Consultant Meeting on the on Compilation of Nuclear Data Experiments for Radiation Characterization (CoNDERC)

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International Atomic Energy Agency

Nuclear Data Section

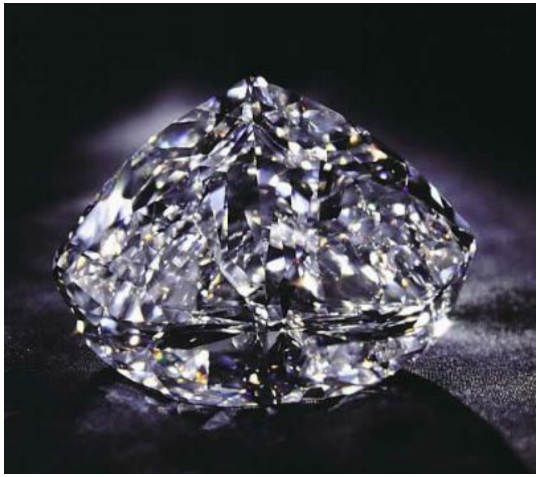
Objectives

- The purpose of the project on Compilation of Nuclear Data Experiments for Radiation Characterization (CoNDERC) is to transfer into technology the experimental integral radiation information that can be used as part of the Validation and Verification processes of nuclear model and code systems, and to provide various schema to perform the V&V
- The IAEA will task, organize institutions to construct several of these databases based on their own extensive V&V activities associated with inventory and source term codes.

Key elements

- Identify and compile a comprehensive set of experimental integral radiation characterization benchmark information: spectral indices, reaction rates, decay heat, resonance integral, particle counts and fluxes, etc…
- Evaluate the data, quantify, compute rank their overall uncertainties then compile the data into computer format for dissemination
- Perform simulations of each experiment with the suitable code system and selected nuclear libraries and produce a database/repository of the necessary input files to repeat those simulations for other nuclear data libraries.

Data mining: from raw to shaped diamond



Blue Zoe

Nuclear Atomic Molecular Material Sciences NAMMS

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

IAEA

Verification & Validation exercises in support of radiation characterisation

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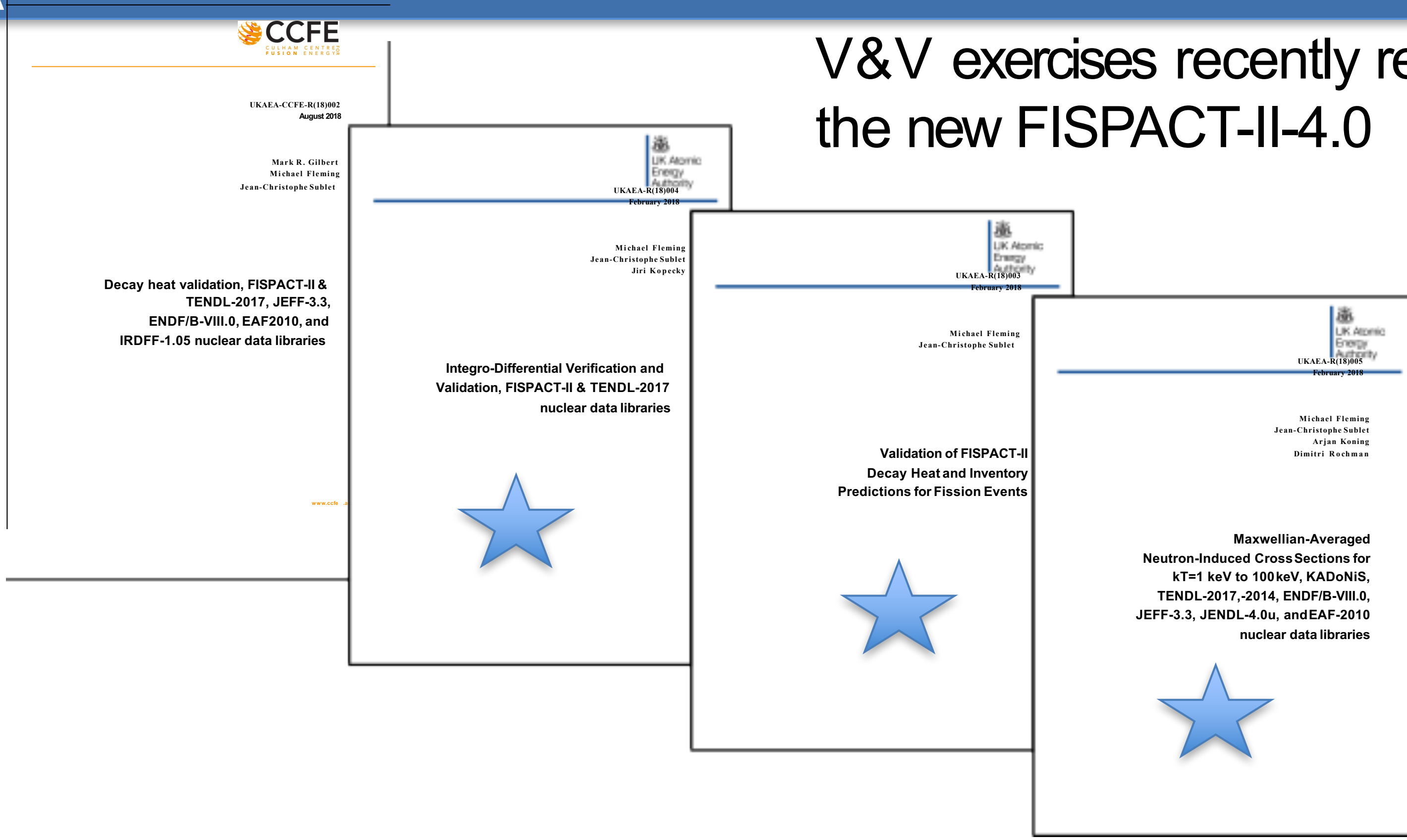
***UKAEA-OECD/NEA**

International Atomic Energy Agency

Nuclear Data Section

Validation with FISPACT-II & Libraries



V&V exercises recently repeated for the new FISPACT-II-4.0

Benchmarking ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0 and TENDL-2017 (and others)

Decay heat validation against (Japan-FNS) fusion experiments

Integral & differential xs validation against EXFOR

Fission events

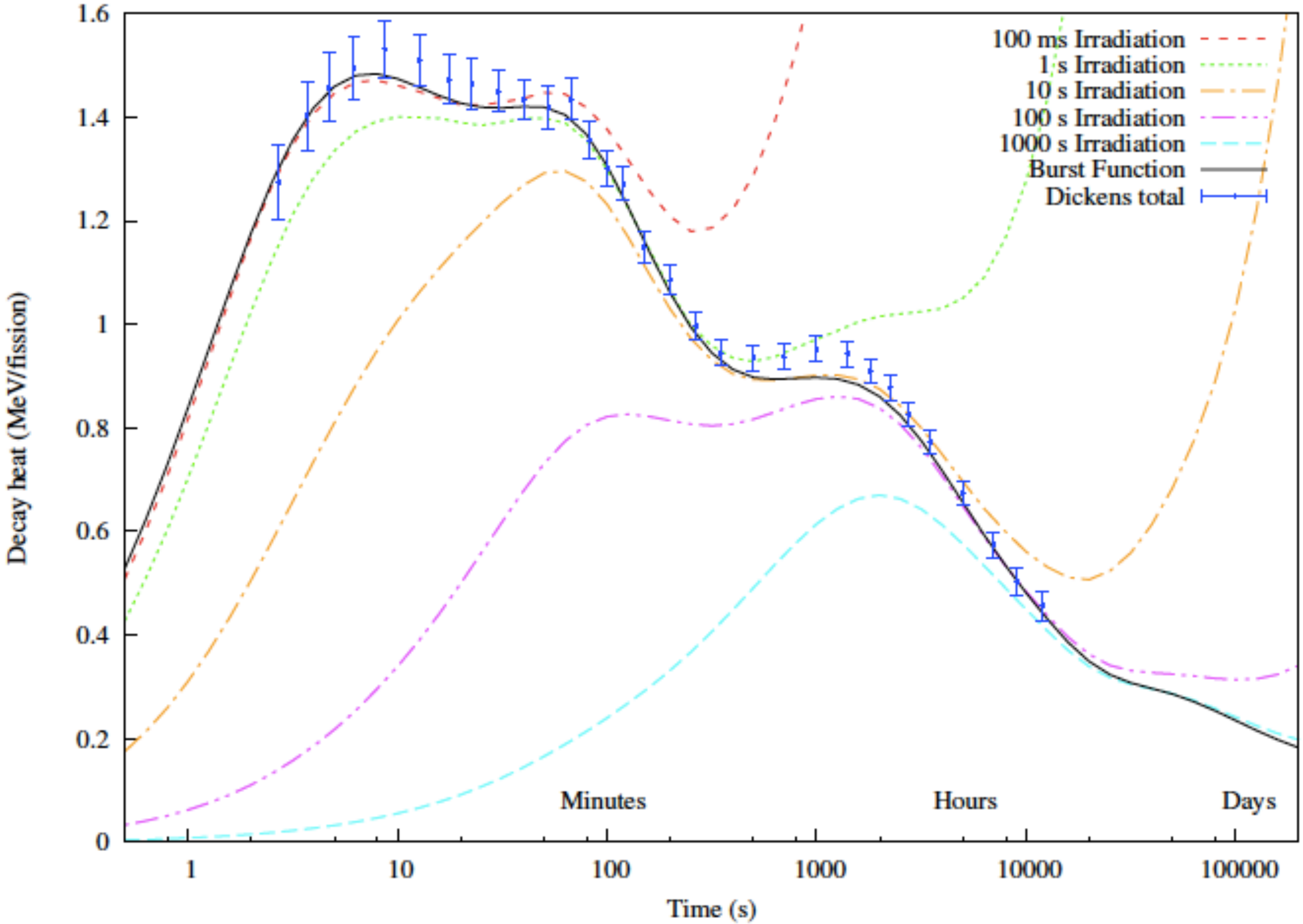
Astrophysics MACS (KADoNiS)

Fission events

Author, Institute	Nuclide(s)	Method	Irrad. (s)	Year
Fisher, LANL	$^{232}Th_f$, $^{233}U_f$, $^{235}U_f$, $^{238}U_f$, $^{239}Pu_f$	γ	< 1	1964
McNair, UKAWRE	$^{235}U_{th}$, $^{239}Pu_{th}$	β	10-1E5	1969
MacMahon, SRRC	$^{235}U_{th}$	β	10-1E4	1970
Scobie, SRRC	$^{235}U_{th}$	β	1E4-1E5	1971
Lott, CEA	$^{235}U_{th}$	Total	1E2-5E3	1973
Yarnell, LANL	$^{233}U_{th}$, $^{235}U_{th}$, $^{239}Pu_{th}$	Total	2E4	1978
Jurney, LANL	$^{233}U_{th}$, $^{235}U_{th}$, $^{239}Pu_{th}$	γ	2E4	1979
Murphy, UKAEA	$^{235}U_f$, $^{239}Pu_f$	β	1E5	1979
Dickens, ORNL	$^{235}U_{th}$, $^{239}Pu_{th}$, $^{241}Pu_{th}$	γ & β	1-100	1980
Baumung, Karlsruhe	$^{235}U_{th}$	Total	200	1981
Akiyama, JAEA	$^{233}U_f$, $^{235}U_f$, $^{238}U_f$, $^{239}Pu_f$	γ & β	10-300	1982
Akiyama, JAEA	$^{232}Th_f$, $^{nat}U_f$	γ	10-300	1983
Johansson, Uppsala	$^{235}U_{th}$	γ & β	4-120	1987
Tobias Berkeley NL	$^{235}U_{th}$, $^{239}Pu_{th}$	Stat.	-	1989
Schier, UM Lowell	$^{235}U_{th}$, $^{238}Pu_f$, $^{239}Pu_{th}$	γ & β	<1	1997
Ohkawachi, JAEA	$^{235}U_f$, $^{237}Np_f$	γ & β	10-300	2002

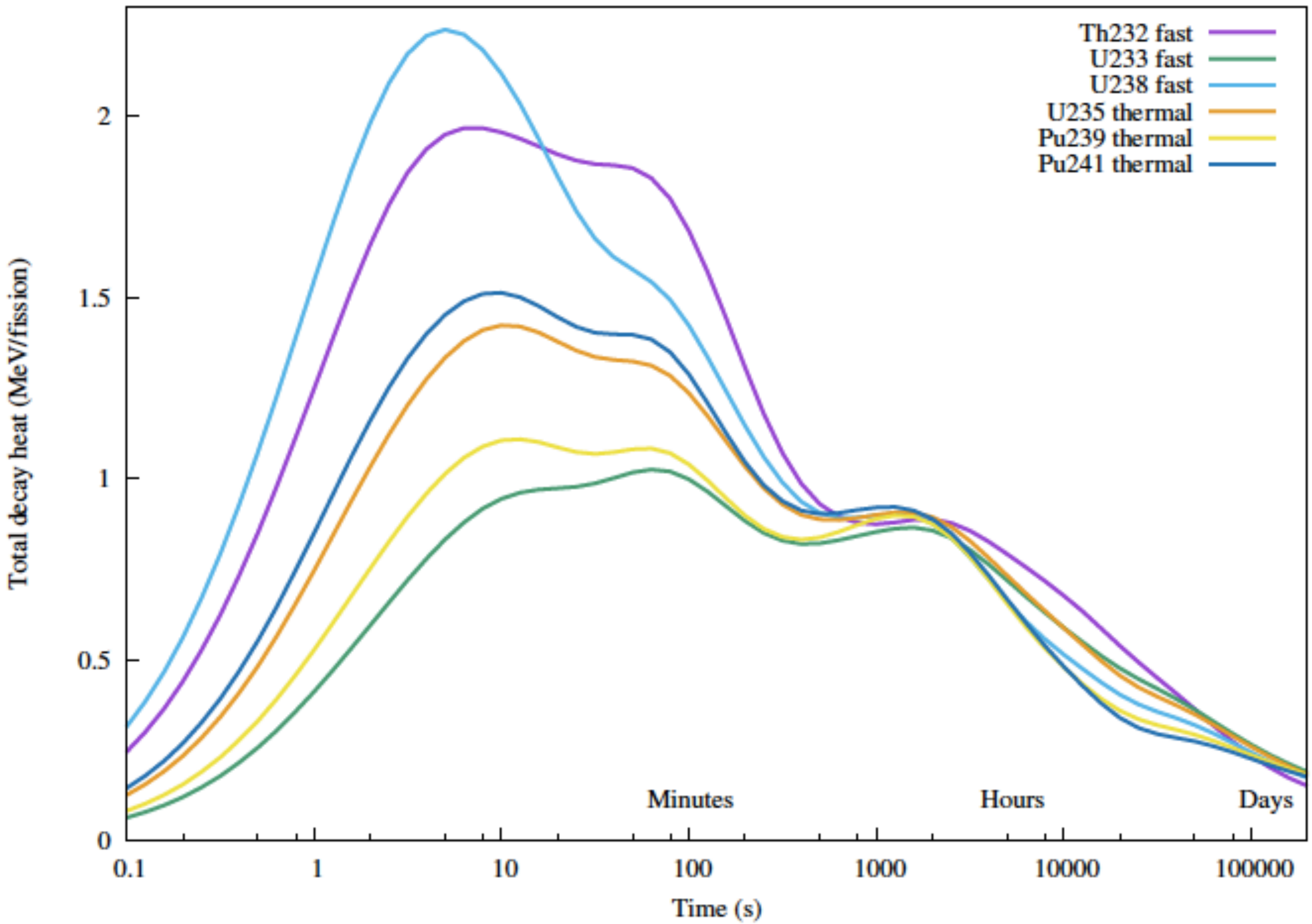
^{241}Pu irradiations against the burst function and Dickens results

The burst function calculated using a 1E^{21} flux over 1 ns and the experimental results from Dickens are included for comparison, capture decay excluded, chain not



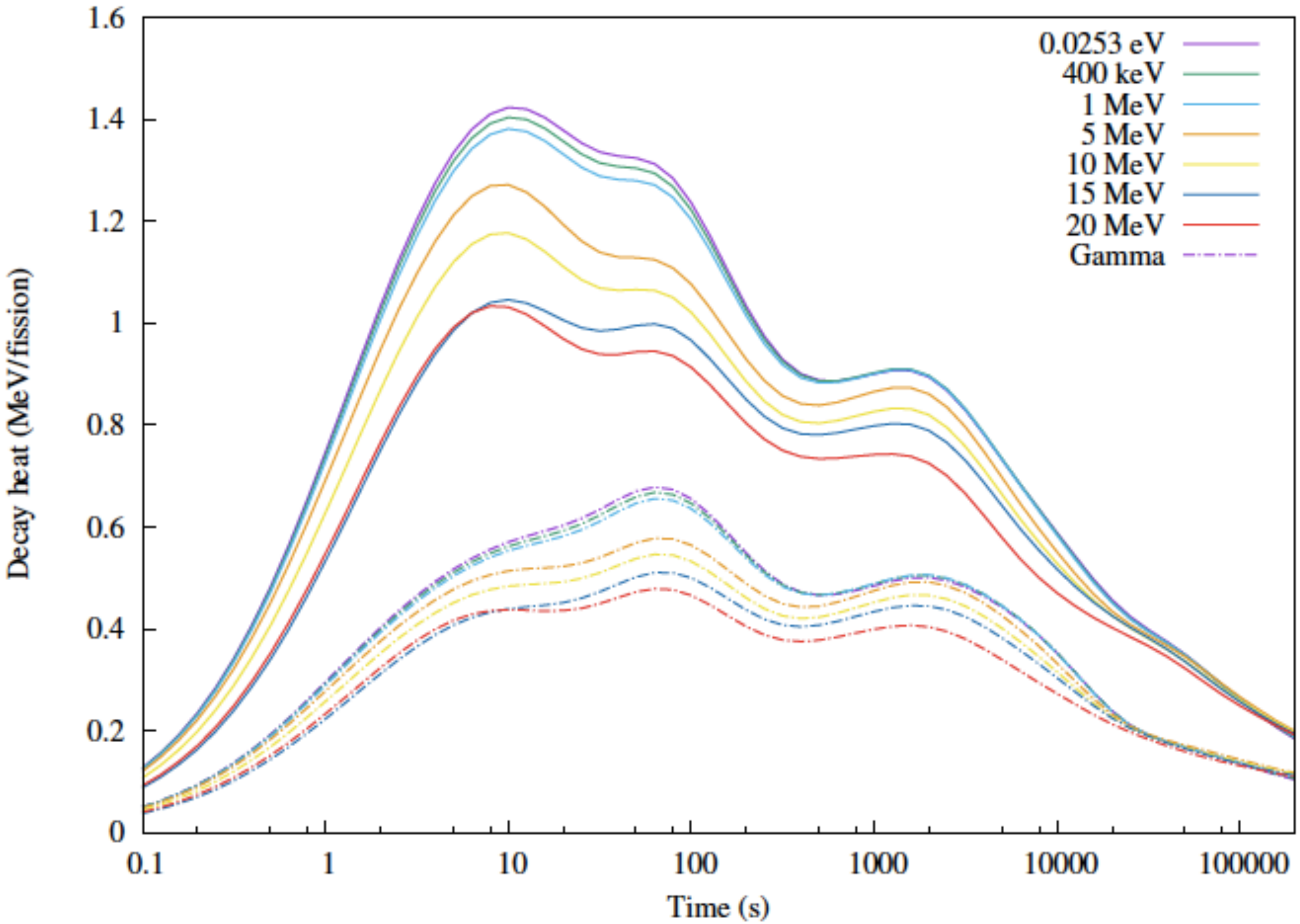
GEF-6.1 nFY with ENDF/B-VII.1 decay data

- Various fissiles, fast and thermal burst



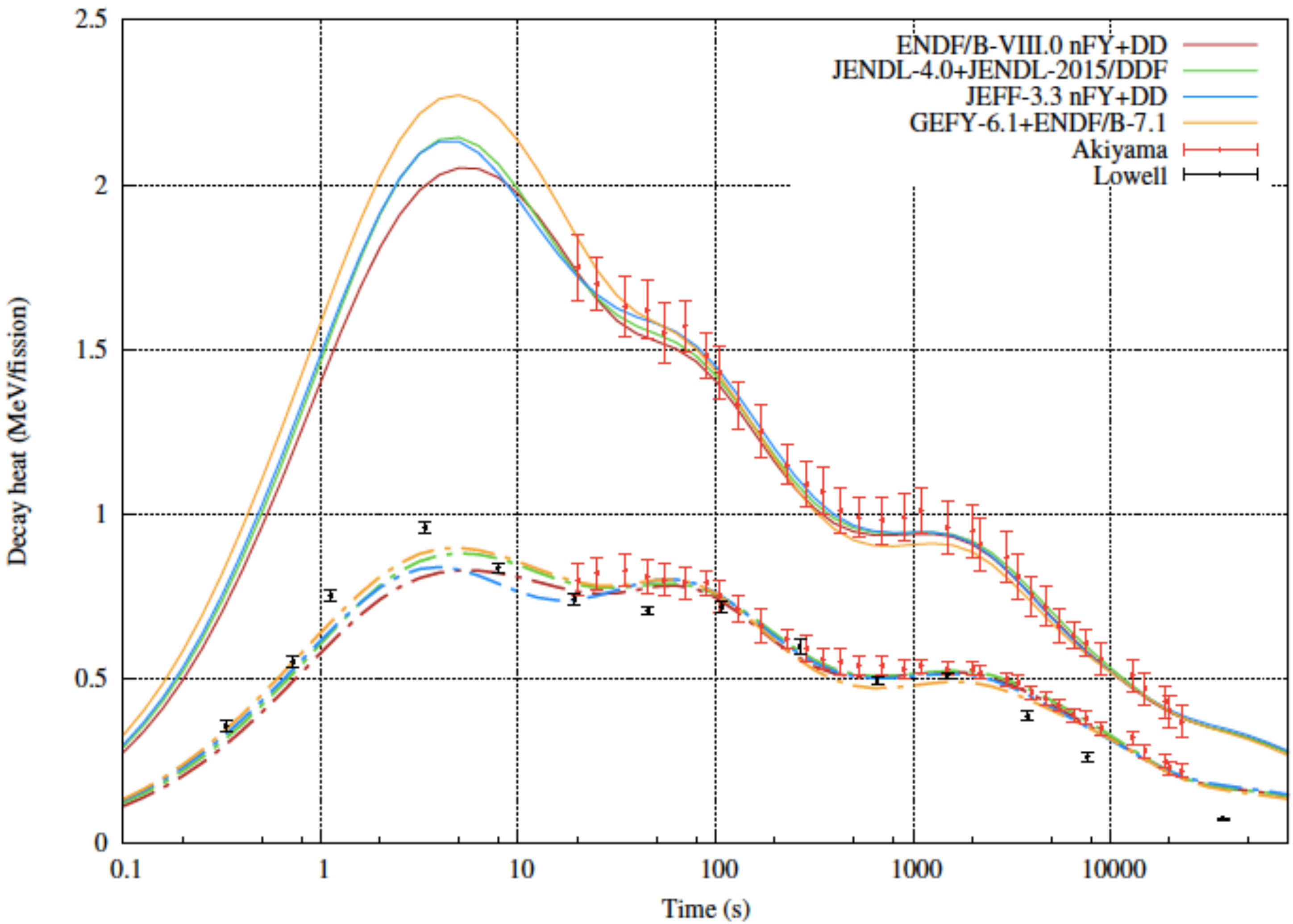
GEF-6.1 nFY with ENDF/B-VII.1 decay data

Decay heat burst functions of ^{235}U for various neutron energies

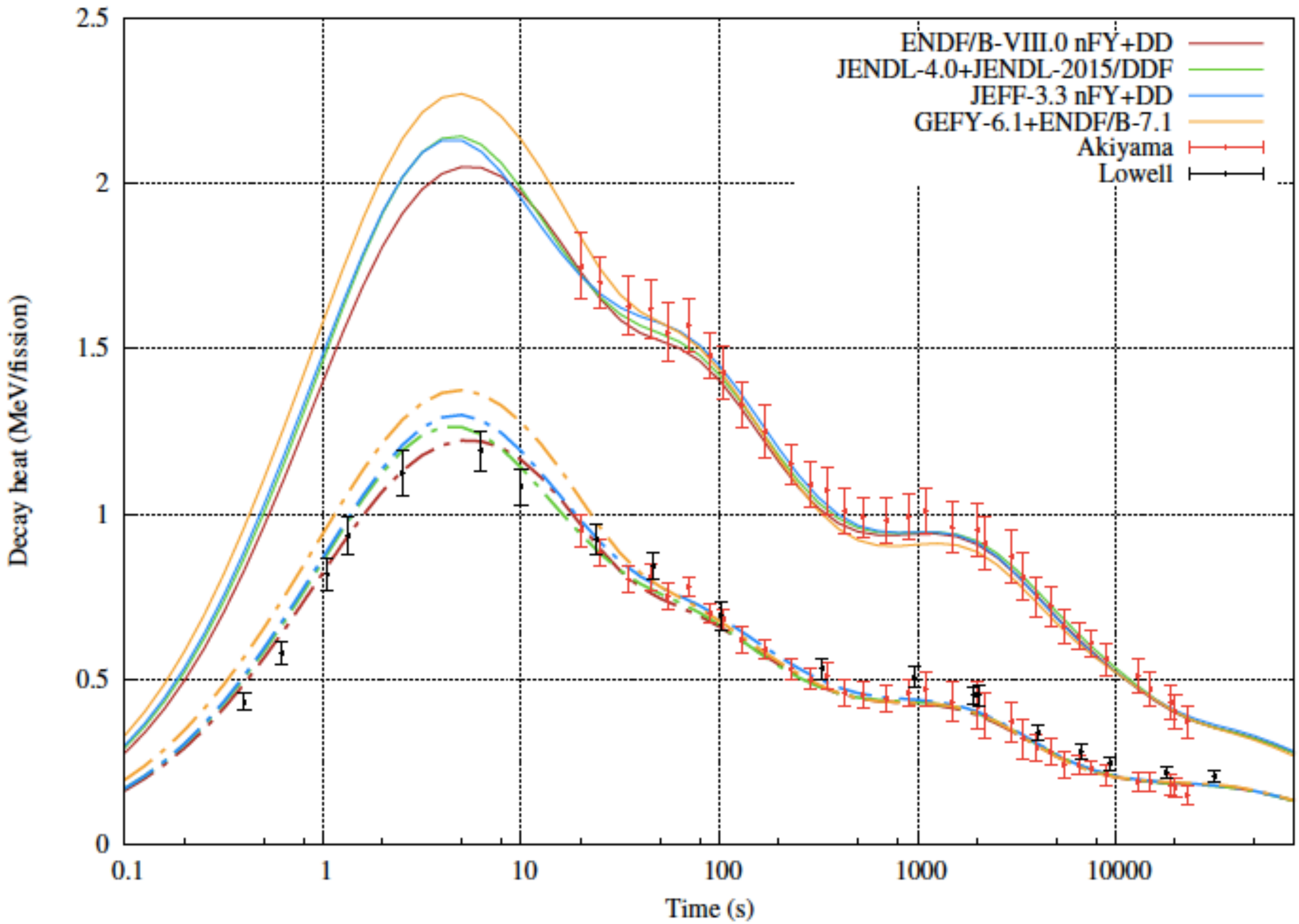


^{238}U fast pulse

Total (solid) and gamma (dash) decay heat from fast pulse ^{238}U

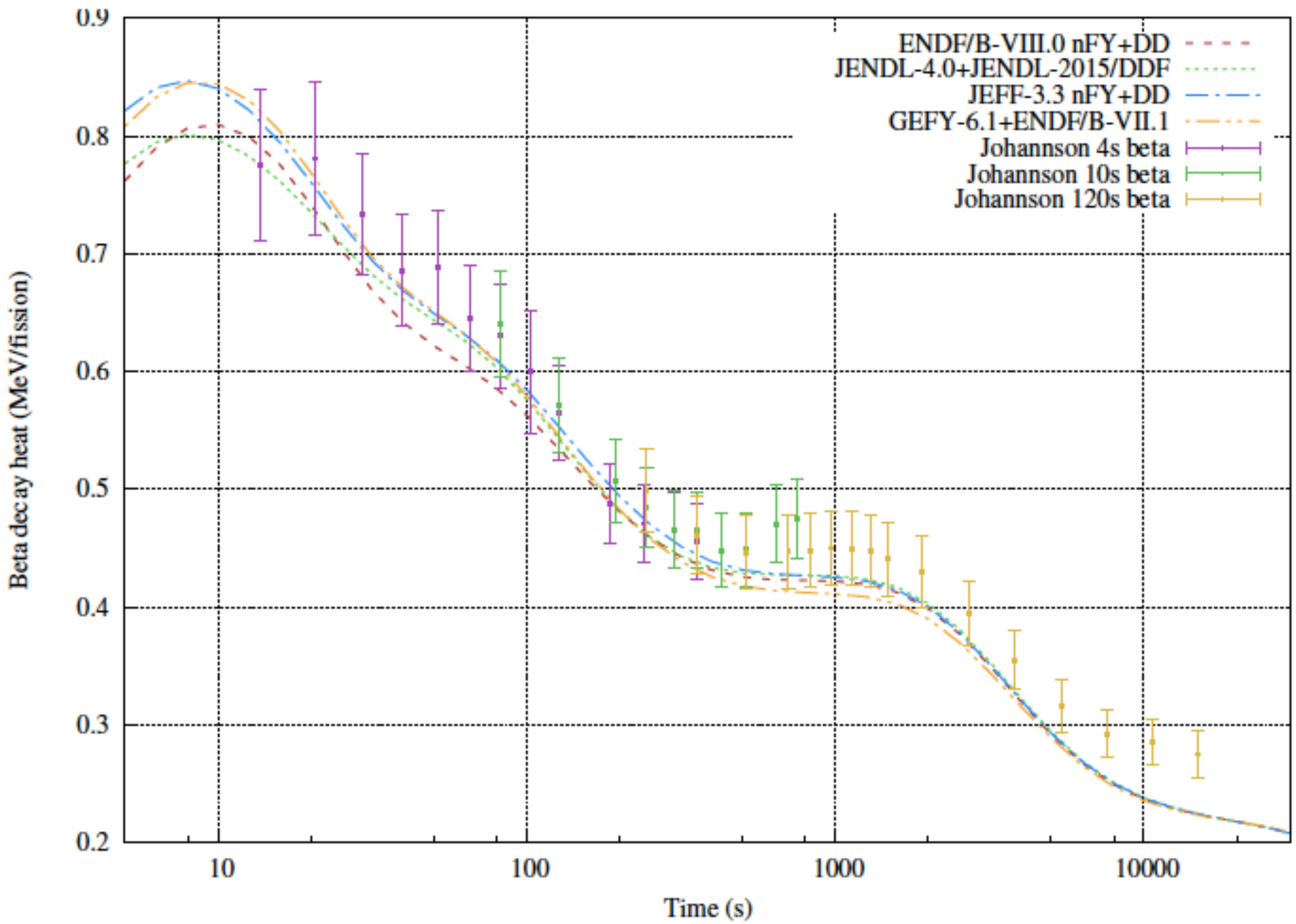


Total (solid) and beta (dash) decay heat from fast pulse ^{238}U



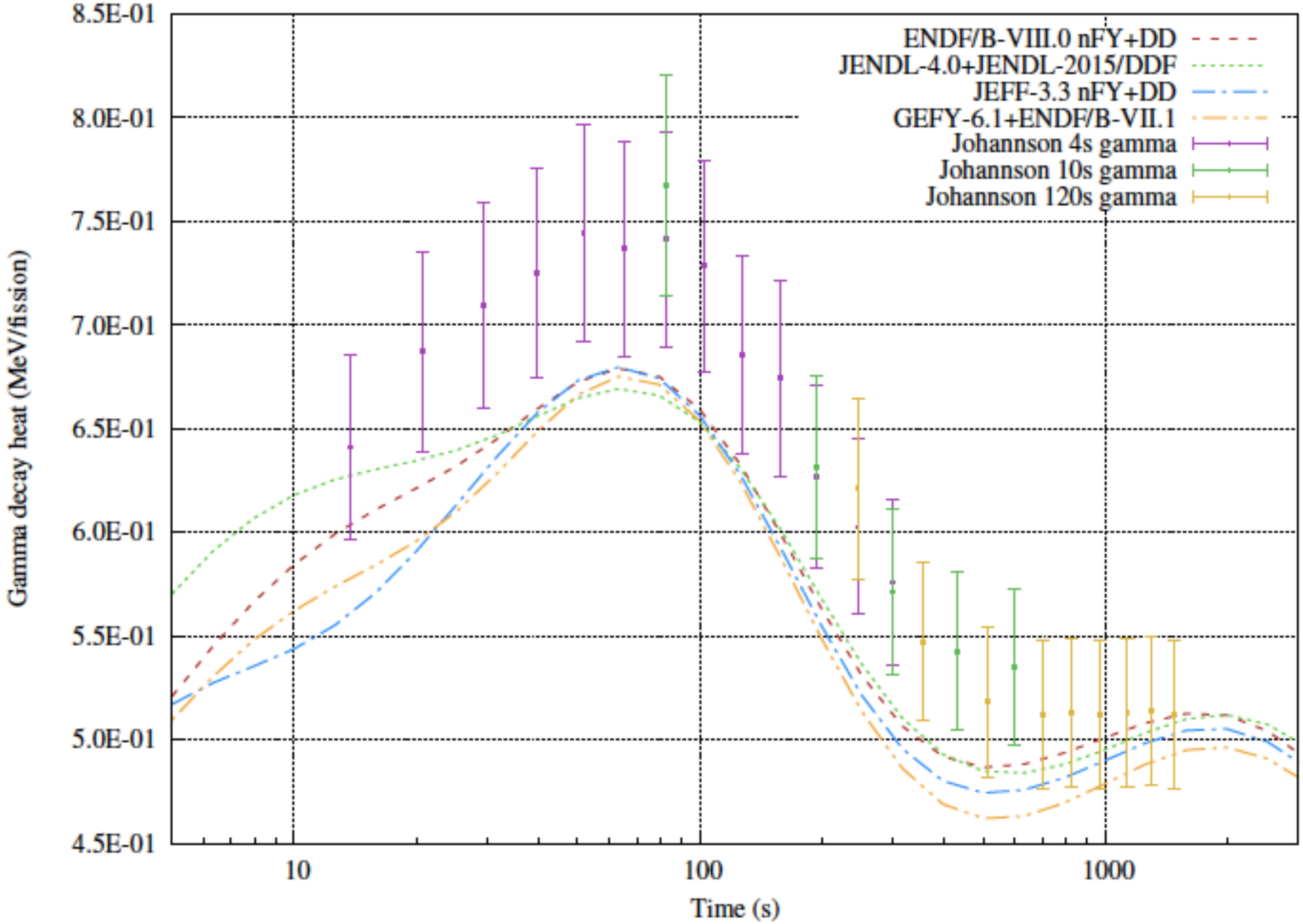
^{235}U Thermal pulse

Beta decay heat from 4-120s irradiation of ^{235}U



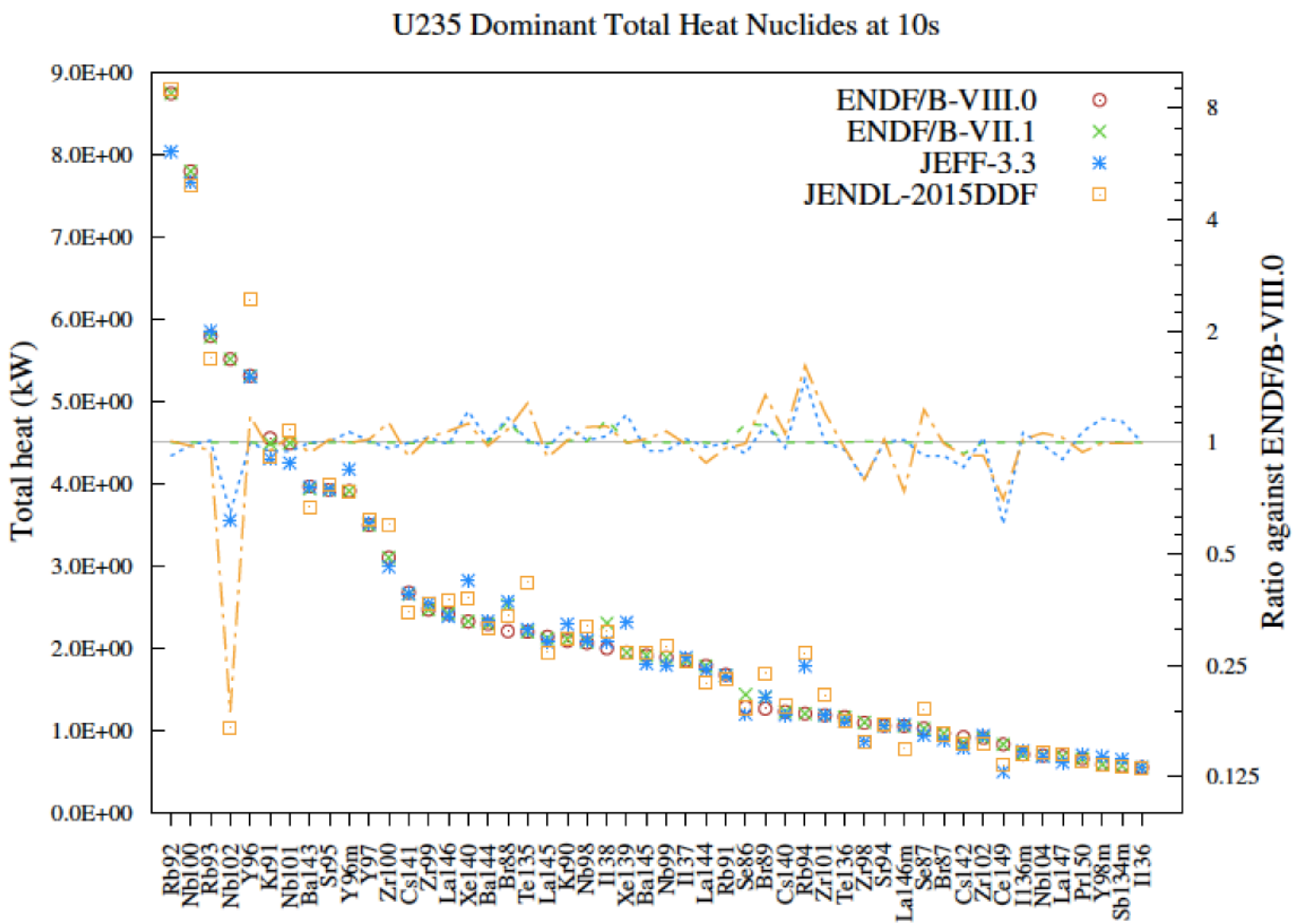
^{235}U Thermal pulse

Gamma decay heat from 4-120s irradiation of ^{235}U



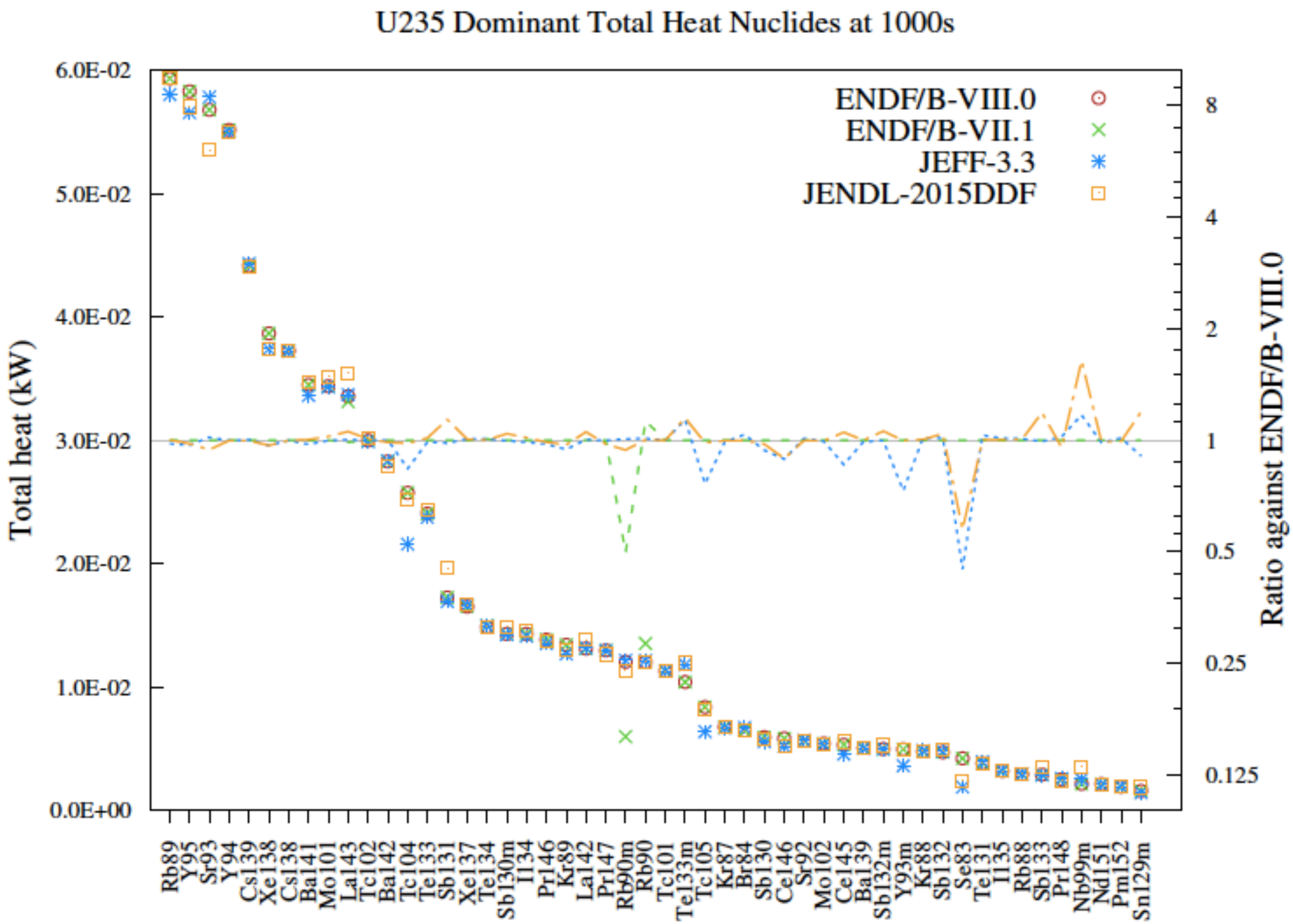
^{235}U 0.0253 eV pulse decay heat

- Nb102 !!



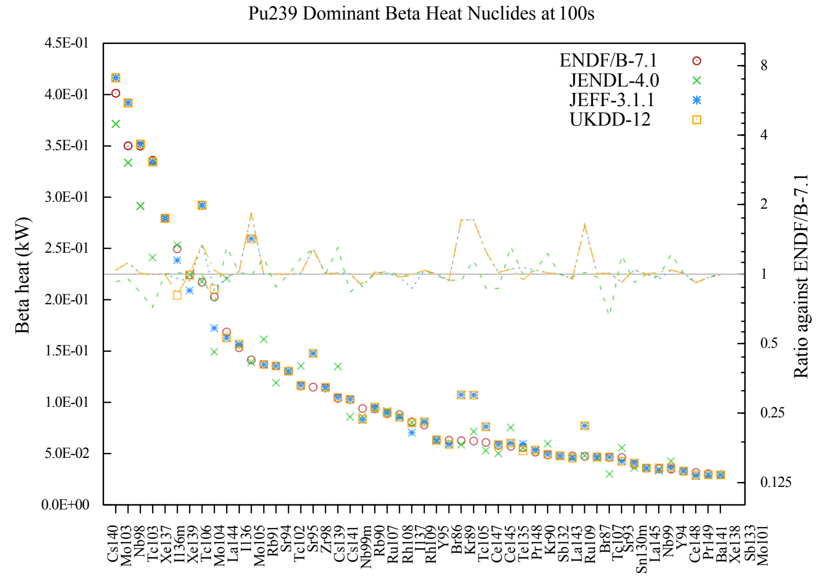
^{235}U 0.0253 eV pulse decay heat

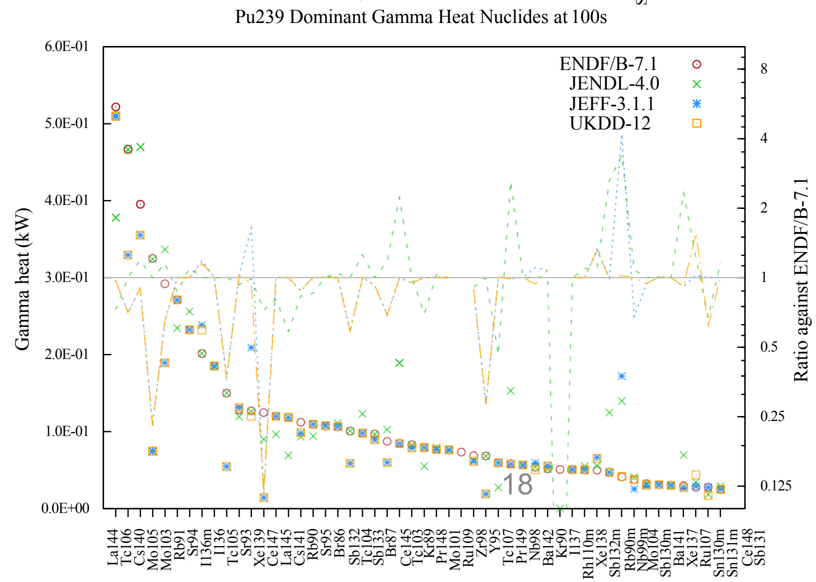
- Too perfect agreement ?? cumulative FY uncertainty



Probe the data: Decay Data

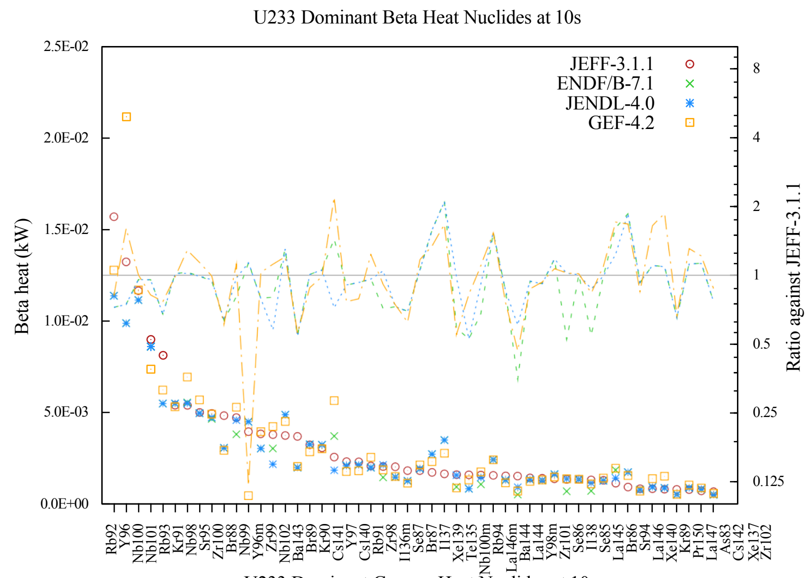
- Fix the nFY and vary the decay data to probe for differences (ENDF/B-VII.1 decay reference)
- Right: ^{239}Pu beta (top) and gamma (bottom) heat at 100 s cooling – note large variation in decay files
  - Nominal values and ratio to one, here ENDF/B-VII.1
- Useful check to see what evaluations have been performed and where some libraries lag behind (or make different evaluations)

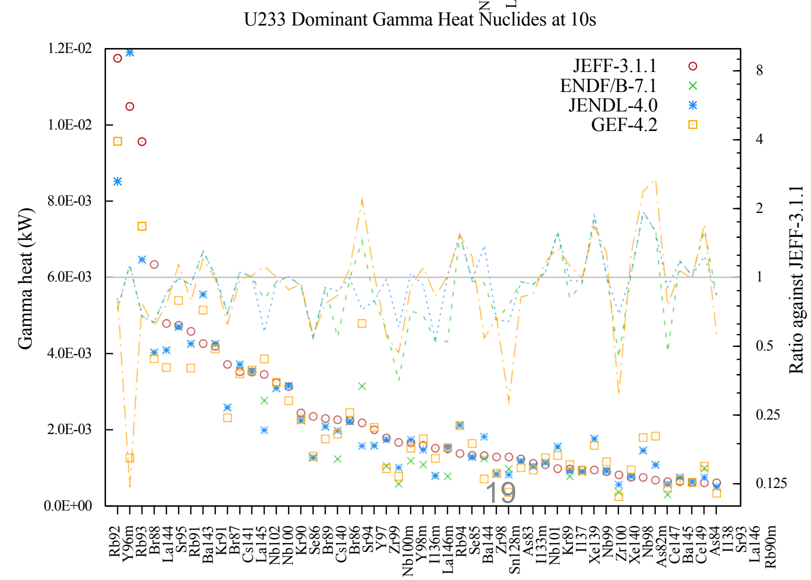




Probe the data: nFission Yields

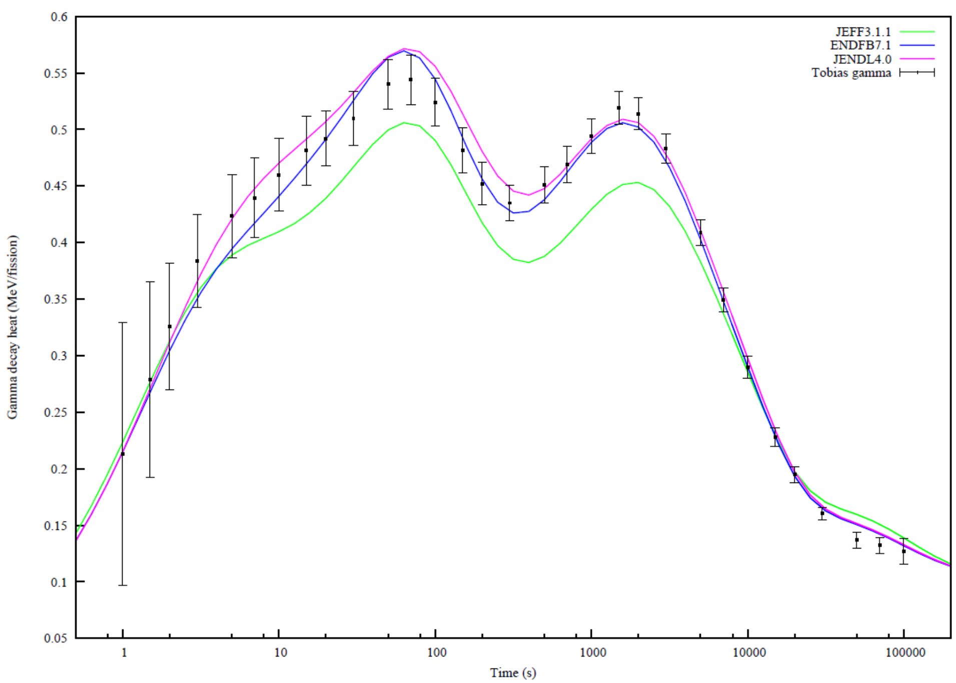
- Other option: use the same DD and vary the nFY
- Right: ^{233}U fast fission pulse beta (top) and gamma (bottom) at 10 s cooling
  - Nominal values and ratio to an example, here JEFF-3.1.1
- This is all over the place! *Note* that the same DD is used in each simulation, but varied independent fission yields
- Minor actinides all show the same pattern

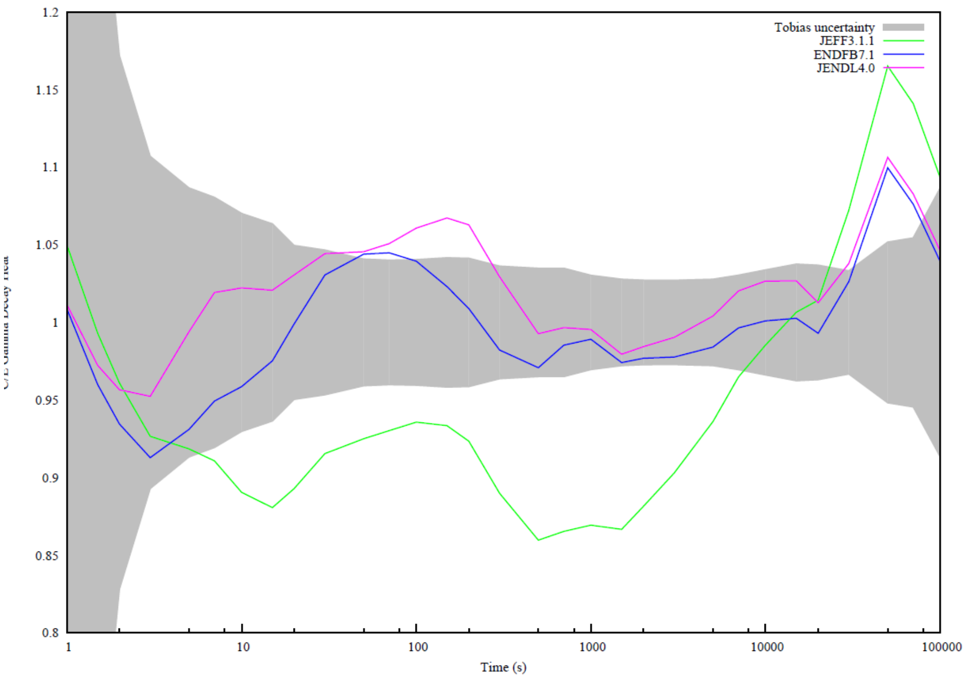




MeV/fission of $^{239}Pu_{th}$ pulse total gamma and C/E

- Underestimation of high-energy gamma feeding due to poor detector efficiency: Pandemonium effect
- Better simulation with TAGS results, recently added in JENDL 4.0 and ENDF/B-VII.1, not JEFF-3.1.1 decay files !!

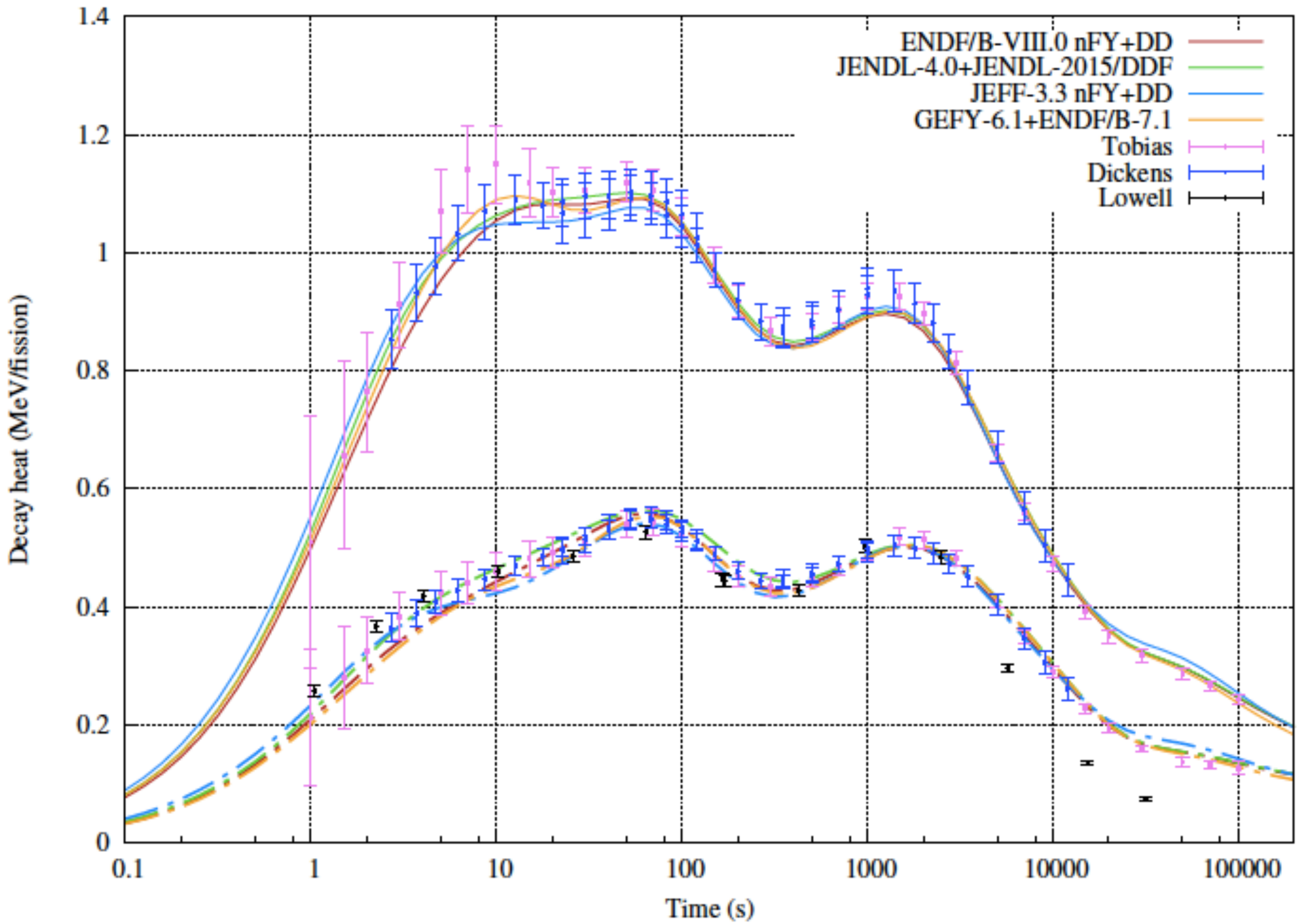




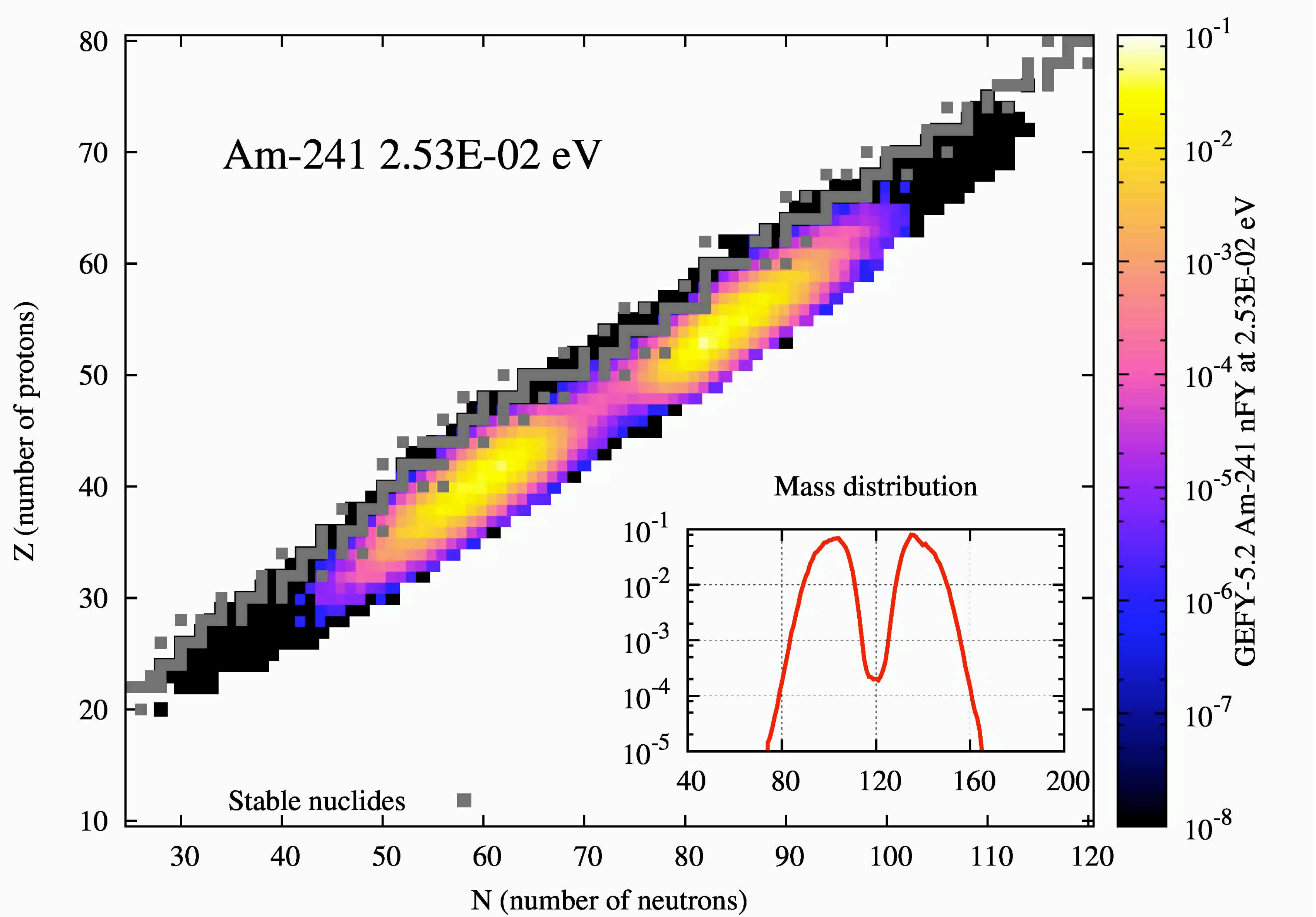
Compensation ➔ too high beta for “fixed” total

MeV/fission of $^{239}Pu_{th}$ pulse total gamma and C/E

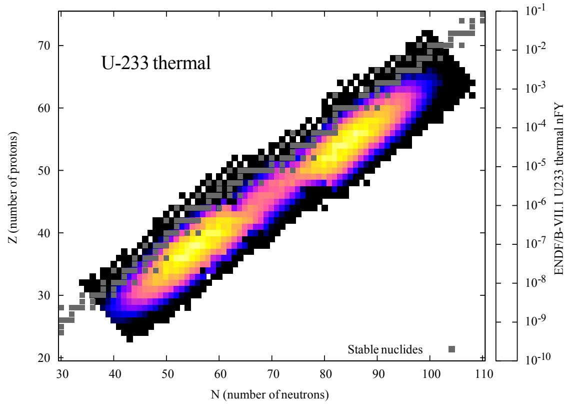
Total (solid) and gamma (dash) decay heat from thermal pulse on ^{239}Pu. Fixed but Tobias metadata @ 1-10 seconds !!



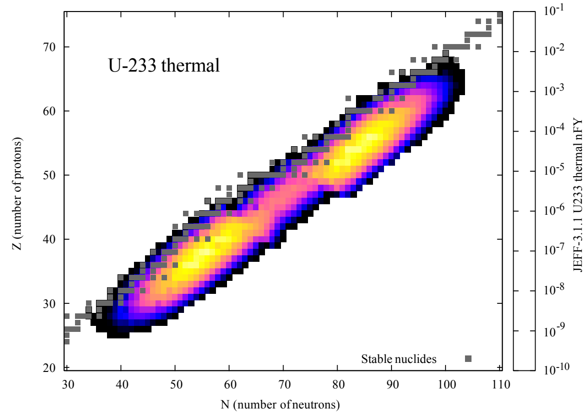
GEFY-5.3 Am241



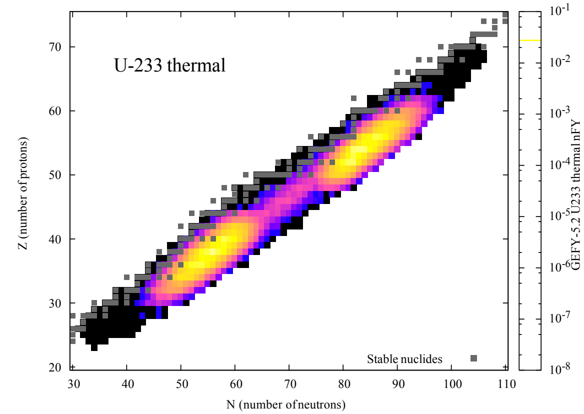
U^{233} nFy examples: yield and uncertainty



ENDF/B-VII.1



JEFF-3.1.1

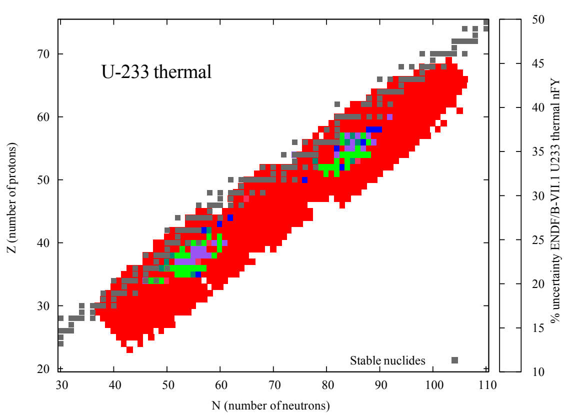


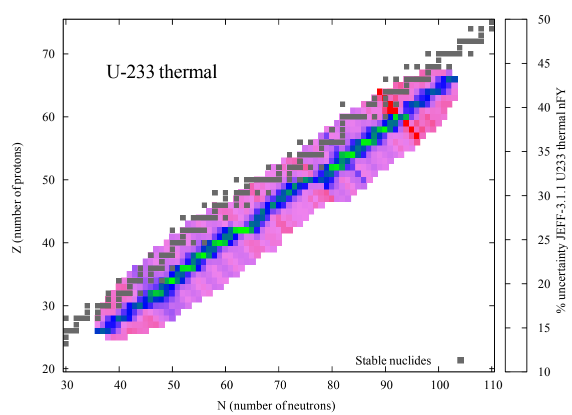
GEFY-5.2

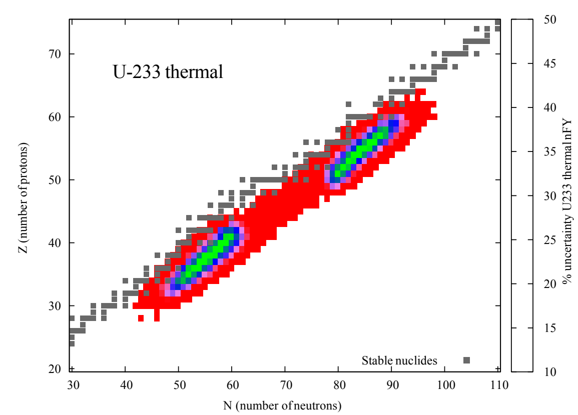
Too far? Man-made bondaries?

N=Z Diagonals?

Far enough?

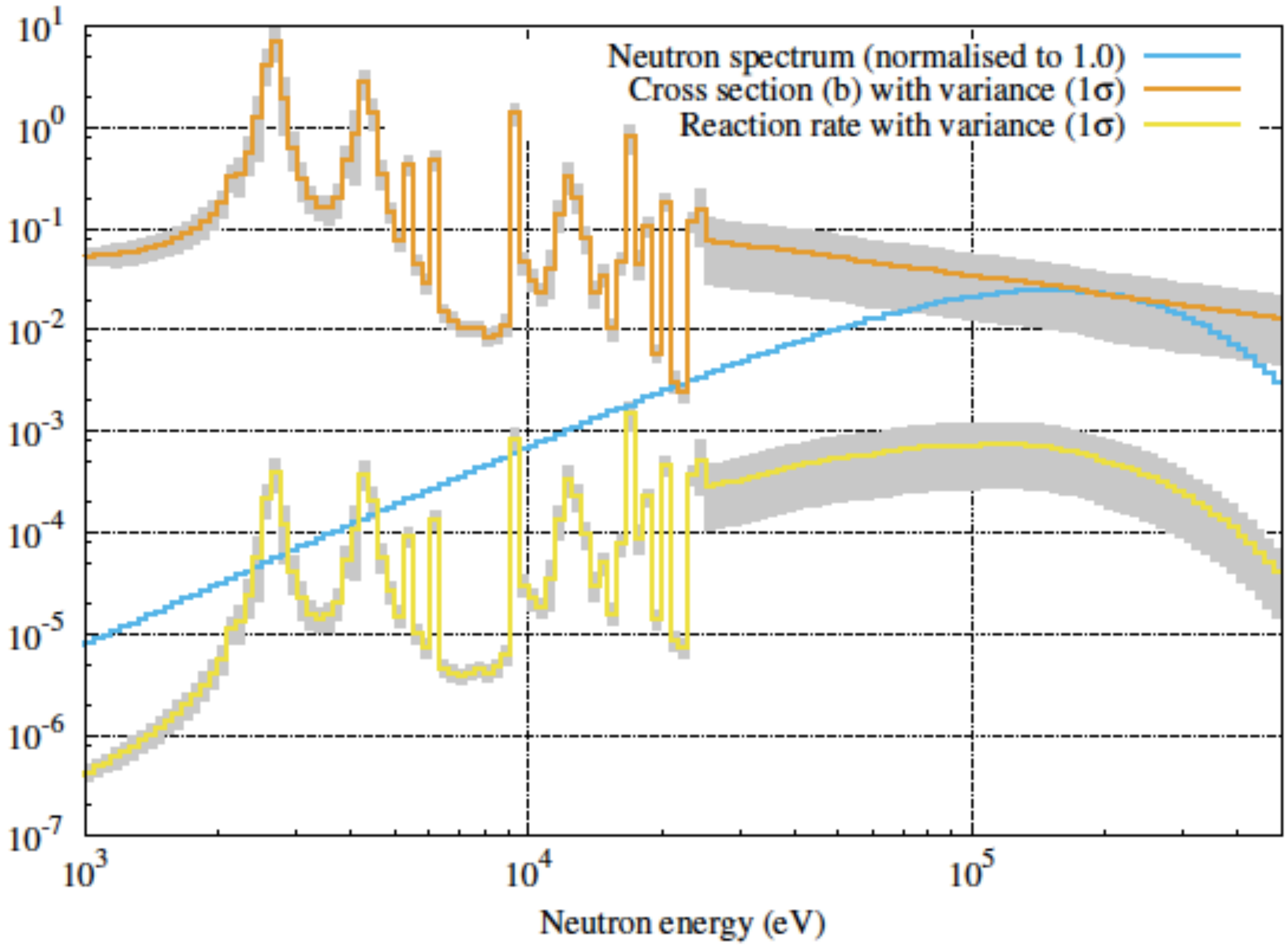






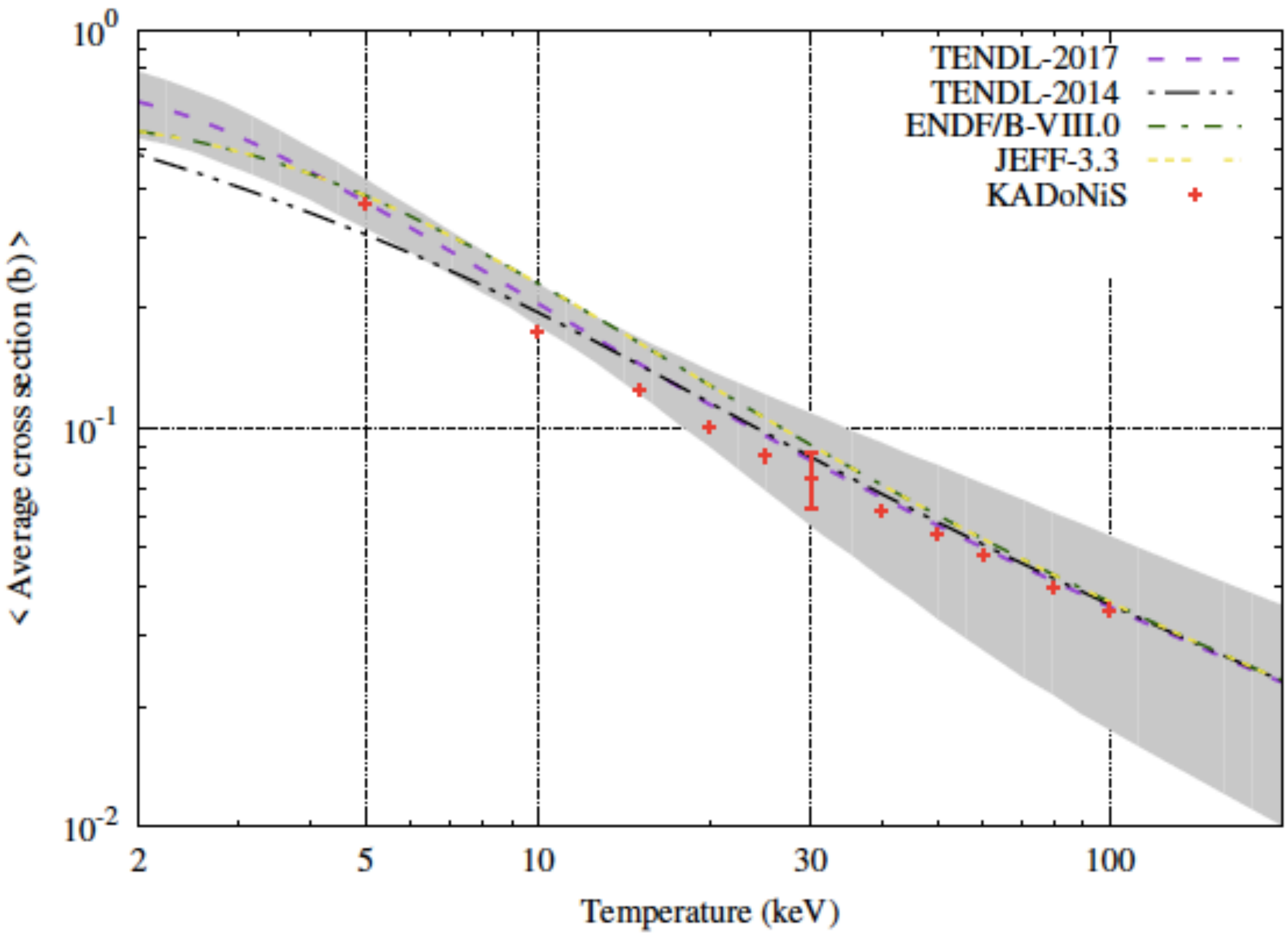
Maxwellian Averaged CS and uncertainty

Fe55 capture 660 group differential cross sections (b) and uncertainties (variances shown) with the kT=30 keV Maxwellian spectrum and resulting, energy-dependent reaction rate with uncertainty



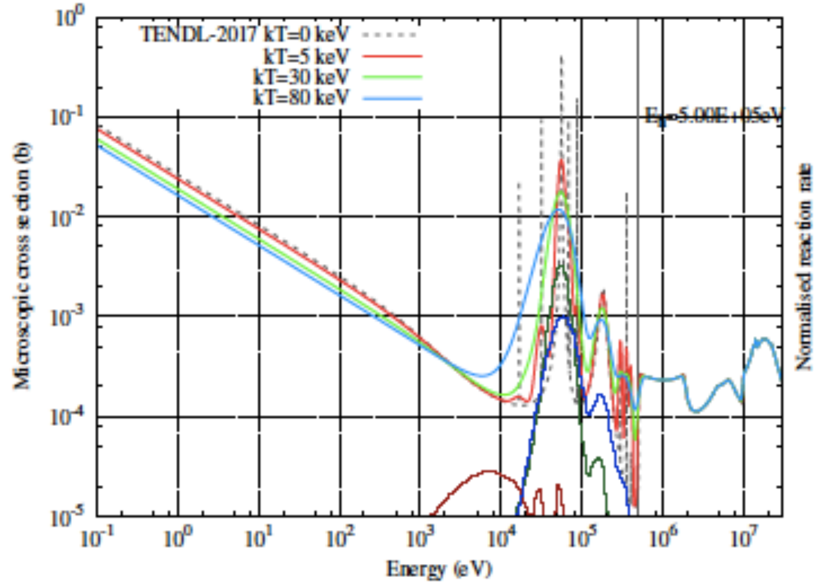
MACS and uncertainty

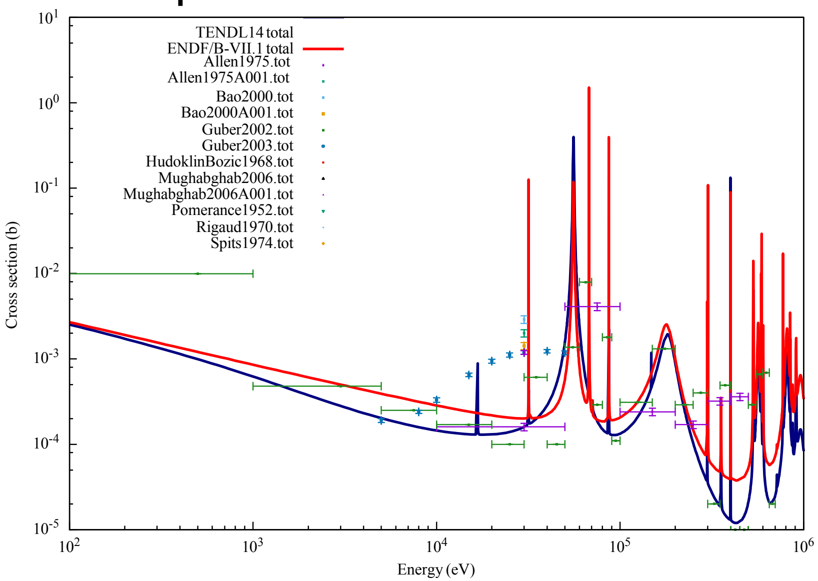
T-dependent MACS for ^{55}Fe + T-dependent uncertainty

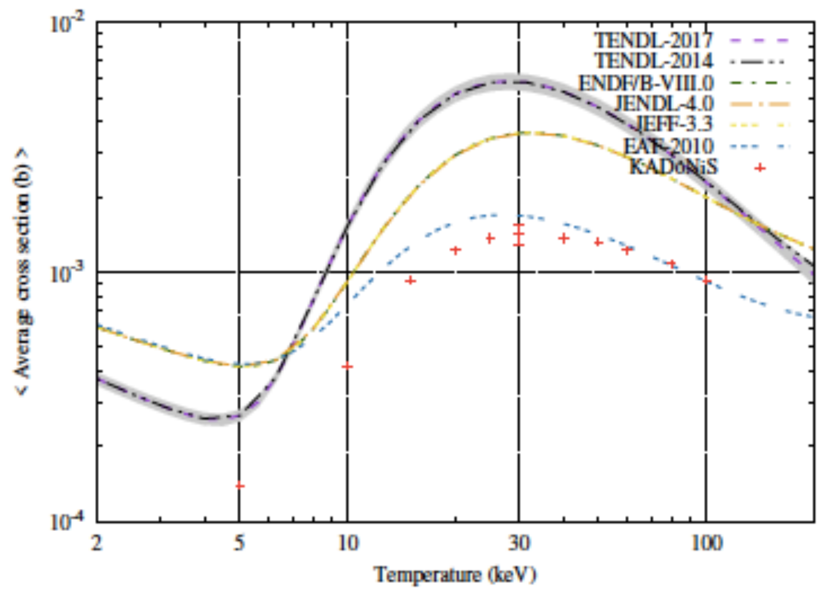


s-Process nucleosynthesis

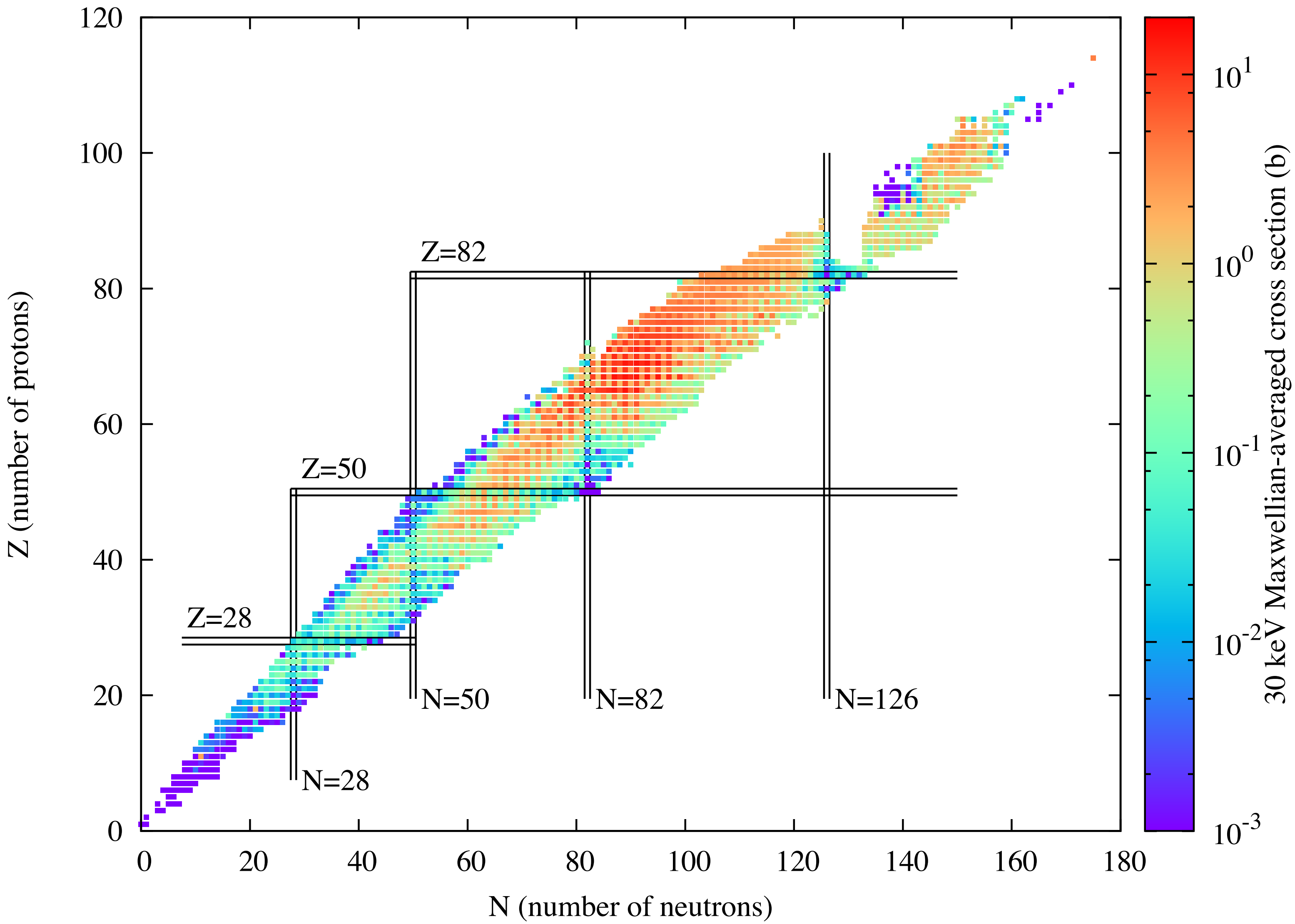
- TENDL adds targets to fully compare against KADoNiS
- A few problematic differences, and several observations from temperature-dep studies
- Often, winner or loser resonance takes it all, ^{28}Si but in that case it is certainly the direct capture competition!!







TENDL 2813 targets @ 30 KeV MACS



KADoNiS probe preferences

In red statistical Kadonis

TENDL-2014: ^{21}Ne, ^{26}Al, ^{36,38}Ar, ^{60}Fe, ^{63}Ni, ^{74,76}Ge, ^{78}Se, ^{126}Sn

JENDL-4.0: ^{140}Ce, ^{206,207,208}Pb

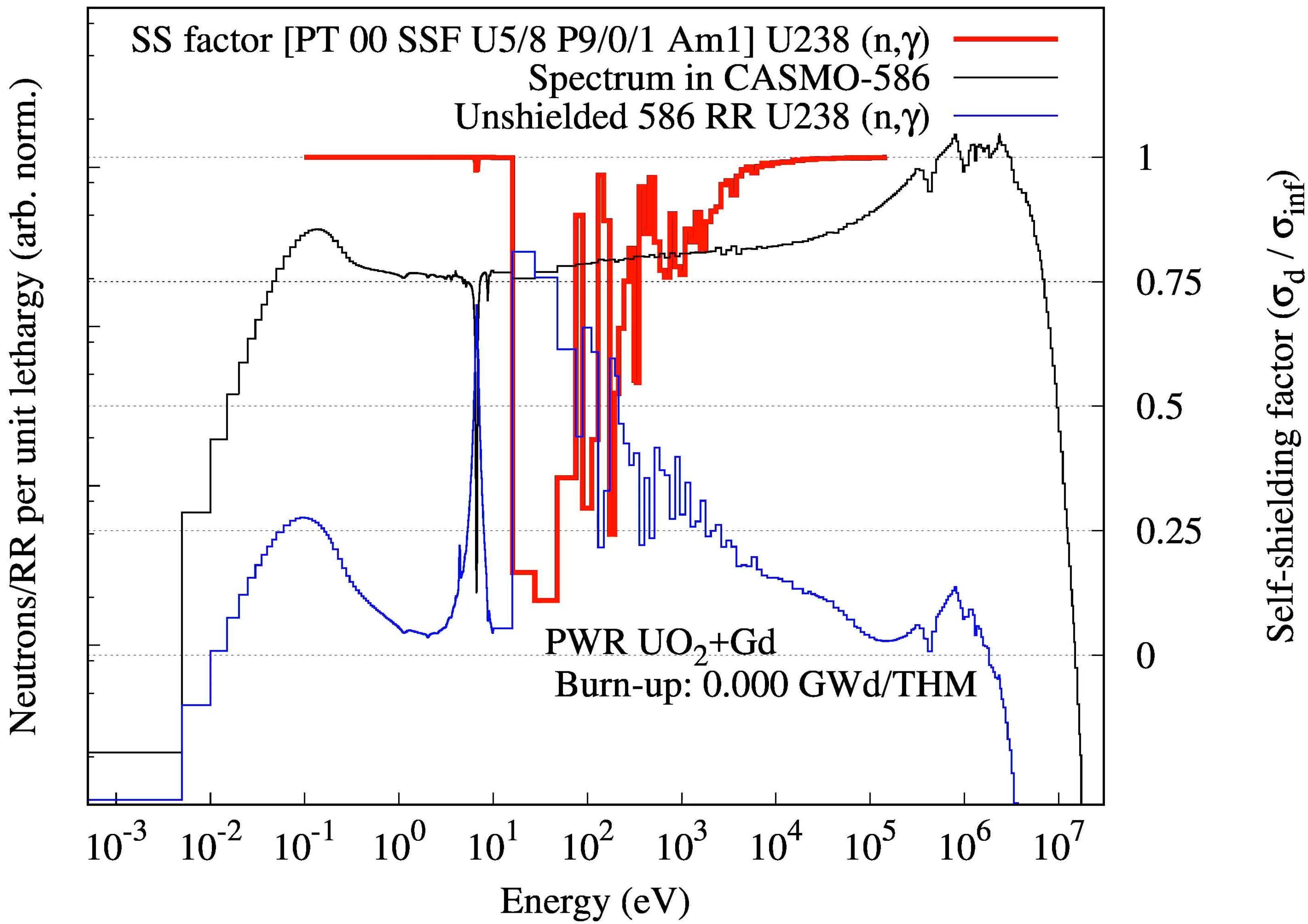
ENDF/B-VIII.0: ^{139}La, ^{205}Tl

JEFF-3.3: ^{192}Pt

EAF-2010: ^{28}Si, ^{36}S

against TENDL-2017

RR time evolution



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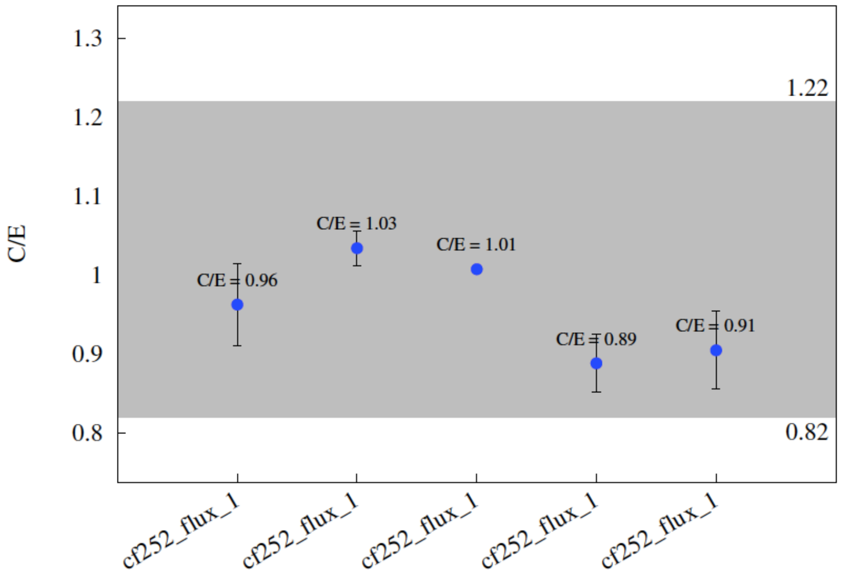
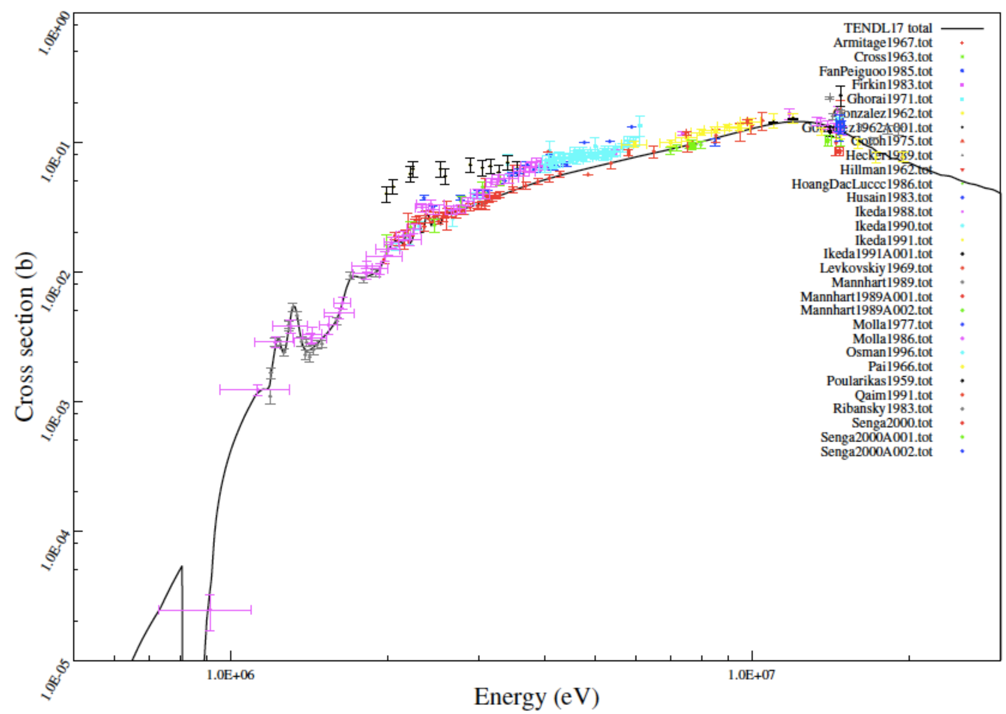
Integro-differential



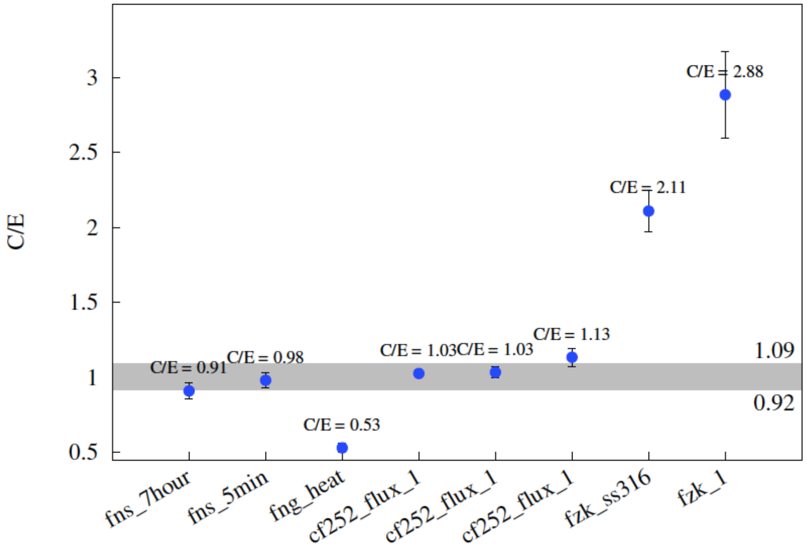
^{47}Ti (n,p) ^{47}Sc

~ 450 channels

UKAEA-R18004



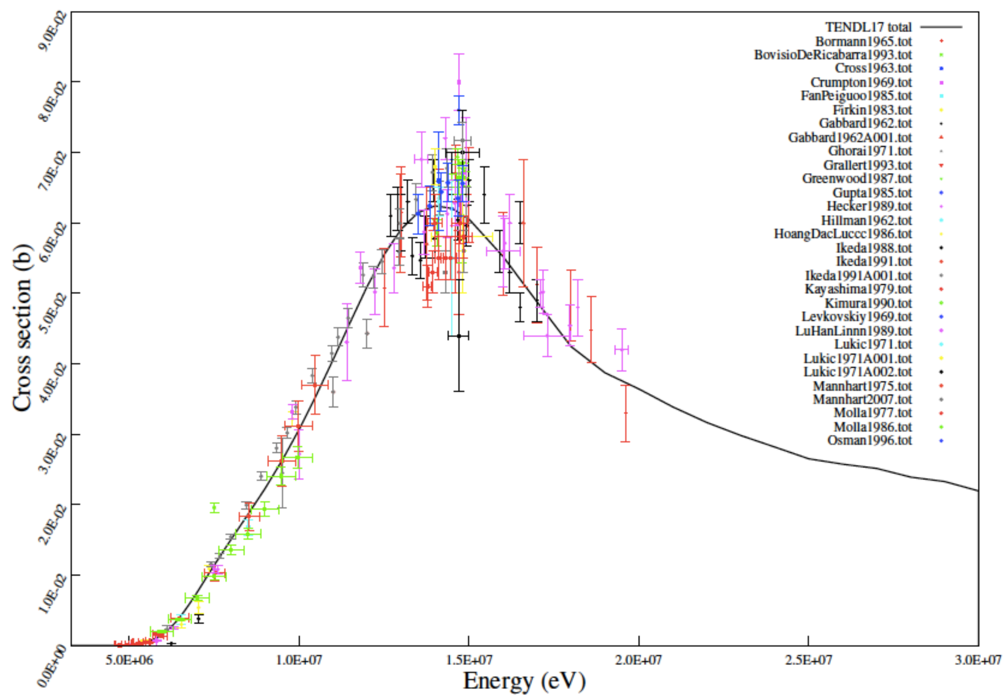
Integro-differential



^{48}Ti (n,p) ^{48}Sc

~ 450 channels

UKAEA-R18004



Work plan

- Uniform, open set of experimental data tables
- Distributed, shared set of inputs decks

- Better, more inquisitive data analytics
- Novel, repeatable visualization techniques
- UQP, uncertainty quantification and propagation
- Open source development

- User’s orientated, but shared by institutions

Spectral indices

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Spectral indices

- Spectral indices embodies direct measurement made in a defined environment

  - Reference source: Cf-252,
  - Experimental reactor, pile: Zoe, Minerve, ZPR, EBR-2…
  - Beam/target experiments: D-Be, D-T, D-Li, P-x,..
  - Astrophysical metrics: MACS

  - Reference input spectra: 1/4 RPV, PWRs, FBRs, SMRs,…Phenix, Paluel, SGHWR, NIF,, etc.

Spectral Indices

- The collapsed cross-sections depend strongly on the nature of the projectile spectra, and so it is important to use the appropriate spectrum together with the appropriately-weighted cross-section data. With the advances of modern simulation software and high resolution spectra the user is reminded of the importance of the tails, low or high-energy ones, on the reaction rates.

- In essence the particle spectrum profile, through the collapsing process, emphasises the energy region of most importance for each application. Transferring data from one application or energy range to another should be done with great care as it can easily lead to misleading and inappropriate numerical results.

Reference input spectra: 50

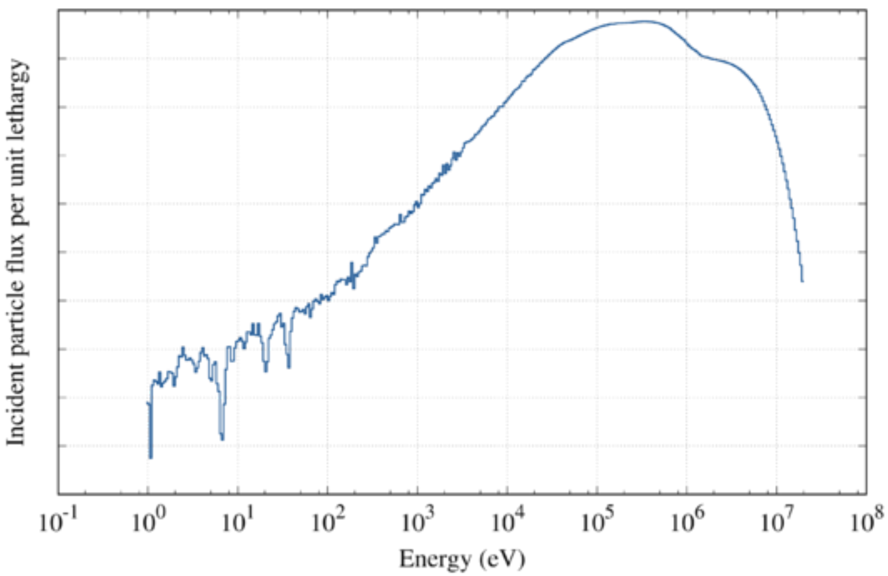
http://fispact.ukaea.uk/wiki/Reference_input_spectra

Reference incident particle spectra

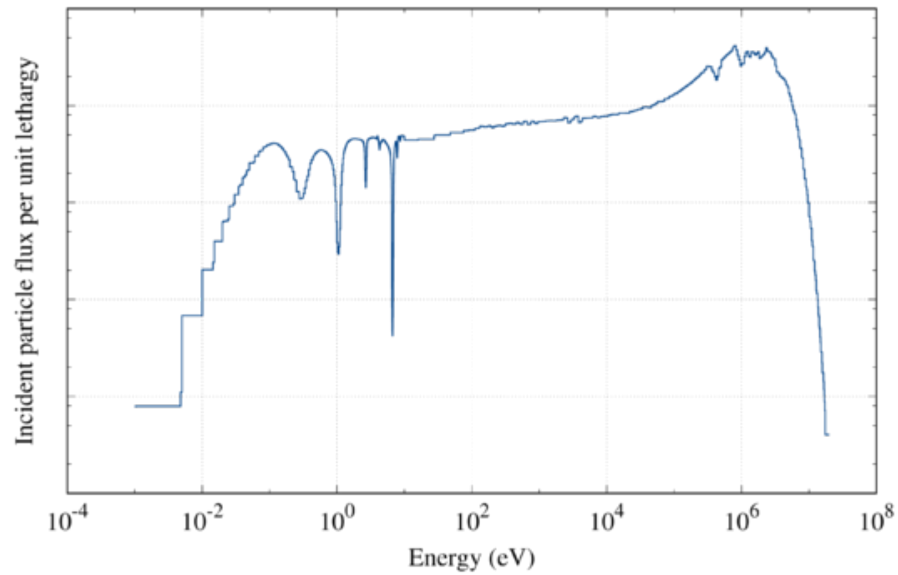
Name	Group	Particle	arb_flux file	Figure	Description
Bigten	407	n	Media:407 Bigten.txt	Bigten	International Criticality Safety Benchmark Experiment, Bigten
BWR-MOX-Gd-0	1102	n	Media:1102 BWR-MOX-Gd-0.txt	BWR-MOX-Gd-0	BWR MOX fuel with Gd, 0 GWd/THM
BWR-MOX-Gd-15	1102	n	Media:1102 BWR-MOX-Gd-15.txt	BWR-MOX-Gd-15	BWR MOX fuel with Gd, 15 GWd/THM
BWR-MOX-Gd-40	1102	n	Media:1102 BWR-MOX-Gd-40.txt	BWR-MOX-Gd-40	BWR MOX fuel with Gd, 40 GWd/THM
BWR-RPV	198	n	Media:198 BWR-RPV.txt	BWR-RPV	Boiling water reactor, 1/4 Thickness reactor pressure vessel
BWR-UO2-Gd-0	1102	n	Media:1102 BWR-UO2-Gd-0.txt	BWR-UO2-Gd-0	BWR UO2 fuel with Gd, 0 GWd/THM
BWR-UO2-Gd-15	1102	n	Media:1102 BWR-UO2-Gd-15.txt	BWR-UO2-Gd-15	BWR UO2 fuel with Gd, 15 GWd/THM
BWR-UO2-Gd-40	1102	n	Media:1102 BWR-UO2-Gd-40.txt	BWR-UO2-Gd-40	BWR UO2 fuel with Gd, 40 GWd/THM
CERN-H4IRRAD	288	n	Media:288 CERN-H4IRRAD.txt	CERN-H4IRRAD	CERN H4IRRAD experiment
Cf252	070	n	Media:070 Cf252.txt	Cf252	Californium-252 spontaneous fission source
DEMO-HCPB-BP	616	n	Media:616 DEMO-HCPB-BP.txt	DEMO-HCPB-BP	DEMO fusion concept He-cooled pebble bed, backplate
DEMO-HCPB-FW	616	n	Media:616 DEMO-HCPB-FW.txt	DEMO-HCPB-FW	DEMO fusion concept He-cooled pebble bed, first wall

Reference spectra

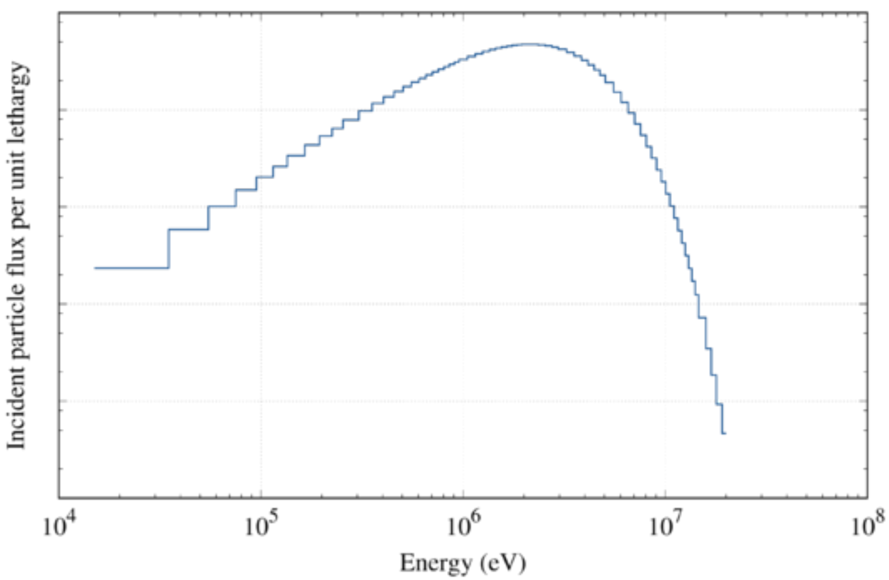
Bigten (407 group)



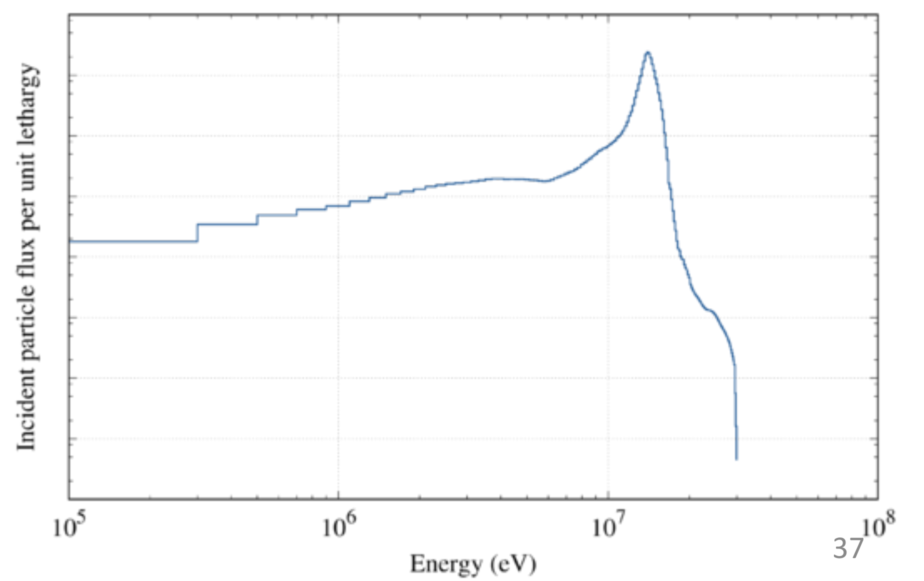
BWR-MOX-Gd-0 (1102 group)



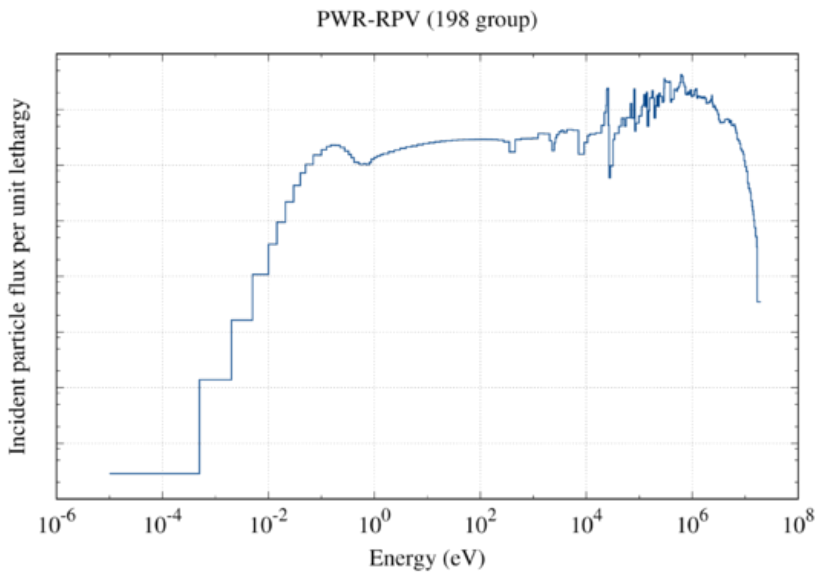
Cf252 (70 group)

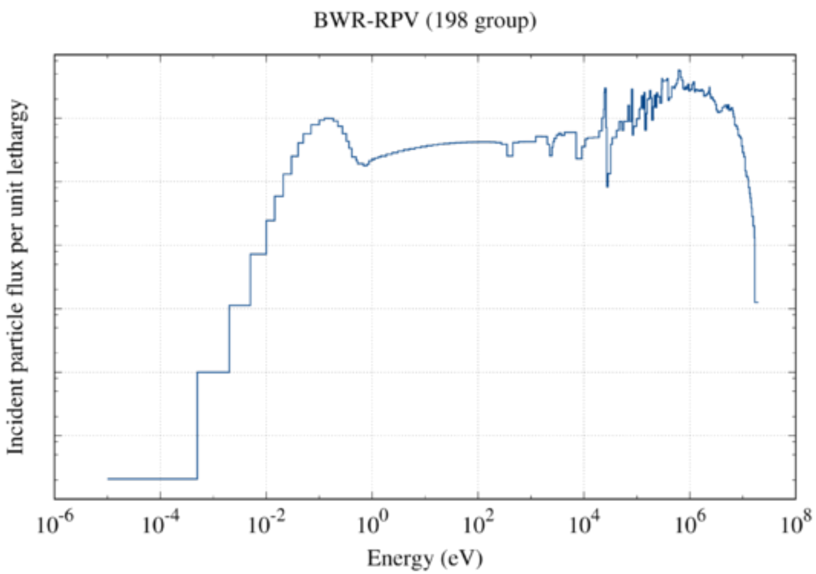


NIF-ignition (150 group)



Background ¼ RPV reference



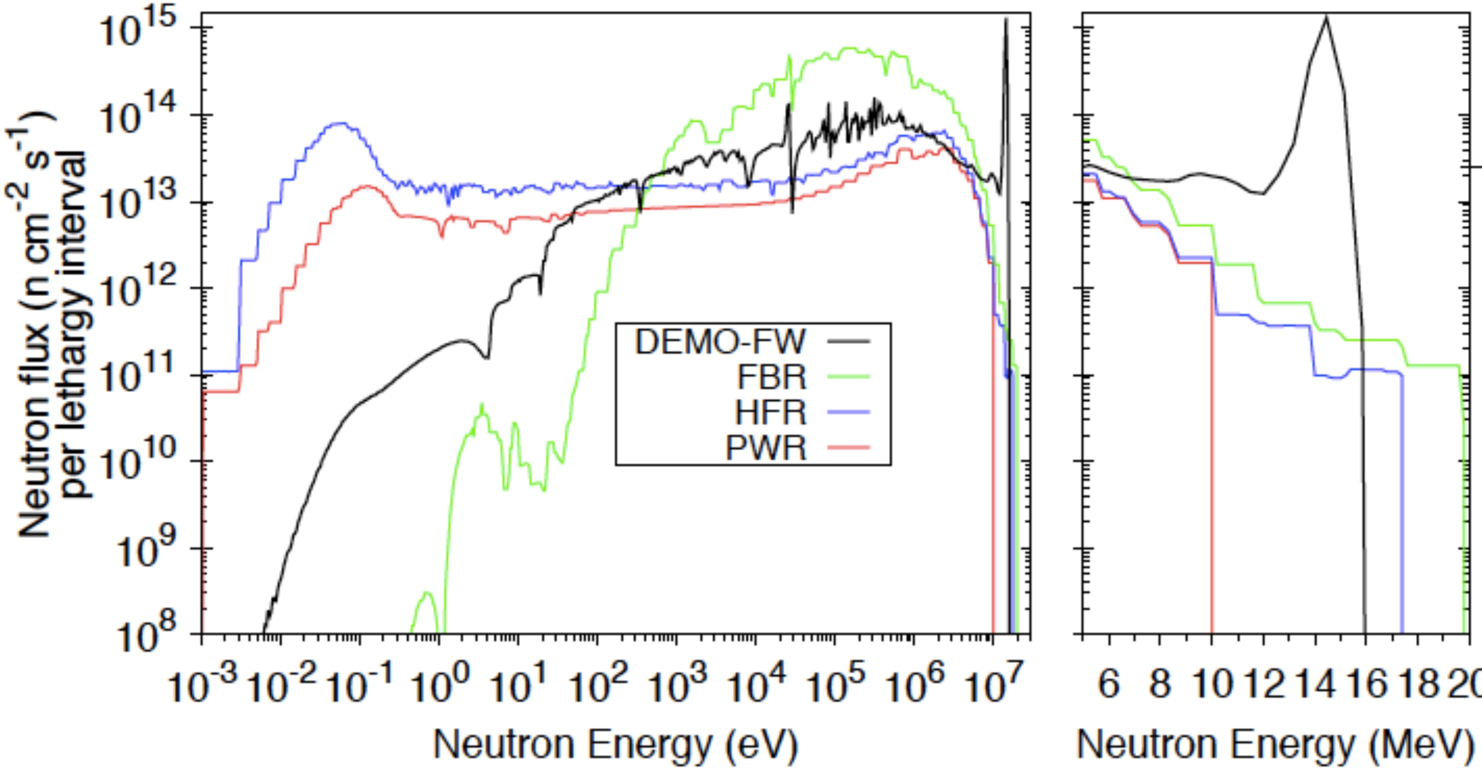


Assuming a 40-year plant operation and a load factor of 0.8, giving an effective lifetime of 32 years, FISPACT-II results

PWR 1.3E-3 x 32 = 0.0416 dpa, total fluence 1.136E+20, > 1 MeV 2.387E+19 n/cm^2
BWR 2.3E-4 x 32 = 0.0073 dpa, total fluence 1.798E+19, > 1 MeV 4.469E+18 n/cm^2

An end-of-life fluence value of 3.0E+19 n/cm^2, is quoted to produces about 0.045+/-0.05 dpa in *G. R. Odette and G. E Lucas, Embrittlement of Nuclear Reactor Pressure Vessels, JOM, 53 (7) (2001), pp 18-22*

Tails: low and high energy



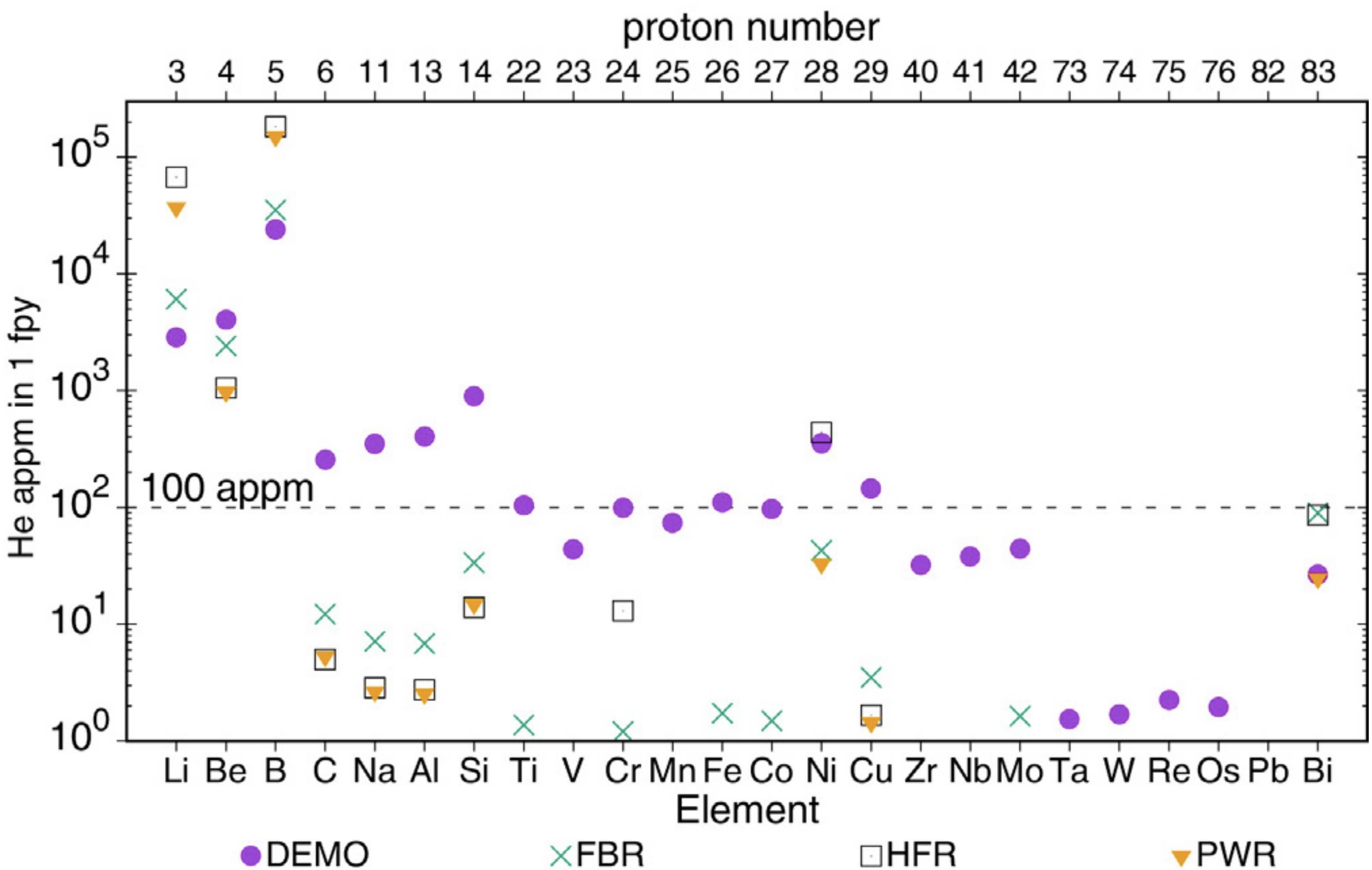
total fluxes ϕ: ($\times 10^{14}$ n cm^{-2} s^{-1})

DEMO	6
FBR	24
HFR	5
PWR	3

- FBR – superphenix Fast Breeder Reactor
- HFR – High Flux Reactor, Petten
- PWR – Pressurized Water-cooled Reactor

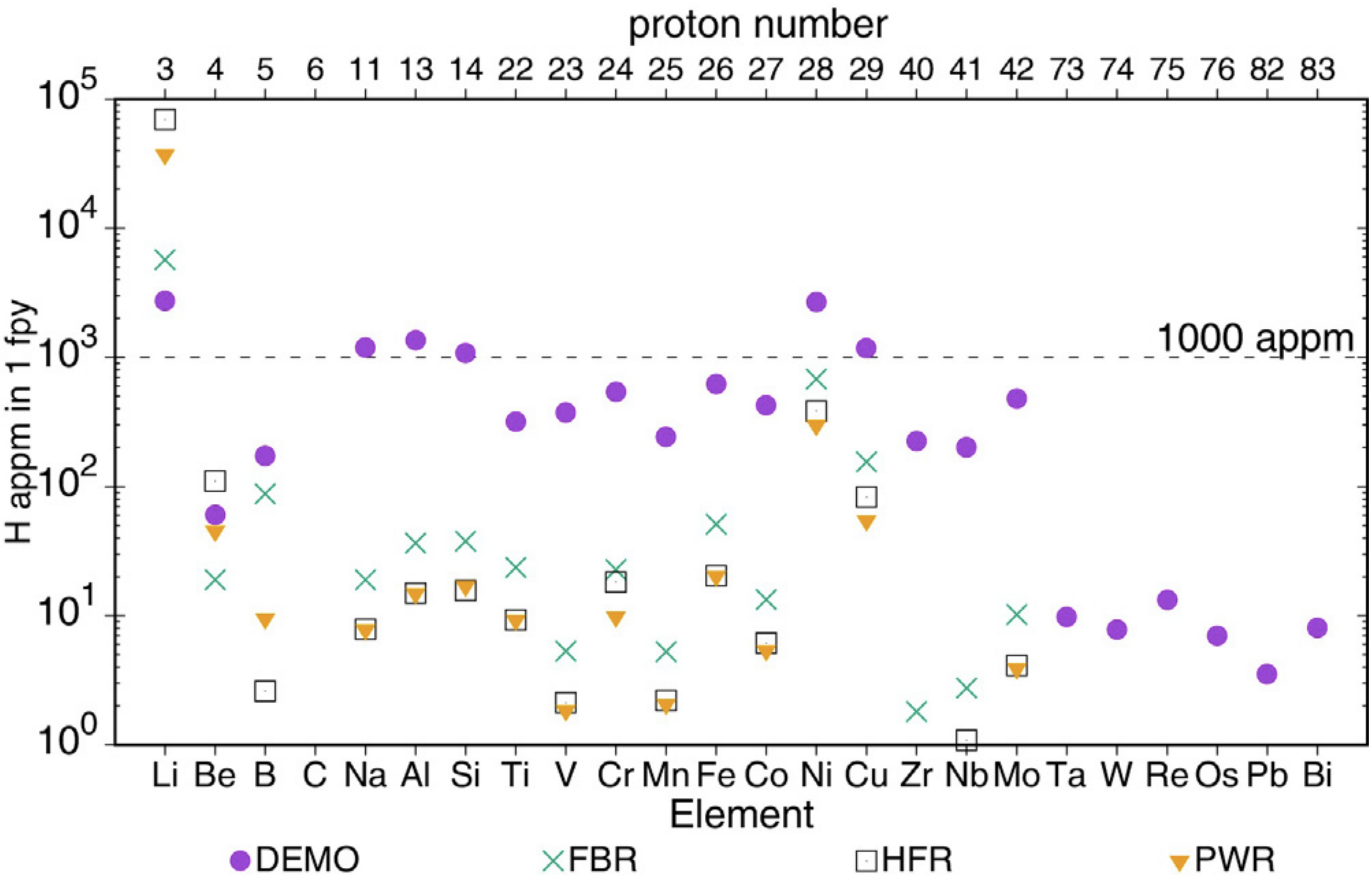
He production in reference spectra

Variation in He production (in atomic parts per million or appm) per fpy as afunction of element and irradiation environment



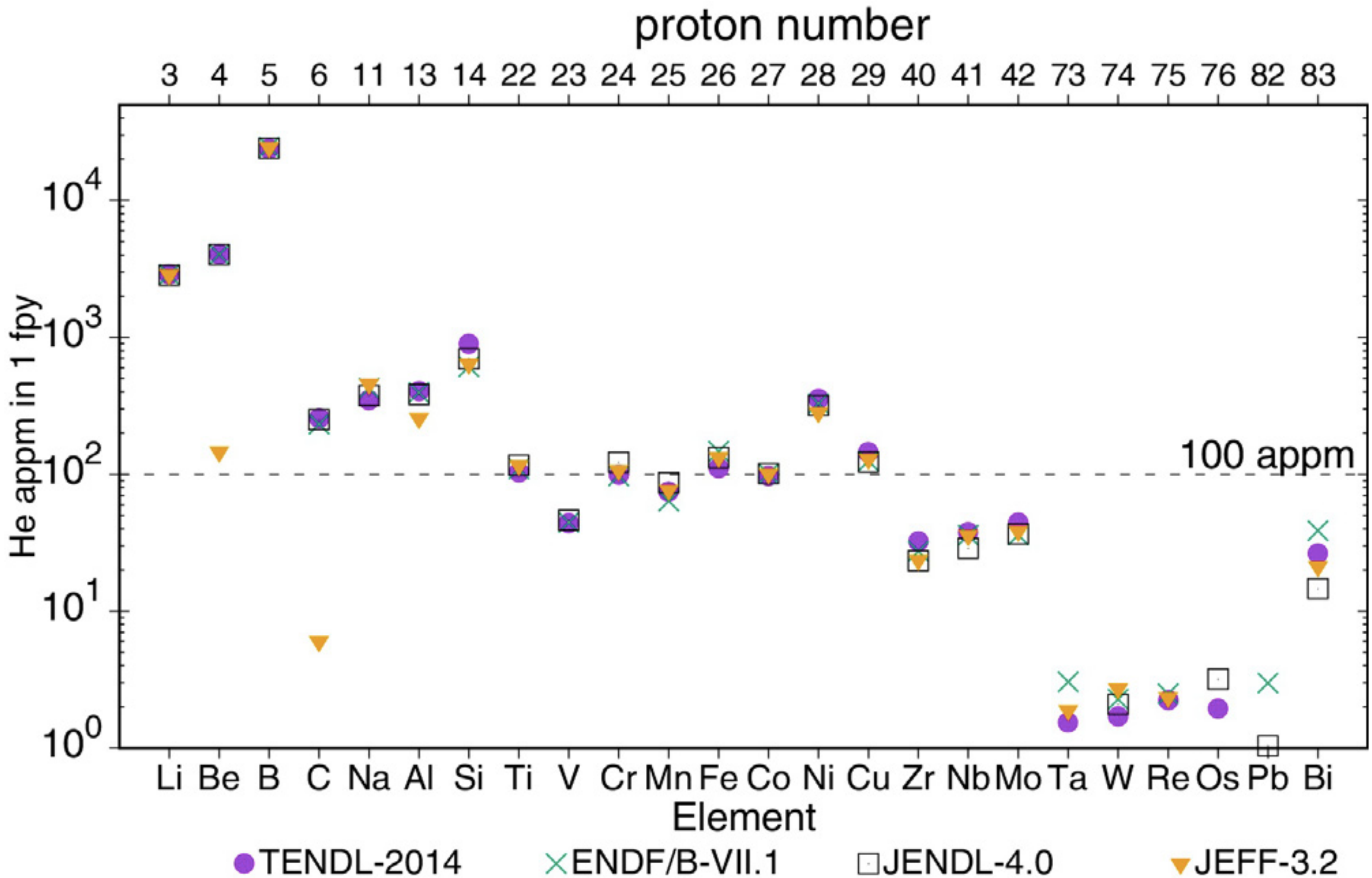
H production in reference spectra

Variation in H appm per fpy as a function of element and irradiation environment.



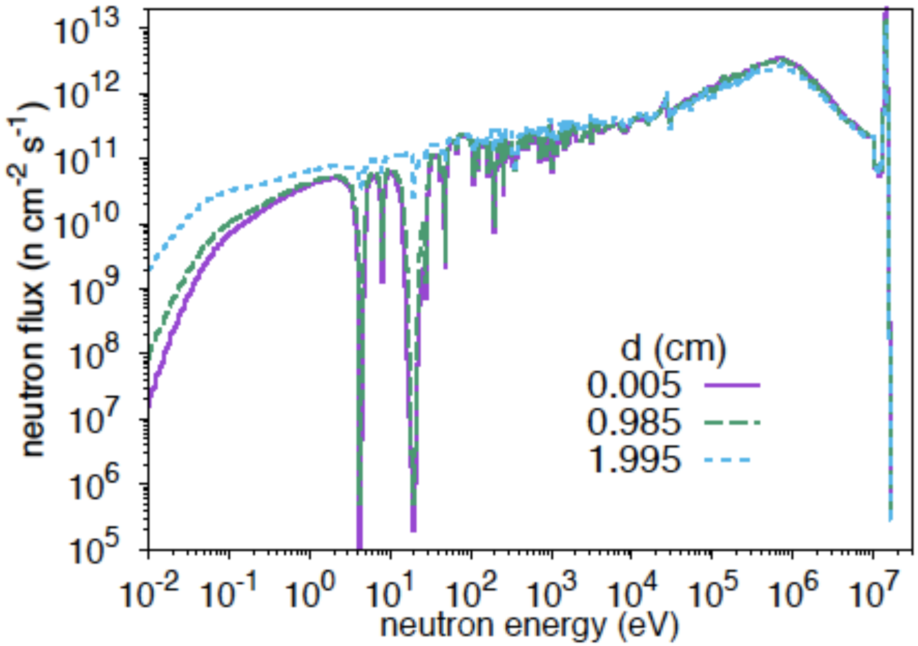
He production from different libraries

Variation in He production per fpy under the DEMO-FW spectrum as a function of element and choice of nuclear data library

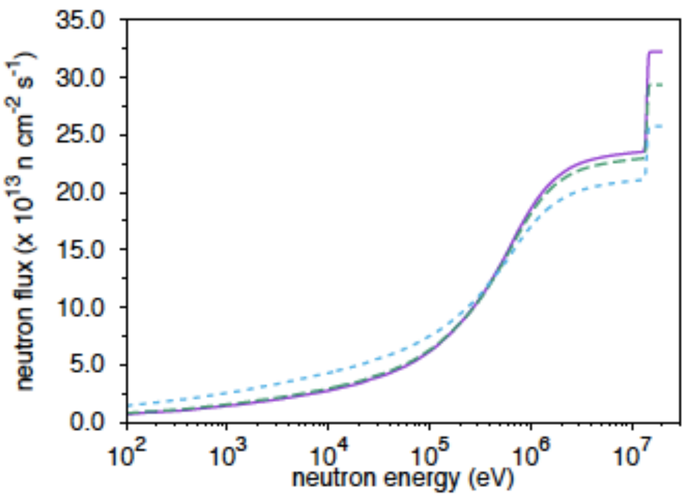


Spherical W shell 2cm thick

- Even in first 0.1 mm the flux depletions due to the giant resonances are present
  - suggesting that self-shielding occurs at all depths because neutron backscattering populates all neutron energies
- Flux depletions are reduced in W layers close to the moderator & thermal component of spectrum is higher
  - potential change in transmutation behaviour

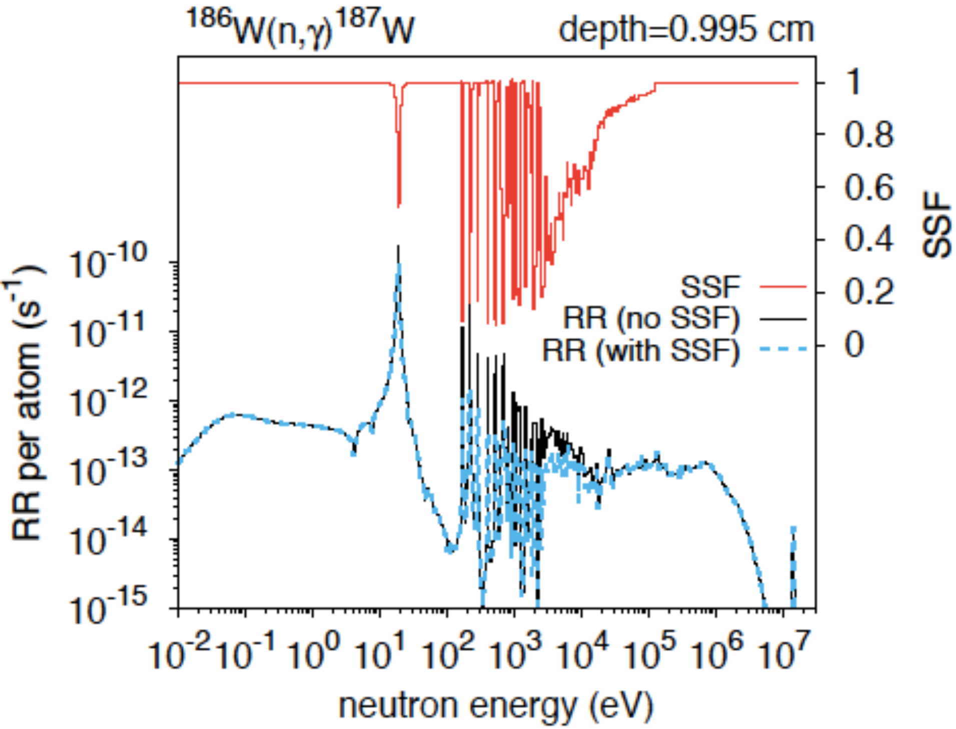


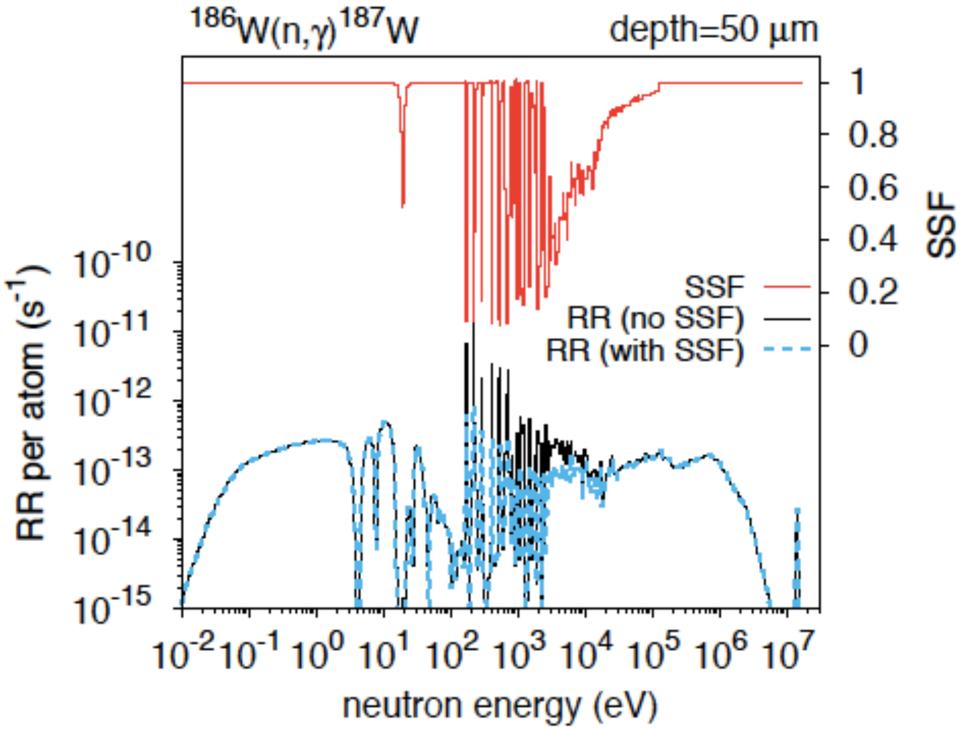
- 20% drop in total flux across 2 cm depth



Spherical W shell 2cm thick

- Probability Table (PT) SSFs used to account for dilution effects associated with both resolved and un-resolved (>∼ 20 keV) resonances





- final 0.1 mm of W
- total SSF: 0.64
- giant resonance dominates RR of ^{186}W (n,γ) (70% of RR)

- first 0.1 mm of W
- total SSF: 0.55
- minor contribution from giant resonance

Spherical W shell 2cm thick

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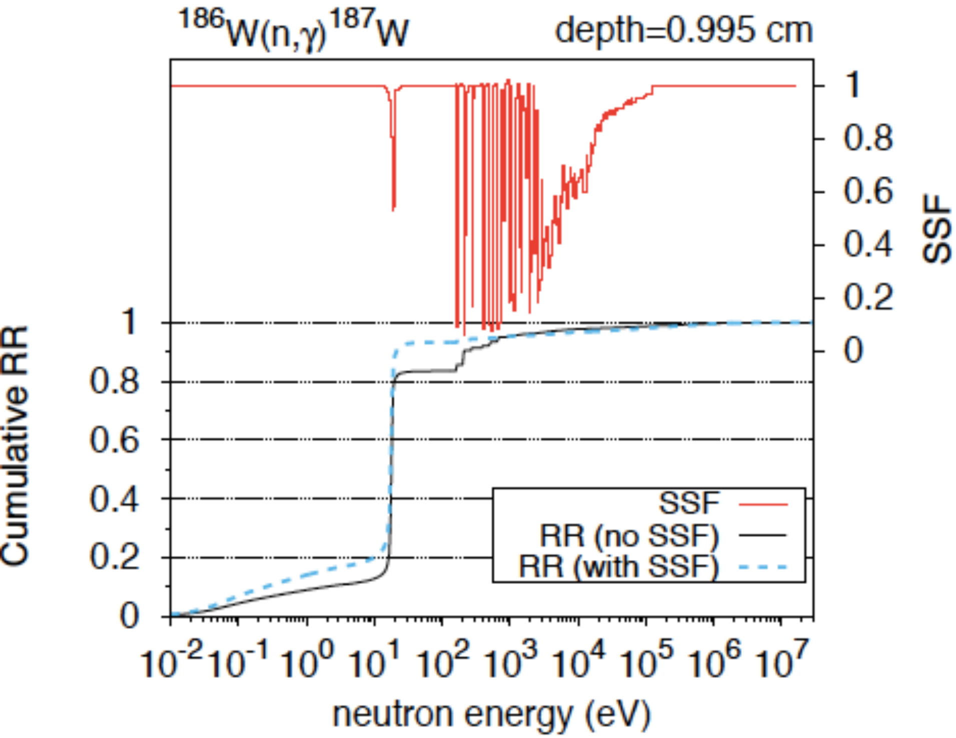

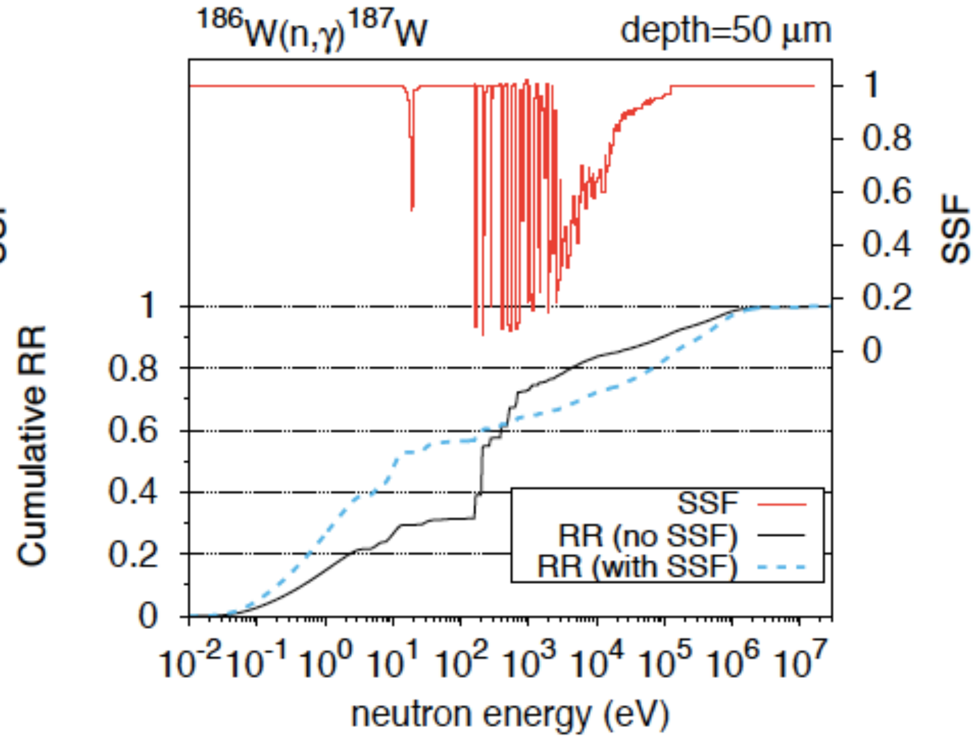

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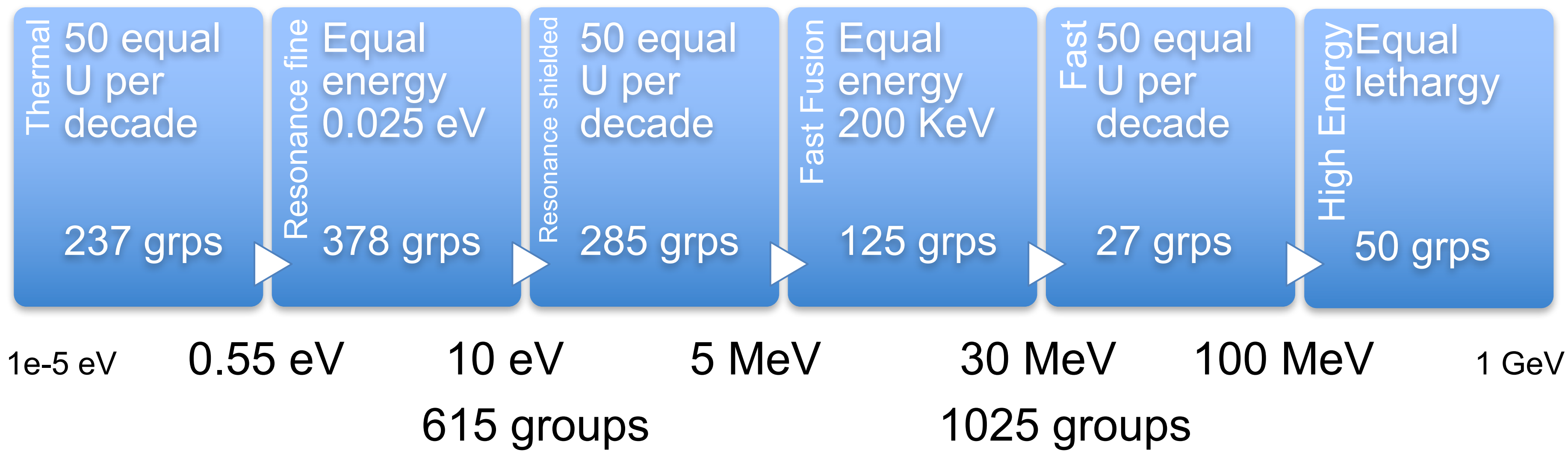
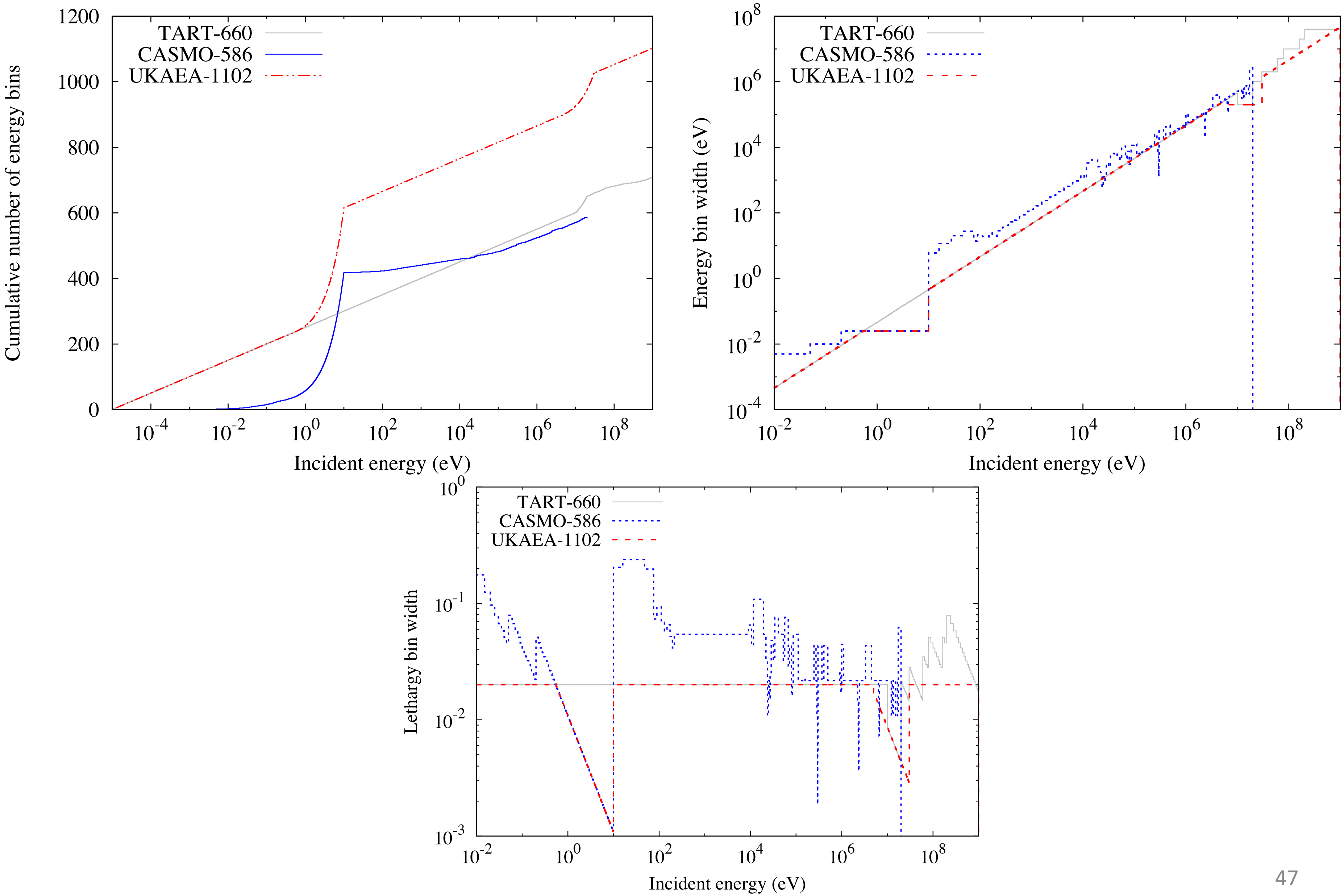
Group structures

- For all target nuclides
- 1102 energy groups for all applications alike

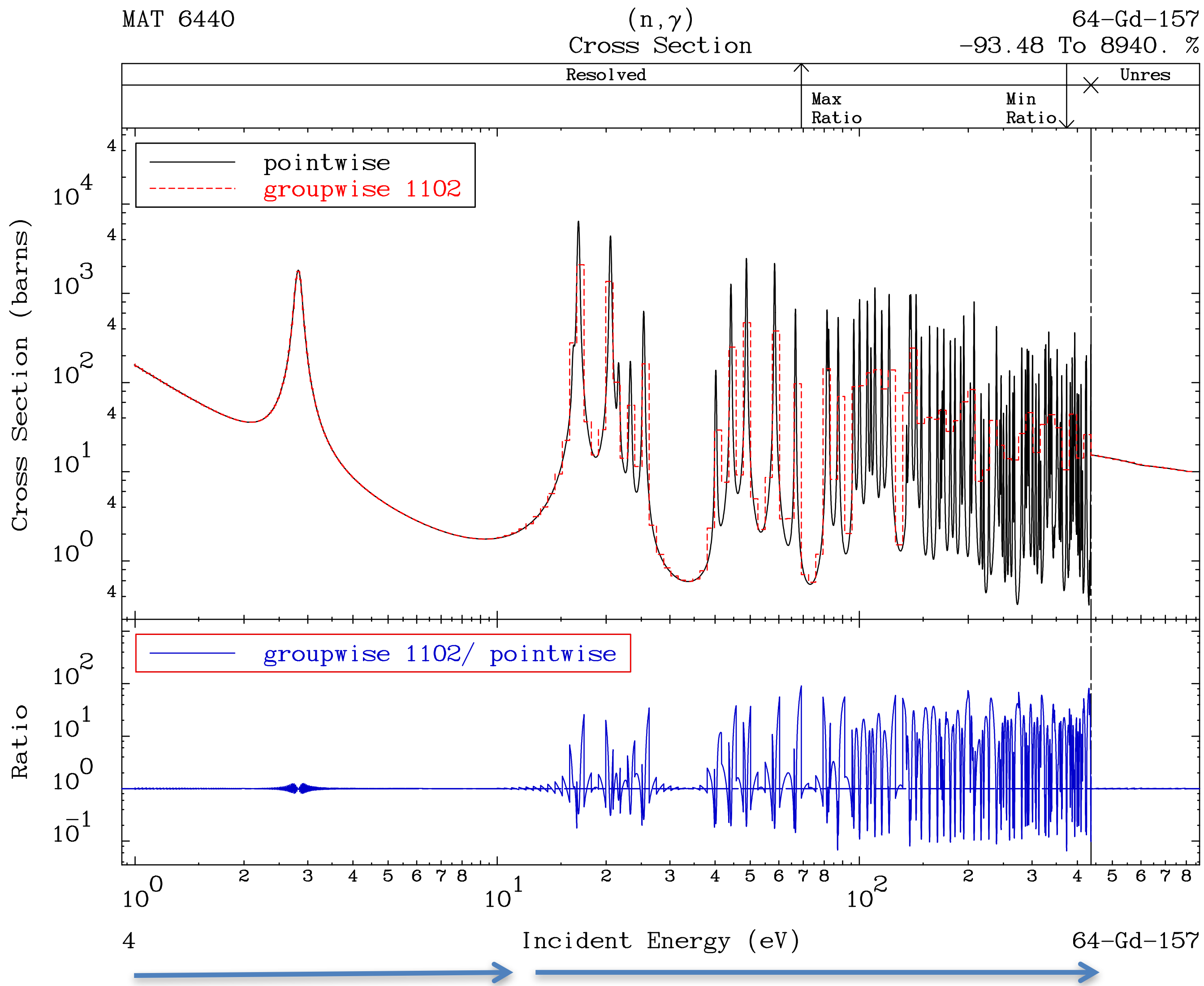


- 378 fine groups in the resonance range
- Resonance shielded data available in the RRR (0.1 eV) up to the end of the URR for all nuclides IDs
- Fast fine structure for accurate threshold reaction rate

Group structures

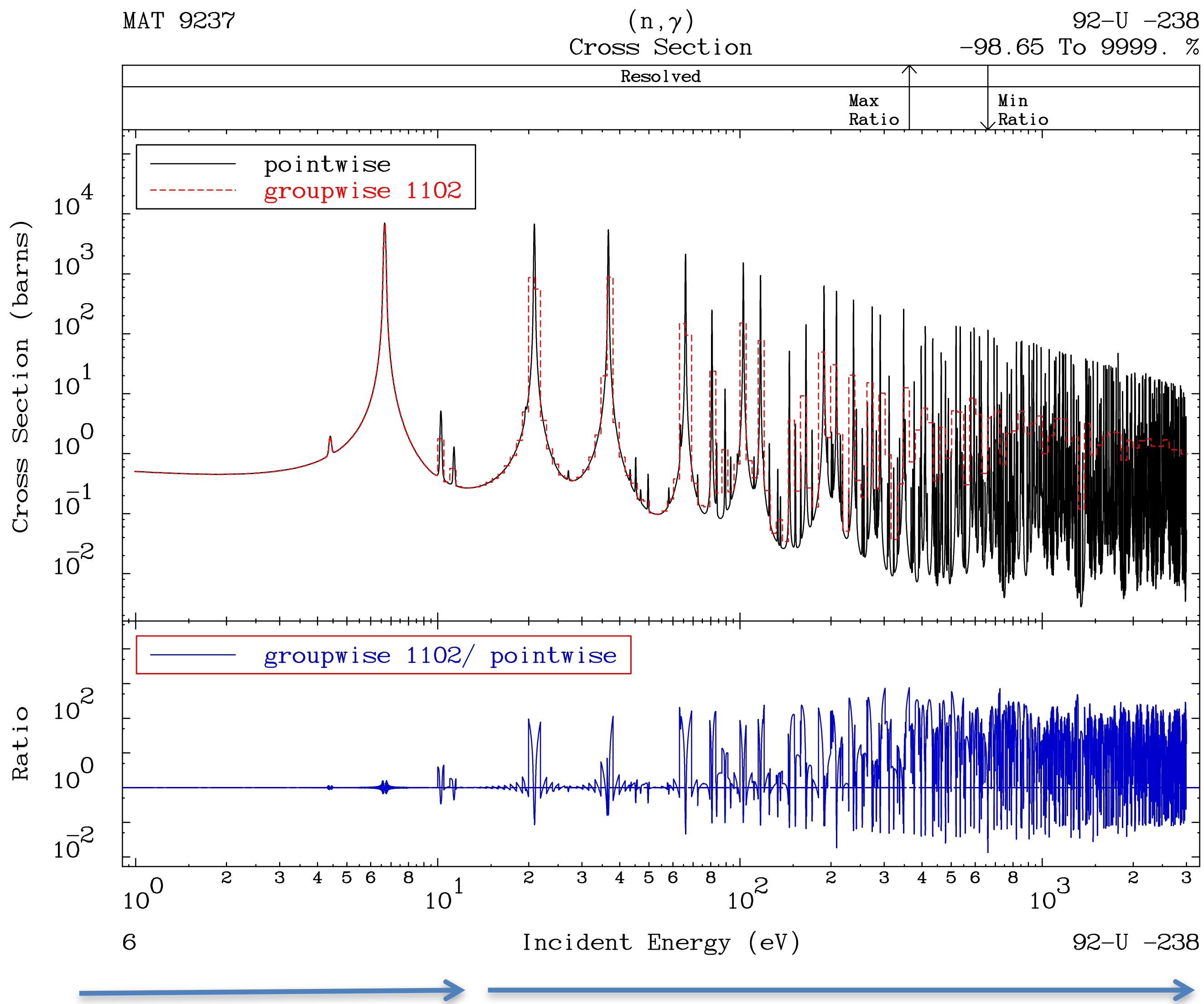


Group structure: 1102



Fine group to 10 eV Resonance shielded to end of URR

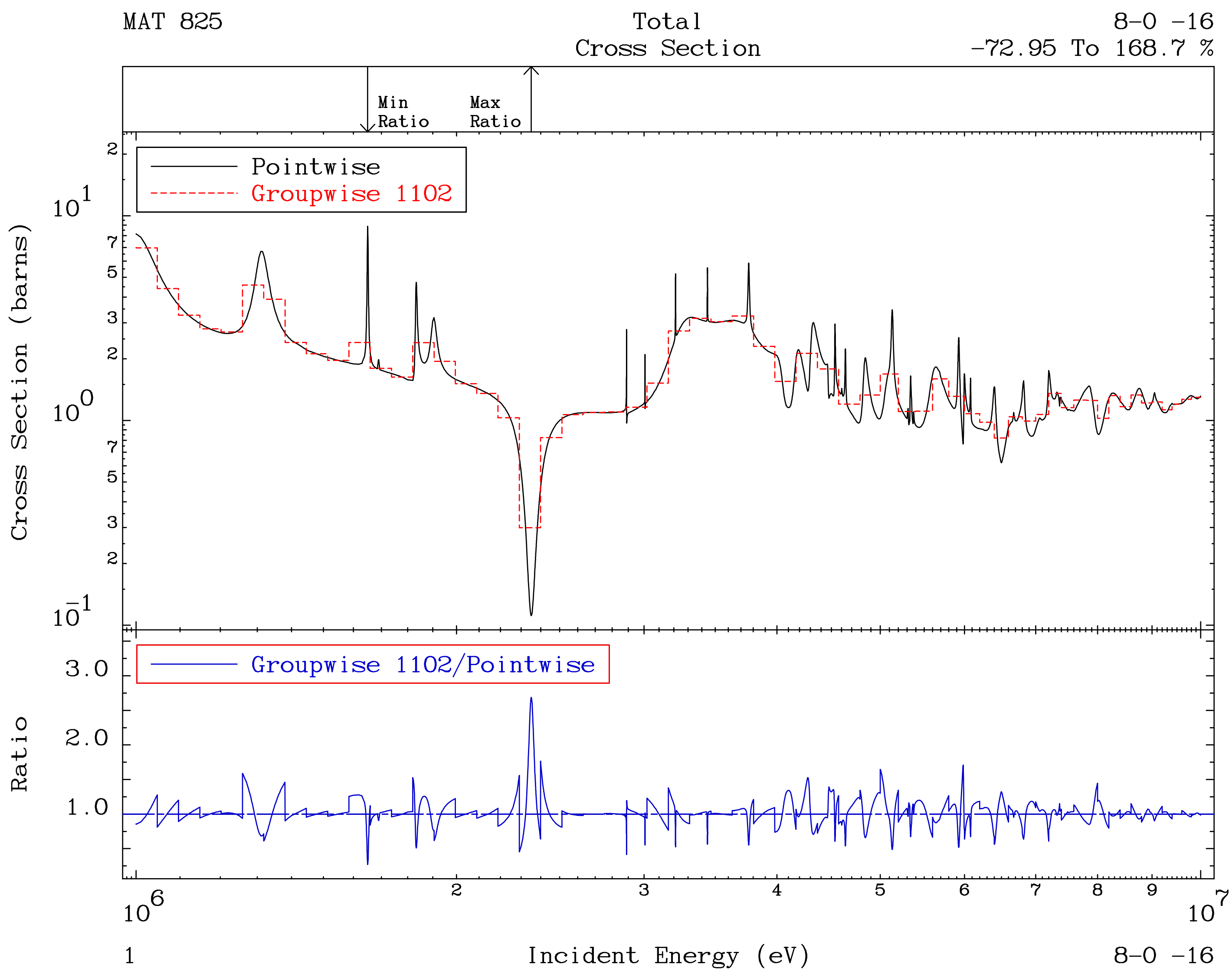
Group structure: 1102



Fine group to 10 eV

Resonance shielded to end of URR

Group structure: 1102



Peak and trough are well described

Work plan

- Clearly spell out the pitfalls
  - Collapsing process
  - Flux tails, high and low, influence on RR
  - It is much more difficult to converge a RR than a Keff

- Reference input spectra database

- UQP reaction rates uncertainty quantification
  - Cross section
  - Effective cross section and SSF (the forgotten factor)
  - Binned flux, standard deviation