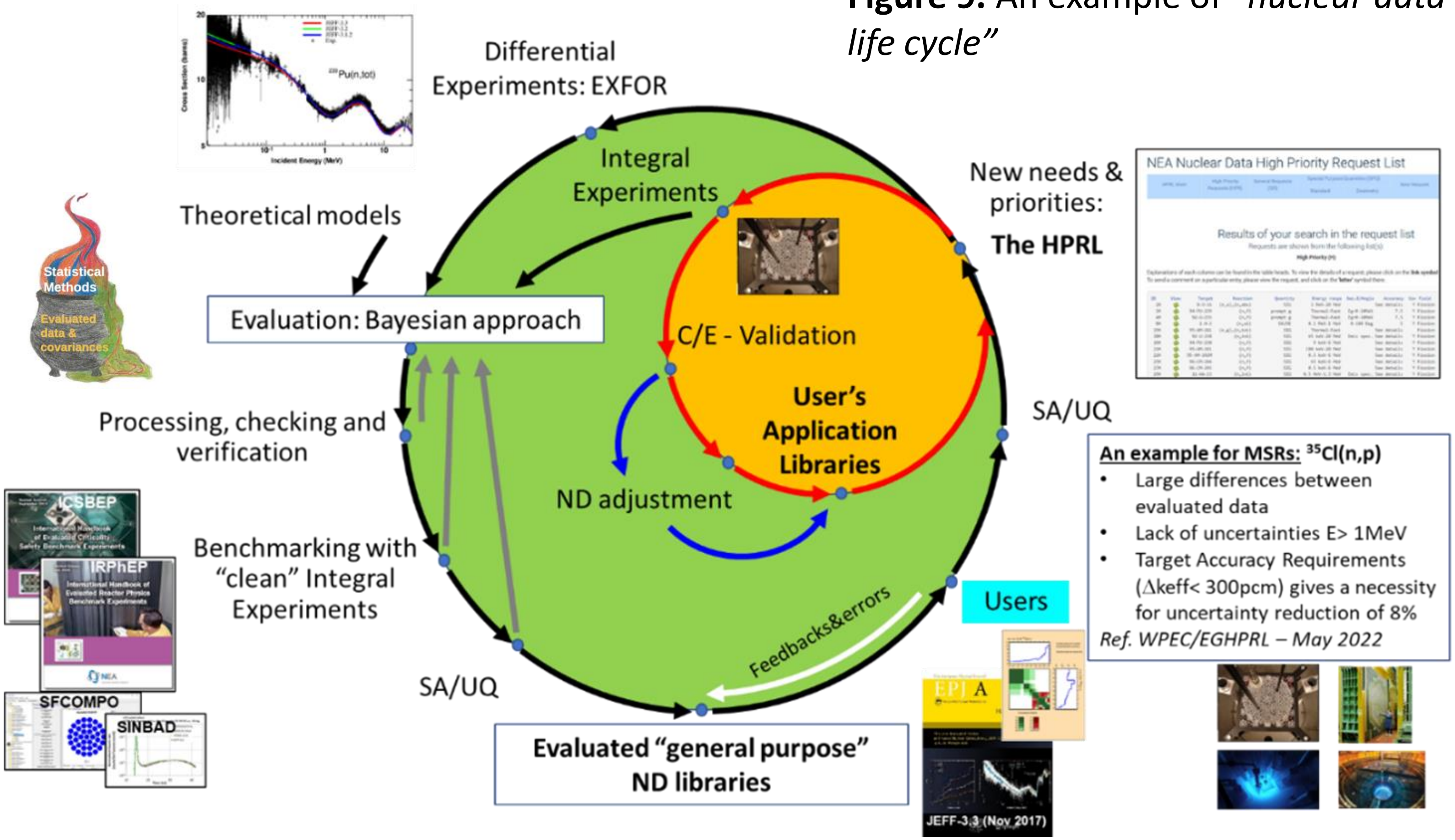


$$\Omega \cdot \nabla\Psi(\mathbf{r},\mathrm{E},\Omega) + \Sigma_T(\mathbf{r},\mathrm{E},\Omega)\Psi(\mathbf{r},\mathrm{E},\Omega) = \int_0^\infty \int_{4\pi} \Psi(\mathbf{r},E',\Omega') \cdot \Sigma_s(\mathbf{r},E' \to E, \Omega' \to \Omega)dE'd\Omega'$$

$$+ \frac{1}{k_{eff}} \frac{\chi_f(E)}{4\pi} \int_0^\infty \int_{4\pi} \Psi(\mathbf{r},E',\Omega') \cdot \overline{\nu_t}(\mathbf{r},E') \cdot \Sigma_f(\mathbf{r},E' \to E, \Omega' \to \Omega)dE'd\Omega'$$

2. Activities associated with nuclear data: *The* ***nuclear data life cycle***

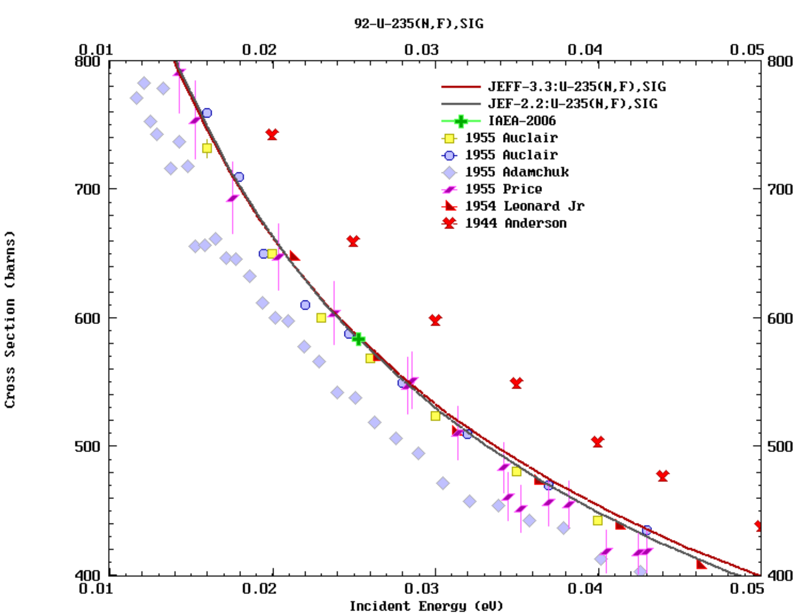
Figure 9. An example of *"nuclear data life cycle"*



2.1 EXFOR: “the mother of all libraries”

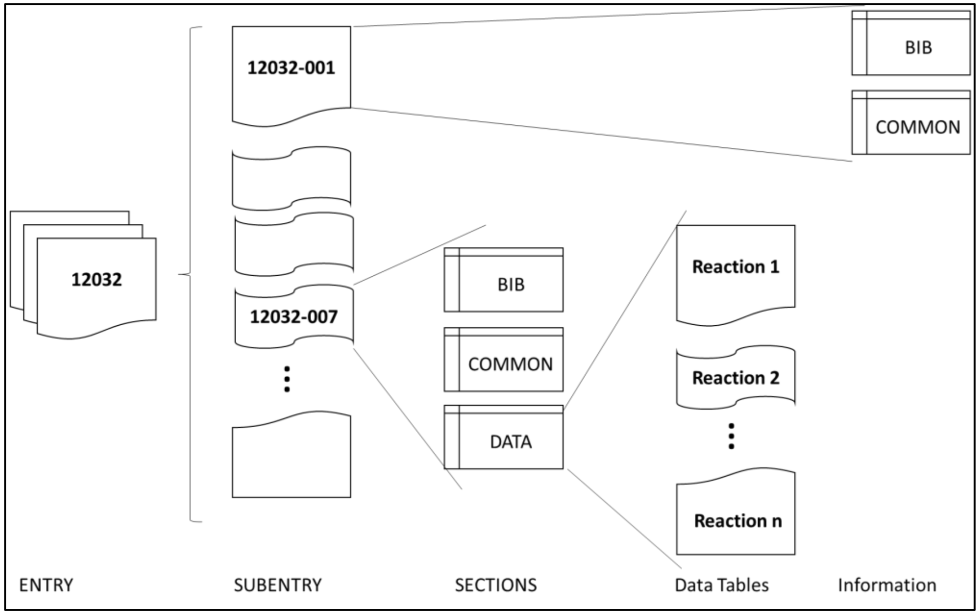
- Currently, EXFOR is the library of experimental nuclear reaction data, cross-sections and other nuclear reaction quantities (e.g. integral resonances, …) … **NOT EVALUATED LIBRARY!!!**
- EXFOR contains nuclear measurements in more than **22 000 experiments**, not only for neutron beam but also for photon, proton and other charged-particle beam.

Figure 10. *Experimental data before 1955 for 235U($n_{thermal}$, fission) cross-section*



- The basic structure of the EXFOR format

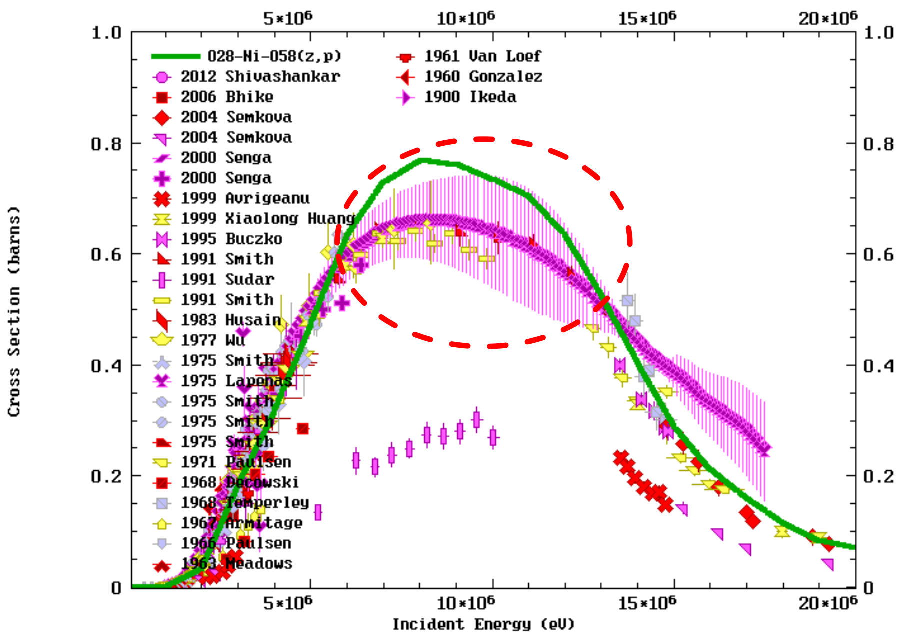
Figure 11. *Structure of information in EXFOR*



2.2 Nuclear reaction models and codes

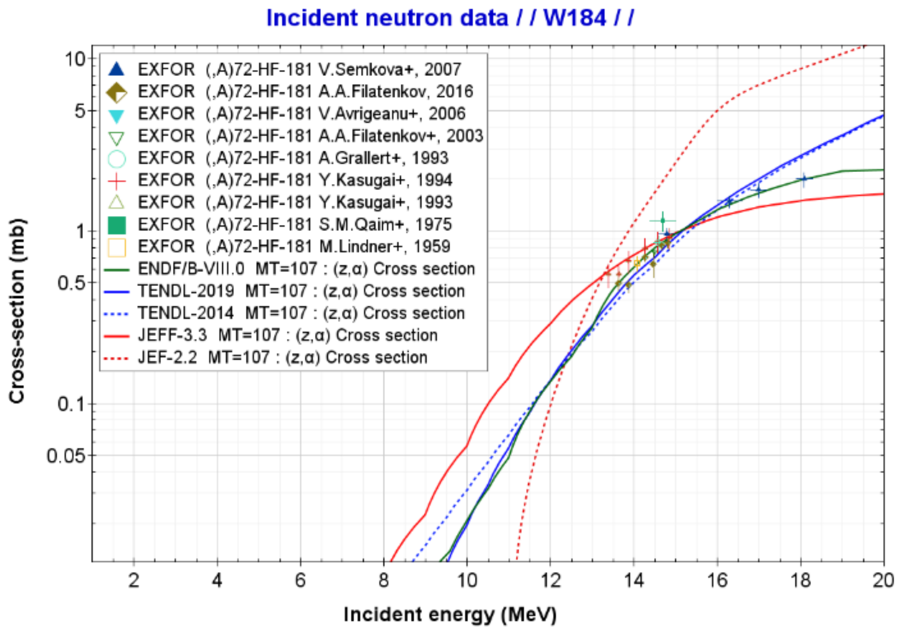
EMPIRE, TALYS, … nuclear reaction codes are used for the simulation of nuclear reactions which provide a complete description of all reaction channels and observable (e.g. cross-sections, angular distributions,…)

Figure 12. *Comparison between EMPIRE code (**green line**) and EXFOR data for 58Ni(n,p)*



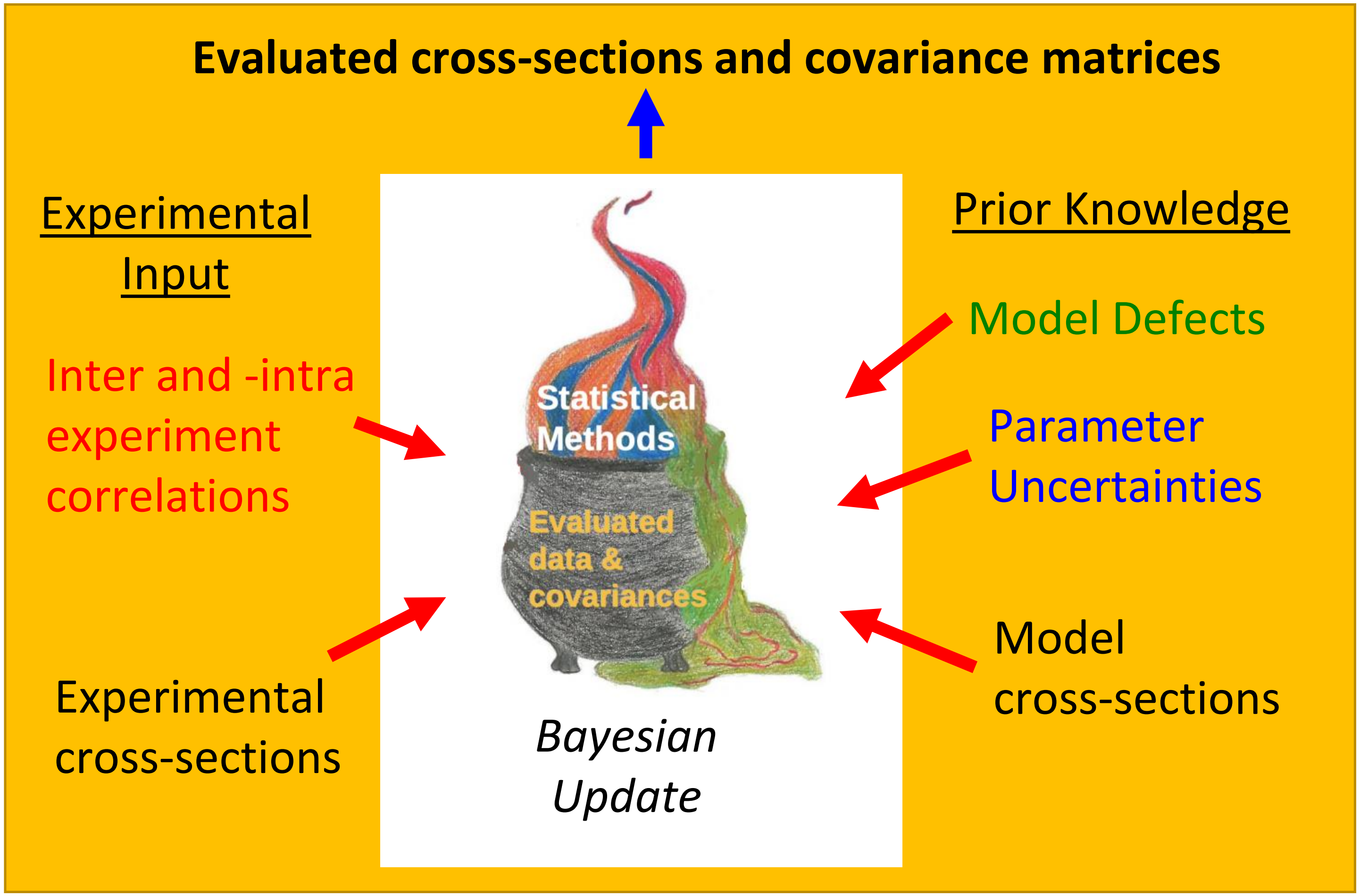
- A good agreement is shown in general except for 10-12 MeV which may reflect deficiencies in the nuclear model parameters for this reaction.

Figure 13. *The cross section 184W(n,alpha)*



- Exp. data are used for calibration of nuclear parameters in models
- But, some nuclear models show lack accuracy for detailed prediction of cross-sections in the whole energy range

3. The Evaluation of ND: The Bayesian's Approach



- Bayesian methods – like "cooking" are very familiar in the evaluation of nuclear data

Figure 14. *Example of the Bayesian procedure to evaluate cross-section and covariances*

Ref. D. Neudecker, S. Gundacker, H. Leeb et al., ND2010 (picture courtesy by D. Neudecker)
… and cooking rice-Paella's photos courtesy by M. Garasa

3. The Evaluation of ND: The Bayesian's Approach

Evaluated cross-sections and covariance matrices

Experimental Input

Inter and -intra experiment correlations

Experimental cross-sections

Bayesian Update

Prior Knowledge

Model Defects

Parameter Uncertainties

Model cross-sections

- Bayesian methods – like "cooking" are very familiar in the evaluation of nuclear data

Figure 14. *Example of the Bayesian procedure to evaluate cross-section and covariances*

Ref. D. Neudecker, S. Gundacker, H. Leeb et al., ND2010 (picture courtesy by D. Neudecker)
… and cooking rice-Paella's photos courtesy by M. Garasa

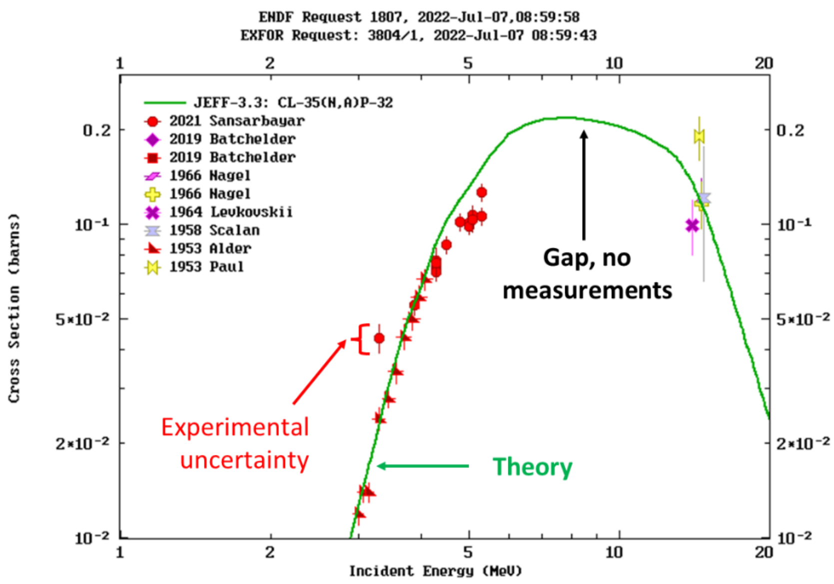
In summary…. the ND evaluation pipeline

Briefly, the nuclear data evaluation "pipeline" can be summarized in the following steps:

- Collection of experimental EXFOR data
- Correction/normalization of experimental data
- Fitting a model to the corrected experimental data:
  - GLLS methods directly to experimental data
  - Nuclear physics model (based on robust fundamental nuclear physics formulation)
    - TALYS
    - EMPIRE
    - …

  Bayesian methods for model fitting are very familiar in the evaluation of nuclear data
- Finally, the last step is the generation of Evaluated Data files:
  - ENDF-6 format
  - GNDS format

Figure 15. *^{35}Cl(n,a) reaction cross section: modelling versus experimental data*



Conclusion

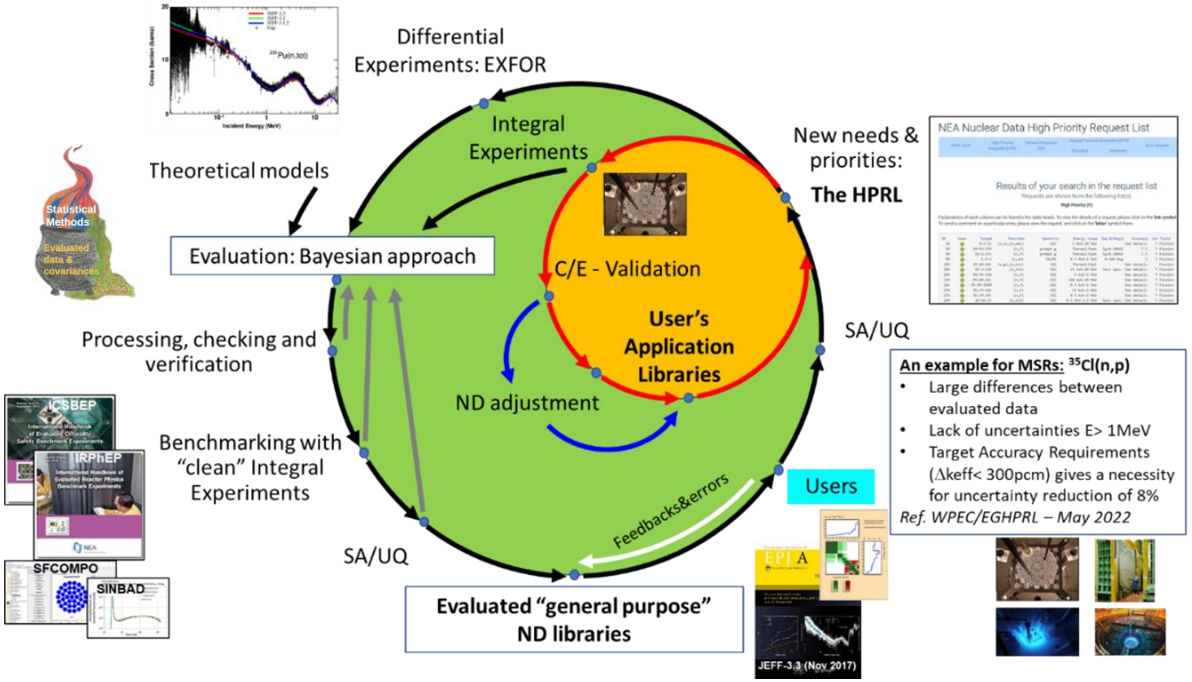


Figure 9. An example of *"nuclear data life cycle"*

An introduction to DATA, DATABASES, MODELS, EVALUATIONS … in the nuclear data field!!! where there is **plenty of room for ML/AI algorithms!**

Next, it is focused on examples of current **ML/AI activities in the nuclear data life cycle**

Background: Nuclear Data Adjustment and ML in Web of Science (WoS)

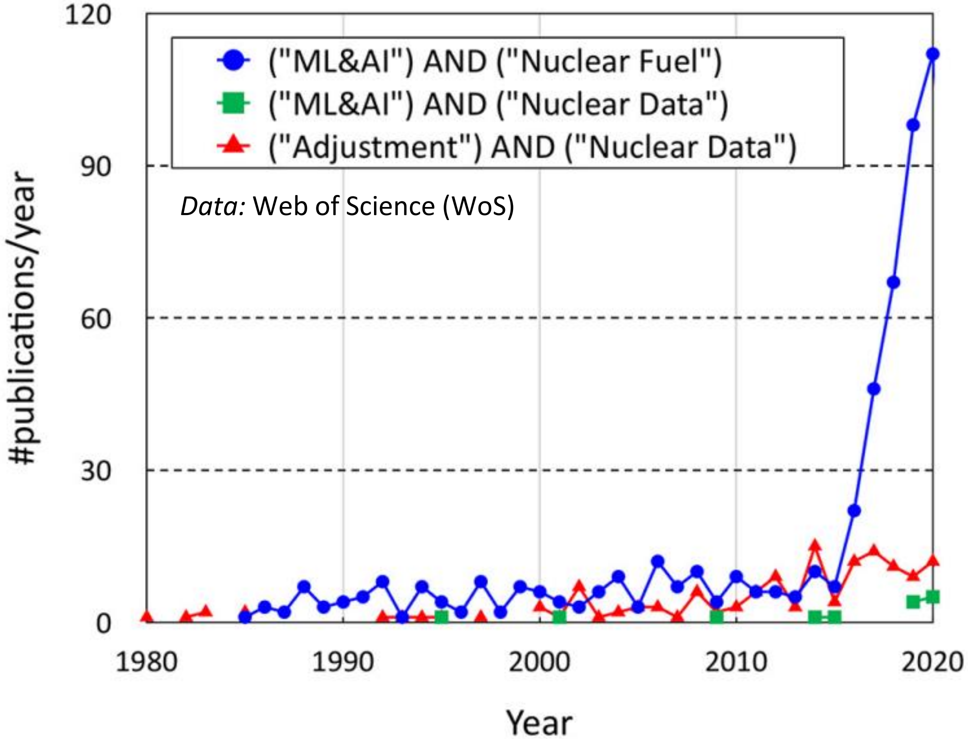


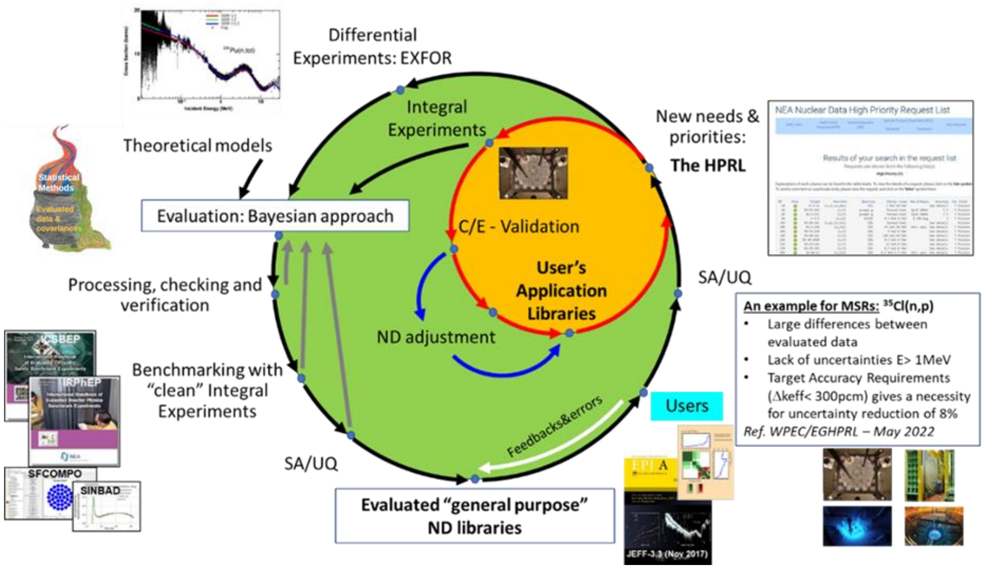
Figure 18. *The number of papers containing terms "ML/AI" and "Nuclear Fuel for in-core management" are plotted in* ***blue****.*

For the topic "nuclear data evaluation", the number of papers shown are for :

- well-stablished adjustment techniques (in **red**)
- ML/AI techniques (in **green**) [1]

Content: Machine Learning Methods
within the Nuclear Data Life Cycle

1. Introduction
2. Experiments/Compilation
3. ND Models
4. Evaluation
5. Validation
6. ML & Optimization
7. Conclusion



Now, we are focusing on examples of current **ML/AI activities** in the nuclear data life cycle

Background: Nuclear data and Integral Experiments (e.g. keff)

Ref.: D. Neudecker et al. , *"Using Machine Learning Algorithms for Large-scale Nuclear data Validation"*, Seminar at UPM (October 2020) LA-UR-2028240

- **The k_{eff}** value is simulated by **20,000 nuclear data values**. Which nuclear data causes difference to predict accurate keff ?

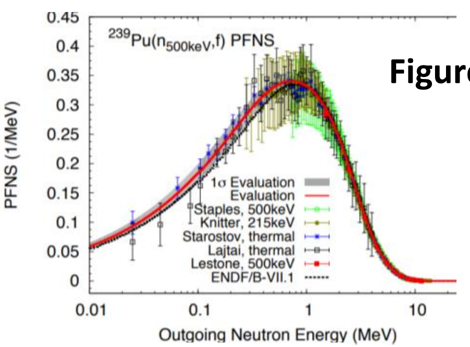


Figure 1. *PFNS*

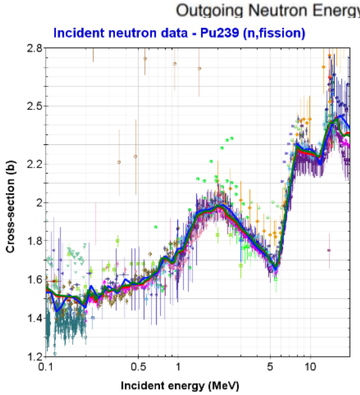


Figure 2. *Fission cross-section*

Figure 3. *The Jezebel 239Pu criticality assembly [1]*

$$\Omega\cdot\nabla\Psi(\mathbf{r},E,\Omega) + \Sigma_T(\mathbf{r},E,\Omega)\Psi(\mathbf{r},E,\Omega) = \int_0^\infty\int_{4\pi}\Psi(\mathbf{r},E',\Omega')\cdot\Sigma_s(\mathbf{r},E'\to E,\Omega'\to\Omega)\,dE'd\Omega'$$
$$+\frac{1}{k_{eff}}\frac{\chi_f(E)}{4\pi}\int_0^\infty\int_{4\pi}\Psi(\mathbf{r},E',\Omega')\cdot\overline{\nu_t}(\mathbf{r},E')\cdot\Sigma_f(\mathbf{r},E'\to E,\Omega'\to\Omega)\,dE'd\Omega'$$

ML/AI .... in nuclear data

- **Problem:** human brain cannot assess which of 20,000 nuclear data are related to imperfect simulation of integral exp
- **Gap:** need systematic method to identify imperfect nuclear data via integral experiments
- **Impact of solving problem**:
  - More targeted (cost-effective) nuclear data research
  - Identify need for integral and differential experiments
  - Better data for application calculations

1. Introduction:
Machine Learning Methods to NDLC

*A summary of main fundings of the nuclear data community identifying the key areas in which AI/ML have already made significant impacts can be found at **WANDA-2020 meeting** [1]*
https://conferences.lbl.gov/event/292/

- **EXPERIMENTS/COMPILATIONS**
    - To identify outlier data points and problematic datasets
    - To identify and quantify missing systematic errors
    - To prioritise new differential measurements
    - …
- **EVALUATIONS/PROCESSING**
    - To develop emulators to incorporate complex physics models into evaluations
    - To extrapolate evaluations to unmeasured nuclei, and to accurately capture the correlations between different nuclear properties
    - To perform a completely new approach to update ENDF files using Gaussian Process
    - To both develop surrogate physics models and use them to sequentially search and optimize over a wide space of experimental design
    - …
- **BENCHMARKING/VALIDATION**
    - To identify systematic trends in nuclear data that were missed by human evaluators
    - To process complex relationships between nuclear data and integral experiments
    - To design and optimize new integral experiments that address nuclear data gaps for particular applications
    - …

Examples in Experiments/Compilation

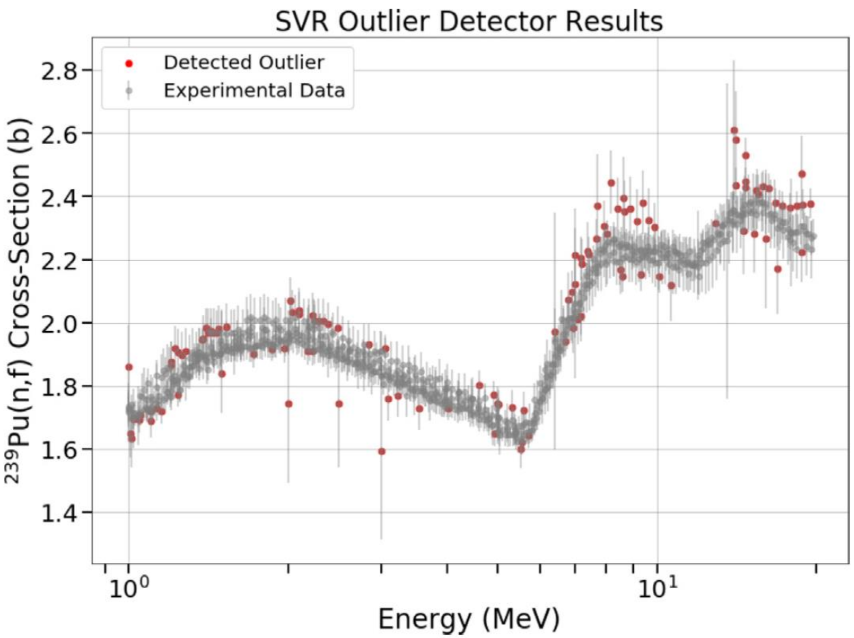
2. Experiments/Compilation: Outlier identification - 239Pu(n,fission)

Ref.: B. Whewell et al. , *"Evaluating 239Pu(n,f) cross sections via machine learning using experimental data, covariances, and measurement features"*, Nuclear Inst. and Methods in Physics Research, A 978 (2020) 164305

Technique: **Hybrid Robust Support Vector Machine (SVM)** is used to identify potential outliers.

Objective: Outlier identification in experimental data for the evaluation of 239Pu. This allows to add penalty uncertainties to the experimental covariances of outlying data points that have outlier measurement features for the evaluation with GLLS technique.

Figure. SVR outlier detector results for 239Pu(n,fission)



Examples in Nuclear Data Models

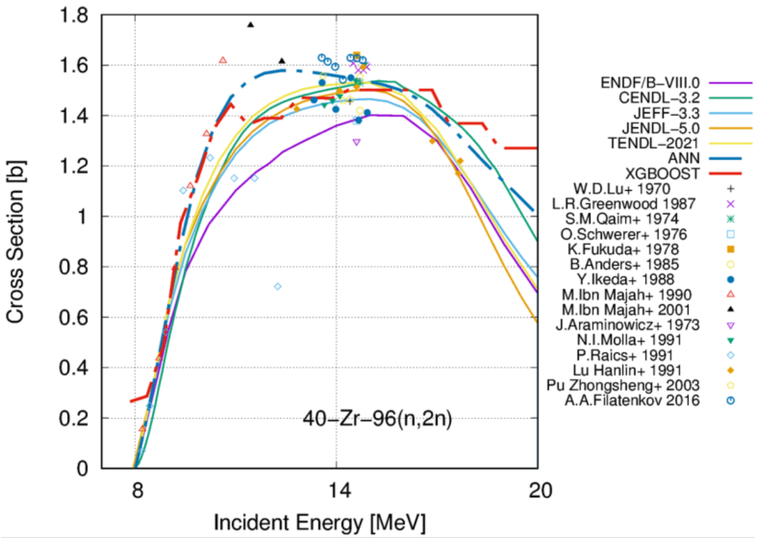
3. ND Models:
Nuclear reactions

Ref.: X. Sun et al. , *"Study of (n,2n) Reaction Cross Section of Fission Product based on Neural Network and Decision Tree Models"*, WONDER 2023, June 5-9, 2023

Technique: **Artificial neural network (ANN) and decision tree (DT) models**

Objective: To predict the (n,2n) reaction cross section, especially those lack of experimental measurements

Figure. Cross-section $^{96}Zr(n,2n)$



- Importance of features assessed
  - Z, A
  - Sn and Sp
  - Shell P-Casten factor, the level density
  - the pairing correction, and the incident energy

- **Results:** $\sigma_{(n,2n)}$ = f(incident neutron energy)

The ML model can predict the nuclear reaction cross section of a large number of nuclei without the requirement for manual and careful parameter optimization.

3. ND Models:
Nuclear reactions

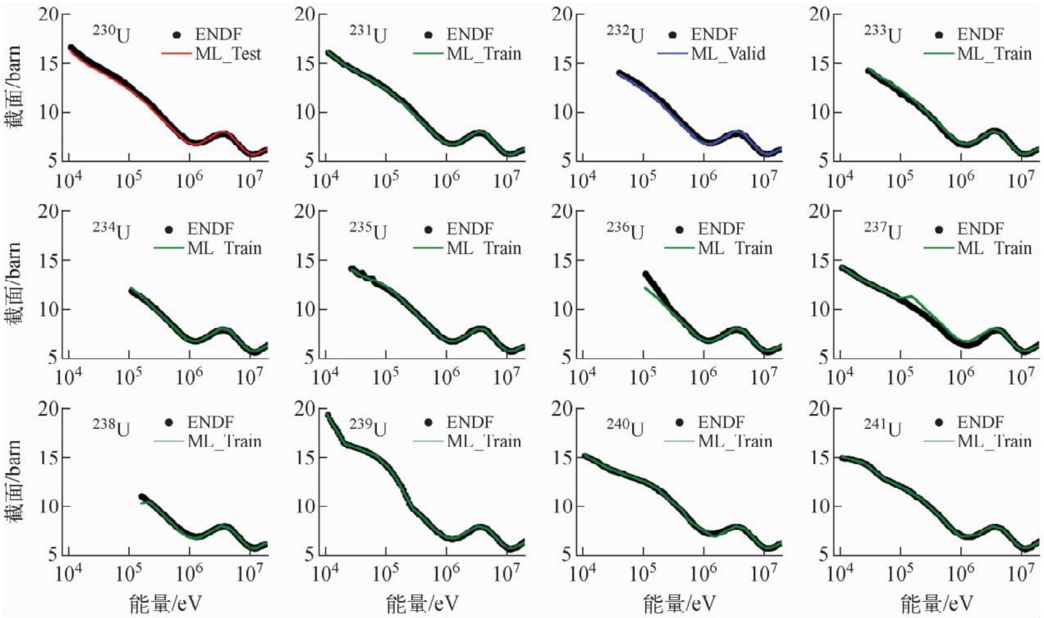
Ref.: HU Zehua et al. , *"Learning Fast Neutron Cross Section by Deep Neural Network"*, Atomic Energy Science and Technology ›› 2023, Vol. 57 ›› Issue (4): 812-817.

Technique: **Deep neural networks**

Objective: Evaluation Uranium files

Results: New U evaluations in the fast energy range

- Features assessed in the model
  - A, Z
  - ENDF data at energy E
  - Sn



- 230U is used as test
- 232U is used for verification
- other 10 U nuclides are used as training data.

Figure. Calculation results, total cross-sections for U

Examples in Evaluation

4. Evaluation: 239Pu(n,fission)

Ref.: B. Whewell et al. , *"Evaluating 239Pu(n,f) cross sections via machine learning using experimental data, covariances, and measurement features"*, Nuclear Inst. and Methods in Physics Research, A 978 (2020) 164305

Technique: Two machine learning methods (**logistic regression with elastic net regularization and random forest regression** with SHAP feature importance metric) are used to highlight measurement features that are common among many of the outlying data points.

Objective: Penalty uncertainties are added to the experimental covariances of outlying data points that have outlier measurement features.

The evaluation is performed with GLLS technique.

Table. Measurement attributes (features) used in the ML analysis

x ** _	Measurement attribute	*x* ** _	Measurement attribute
0	GMA-number	19	Neutron Flux Detector
1	Observable	20	Neutron Flux associated Particle measured
2	Absolute	21	Sample re-used
3	Ratio Isotope	22	Neutron Producing Reaction
4	Background Corrected	23	Incoming Neutron Source
5	Multiple Scattering Corrected	24	Target Backing Material
6	Attenuation Corrected	25	Target Backing Thickness
7	Stopping Power Corrected	26	Target Thickness (mg/cm^2)
8	Sample Roughness Corrected	27	Target Diameter (mm)
9	Ang. Dist. Fission Frag. Corrected	28	# atoms sample determination technique
10	Forward Boost Corrected	29	Neutron flux determination method
11	Deadtime Corrected	30	Energy Determination Method
12	Impurities Corrected	31	Background determination method
13	Random Coincidence Correction	32	Multiple scattering determination method
14	Spectrum extrapolation	33	Attenuation determination method
15	Geometry	34	Detector efficiency determination
16	Neutron flux variation	35	Impurity determination method
17	Fission Detector Type	36	Configuration of Samples
18	Reference Detector Type	37	Sample Fabrication

4. Evaluation: 239Pu(n,fission)

Ref.: B. Whewell et al. , *"Evaluating 239Pu(n,f) cross sections via machine learning using experimental data, covariances, and measurement features"*, Nuclear Inst. and Methods in Physics Research, A 978 (2020) 164305

- **Results:** GLLS evaluation with penalties due to outlying data

Figure. SHAP regression indexes. Red points on the positive *x*-axis indicate the feature is considered as related to outlying data.

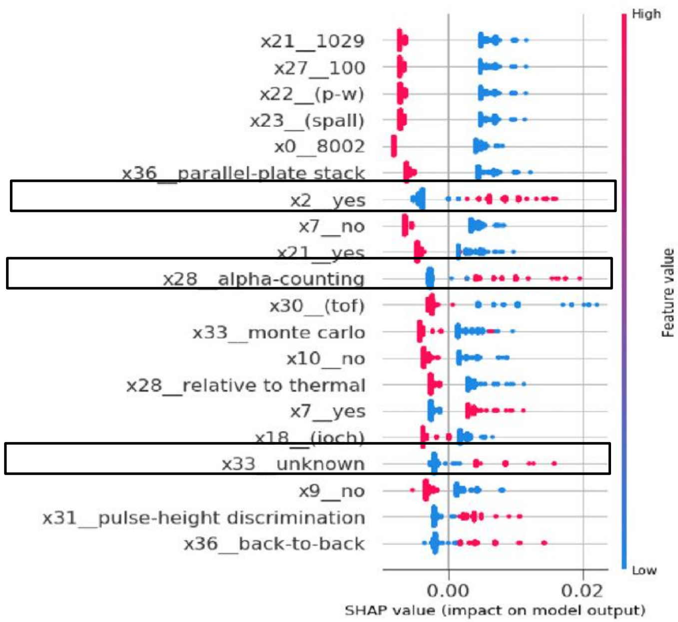
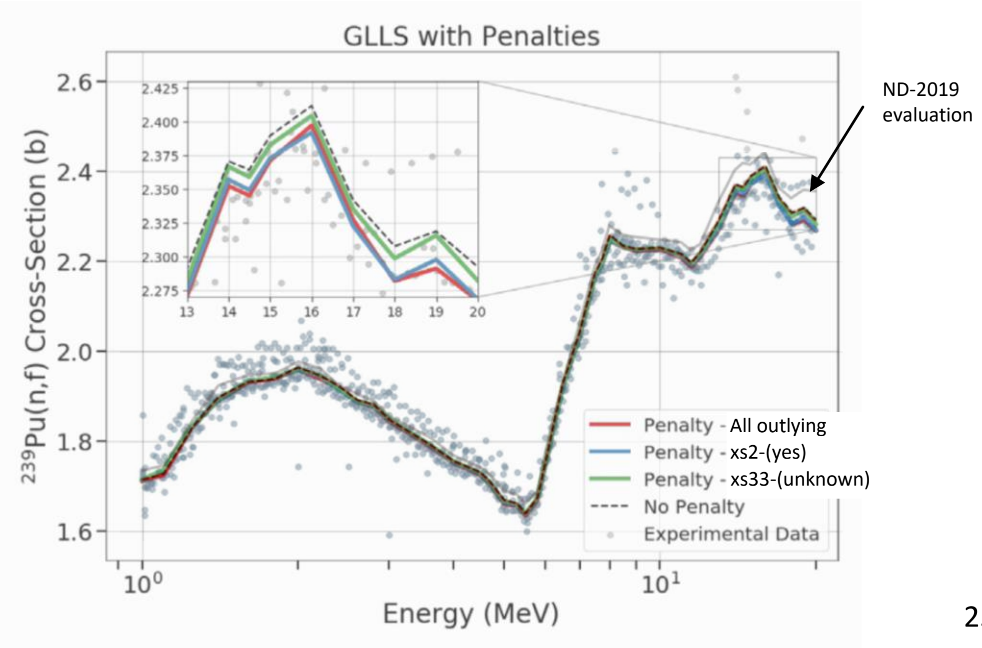


Figure. A comparison between different penalized options using GLLS technique.



Examples in Validation

5. Validation:
Enhancing Nuclear Data Validation - 19F

Ref.: D. Neudecker et al. , *"Enhancing nuclear data validation analysis by using machine learning"*, Nuclear Data Sheets, Volume 167, pp 36-60 (2020)

Technique: **Random forests**

Objective: Build a prediction model for the bias as a non-linear function of the large set of potentially informative features:

$$\text{Bias} = \text{C-E} = f(X_1, \ldots X_N) + \varepsilon$$

- Importance of features assessed with SHAP metric
  - Δkeff values for 875 Benchmarks with ENDF/B-VII.1 and ENDF/B-VIII.0
  - Features for each benchmark:
    - sensitivity coefficients ($\Delta k_{eff}/\Delta\sigma$)
    - engineering/measurement data (reflector material, spectrum, etc…)

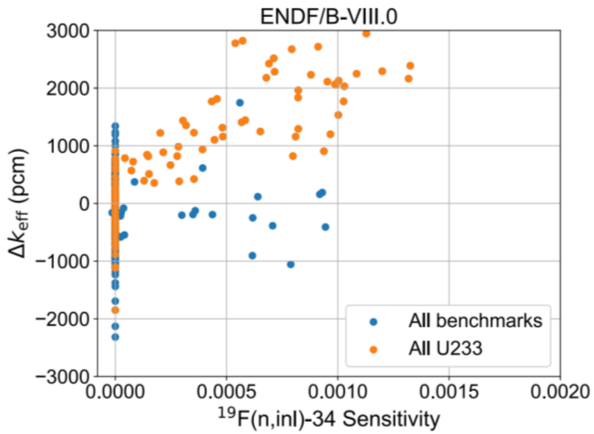


Figure. Δkeff is shown as a function of sensitivity of keff to 19F(n,inl)

Results: ML point towards potential issue in "19F(n,inelastic)"- ENDF/B-VII.1 and VIII.0

5. Validation:
Enhancing Nuclear Data Validation - 19F

Ref.: D. Neudecker et al. , *"Enhancing nuclear data validation analysis by using machine learning"*, Nuclear Data Sheets, Volume 167, pp 36-60 (2020)

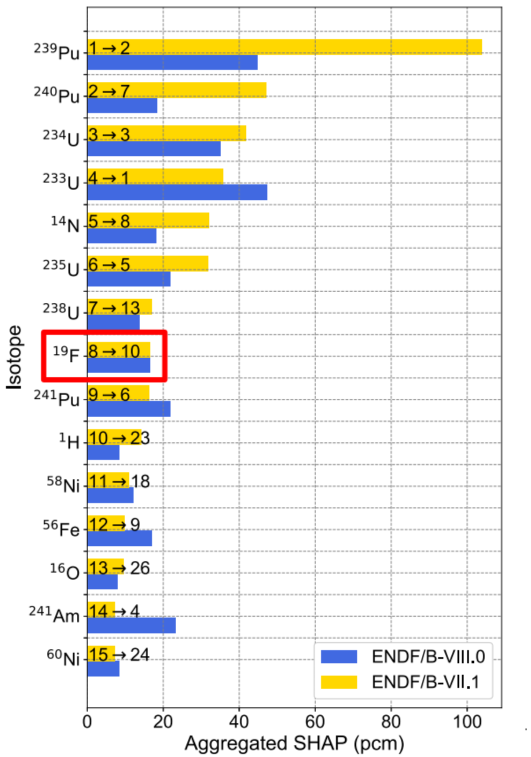


Figure. The 15 most important isotopes to predict Δkeff are shown versus their aggregated SHAP values

ML correctly identifies unknown issues in 19F(n,inelastic) current nuclear data libraries.

why this issue was hiding in plain sight?

- Large amount of data to look trough
- Expert judgment overlooked it because lesser importance for simulating keff

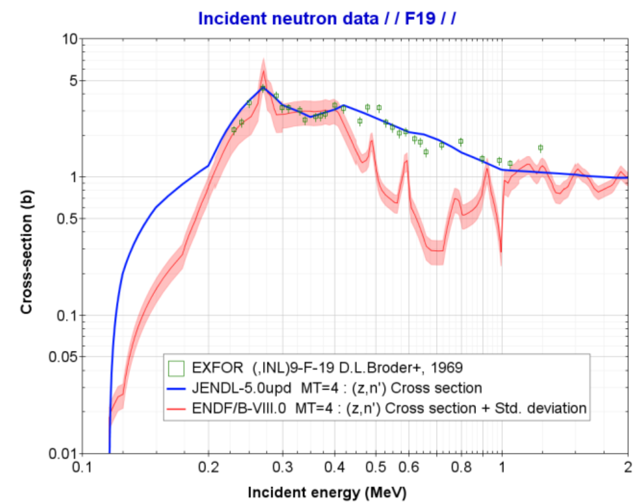


Figure. Comparison of ENDF/B-VII.1=VIII.0 and JENDL-5.0 evaluations for the 19F(n,inl) reaction with experimental data.

See also Ref.: P. Grechanuk et al, *"Application of Machine Learning Algorithms to Identify Problematic Nuclear Data"*, Nuclear Science and Engineering , Vol 195- Issue 12 (2021)

5. Validation:
Designing Critical Experiments

Ref.: N.A. Kleedtke et al. , *"Designing Critical Experiments using Gaussian Process Optimization"*, LA-UR-19-27536 (2019)

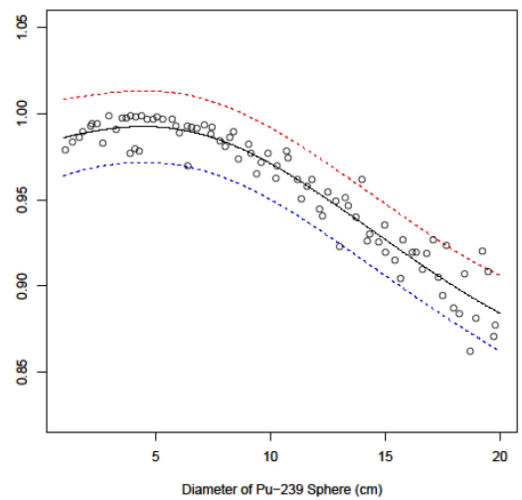
Technique: **Gaussian Process**

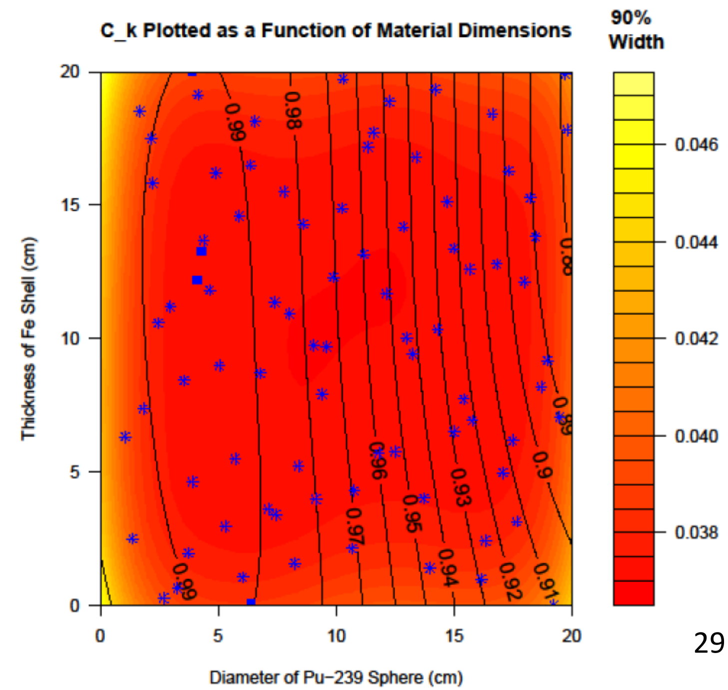
Objective: Create algorithm to optimally design critical experiments that match cross-section sensitivities of an application model while minimizing the number of simulation runs in the optimization

Results:

Find ideal material, dimensions by optimizing over ck-values

Figure. An example of optimization results





7. Conclusions

- *"The design and incorporation of artificial intelligence and machine learning tools to improve the nuclear data evaluation process"*
  (by Lee Bernstein, Briefing to NSAC, March 7, 2023)

- *"Machine learning helps us where human brain is overwhelmed with wealth of data. Conversely, we can integrate "expert knowledge" in these methods (*RATHER THAN REPLACE IT*).*
  …
  It is critical to feed it expert knowledge and use physics intuition to interpret results"
  (by Denise Neudecker, WANDA 2021, February 1, 2021)

Fostering collaborations between nuclear data researchers and experts in the ML/AI community (experts to feed the algorithms carefully curated data and correctly interpret the result) and attracting young talent to this scientific area will be critical for a successful outcome [3].

Questions?

References

[##] Some slides taken from Gre@t-Pioneer (https://great-pioneer.eu/) course on *"Nuclear Data for Energy and non-Energy Applications".* European Union's Euratom research and training programme 2019-2020 under the Grant Agreement nº 890675. (2019-2024)

Other suggested references:

[1] P. Bedaque et al, *"A.I. for nuclear physics", Eur. Phys. J.A: (2021) 57:100*

[2] A. Boehnlein et al., "Machine Learning in Nuclear Physics", https://arxiv.org/abs/2112.02309v2 (Dec. 2021)

[3] O. Cabellos, D. Neudecker, Machine Learning in Nuclear Science and Engineering Applications, Revista Nuclear España (September 2021) - LA-UR-21-28449

https://www.revistanuclear.es/wp-content/uploads/2021/09/Art.-Oscar-Cabellos.pdf

Acknowledgment

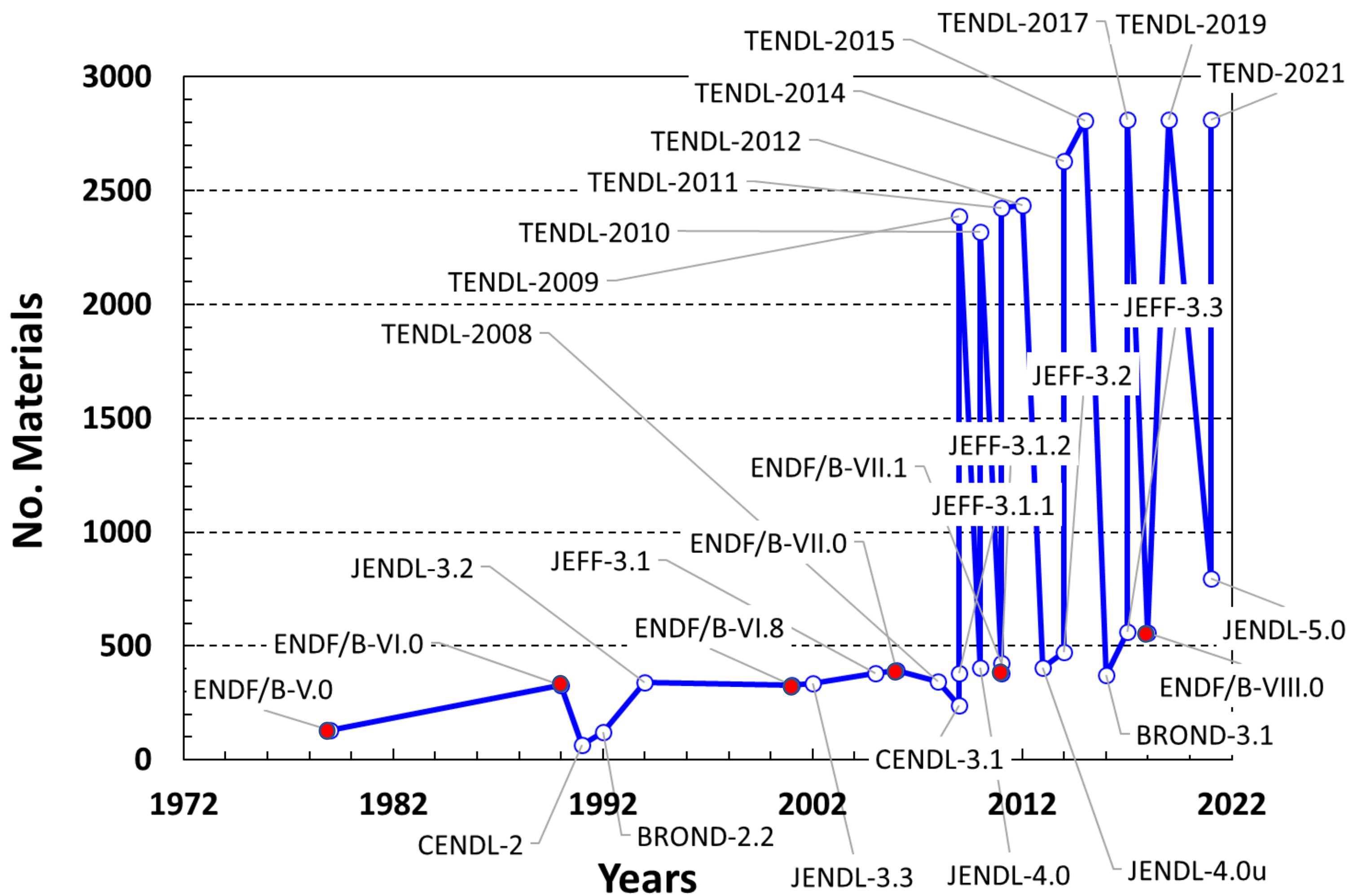
- *Some slides taken from Gre@t-Pioneer course on "Nuclear Data for Energy and non-Energy Applications". GREaT-PIONEeR Project ("Graduate Education Alliance for Teaching the Physics and safety of Nuclear Reactors") has received funding from the European Union's Euratom research and training programme 2019-2020 under the Grant Agreement nº 890675.*

- *Slides of this presentation were also given at the Frédéric Joliot and Otto Hahn (FJOH) Summer School, August 2023 held in Karlsruhe, Germany.*

Back-up slides

3.1 International efforts on evaluation of ND

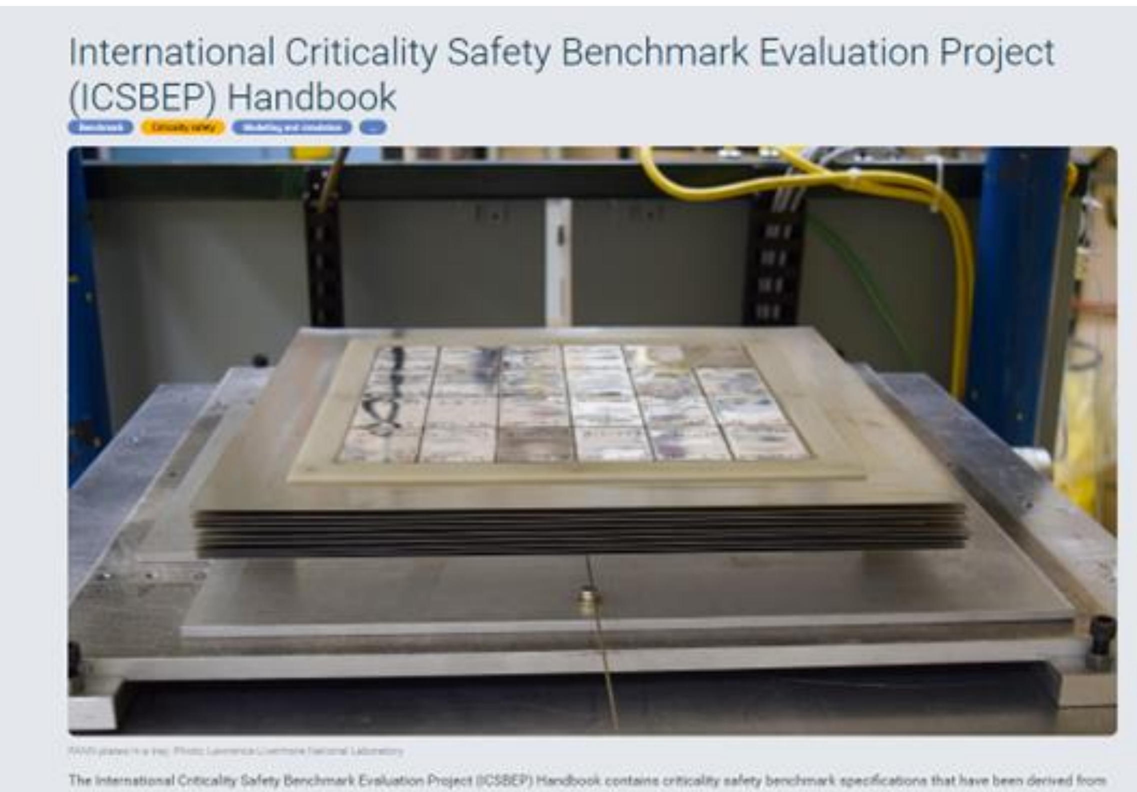
Figure 16. *Nuclear data libraries (for NEUTRONS) of today versus MAT*



4. Integral Databases for B&V: ICSBEP

- ❑ ICSBEP is the International Criticality Safety Benchmark <u>Evaluation</u> Project

Figure 17. *Official OECD/**ICSBEP Handbook** web-site*



ICSBEP contains thorough evaluations (**5053** cases in 2020) of critical and subcritical benchmark experiments (e.g keff) at room temperature. Each evaluation contains four different sections:

- Description of Measurements
- Evaluation of Experimental Data
- Benchmark Specifications
- Sample Calculations

Examples in Experiments/Compilation

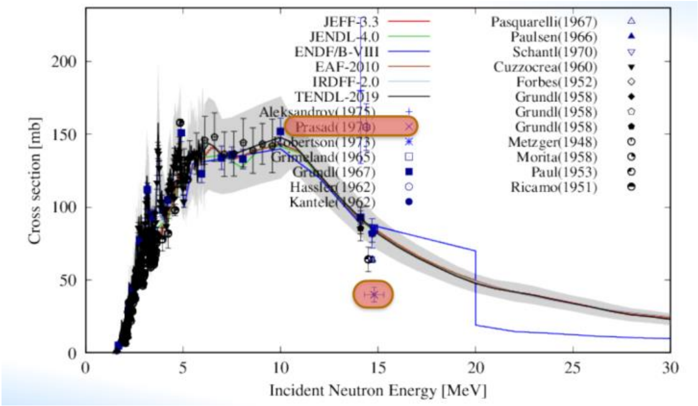
2. Experiments/Compilation: Outlier identification in EXFOR

Ref.: A. Koning, *“EXFOR and outliers”, JEFF meeting on Machine Learning, November 23, 2021, NEA, Paris. JEFDOC-2085*

Technique: Traditional outlier detection in EXFOR

- Quality scoring
- Numerical goodness-of-fit estimators (F, χ^2,…)
- Graphical estimation

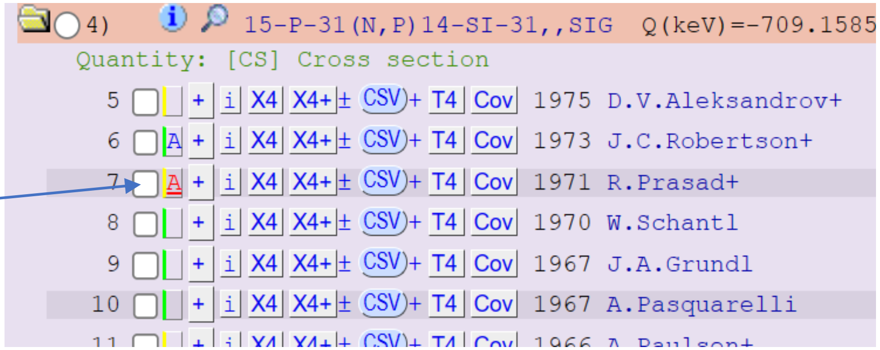
Figure. Cross-section $^{31}P(n,p)^{31}Si$



Ref: Arjan Koning, “Statistical verification and validation of the EXFOR database: (n,gamma), (n,n’), (n,2n), (n,p), (n,alpha) and other neutroninduced reaction cross sections”, NEA/DB/DOC(2017)1.

Objective: Outlier identification and *quality assignment of EXFOR data*

Arjan Koning Statistical Verification of EXFOR neutron-ind. Reactions XS (2020) #flag=R2 #[R]Reviewed #[2] Doubtful



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

2. Experiments/Compilation: Outlier identification in EXFOR

Ref.: P. Vicente Valdez, https://pedrojrv.github.io/nucml/notebooks/0_Evaluating_Dataset_Quality.html

Technique: Isolation Forest, One Class SVM, Local Outlier Factor, Elliptic Envelope

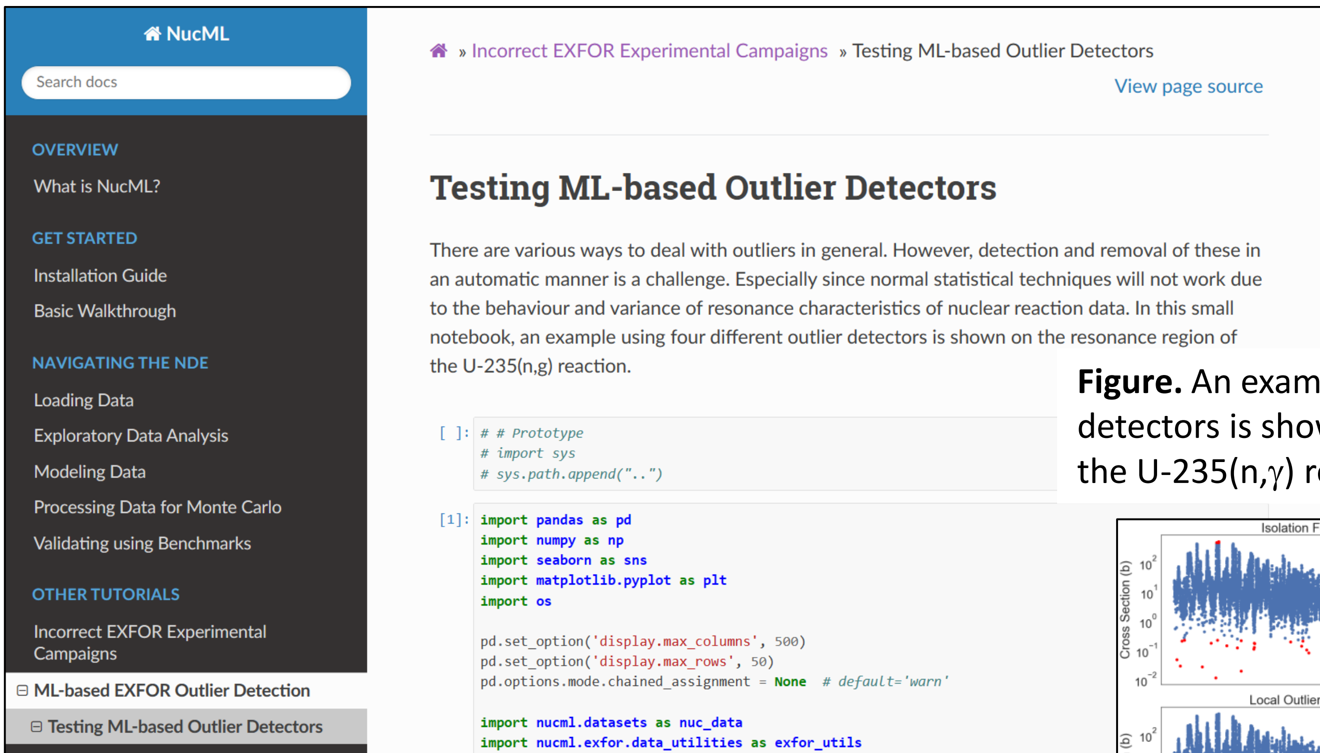
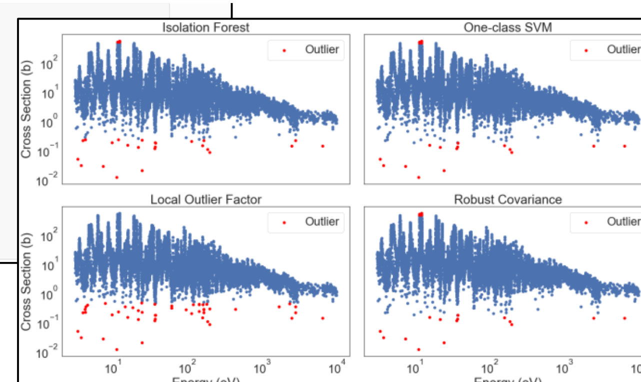


Figure. An example using four different outlier detectors is shown on the resonance region of the U-235(n,γ) reaction



Objective: Outlier identification

2. Experiments/Compilation: Outlier identification in EXFOR

Ref.: M. González-Torre et al., “Feedbacks on Processing and Verification for JEFF-4T2.2”, JEFF Nuclear Data Week April 2023.JEFDOC-224

Technique: Unsupervised ML algorithm - DBSCAN (Density-Based Spatial Clustering of Applications with Noise)

Objective: To identify anomalous data in EXFOR database

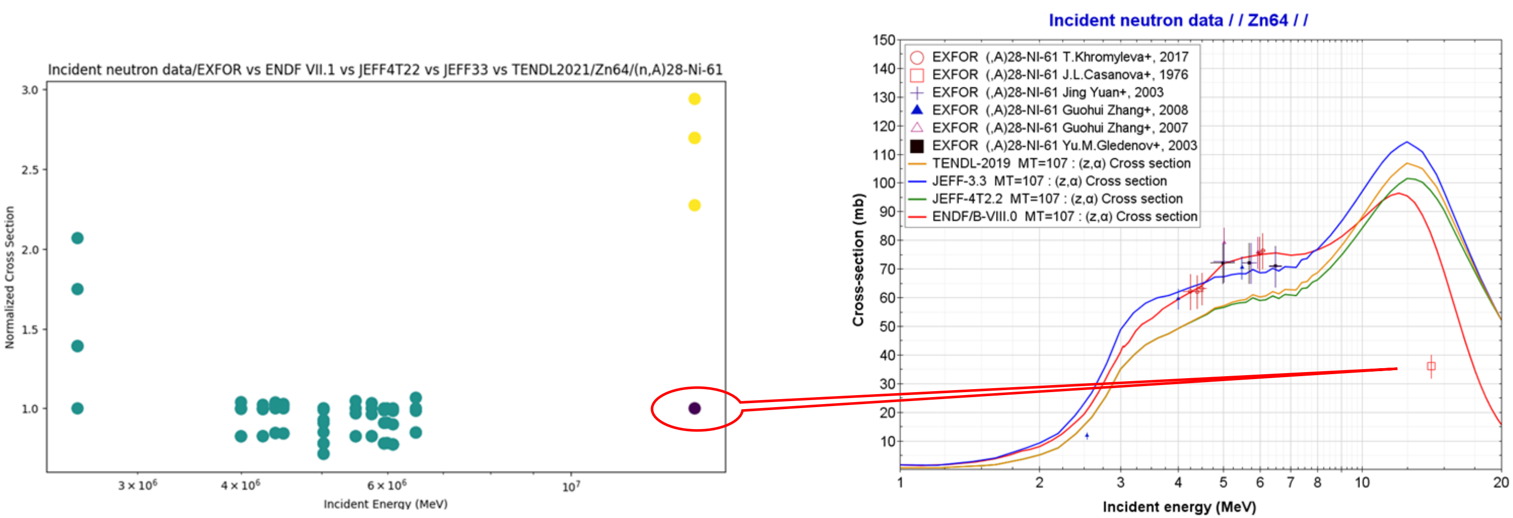


Figure. Comparison between EXFOR and recent evaluated data for the 64Zn(n,alpha) reaction cross-section as a function of neutron energy

Objective: Outlier identification

2. Experiments/Compilation: "Analysis of ND Measurements"

Ref.: A. Sánchez et al. , *"Deep Learning applied to Capture Cross Section Data Analysis", JEFF meeting on Machine Learning, November 23, 2021, NEA, Paris. JEFDOC-2088*

Technique: Artificial neural network classifier (ANN): 0=capture , 1=non-capture

Objective: Deep Learning model for classification of capture/non capture events from Total Absorption Calorimeter (TAC) signals

^{197}Au with aluminum canning

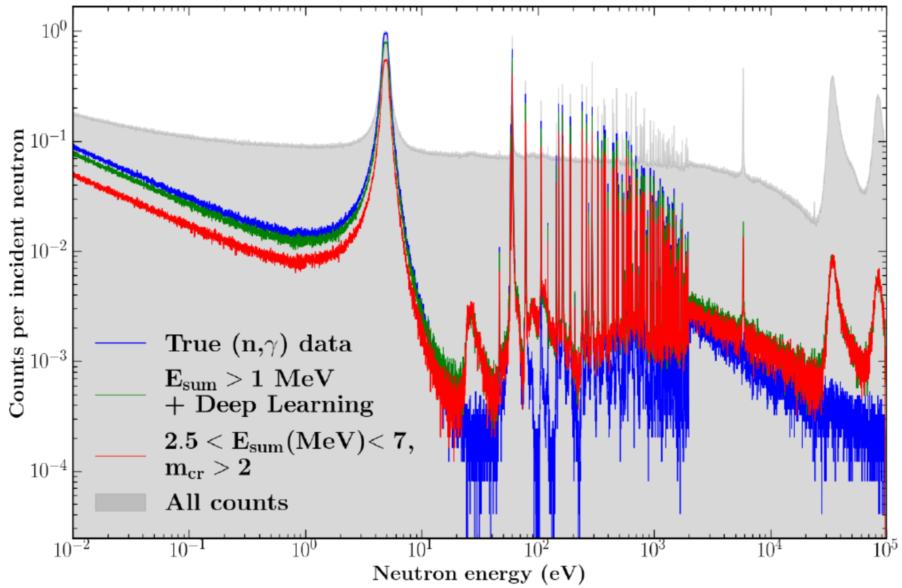


Figure. Example of capture spectra with and without Deep Learning

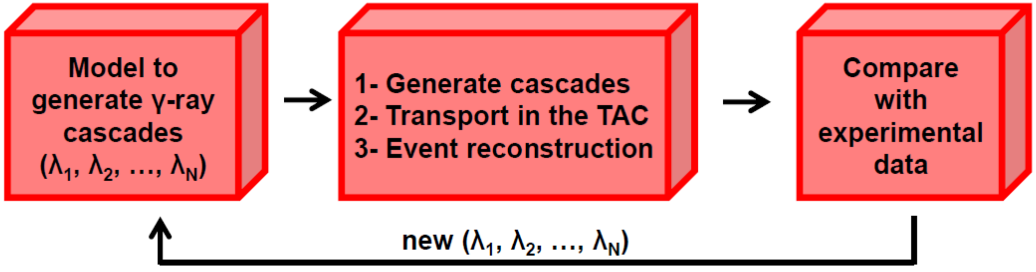
Results: Available to discriminate most of the capture events, improving the capture efficiency in some regions

2. Experiments/Compilation: "Analysis of ND Measurements"

Ref.: E. Mendoza et al. , *"Machine learning applied to the modelling of nuclear deexcitation cascades"*, Workshop on ML - UPM/*CEIDEN (May 2021)*
https://ceiden.com/wp-content/uploads/2021/12/06_ML_EMendoza_v01.pdf

Technique: Differential evolution (genetic) algorithm

Objective: To find the minimum of FOM(λ_1, λ_2, ..., λ_N) in order to generate reliable γ-ray cascades emitted after neutron capture



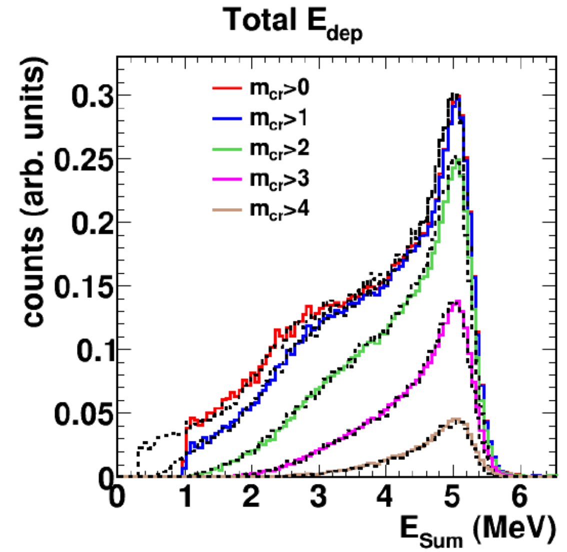


Figure. Example of the detection efficiency in 240Pu(n,γ)

Results: The methodology has been used to calculate the detection efficiency of the Total Absorption Calorimeter (TAC) at n_TOF(CERN) to 240Pu(n,γ) and 244Cm(n,γ) cascades.

See also Ref.: E. Mendoza et al. , EPJ Web of Con. 239, 01015 (2020)

Examples in Nuclear Data Models

3. ND Models: Level densities

Ref.: H. Ozdogan et al. , *"Estimations of level density parameters by using artificial neural network for phenomenological level density models"*, Applied Radiation and Isotopes 169 (2021) 109583

Technique: Artificial neural network (ANN) jointly with an efficient Bayesian-based algorithm is presented for classification algorithms.

Objective: To estimate nuclear level density parameters for Gilbert Cameron Model (GCM), Back Shifted Fermi Gas Model (BSFGM) and Generalised Super Fluid Model (GSM)

- Importance of features assessed for the BSFGM model
  - atomic number of the compound nucleus (Z)
  - mass number of the compound nucleus (A)
  - spin of the ground state for the target nucleus (Io)
  - neutron binding energy of the compound nucleus (Bn)
  - evaluated average resonance spacing in keV (Do)
  - uncertainty of the resonance spacing in keV (Derr)
  - evaluated cumulative number of low-lying levels (No)
  - excitation energy in MeV that corresponds to No

- **Results:** Level densities

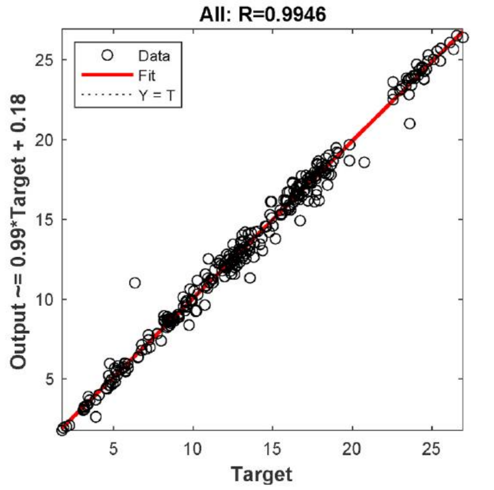


Figure . Level Density parameter calculations performed by the ANN for the BSFGM versus RIPL-2

Examples in Evaluation

4. Evaluation:
Photo-reaction cross-sections

Ref.: R.-D Lasseri et al , *“Using neural approaches to refine photo-reaction cross section estimation.”, JEFF meeting on Machine Learning, November 23, 2021, NEA, Paris. JEFDOC-2089*

Technique: Artificial neural network (ANN) and Gradient boosting approaches.

Objective: Evaluation of photo-reaction cross-section

- Importance of features assessed for the BSFGM model
  - atomic number of the compound nucleus (Z)
  - mass number of the compound nucleus (A)
  - Nuclear models … β_{HFB}

  - **EXFOR:** Few experimental data

  (for light Z<28 nuclei only
  26 experimental data available),
  154 sets available overall

- **Results:** Photo reaction prediction

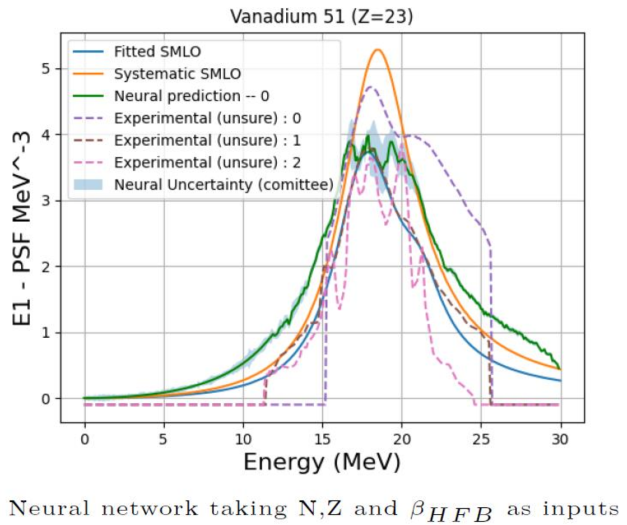


Figure 13. Photo reaction cross-section for 51V(γ,n)

4. Evaluation: G. Schnabel

Ref.: G. Schnabel et al. , *“Nuclear Data Evaluation with Bayesian Networks”*, arXiv:2110.10322, pp-1-38 (2021)

Technique: Bayesian networks based on graphical models to represent the probabilistic relationships between variables in the Bayesian framework.

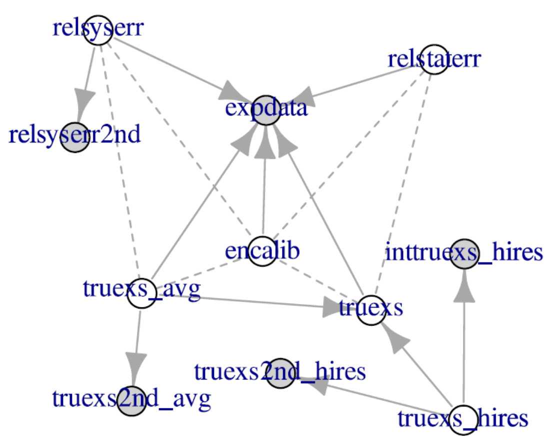


Figure. Bayesian network for the evaluation of the 235U(n,f) cross section

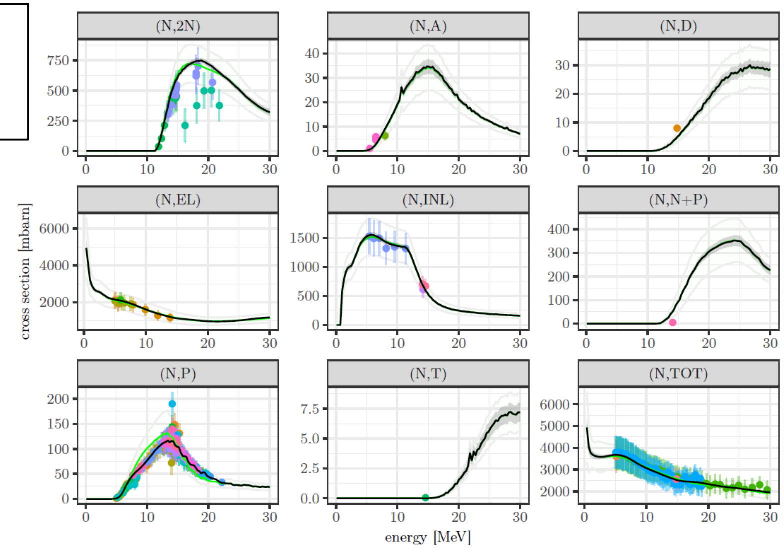


Figure. Most likely true cross section (**black**) of the neutron-induced reaction channels of 56Fe between 5 and 30 MeV. The prior curves (green) and associated uncertainty band (pale green) are also displayed.

Objective: Evaluation of nuclear data

- Importance of features assessed
  - EXFOR data
  - Nuclear parameters in models (e.g. TALYS code)

Results: Examples emerged in the context of the neutron data standards project and the INDEN evaluation efforts of structural materials

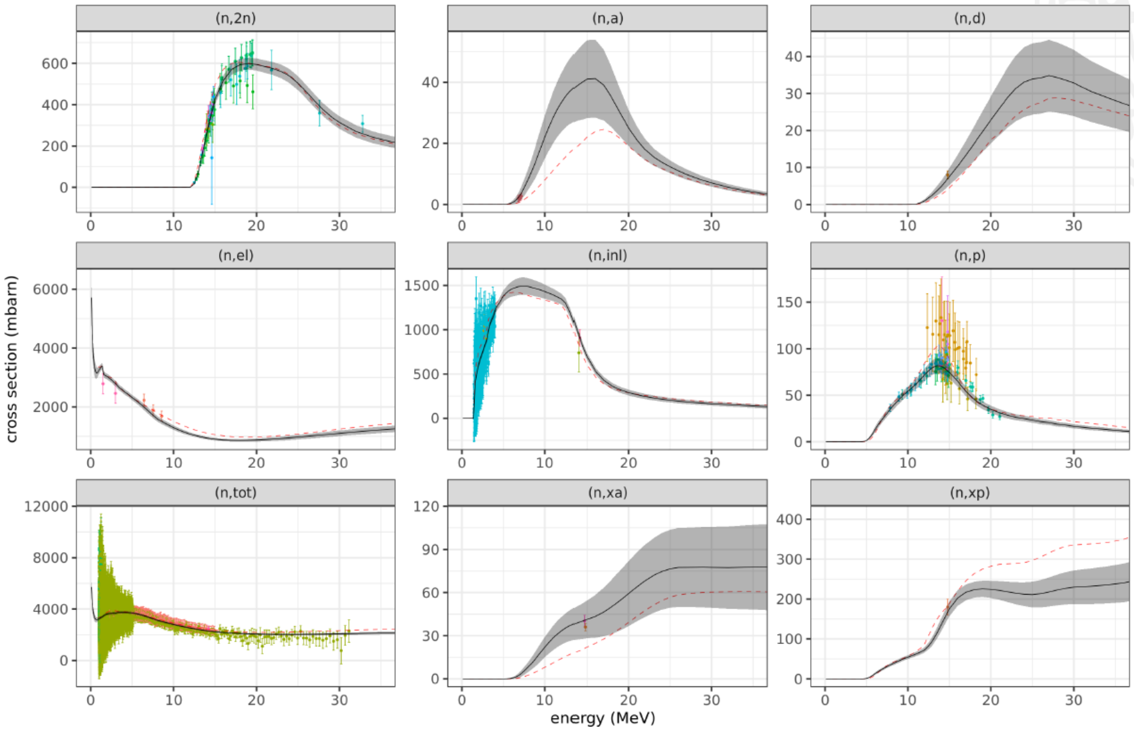
4. Evaluation: 52Cr

Ref.: A. Göök et al. , *“A Nuclear Data Evaluation Pipeline for the Fast Neutron Energy Range”*, WONDER 2023, Aix-en-Provence (France) June 2023.

Technique: Gaussian Process

Objective: Treatment of random uncertainties -> GP, Treatment of Model Defects -> GP

Figure. Results –all fitted channels for the 52Cr induced cross-sections



Results: New evaluations in the fasts energy range: EXFOR+TALYS+ML

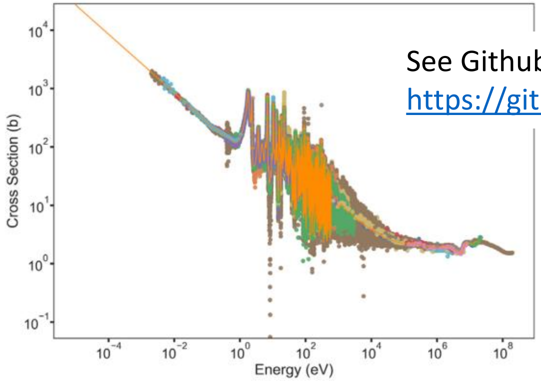
4. Evaluation: Nuclear reactions

Ref.: P. Vicente-Valdez et al. , *"Nuclear data evaluation augmented by machine learning"*, Annals of Nuclear Energy 163 (2021) 108596

Technique: Decision Tree and K-Nearest-Neighbor to fit EXFOR data to infer neutron induce reaction cross sections

Objective: To predict the nuclear reaction cross-sections for :233U(n,tot), (n,γ), (n,inelastic), (n,elastic), and (n,fission) and 35Cl(n,p)

Figure. 233U(n,fission) X reaction channel experimental datapoints in EXFOR vs. the ENDF/B-VIII.0 evaluation



See Github link at: https://github.com/pedrojrv/nucml

Table. Dataset features – measurable properties or characteristics

Feature Name	Values (min, max)
Incident energy (eV)[a]	5.7630e-10, 1.0170e + 11
Number of protons	1, 99
Number of neutrons	0, 156
Atomic mass number	1, 255
Reaction number (MT) [b]	1–4, 16–18, 22, 24, 28–29 32–33, 37, 41, 51, 101–108 111–113, 152–153, 155 158–161, 203, 1003, 1108 2103, 9000, 9001
Center of mass flag [b]	Lab, Center of mass
Target type [b]	Isotope, Natural
Atomic Mass (micro-amu)	1.0070e+06, 2.5509e+08
Target Atomic Radius (fm)	1.25–7.92
Neutron/Target Atomic Radius Ratio (fm)	1.0092e-01, 6.4000e-01
Mass Excess (keV)	-9.1652e+04, 8.4089e+04
Binding Energy (keV)	0.0000e+00, 8.7945e+03
β^- Decay Energy (keV)	−2.2898e+04, 1.8244e+04
S(2n) Energy (keV)	2.0254e+03, 3.7512e+04
S(2p) Energy (keV)	7.7180e+03, 3.6635e+04
S(n) Energy (keV)	1.0969e+03, 2.0577e+04
S(p) Energy (keV)	0.0000e+00, 2.0831e+04

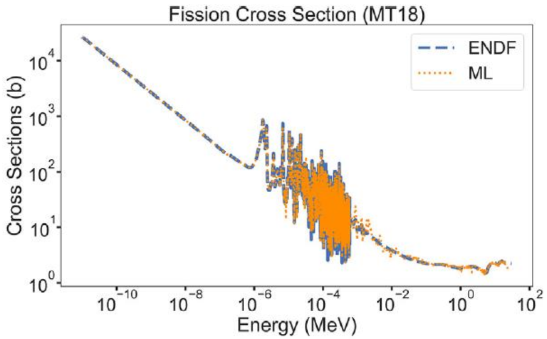
[a]85% and 17% of the energy and cross section values respectively either did not report uncertainties or were not readily accessible, therefore, uncertainty for these features was not included. [b]Treated as categorical features.

4. Evaluation:
Nuclear reactions

Ref.: P. Vicente-Valdez et al. , *“Nuclear data evaluation augmented by machine learning”*, Annals of Nuclear Energy 163 (2021) 108596

Results: Evaluations 233U and 35Cl

Figure. Comparison of KNN generated and ENDF/B-VIII.0 cross sections for fission and radioactive capture



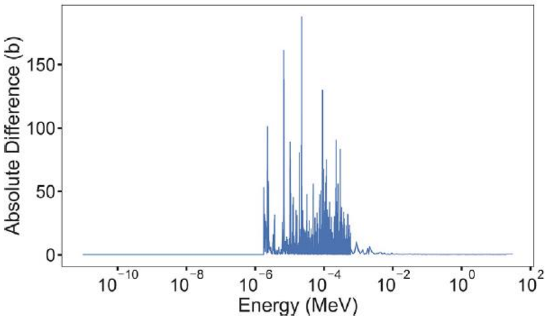


Figure. KNN and DT generated cross section for the 35Cl(n,p)35S reaction vs the ENDF/B-VIII.0 library and the available EXFOR experimental datapoints

Both the KNN and DT model, reliant on learned patterns and behaviors of other X(n,p) Y reactions

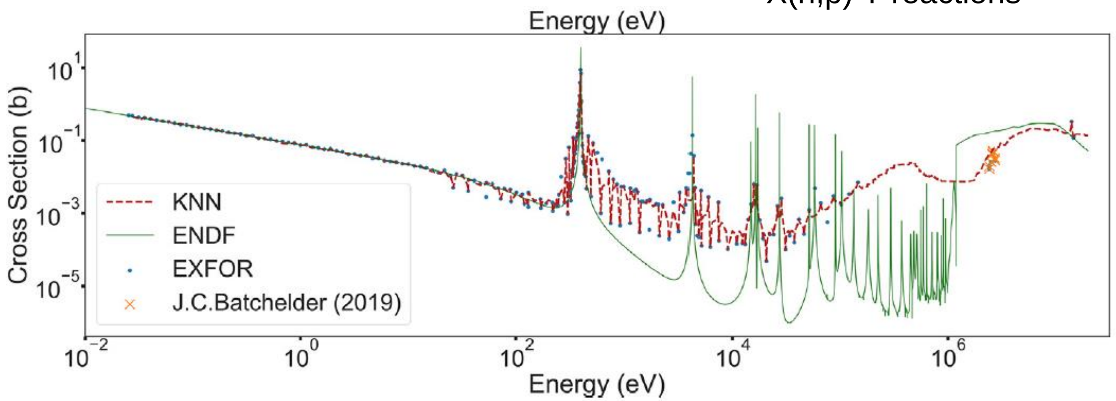


Table 3. 233U Jezebel Benchmark Criticality Results with SERPENT code.

Library	k_{eff}	Uncertainty	Error (%)
ENDF	1.0002	+/- 0.0011	0.02
KNN[a] ($k = 9$)	1.0038	+/- 0.0004	0.38
KNN[b] ($k = 20$)	0.9934	+/- 0.0004	0.66
KNN[c] ($k = 18$)	1.0000	+/- 0.0004	0.00
DT[a, d]	0.9971	+/- 0.0004	0.29
DT[b, e]	1.0023	+/- 0.0004	0.23
DT[c, f]	0.9999	+/- 0.0004	0.01

Examples in Validation

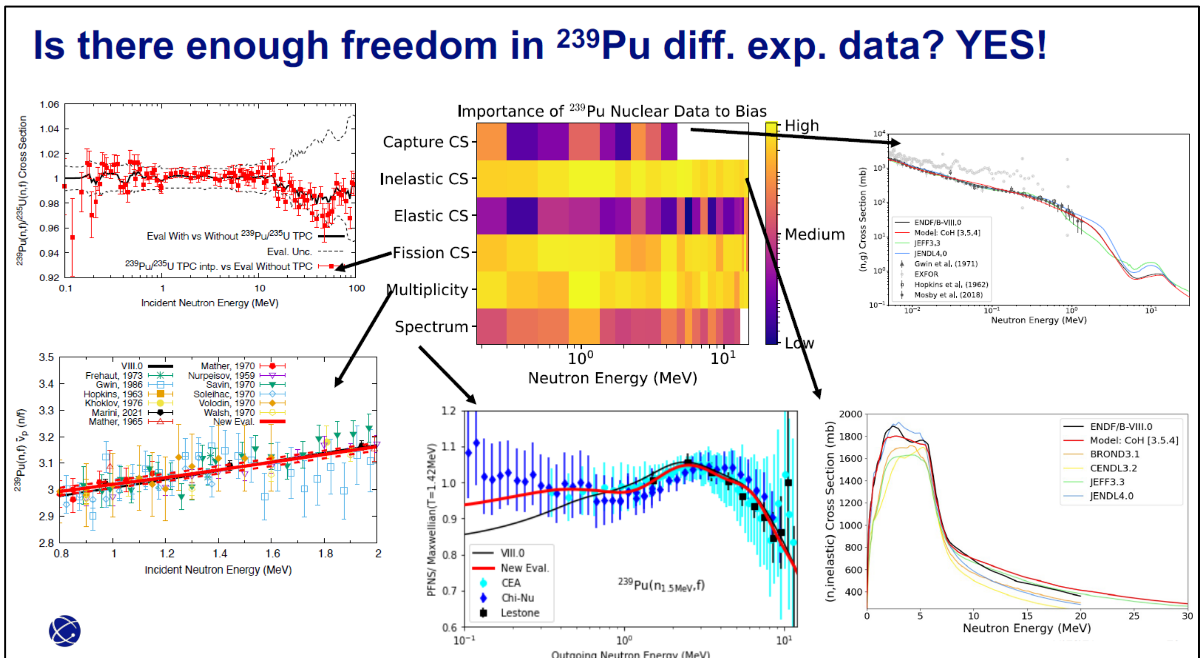
5. Validation:
Unconstrained physics space -239Pu

Ref.: D. Neudecker et al. , *"Using ML and various integral responses to identify unconstrained physics spaces in nuclear data"*, JEFF meeting on Machine Learning, November 23, 2021, NEA, Paris. JEFDOC-2086

Technique: Random forests + SHAP metric to highlight relationships between ND and bias

Objective: To identify unconstrained physics spaces between different nuclear data observables occurs due to freedom in differential data and integral values

Results:
Unconstrained ND
for 239Pu
in the high energy range



See also Ref : D. Neudecker et al., *"Informing Nuclear Physics via Machine Learning Methods with Differential and Integral Experiments"*, Phys. Rev. C 104, 034611 – (2021)

Examples in Optimization

6. ML & Optimization: Uncertainty Reduction – inverse problem

Ref.: K. Qin et al. , *"Uncertainty quantification and target accuracy assessment of nuclear data to effective neutron multiplication factor of heat pipe cooled reactor"*, Annals of Nuclear Energy 190 (2023) 109866

Technique: The differential evolution algorithm applied for optimization – the inverse problem

Objective: Uncertainty reduction in nuclear data to achieve the target accuracy requirements of the heat pipe cooled reactor

Results: Optimization

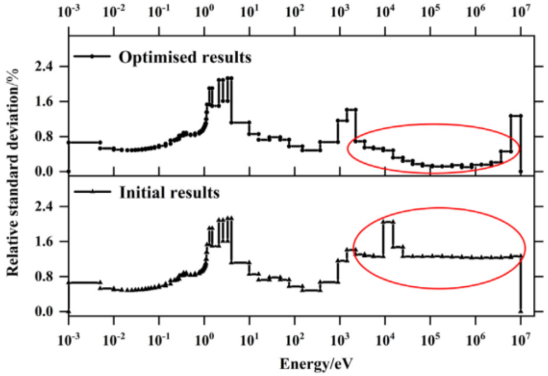


Figure. An example of optimization results for the 235U fission reaction cross section

Table. Ranking the importance of nuclear data for improvement in heat pipe cooled reactors

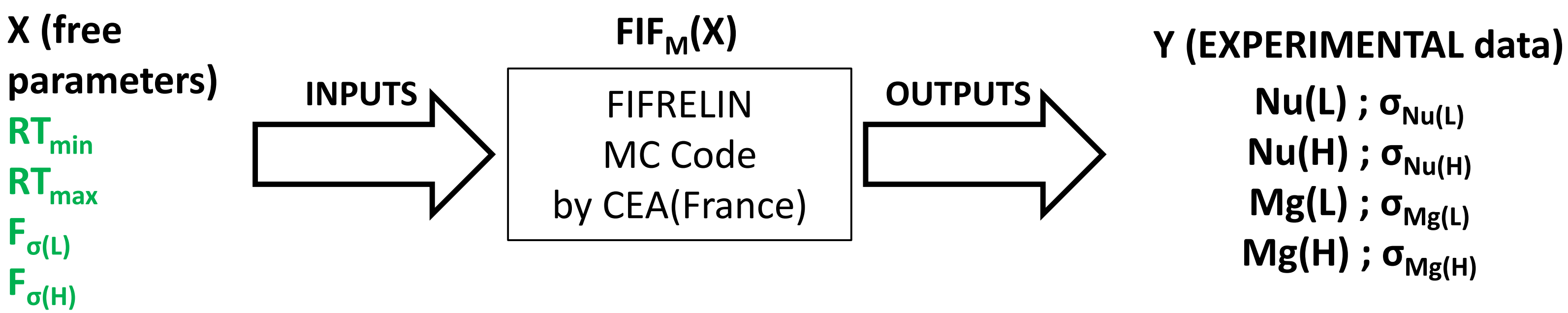
Reaction type	Energy range/eV	Initial relative standard deviation/%	Optimized relative standard deviation/%	ξ/%
^{235}U $\sigma(n, f)$	$1.11\times10^5 \sim 1.83\times10^5$	1.266	0.116	5.353
^{235}U $\sigma(n, f)$	$1.83\times10^5 \sim 3.025\times10^5$	1.253	0.118	5.028
^{235}U $\sigma(n, f)$	$5\times10^5 \sim 8.21\times10^5$	1.238	0.099	4.902
^{235}U $\sigma(n, f)$	$6.734\times10^4 \sim 1.11\times10^5$	1.260	0.134	4.694
^{235}U $\sigma(n, f)$	$4.085\times10^4 \sim 6.734\times10^4$	1.258	0.170	3.994
^{235}U $\sigma(n, f)$	$3.025\times10^5 \sim 5\times10^5$	1.247	0.145	3.701
^{235}U $\sigma(n, f)$	$2.231\times10^6 \sim 3.679\times10^6$	1.252	0.110	2.937
^{235}U $\sigma(n, f)$	$3.679\times10^6 \sim 6.0655\times10^6$	1.254	0.114	2.812
^{235}U $\sigma(n, f)$	$2.478\times10^4 \sim 4.085\times10^4$	1.260	0.242	2.715
^{235}U $\sigma(n, \gamma)$	$6.734\times10^4 \sim 1.11\times10^5$	7.988	1.137	2.697

6. ML & Optimization: FIFRELIN code

Ref.: G. Bazelaire et al. , *"Assimilating fission-code FIFRELIN using Machine Learning"*, WONDER 2023, June 5-9, 2023

Technique: Gaussian Process Regression (Kriging) with a Matern Kernel (used for problems where the data may not be smooth)

Objective: Find a suitable list of free parameters that would give the desired output data using FIFRELIN code (predicting fission observables, e.g., prompt neutron and γ -ray multiplicities … using nuclear models).



Results:

GP Optimization

X (free parameters)

RT_{min} **=0.182**
RT_{max} **=1.580**
$F_{\sigma(L)}$ **=1.381**
$F_{\sigma(H)}$ **=1.369**

Values in VEXPA experiment:

Nu(L) : neutron multiplicity (light fragment) =2.06
Nu(H) : neutron multiplicity (heavy fragment) =1.70
Mg(L) : gamma multiplicity (light fragment) =4.56
Mg(H) : gamma multiplicity (heavy fragment) =3.82

with σNu(L), σNu(H) ≤ 0.01 and σMg(L), σMg(H) ≤ 0.03