IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Introduction to nuclear data and applications

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Joint ICTP/IAEA School on AI for Nuclear, Plasma and Fusion Science
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Outline

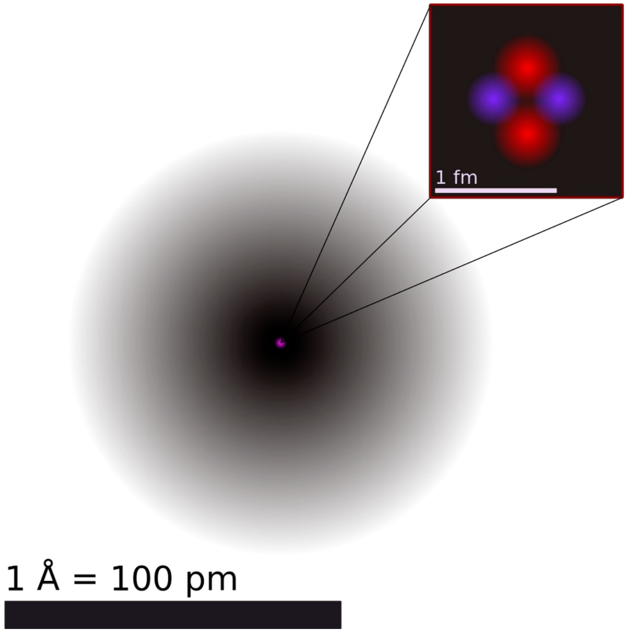
- What are nuclear data?
- Where is nuclear data needed?
- How are nuclear data produced?
- Where are nuclear data maintained and stored?

Simple definition of Nuclear Data

Nuclear data represents a collection of information and properties related to the atomic nuclei and their interactions.

Object	Size	Binding energy
Atom	10^{-10} m	$\sim$ eV
Nucleus	$\sim 10^{-15}$ m	$\sim$ MeV
Quark	$< 10^{-18}$ m	$>$ TeV

1 MeV ≈ 1.602×10^{-13} Joules

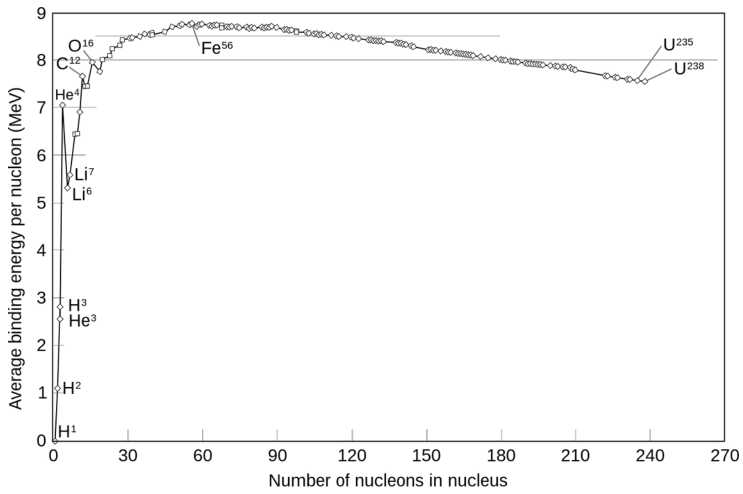


Wikipedia, User Yzmo (CC BY-SA 3.0)

Some properties of the nucleus

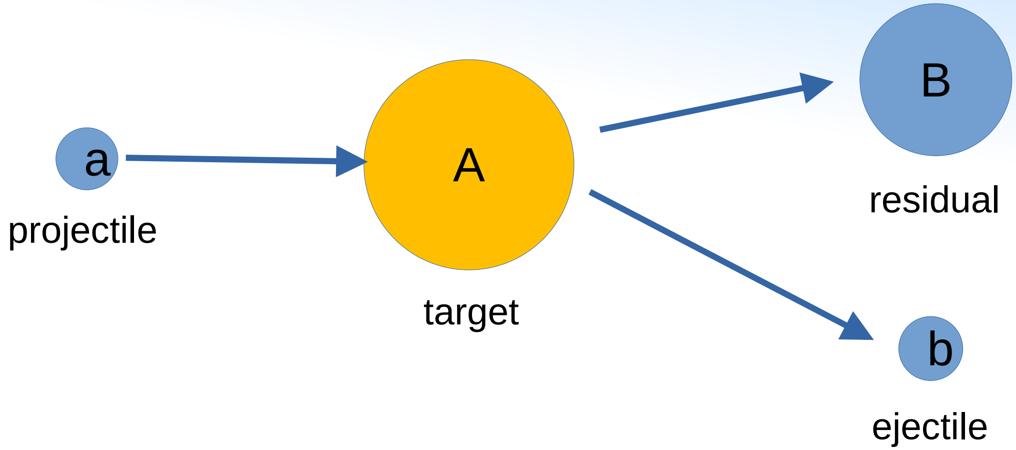
- Atomic number (Z): number of protons
- Mass number (A): number of nucleons
- Binding energy
- Spin and parity

Example specification: ^{197}Au



$$BE(N,Z) = M(N,Z)c^2 - Zm_pc^2 - Nm_nc^2$$

Nuclear reaction



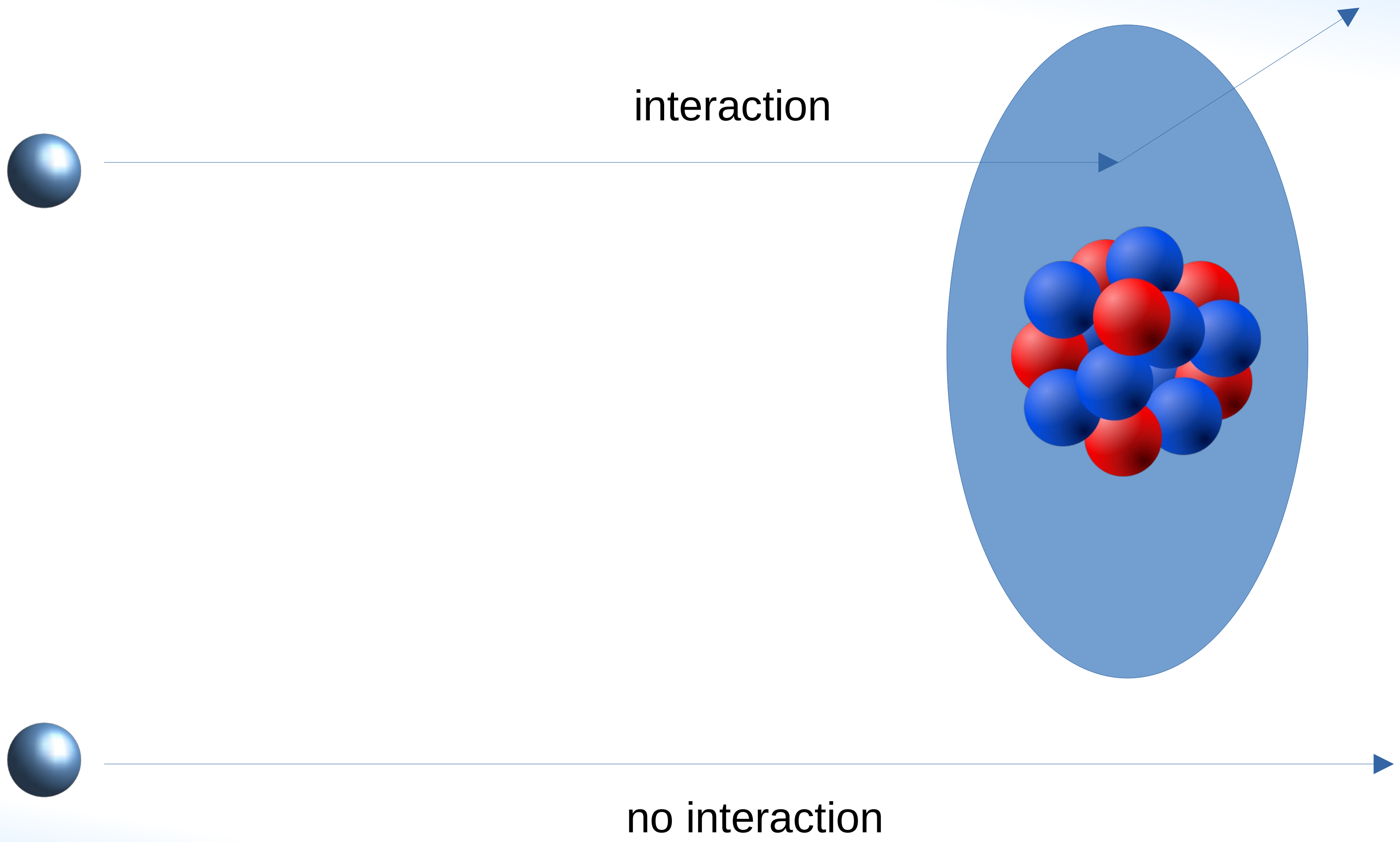
$$a + A \rightarrow b + B$$

$$A(a,b)B$$

Q-value: amount of energy released in reaction

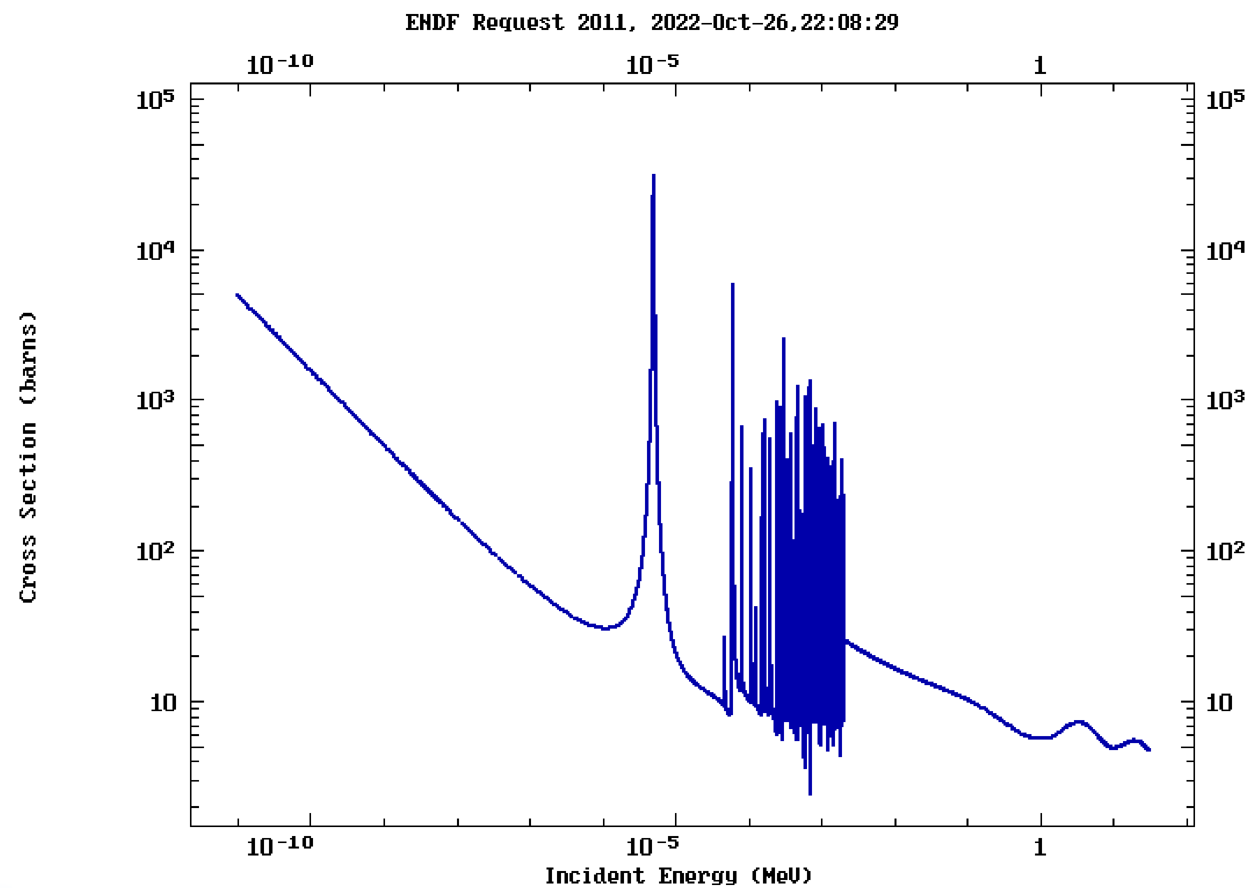
$$Q = \text{masses (before)} - \text{masses (after)}$$
$$= M_a + M_A - M_B - M_b$$

Total cross section



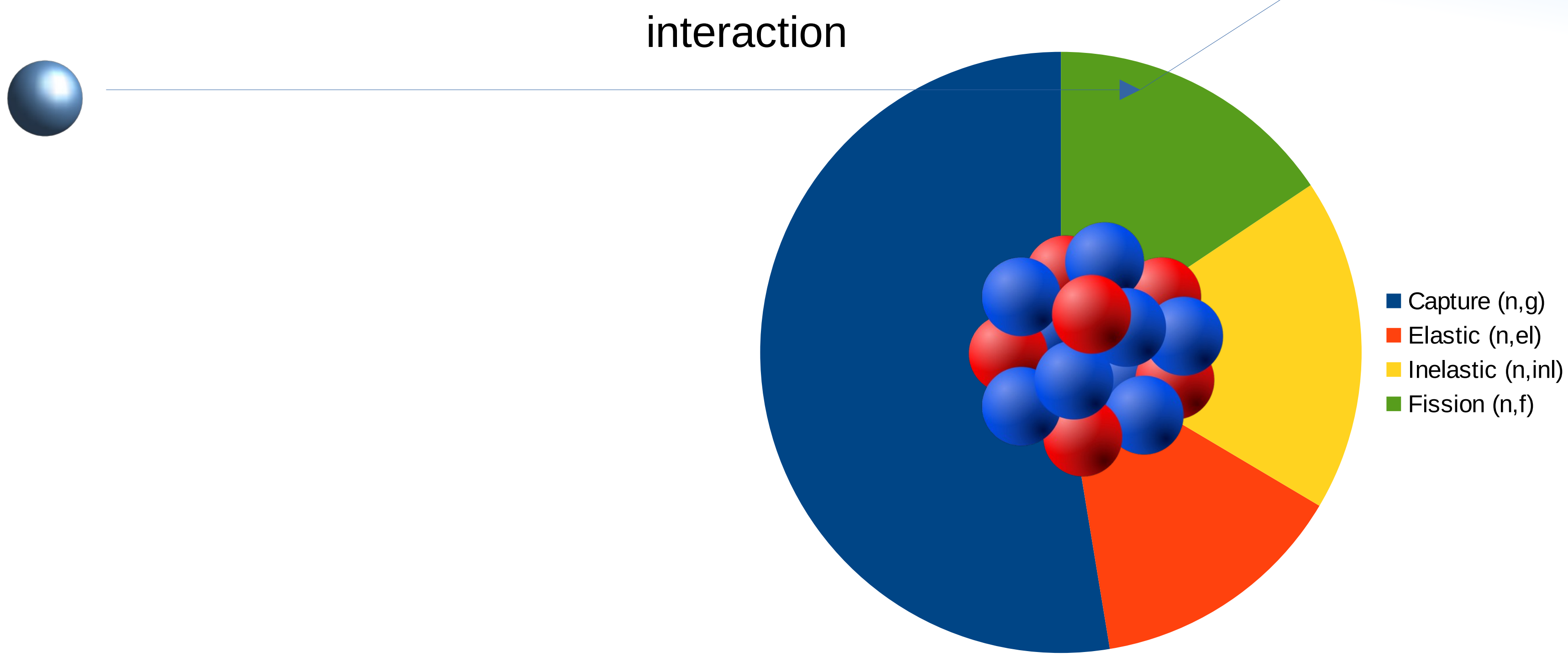
Energy dependence of total cross section

Total neutron-induced cross section of Au-197

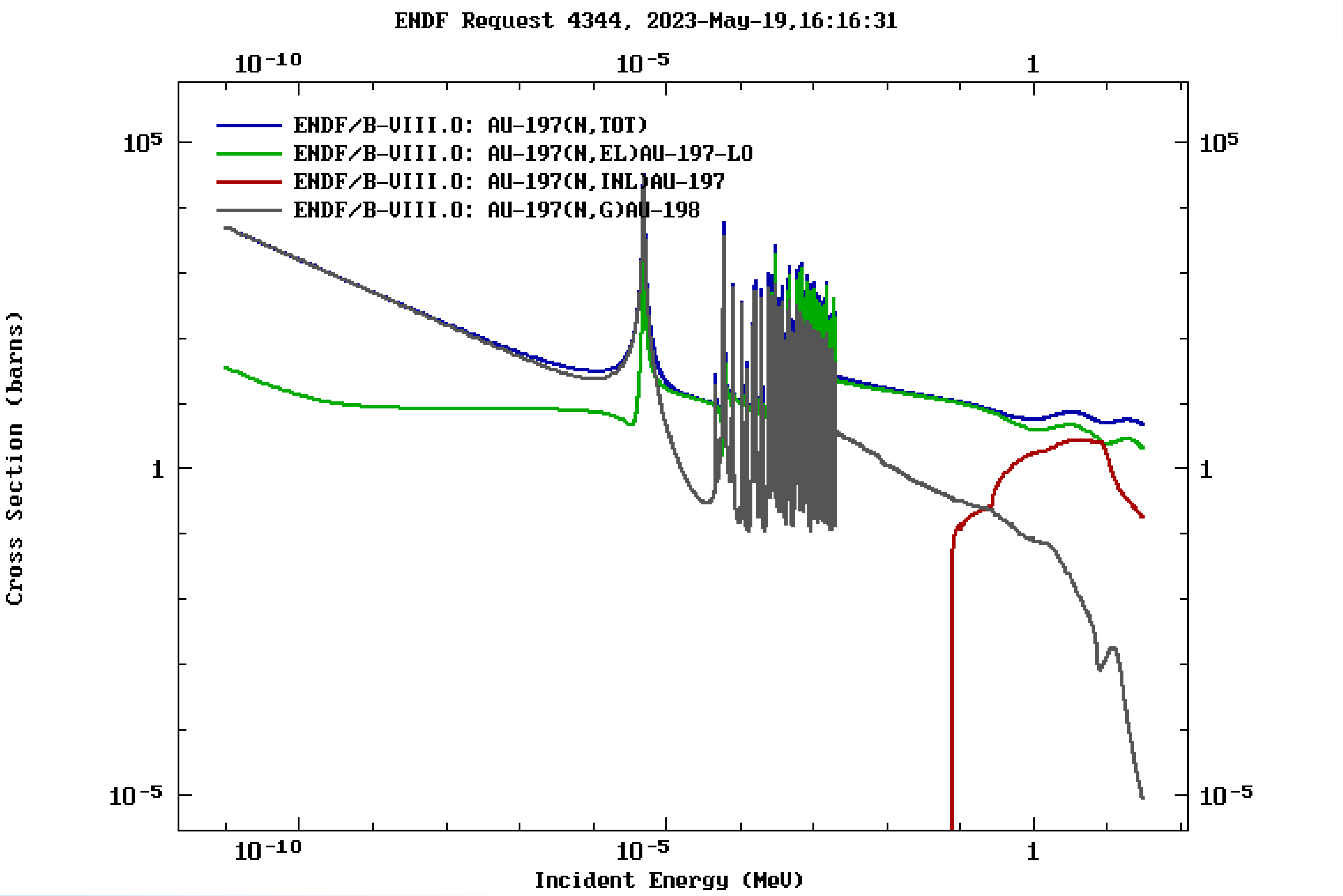


1 barn = 10^{-28} m^2

Other essential cross sections

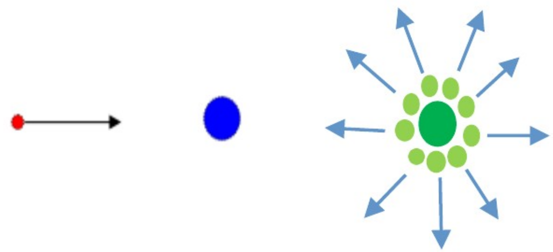


Competition of reaction channels

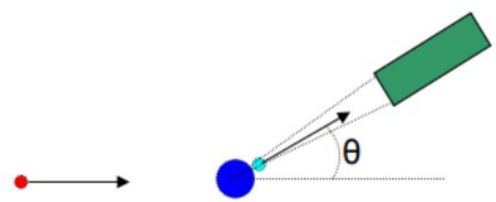


Different types of cross sections

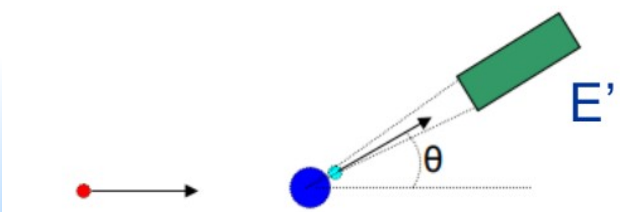
- Angle-integrated cross sections



- Angular distribution $d\sigma/d\Omega$

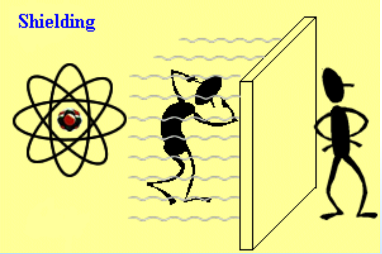


- Double-differential cross section $d^2\sigma/dEd\Omega$



Where are cross section data needed?

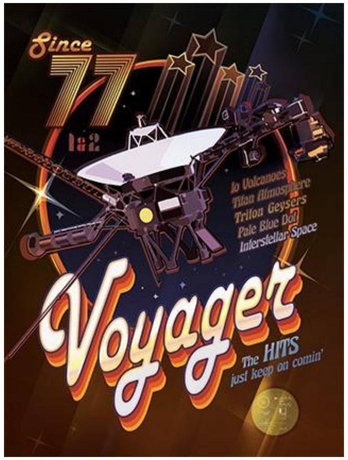

PSI Gantry 2 facility



- Design of nuclear reactors and accelerators
- Nuclear medicine and radiation therapy
- Nuclear astrophysics
- Radiation protection
- Fusion research
- Space applications
- Radioactive waste management

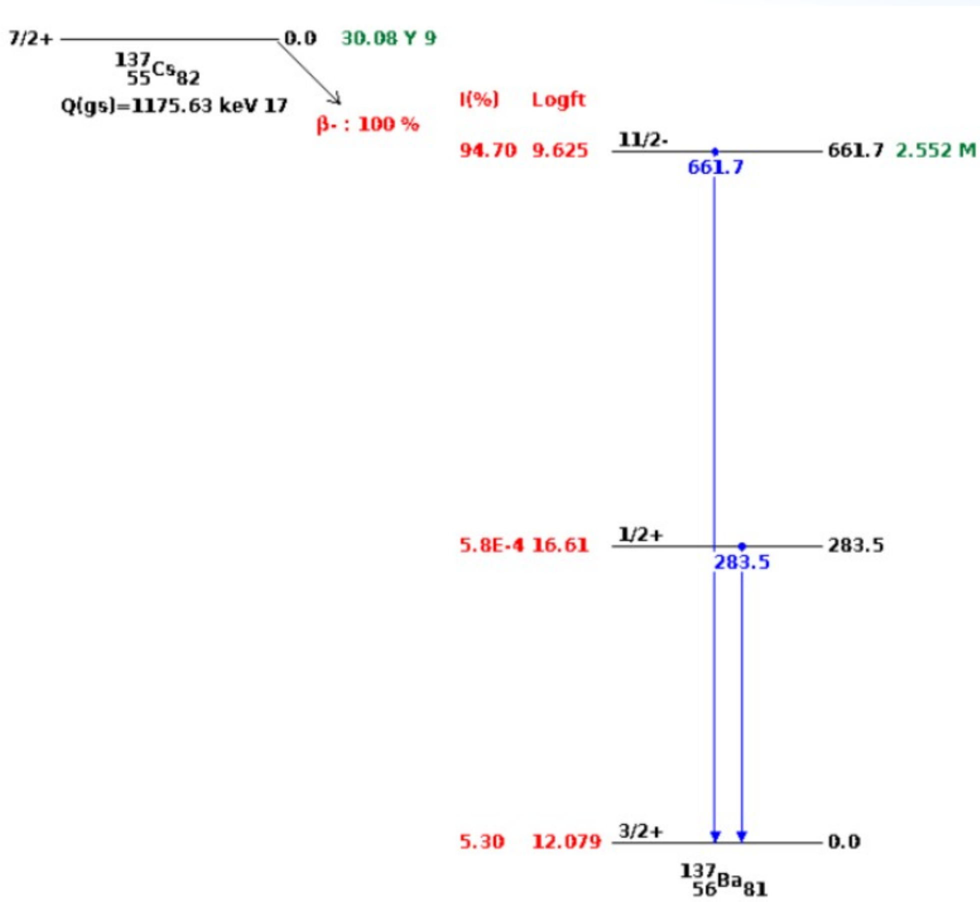

Palisades Nuclear Generating Stations


Joint European Torus



Nuclear structure data

- **Half-lives**
- **Decay modes**: alpha, beta, gamma, etc.
- **Decay radiation**: alphas, electrons, positrons, gammas, etc.
- **Branching ratios**
- **Levels, spins, parities**
- **Other:** multipolarities, conversion coefficients, magnetic moments, Q-values, transition strengths



Ion beam analysis

Example: Nuclear Reaction Analysis (NRA)

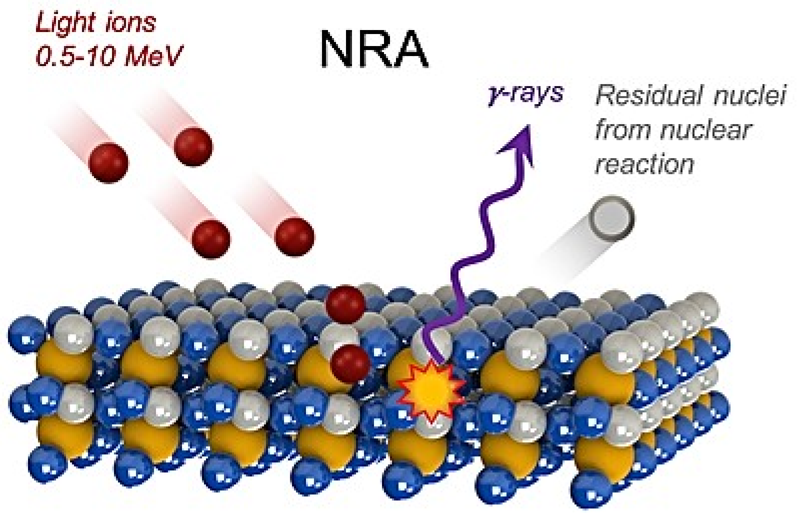
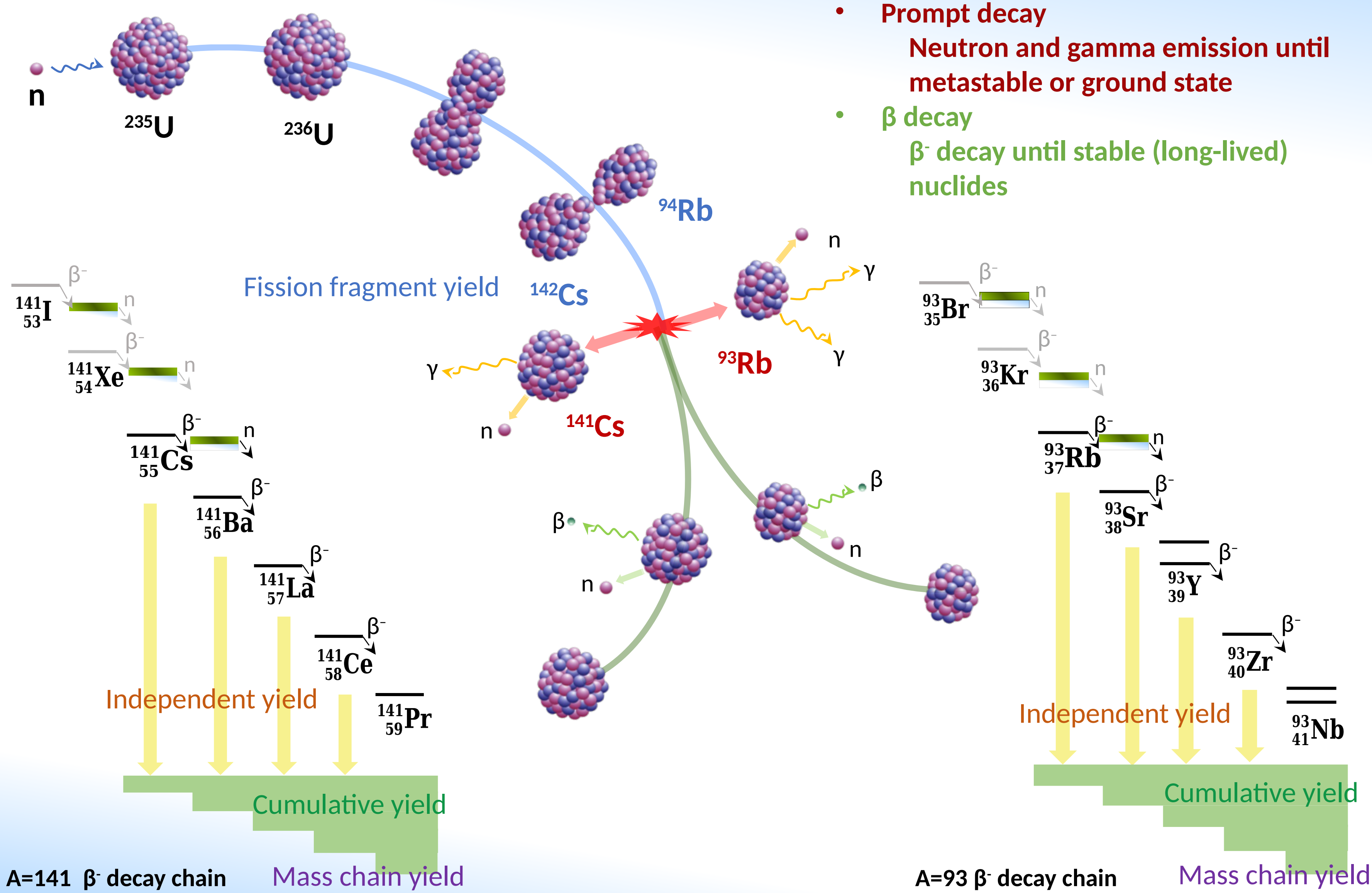


Image credit: Helmholtz-Zentrum Dresden Rossendorf (HZDR)
https://www.hzdr.de/db/Cms?pOid=10633&pNid=597

$$^{15}N + ^{1}H \rightarrow ^{12}C + ^{4}He + \gamma \text{ (4.43 MeV)}$$

Fission process & fisison yields

- **Prompt decay**
  Neutron and gamma emission until metastable or ground state
- **β decay**
  β^- decay until stable (long-lived) nuclides



Example of fission product yields

IAEA

Fission products from U-235 [edit]

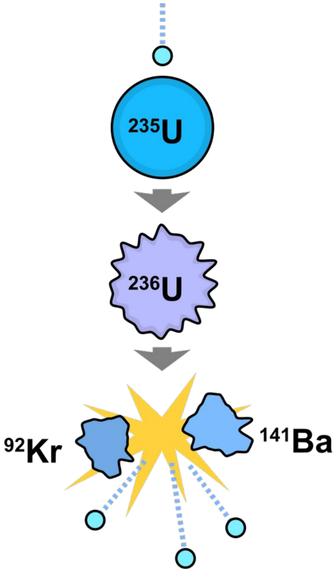
Yield	Element	Isotope	Halflife	Comment
6.7896%	Caesium	$^{133}Cs \rightarrow ^{134}Cs$	2.065 y	Neutron capture (29 barns) slowly converts stable ^{133}Cs to ^{134}Cs, which itself is low-yield because beta decay stops at ^{134}Xe; can be further converted (140 barns) to ^{135}Cs.
6.3333%	Iodine, xenon	$^{135}I \rightarrow ^{135}Xe$	6.57 h	Most important neutron poison; neutron capture converts 10–50% of ^{135}Xe to ^{136}Xe; remainder decays (9.14h) to ^{135}Cs (2.3 My).
6.2956%	Zirconium	^{93}Zr	1.53 My	Long-lived fission product also produced by neutron activation in zircalloy cladding.
6.1%	Molybdenum	^{99}Mo	65.94 h	Its daughter nuclide ^{99m}Tc is important in medical diagnosing.
6.0899%	Caesium	^{137}Cs	30.17 y	Source of most of the decay heat from years to decades after irradiation, together with ^{90}Sr.
6.0507%	Technetium	^{99}Tc	211 ky	Candidate for disposal by nuclear transmutation.
5.7518%	Strontium	^{90}Sr	28.9 y	Source of much of the decay heat together with ^{137}Cs on the timespan of years to decades after irradiation. Formerly used in radioisotope thermoelectric generators.
2.8336%	Iodine	^{131}I	8.02 d	Reason for the use of potassium iodide tablets after nuclear accidents or nuclear bomb explosions.
2.2713%	Promethium	^{147}Pm	2.62 y	beta decays to very long lived Samarium-147 (half life>age of the universe); has seen some use in radioisotope thermoelectric generators
1.0888%	Samarium	^{149}Sm	virtually stable	2nd most significant neutron poison.

From https://en.wikipedia.org/wiki/Fission_product_yield

Need for fission yield data

- Fuel burnup
- Fuel design optimization
- Radioactive waste management
- Transmutation
- Nuclear forensics
- ...

Wikipedia, User Avda (CC BY-SA 3.0)



Generation of nuclear data (ideal world)

- "The high-level strategy is to solve the non-relativistic many-nucleon Schrödiner equation with the inter-nucleon interactions as the only input"

$$\hat{\mathrm{H}}\,|\Psi\rangle = E|\Psi\rangle$$

$$\hat{H} = \hat{T}_{\mathrm{int}} + \hat{V}$$

$$\hat{H} = \frac{1}{A}\sum_{i<j=1}^{A}\frac{(\hat{\vec{p}}_i - \hat{\vec{p}}_j)^2}{2m} + \sum_{i<j=1}^{A}\hat{V}_{ij}^{NN} + \sum_{i<j<k=1}^{A}\hat{V}_{ijk}^{3N} + \ldots$$

From P. Navratil et al, "Unified ab initio approaches to nuclear structure and reaction" (arXiv:1601.03765)

Generation of nuclear data (reality)

Compilation

Collecting experimental data and ingesting them into databases

Evaluation

Combining models and experimental data by statistical techniques (Bayesian inference)

Validation

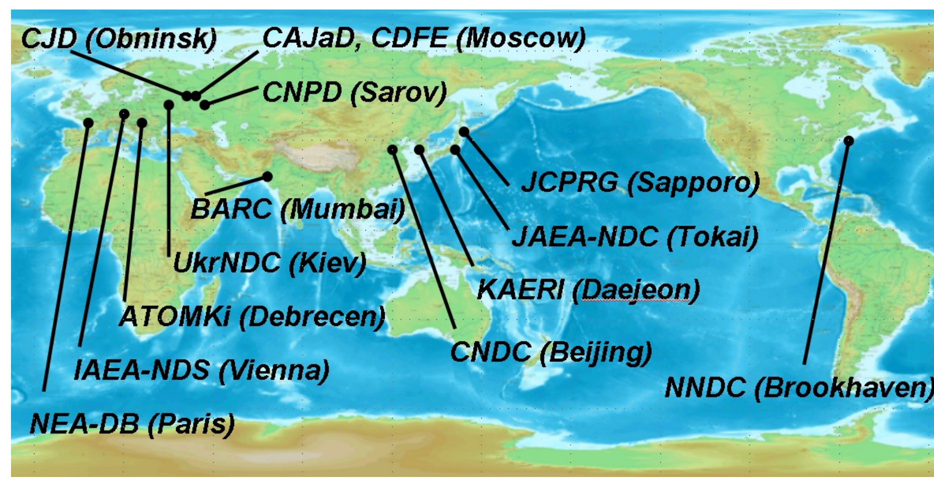
Assessing the performance of evaluated nuclear data by using them in simulations of benchmark experiments (criticality, shielding, etc.)

Nuclear Reaction Data Centre Network (NRDC)

NNDC
OECD NEA Data Bank
IAEA NDS
CJD, CDFE, CNPD
ATOMKI
UkrNDC
JCPRG
CNDC
NDPCI
KAERI

Coordinated by IAEA-NDS (Nuclear Data Section)

Each centre compiles data measured in its geographical area
(e.g., Data measured in Spain are compiled by NEA Data Bank in Paris)



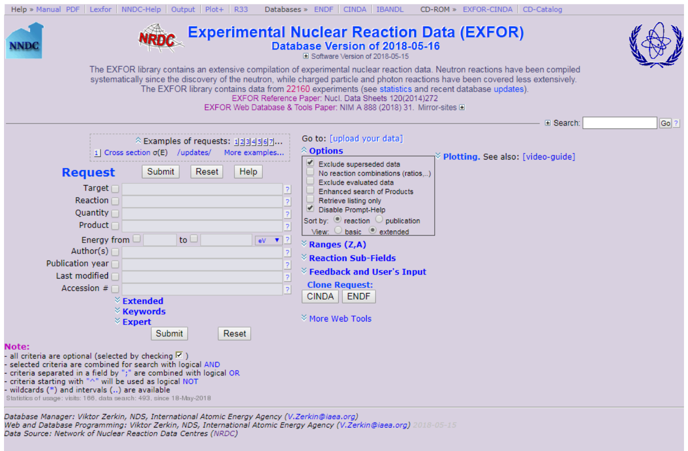
EXFOR – Library of exp. cross sections

- Collection of numerical experimental data and other quantities
- Not only neutrons but also photons, protons, and other charged particles

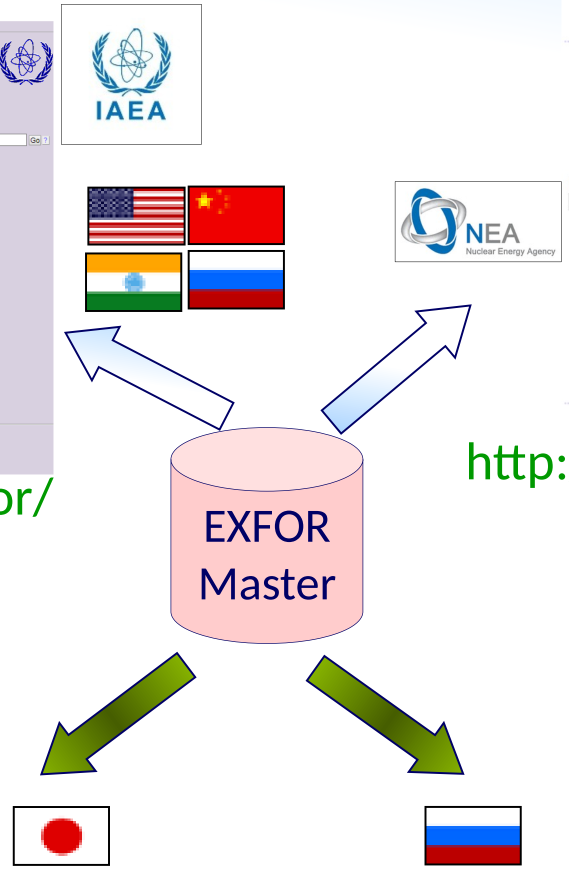
```
SUBENT         22006049   20081028
BIB                   4          8
REACTION    (92-U-238(N,G)92-U-239,,SIG)
SAMPLE       Metallic disk  29.872 gram, 50 mm diameter,
             0.9  mm thick
STATUS      (TABLE) Data submitted by Dr. J.Voignier .
                   Table  V of main reference.
HISTORY     (19910125C) S.W.
            (19910205E)
            (20050716A)  Sample data added .
ENDBIB                8
NOCOMMON              0          0
DATA                  3          4
EN          DATA        ERR-T
MEV         MB          MB
 5.0000E-01 1.2200E+02 9.0000E+00
 7.2000E-01 1.2770E+02 9.0000E+00
 9.0000E-01 1.3160E+02 9.0000E+00
 1.1000E+00 1.1440E+02 8.0000E+00
ENDDATA               6
ENDSUBENT            19
```

^{238}U(n,γ)^{239}U cross section measured in France in 1980s in EXFOR

Various access options to EXFOR

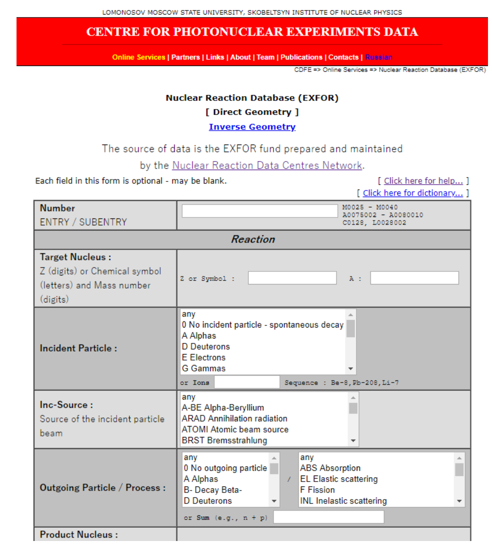


http://www-nds.iaea.org/exfor/



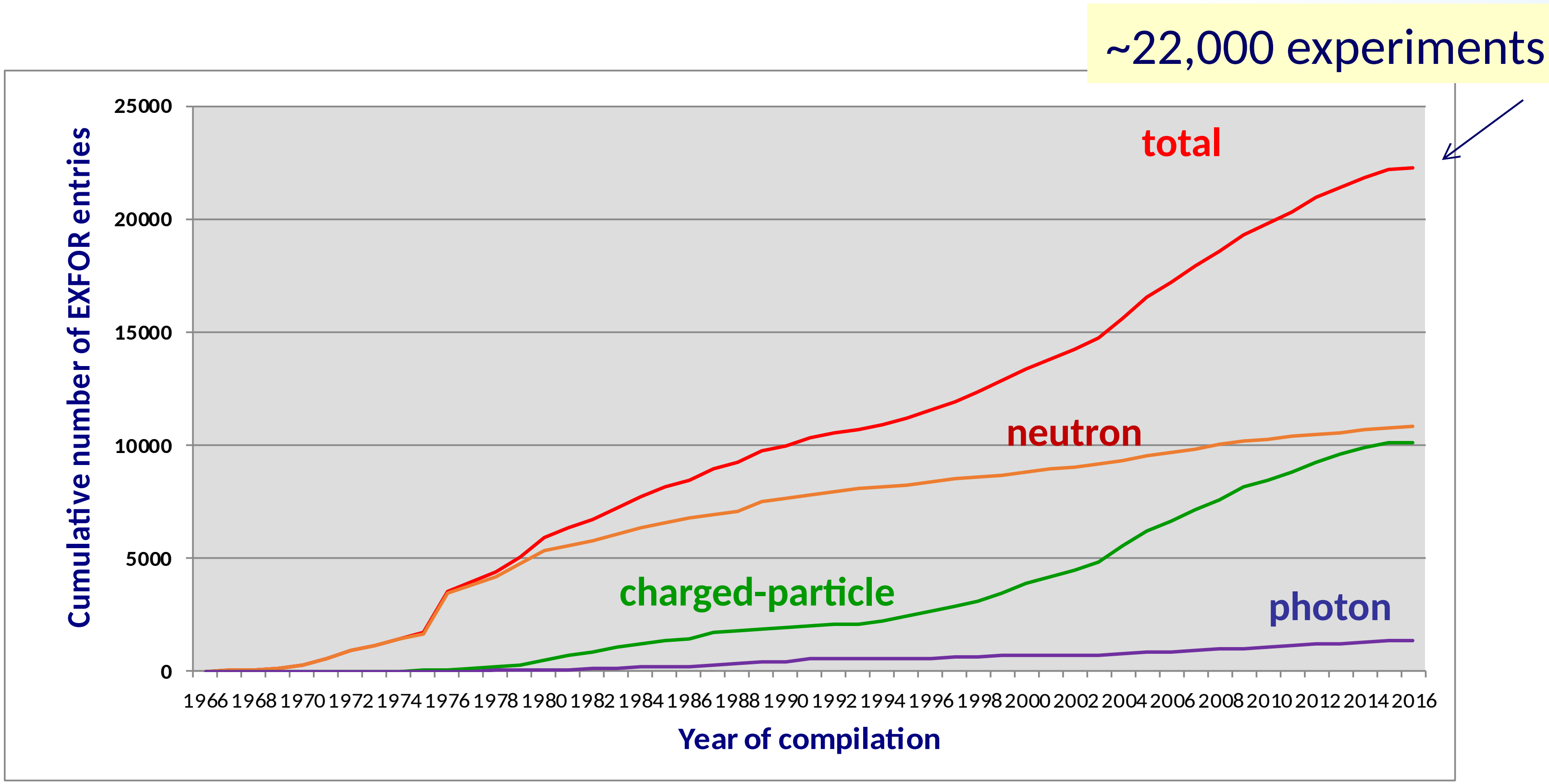
http://www.oecd-nea.org/janis/

http://www.jcprg.org/exfor/



http://cdfe.sinp.msu.ru/exfor/

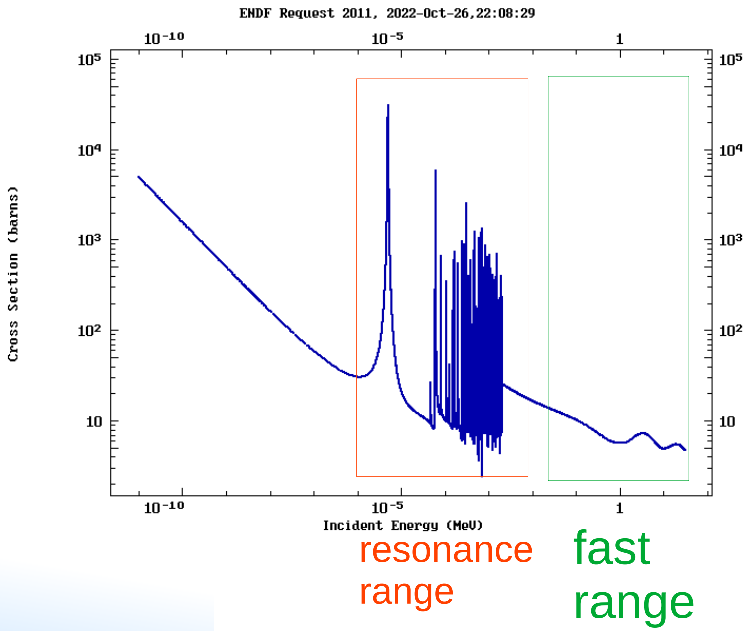
Evolution of EXFOR over time



Nuclear data evaluation

Different approaches depending on energy range and objective of evaluation, e.g.,

- R-matrix fits in the resonance range
- Fits of nuclear models in the fast energy range
- “No-model” fits if lots of data available and accuracy is essential (e.g., neutron data standards)



Nuclear reaction codes

- R-matrix analysis codes:

  AZURE2, SAMMY (ORNL), EDA (LANL), CONRAD (CEA Cadarache), AMUR (JAEA), FRESCO (LLNL), RAC (Tsinghua), REFIT (GEEL), ...

- Nuclear Reaction Codes
  - Empire: https://nds.iaea.org/empire/
  - TALYS: https://www-nds.iaea.org/talys
  - CCONE
  - CoH_3
  - ...

"Compound Nuclear Reactions,", Proceedings of the 6th International Workshop on Compound-Nuclear Reactions and Related Topics, CNR*18

https://link.springer.com/book/10.1007/978-3-030-58082-7

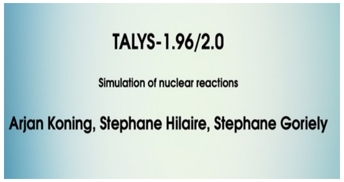
Components in TALYS

Input → Physical parameters → Reaction models → Multiple emission → Output

Input

projectile n
element Fe
mass 56
energy 14.0

+ some 400 keywords



Physical parameters

Nuclear Structure (RIPL-3)

- Masses
- Discrete levels
- Level densities
- Resonance parameters
- Photon strength functions
- Optical model parameters
- Fission barrier parameters

Other

- Fission fragment distributions
- 'Best' nuclear model parameters optimised to experimental reaction data

- Phenomenological parameters
- Microscopic tables

Reaction models

Optical model (ECIS)

- Local/global OMP
- Phenomenological
- Semi-microscopic (JLM)

Direct reaction

- Spherical OMP
- DWBA
- Coupled-channels
  - Rotational
  - Vibrational
- Giant resonances
- Weak-coupling

Compound reactions

- Hauser-Feshbach
- Width fluctuations
- Blatt-Biedenharn ang. dis.
- Particle, photon and fission transmission coeff.
- γ-ray emission

Multiple emission

Multiple emission

- Hauser-Feshbach
- Multiple preeq. exciton
- Fission competition
- γ-ray cascade
- Exclusive channels
- Recoils
- Fission fragment de-excitation

Pre-equilibrium reactions

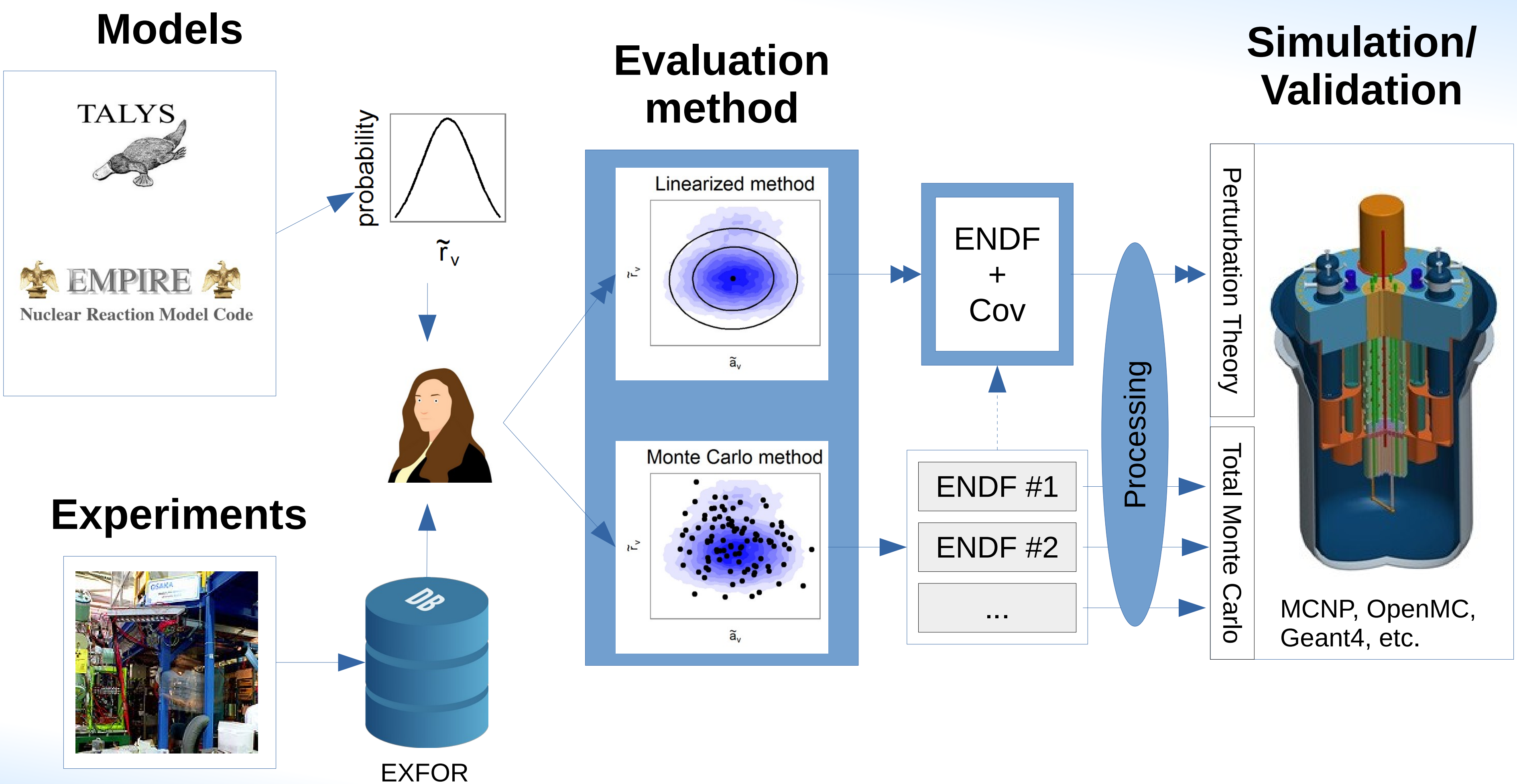
- Exciton model
- Particle hole level density
- Kalbach systematics
  - Angular distribution
  - Cluster emission
- γ-ray emission

Output

Output files per reaction channel

- Cross sections
  - Total
  - Exclusive: (n,γ), (n,f), (n,n'), (n,2n), (n,p) etc.
  - Per level
  - Residual production
  - Particle production
  - γ-ray production
- Emission spectra
  - Single-differential
  - Double differential
  - Recoils
- Angular distributions
  - Elastic
  - Per level
- Particle multiplicities
- Fission yields, neutron observables
- Astrophysical reaction rates, MACS
- …

Model-based evaluation



Evaluation example without nuclear models

IAEA

Available online at www.sciencedirect.com

ScienceDirect

Nuclear Data Sheets 148 (2018) 143–188

Nuclear Data Sheets

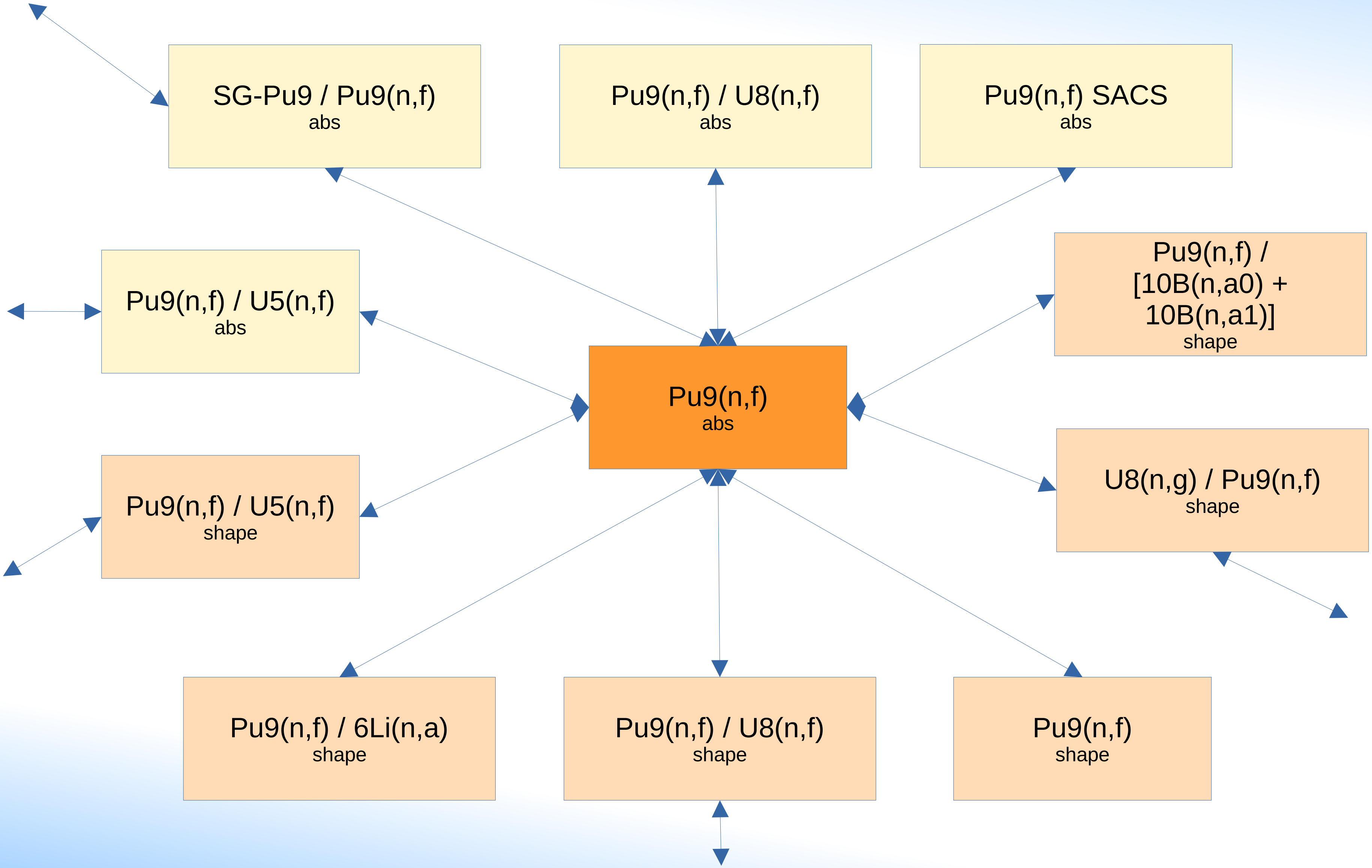
www.elsevier.com/locate/nds

Evaluation of the Neutron Data Standards

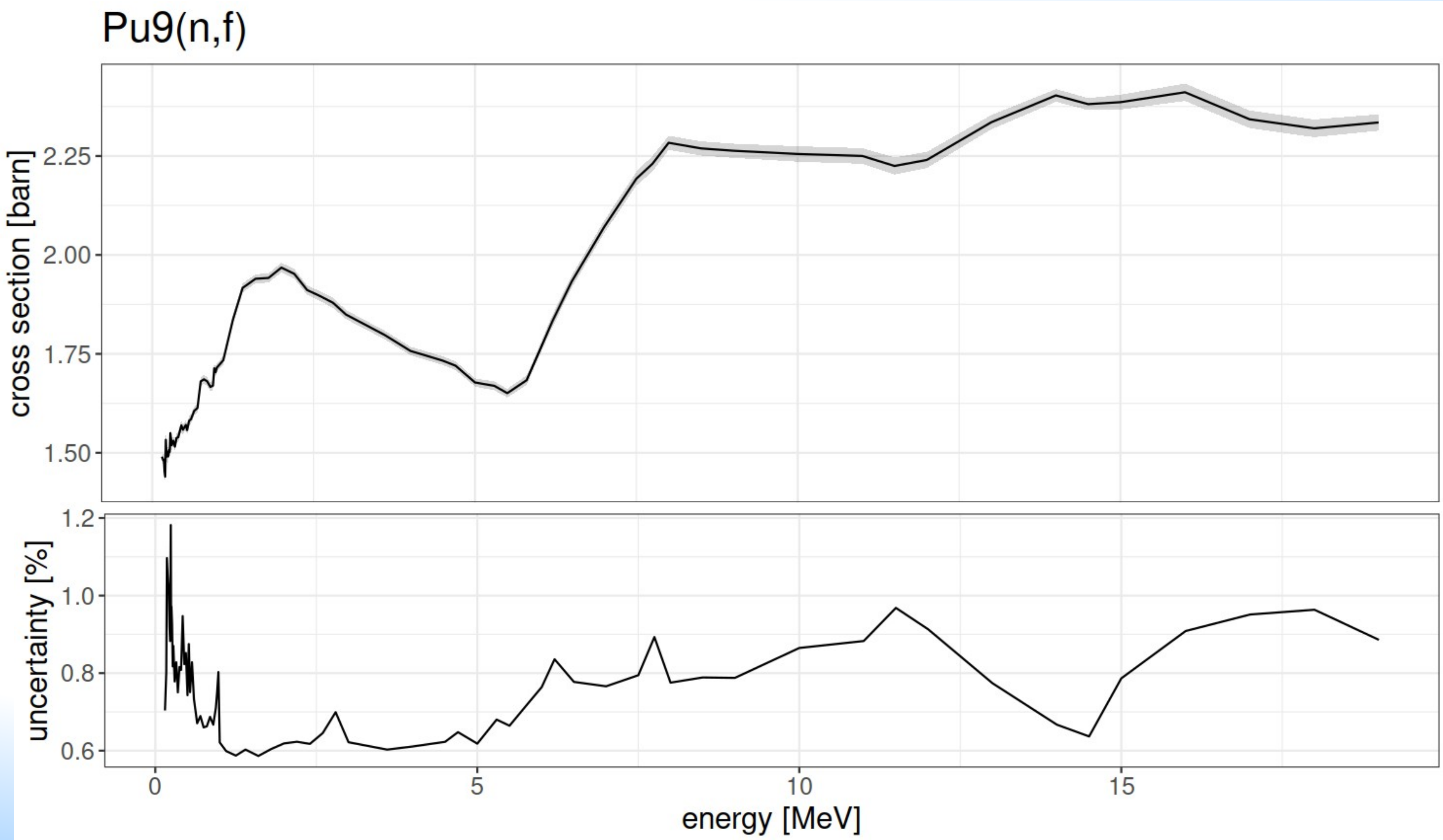
A.D. Carlson,[1,*] V.G. Pronyaev,[2] R. Capote,[3] G.M. Hale,[4] Z.-P. Chen,[5] I. Duran,[6] F.-J. Hambsch,[7] S. Kunieda,[8] W. Mannhart,[9] B. Marcinkevicius,[3,10] R.O. Nelson,[4] D. Neudecker,[4] G. Noguere,[11] M. Paris,[4] S.P. Simakov,[12] P. Schillebeeckx,[7] D.L. Smith,[13] X. Tao,[14] A. Trkov,[3] A. Wallner,[15,16] and W. Wang[14]

With the need for improving existing nuclear data evaluations, (*e.g.*, ENDF/B-VIII.0 and JEFF-3.3 releases) the first step was to evaluate the standards for use in such a library. This new standards evaluation made use of improved experimental data and some developments in the methodology of analysis and evaluation. In addition to the work on the traditional standards, this work produced the extension of some energy ranges and includes new reactions that are called reference cross sections. Since the effort extends beyond the traditional standards, it is called the neutron data standards evaluation. This international effort has produced new evaluations of the following cross section standards: the H(n,n), ^{6}Li(n,t), ^{10}B(n,α), ^{10}B(n,$\alpha_1\gamma$), ^{nat}C(n,n), Au(n,γ), ^{235}U(n,f) and ^{238}U(n,f). Also in the evaluation process the ^{238}U(n,γ) and ^{239}Pu(n,f) cross sections that are not standards were evaluated. Evaluations were also obtained for data that are not traditional standards: the Maxwellian spectrum averaged cross section for the Au(n,γ) cross section at 30 keV; reference cross sections for prompt γ-ray production in fast neutron-induced reactions; reference cross sections for very high energy fission cross sections; the ^{252}Cf spontaneous fission neutron spectrum and the ^{235}U prompt fission neutron spectrum induced by thermal incident neutrons; and the thermal neutron constants. The data and covariance matrices of the uncertainties were obtained directly from the evaluation procedure.

Consistent evaluation of multiple reaction channels (without nuclear model)



Evaluation: Estimated excitation function with uncertainty band



Validation with Integral benchmarks

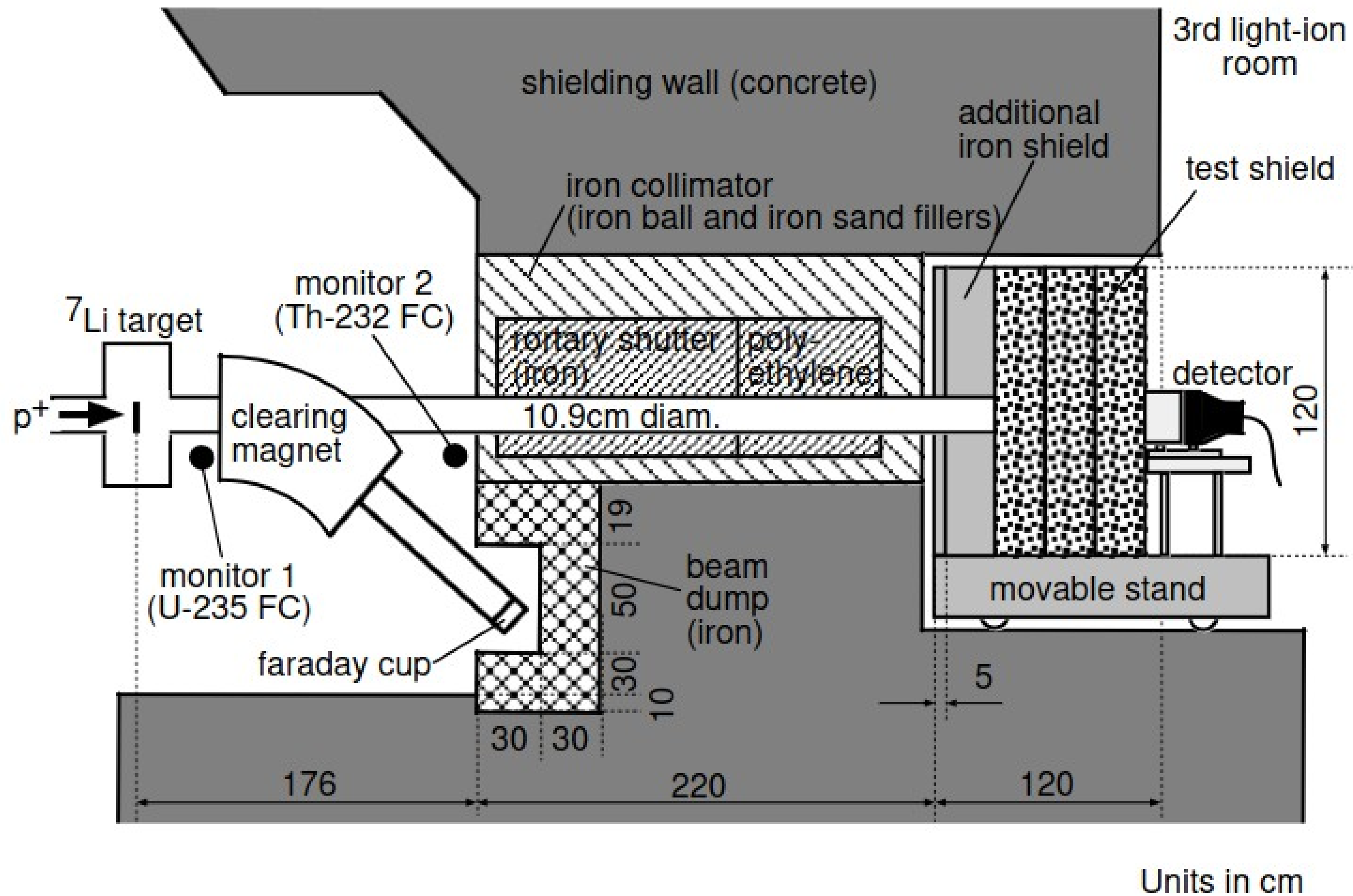


Fig. 1 Experimental arrangement of shielding experiments at JAERI/TIARA.

From: C. Konno, Y. Ikeda, K. Kosako, “DORT Analysis of Iron and Concrete Shielding Experiments at JAERI/TIARA with P_7 and P_9 Approximated LA150 Multigroup Libraries” (2000)

Nuclear Data Libraries

Storage and dissemination of nuclear data

Libraries associated with regions/countries:

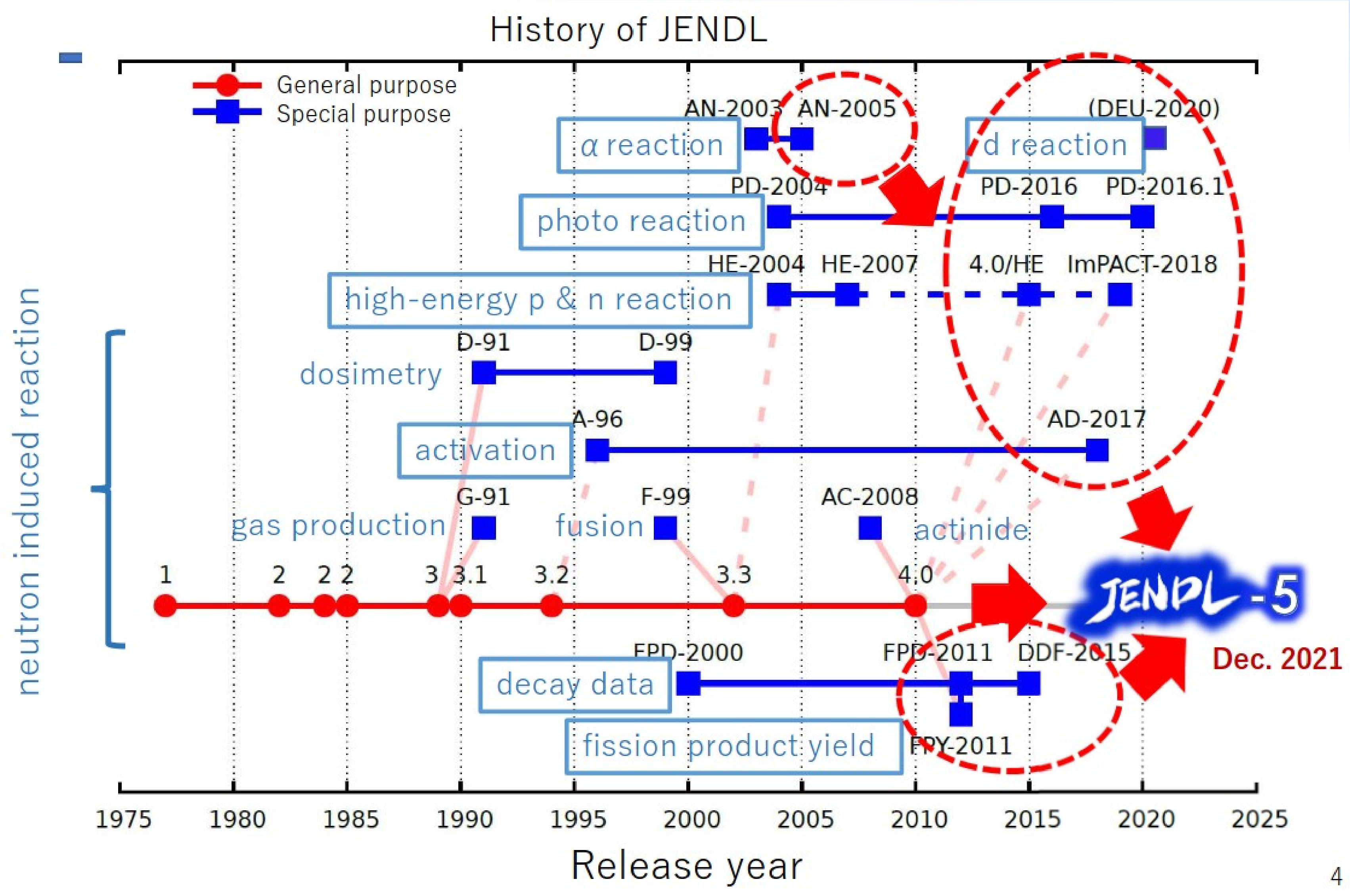
ENDF/B (USA), JEFF (Europe), JENDL (Japan), CENDL (China), BROND (Russia)

Other/Project based libraries:

FENDL, IRDFF-II, Neutron Data Standards, Photonuclear (IAEA), TENDL (TALYS), ...

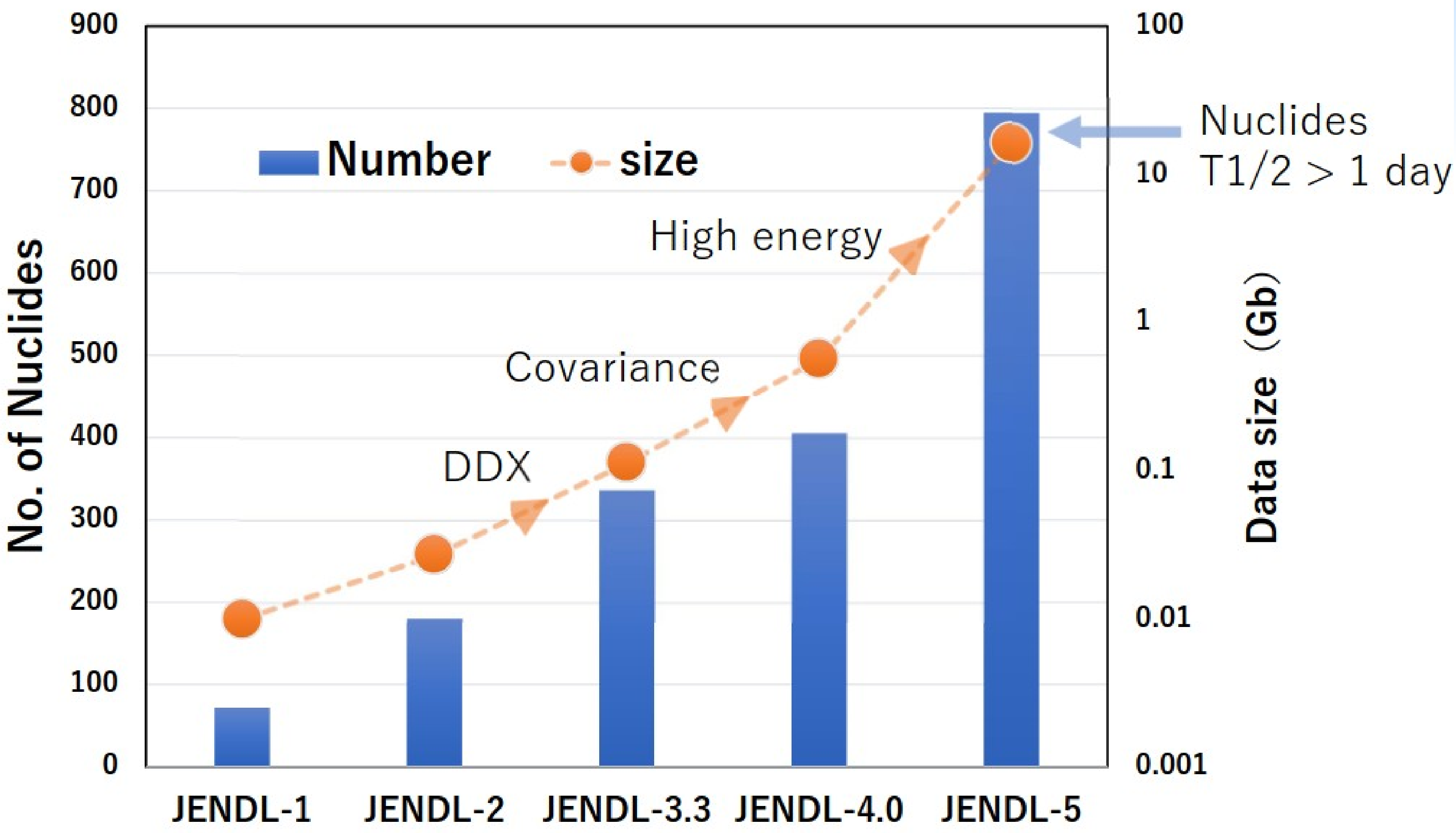
Graphical interface to content of libraries:
https://nds.iaea.org/exfor/endf.htm

Example JENDL



Slide: Courtesy of Osamu Iwamoto

Example JENDL



- Inclusion of all nuclides in natural abundance
- Sufficient number of nuclei for neutron activation calculation

Slide: Courtesy of Osamu Iwamoto

Summary

- Nuclear data: quantities associated with nuclear reactions (cross sections, Q-values, etc.) and nuclear structure (level energies, spin, parity, etc.)
- Wide range of applications (e.g., nuclear medicine, reactor design, fusion research)
- Ab-initio calculations challenging, therefore production of nuclear data relies on experimental data and nuclear models
- Statistical methods are used for an evaluation to combine various sources of data (models and measurements)

Acknowledgments

Thanks to my colleagues Daniel Lopez Aldama, Vivian (Paraskevi) Dimitriou, Osamu Iwamoto, Arjan Koning, Shin Okumura, Naohiko Otsuka and Jean-Christophe Sublet for sharing parts and visuals of some of their presentations