WANDA
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IAEA

Databases for an automated nuclear data pipeline and the role of AI/ML

Arjan Koning

Head of **Nuclear Data Section**, Division of Physical and Chemical Sciences, Department of Nuclear Sciences and Applications, International Atomic Energy Agency

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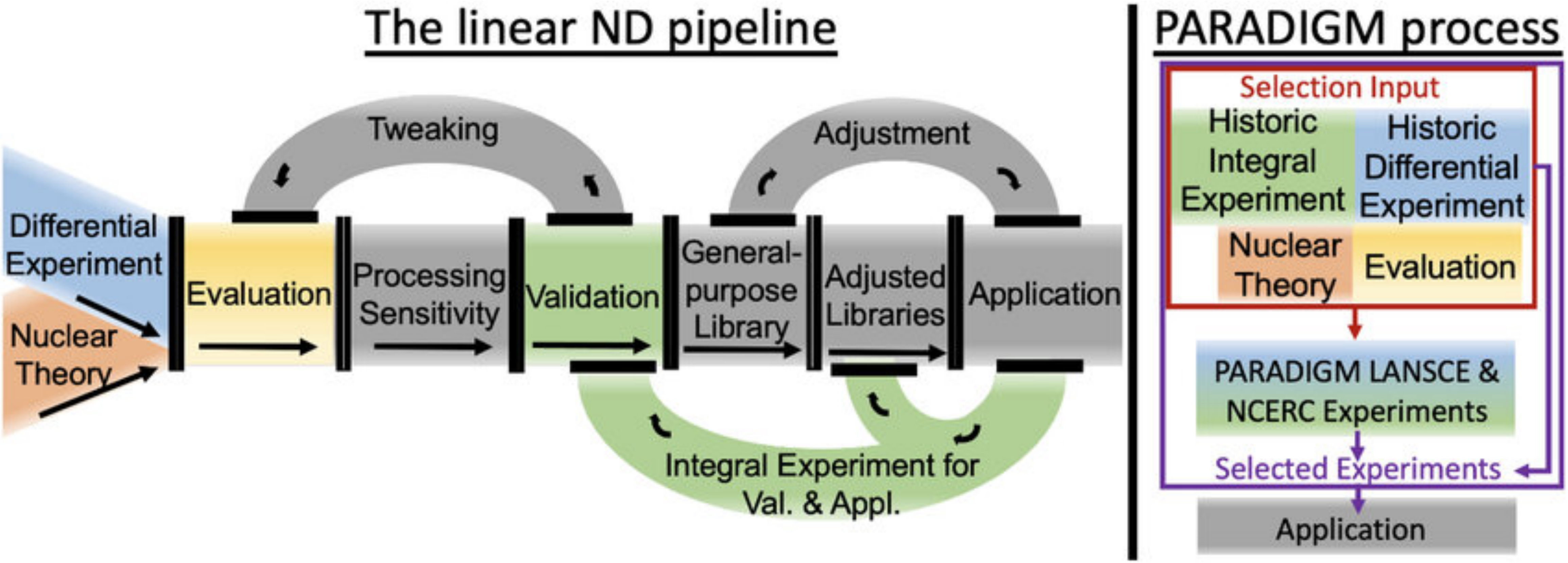
The linear ND pipeline
Tweaking
Adjustment
Differential Experiment
Nuclear Theory
Evaluation
Processing Sensitivity
Validation
General-purpose Library
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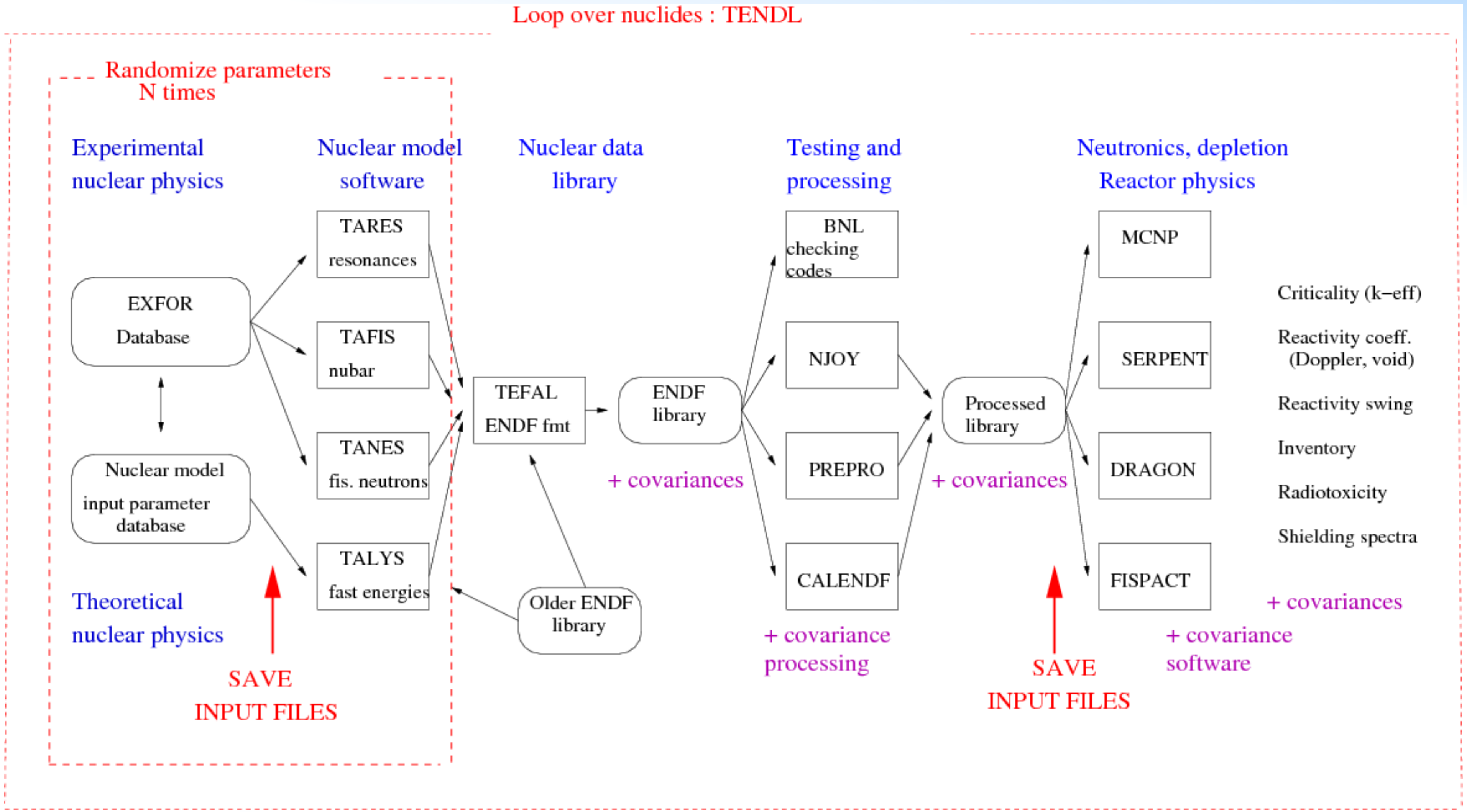
Application
Integral Experiment for Val. & Appl.
PARADIGM process
Selection Input
Historic Integral Experiment
Historic Differential Experiment
Nuclear Theory
Evaluation
PARADIGM LANSCE & NCERC Experiments
Selected Experiments
Application

TENDL: A nuclear reaction data pipeline



Once the system (**autotalys**) works, only the input files (= "the evaluation") are important

Reproducibility

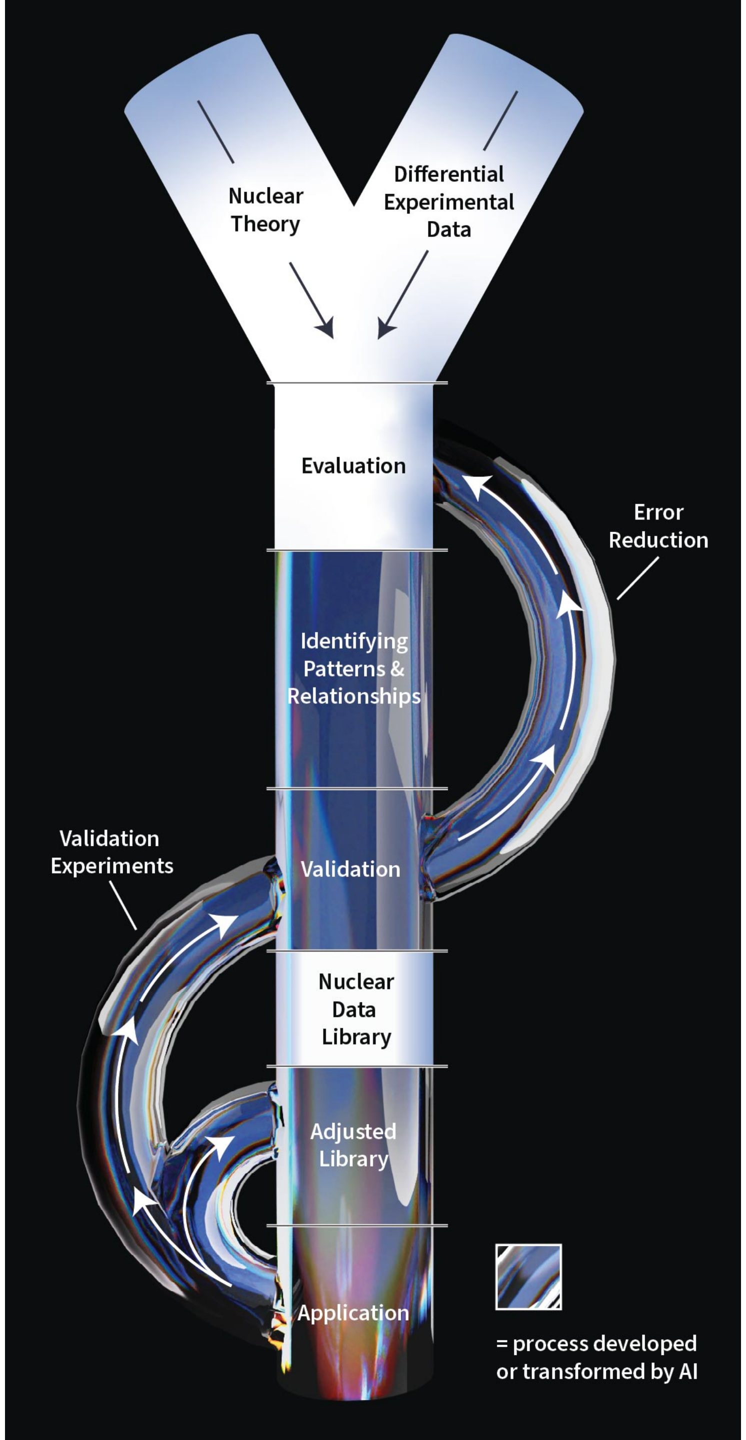
tendl.imperial.ac.uk

TENDL popular for:

- Medical isotope production
- Activation library
- Neutron applications beyond crit-safety
- Astrophysics
- Anything beyond neutrons
- JEFF-4.0 (80% of isotopes)
- Input to AI applications

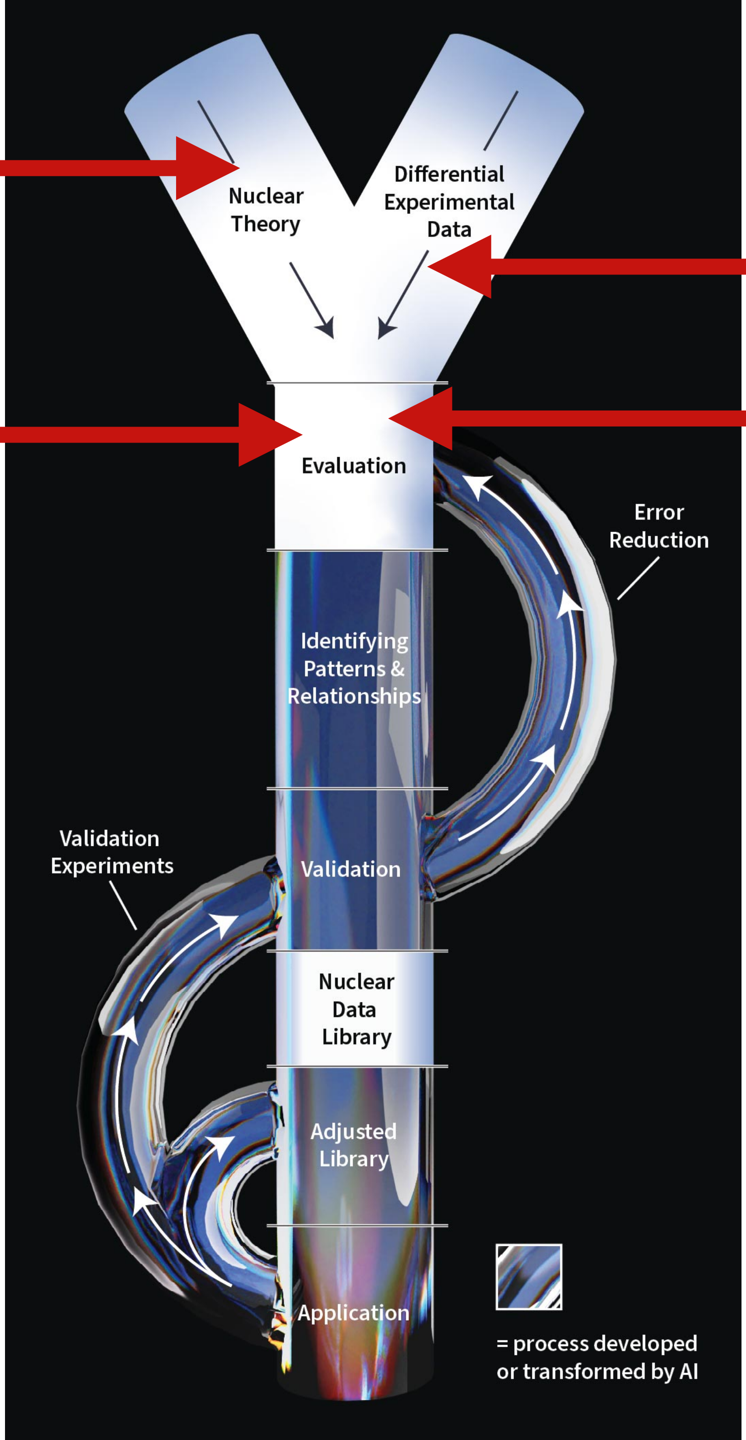
Not (yet) competitive for:

- Major actinides
- Major structural materials
- Light nuclides


Nuclear Theory
Differential Experimental Data
Evaluation
Error Reduction
Identifying Patterns & Relationships
Validation Experiments
Validation
Nuclear Data Library
Adjusted Library
Application
= process developed or transformed by AI

Theoretical model parameters: IAEA Reference Input Parameter Library (RIPL)

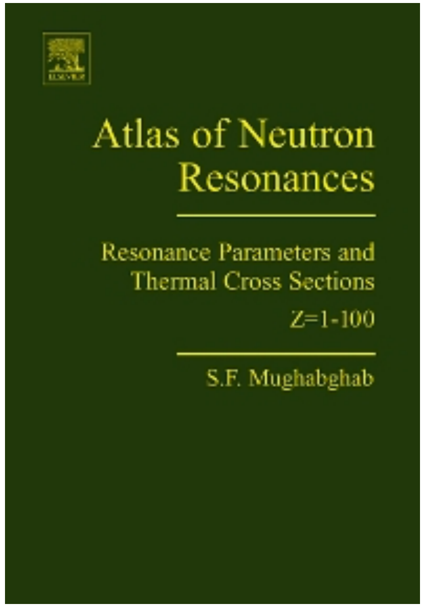
Existing high-quality ENDF evaluations



Experimental reaction data: EXFOR

Evaluated (average) resonance parameters: Various Atlases

Thermal cross sections, resonance integrals, MACS and (average) resonance parameters: several sources of information



Mughabghab Atlas 2018
Mughabghab Atlas 2006

Sukhoruchkin 2015

Neutron Activation Analysis: http://www.kayzero.com/k0naa

ELSEVIER
Available online at www.sciencedirect.com
ScienceDirect
Nuclear Data Sheets 110 (2009) 3107–3214
Nuclear Data Sheets
www.elsevier.com/locate/nds

The major nuclear data libraries

RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations

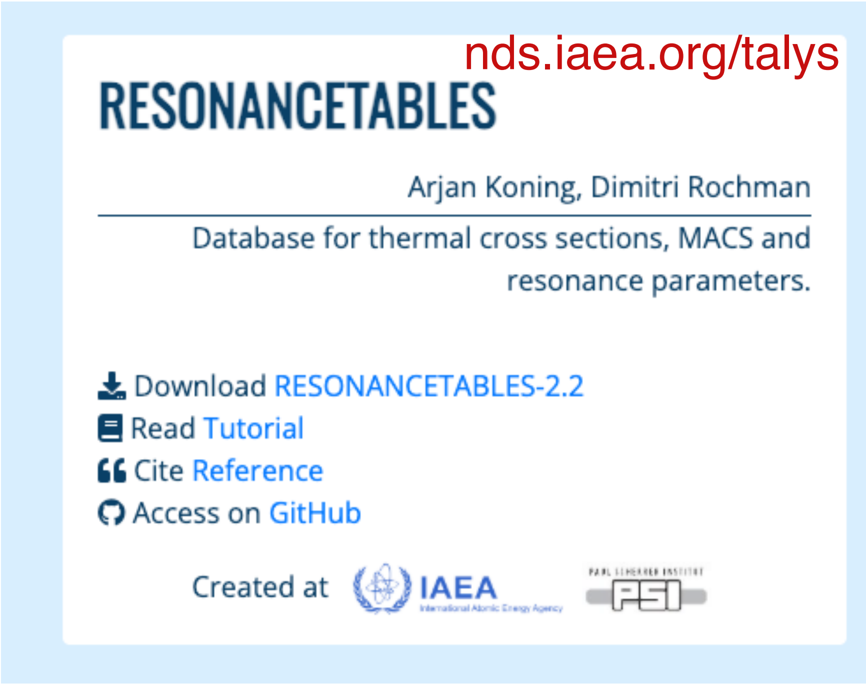
R. Capote,[1*] M. Herman,[1,2] P. Obložinský,[1,2] P.G. Young,[3] S. Goriely,[4] T. Belgya,[5] A.V. Ignatyuk,[6] A.J. Koning,[7] S. Hilaire,[8] V.A. Plujko,[9] M. Avrigeanu,[10] O. Bersillon,[8] M.B. Chadwick,[3] T. Fukahori,[11] Zhigang Ge,[12] Yinlu Han,[12] S. Kailas,[13] J. Kopecky,[14] V.M. Maslov,[15] G. Reffo,[16] M. Sin,[17] E.Sh. Soukhovitskii,[15] P. Talou[3]

EXFOR

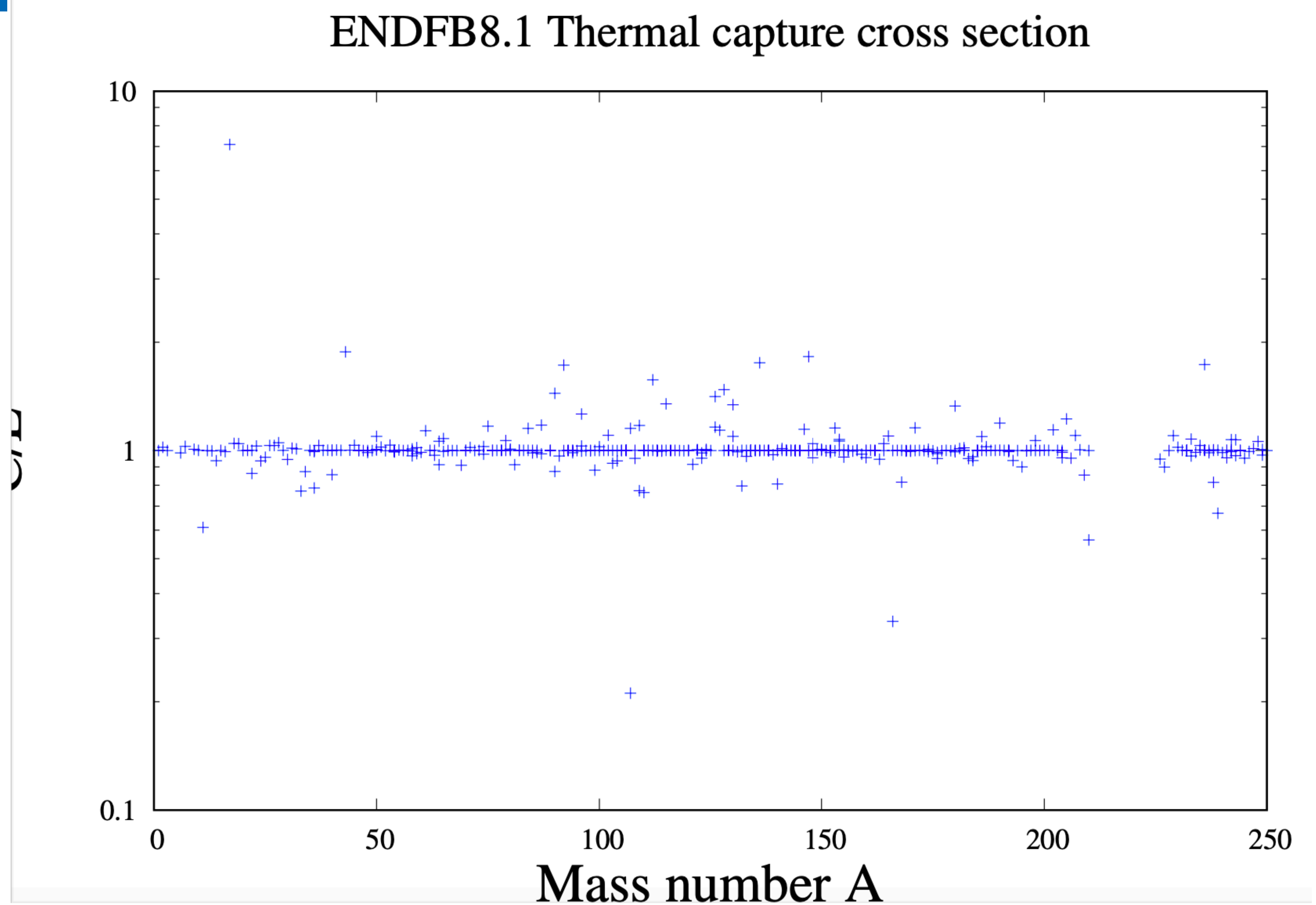
Resonance parameter database

- Unify data from all evaluations and compilations into one consistent structure:
  - all individual resonance parameters of the major nuclear data libraries, decrypted from ENDF (using TARES code of Dimitri Rochman), including uncertainties
  - Average resonance parameters: D_0 , D_1 , $\Gamma\gamma$, S_0, S_1 , R
  - Resonance integrals I_g and I_f
  - Thermal cross sections for all channels, nubar
  - Maxwellian-averaged cross sections
- …so the final database is available for trend analysis, outlier detection, automated inclusion in evaluation pipeline etc.

A meeting (IAEA?) is required to decide on the RECOMMENDED values



Assess ‘horizontal’ quality of the library



	Frms
CENDL-3.2:	1.034
JENDL-5.0:	1.020
ENDF/B-8.1:	1.021
TENDL-2025:	1.011
JEFF-3.3:	1.024
JEFF-4.0:	1.015

Example: MACS for Xe132

```
# header:
#   title: Xe132(n,g) MACS
#   source: Resonancetables
#   date: 2026-02-02
# target:
#   Z: 54
#   A: 132
#   nuclide: Xe132
# reaction:
#   type: (n,g)
# observables:
#   selected value [b]:  5.832863E-02
#   selected value uncertainty [b]:  2.663930E-03
#   selected value source: Astral
#   number of values: 10
#   average value [b]:  5.861926E-02
#   relative standard deviation [%]:     10.671627
#   quantity:
#     type: Compilation spectrum-averaged
#     average value:  5.998573E-02
#     relative standard deviation [%]:     11.628228
#   datablock:
#     columns: 11
#     entries: 5
##    Author                        Type          Year          Value         dValue        Reference        Ratio
##      []             []             []            []            [b]           [b]           []              []
      Bao                    Compilation          2000     6.460000E-02  5.300000E-03                    1.107518
      Kadonis                Compilation          2010     6.460000E-02  5.300000E-03                    1.107518
      Sukhoruchkin           Compilation          2015     4.700000E-02  9.000000E-03                    0.805779
      Mughabghab-2018        Compilation          2018     6.540000E-02  4.800000E-03                    1.121233
      Astral                 Compilation          2020     5.832863E-02  2.663930E-03                    1.000000
#   quantity:
#     type: Nuclear data library
#     average value:  5.725280E-02
#     relative standard deviation [%]:      8.885033
#   datablock:
#     columns: 11
#     entries: 5
##    Author                        Type          Year          Value         dValue        Reference        Ratio
##      []             []             []            []            [b]           [b]           []              []
      cendl3.2               NDL                  2019     5.769400E-02  0.000000E+00                    0.989120
      jendl5.0               NDL                  2021     6.188300E-02  0.000000E+00                    1.060937
      endfb8.1               NDL                  2024     4.743100E-02  0.000000E+00                    0.813168
      tendl.2025             NDL                  2025     5.962800E-02  0.000000E+00                    1.022277
      jeff4.0                NDL                  2025     5.962800E-02  0.000000E+00                    1.022277
```

Example: ENDF/B-VIII.1 Cr-052 resonance range

```
# D. Rochman  TARES version 1.71, Villigen    , Switzerland
# Time: Tue Dec  2 16:18:52 2025
#
# Element                             : Cr
# Z                                   : 24
# A                                   : 52
# I                                   : 0
# Abundancy                        [%]: 83.789
# Data origin                         : endfb8.1
# Formalism                           : Reich-Moore
# Emin (RRR)                      [eV]: 1e-5
# Emax (RRR)                      [eV]: 1.430000E+06
# Emax2 (background)              [eV]: 2.000000E+07
# Number of resonances (<Emax)        : 352
# Number of resonances (<Emax2)       : 392
# Thermal  (n,g) xs (calculated)  [b.]: 5.453590E-01
# Res. Int (n,g) (calculated)     [b.]: 3.538890E-01
# MACS 30 keV (calculated)        [b.]: 8.638700E-03
# Westcott factor (calculated)        : 1.000560E+00
#
# Thermal (n,el) xs (calculated)  [b.]: 3.047100E+00
# Res. Int (n,el) (calculated)    [b.]: 4.677530E+01
#
# Scattering radius               [fm]: 5.34
# Scattering radius L= 0          [fm]: 5.34 +/- 5.00 %
# Scattering radius L= 1          [fm]: 5.34 +/- 5.00 %
# Scattering radius L= 2          [fm]: 5.34 +/- 5.00 %
#
# Average reduced (Gn^0) Gn l=0   [eV]: 1.139980E+01
# Average Gg        l=0           [eV]: 1.297510E+00
# Average level spacing D0 (l=0)  [eV]: 3.177780E+04
# Neutron strength function S0 (l=0)  : 3.667070E-04
#
# Average reduced (Gn^1) Gn l=1   [eV]: 1.026610E+00
# Average Gg        l=1           [eV]: 5.765870E-01
# Average level spacing D1 (l=1)  [eV]: 1.243480E+04
# Neutron strength function S1 (l=1)  : 3.945350E-05
#
# Average reduced (Gn^2) Gn l=2   [eV]: 3.676160E+00
# Average Gg        l=2           [eV]: 6.683710E-01
# Average level spacing D2 (l=2)  [eV]: 8.362570E+03
# Neutron strength function S2 (l=2)  : 2.352030E-04
```

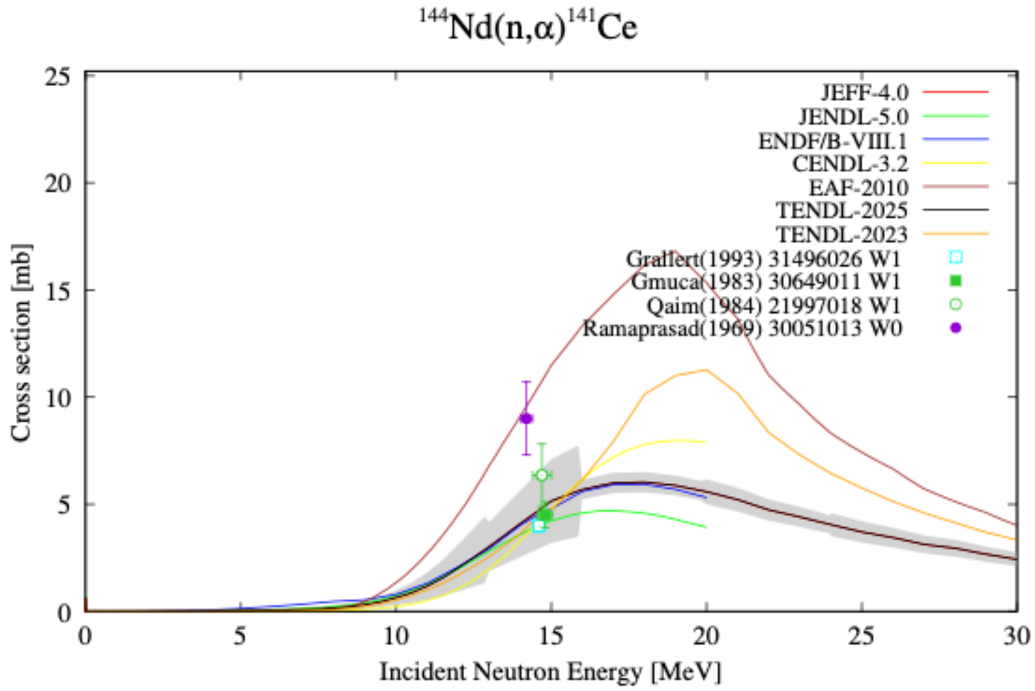
(continued)

#

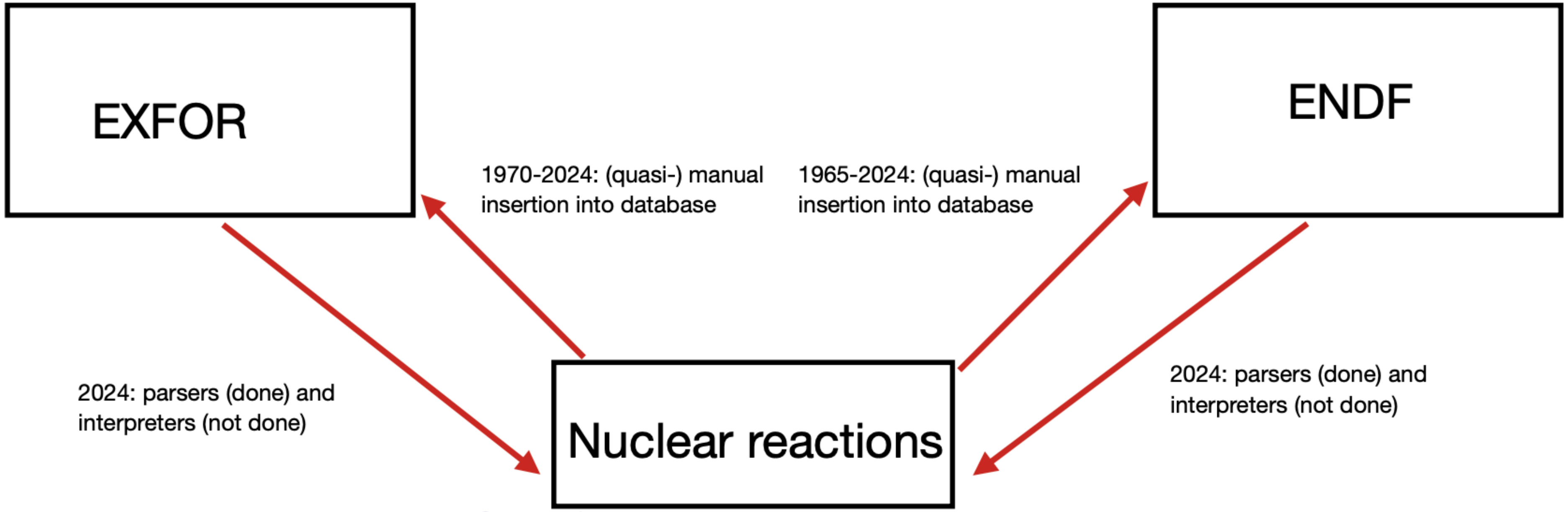
# Energy (eV)	+/- DE (eV)	l	J	Gn (eV)	+/- DGn (
-8.205200E+05	1.670579E+02	0	+0.50	1.006500E+02	5.123010E
-8.018700E+05	1.632607E+02	0	+0.50	7.690200E+03	3.914258E
-7.554900E+05	1.538178E+02	0	+0.50	2.150500E+04	1.094589E
-7.302400E+05	1.486769E+02	0	+0.50	2.003200E+03	1.019615E
-7.115500E+05	1.448716E+02	0	+0.50	1.628700E+04	8.289969E
-5.870700E+05	1.195275E+02	0	+0.50	3.839600E+02	1.954329E
-5.260200E+05	1.070977E+02	0	+0.50	1.084000E+04	5.517484E
-4.852800E+05	9.880301E+01	0	+0.50	5.651200E+03	2.876421E
-4.496800E+05	9.155485E+01	0	+0.50	2.072900E+04	1.055092E
-4.293700E+05	8.741973E+01	0	+0.50	2.289900E+03	1.165543E
-3.887500E+05	7.914950E+01	0	+0.50	1.444100E+04	7.350368E
-3.584500E+05	7.298042E+01	0	+0.50	1.660100E+02	8.449790E
-3.189000E+05	6.492804E+01	0	+0.50	4.766700E+03	2.426217E
-2.394600E+05	4.875406E+01	0	+0.50	1.319100E+04	6.714127E
-1.399100E+05	2.848568E+01	0	+0.50	2.641700E+03	1.344607E
-1.137100E+05	2.315136E+01	0	+0.50	1.029400E+04	5.239574E
-7.969900E+04	1.622672E+01	0	+0.50	1.756500E+03	8.940462E
-3.006818E+04	6.121881E+00	0	+0.50	1.763600E+03	8.976601E
+1.625867E+03	3.310270E-01	1	+1.50	3.120000E-02	1.590000E
+1.935777E+04	3.941242E+00	1	+0.50	4.265000E-03	2.200000E
+2.295014E+04	4.672648E+00	1	+1.50	3.500000E+00	1.781500E
+2.485516E+04	5.060511E+00	1	+0.50	6.925000E-03	3.500000E
+2.759859E+04	5.619073E+00	1	+1.50	8.156300E-01	4.151000E
+3.163829E+04	6.441556E+00	0	+0.50	2.610100E+01	1.328520E
+3.391804E+04	6.905713E+00	1	+0.50	7.411800E-01	3.773000E

Making EXFOR computer accessible

- WPEC SG-50 (Neudecker, Lewis), SG54 (Pritychenko)
- Several EXFOR parsers and dissemination mechanisms now available, see Section 4.4.4 of IAEA report INDC-NDS-0926, Neutron-induced Reactions on Short-lived Nuclide (December 2025) for a full list:
  - EXFOR in JSON, parsers on github.com/IAEA-NDS
  - 'Standard' IAEA retrieval system, Data Explorer, web API's etc.
  - Outlier database (for 24000 data sets, JSON)
    - https://github.com/arjankoning1/EXFOR_outliers/.
    - Binary weight, 0 or 1, improves automatic optimisation



Check out nds.iaea.org/talys
Libraries-2025 plots.tar for 30 000 of such plots



Cross sections

- Cumulative: total, elastic, non-elastic
- Exclusive: (n,n'), (n,2n), (n,g), (n,f), n,p),….to ground state and isomer
- Discrete level: (n,n'_1), (n,n'_2),…(n,p_0),….
- Particle production: (n,xn), (n,xp),….
- Residual production: (n,x), (p,x),….to ground state and isomer

Angular distributions

- Elastic
- Inelastic

Single-differential emission spectra (energy)

Double-differential emission spectra (energy-angle)

Gamma-ray production cross sections

Fission yields

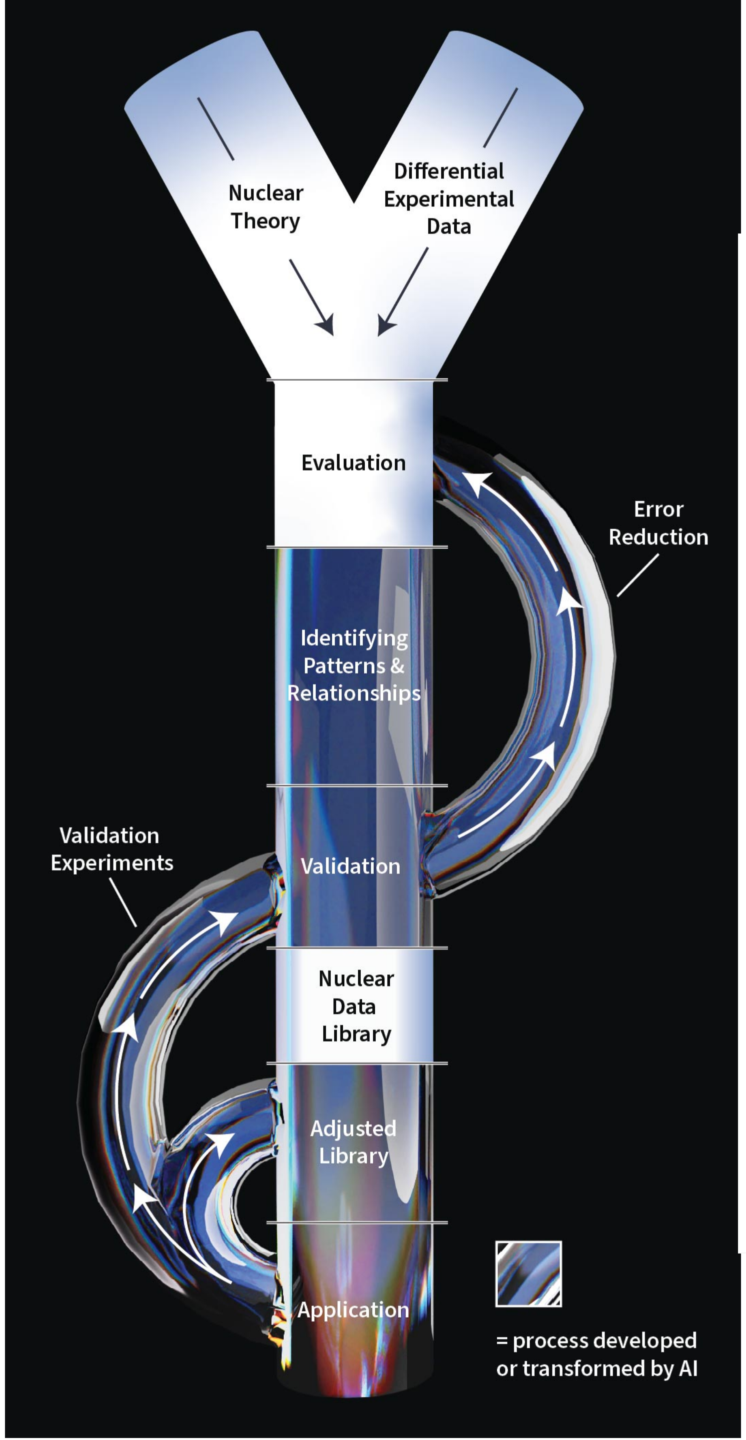
Fission neutron observables (nubar, nu(A), PFNS, etc.)

…………

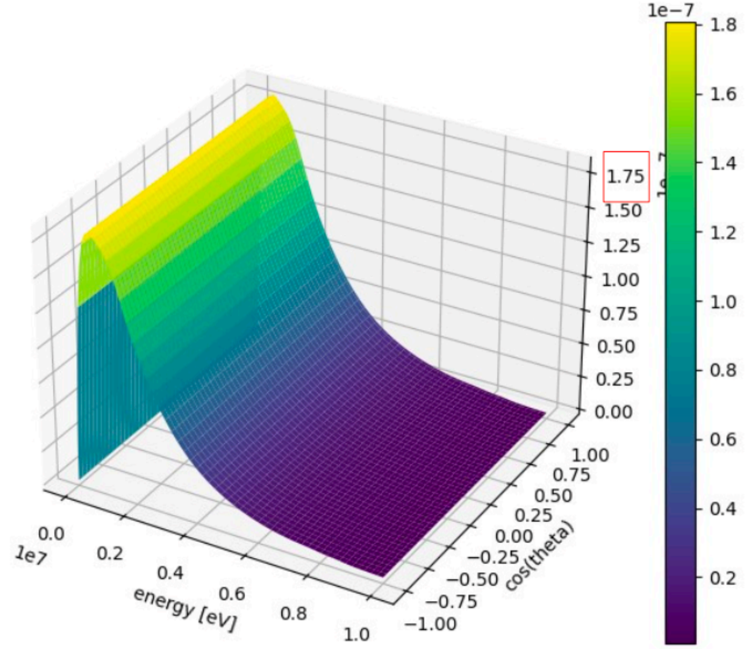
Turning ENDF into observables

Parsing: endf_parserpy
Observables: endf_userpy

(Georg Schnabel, IAEA)



U-235(n,f) double-differential *distribution* of emitted neutrons



$$\sigma_i(\mu, E, E') = \sigma(E)\; y_i(E)\; f_i(\mu, E, E')/2\pi$$

compute_dist2d_values(endf_dict, mt=18, zap=1, energies_in=14.1, energies_out, angle_cosines_out)

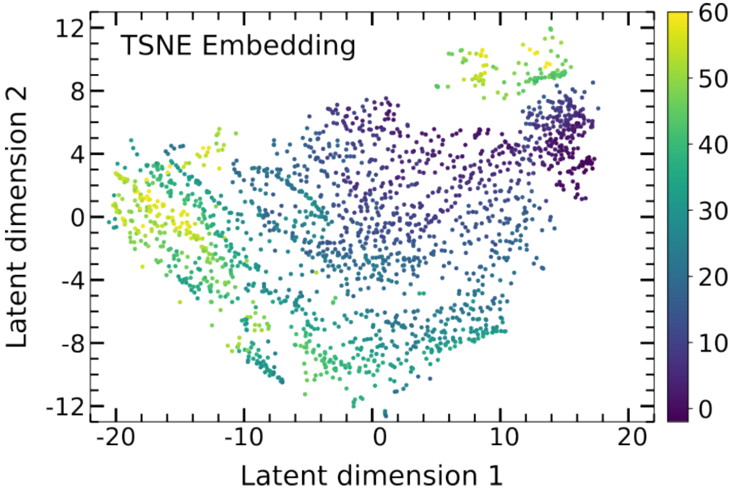
Combines MF4 and MF5 information

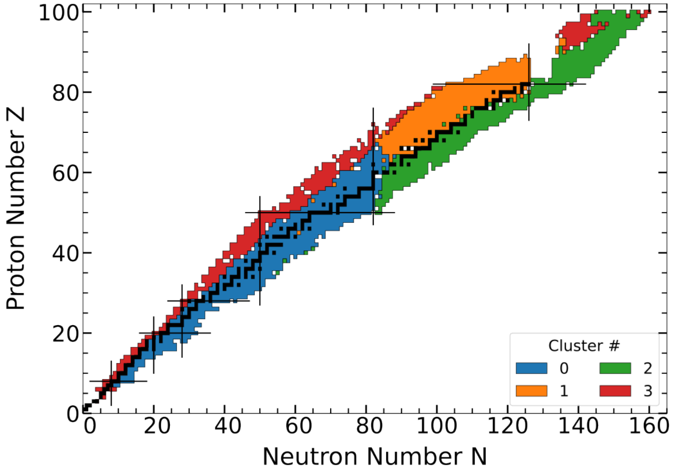
Implicit neural representations are an extremely powerful tool to encode complex signals

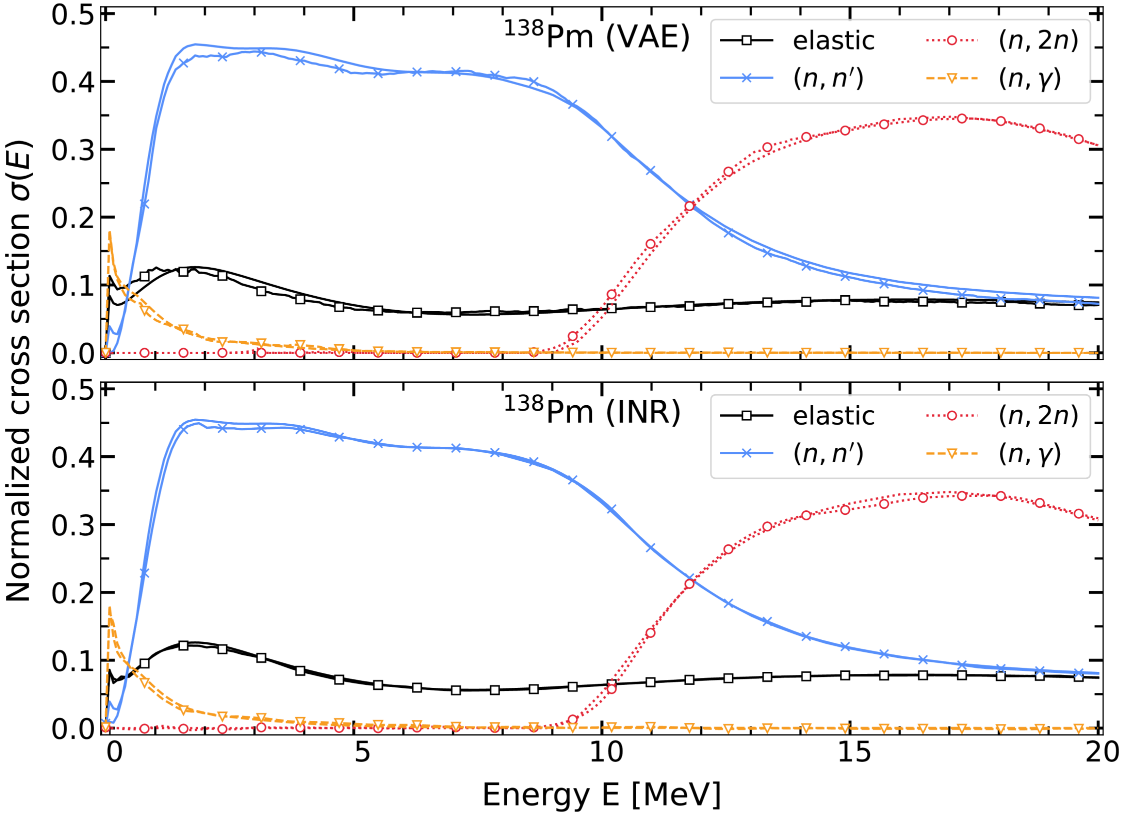
Deep Learning versus TALYS/TENDL

- Simultaneous encoding of 4 different channels with factor ~30x compression
- AI/ML can learn physical properties from encoding alone!

Mitra, Choi, Liu, Glatt, Wendt and Schunck, arXiv:2404.02332 - Lawrence Livermore + Arizona state Univ.







Precision of reconstruction is superior to typical experimental/model uncertainties

Summary

- IAEA Nuclear Data Section core business:
  - Maximize quality of nuclear data through networks
  - Data dissemination
    - Efficient, flexible GUI’s, API’s (EXFOR, ENDF, ENSDF and others)
    - Data archaeology and cleanup to allow **you** to do your AI magic

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Thank you for your attention!