AWE NUCLEAR SECURITY TECHNOLOGIES

How do end-users use the outputs from academic nuclear physics research?

Institute of Physics Early Career Researcher forum, 16th April 2026

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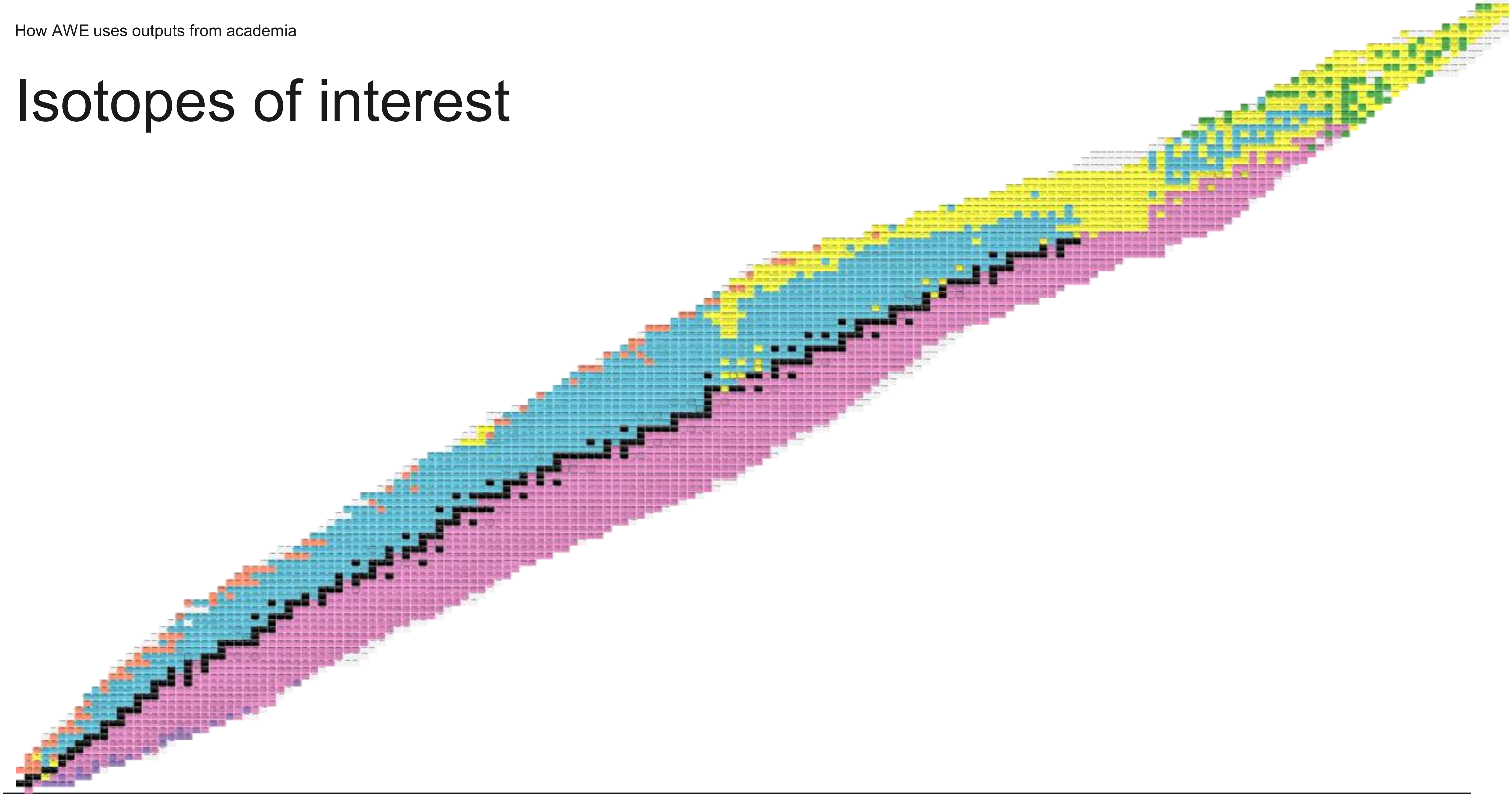
Introduction

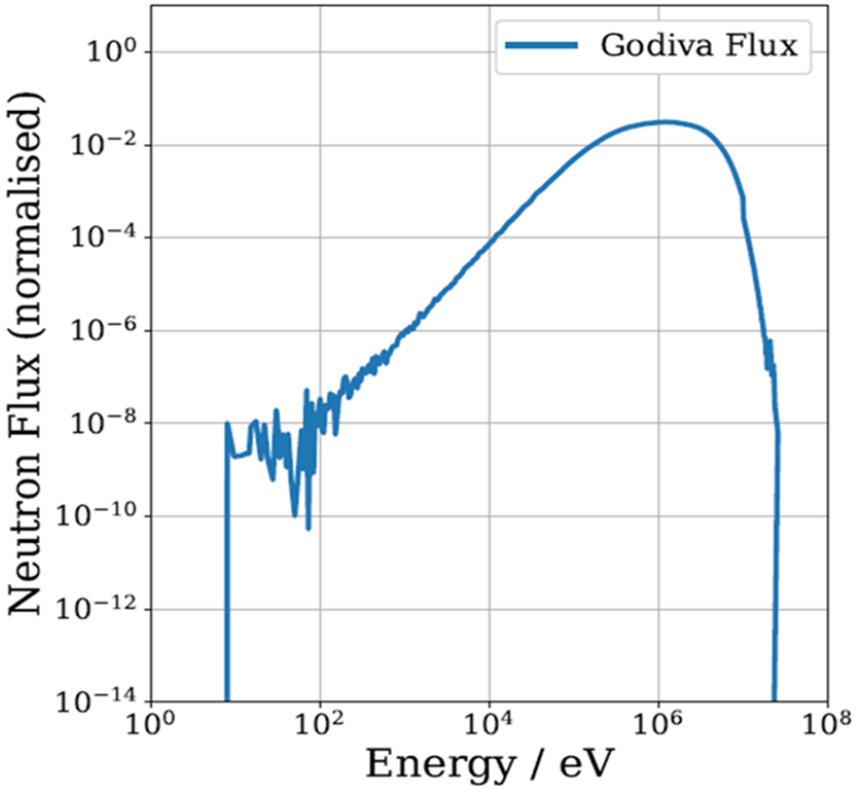
- Who am I?
- AWE?
- End-users utilise *nuclear data* in a wide range of modelling calculations.
  - Which outputs from academic nuclear physics experiments or theoretical studies are useful?
  - How do users incorporate these into models?

Isotopes of interest



Regimes of interest

- Generally incident neutrons of most interest.
  - But, other incident particle data also of interest, as well as outgoing spectra.
  - For example, research into predictions of gamma-ray spectra from light-ion fusion reactions.
    - See e.g. N. Timofeyuk et al, PRC 110(1)014612.
- Neutrons from different sources;
  - e.g. fission (example shown right), DD (2.45 MeV) and DT (14.1 MeV), and RIF (>20 MeV).



What is the working level?

- Most end-users of nuclear physics properties are several steps removed from fundamental calculations or measurements.

Codes (e.g. MCNP, OpenMC, MONK, GEANT4, FISPACT-II) that perform calculations of nuclear systems, e.g. reactors, nuclear waste, accelerators.

Nuclear data available for practical calculations, e.g. ENDF/B-VIII, JENDL-4.0.

Codes that calculate reaction properties, e.g. TALYS, YAHFC, EMPIRE.

Libraries of nuclear properties, e.g. RIPL, ENSDF.

Explicitly solving the Schrödinger equation, explicitly working with Hamiltonians, nuclear DFT, TDHF, ab initio calculations, etc.

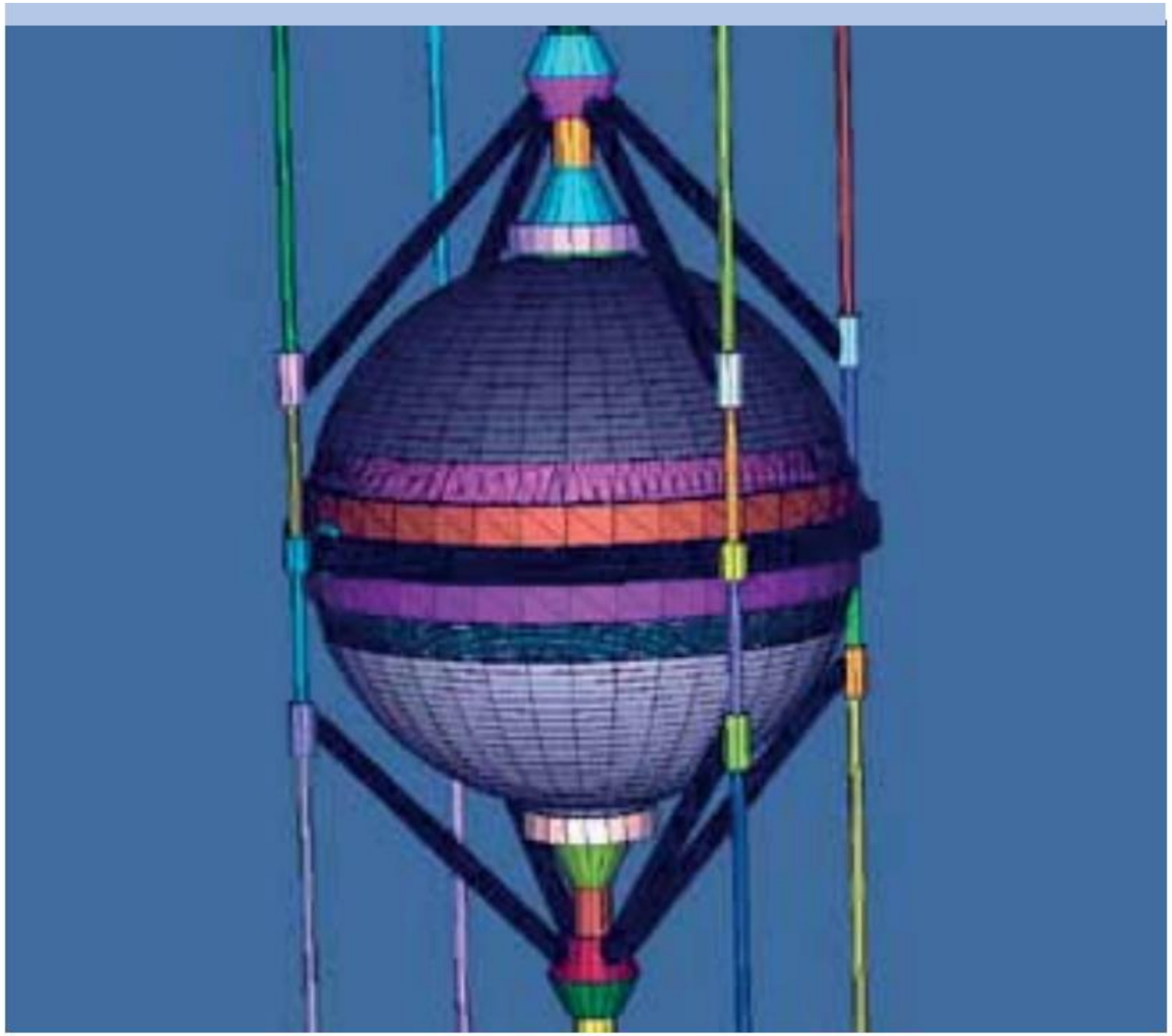
Example applications: Criticality

TABLE 1

Experiment	1.0000 ± 0.0020	
	$k_{effective}$	$\pm 1\sigma$
ENDF/B-VII	0.9986	0.0001
JEFF 3.1	0.9986	0.0001
JENDL 3.2	0.9964	0.0001

Plutonium-239 'Jezebel' $k_{effective}$ values.

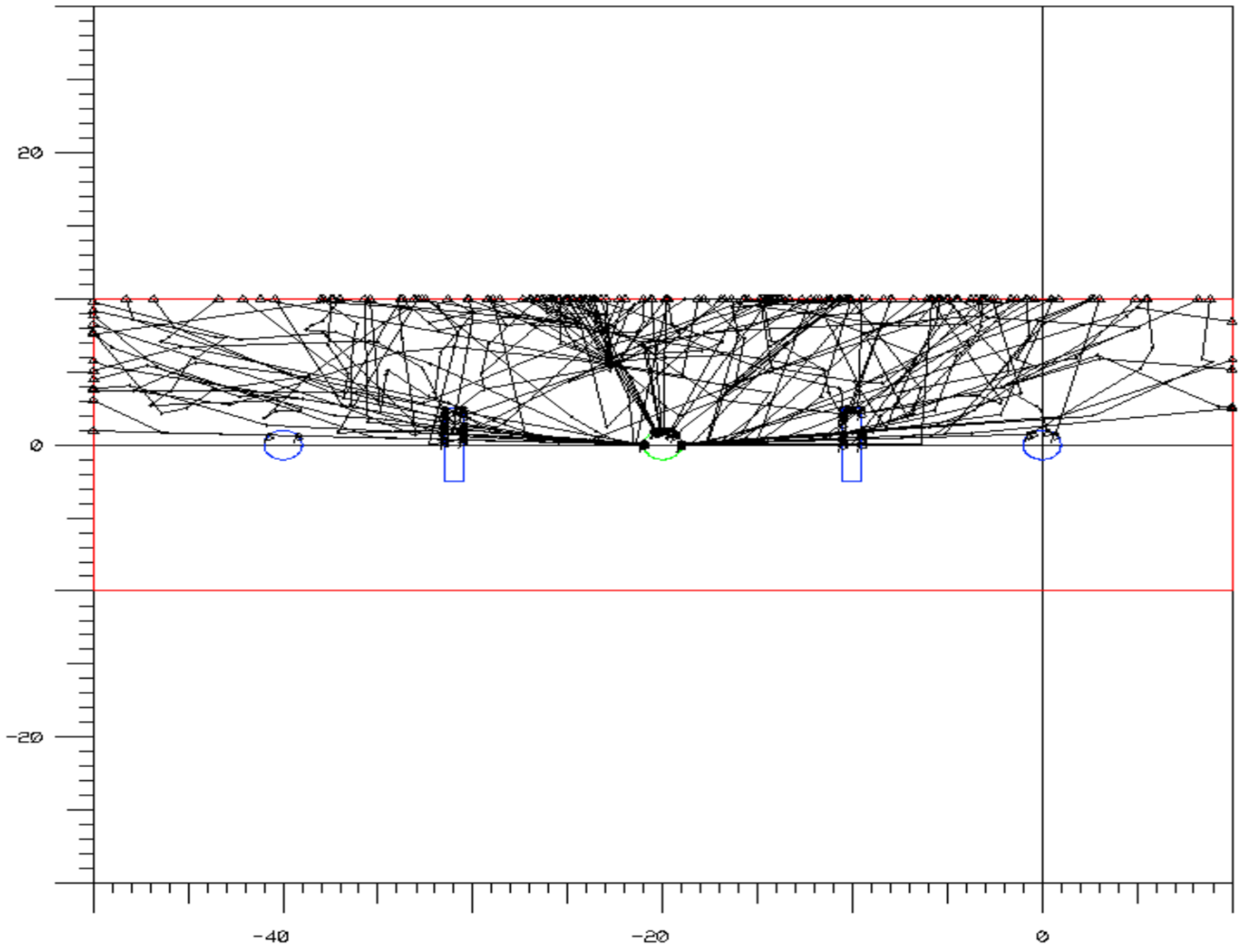
- Important for reactors, nuclear material storage, nuclear waste, etc.
- Neutrons are transported through a geometry, undergoing reactions and the neutron *multiplicity* calculated.
- Usually, Monte Carlo codes such as MONK or MCNP are used.
- Deterministic codes are also available, e.g. PARTISN.



Plutonium-239 'Jezebel' Critical Assembly – complete.

Transport and shielding

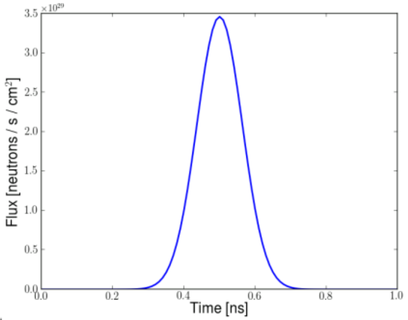
- The transport of neutrons, or other forms of radiation, from a source to specific locations must be understood for a number of applications.
  - e.g. shielding of operators around an accelerator or reactor.
- Monte Carlo codes such as MCNP, GEANT4, OpenMC are often used.
- Deterministic options also available.

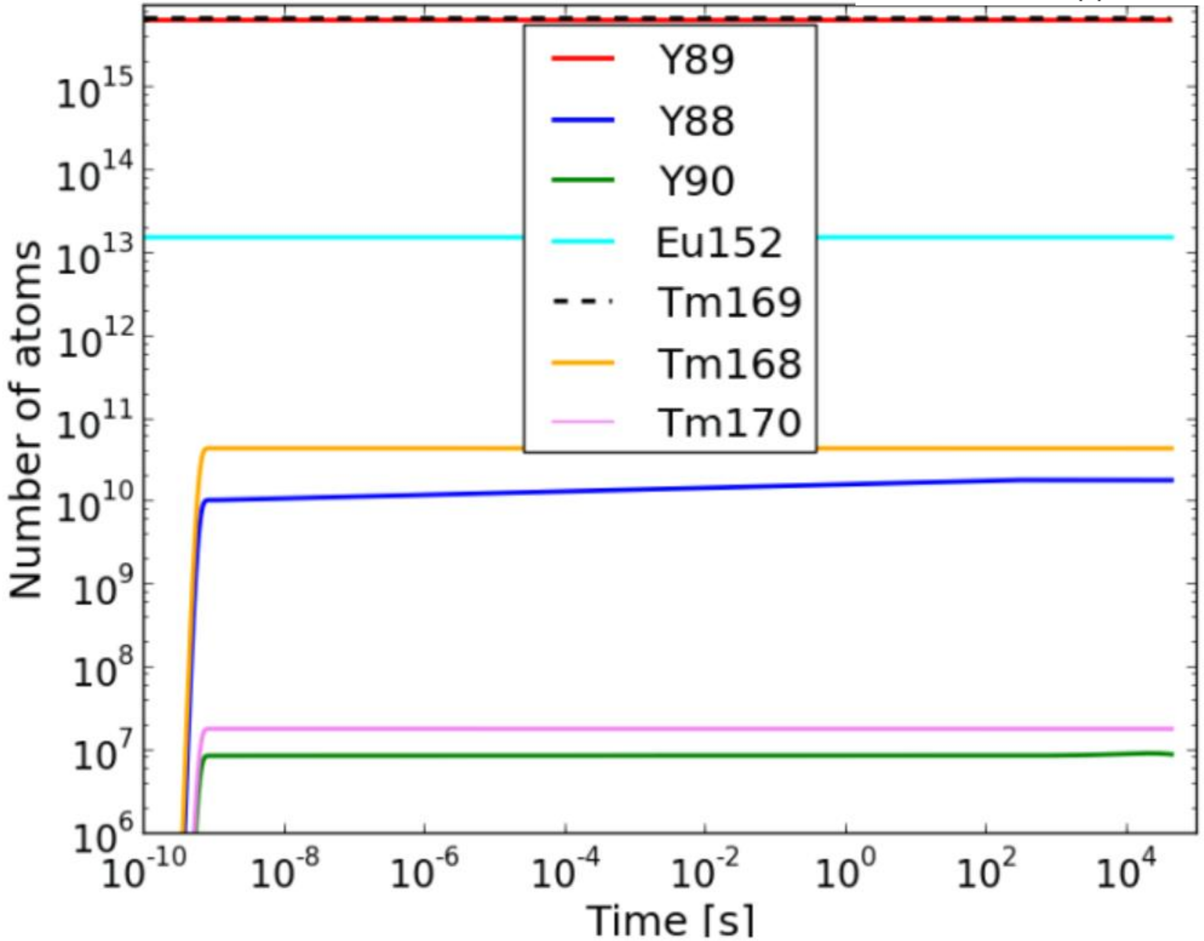


Activation / Burn-up

- Calculations of the number of atoms present at different times during or following irradiation are important, for e.g. dose rate calculations, waste transmutation, etc.

- Activation codes which solve the Bateman equations (a set of coupled differential equations) are used, e.g. FISPACT-II.



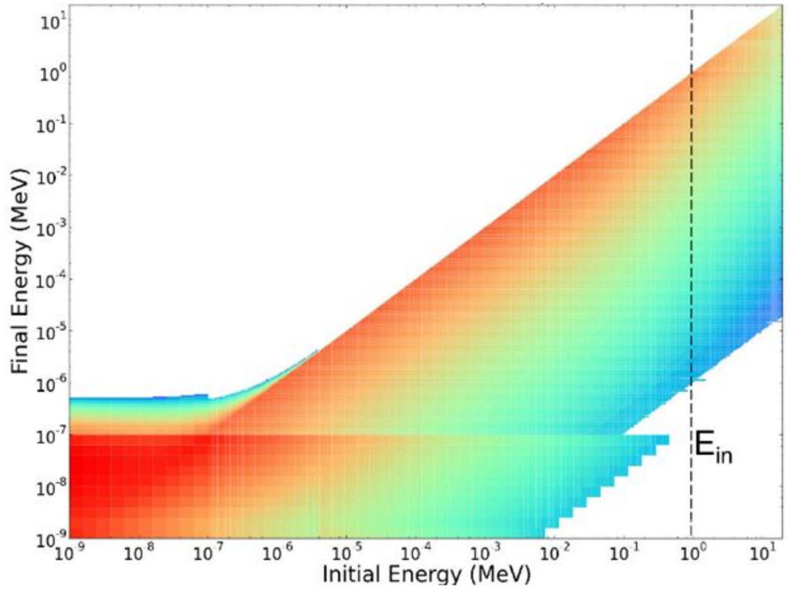


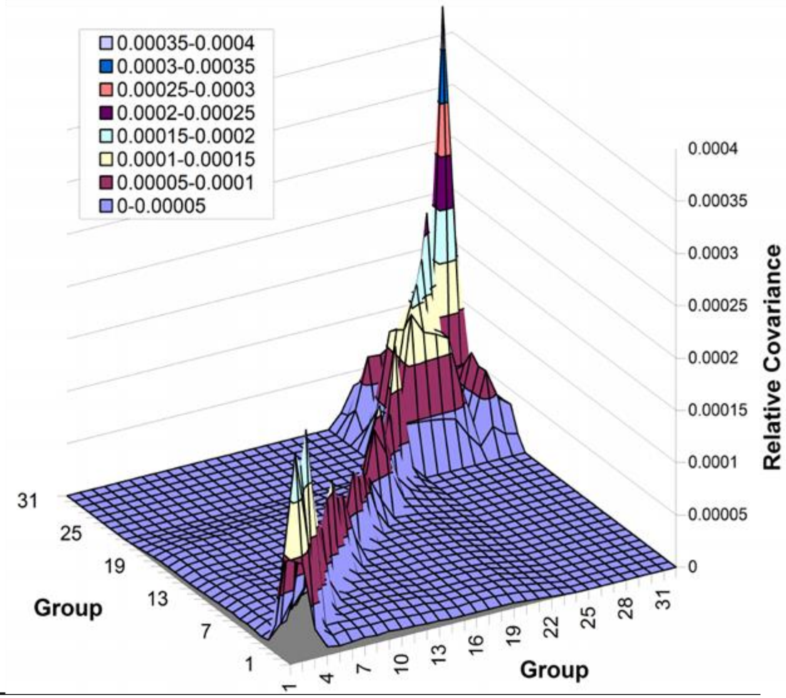
Where can data enter the modelling “work stream”?

- Within a full evaluated nuclear data library.
- As an individual cross sections or similar property.
- As some underlying property used to calculate other nuclear data.

Evaluated nuclear data files

- For a neutron-induced nuclear data file the following parts may be present:
  - Low energy cross sections stored as resonance parameters.
  - Higher energy cross sections stored as pointwise values.
  - Secondary distributions,
    - i.e. angular or energy dependent distributions of outgoing particles.
  - Fission product data and other fission-related data.
  - Uncertainty information.
    - Generally stored as covariance matrices





Available open libraries include…

- US-led (NNDC / CSEWG), ENDF/B-VIII.1
- European-led (JEFF), JEFF-4.0
- Japanese-led (JAEA), JENDL-5
- Chinese-led (CNDC), CENDL-3.2

ENDF format

- Legacy 80-character punch card inspired format.
- Each evaluation is split into separate files (MF) with each storing a different kind of data, e.g.
  - MF2 resonance data.
  - MF3 cross section curves.
  - MF33 covariance data.

```
 1.400000+4 2.784400+1          0          0          0          01400 3 16
-8.473800+6-8.473800+6          0          0          1         121400 3 16
         12          2                                            1400 3 16
 8.778100+6 0.000000+0 1.000000+7 6.166000-3 1.100000+7 1.564000-21400 3 16
 1.200000+7 2.589000-2 1.300000+7 3.650000-2 1.400000+7 4.663000-21400 3 16
 1.500000+7 5.400000-2 1.600000+7 5.620000-2 1.700000+7 5.734000-21400 3 16
 1.800000+7 5.830000-2 1.900000+7 5.870000-2 2.000000+7 5.892000-21400 3 16
 0.000000+0 0.000000+0          0          0          0          01400 3  0
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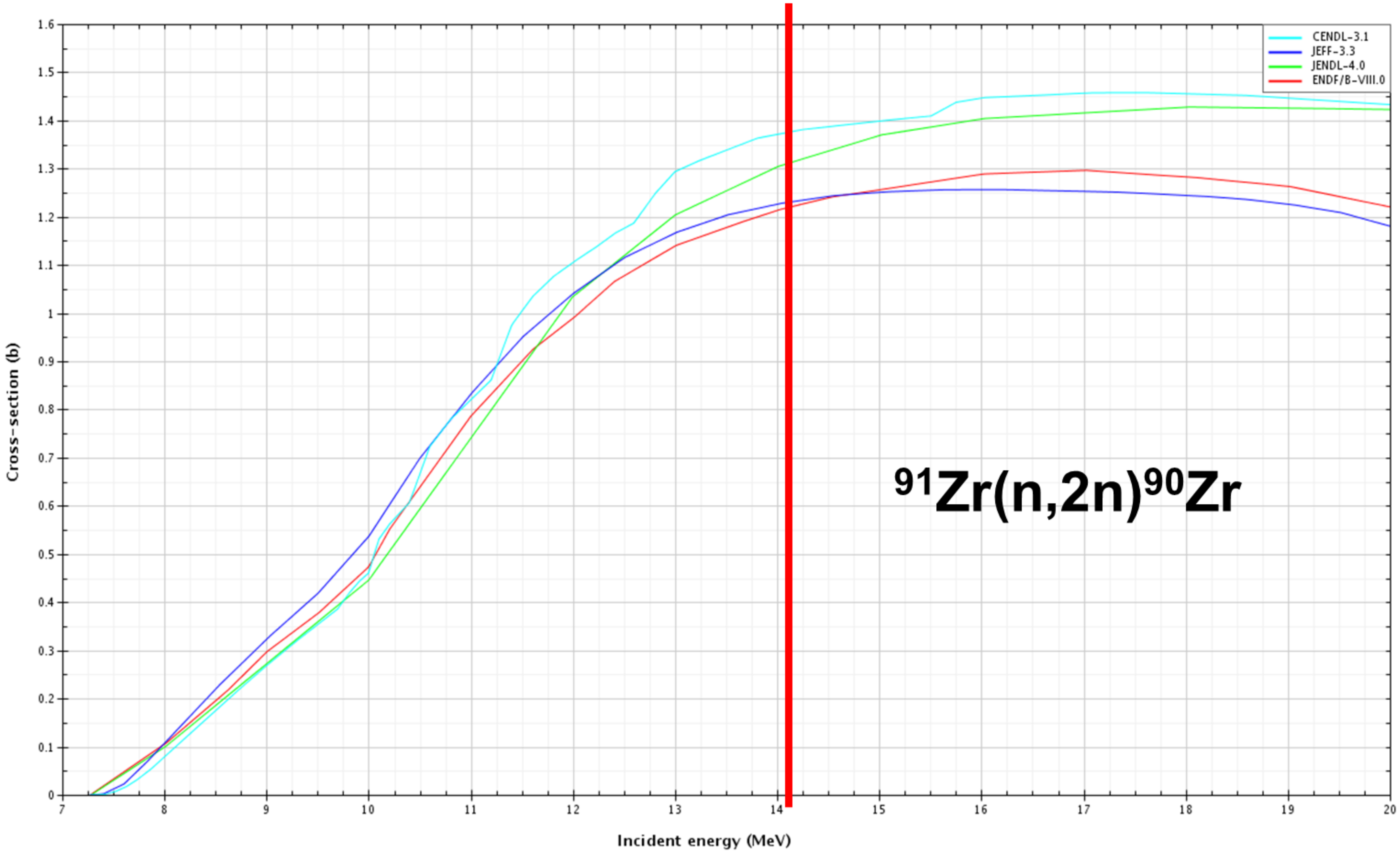
- Gradually being replaced with more human-readable *GNDS*.
  - XML-based.
  - LLNL-led international project.

Using an individual measured cross section



Overview of nuclear reaction code inputs

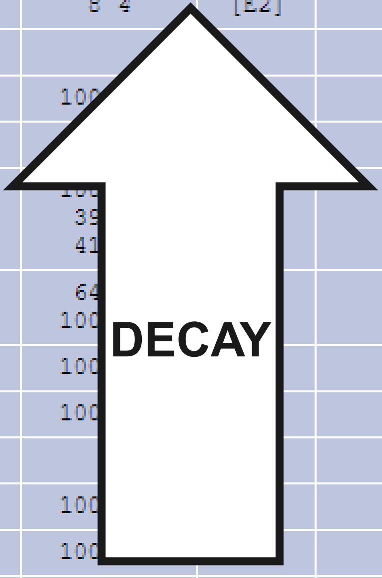
- Example codes are; TALYS, EMPIRE, YAHFC.
- Discrete level schemes.
- Level density models.
- Optical Model Potentials

Discrete levels

^{88}Y level scheme as an example
(taken from NNDC Chart of the Nuclides)

E(level) (keV)	XREF	Jπ(level)	$T_{1/2}$(level)	E(γ) (keV)	I(γ)	M(γ)	Final level	
0.0	ABCDEFGHI KLMNOPQRST	4-	106.626 d 21 % ε = 100					
231.927 25	CDEFGHI KLMNOPQRS	5-	0.8 ns 1	231.929 25	100	M1	0.0	4-
392.86 9	AB FGH LMNOPQRS	1+	0.301 ms 3 % IT = 100	392.87 9	100	E3	0.0	4-
674.55 4	CDEF H KLMNOP	8+	13.98 ms 17 % IT = 100	442.62 3	100	E3	231.927	5-
703.83 14 ?	D K M	(7)+						
706.79 13	FG L N PQRS	2-	> 10 ps	313.93 10 706.3 5	100 6 8 4	 [E2]	392.86 0.0	1+ 4-
707.4 4	N Q S	1+,2+,3+						
715.12 13	F H K M P R	(6)+		483.50 20	100		231.927	5-
766.22 16	FG LMN PQR	(0)+	2.4 ps +13-6	373.30 15	100	(M1)	392.86	1+
843.04 12	FGH KLMN P RS	(5)+	1.8 ps +9-3	128.0 1 611.0 2 842.5 3	100 5 39 3 41 4	M1 [E1] [E1]	715.12 231.927 0.0	(6)+ 5- 4-
984.66 13	FG KLMN P R	(4)+	0.82 ps 8	141.6 1 984.6 4	64 5 100 6	(M1) [E1]	843.04 0.0	(5)+ 4-
1088.21 10	FG KLMN P RS	(4,5,6)-		1088.20 10	100		0.0	4-
1128.6 6	K MN PQRS	3-,4-,5-	< 0.25 ps	896.7 6	100		231.927	5-
1215 3 ?	N							
1220.83 20	FG KLMN QR	(0,1)+	0.44 ps 4	828.3 3	100		392.86	1+
1234.0 20	L			1234 2	100		0.0	4-
1262.0 20	L S	(2,3,4)-		1262 2	100		0.0	4-
1275.09 18	FG L N QRS	(1,2)+		508.85 10 882.1 23	100 6 22 3		766.22 392.86	(0)+ 1+
1283.81 15	FGH KLM P R	(3,4,5)+	0.19 ps 2	299.1 1 1284.2 3	100 6 28 6	(M1) [E1]	984.66 0.0	(4)+ 4-
1315 4	N S	(4,5,6)-						
1320.13 10	F K MN S	-	0.24 ps 3	1088.2 1	100		231.927	5-
1461.6 3	EF H S	(6-,7-)	1.8 ps +6-4	1229.7 3	100		231.927	5-
1475 4 ?	G S	2-,3-,4-						
1476.86 13	DEF HI K MN	9+	0.11 ps 3	802.25 16	100	(M1+E2)	674.55	8+

E(level) (keV)	XREF	Jπ(level)	$T_{1/2}$(level)	E(γ) (keV)	I(γ)	M(γ)	Final level	
0.0	ABCDEFGHI KLMNOPQRST	4-	106.626 d 21 % ε = 100					
231.927 25	CDEFGHI KLMNOPQRS	5-	0.8 ns 1	231.929 25	100	M1	0.0	4-
392.86 9	AB FGH LMNOPQRS	1+	0.301 ms 3 % IT = 100	392.87 9	100	E3	0.0	4-
674.55 4	CDEF H KLMNOP	8+	13.98 ms 17 % IT = 100	442.62 3	100	E3	231.927	5-
703.83 14 ?	D K M	(7)+						
706.79 13	FG L N PQRS	2-	> 10 ps	313.93 10 706.3 5	100 6 8 4	 [E2]	392.86 0.0	1+ 4-
707.4 4	N Q S	1+,2+,3+						
715.12 13	F H K M P R	(6)+		483.50 20	100		231.927	5-
766.22 16	FG LMN PQR	(0)+	2.4 ps +13-6	373.30 15			392.86	1+
843.04 12	FGH KLMN P RS	(5)+	1.8 ps +9-3	128.0 1 611.0 2 842.5 3	100 39 41		715.12 231.927 0.0	(6)+ 5- 4-
984.66 13	FG KLMN P R	(4)+	0.82 ps 8	141.6 1 984.6 4	64 100		843.04 0.0	(5)+ 4-
1088.21 10	FG KLMN P RS	(4,5,6)-		1088.20 10	100		0.0	4-
1128.6 6	K MN PQRS	3-,4-,5-	< 0.25 ps	896.7 6	100		231.927	5-
1215 3 ?	N							
1220.83 20	FG KLMN QR	(0,1)+	0.44 ps 4	828.3 3	100		392.86	1+
1234.0 20	L			1234 2	100		0.0	4-
1262.0 20	L S	(2,3,4)-		1262 2	100		0.0	4-
1275.09 18	FG L N QRS	(1,2)+		508.85 10 882.1 23	100 6 22 3		766.22 392.86	(0)+ 1+
1283.81 15	FGH KLM P R	(3,4,5)+	0.19 ps 2	299.1 1 1284.2 3	100 6 28 6	(M1) [E1]	984.66 0.0	(4)+ 4-
1315 4	N S	(4,5,6)-						
1320.13 10	F K MN S	-	0.24 ps 3	1088.2 1	100		231.927	5-
1461.6 3	EF H S	(6-,7-)	1.8 ps +6-4	1229.7 3	100		231.927	5-
1475 4 ?	G S	2-,3-,4-						
1476.86 13	DEF HI K MN	9+	0.11 ps 3	802.25 16	100	(M1+E2)	[illegible]	

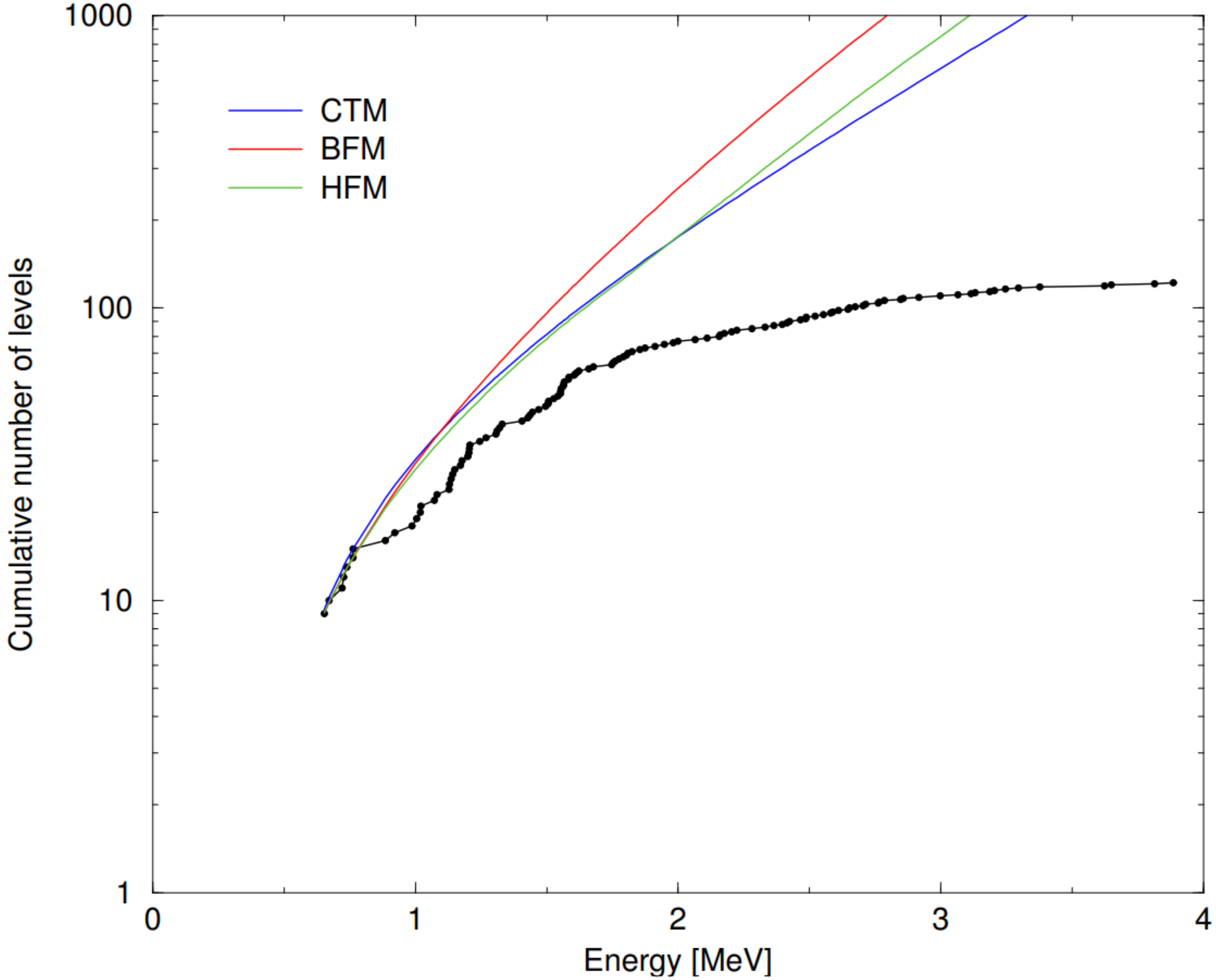


Many level assignments uncertain.

E_{thres} for $^{89}Y(n,2n)$ ~ 11.5 MeV

-> Excitations in ^{88}Y ~3MeV

Level density functions



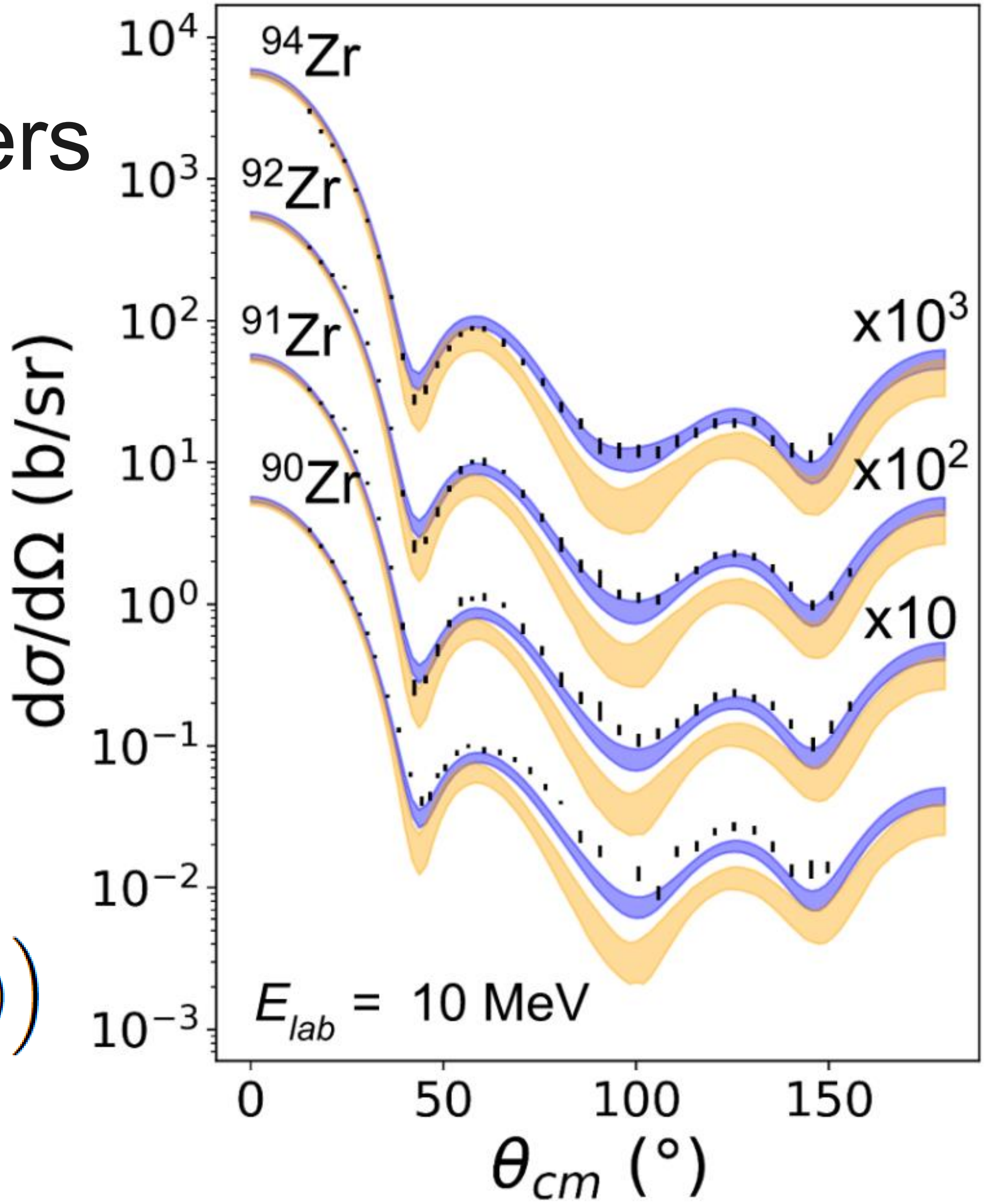
Taken from TALYS manual:
nds.iaea.org/talys

A.J. Koning, S. Hilaire, S. Goriely, "TALYS: modeling of nuclear reactions", Eur. Phys. J. A 59, 131 (2023).

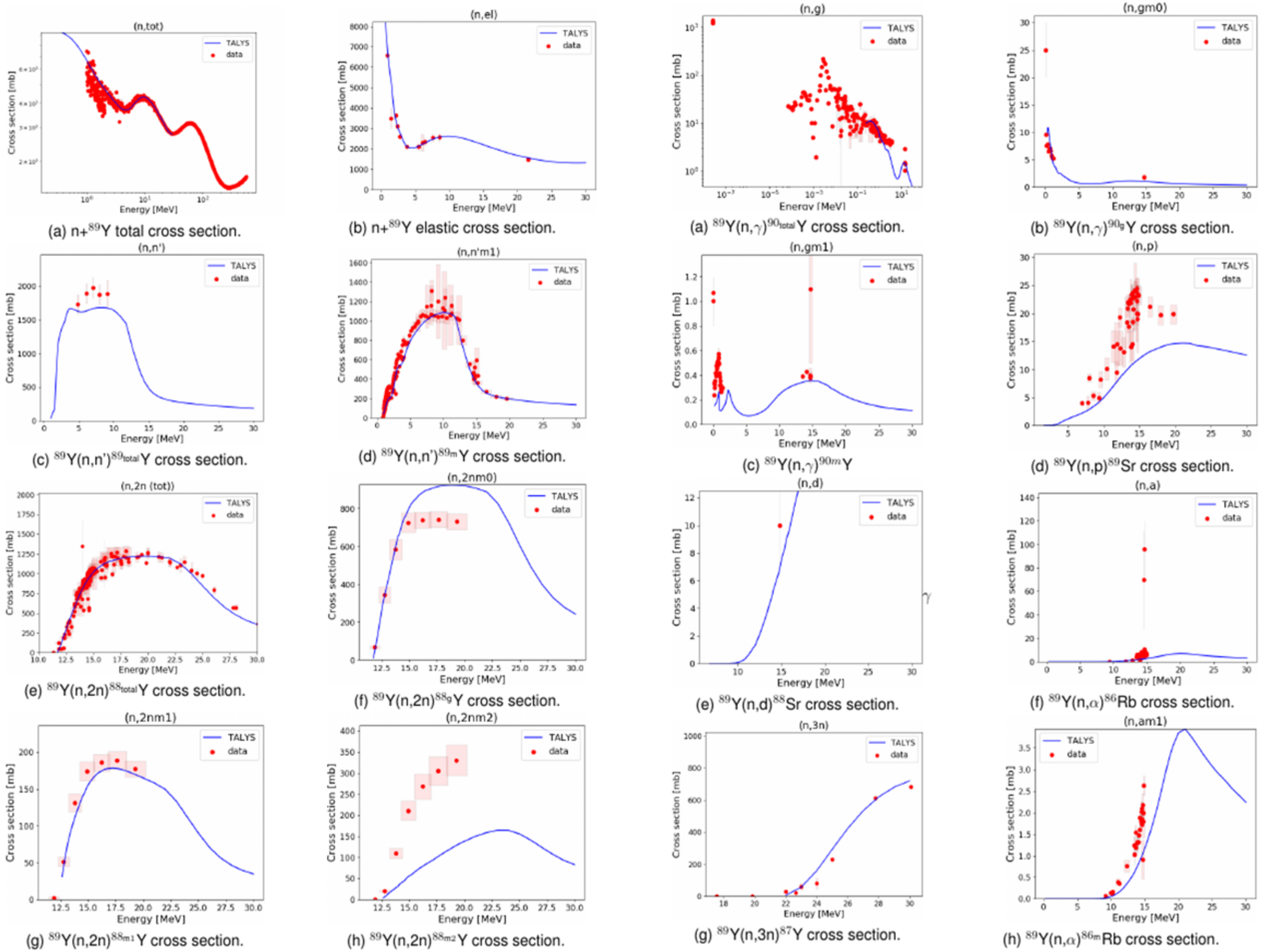
Optical Model Potential parameters

- OMP potentials determine reaction cross sections in most theoretical calculations.
- *Local*, *regional* or *global*.
- Fitted to scattering data or calculated from microscopic models.

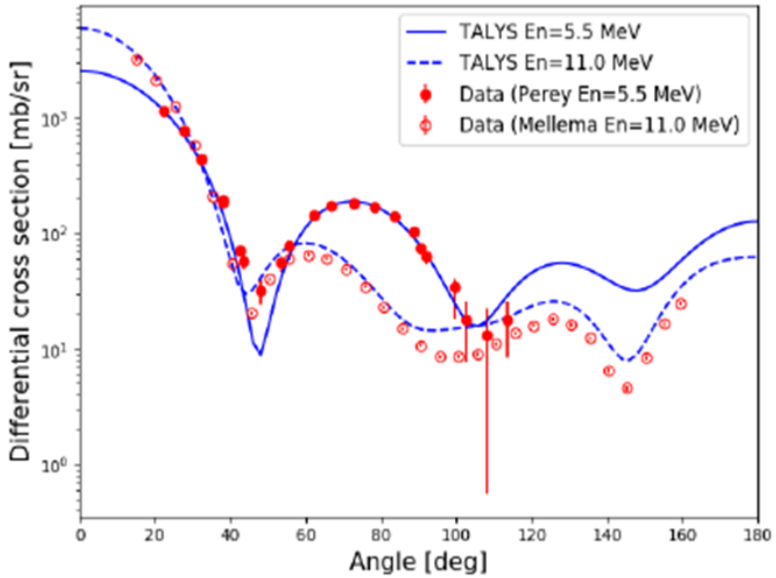
$$U(r,E) = -\mathcal{V}_r(r,E) - i\Big(\mathcal{W}_v(r,E) + \mathcal{W}_s(r,E)\Big) - \mathcal{V}_{so}(r)(\ell \cdot \sigma) + \mathcal{V}_C(r)$$



Example theory calculations



(a) n+^{89}Y total cross section.
(b) n+^{89}Y elastic cross section.
(a) ^{89}Y(n,γ)$^{90_{total}}$Y cross section.
(b) ^{89}Y(n,γ)^{90_g}Y cross section.
(c) ^{89}Y(n,n')$^{89_{total}}$Y cross section.
(d) ^{89}Y(n,n')^{89m}Y cross section.
(c) ^{89}Y(n,γ)^{90m}Y
(d) ^{89}Y(n,p)^{89}Sr cross section.
(e) ^{89}Y(n,2n)$^{88_{total}}$Y cross section.
(f) ^{89}Y(n,2n)^{88_g}Y cross section.
(e) ^{89}Y(n,d)^{88}Sr cross section.
(f) ^{89}Y(n,α)^{86}Rb cross section.
(g) ^{89}Y(n,2n)$^{88_{m1}}$Y cross section.
(h) ^{89}Y(n,2n)$^{88_{m2}}$Y cross section.
(g) ^{89}Y(n,3n)^{87}Y cross section.
(h) ^{89}Y(n,α)^{86m}Rb cross section.



Questions?