The nuclear observables of the lesser Gods

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Exploring the nuclear and technology landscapes

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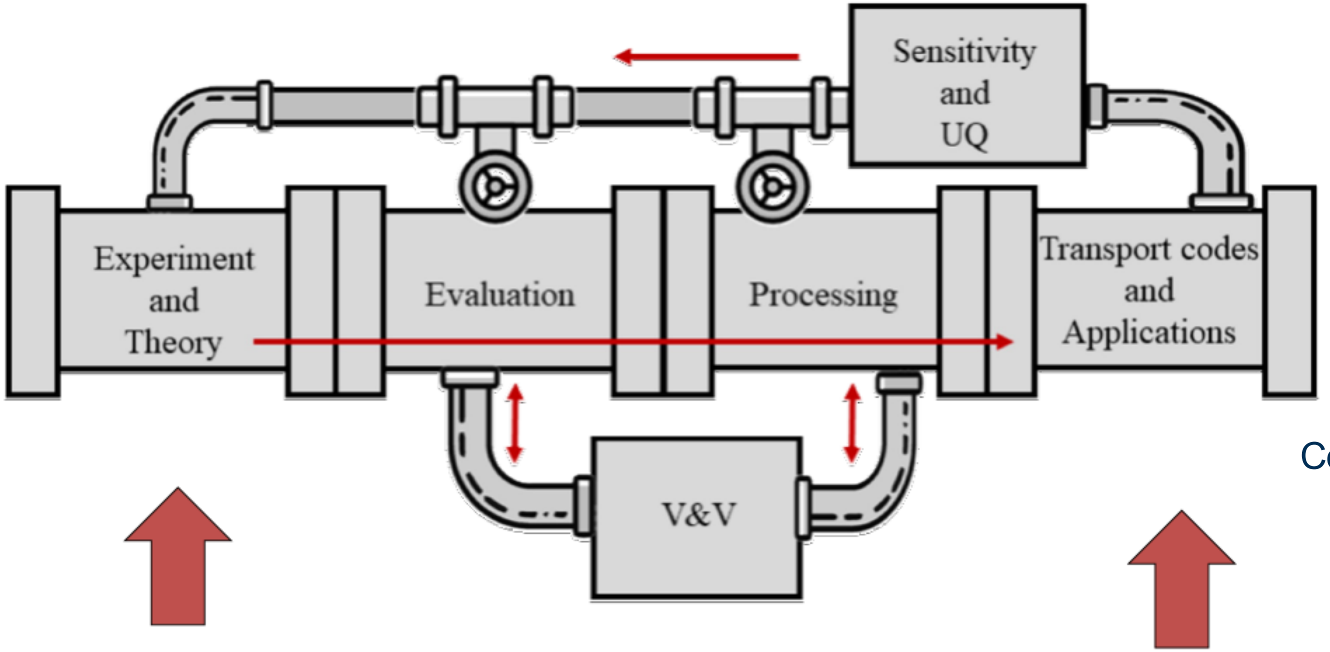
Preamble

- Nuclear data are provided in **ENDF-102 or GNDS** format
- Nuclear data processing systems are used to **convert** evaluations in the Evaluated Nuclear Data Files (ENDF) format into **forms useful for practical applications** such as fission, fusion, space, astrophysics, earth and life sciences, technology for criticality safety, radiation shielding, power, propulsion, stockpile stewardship, nuclear material damage, fuel and waste management, nuclear medicine, radioisotope production, health physics, and more…
- Each application, dedicated analysis that relies on particle transport, **material Inventory and radiation Source Term simulation**, have **specific, sometimes unique nuclear data form needs,** requirements and priority that depends on the type of results envisaged.
- **Processing codes, methods and protocols allow the required data forms to be extracted.**

Nuclear data pipeline

The nuclear data pipeline moves data from **basic science model to evaluated libraries,** application libraries and then simulation tools & results



Courtesy: D. Brown

Foundational Sciences

Applications

- build a **modern durable partnership between** fundamental sciences and applications needs

Inventory, radiation source term models

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- The **Bateman** equation is a (1910) mathematical model describing abundances and activities in a decay chain as a function of time, based on the decay rates and initial abundances.
- Inventory requires a set of stiff Ordinary Differential Equations to be solved

$$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i \phi) + \sum_{j \neq i} N_j(\lambda_{ij} + \sigma \phi)$$

  - Here λ_i and σ_i are respectively the total decay constant and cross-section for reactions on nuclide i
  - σ_{ij} is the cross-section for reactions on nuclide j producing nuclide i, and for fission it is given by the product of the fission cross-section and the fission yield fractions, as for radionuclide production yield
  - λ_{ij} is the constant for the decay of nuclide j to nuclide i

Backward Differentiation Formula; Exponential, Matrix Exponential, Newton-Krylov implicit integrators, Markovian chains, first to fifth-order Runge-Kutta, Chebyshev Rational Approximation, …

Nuclear data forms e.g., FISPACT-II

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- FISPACT-II is an **enhanced Multiphysics time inventory, radiation, source term** code system providing a wide variety of advanced, predictive, spectral and and temporal simulation methods.
- The system needs to rely on **complete nuclear data forms**: reaction and decay covering neutron, gamma and charged-particle interactions.
- The data forms encompass energy dependent **reaction cross-sections**, **productions cross-sections** for radionuclides, **multiplicity, branching, fission and radionuclides yields, decay** for all radioactive products, gas production, Kerma and dpa and biological **responses**
- The processing steps need to be able to handle both **explicit and implicit** ENDF-6 data format: **two-bodies, multi-bodies, complex, breakup and isomeric channels and all (28) decay types.**
- To account for **all projectile, target, emitted, residual possible events with time.**

Projectile **b** on target **a** -> **[compound]**$^{(*)}$ -> emitted **c** and residual **d**

a + b -> c + d + Q - a(b,c)d - $_{Z}A(b,c)_{Z}D$ - with $^{A}D > {}^{A}c$

Grid of reactions, MTs in ENDF-6 format

Explicit ENDF notation

n in ➔ Z_{res} = or decrease
α, p in ➔ Z_{res} increase

The emitted particles may differ, not the residual

The residual product could be another element, stable isomeric or radioactive

Z_{res} = activation
Z_{res} ≠ transmutation
Z_{res} = 0 disappearance, mt18 sum of 19,20,21 and 28; mt5; breakup

Z < 4 gas production
emitted particle Z < 4

Proton number Z

Ni	Z+2			(α,3n)	(α,2n)	(α,n)	
Co	Z+1			(p,n) β^-	(p, γ) (d,n)	(t,n)	
Fe	Z	(n,4n) 37	(n,3n) (γ,2n) 17	(n,2n) (γ,n) 16	(n,n') 4	(n,γ) 102	(t,p)
Mn	Z-1	(n,2nt) 154	(n,nt; 3np) 33, 42	(n,t; nd; 2np) 105, 32, 41	(n,d; np) 104, 28	(n,p); β^+ 103	
Cr	Z-2	(n,2na) 24	(n,n'a) 22	(n,a; nh; pt) 107, 34, 116	(n,h; n2p; pd) 106, 44, 115	(n,2p) 111	
V	Z-3	(n,2npa) 159	(n,da; npa) 117, 45	(n,pa) 112		(n,3p) 197	
Ti	Z-4	(n,2a) 108					
		N-3	N-2	N-1	N	N+1	N+2
		53	54	55	56	57	58

target Fe^{56}

Neutron number N

At high energy, above 30 MeV generally, the **implicit ENDF** notation is used: MF3-mt5*MF6

Grid of reactions, decays (some) & CPs

Proton number Z

0	**8**		Decay			α in				^{16}O	^{17}O	^{18}O
N	**7**		β^-	p in	d in	t in			^{14}N	^{15}N		
C	**6**		n	^{A}Z	n in			^{12}C	^{13}C			
B	**5**				β^+		^{10}B	^{11}B				
Be	**4**	α				^{8}Be $10^{-17}s$	^{9}Be		(p,n)	(d,n)	(t,n)	
Li	**3**				^{6}Li	^{7}Li			(n,2n) (γ,n)	^{A}Z (n,n’)	(n,γ) (d,p)	
He	**2**		^{3}He	^{4}He	^{5}He $10^{-22}s$				(n,t)	(n,d) (γ,p)	(n,p)	
H	**Z=1**	^{1}H	^{2}H	^{3}H 12.3y					(n,α)	(n,^{3}He)		
			^{1}n									
		0	**N=1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**

Neutron number N

Nuclear breakup

$Be^9(n,2n)Be^8$

$C^{12}(n,n')3He^4$

$Li^6(n,t)He^4$

$Li^7(n,n't)He^4$

…

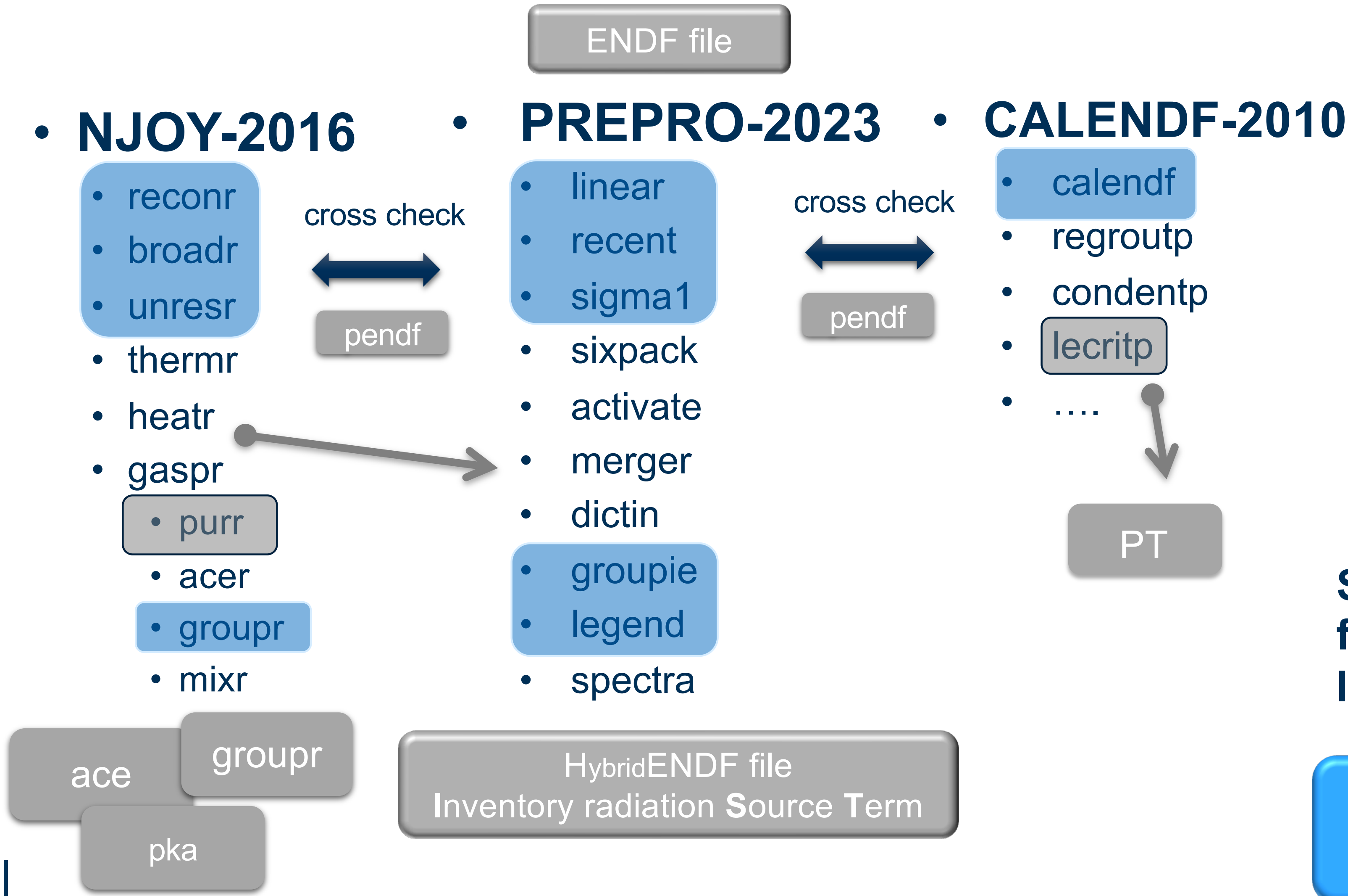
$T(d,\gamma)^5He^*$

Inelastic levels

FISPACT-II – Inventory radiation Source Terms data

Solver	Numerical - LSODES
Incident particles (5)	✓ α, γ, d, p, n
ENDF's style libraries: TENDL-2025 & GEFY, JEFF-4.0 , JENDL-5, ENDF/B-VIII.1, CENDL-3.2,… **s30** MF-1-2-3-8-10 & MF-33-40 & PTs & breakup LR *The European Activation File EAF-2010 neutron-induced cross section library	XS data Decay data nFY, sFY, otherFY **Biological hazard, clearance indices, A2**
Dpa, Kerma, Gas production, **s0** style high energy radionuclide yields	✓
PKA, primary recoils and emitted particles spectra	✓
Uncertainty Quantification and Propagation - UQP	✓ Variance-covariance
Temperatures (from reactor Kelvin to astrophysics KeV) 1 KeV ~ 12 million Kelvin	✓ 0, 294, 600, 900K,…5, 30, 80 KeV
Self-shielding with probability tables or with resonance parameters	✓ Resolved and Unresolved Resonance Range
Energy range	✓ 10^{-5} eV – 30, 200 MeV, 1GeV
Sensitivity	✓ Monte Carlo
Pathways analysis, routes of production	✓ multi steps
Thin, thick targets yields	✓

Processing trails: three interlinked codes



Single script for an entire library

Done over the week-end

Processing trails: Inventory, Source Terms

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ENDF file

- **NJOY-2016**
  - reconr
  - broadr
  - unresr
  - heatr
  - gaspr
    - groupr
    - mixr
- **PREPRO-2023**
  - linear
  - recent
  - sigma1
  - sixpack
  - activate
  - merger
  - dictin
  - groupie
- **CALENDF-2010**
  - calendf
  - condentp

pendf

Probability Table

Element

MF6 recoil matrix
Legendre order 0,1
all proton, alpha, A>4
MF3 capture

HENDF file
Inventory radiation **S**ource **T**erm

Spectra-PKA
80 grps

FISPACT-II - 1102 grps
@ Temperature
@ Dilution

MF=1
MF=2 res. parameters
MF=3 channels, kerma, dpa, gaz, radionuclide prod., alpha, eta,…
MF=8 dictionary
MF=10 partials
MF=33 channels cov.
MF=40 radionuclide cov.
Probability table: 01. eV to Eh

Processing trails: charge particles

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ENDF file

- **NJOY-2016**
  - reconr
  - acer
  - groupr

pendf

gendf

- **PREPRO-2023**
  - linear
  - sixpack
  - activate
  - dictin
  - groupie
  - legend

$-p$ $-d$ $-\alpha$
$-\gamma$

MCNP6

Spectra-PKA

IrST HENDF 162 grps

FLUKA

PHITS

FISPACT-II

GEANT4

283 stable targets
Light targets
CM LAB conversion
Multiscale simulation

Single script for an entire library

Nuclear landscape: isotopic targets range

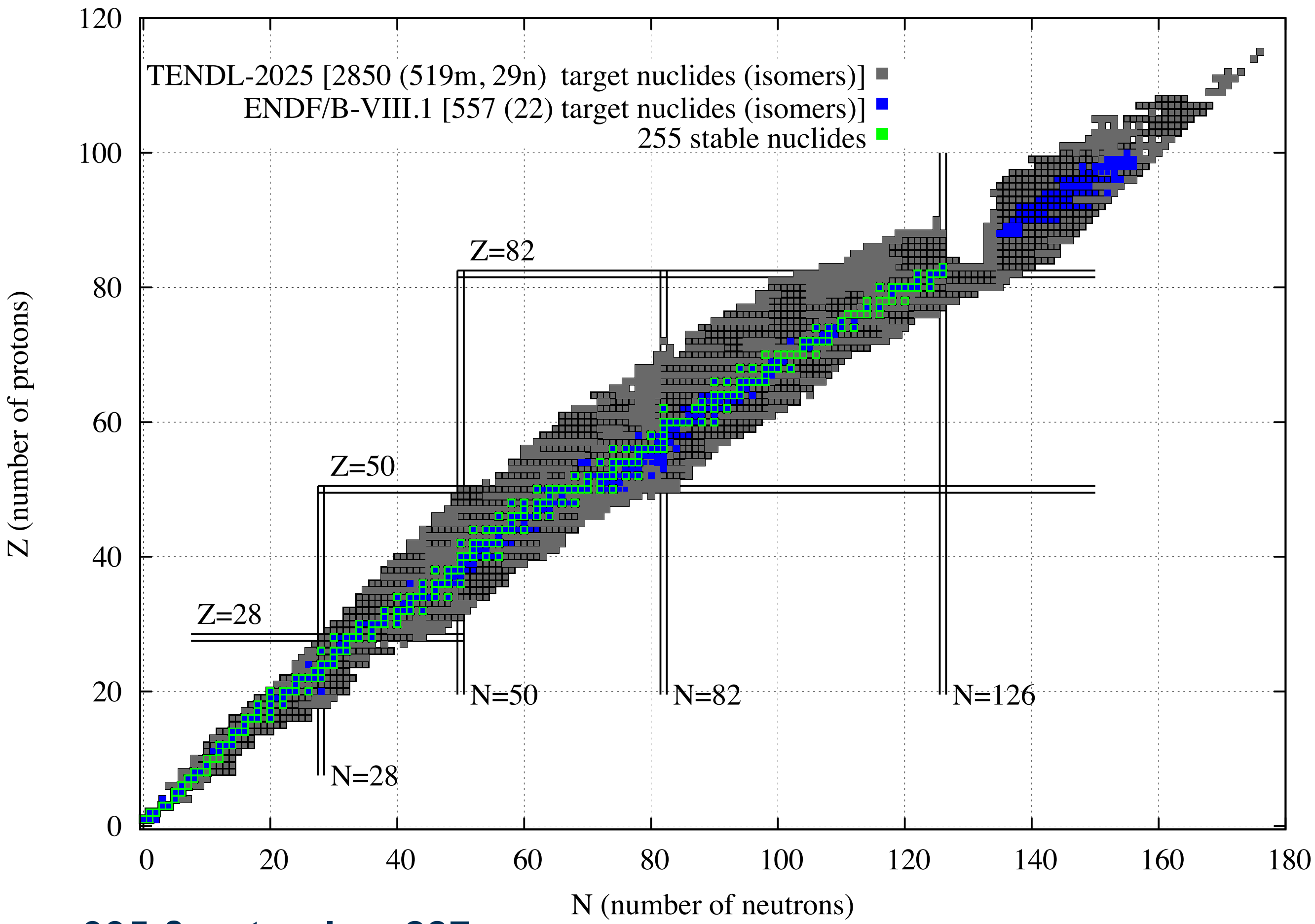
TENDL 7 incident particles ~2850 targets

- neutron*
- gamma
- proton
- deuteron
- alpha
- *helion, triton*

*complete for transport, inventory, source term, material sciences in term of MF's, targets (>1 s.) and daughters (>0.1 s.)

816 in EAF-2010
795 in JENDL-5
818 in CNAF
593 in JEFF-4

1036 in IrST for $T_{1/2}$ > 1 hr. + inclusive of all "special" from the above legacy libraries - **117m, 7n isomers**



$T_{1/2}$ > 1 hr. = 995 & naturals = 287

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Nuclear landscape: isotopic residuals & decays

Radioactive decay products: **4035** “daughters” or “residuals”

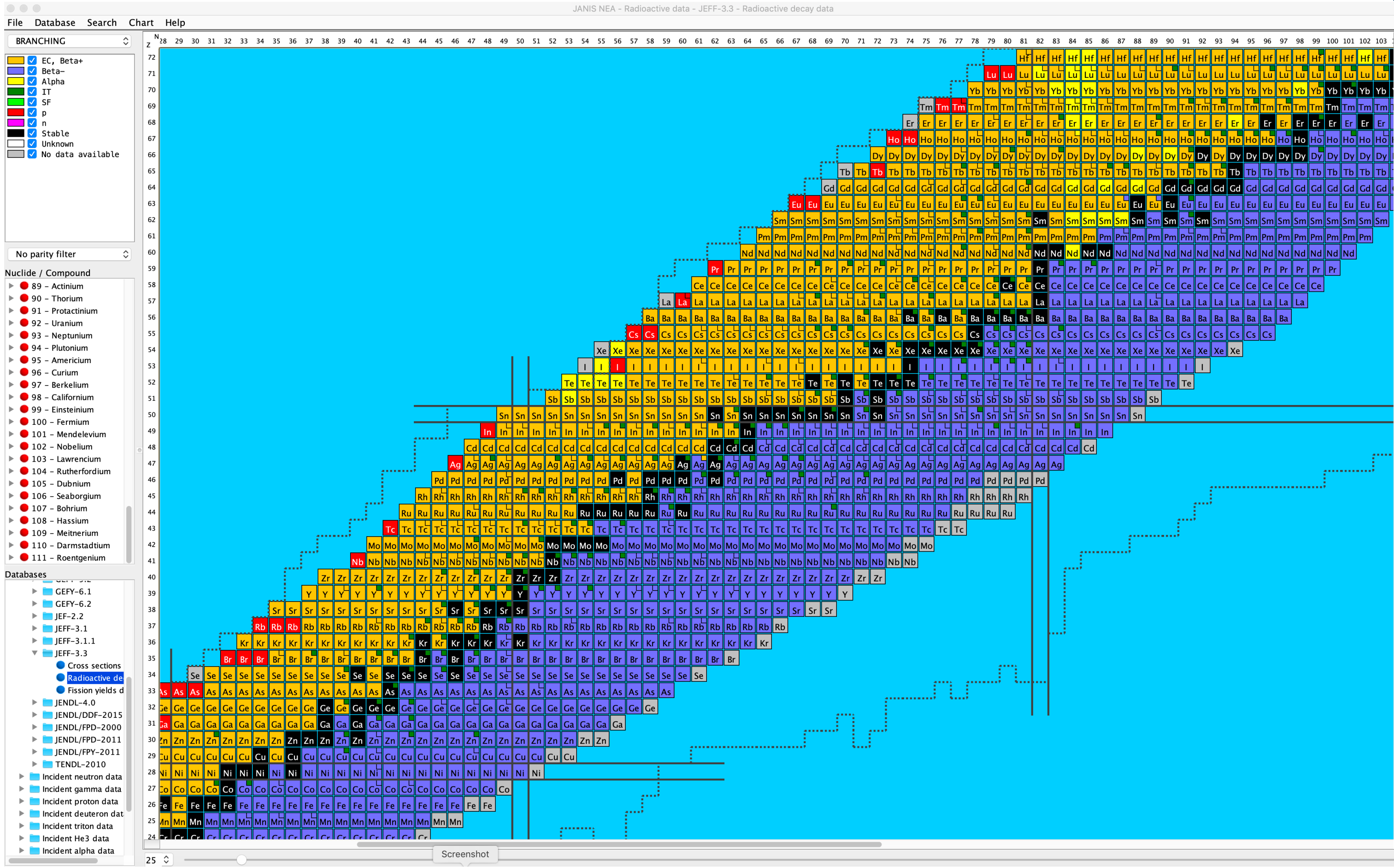
UK Decay Data series
EAF series to 2007 ✗
Decay_2012
Decay_2020

Ground and isomeric daughters. **Subtle** difference between **discrete** level, **excited and isomeric** state

Uniquely defined by the **Elevel** and **T$_{1/2}$**

MF8 contains the unique daughter metastable **Elevel** from mainly RIPL-4

ENDF # ENSDF



NJOY-2016 & CALENDF-2010 processing steps

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- 0 Kelvin run
- Single temperature pendf, 294 Kelvin to… 100 KeV
- **UNRESR**: URR processing, because…
- *PURR: URR PTs processing*
- **GASPR**: independent gas production
- **HEATR**: n only **or** n + g heating, two runs 7 + 4 responses
- MIXR: elemental reconstruction
- ACER: energy-angle outgoing, graphical checks
- GROUPR: MF3-mt5*MF6 implicit processing

PENDFs, GENDFs
Ace c, t, y, u & h, o, a
Group data MF3,10, 8, 9

- 0 Kelvin run
- Single temperature pendf, 294 to… 1200K
- **CALENDF**: RRR & URR PTs from 0.1 eV to E_h

PTs in MF50

PREPRO-2023 processing steps

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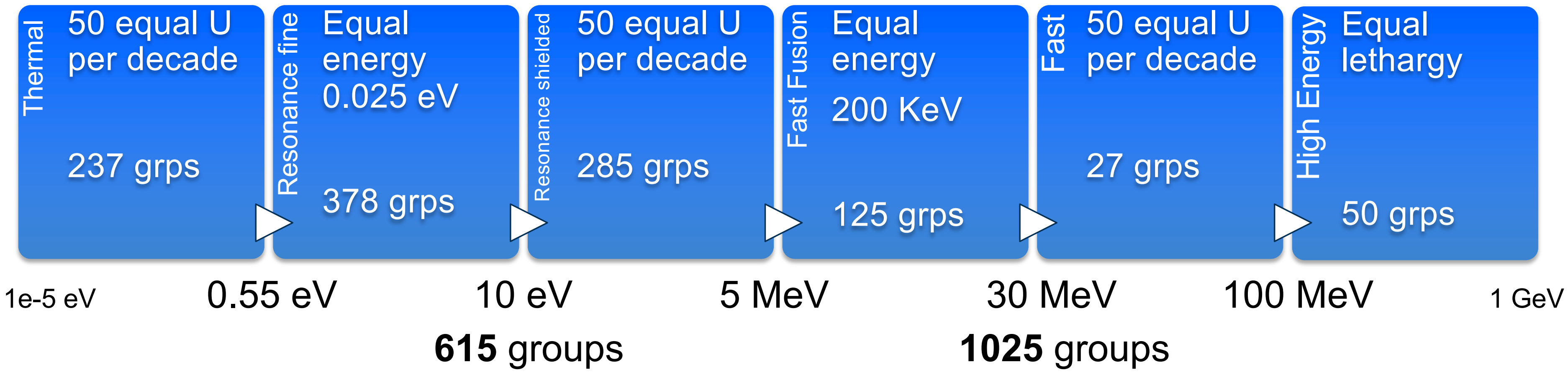
- 0 Kelvin run
- Single temperature pendf, 294 Kelvin to… 100 KeV
- ***SIXPACK***: *MF3-mt5*MF6 "implicit" processing*
- ***ACTIVATE***: *MF9 processing*
- *LEGEND: tabulated angular distribution*
- *SPECTRA: tabulated outgoing energy distribution*
- **MERGER**: merge NJOY2016 dpa, kerma, pendf responses on pendf
- *GROUPIE:*
  1102 grps @ 1 GeV
  1067 grps @ 200 MeV
  1025 grps @ 30 MeV
  615 grps @ 10 eV
  162 gprs @ 200 MeV (for charge particle)

- MF2 processed, but also **kept** in for further usage (target yield)

The resulting **hendf or pendf** or **gendf** "tape" fully comply to the ENDF-6 format frame and many utilitarian process (display, merge, concatenate, etc.) can be performed on such data forms

Group structure - 1102 groups

For all target nuclides, applications, libraries alike



- **237 fine groups** for proper 1/E < 0.55 eV
- **378 fine groups** in the resonance range < 10 eV
- Resonance shielded data available in the RRR (>0.1 eV) up to the end of the URR for all nuclides IDs
- Fast fine enough structure for **accurate threshold reaction rate**

They pave the way - Harry Bateman mathematician FRS

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EAF series:
1, 2, 3, 4 ✗ -99,
2001, 2003,
2005, 2007,
2010 ✗

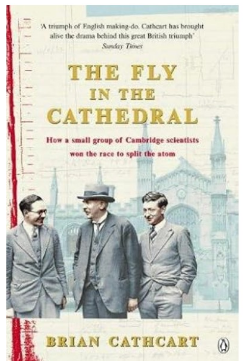
TENDL series:
2008, 2009,
2010, 2011,
2012, 2014,
2015, 2017,
2019, 2021,
2023, **2025…**

GEFY series:
4.2, 5.2, 5.3, 6.1,
6.2, 7.1, 7.2, 8.1,
9.1, **10.1…**

Robin Forrest
Marshall Blann
Dimitri Rochman
Jose Manuel Perlado
Dave Endacott
Neill Jarvis
Arjan Koning
Carlo Ponti
Ian Gauld
Fred Mann
Rodney Martineau Burstall
William Bradley Wilson
Harm Gruppelaar
Jura Kopecky
Javier Sanz

The model codes:

ALICE
STAPRE
SAFEPAQ
GEF
TALYS
…



The 1920s

Jarvis O. N., "Description of the Transmutation and Activation Data Library UKCTR-III-A", **(1980), AERE-R9601**

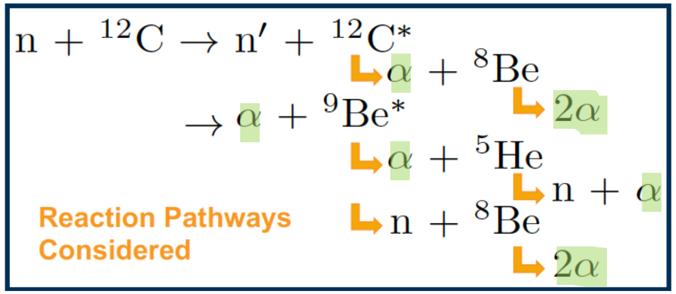
Reactions – ENDF rules – n entrance

Reaction	MT	LR
^{6}Li(n,n$_1$) ^{6}Li $\rightarrow$ d+α	51	32
^{7}Li(n,n$_c$) ^{7}Li $\rightarrow$ t+α	91	33
^{10}B(n,n$_{12}$) ^{10}B $\rightarrow$ d+2α	62	35
^{12}C(n,n$_2$) ^{12}C $\rightarrow$ 3α	52	23
^{16}O(n,n$_1$) ^{16}O $\rightarrow$ e$^+$+e$^-$+^{16}O	51	40
^{16}O(n,n$_6$) ^{16}O $\rightarrow$ α+^{12}C	56	22

neutron production MTs to **ground, exited states or continuum** with **further breakup**

- Particle transport code generally handles **prompt** outgoing n, γ, e,.. < 10^{-16} s
- Materials sciences tends to follows **elemental residual and emitted** Z<4 production
- Inventory code need to be able to follows all **possible combinations**: parent, daughter, emitted, through **nuclear chain reactions, breakup and decays**
- Time matters **10^{-6}s to millennia, isomeric states (# excited levels)**

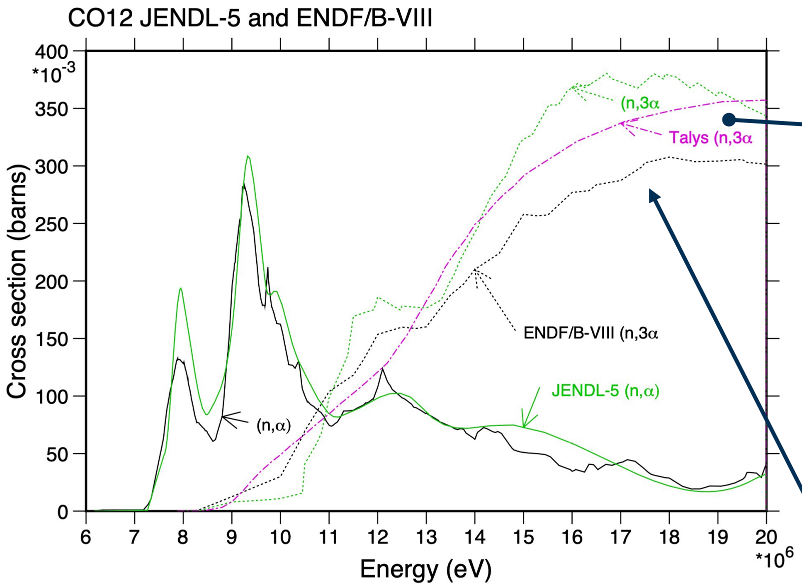
Processing steps, breakup, LR flags

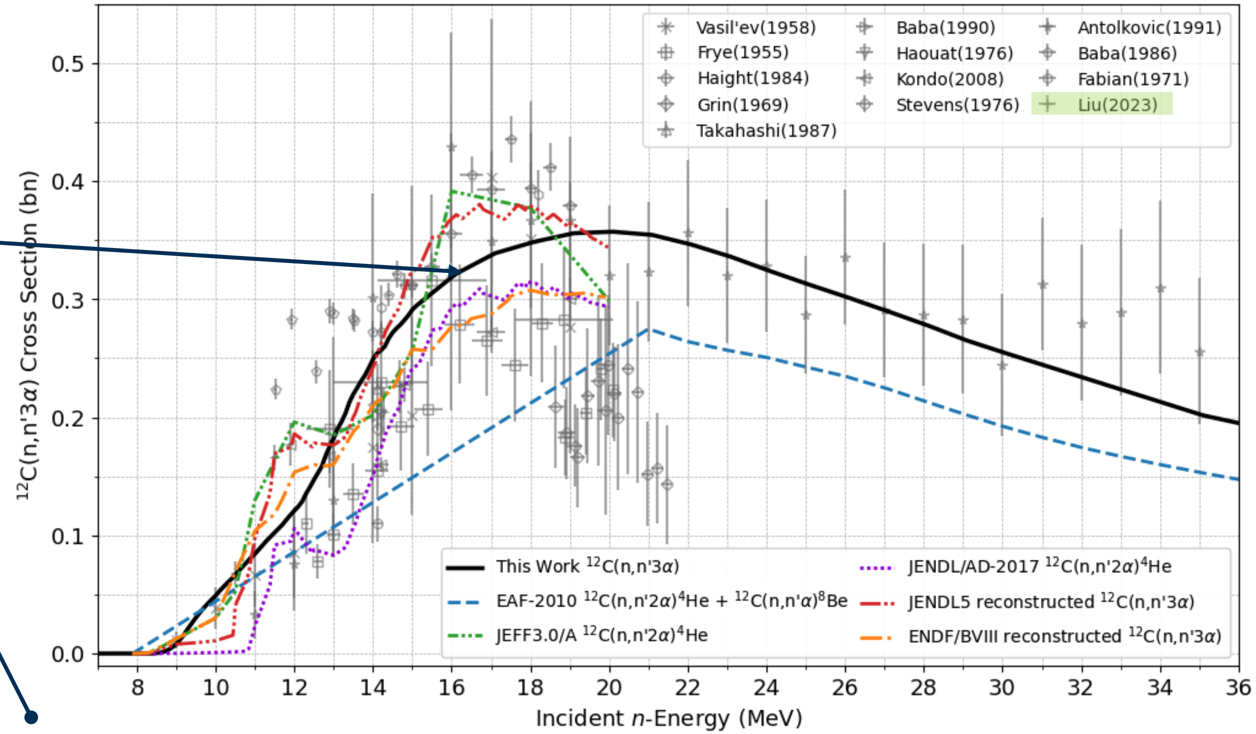


$^{12}C(0_2^+)(n_2,n_{0,1})$
Hoyle state
$^{12}C\ (n,n_2)3\alpha$

EXFOR recorder quantity ??
EXFOR $^{12}C(n,2a+n)^4He$ and $^{12}C(n,X)^4He$??
Compiled as MT=29, n2α !!! one α residual ??
EXFOR data, not particularly reliable !!!

^{12}C full breakup: (n,3α





Inelastic channels LR=23 flag ➔ **derived form MT=23,** constructed during processing
Energy range well above **R-matrix** code capability so HF **TALYS**, no discrete level on ^{12}C, ^9Be and ^8Be

LR's flag processing steps

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JENDL-5, JEFF-4.0 and **ENDF/B-VIII.1** "additional" channels

Targets	JENDL-5	JEFF-4.0	ENDF/B-VIII.1
Li006	32=+(51, 56)+(58, 86)	32=+(51, 56)+(58, 86)	
Li007	33=+(52, 84)	33=+(52, 82)	33=+(52, 82)
Be009		30=+(875,885)	
B010	35=+(61, 89)	*	*
C012	23=+(52, 91)		23=+(52, 91)
O016	22=(22, 22)+(55, 79)		

JEFF-4.0 C012 MT=23 explicit, from TALYS
JEFF-4.0 Be009 MT=30 from partials (n,2n$_x$)

Complex sums, sometimes only clearly described in MF1-mt451

*	
20=+(55, 56)+(58, 61)+(63, 63)+(66, 67)+(69, 69)	temp.
21=+(72, 72)+(75, 75)+(82, 82)+(85, 85).	temp.
22=+(20, 21)	α emitted
28=+(65, 65)+(78, 78)	p emitted
33=+(62, 62)+(68, 68)+(71, 71)+(73, 74)+(76, 77)	t emitted
34=+(79, 81)+(83, 84)	^{3}He emitted
35=+(33, 34)	d2α emitted

LRs flags impact & subtility

- Usually transport codes do not **transport, track** all breakup secondaries.
- NJOY-gaspr keeps track of the **total** production of light particles $^{1,2,3}H$ & $^{2,4}He$ as residual $^{1}H(n,2n)^{2}H$, $^{9}Be(n,2n)2\alpha$ and emitted **but** as single responses: MT203 to 207, **no residual tracking possible**
- Traditionally inventory codes only processes the inelastic partials when **super-elastic**: the residual is an isomer ($T_{1/2}$ > 10^{-3}s ≠ discreet state, level).
- **Reduced chains inventory** simulations only accept simple MTs with residual: (n,2a)^{4}He instead of breakup (n,3a , e.g. SERPENT CRAM solver.
- Breakup usually means **burnup**, **target disappearance event,** like handling fission target inventory in a way
- In cases, the yield per reaction for the light product, breakup residual may be tabulated directly (and even fractional) when a MF6 is used.

Conclusions

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- **Reactions: MF3** cross-section, **MF10** partials, **MF9** branching ratio, **MF8** dictionary for mt5*MF6 radionuclide production, **MF12** photon production
- **Decays & Fission product yields**: **MF8** subtility**,** correspondence between excited and isomeric state
- **Covariances: MF33-40 (-34,35?)**
- Rather complex, unique to a target, **processing steps are necessary** to account for the **LR** flags in **I**nventory, radiation **S**ource **T**erm simulations.
- Without such **additional steps** inventory systems **cannot account for breakup**, burn, deplete properly, have the target disappear when it should.
- In the major libraries it impacts **^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{12}C** and **^{16}O** inventory under n-irradiation.
- **JENDL-5, ENDF/B-VIII.1** and **JEFF-4.0** Multiphysics **I**nventory, radiation **S**ource **T**erms **IrST** application libraries for **FISPACT-II** now includes these additional steps.

The Nuclear Observables of the Lesser Gods

a playful mythological analogy for inventory, radiation source terms observables

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In the grand pantheon of nuclear physics, all observables live on mount **NucleOlympus**, but not all enjoy the same fame.

⚡ The "Major Gods" at the summit sit the well-known, **mighty deities**:

- *Elastic scattering*, **Zeus** himself - ruler of reaction channels, consulted by all.
- *Prompt gammas*, **Apollo** - bright, immediate, shining with clarity.
- *Fission observables*, **Poseidon** - powerful, dramatic, sometimes destructive.
- *Neutron multiplicities and spectra*, **Hera -** ever-watchful, essential to the harmony of the realm.

These are the observables that everyone quotes, measures, models, argues about, and builds facilities for. **They get the temples, the offerings, the citations**.

The Nuclear Observables of the Lesser Gods

a playful mythological analogy for inventory, radiation source terms observables

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And then, a little further down mount **NucleOlympus**, dwell the humble radiation observables. **Not weak — just quietly powerful**.

🔥 The “Lesser Gods” :

- *Activities and radiations*, the tireless **Hephaestus**, hammering away in the workshop long after the beam is off.
- *Decay gammas*, the **Hestia** of the family — steady, constant, the warm glow at the hearth.
- *Cumulative and independent yields*, the **Fates**, weaving the threads of fissions events.
- *Isomeric ratios*, the mysterious **Hermes**, messenger between ground states and metastable realms.
- *Integral reaction rates*, the **Demeter** of the group — nourishing the fields of dosimetry, radionuclides production and diagnostics.

They don’t draw lightning or split mountains, **but when the great Gods are silent or unreachable, it is the lesser Gods who speak.**

Playwright: G. Schnabel & Co

Complementary slides

Software - https://github.com/fispact/PATHFINDER

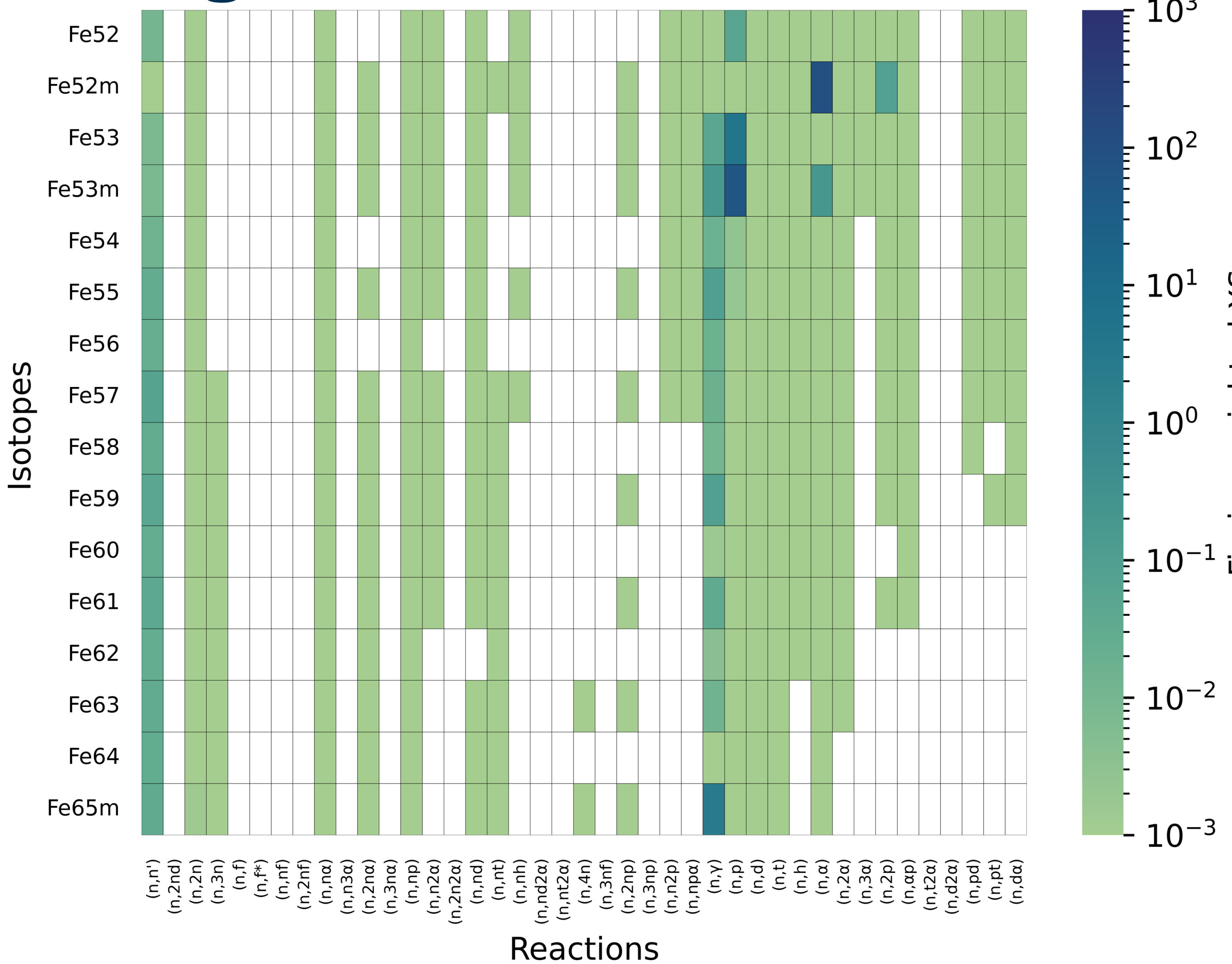
PATHFINDER

Paper reference -> P. Kanth, M.R. Gilbert, D. Foster, PATHFINDER: A tool for calculating pathways for fusion-activated materials, in: 31st International Conference Nuclear Energy for New Europe, 2022.

Fission weighted XS – TENDL-2025

Fe isotopes
$T_{1/2}$ > 1. s

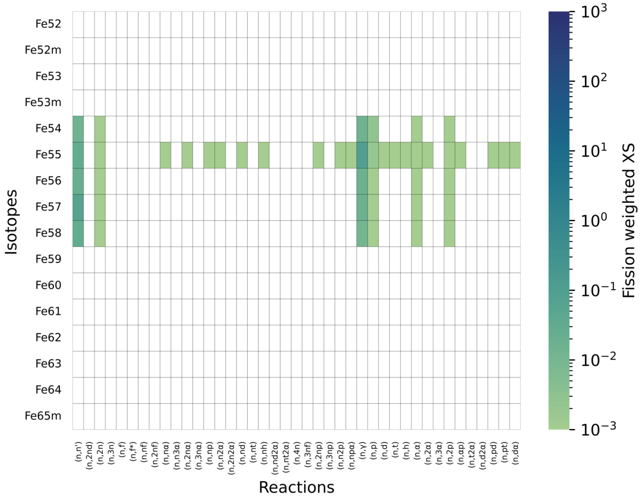
white box
=
no xs data



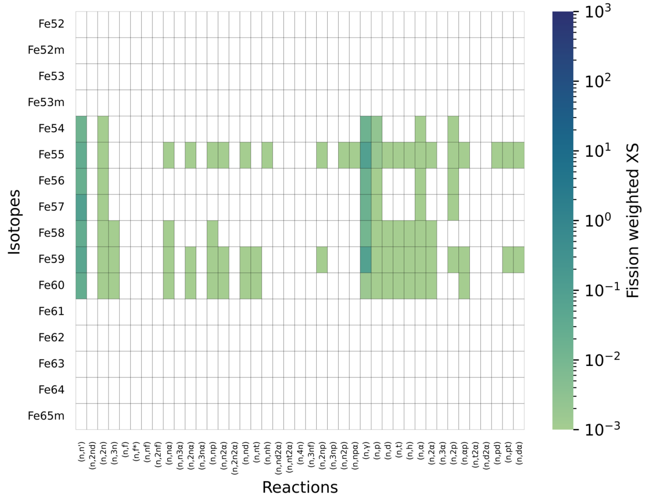
Courtesy: P. Kanth

Fission weighted XS

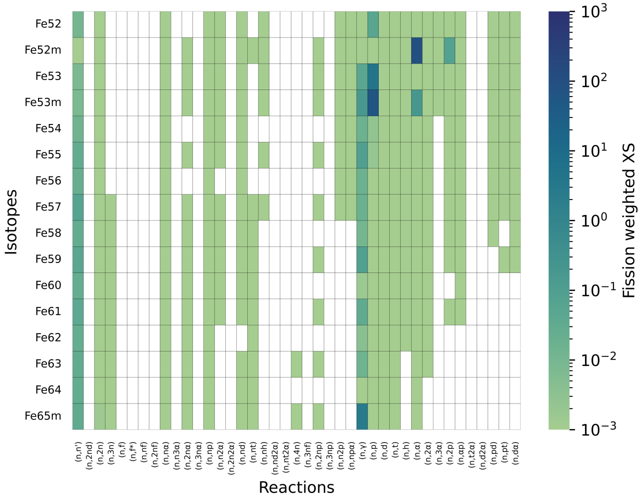
ENDB/B-VIII.1



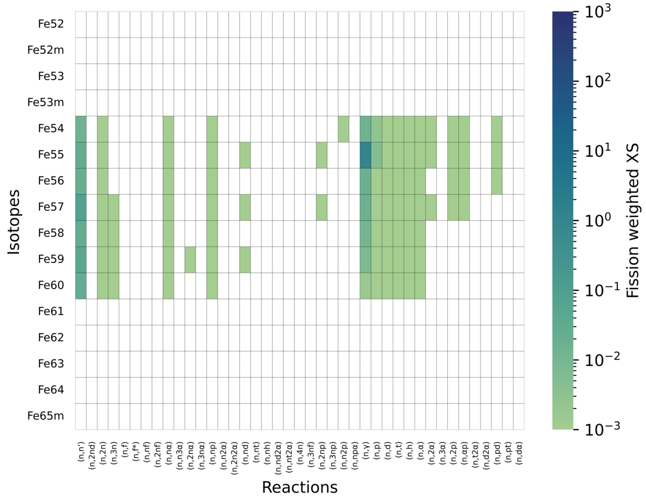
JEFF-4.0



TENDL-2025



JENDL-5



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