IAEA 60 Years
Atoms for Peace and Development

Fission applications: reactor physics

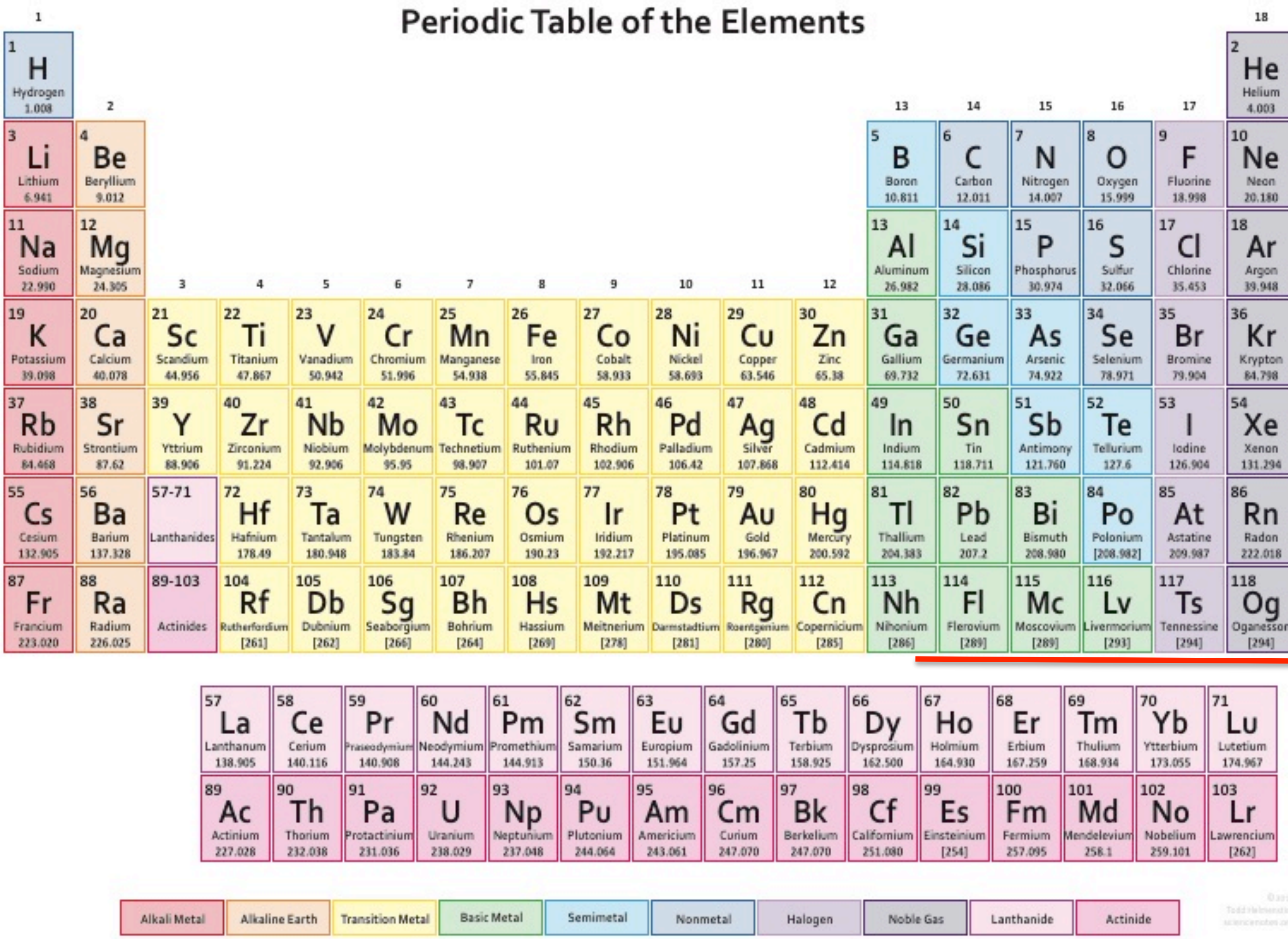
Dr.Eng. Jean-Christophe C. Sublet

International Atomic Energy Agency
Nuclear Data Services Unit Head
Nuclear Data Section

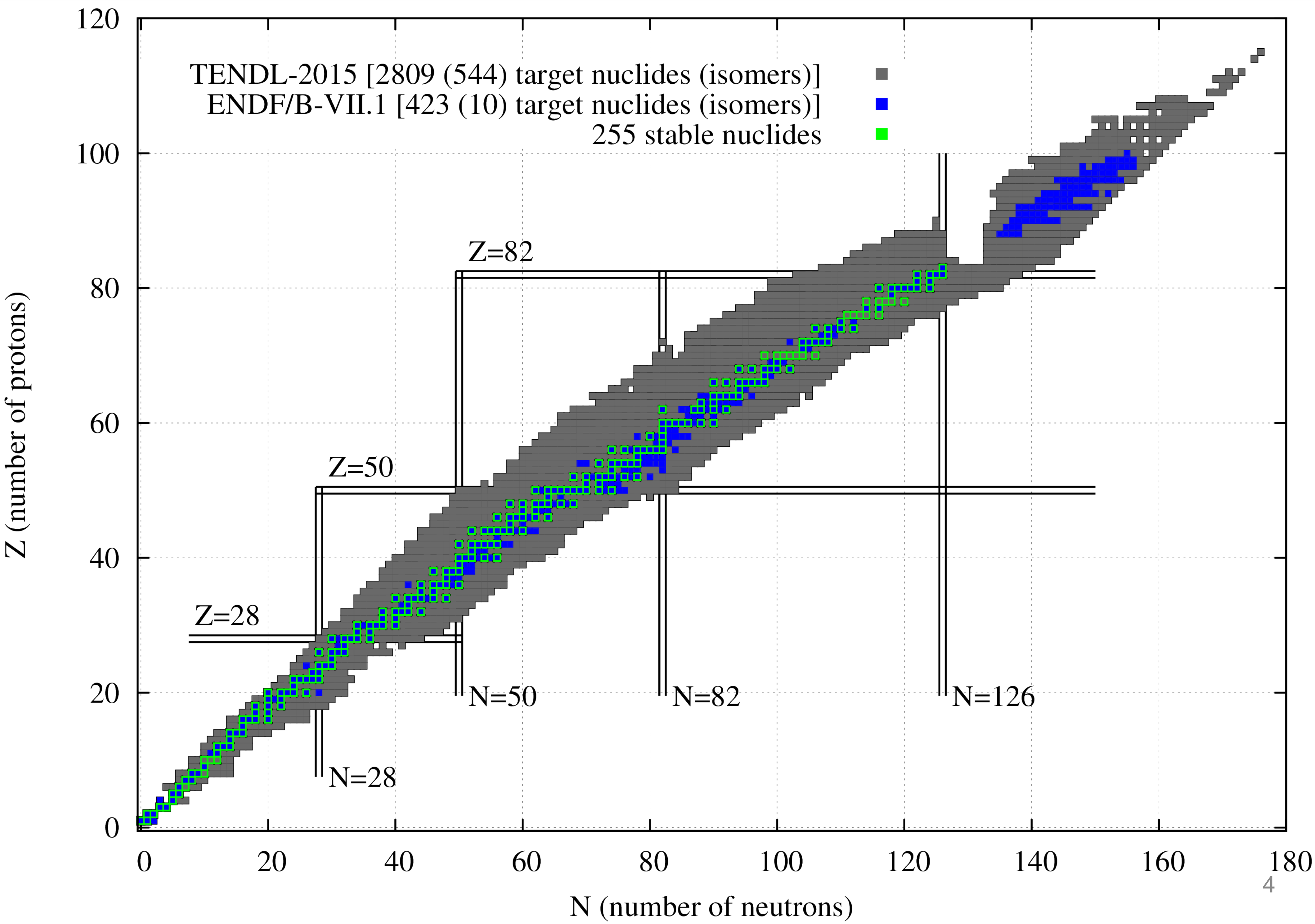
Outline

- Introduction
- Fission processes
  - Spontaneous, particle induced
  - Cross sections
    - Total and partials
  - Emitted particle yields and spectra
    - Prompt, delayed; independent and cumulative
    - Nu, nubar, prompt fission neutron spectra
  - Fast and thermal
- Nuclear data libraries and processing issues
- Reactor parameters and associated uncertainty
- Fissions processes modelling in reactor physics:
  - Neutronics; reactor engineering
  - Terminologies: pcm, mill-k, millinile, millirho
- Reactor types, piles, criticality issues
  - Deterministic
  - Monte Carlo
- Neutron balance and neutron maps
  - Pin power, Power maps
  - Production, absorption and leakage
- Reactor anti-neutrino anomaly

Nuclear landscape: elemental periodic table

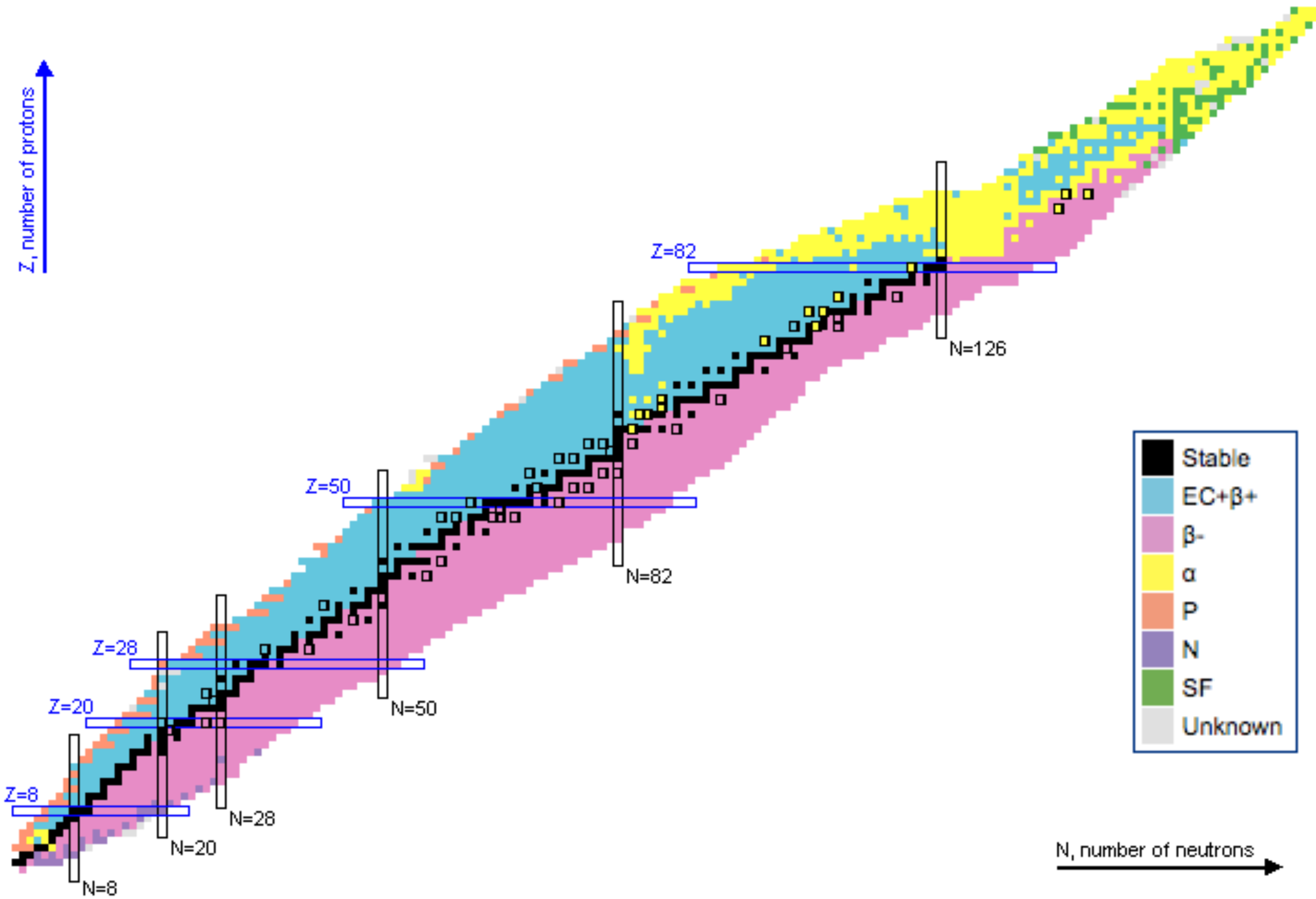


Nuclear landscape: Isotopic targets



Nuclear landscape: decay data

3873 isotopes (23 decay modes; 7 single and 16 multi-particle ones)



Some LWR parameters

- 1000 MWe, 2900 MWth Typical, 3-4 M€
- Fuel enrichment: 1.8 – 2.4 – 3.1 % mass, 82 ton of $U0_2$
- 3.1 10^{10} fission/s = 624 10^{10} MeV/s ~ 1 Watt
- Heavy isotope production: in order Pu239, U236, Pu240, Pu241, Np-237, Pu242,…
- Pressure 155 bar, T_{in} 292 C, T_{out} +53 C
- Combustion: 33 – 45.000 Mwd/Te
- Mean power
  - assembly 17.7 MW
  - pin 67,2 kW
  - Linear 180 W/cm
  - Surface 60 W/cm2
  - Volume 338.6 W/cm3

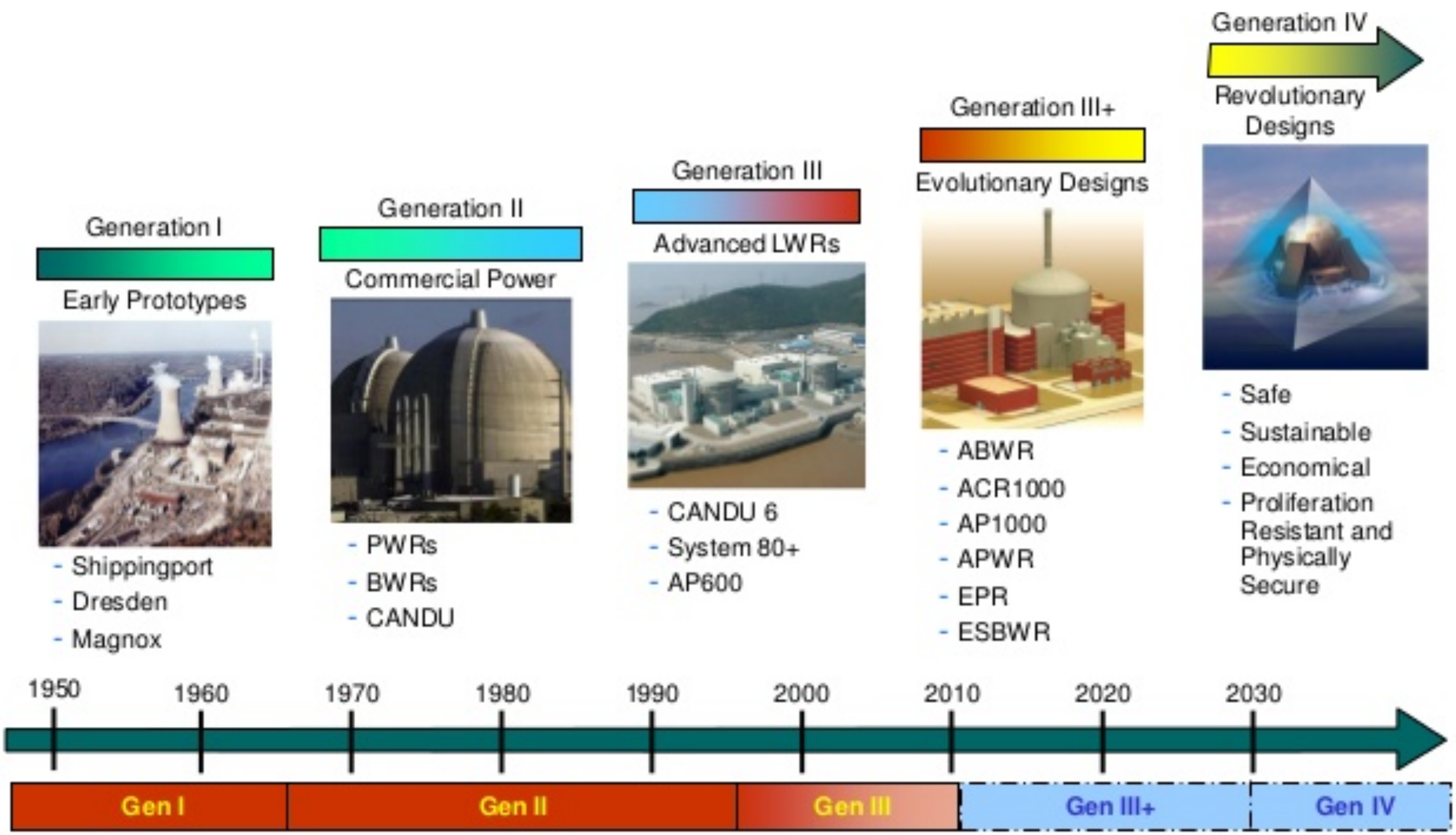
444 (96) power reactors in the World (March 2017)

LWR types

Types:	Operating	Planned
– LWR's:		
• PWR	287	77
• BWR	78	6
– Gas cooled, GCR's:	14	1
– Heavy water, PHWR's:	48	9
– Graphite moderated, LGR's	15	0
– Liquid metal cooled, LMFBR, LMR	2	3
– Total	444	96
– No longer in service	156	
– Research reactors, piles 768 (-360)	216	11

Generation of reactors

- GEN IV = Sodium Fast R's, Very High Temperature R (triso), Small Modular R's, Molten Salt R's



Introduction

- The importance, treatment of the fission processes differs depending on the applications, but the physic principles underlying them do not
  - fission cross-sections
  - energy dependence, fission chances
  - prompt, delayed neutron multiplicities
  - prompt, delayed emitted neutron spectra
  - fission products yields for typical reactor applications @ thermal
  - prompt, delayed gamma radiations
- For reactor physics fission is a must (to bank 200 MeV per event) but it faces stiff competition (fortunately) from another usually open channel in the same energy range: radiative capture
- In the fuel $U0_2$, fission is on U^{235}, while capture is on U^{238}

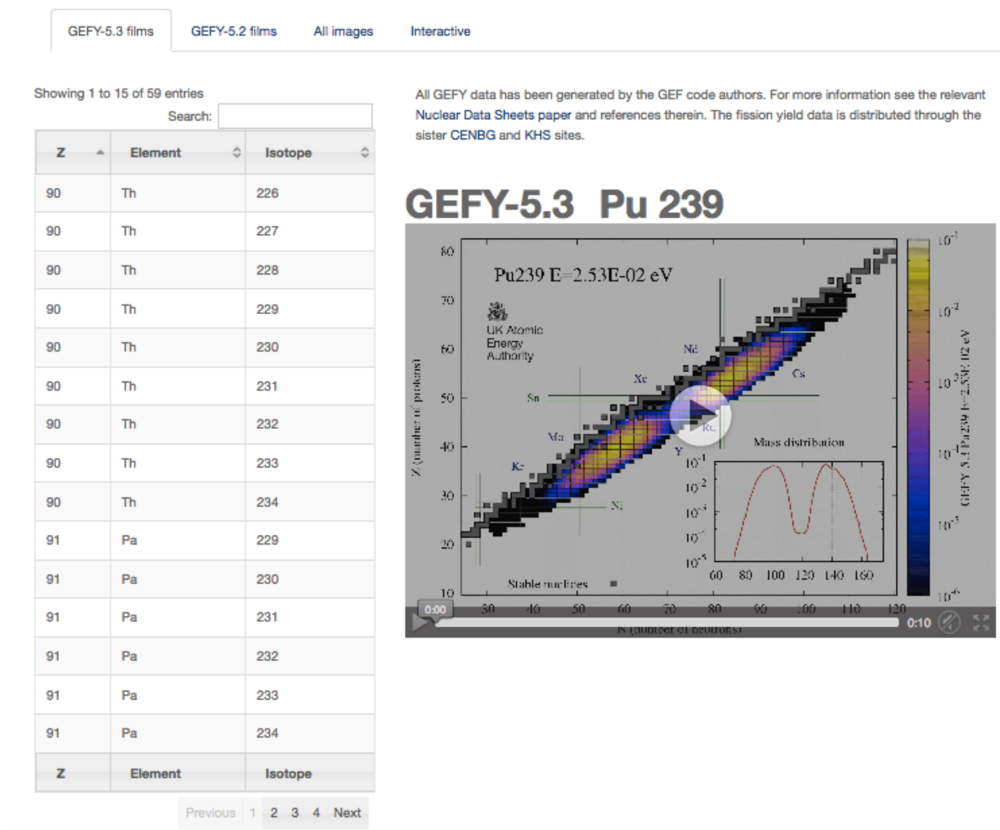
Introduction

- The importance, treatment of the fission processes differs depending on the applications, what is missing:
  - isotropic, really all events !!
  - fission fragments angular/energy distributions
  - time dependent energy release rates
  - multi-chance fission (n,n'f), (n,2n'f),….
  - fission on non-actinides, the lesser fissile
- For reactor physics fission, all the above are of little interest, what is in fact important are
  - the energy release(s) and fission neutron maps during operation and shortly thereafter (accidental scenarios also)
  - the fuel burnup rate, the poisonous fission fragments that capture the neutron that should induce another fission

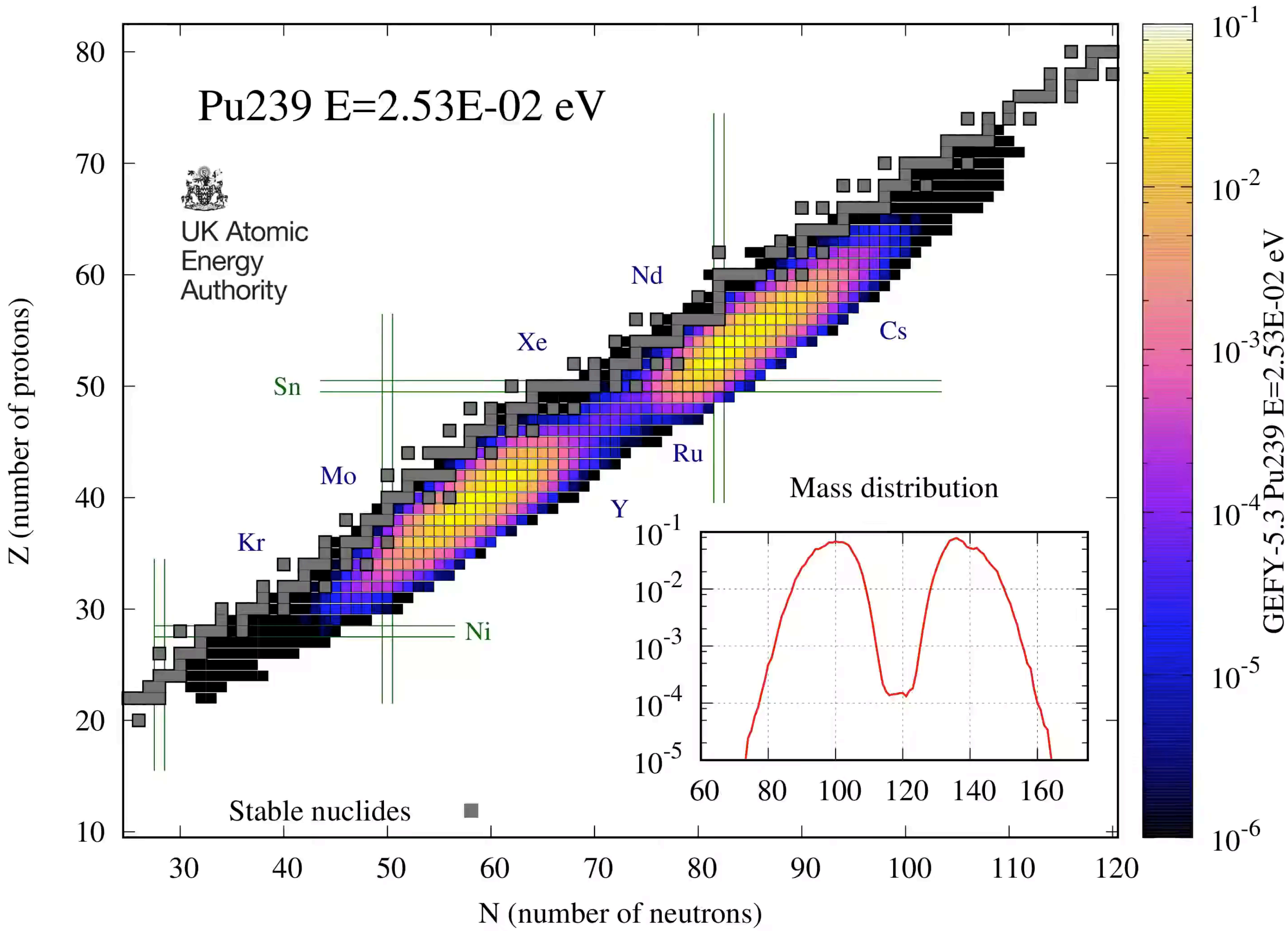
IAEA 60 Years Atoms for Peace and Development

Visualization tools: fission yields

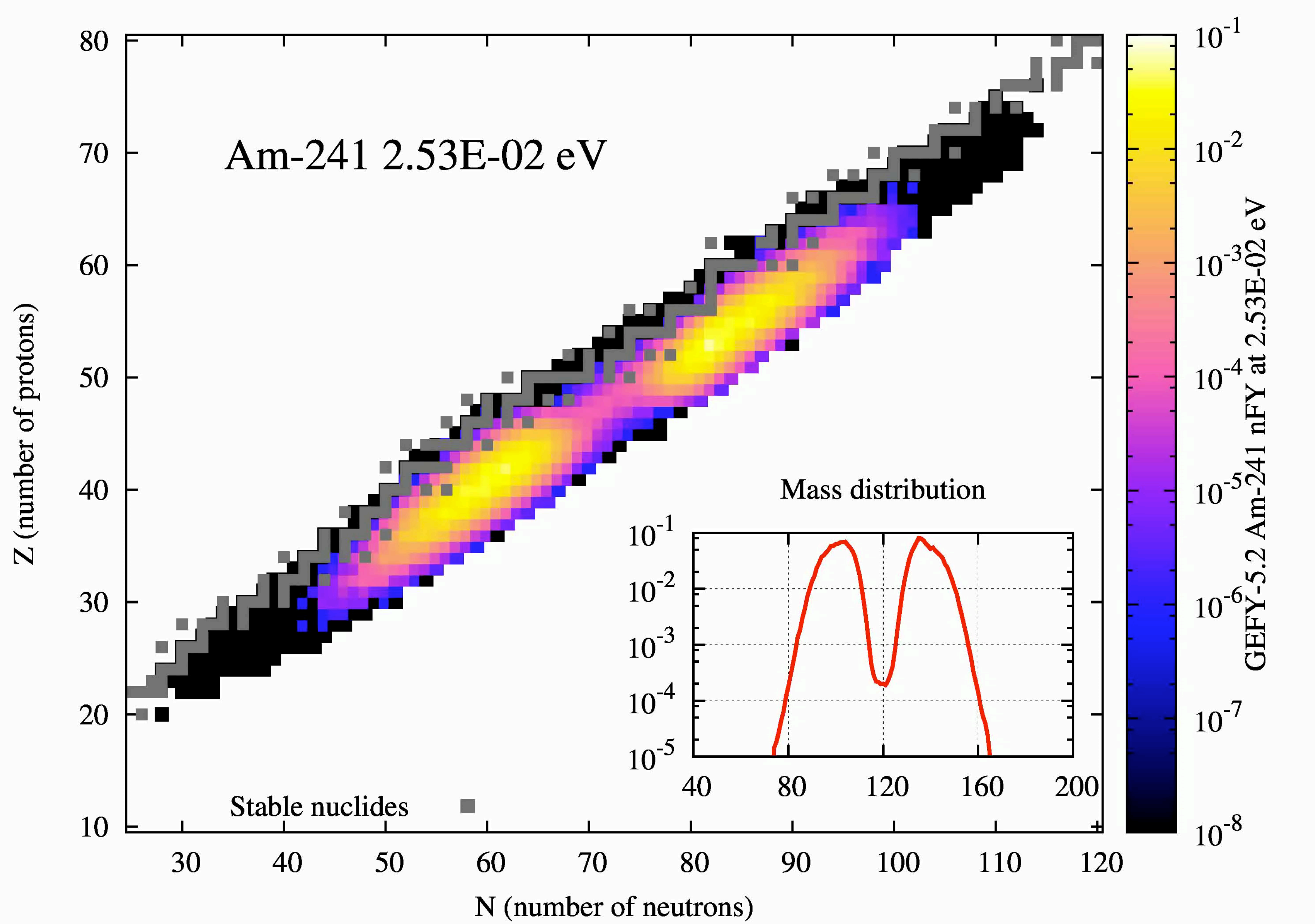
- Searchable database of fission yield data with visualizations
- Plotly based interactive data interrogation in development
- There are some benefits in scrutinizing the data



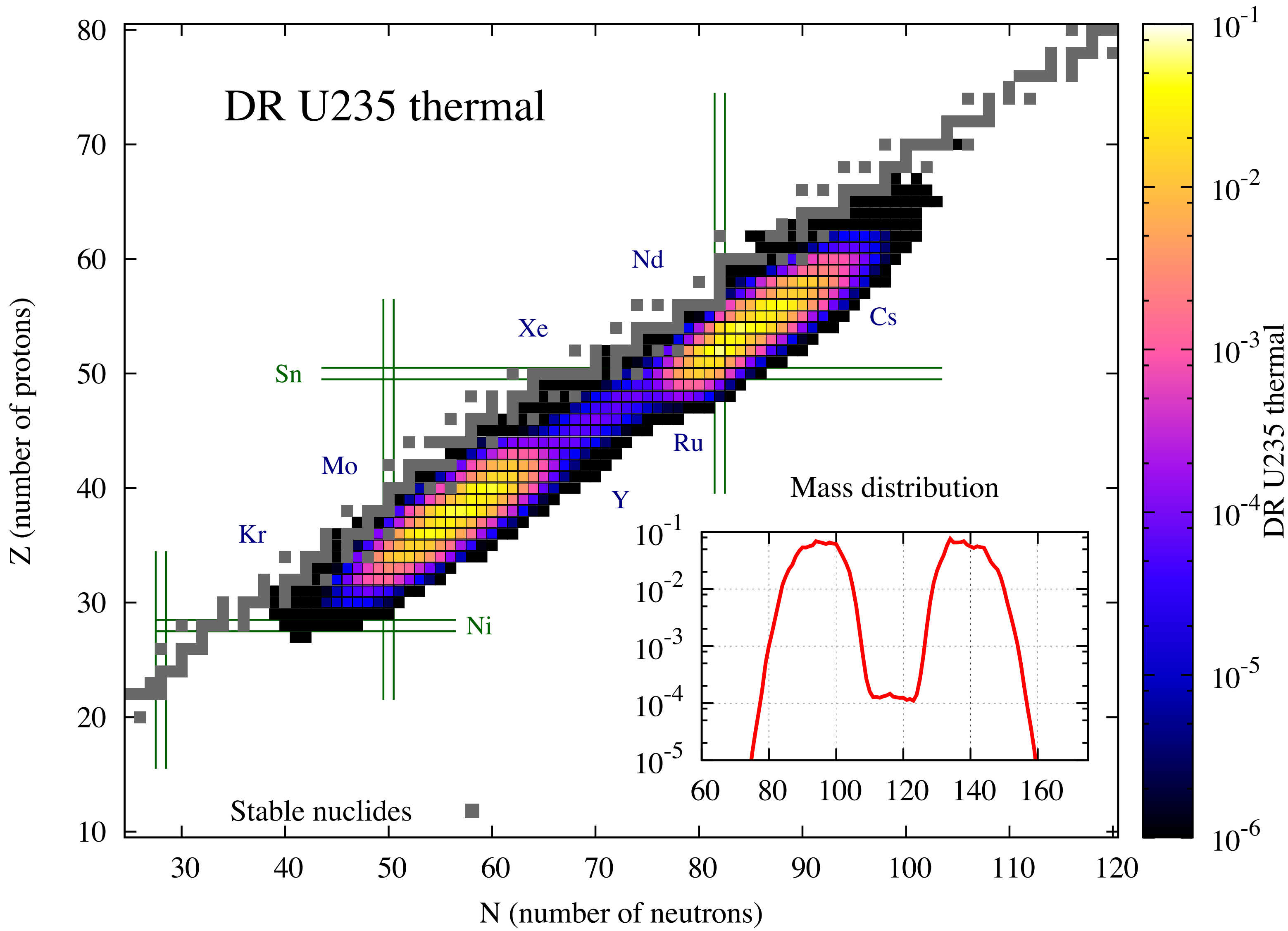
GEFY-5.3 Pu239



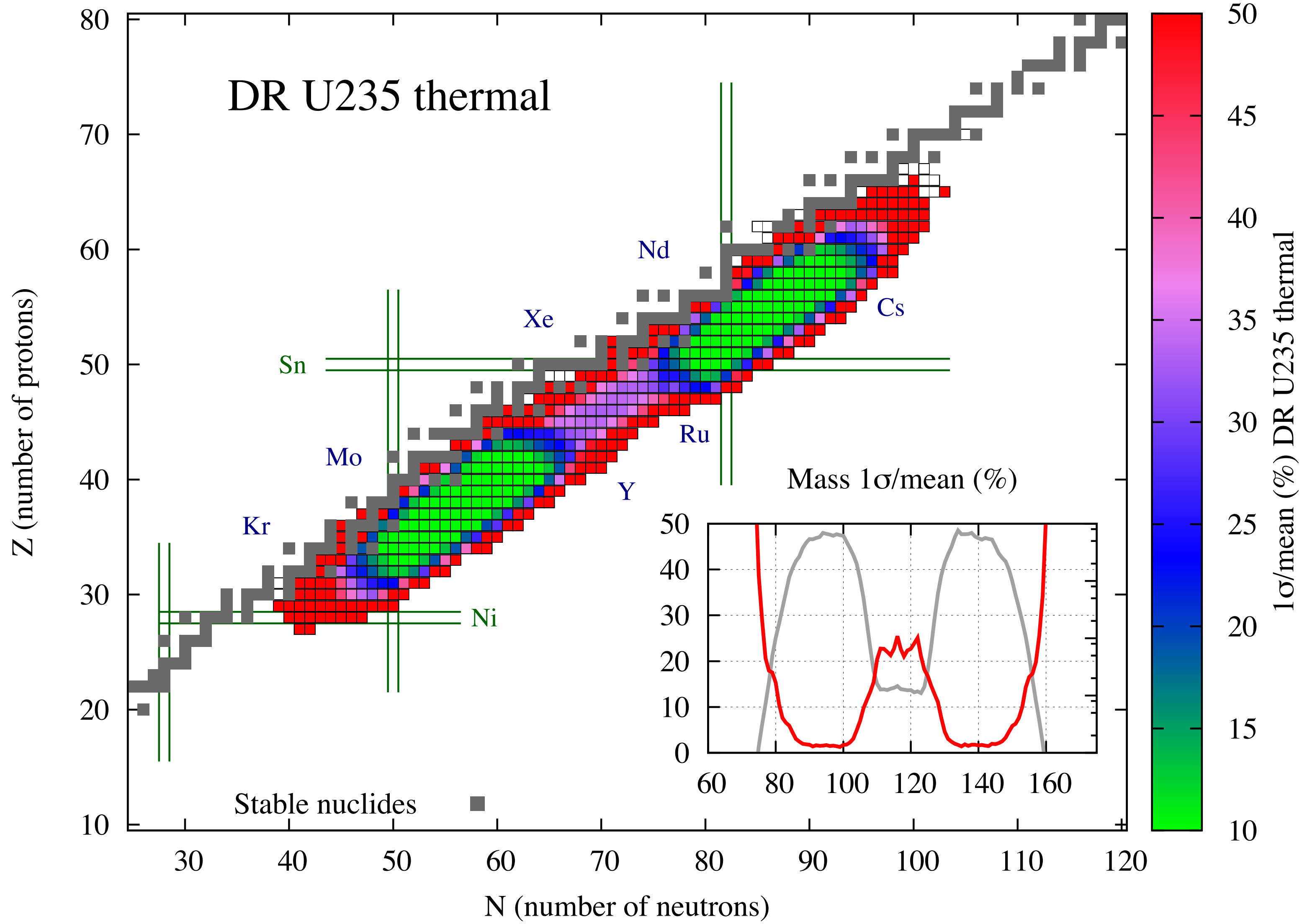
GEFY-5.3 Am241



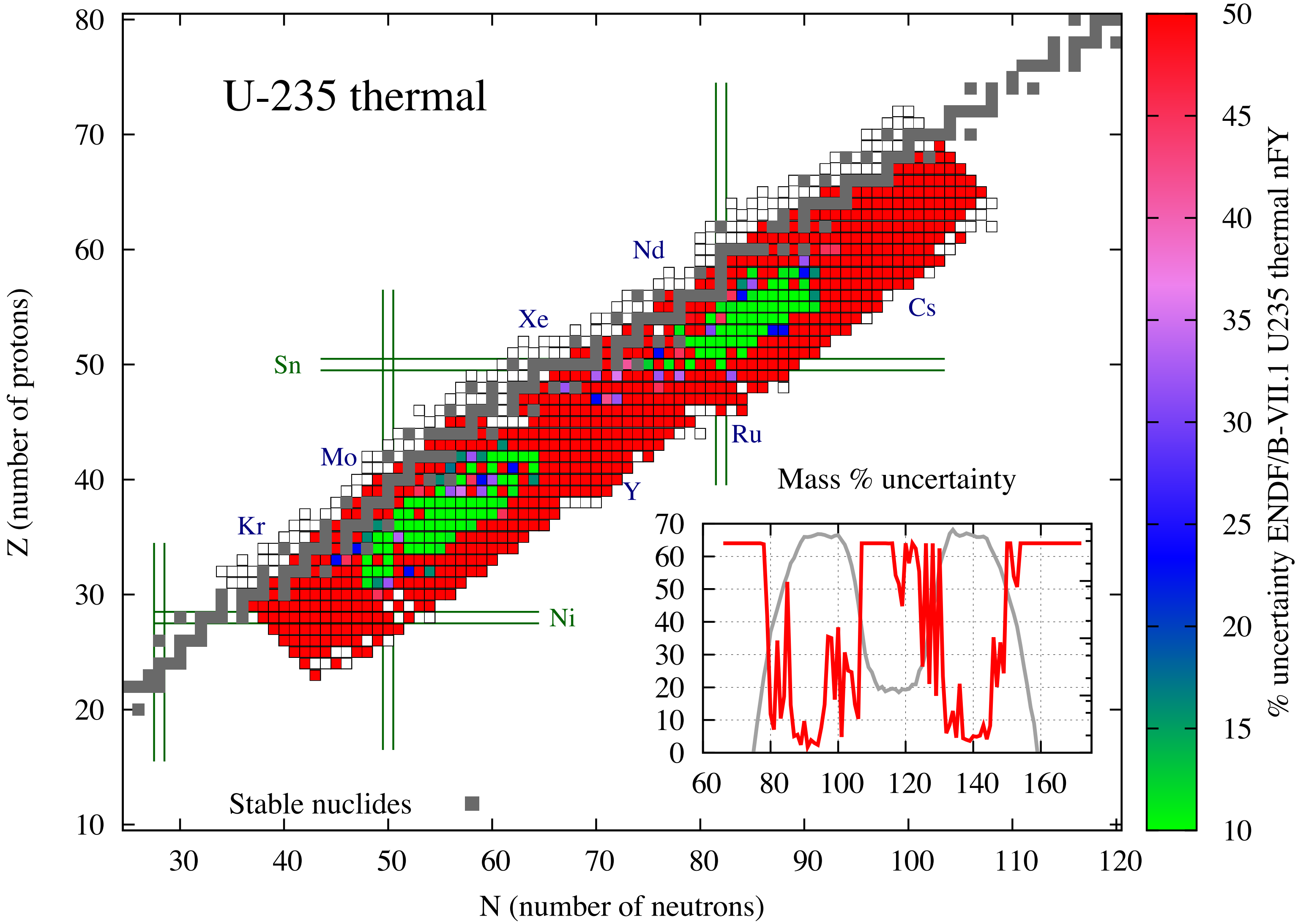
U235 FY's @ 0.0253 eV



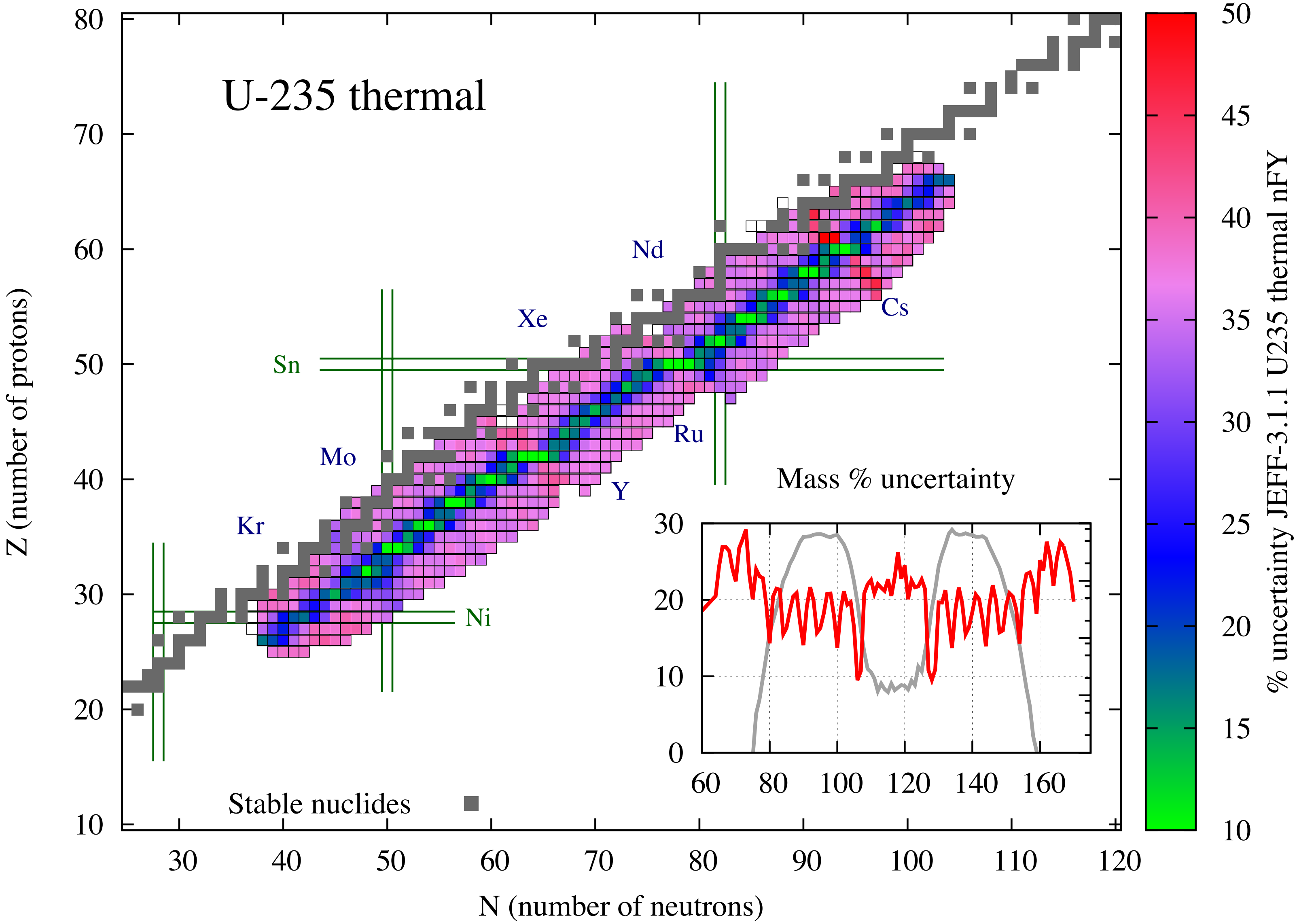
U235 FY's uncertainty @ 0.0253 eV



U235 FY's uncertainty @ 0.0253 eV



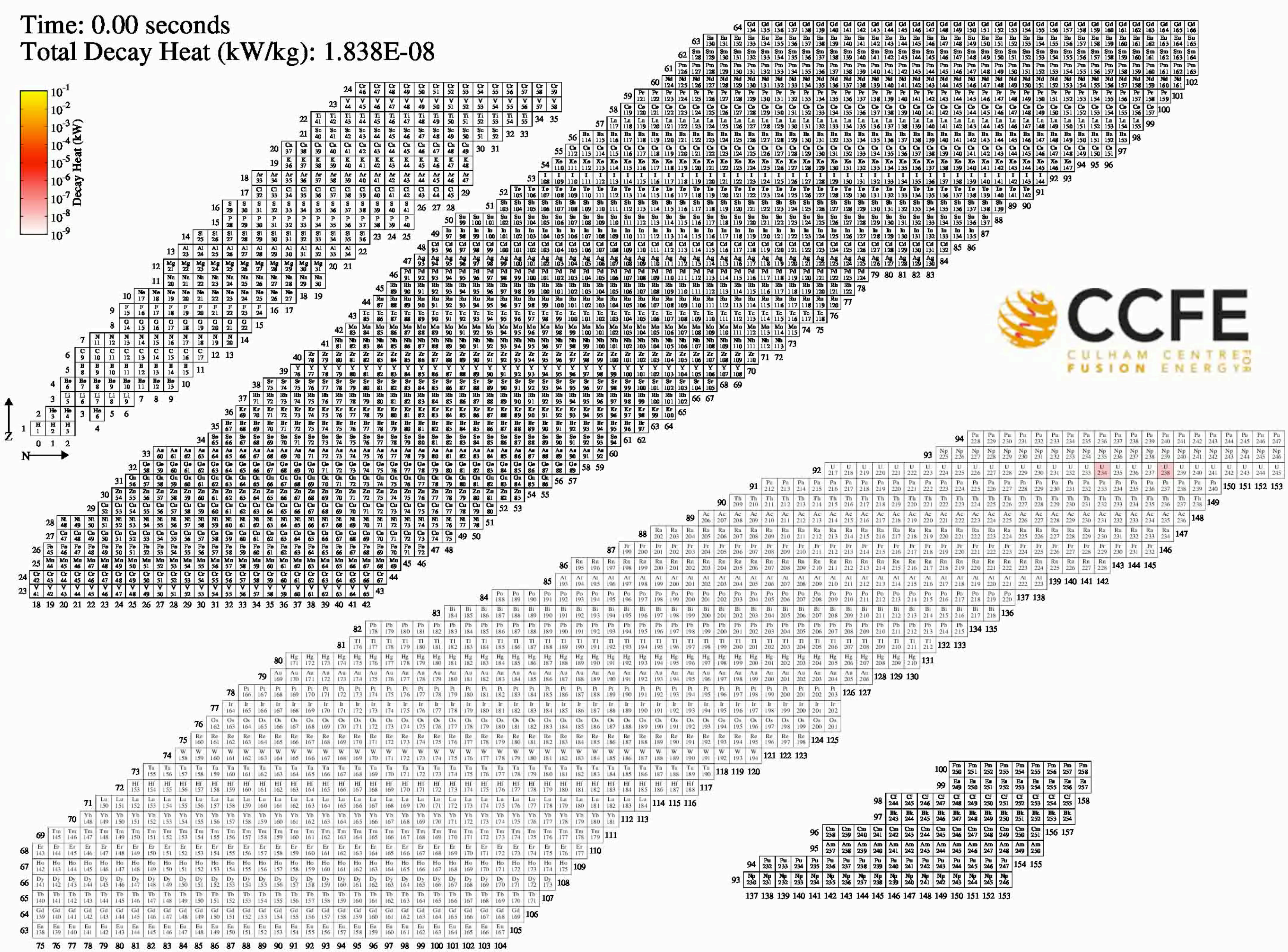
U235 FY's uncertainty @ 0.0253 eV



Pu^{239} fission pulse

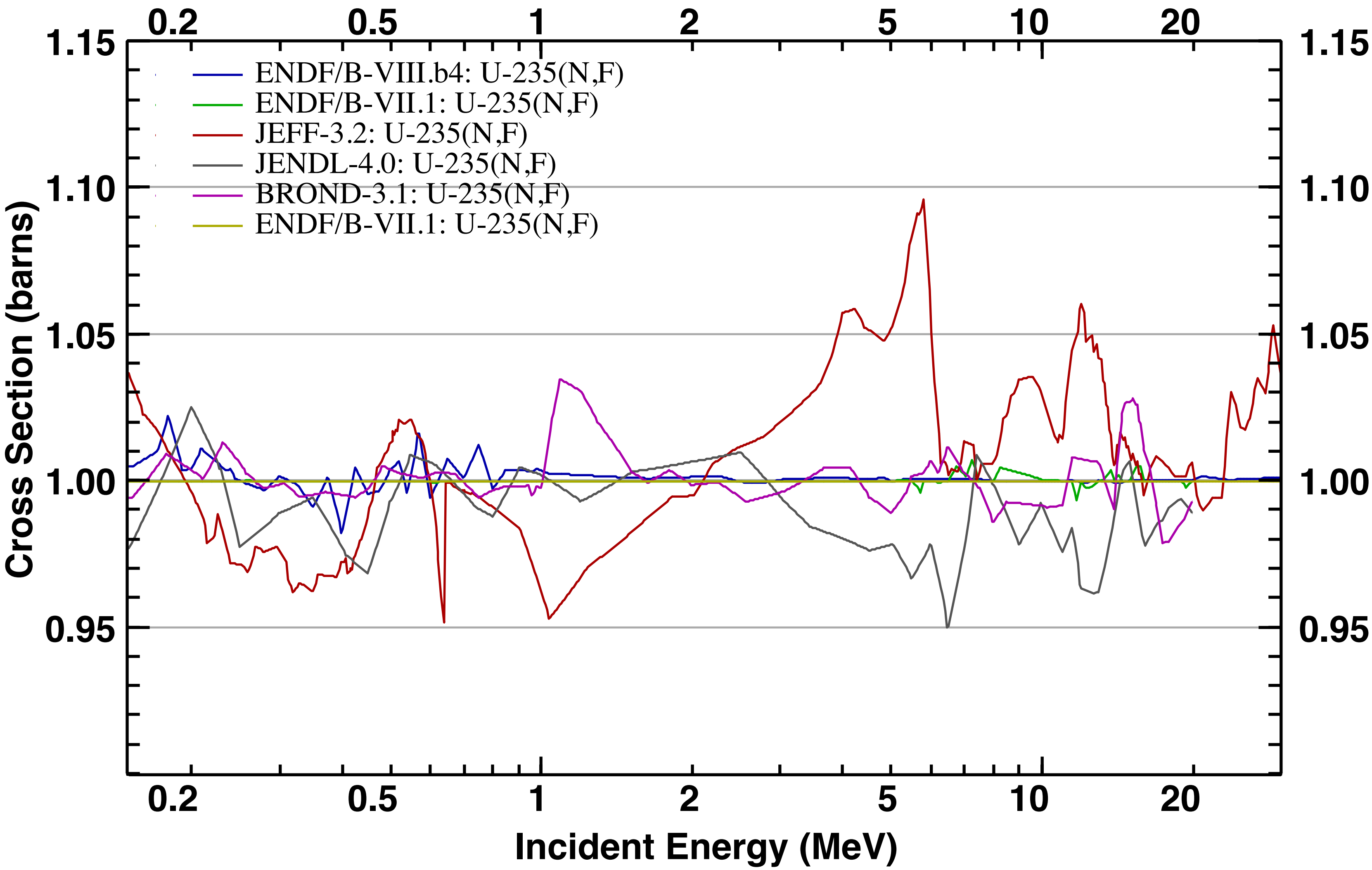
CCFE
CULHAM CENTRE FOR FUSION ENERGY

U^{235} Fission, 1 year



CCFE
CULHAM CENTRE FOR FUSION ENERGY

Fission cross section(s) in files



Nuclear data libraries and processing issues

- ENDF/B-VII.1, JENDL-4.0, JEFF-3.2, TENDL-2015, GEFY…
  - fission cross sections mf-3 mt-18,19-21,38
  - multiplicities mf-1 mt-452, 455 delayed,456 prompt
  - energy releases for fission mf-1 mt-458
  - neutrons spectra mf-5 or mf-6

  - nFYs and sFYs mf-8 mt-454,459
    - independant and cumulative fission yields
    - Incident-grid usually 0.0253 eV, 400 KeV, 14 MeV
    - tabulated 59 incident energies (GEF)
    - with uncertainties !!! on the fitted (to experiments) cumulative yields

Nuclear data libraries and processing issues

- Using NJOY, PREPRO or CALENDF
  - from mf-2 parameters to pointwise data in mf-3
  - from mf-2 parameters in the URR to PT's SSF (Monte Carlo)
  - from mf-5 distributions laws to tabulated
  - from mf-3 to groupwise data
  - from mf-2 parameter to SSF's (Bondarenko)
  - from mf-3, mf-4/mf-5 or mf6 group matrices

- This of course assumes that the evaluator, then the processor are aware of what the reactor physicist needs exactly or can cope with. Usually the latter need to know, but not the first !

Processing steps: three codes

ENDF file

- **NJOY12-099**
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
    - purr
    - acer
    - groupr

ACE file

cross-check

- **PREPRO-2017**
  - **linear**
  - **recent**
  - **sigma1**
  - **sixpack**
  - **activate**
  - **merger**
  - **dictin**
  - **groupie**

Processed ENDF file

cross-check

- **CALENDF-2010**
  - calendf
  - regroutp
  - lecritp
  - ….

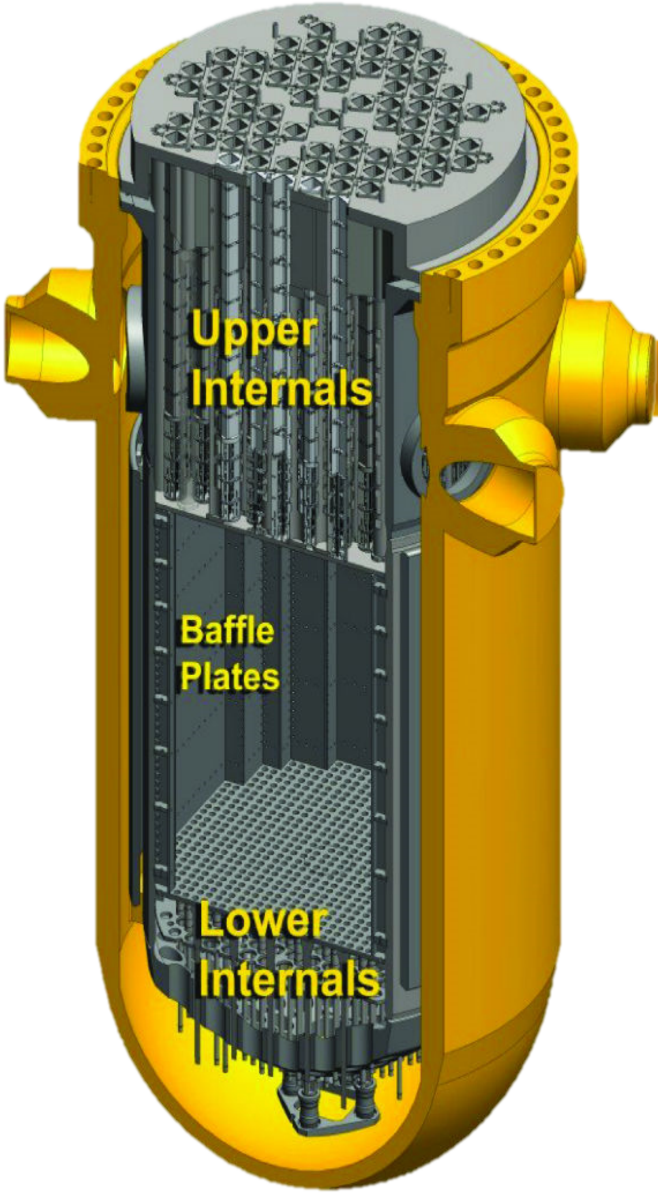
PT file

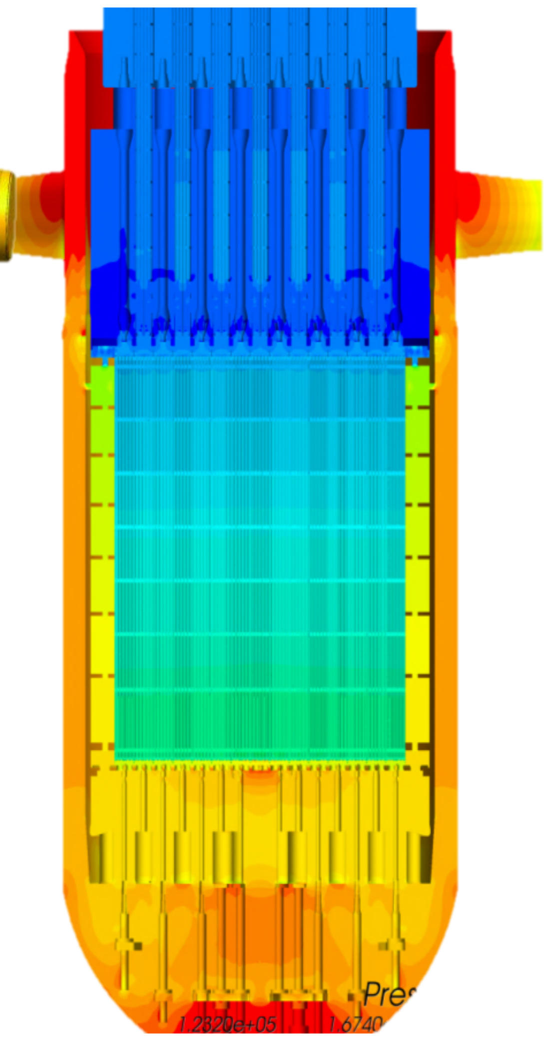
Single script for an entire library

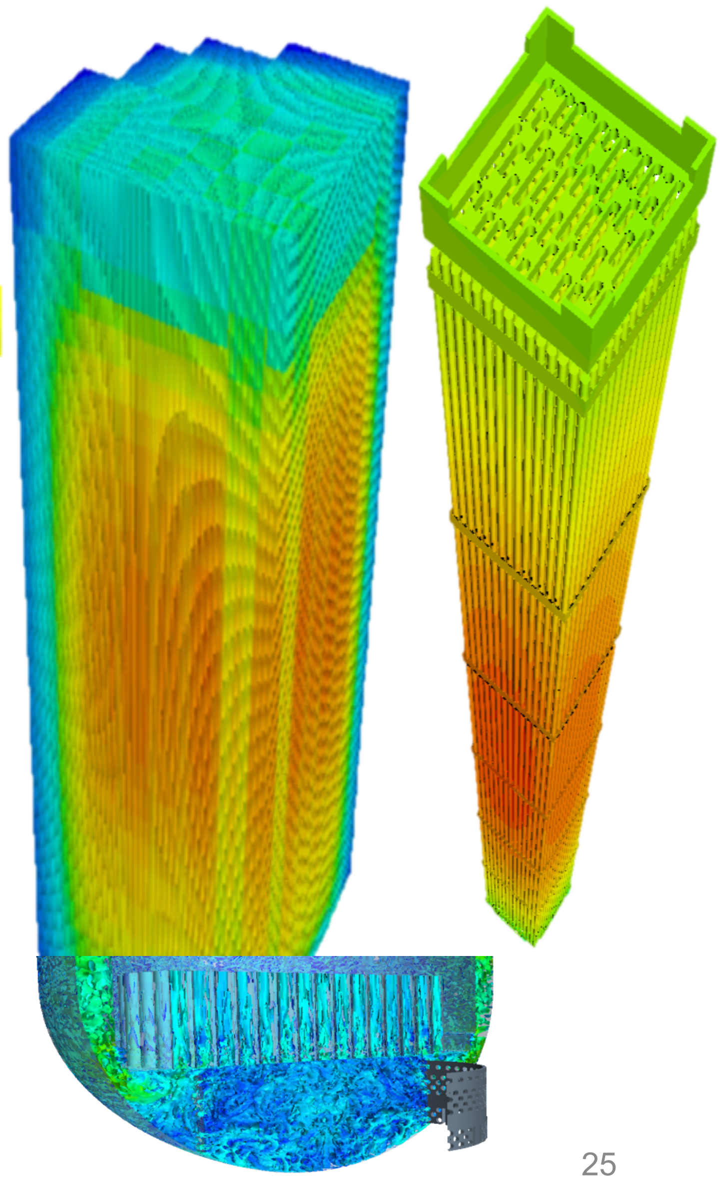
Processing codes

- Reactor simulation software, usually proprietary (non exhaustive list)
  - Pin cell, collision probability, lattice codes: WIMS, APOLLO, CASMO, …
  - Nodal core, MOC (Method of Characteristic): PANTHER, CRONOS, SIMULATE, ...
  - Transmutation: FISPIN, ORIGEN, FISPACT-II, ….
  - Monte Carlo: MONK, MCNP, TRIPOLI, SERPENT, MC21, ….
  - Integrated system: VERA (Consortium for Advanced Simulation of LWR), SCALE (ORNL), ERANOS (CEA), …
  - …
- None of the above can use non-processed, raw nuclear data, so they all rely in parts or in all on the data form(s) outputted by one or more of the processing codes

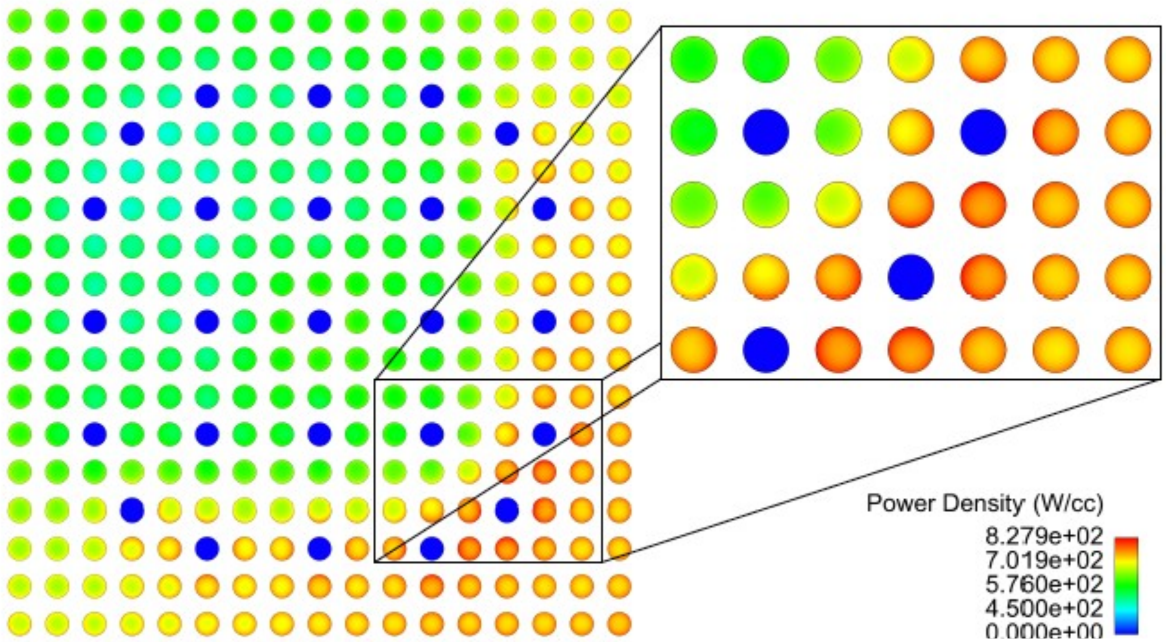
Reactor, pile criticality issues



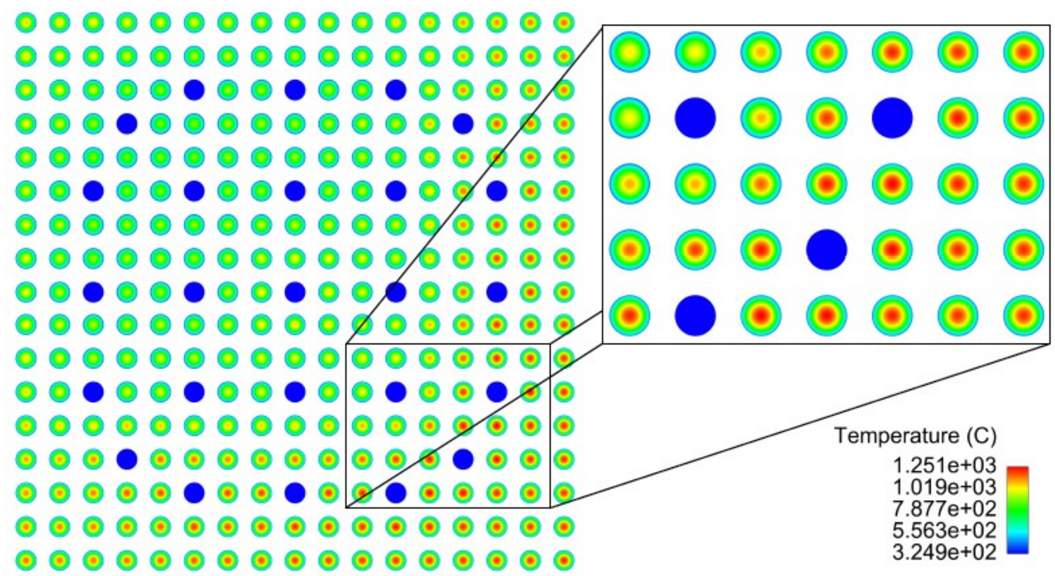




High-Resolution Reactor Core Simulations

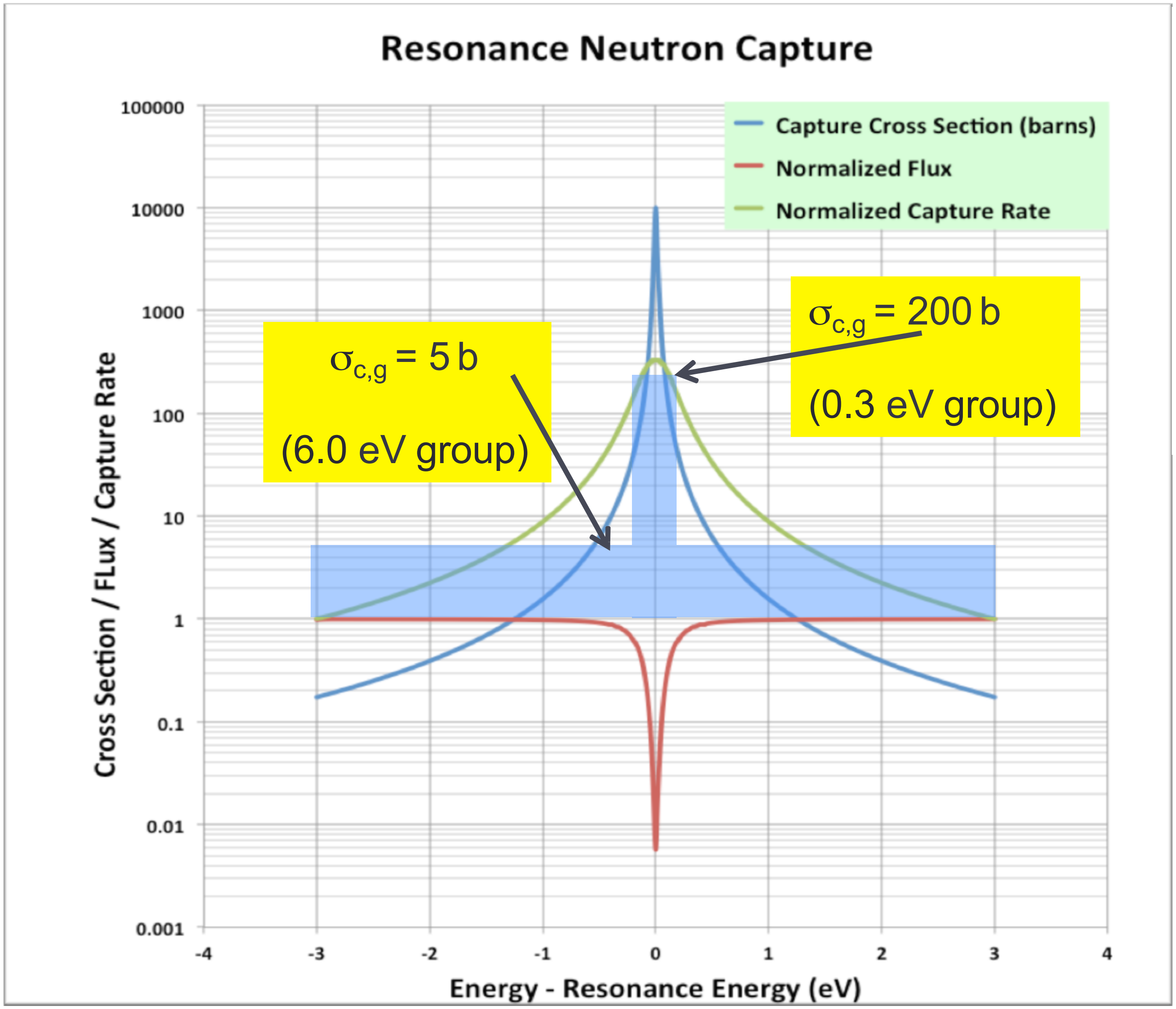


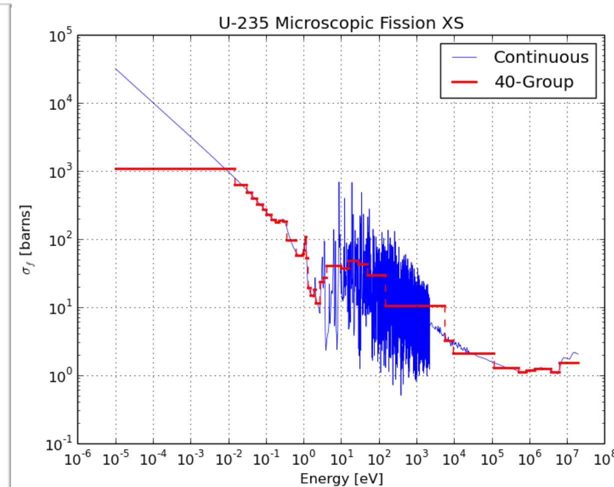
Radial Fission Rates
and
Fuel Temperatures



High-resolution requires full local detail

200 pcm jungle: multi-group resonance XS





$$\sigma_{c.g} \equiv \frac{\int_{E_{g-1}}^{E_g} \sigma_c(E)\,\phi(E)\,dE}{\int_{E_{g-1}}^{E_g} \phi(E)\,dE}$$

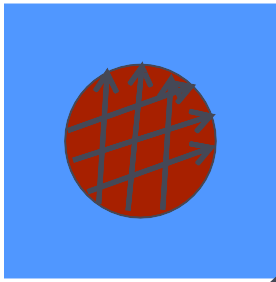
$$\phi_g^{N.R.} = \frac{\left(\sigma_{pot,f}+\sigma_e\right)}{\sigma_{c,g}+\left(\sigma_{pot,f}+\sigma_e\right)}$$

$$\phi_g^{N.R.} \cong \frac{75b}{\sigma_{c,g}+75b}$$

As group width increases, resonance absorption has smaller impact on multi-group flux

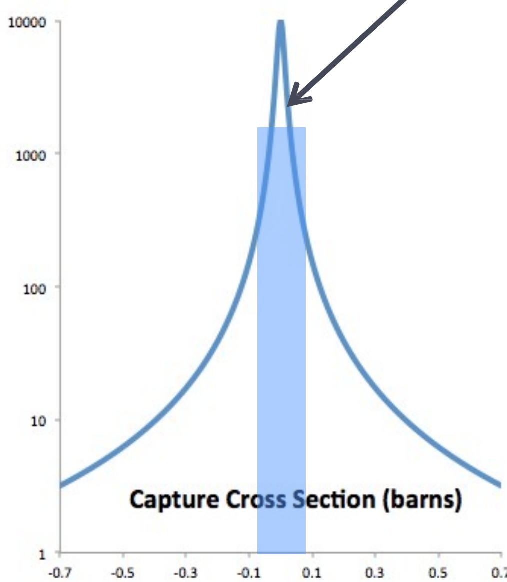
Equivalence for multi-group XS

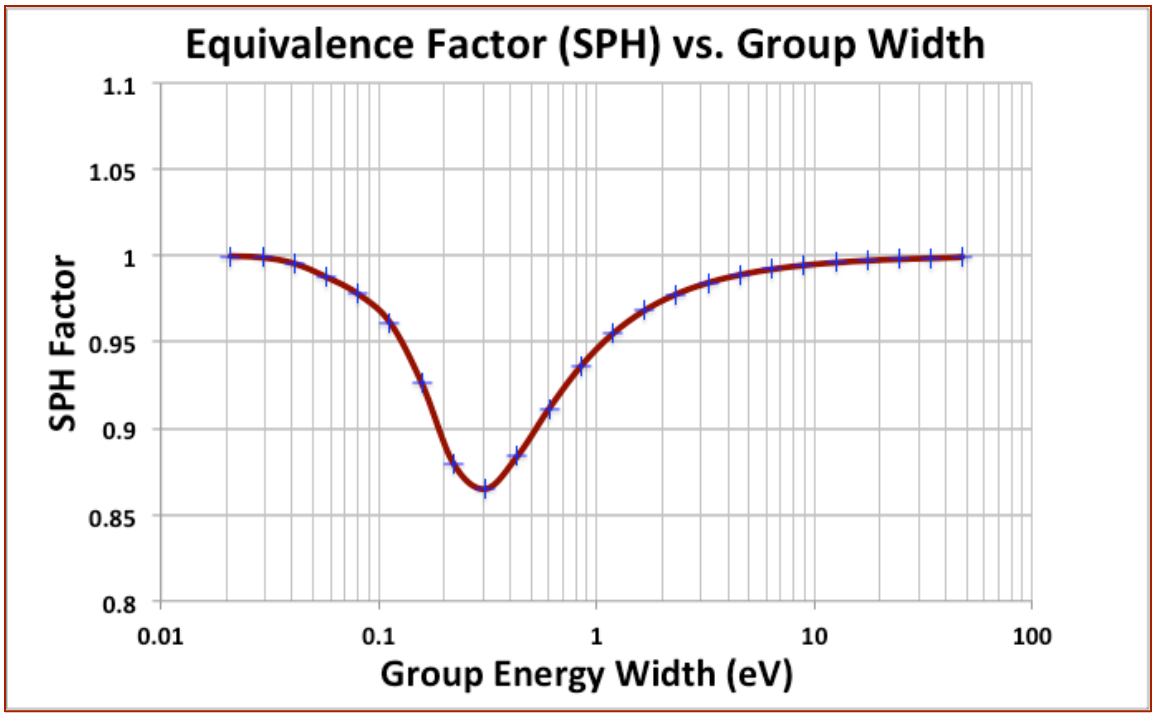
$$\int_{E_{g-1}}^{E_g} \Sigma(E)\,\phi^{MC}(E)\,dE = \Sigma_g\phi_g^{MC} \neq \Sigma_g\bar{\phi}_g^{Multi-group}$$



$$\int_{E_{g-1}}^{E_g} e^{-\Sigma(E)\tau/\propto}\,dE \neq e^{-\Sigma_g\tau/\propto}\int_{E_{g-1}}^{E_g} dE$$

$$\int_{E_{g-1}}^{E_g} e^{-\Sigma(E)\tau/\propto}\,dE \equiv e^{-SPH\cdot\Sigma_g\tau/\propto}\int_{E_{g-1}}^{E_g} dE$$

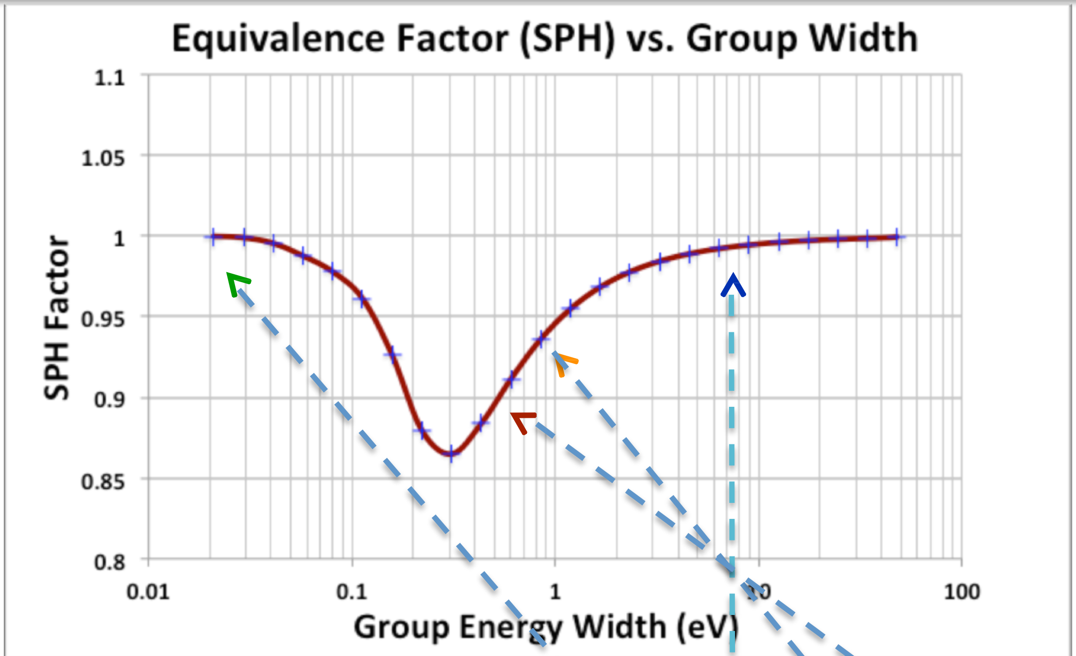


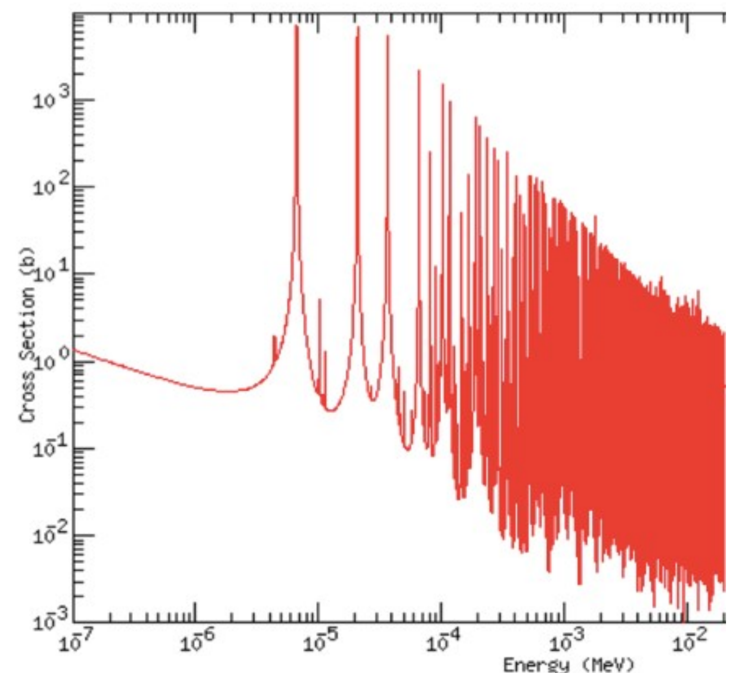


$$\hat{\Sigma}_g \equiv SPH\cdot\Sigma_g$$

$$\Sigma_g\phi_g^{MC} = \hat{\Sigma}_g\bar{\phi}_g^{Multi-group}$$

Selecting Multi-Group Energy Boundaries



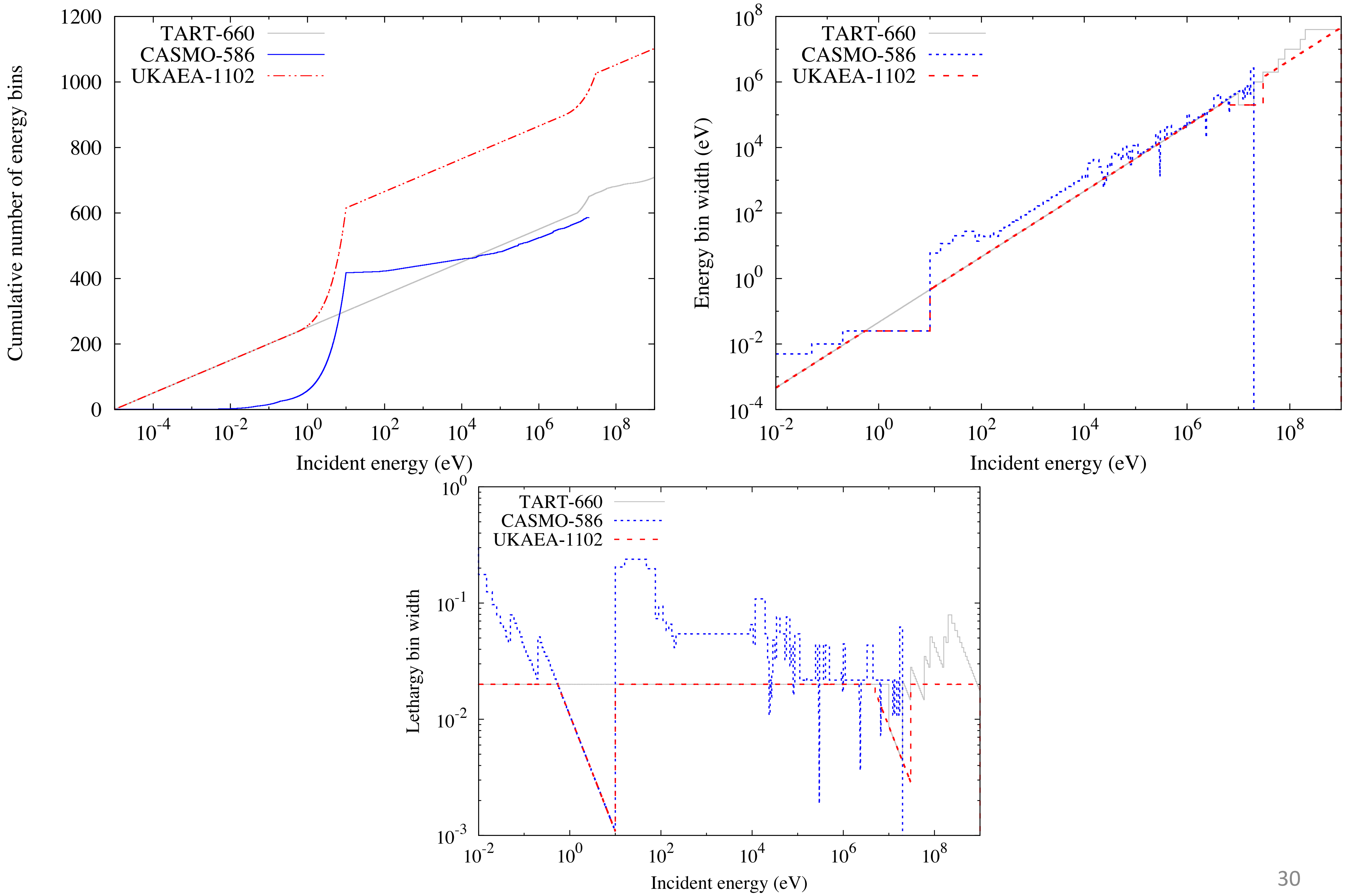


U-238 res.	Energy group width (eV) near resonance peak			
Energy eV	WIMS- 69	SHEM-361	Xmas-172	CASL-51
36.68	10.30	~0.05	3.50	18.30
20.87	11.70	~0.01	3.15	16.60
6.67	5.90	~0.01	0.8 -1.4	0.3 – 0.8

1000's of energy groups are needed to blindly overcome group boundary sensitivities

Intermediate group widths produce results that are sensitive to "equivalence factors"

Group structures 586 to 1000+



Group structure 1000+

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

Thermal	Resonance fine	Resonance shielded	Fast Fusion	Fast	High Energy
50 equal U per decade	Equal energy 0.025 eV	50 equal U per decade	Equal energy 200 KeV	50 equal U per decade	Equal lethargy
237 grps	378 grps	285 grps	125 grps	27 grps	50 grps

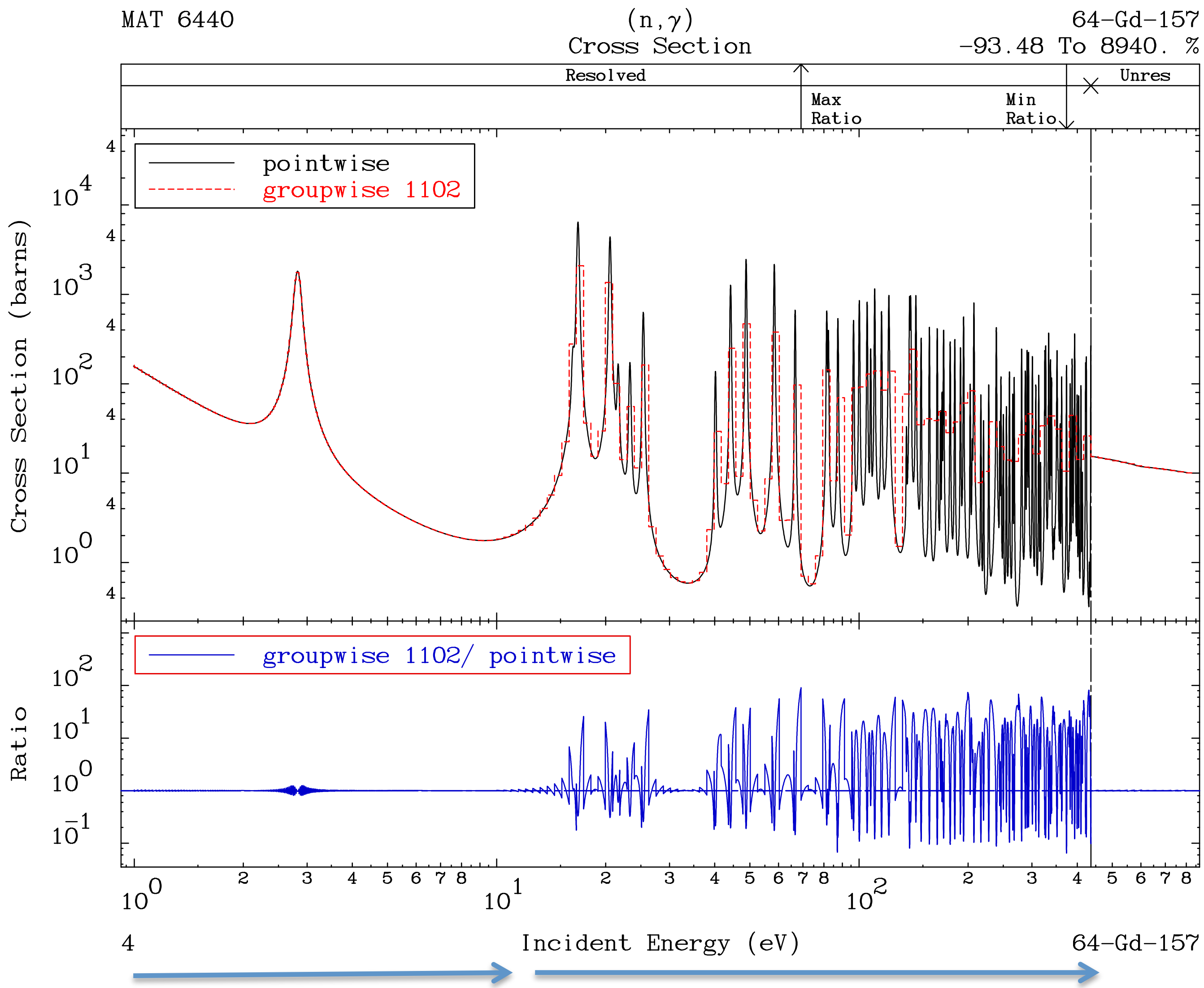
1e-5 eV — 0.55 eV — 10 eV — 5 MeV — 30 MeV — 100 MeV — 1 GeV

615 groups

1025 groups

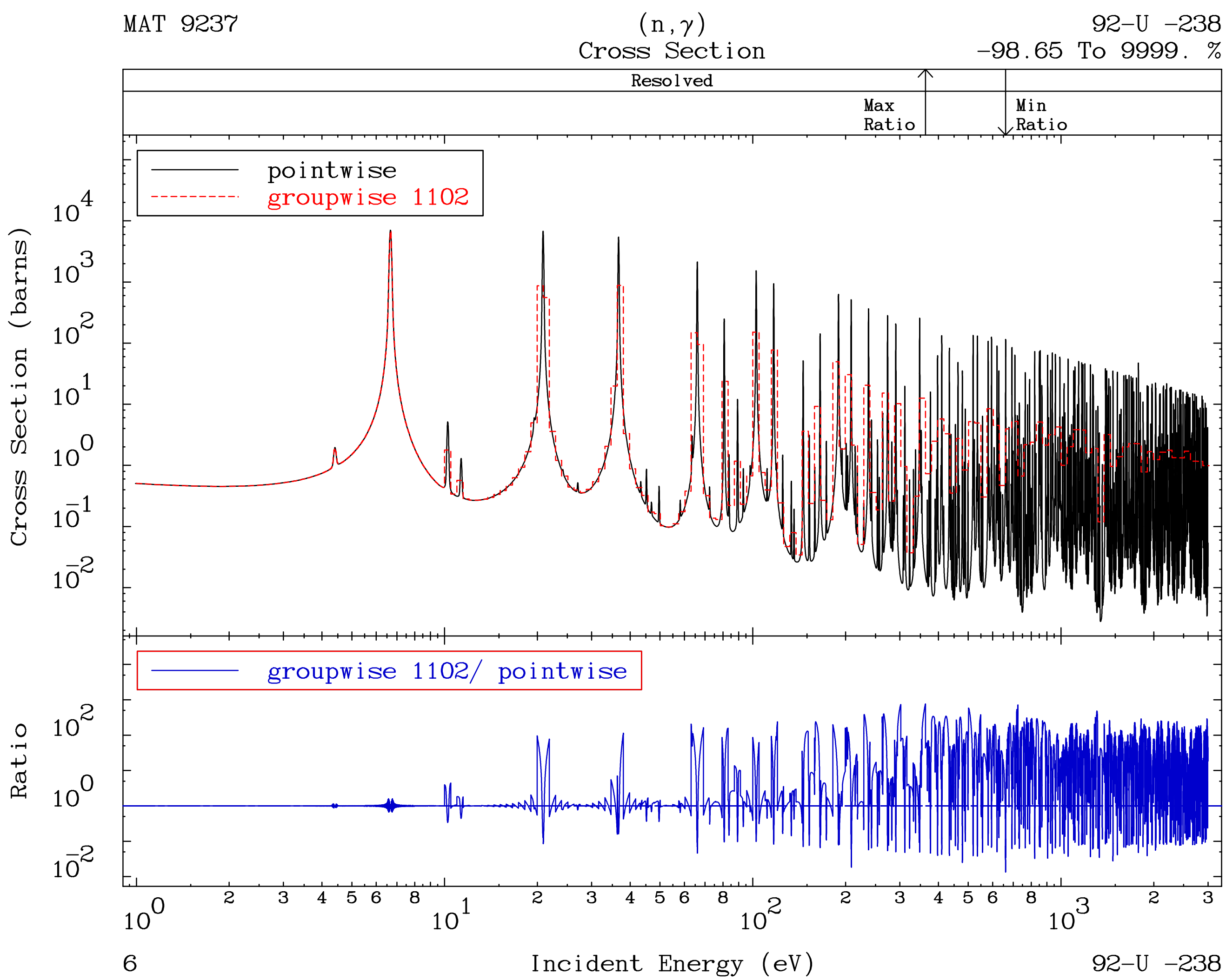
- 378 fine groups in the resonance range
- Resonance shielded data available in the RRR (0.1 eV) up to the end of the URR for all nuclides IDs
- Fast fine structure for accurate threshold XS reaction rate

Group structure: 1102



Fine group to 10 eV Resonance shielded to end of URR

Group structure: 1102



Fine group to 10 eV

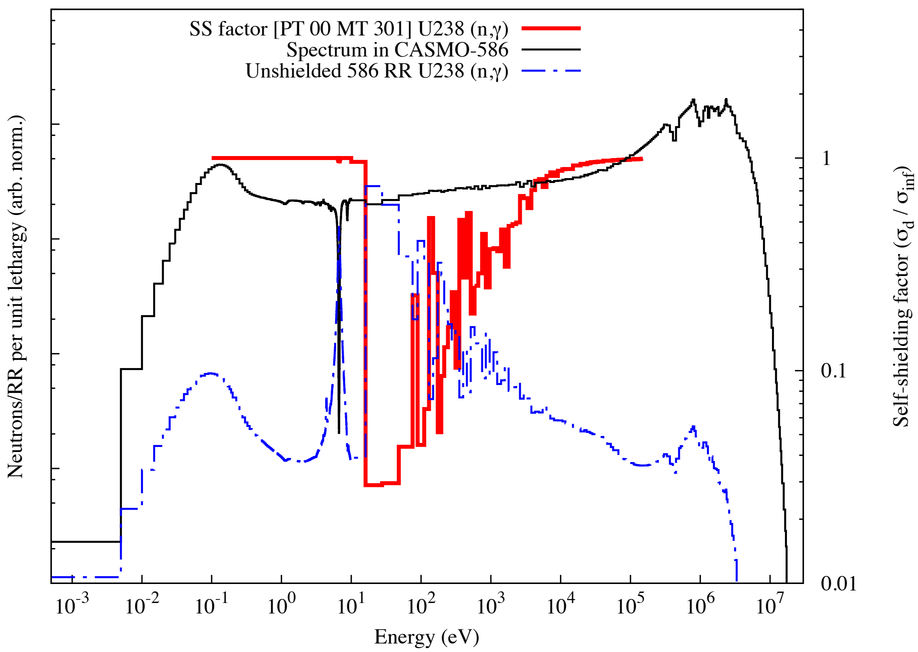
Resonance shielded to end of URR

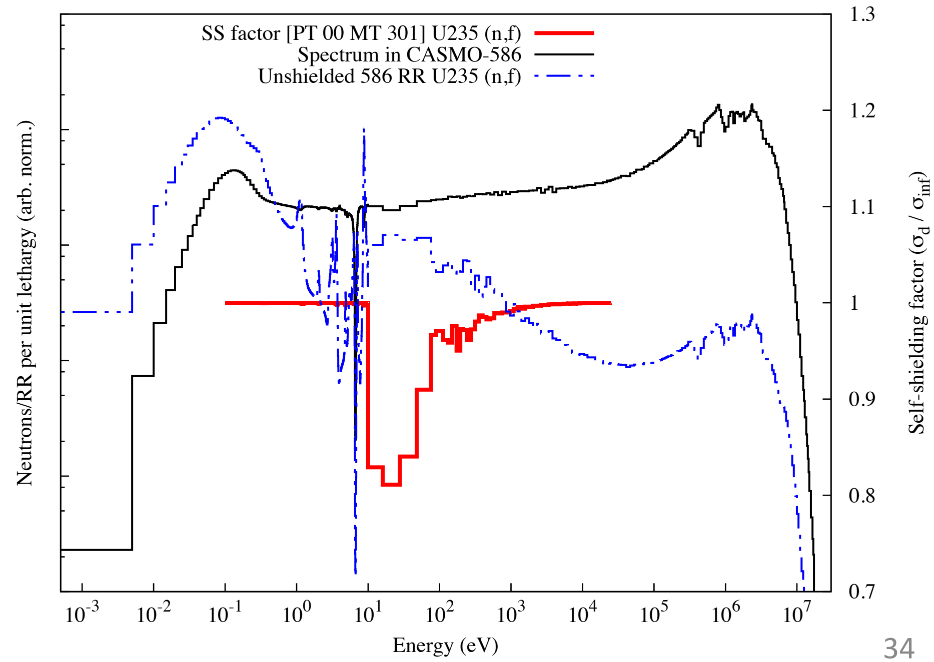
LWR assembly simulations

- 586 gprs CASMO data for ENDF/B-VII.1, with CALENDF PTs for self-shielding. Applied to major actinides

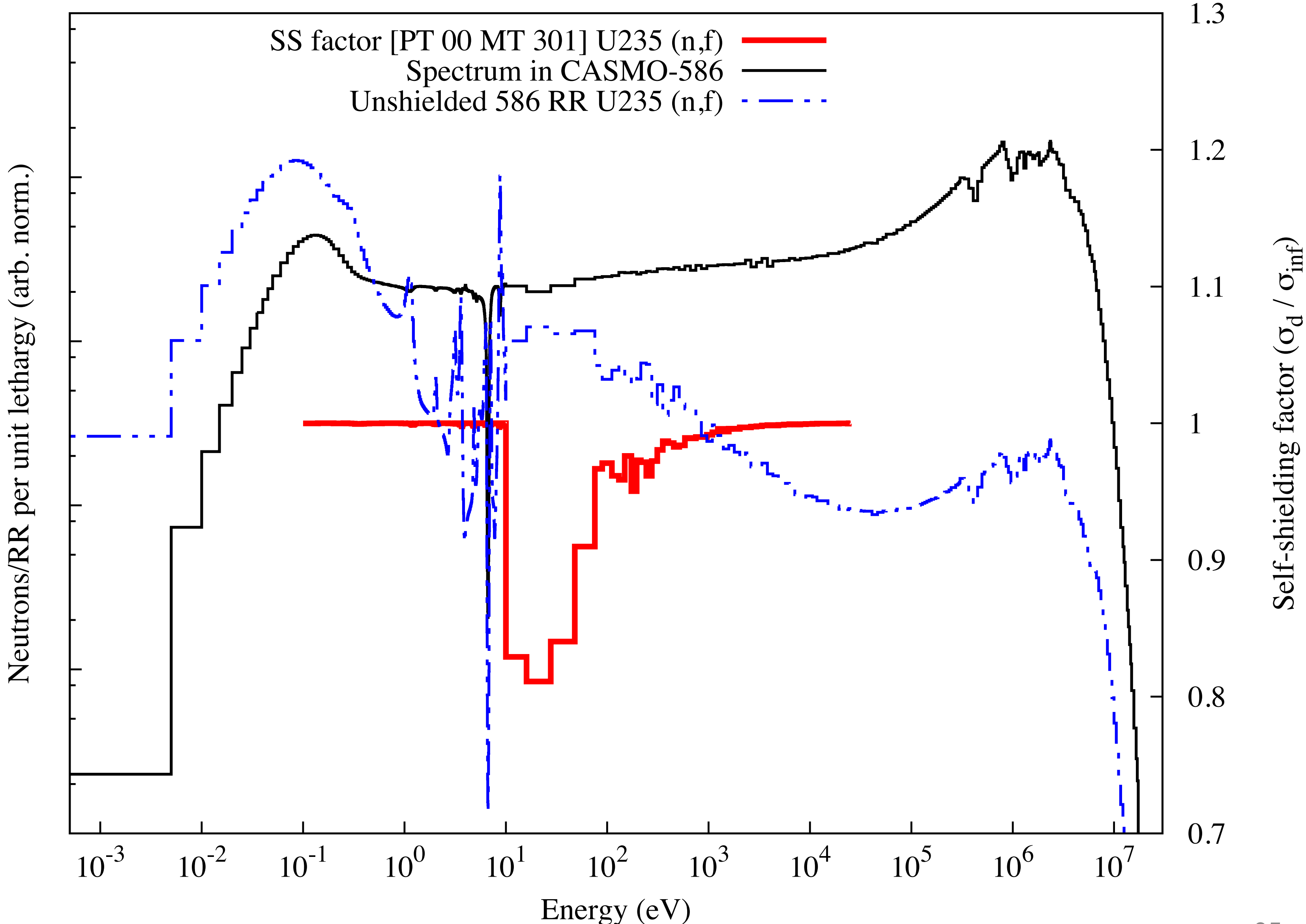
- **Left**: U8 capture RR and SSFs **Right**: U5 fission RR+SSFs

Note: 586 gprs treatment of <10 eV requires no SSFs! No so for >10 eV, where significant SS occurs and must be accounted for.

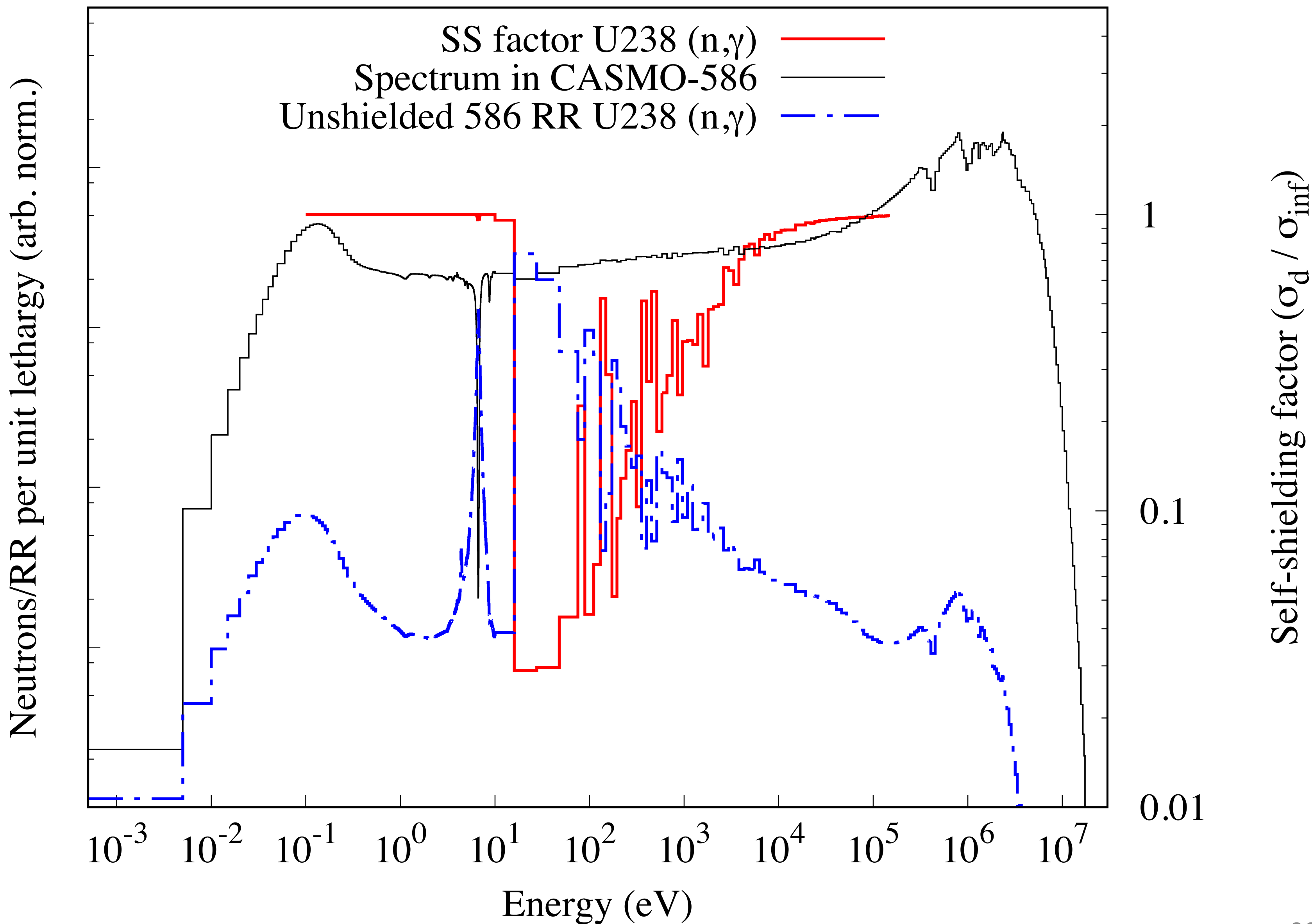




U^{235} fission

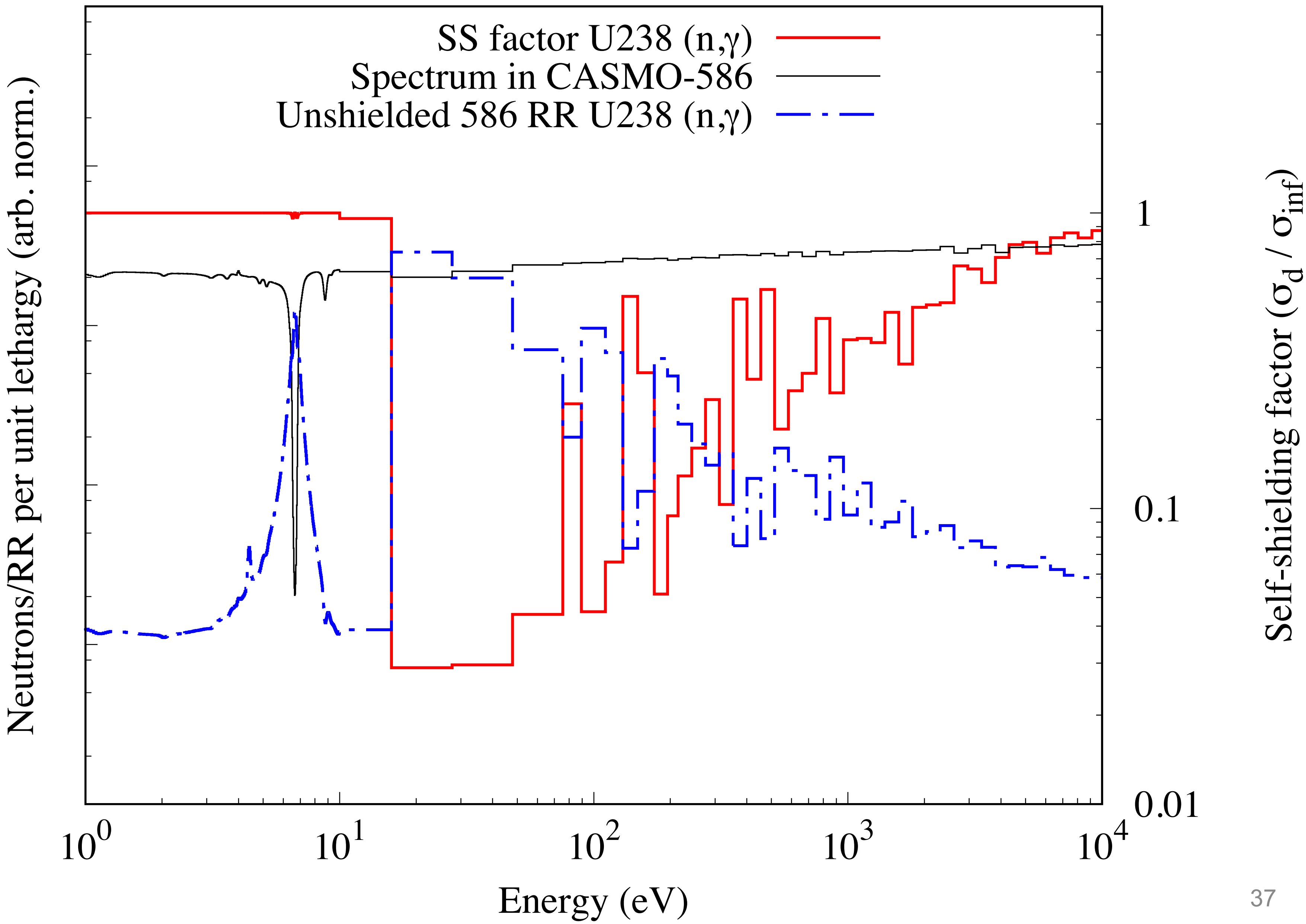


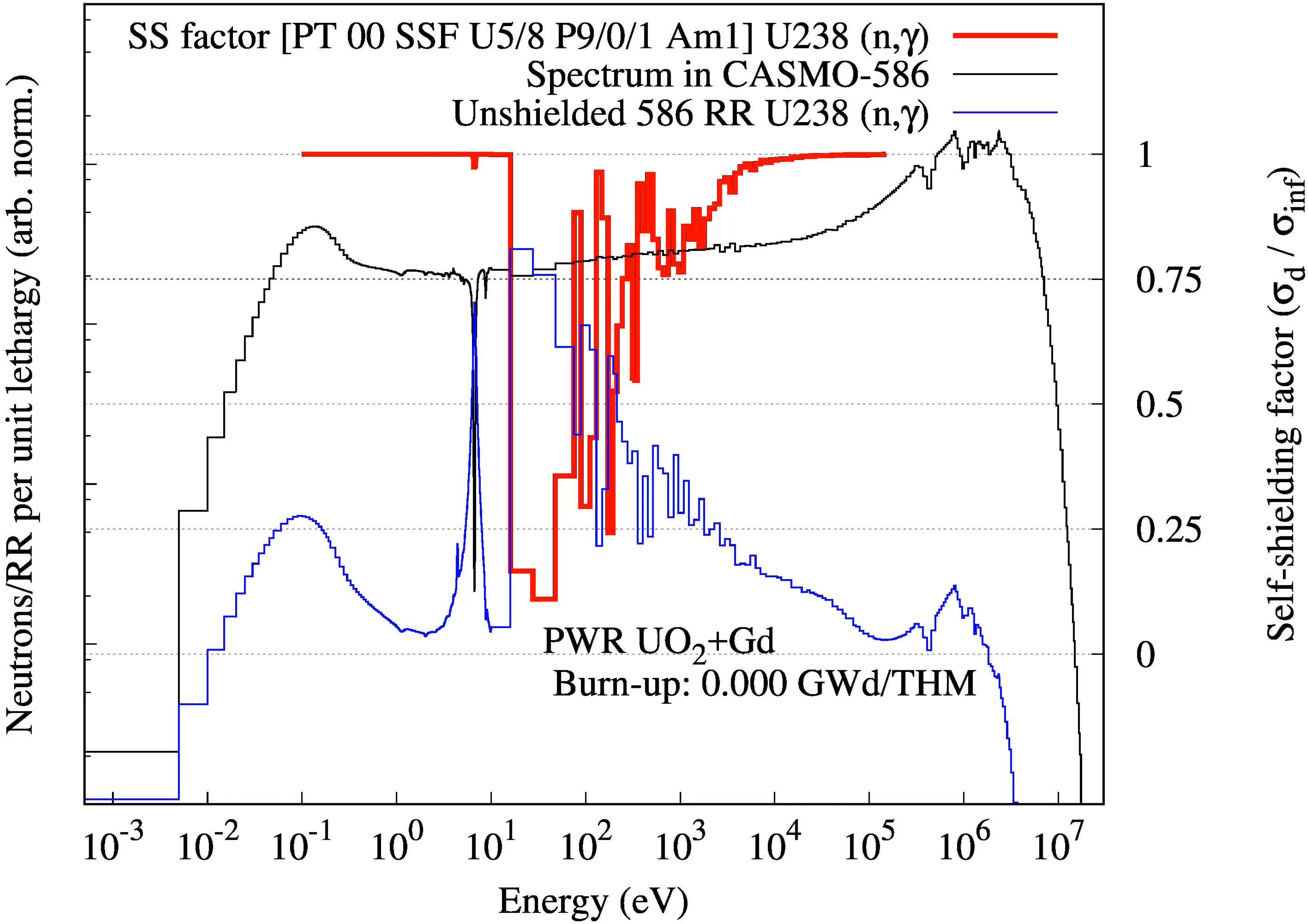
U^{238} reaction rate



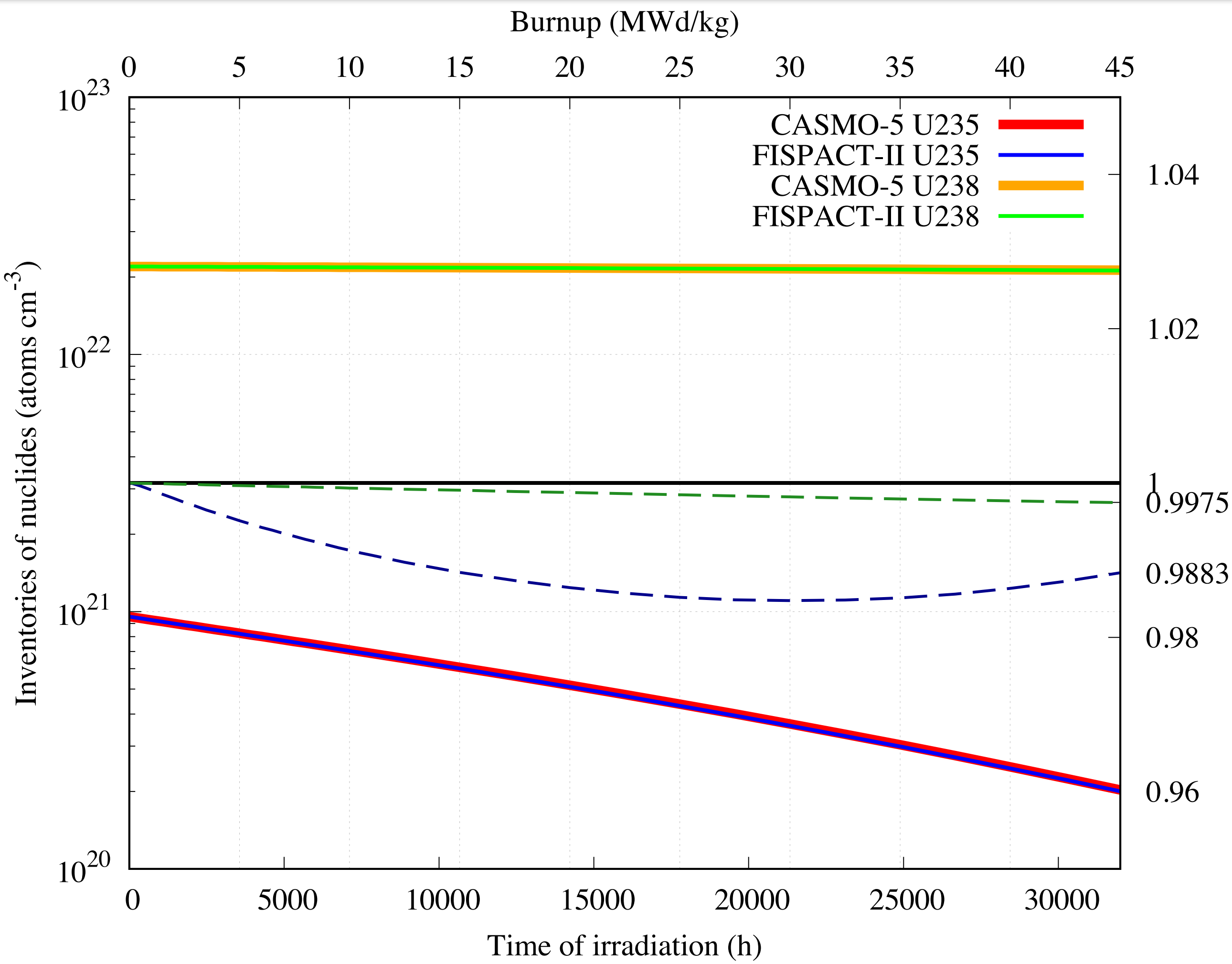
60 Years
IAEA Atoms for Peace and Development

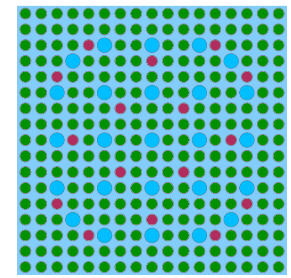
U^{238} reaction rate




SS factor [PT 00 SSF U5/8 P9/0/1 Am1] U238 (n,γ)
Spectrum in CASMO-586
Unshielded 586 RR U238 (n,γ)
PWR UO_2+Gd
Burn-up: 0.000 GWd/THM
Neutrons/RR per unit lethargy (arb. norm.)
Self-shielding factor (σ_d / σ_{inf})
1
0.75
0.5
0.25
0
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
Energy (eV)

17x17 lattice Inventories





Takahama-3

Takahama-3 assembly uranium inventories from CASMO-5 and FISPACT-II simulations over a 45 GWd/THM simulation. Ton of Heavy Metal
The ratio of 235U (ending at 1.2% difference) and 238U (ending at 0.25% difference) are also shown.

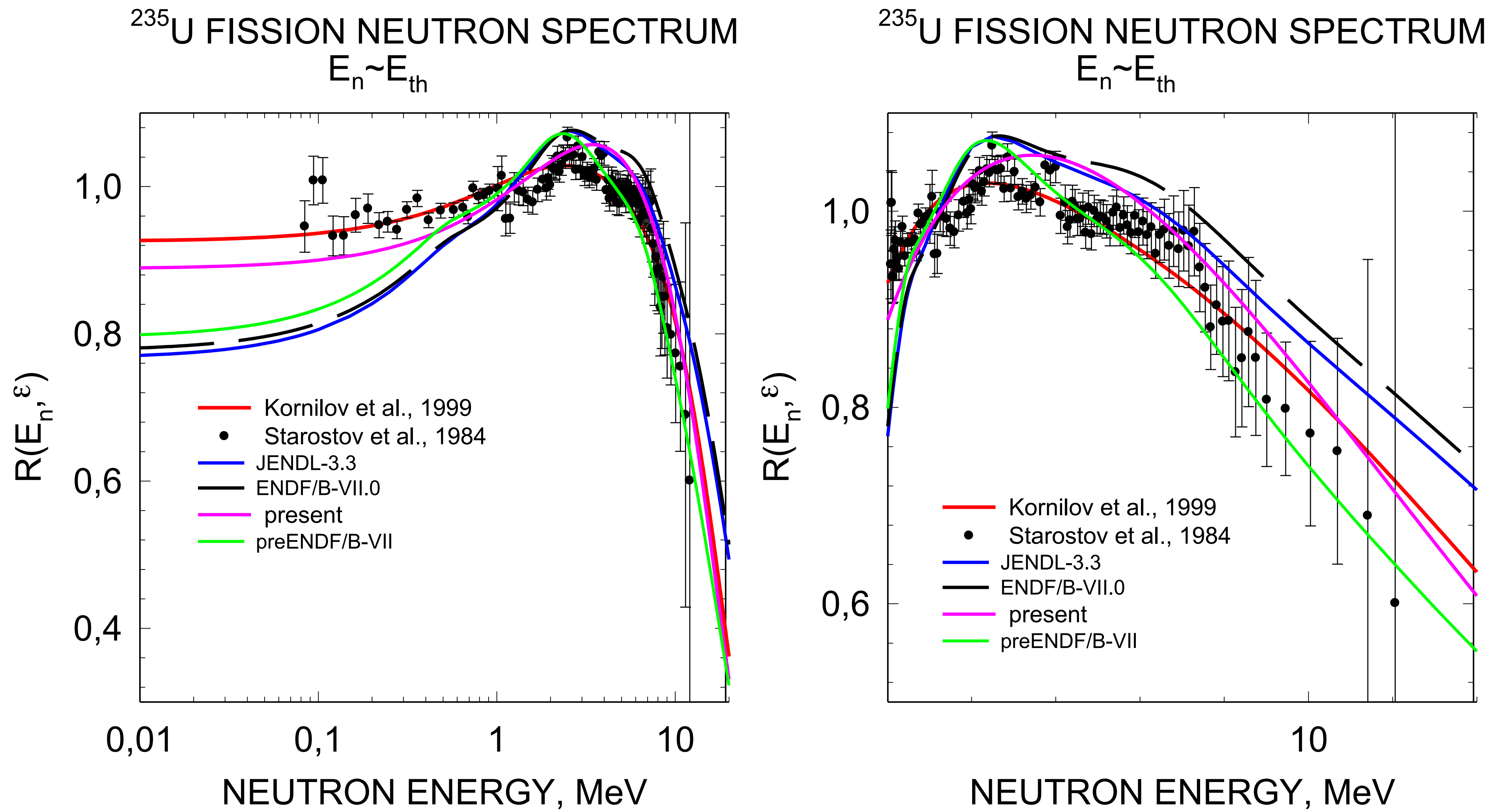
Benchmarking scope

- Are emitted particle spectra important for LWR ?
  - energy dependence, E_n
  - energy profile

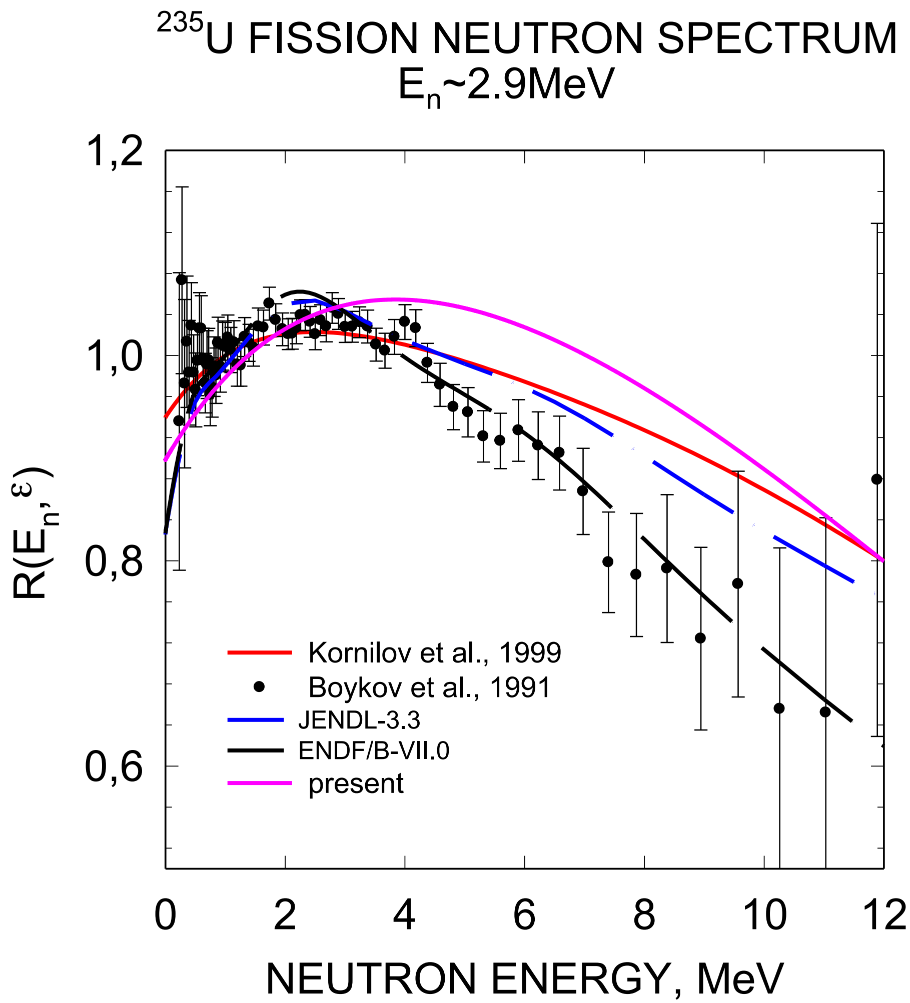
Let us look at fission, but think also inelastic,…

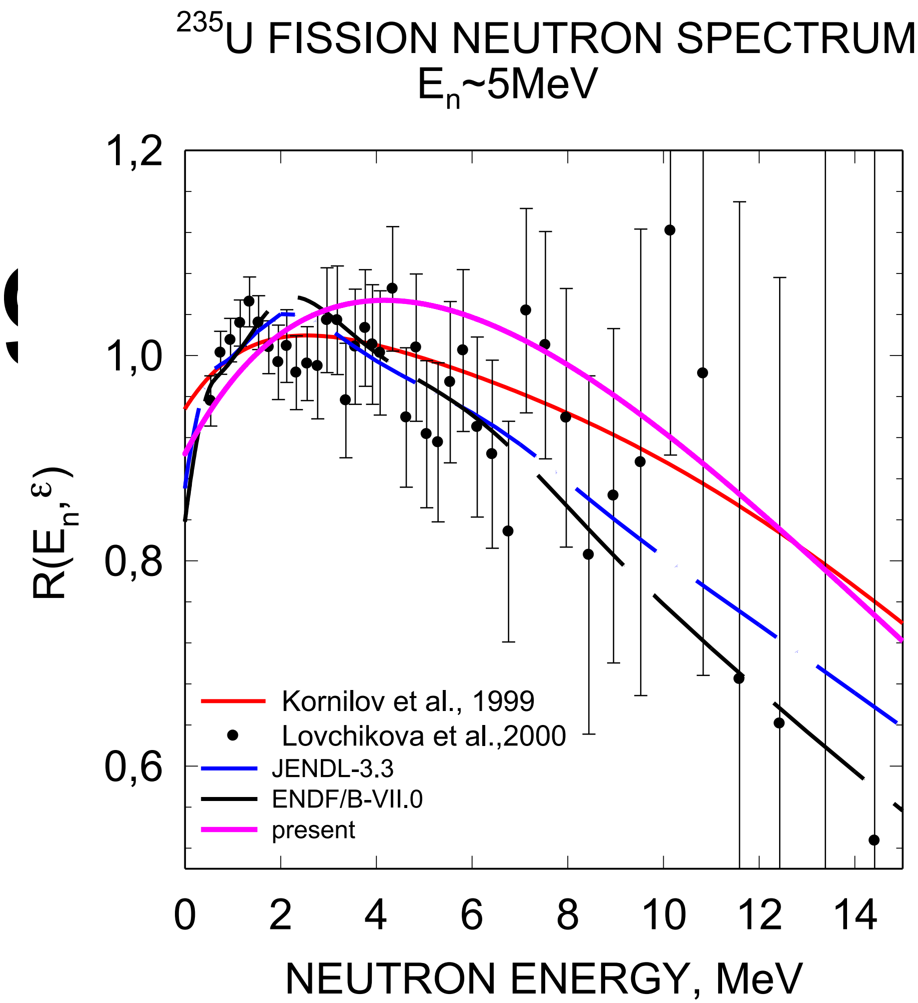
- Single MF-5 MT-18 !! and a tuned thermal nu..
- MF-5 have been better evaluated over the years and we look at the impact on well established ICSBEP benchmarks with the Monte Carlo code TRIPOLI

$U^{235}(n_{th}, f)$, PFNS, ~50 keV shift in <E>

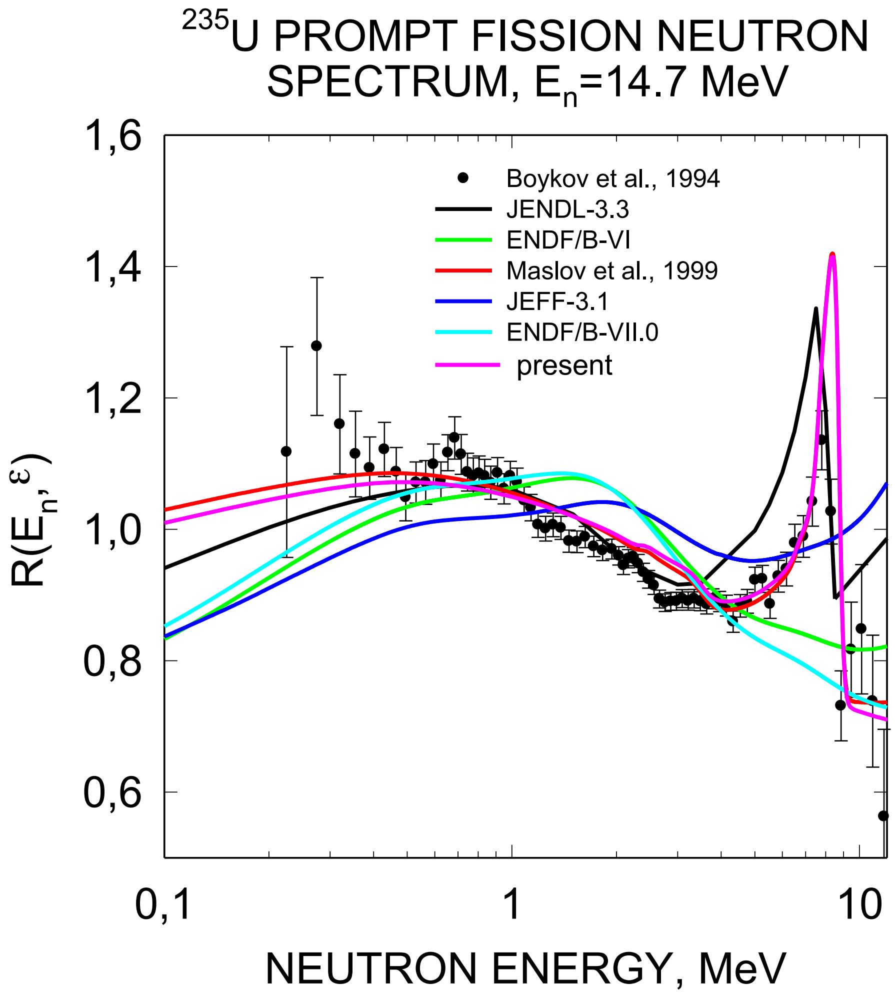


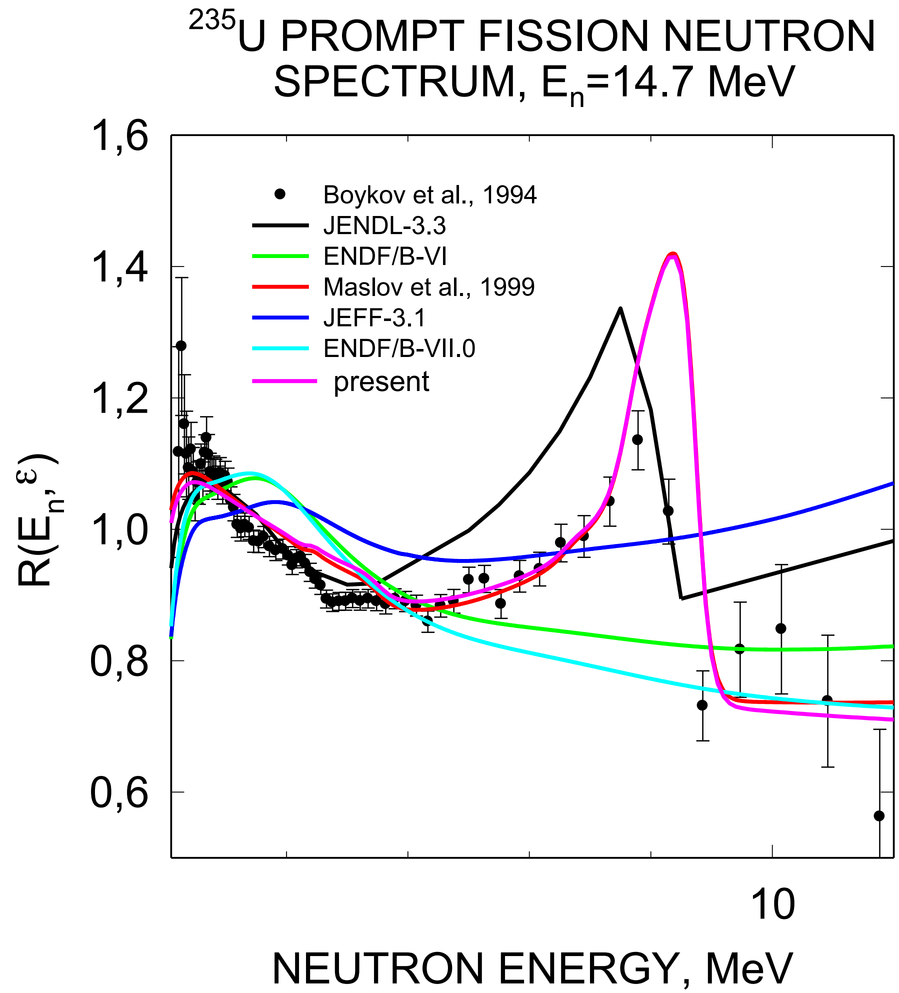
U^{235} PNFS


^{235}U FISSION NEUTRON SPECTRUM
E_n~2.9MeV
R(E_n, ε)
NEUTRON ENERGY, MeV
Kornilov et al., 1999
Boykov et al., 1991
JENDL-3.3
ENDF/B-VII.0
present

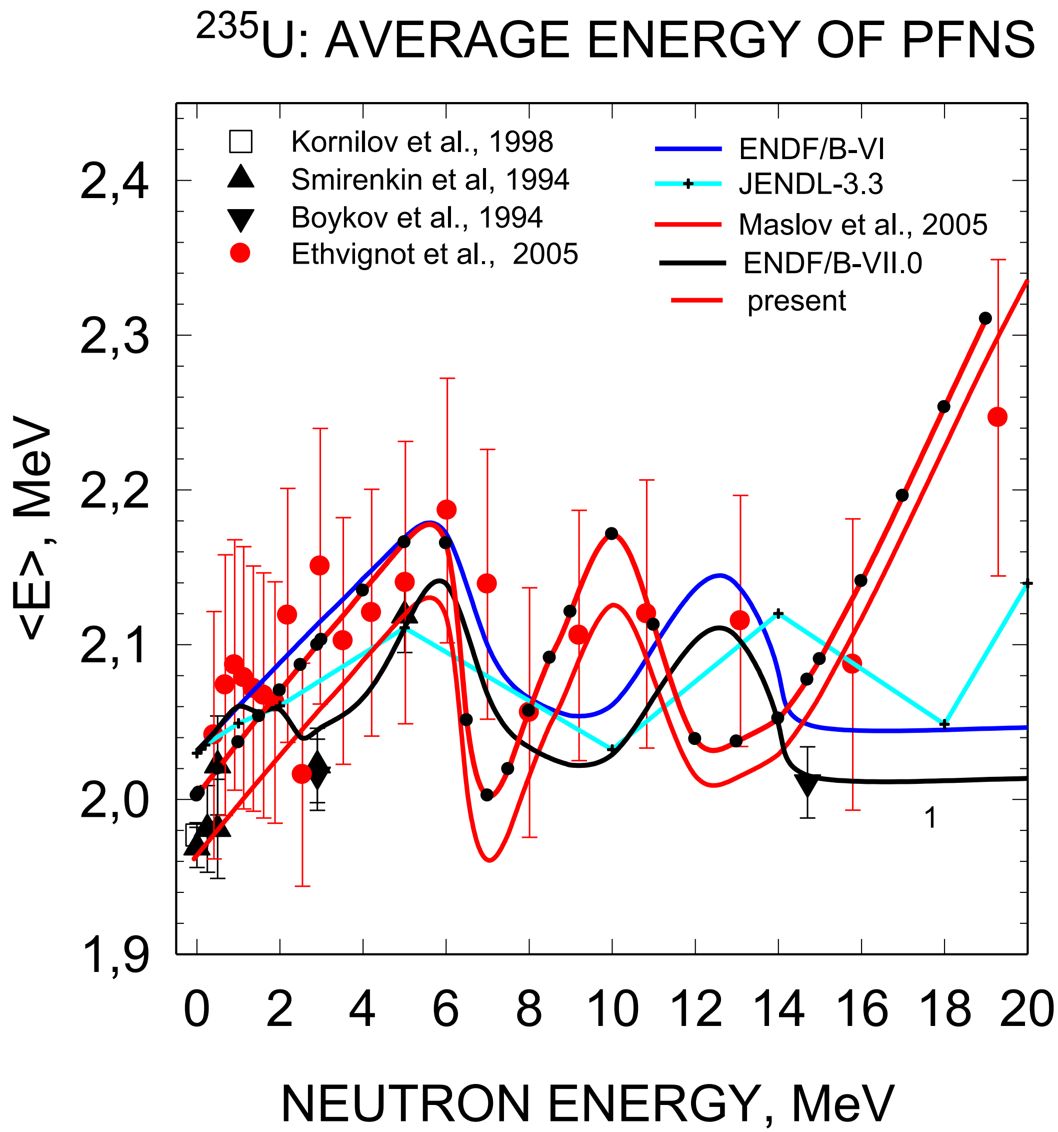

^{235}U FISSION NEUTRON SPECTRUM
E_n~5MeV
R(E_n, ε)
NEUTRON ENERGY, MeV
Kornilov et al., 1999
Lovchikova et al.,2000
JENDL-3.3
ENDF/B-VII.0
present

U^{235} E_n 14.7 MeV

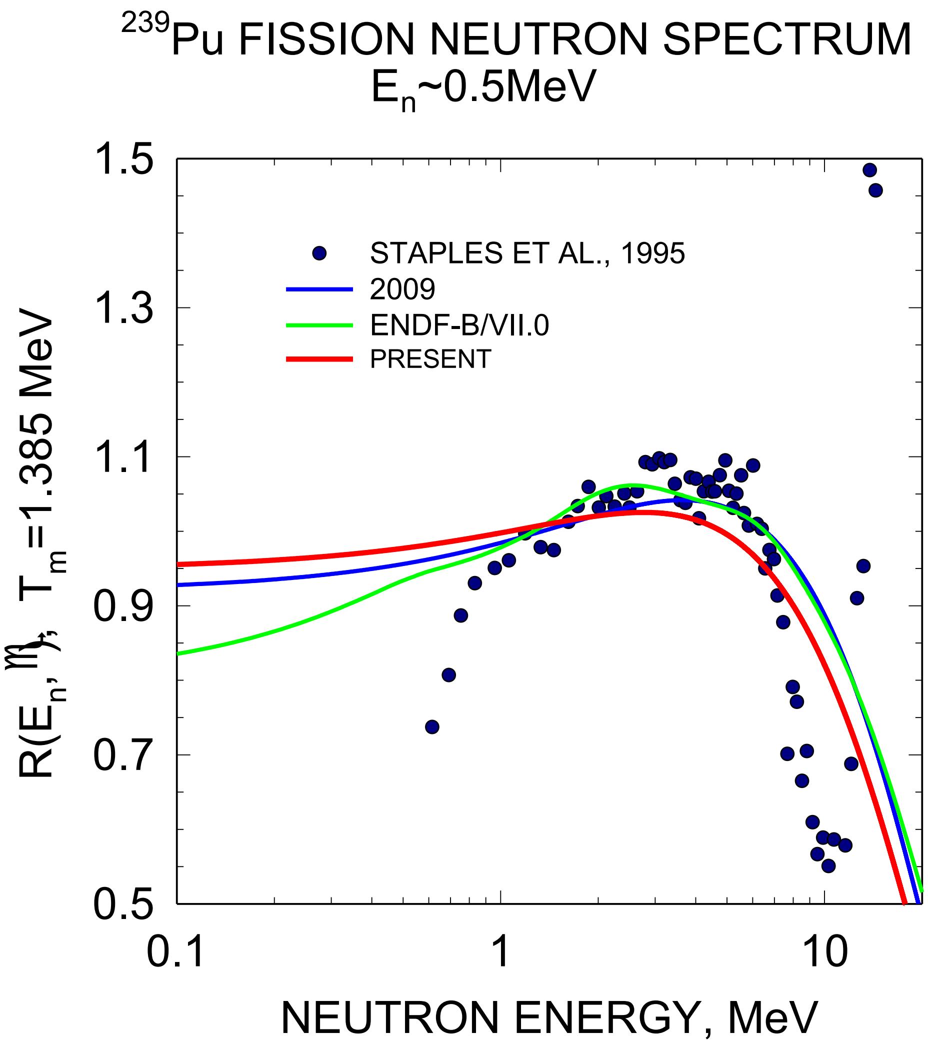


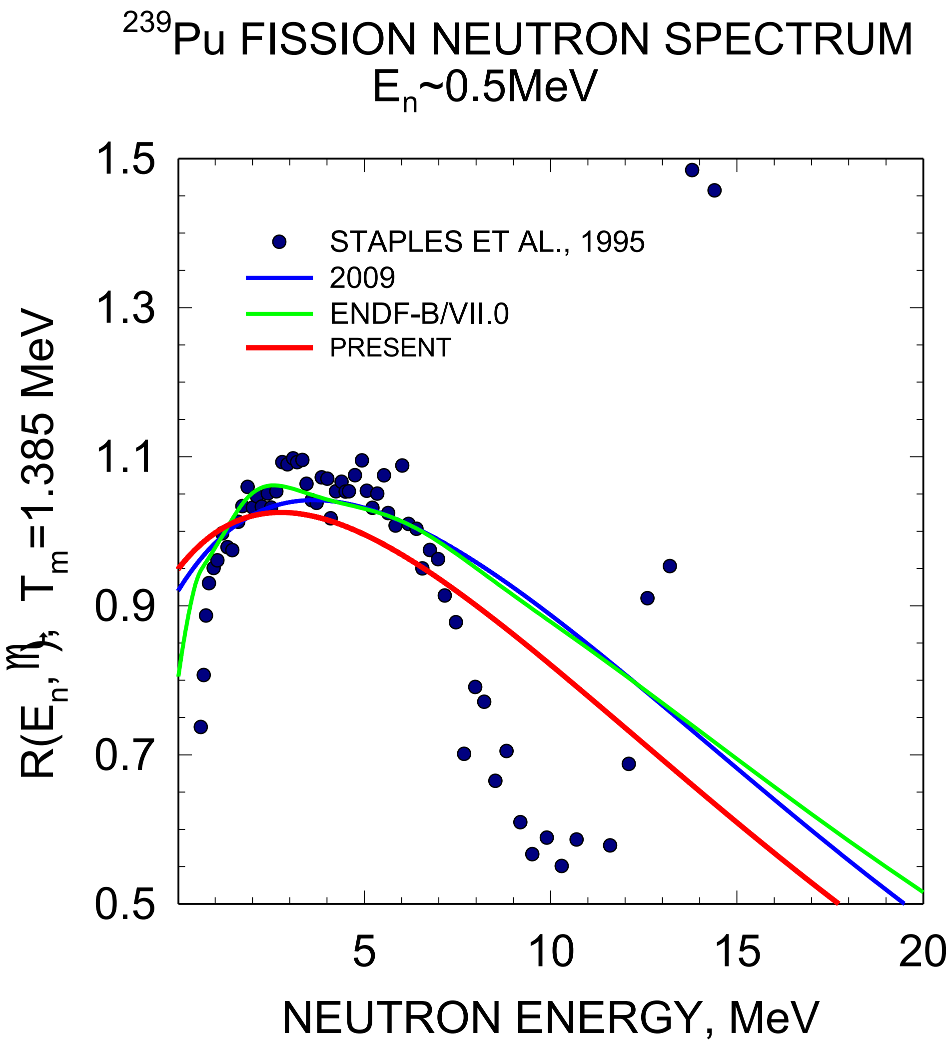


Average Energy

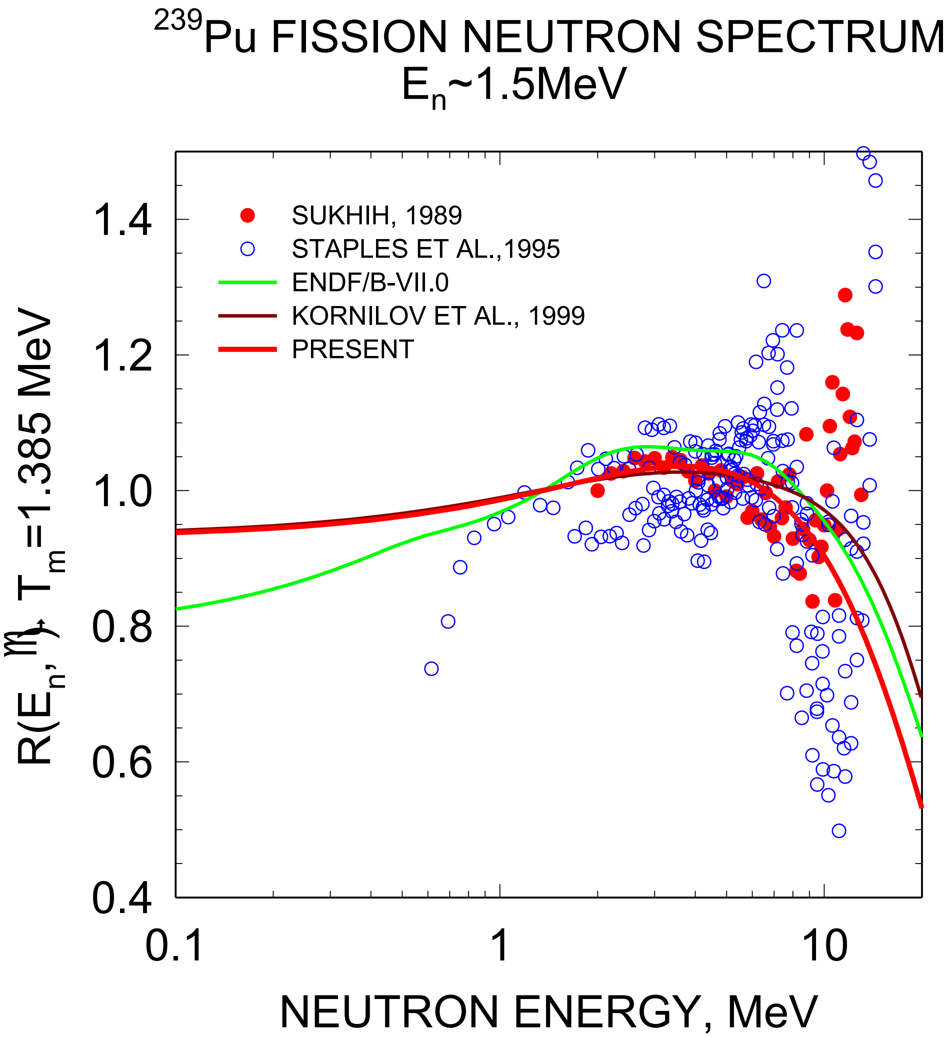


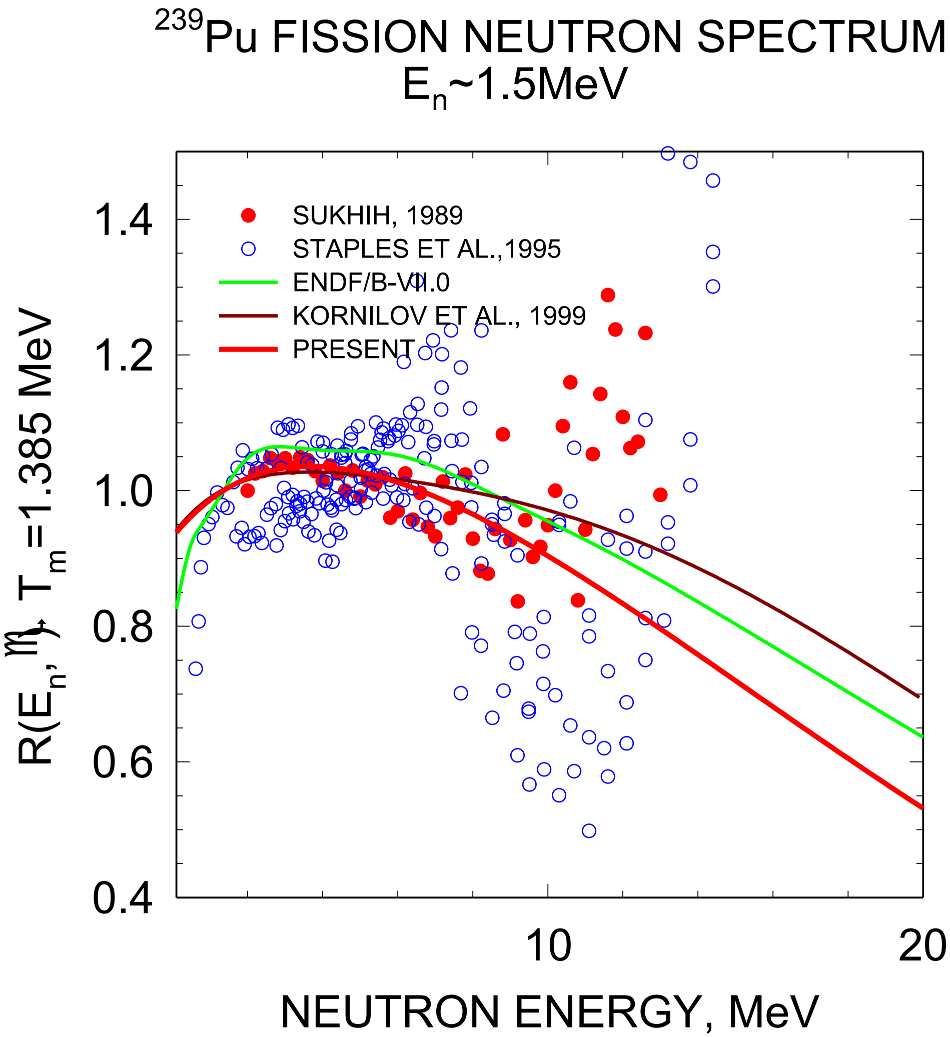
Pu^{239} PNFS


239Pu FISSION NEUTRON SPECTRUM
En~0.5MeV
STAPLES ET AL., 1995
2009
ENDF-B/VII.0
PRESENT
R(En, Tm), Tm=1.385 MeV
NEUTRON ENERGY, MeV
1.5
1.3
1.1
0.9
0.7
0.5
0.1
1
10

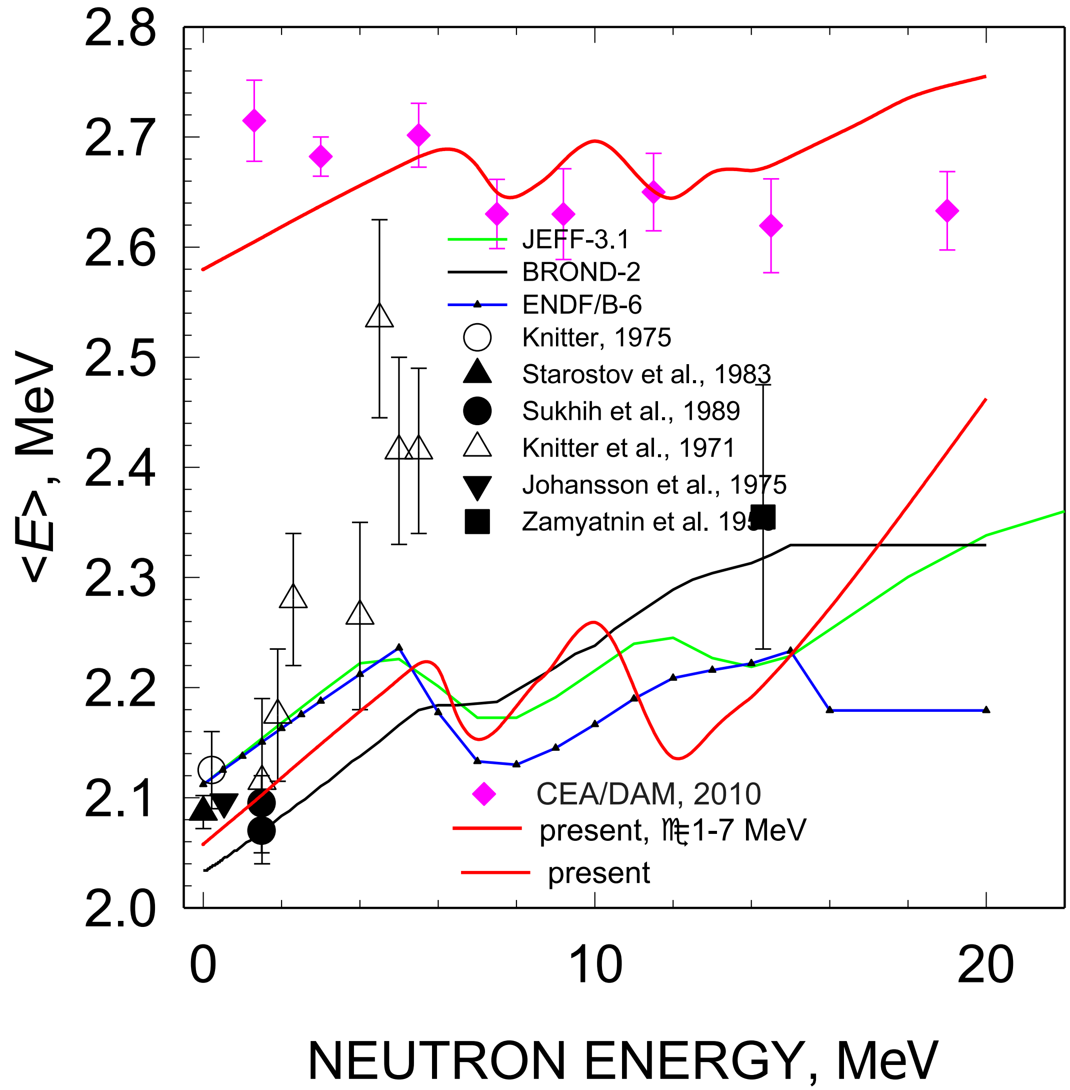

239Pu FISSION NEUTRON SPECTRUM
En~0.5MeV
STAPLES ET AL., 1995
2009
ENDF-B/VII.0
PRESENT
R(En, Tm), Tm=1.385 MeV
NEUTRON ENERGY, MeV
1.5
1.3
1.1
0.9
0.7
0.5
5
10
15
20

Pu^{239} PNFS


239Pu FISSION NEUTRON SPECTRUM
En~1.5MeV
SUKHIH, 1989
STAPLES ET AL.,1995
ENDF/B-VII.0
KORNILOV ET AL., 1999
PRESENT
R(En,<E>), Tm=1.385 MeV
1.4
1.2
1.0
0.8
0.6
0.4
0.1
1
10
NEUTRON ENERGY, MeV


239Pu FISSION NEUTRON SPECTRUM
En~1.5MeV
SUKHIH, 1989
STAPLES ET AL.,1995
ENDF/B-VII.0
KORNILOV ET AL., 1999
PRESENT
R(En,<E>), Tm=1.385 MeV
1.4
1.2
1.0
0.8
0.6
0.4
10
20
NEUTRON ENERGY, MeV

Pu^{239} Average Energy



Jargon: reactor physics

- Integral results are requested to enable the following system total results to be calculated: flux; production as a sum of fission production, (n,2n) production, and (n,3n) production; absorption as a sum of fission, capture, (n,2n), and (n,3n); and leakage from the outer edge of the system.

- The normalization of these results is not important, because a reactor can be critical at any power level. Specifically we consider the definition:

➔ Keff = production / absorption + leakage

Jargon: reactor physics

- Nota Bene: since the **inhour**, **dollar**, and **cent** all depend upon the constituents and even structure of a reactor, reactivity is also measured in units defined as decimal fraction of unity. There are varying degree of usage and appropriation of the Canadian **mill-k**, equal to, the British **millinile**, the French “**pour cent mille**”, the Italian “**per centomila**”, the US percent **millirho**, all equal to and abbreviated **pcm**

- **LCT** Low Enriched Uranium-Compound-Thermal spectrum
- **PST** Plutonium-Solution-Thermal spectrum
- **HST** High Enriched Uranium-Solution-Thermal spectrum

IAEA 60 Years *Atoms for Peace and Development*

U^{235} fast range

Code				Tripoli-4.5		Tripoli-4.5		Tripoli-4.5	
Library				JEFF-3.1		JEFF-3.1.1		Maslov	
		Experiment		Calc.		Calc.	Δ	Calc.	Δ
		Keff	Unc.	Kcalc	S.D.	Kcalc	(C-C)	Kcalc	(C-C)
ICSBEP	Name			Fast Range					
IMF-007	Cyl. U Metal (10% 235U), thick 238U Reflector								
Big Ten	deta.	1.0045	70	0.99863	13	0.99878		0.99582	
	simp.	1.0045	70	0.99790	13	0.99770		0.99511	
Δ (C-E)				-623		-626	-2	-903	-278
	t.z.h.	0.9948	130	0.98830	13	0.98838		0.98556	
Δ (C-E)				-650		-642	8	-924	-282
IMF-012	Cyl. U Metal (16% 235U), Al and Steel, Reflected by Depleted-U								
ZPR(16%)	c-1	1.0007	270	1.00261	13	1.00262		1.00050	
Δ (C-E)				191		192	1	-20	-212
IMF-10	Cyl U Metal (9% 235U), thick Depleted U Reflector								
ZPR-U9	c-1	0.9954	240	0.99181	13	0.99191		0.98880	
Δ (C-E)				-359		-349	10	-660	-311
IMF-002	Nat. U Reflected Assembly of Enriched U Plates								
	c-1	1.0000	300	0.99216	10	0.99207		0.98997	
Δ (C-E)				-784		-793	-9	-1003	-210
IMF-001	Bare Cyl. Conf. of Enriched and Natural U								
Jemima	c-2	1.0000	120	0.99837	12	0.99797		0.99725	
	c-3	1.0000	100	0.99741	12	0.99779		0.99622	
	c-4	1.0000	100	0.99850	12	0.99821		0.99691	
Average				0.99809		0.99799		0.99679	
Δ (C-E)				-191		-201	-10	-321	-120
HMF-028	235U Sphere Reflected by Normal U using Flattop								
Flattop-25		1.0000	300	1.00210	11	1.00199		1.00150	
Δ (C-E)				210		199	-11	150	-49
HMF-001	Bare, Highly Enriched U Sphere								
Godiva	c1	1.0000	100	0.99645	11	0.99668		0.99663	
	c2	1.0000	100	0.99660	11	0.99647		0.99645	
Average				0.99653		0.99658		0.99654	
Δ (C-E)				-347		-342	5	-346	-4

up to ~ - 300 pcm and Godiva, Flattop intact

!! for JEFF-3.1.1

- ENDF/B-VII much better there than !! too much better??

Shaded grey means C/E outside the exp. Uncertainty (quoted)

U^{235} Thermal

Code				Tripoli-4.5		Tripoli-4.5		Tripoli-4.5	
Library				JEFF-3.1		JEFF-3.1.1		Maslov	
	Experiment			Calc.		Calc.	Δ	Calc.	Δ
		Keff	Unc.	Kcalc	S.D.	Kcalc	(C-C)	Kcalc	(C-C)
ICSBEP	Name			Thermal range U					
LCT-006	Low Enriched UO2 Fuel Rods with # Water-to-Fuel Volume Ratios								
	c-1	1.0000	200	0.99998	12	1.00071		1.00172	
	c-3	1.0000	200	1.00051	9	1.00127		1.00227	
	c-4	1.0000	200	0.99987	12	1.00082		1.00175	
	c-8	1.0000	200	1.00059	12	1.00118		1.00260	
	c-9	1.0000	200	1.00011	12	1.00067		1.00228	
	c-13	1.0000	200	0.99994	12	1.00042		1.00210	
	c-14	1.0000	200	0.99958	12	1.00036		1.00185	
	c-18	1.0000	200	0.99978	12	1.00049		1.00195	
Average				1.00005		1.00074		1.00206	
Δ (C-E)				5		74	69	206	133
LCT-007	Water Reflected 4.738 Wt.% Enriched UO2 Fuel Rod Arrays								
Valduc	c-1	1.0000	160	0.99780	10	0.99844		1.00021	
	c-2	1.0000	160	0.99932	10	0.99975		1.00250	
	c-3	1.0000	160	0.99749	10	0.99821		1.00019	
	c-5	1.0000	160	0.99753	10	0.99806		1.00002	
	c-6	1.0000	160	0.99915	10	0.99988		1.00238	
	c-7	1.0000	160	0.99843	10	0.99915		1.00132	
Average				0.99829		0.99891		1.00110	
Δ (C-E)				-171		-109	62	110	219
LCT-039	Incomplete Arrays of Water Reflected 4.738 Wt.% Enriched UO2 Fuel Rods								
Valduc	c-1	1.0000	140	0.99761	12	0.99799		1.00025	
	c-4	1.0000	140	0.99665	12	0.99723		0.99969	
	c-6	1.0000	140	0.99767	12	0.99831		1.00073	
Average				0.99731		0.99784		1.00022	
Δ (C-E)				-269		-216	53	22	238
Hector	k∞ Experiments in Intermediate Neutron Spectra for 235U								
Hiss		1.0000	600	1.01003	13	1.00978		1.00986	
Δ (C-E)				1003		978	-26	986	9
	Enriched Uranium Hydride sphere								
Topsy-NI		1.0000	400	1.00201	17	1.00182		1.00487	
Δ (C-E)				201		182	-19	487	305
Topsy-UR		1.0000	400	1.00687	16	1.00733		1.00861	
Δ (C-E)				687		733	46	861	128

up to ~ + 300
and Hiss intact
not Topsy

Better Valduc LCT-039
unique …

Thermal Pu^{239}

Code				Tripoli-4.5		Tripoli-4.5		Tripoli-4.5	
Library				JEFF-3.1		JEFF-3.1.1		Maslov	
	Experiment			Calc.		Calc.	Δ	Calc.	Δ
		Keff	Unc.	Kcalc	S.D.	Kcalc	Δ (C-C)	Kcalc	(C-C)
ICSBEP	Name			Thermal range Pu					
PST-009	48" sphere, Al vessel, bare								
9.54 gPu/l	c-2A	1.0003	330	1.01893	11	1.01105		1.01272	
9.46 gPu/l	c-3A	1.0003	330	1.01927	11	1.01466		1.01634	
Average				**1.01910**		**1.01285**		**1.01453**	
Δ (C-E)				**1880**		**1255**	**-625**	**1423**	**168**
MCT-004	Mox 3.01 wt% PuO2-UO2 fuel rods,								
2.4 w/f ratio	c-1	1.0000	460	0.99683	13	0.99601		0.99882	
2.9 w/f ratio	c-4	1.0000	390	0.99707	13	0.99605		0.99922	
4.2 w/f ratio	c-7	1.0000	400	0.99779	13	0.99654		0.99938	
5.5 w/f ratio	c-10	1.0000	510	0.99783	13	0.99631		0.99870	
Average				**0.99738**		**0.99622**		**0.99903**	
Δ (C-E)				**-262**		**-378**	**-116**	**-97**	**281**
PST-001	11.5" sphere, water reflected								
73.0 gPu/l	c-1	1.0000	500	1.00186	12	1.00218		1.01057	
96.0 gPu/l	c-2	1.0000	500	1.00356	12	1.00403		1.01236	
119.0 gPu/l	c-3	1.0000	500	1.00665	12	1.00713		1.01539	
132.0 gPu/l	c-4	1.0000	500	1.00104	12	1.00144		1.00969	
140.0 gPu/l	c-5	1.0000	500	1.00505	12	1.00552		1.01354	
268.7 gPu/l	c-6	1.0000	500	1.00681	12	1.00732		1.01499	
Average				**1.00416**		**1.00460**		**1.01275**	
Δ (C-E)				**416**		**460**	**44**	**1275**	**815**
PST-011	16&18" sphere, bare								
34.9 gPu/l	16-1	1.0000	520	1.00669	13	1.00736		1.01498	
43.4 gPu/l	16-5	1.0000	520	1.00337	13	1.00370		1.01172	
Average				**1.00503**		**1.00553**		**1.01335**	
Δ (C-E)				**503**		**553**	**50**	**1334**	**781**
22.3 gPu/l	18-1	1.0000	520	0.99134	13	0.99160		0.99796	
27.5 gPu/l	18-6	1.0000	520	0.99708	13	0.99761		1.00428	
Average				**0.99421**		**0.99460**		**1.00112**	
Δ (C-E)				**-579**		**-540**	**39**	**112**	**652**

up to ~ + 800 pcm

More impact on its own than the thermal xs adjusted JEFF-3.1.1
- artificial neg. res.
-reduced nu prompt

Remark: which benchmarks you choose to fit ?? and why ??

Is this code, method, continent dependent ??

Pu^{239} Thermal and Fast

60 Years IAEA Atoms for Peace and Development

Code				Tripoli-4.5		Tripoli-4.5		Tripoli-4.5	
Library				JEFF-3.1		JEFF-3.1.1		Maslov	
	Experiment			Calc.		Calc.	Δ	Calc.	Δ
		Keff	Unc.	Kcalc	S.D.	Kcalc	Δ (C-C)	Kcalc	(C-C)
PST-013	256-mm cyl, in air								
115 gPu/l	c-1	0.9980	400	1.00169	12	1.00203		1.00600	
115 gPu/l	c-2	0.9980	400	1.00157	12	1.00200		1.00623	
Average				1.00163		1.00202		1.00611	
Δ (C-E)				363		402	38	811	420
115 gPu/l	c-4	0.9965	520	0.99419	12	0.99460		0.99852	
Δ (C-E)				-231		-190	41	202	391
PMF-001	Bare Sphere of Pu-239 Metal								
Jezebel	c-1	1.0000	200	1.00025	15	0.99999		0.99889	
Δ (C-E)				25		-1	-26	-111	-110
PMF-002	Bare Sphere of Pu-239 Metal								
Jez. 240	c-1	1.0000	200	1.00430	15	1.00426		1.00332	
Δ (C-E)				430		426	-4	332	-94

Quite and impact

Pu-239 PNFS impact on jezebel 240 !!, but every body think only Pu-240 in Jezebel 240 analysis.

Thermal Solutions

Code				Tripoli-4.5		Tripoli-4.5		Tripoli-4.5	
Library				JEFF-3.1		JEFF-3.1.1		Maslov	
		Experiment		Calc.		Calc.	Δ	Calc.	Δ
		Keff	Unc.	Kcalc	S.D.	Kcalc	Δ (C-C)	Kcalc	(C-C)
ICSBEP	Name			Solutions					
HST001									
Mid	c-1	1.0004	600	0.99908	16	0.99917		1.00493	
Leakage	c-2	1.0021	720	0.99666	16	0.99695		1.00221	
Nitrate	c-3	1.0003	350	1.00237	16	1.00263		1.00809	
	c-4	1.0008	530	0.99929	16	0.99930		1.00448	
	c-5	1.0001	490	0.99974	16	1.00024		1.00470	
	c-6	1.0002	460	1.00314	16	1.00375		1.00802	
	c-7	1.0008	400	0.99882	16	0.99909		1.00456	
	c-8	0.9998	380	0.99890	16	0.99929		1.00471	
	c-9	1.0008	540	0.99483	16	0.99477		1.00069	
Average		**1.0006**		**0.99920**		**0.99947**		**1.00471**	
Δ (C-E)				**-139**		**-112**	**26**	**412**	**524**
HST009									
High	c-1	0.9990	430	1.00064	16	1.00143		1.00623	
Leakage	c-2	1.0000	390	1.00144	16	1.00163		1.00694	
Fluoride	c-3	1.0000	360	1.00099	16	1.00134		1.00669	
	c-4	0.9986	350	0.99559	16	0.99573		1.00099	
Average		**0.9994**		**0.99966**		**1.00003**		**1.00521**	
Δ (C-E)				**26**		**63**	**37**	**581**	**518**
HST010									
Fluoride	c-1	1.0000	290	1.00104	16	1.00108		1.00615	
	c-2	1.0000	290	1.00122	16	1.00156		1.00616	
	c-3	1.0000	290	0.99872	16	0.99896		1.00360	
	c-4	0.9992	290	0.99666	16	0.99700		1.00203	
Average		**0.9998**		**0.99941**		**0.99965**		**1.00448**	
Δ (C-E)				**-39**		**-15**	**24**	**468**	**483**

up to ~ + 500 pcm
a first !!

For those
ENDF/B-VII ~
JEFF-3.1 ~
JENDL-3.3

Are solution more sensitive to spectral data ??

Really reliable ??

Fluor, Nitrogen data impact ?

60 Years

IAEA Atoms for Peace and Development

Thermal solutions

HST010									
Fluoride	c-1	1.0000	290	1.00104	16	1.00108		1.00615	
	c-2	1.0000	290	1.00122	16	1.00156		1.00616	
	c-3	1.0000	290	0.99872	16	0.99896		1.00360	
	c-4	0.9992	290	0.99666	16	0.99700		1.00203	
Average		**0.9998**		**0.99941**		**0.99965**		**1.00448**	
Δ (C-E)				**-39**		**-15**	**24**	**468**	**483**
HST011									
Fluoride	c-1	1.0000	230	1.00473	16	1.00519		1.00922	
	c-2	1.0000	230	1.00062	16	1.00142		1.00544	
Average				**1.00267**		**1.00331**		**1.00733**	
Δ (C-E)				**267**		**331**	**63**	**733**	
HST012									
	c-1	0.9999	580	1.00115	15	1.00126		1.00346	
Δ (C-E)				**125**		**136**		**356**	**220**
HST013									
ORNL-1	c-1	1.0012	260	0.99880	16	0.99816		1.00117	
ORNL-2	c-2	1.0007	360	0.99791	16	0.99962		1.00008	
ORNL-3	c-3	1.0003	360	0.99416	16	0.99452		0.99654	
ORNL-4	c-4	1.0003	360	0.99591	16	0.99641		0.99811	
Average		**1.0006**		**0.99669**		**0.99718**		**0.99897**	
Δ (C-E)				**-393**		**-345**	**48**	**-165**	**179**
HST018									
Nitrate	c-1	1.0000	340	0.98956	16	0.98980		0.99483	
	c-2	1.0000	460	0.98503	16	0.98535		0.99030	
	c-3	1.0000	420	0.98832	16	0.98877		0.99369	
Average				**0.98764**		**0.98797**		**0.99294**	
Δ (C-E)				**-1236**		**-1203**	**34**	**-706**	**497**
HST019									
	c-1	1.0000	410	0.99691	16	0.99708		1.00204	
Δ (C-E)				**-309**		**-292**	**17**	**204**	**495**
HST032									
ORNL-10		1.0015	260	0.99881	16	0.99921		1.00036	
Δ (C-E)				**-269**		**-229**	**41**	**-114**	**114**

up to ~ + 500 pcm
a first !!

More attention need to be pay to solution benchmarks

495 pcm swing

Résumé

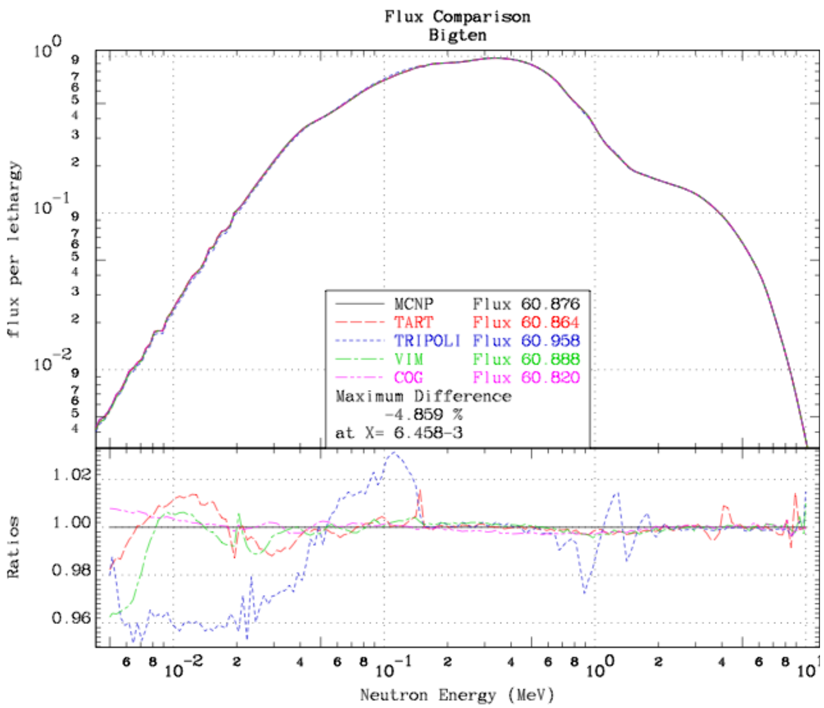
- Contrary to common (reactor physicist) belief PFNS were
  - poorly described, evaluated and certainly used (only one thermal spectra to create a matrix)
  - in essence questionable

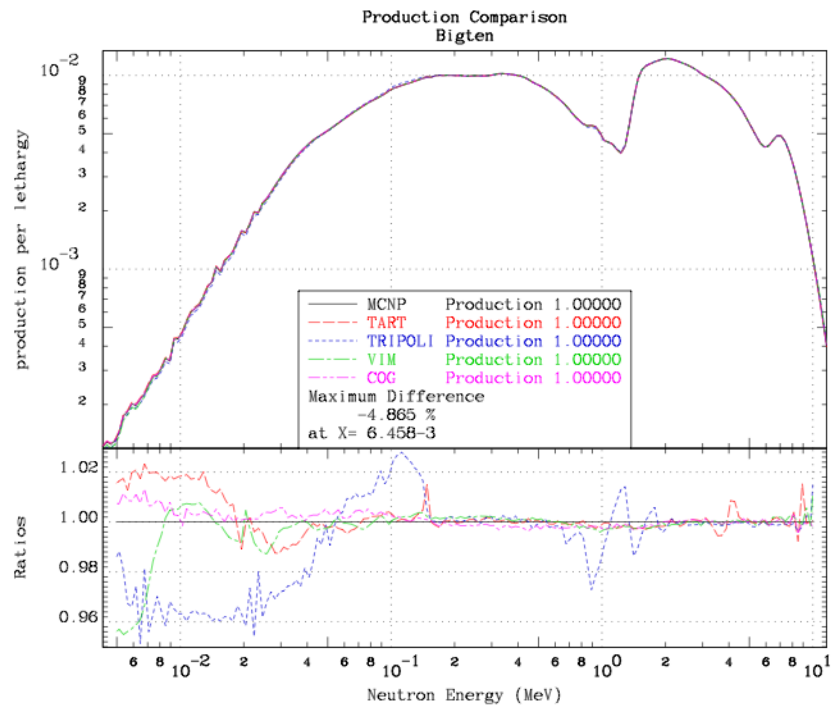
- PFNS can impact benchmarks Keff as potently as cross section, i.e.
  - ☞ + 500 pcm for solutions (unique amongst all libraries)
  - ☞ - 300 pcm for thermal U but + 300 pcm for fast U
  - ☞+ 800 pcm for thermal Pu but -300 for fast Pu

- Emitted spectra are as important as cross section or even angular distribution but not for fission

Keff on Bigten

- Neutron fluxes and production, 660 groups

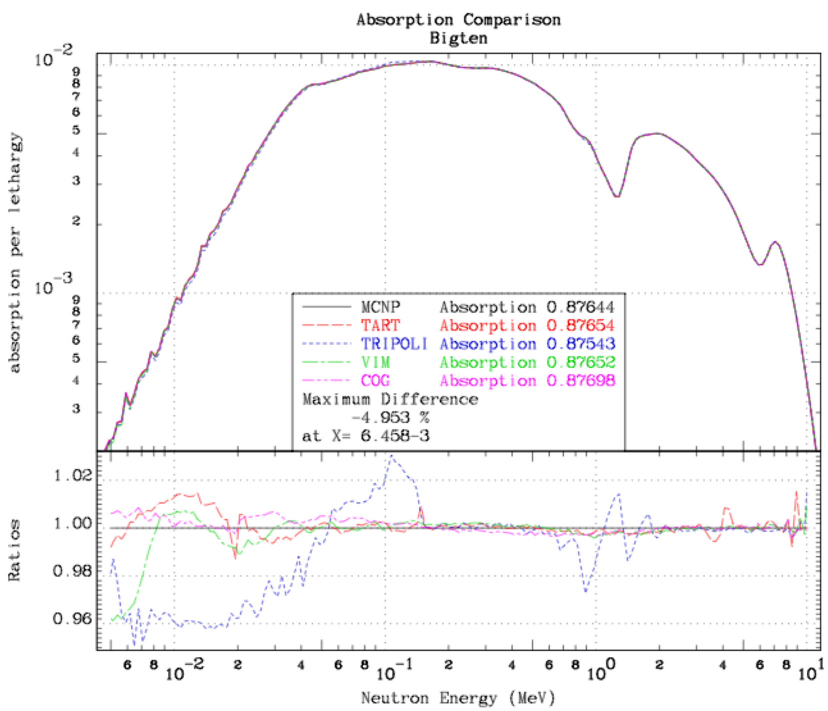


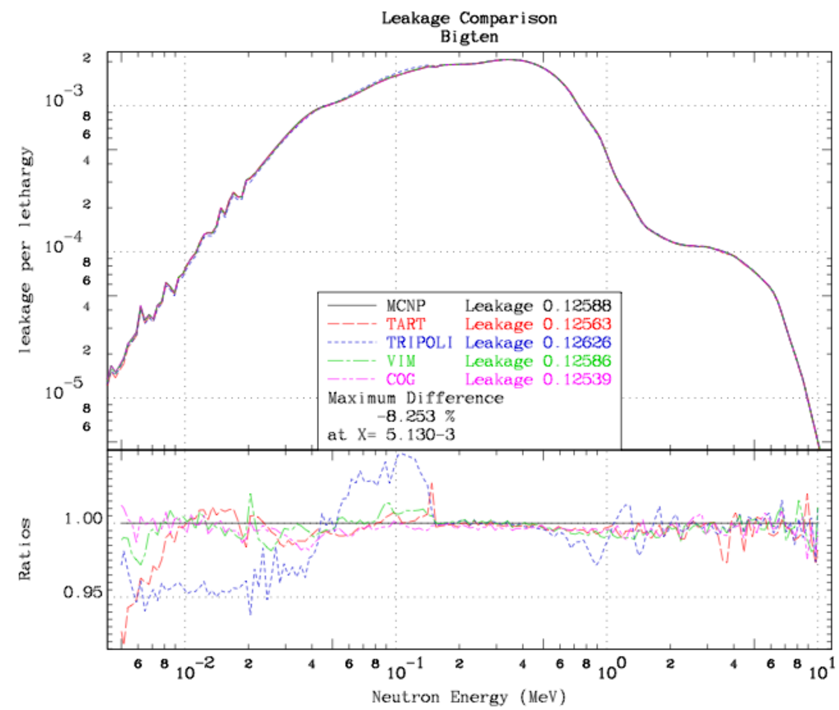


	Absorption	Leakage	K-eff
MCNP	.884520	.121459	0.99406
TART	.884691	.121389	0.99402
TRIPOLI	.884657	.121288	0.99409

Keff on Bigten

- Absorption and leakage, 660 groups





	Absorption	Leakage	K-eff
MCNP	.884520	.121459	0.99406
TART	.884691	.121389	0.99402
TRIPOLI	.884657	.121288	0.99409

Résumé

- The biases induced by the actual pretty much identical (ENDF/B, JEFF or JENDL) U's and Pu's PNFS are
  - rarely accounted for and certainly not negligible
  - parts of the compensating effects
  - now understandable, having been probed by Monte Carlo codes analysis

- New, more physical and better described prompt fission spectra have been, are been produced and need to be accounted for, particularly when cross section fitting or adjustment are foreseen or have been already imbedded in a given library (nu, inelastic level,…)

Résumé : integral trends

- Mostly form deterministic simulation results
- Monte Carlo and Deterministic results do not always agree on fast ICSBEP benchmark and good Monte Carlo on thermal are rare
- Monte Carlo results on big power full core are rare
- Big power core differs feedbacks from little leaky ones, but both are interpreted in the same way
- Simulation methods data forms interpretation issues exists

- Indubitably, all nuclear data contains compensating data, but the past 20 years revealed, interpretation issues
  - U^{238} capture, U238 inelastic
  - O^{16} capture above 2.4 MeV !! For UOx and not H_2O
  - U^{235} pnfs and their interpretation
  - H_2O thermal below 10 eV

Reminding all that rectors are made of real materials, molecules (UOx, H_2O, etc..) and not pure isotope

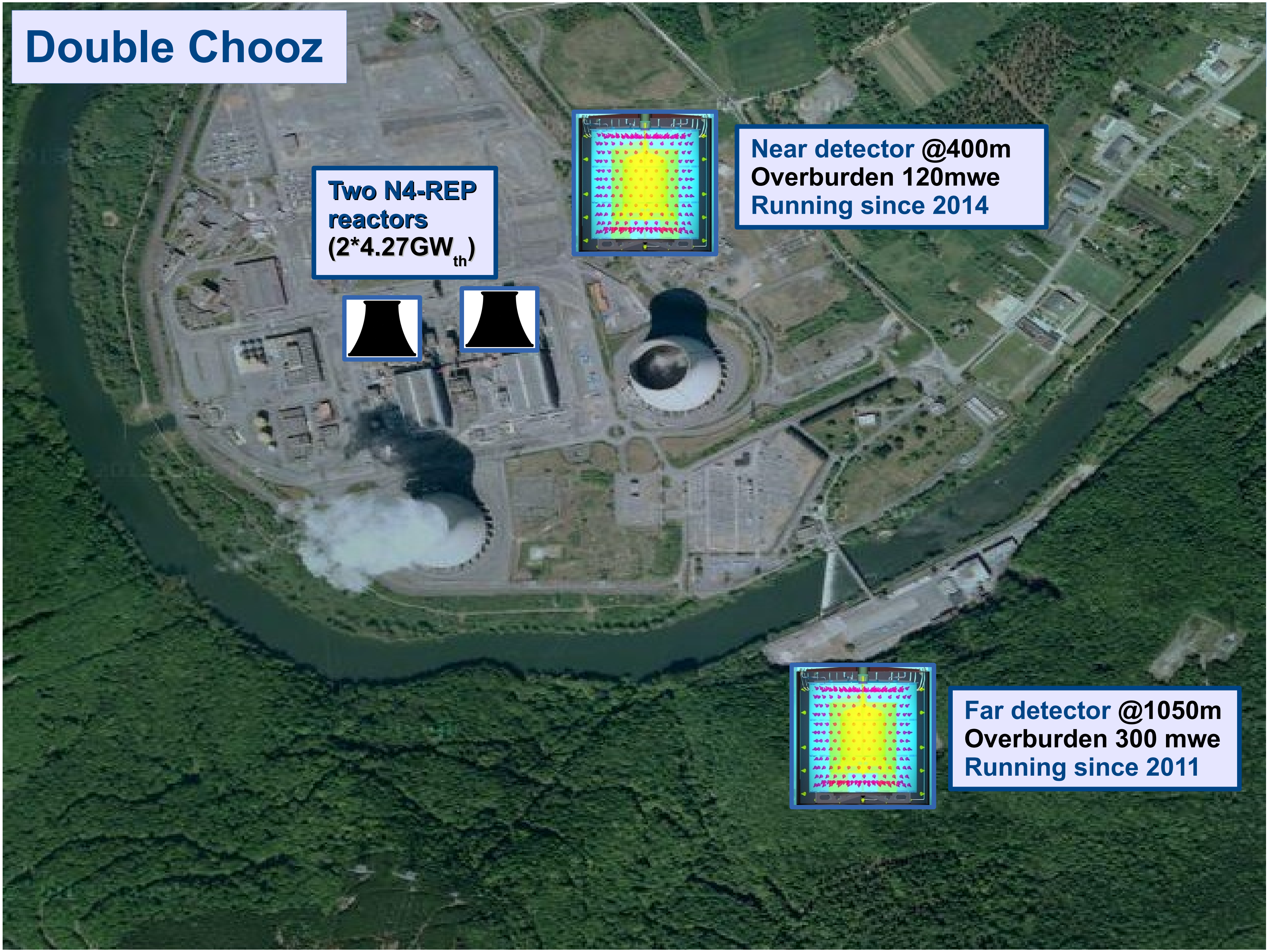
Reactor physics needs

- For pure reactor physics applications, and by that I mean reactor operational simulations, it is now clear that “they” have all the nominal data needed, 444 power reactors running but ^{239}Pu C/E 10% & ^{235}U number density # 5%

- In the light of reactor physics latest software and analysis tools development what clearly missing are
  - The use of nuclear data forms variance-covariance information:
    - Energy wise
    - Channel wise, Isotope wise
    - Matrix wise; nu, sigma, spectra
  - The true, realistic software/methods biases (The jungle..)
  - The correlation between the macro-quantities, data forms used by the simulation tools (macro # micro)

- Solely new fuels, claddings, operational (energy) regimes may change, modify those requirements

Double Chooz



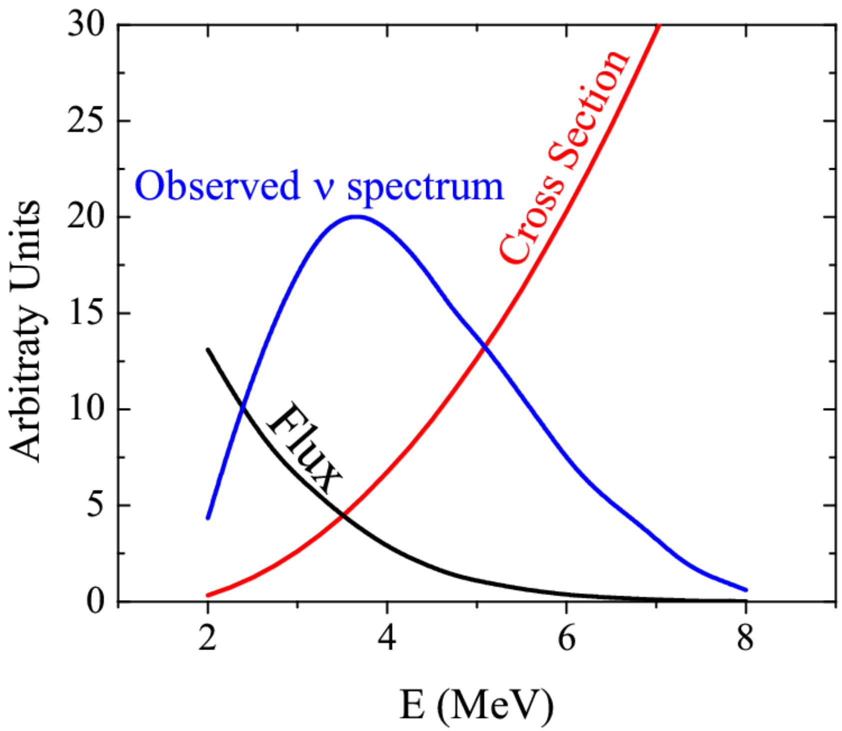
Reactor anti-neutrino issue(s)

- In a nuclear reactor there are about 6 β-decays, and hence neutrinos, per fission or about 2×10^{20} neutrinos per second per GW of thermal power.
- Fortunately, there are only four isotopes whose fission make up more than 99% of all reactor neutrinos with an energy above the inverse β-decay threshold: ^{235}U, ^{239}Pu, ^{241}Pu and ^{238}U
- Nonetheless, the resulting neutrino flux is a superposition of thousands of β-decay branches of the fission fragments of those four isotopes and thus, a first principle calculation is challenging, even with modern nuclear structure data
  - Inverted measured@ILL total β-spectra for thermal fission of ^{235}U, ^{239}Pu and ^{241}Pu (no fast ^{238}U) conversion method
  - Summation method

The reactor ν_e anomaly

Flux $\sim 5 \cdot 10^{20}\ \overline{\nu}_e / s$

$\langle N_\nu \rangle \sim 6$



Principal originators of contributors

^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu

Detection through inverse β decay on proton

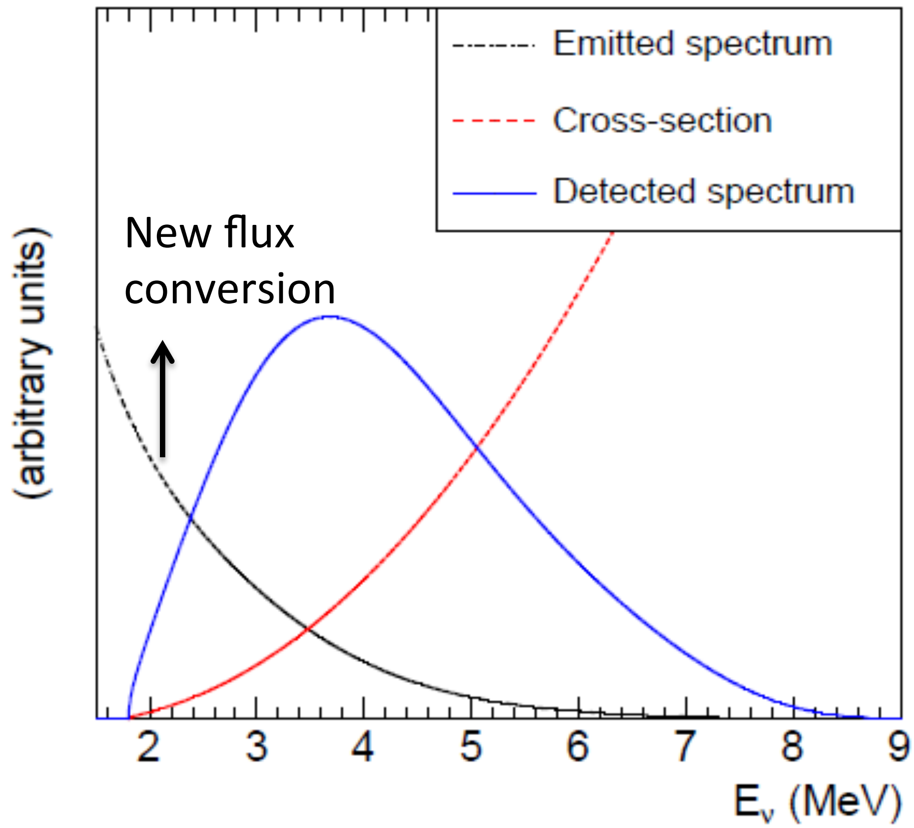
$$\overline{\nu}_e + p \rightarrow e^+ + n$$

Reaction threshold : ~1.8 MeV

$$\langle \sigma \rangle \sim 10^{-43} cm^2$$

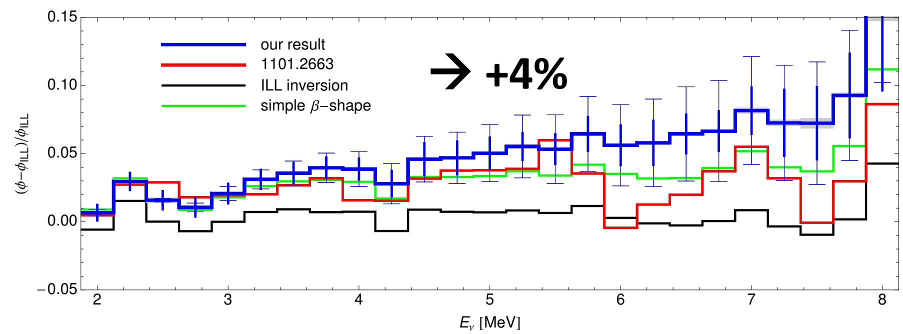
The reactor ν_e anomaly, appeared in 2011

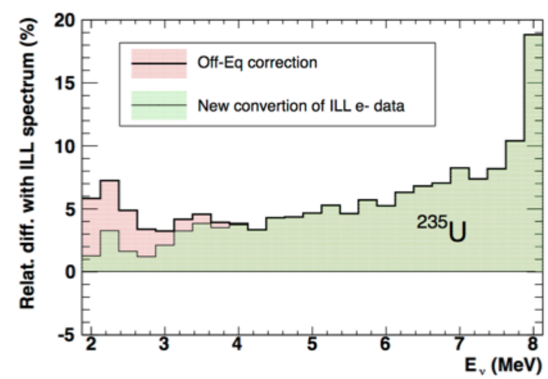
New conversion of ILL beta spectra



Th. Mueller et al, Phys. Rev. C83,054615 (2011)

P. Huber, Phys. Rev. C84, 024617(2011)



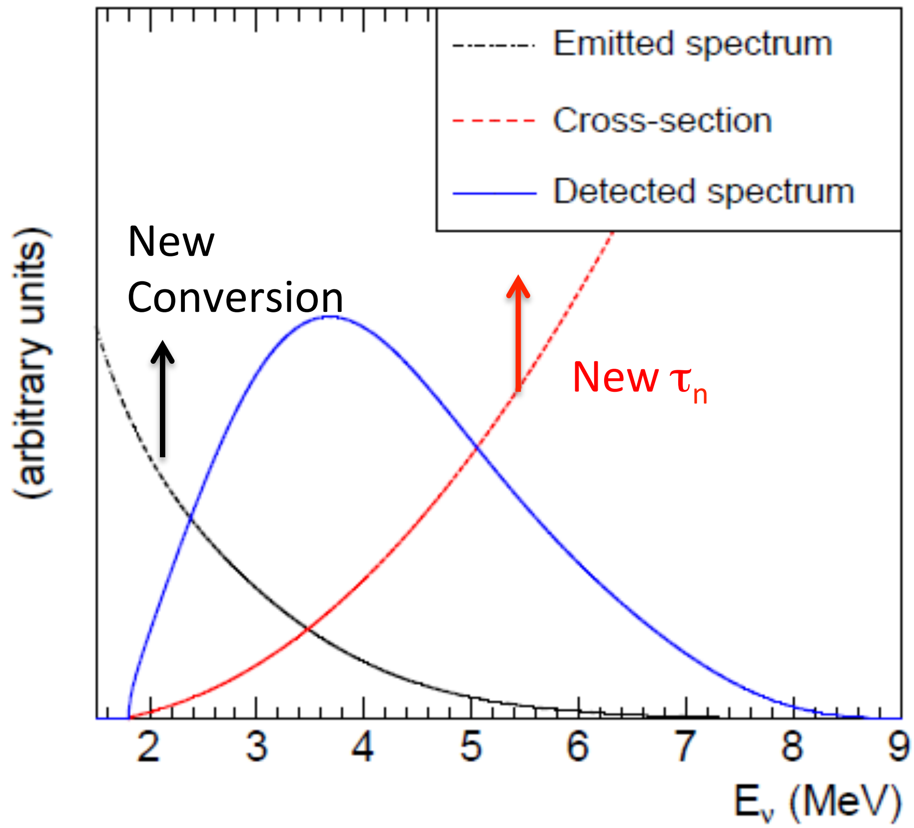


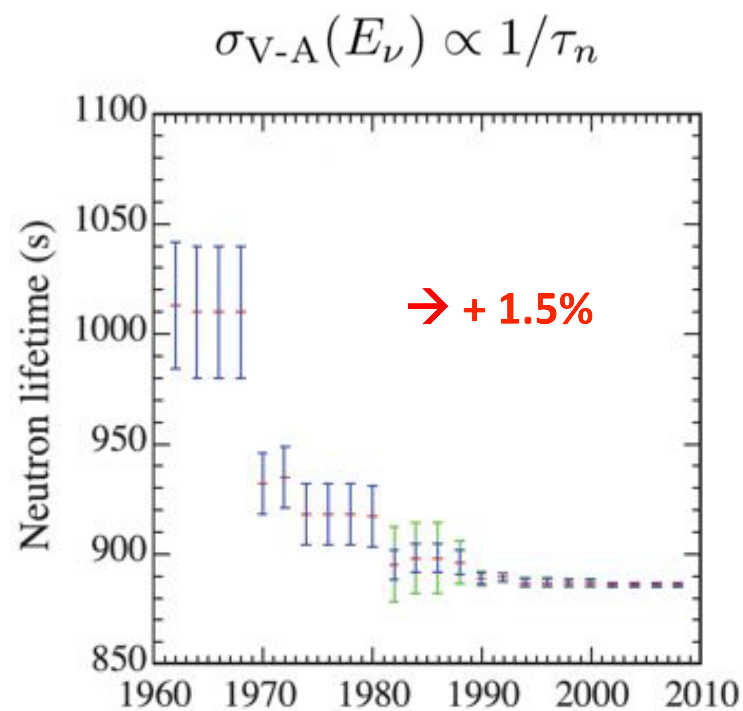
Accumulation of long lived isotopes

→ +1%

The reactor ν_e anomaly

Re-evaluation of $s_{interaction}$

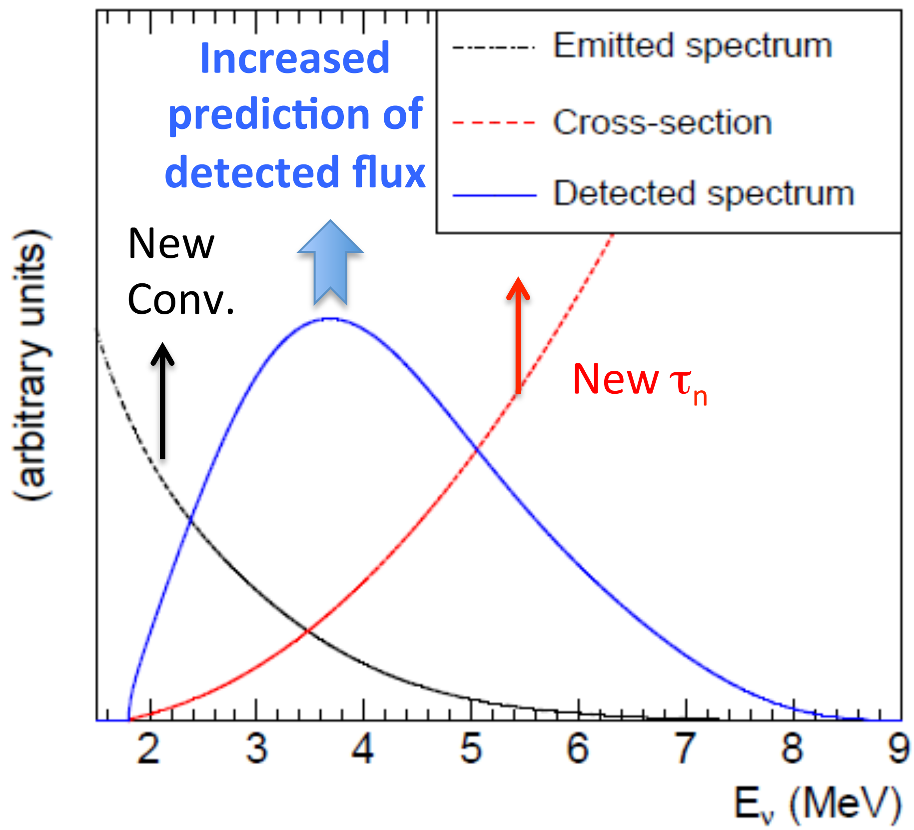




PRD 83, 073006 (2011)

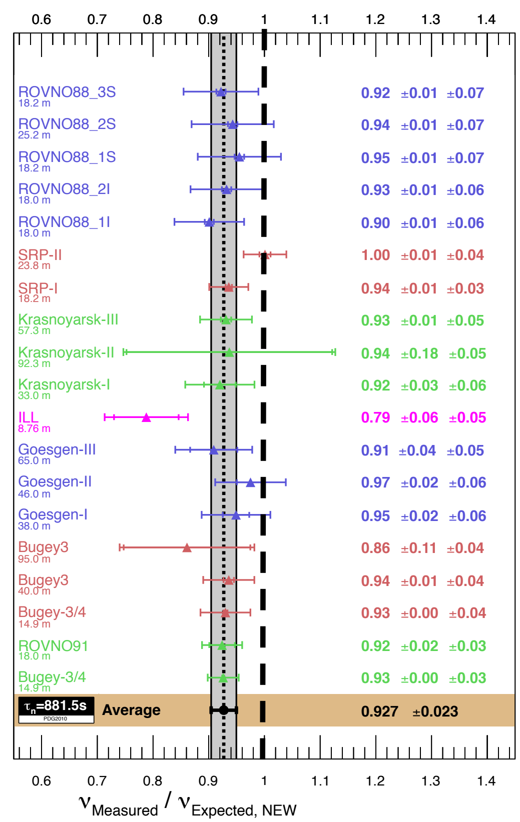
The reactor ν_e anomaly

Reanalysis of reactor short baselines experiments



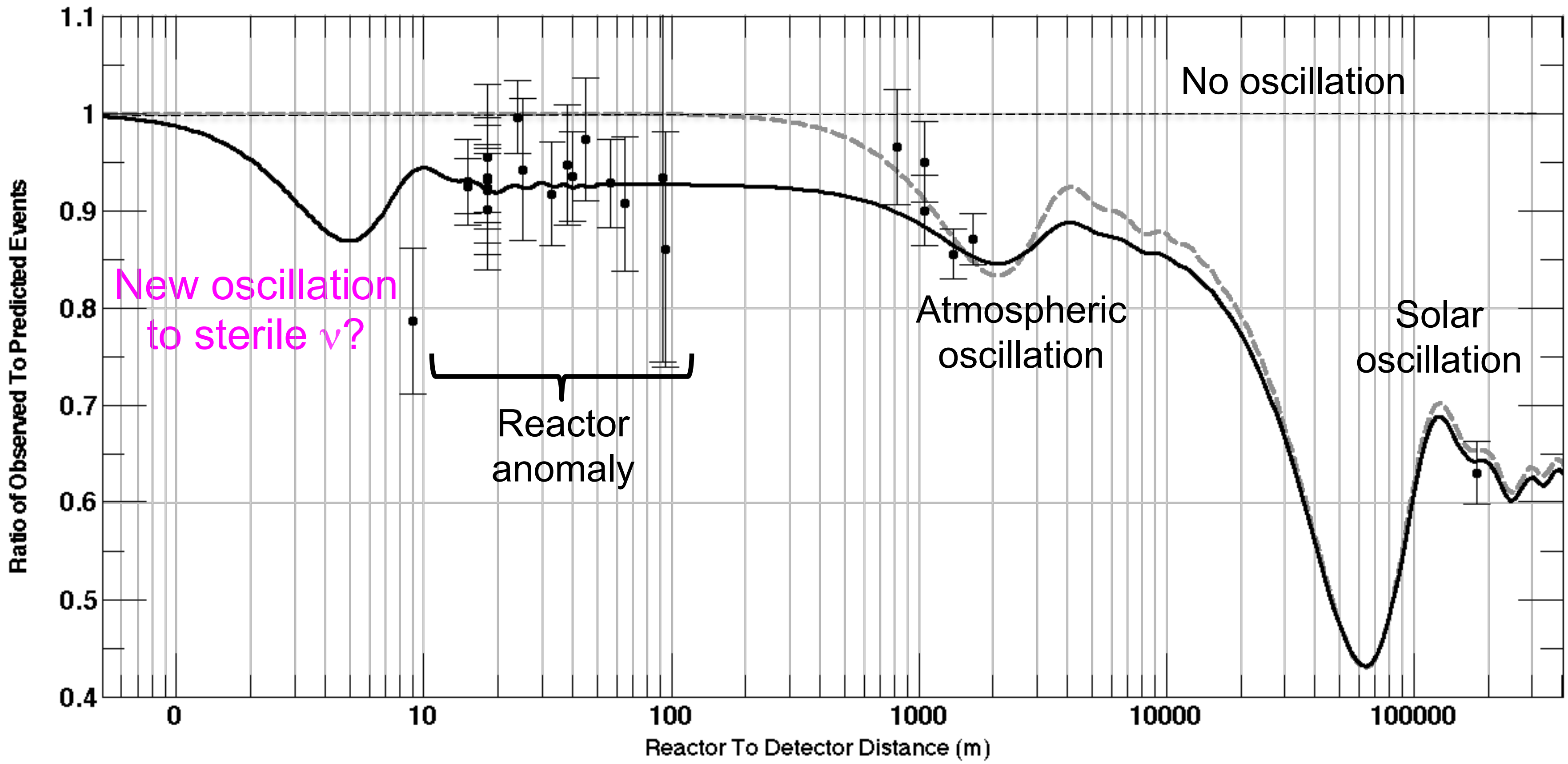
Significant increase of the prediction by 6.5%

G. Mention et al., Phys. Rev. D83, 073006 (2011)



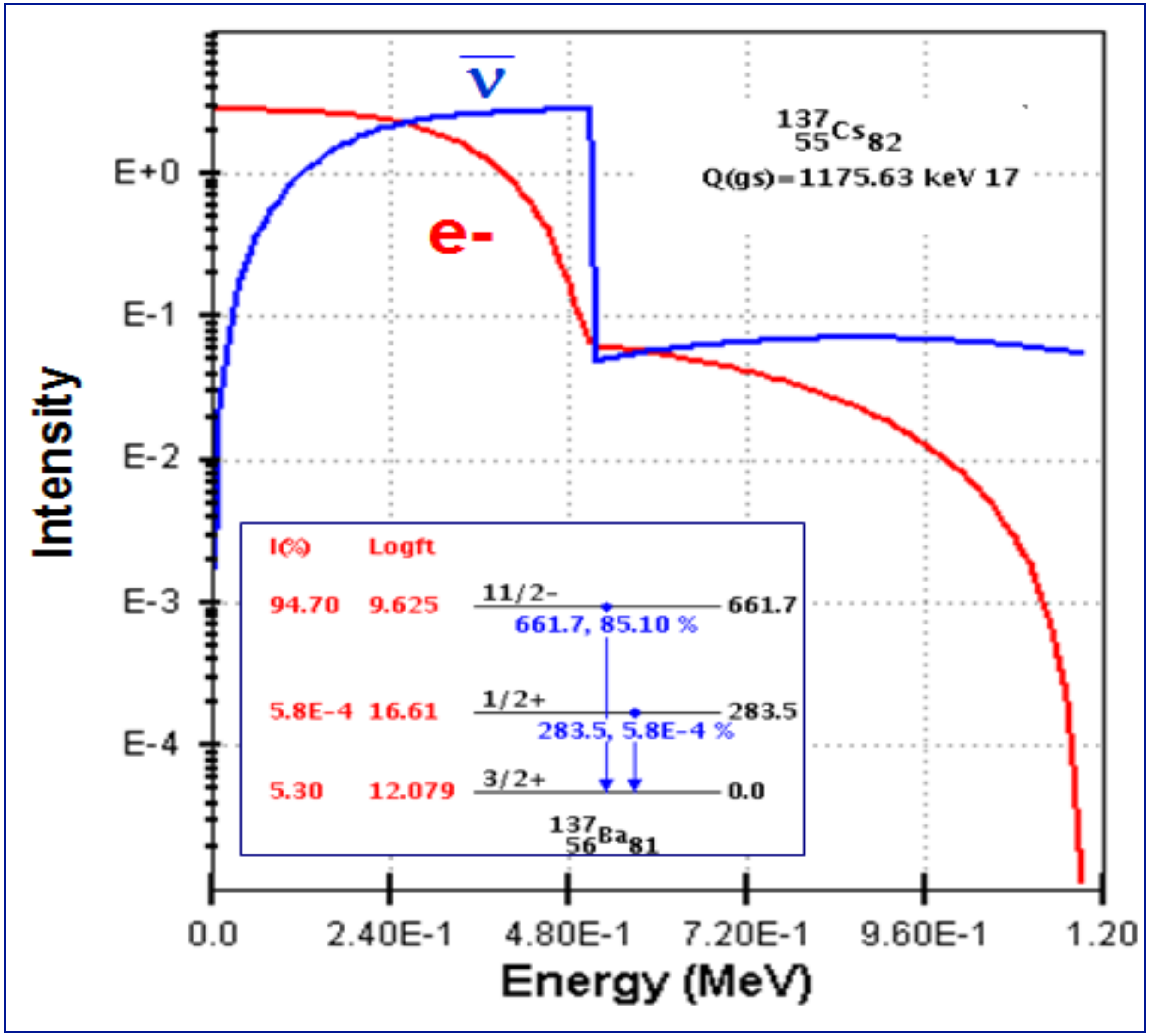
The reactor ν_e anomaly

Survey of 19 short baseline (<100 m) reactor antineutrino experiments
Observed/predicted averaged event ratio: R=0.935±0.024

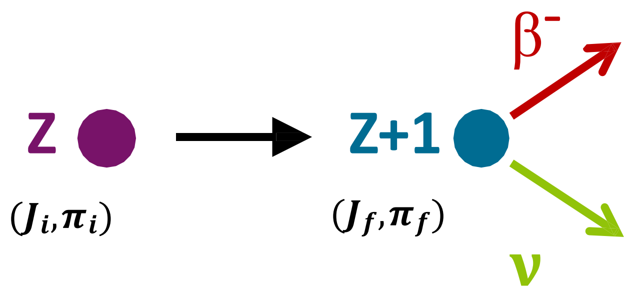


Deficit of ~6.5%, or 3 times the calculated uncertainty
In the spectrum

^{137}Cs β^- & ν_e spectra



Basic of beta decay



ΔJ	$\pi_i \pi_f$	Classification
$0, 1$	1	Allowed
$0, 1$	-1	1st fnu
> 1	$(-1)^{\lvert \Delta J \rvert}$	$\lvert \Delta J \rvert$ th fnu
> 1	$(-1)^{\lvert \Delta J \rvert - 1}$	$(\lvert \Delta J \rvert - 1)$th fu

$\Delta J = \lvert J_f - J_i \rvert$

fnu: forbidden non-unique
fu: forbidden unique

Basics of beta decay, the **most common assumption**

- **Systematic comparison** with 130 **experimental shape factors**

Recent precise measurements of **^{63}Ni** and **^{241}Pu** beta spectra

- **Improvements** of the calculation to include **atomic effects**

Basic of beta decay

Similarly we obtain for the space components

$$\langle p|\,\mathbf{V}+\mathbf{A}\,|n\rangle = \mathrm{i}u_{\mathrm{p}}^{+}\underbrace{\gamma_4\gamma_\mu}_{\begin{pmatrix}0 & \mathrm{i}\boldsymbol{\sigma}\\ \mathrm{i}\boldsymbol{\sigma} & 0\end{pmatrix}}(1+\underbrace{\lambda\gamma_5}_{\lambda\begin{pmatrix}0&1\\1&0\end{pmatrix}})u_{\mathrm{n}} = \sqrt{\frac{(W_{\mathrm{n}}+M_{\mathrm{n}})}{2W_{\mathrm{n}}}}\sqrt{\frac{(W_{\mathrm{p}}+M_{\mathrm{p}})}{2W_{\mathrm{p}}}}$$
$$\times\left\{\left(\frac{\boldsymbol{\sigma}\mathbf{p}}{W_{\mathrm{p}}+M_{\mathrm{p}}}\chi_{\mathrm{p}}^{m'}\right)^{+}\boldsymbol{\sigma}\chi_{\mathrm{n}}^{m}+(\chi_{\mathrm{p}}^{m'})^{+}\boldsymbol{\sigma}\frac{\boldsymbol{\sigma}\mathbf{p}}{W_{\mathrm{n}}+M_{\mathrm{n}}}\chi_{\mathrm{n}}^{m}-\lambda(\chi_{\mathrm{p}}^{m'})^{+}\boldsymbol{\sigma}\chi_{\mathrm{n}}^{m}\right.$$
$$\left.-\lambda\left[\left(\frac{\boldsymbol{\sigma}\mathbf{p}}{W_{\mathrm{p}}+M_{\mathrm{p}}}\chi_{\mathrm{p}}^{m'}\right)^{+}\boldsymbol{\sigma}\frac{\boldsymbol{\sigma}\mathbf{p}}{W_{\mathrm{n}}+M_{\mathrm{n}}}\chi_{\mathrm{n}}^{m}\right]\right\}. \quad (6.38)$$

This equals to

$$\langle p|\,\mathbf{V}+\mathbf{A}\,|n\rangle = \sqrt{\frac{(W_{\mathrm{n}}+M_{\mathrm{n}})}{2W_{\mathrm{n}}}}\sqrt{\frac{(W_{\mathrm{p}}+M_{\mathrm{p}})}{2W_{\mathrm{p}}}}\left\{(\chi_{\mathrm{p}}^{m'})^{+}\underbrace{\frac{\boldsymbol{\sigma}\mathbf{p}_{\mathrm{p}}}{W_{\mathrm{p}}+M_{\mathrm{p}}}\boldsymbol{\sigma}}_{\frac{\mathbf{p}_{\mathrm{p}}+\mathrm{i}(\boldsymbol{\sigma}\times\mathbf{p}_{\mathrm{p}})}{W_{\mathrm{p}}+M_{\mathrm{p}}}}\chi_{\mathrm{n}}^{m}\right.$$
$$+(\chi_{\mathrm{p}}^{m'})^{+}\underbrace{\boldsymbol{\sigma}\frac{\boldsymbol{\sigma}\mathbf{p}_{\mathrm{n}}}{W_{\mathrm{n}}+M_{\mathrm{n}}}}_{\frac{\mathbf{p}_{\mathrm{n}}-\mathrm{i}(\boldsymbol{\sigma}\times\mathbf{p}_{\mathrm{n}})}{W_{\mathrm{n}}+M_{\mathrm{n}}}}\chi_{\mathrm{n}}^{m}-\lambda(\chi_{\mathrm{p}}^{m'})^{+}\boldsymbol{\sigma}\chi_{\mathrm{n}}^{m}$$
$$\left.-\lambda\left[(\chi_{\mathrm{p}}^{m'})^{+}\underbrace{\frac{\boldsymbol{\sigma}\mathbf{p}_{\mathrm{p}}}{W_{\mathrm{p}}+M_{\mathrm{p}}}\boldsymbol{\sigma}\frac{\boldsymbol{\sigma}\mathbf{p}_{\mathrm{n}}}{W_{\mathrm{n}}+M_{\mathrm{n}}}}_{\frac{-(\mathbf{p}_{\mathrm{p}}\mathbf{p}_{\mathrm{n}})\boldsymbol{\sigma}+(\boldsymbol{\sigma}\mathbf{p}_{\mathrm{p}})\mathbf{p}_{\mathrm{n}}+\mathbf{p}_{\mathrm{p}}(\boldsymbol{\sigma}\mathbf{p}_{\mathrm{n}})-\mathrm{i}(\mathbf{p}_{\mathrm{p}}\times\mathbf{p}_{\mathrm{n}})}{(W_{\mathrm{p}}+M_{\mathrm{p}})(W_{\mathrm{n}}+M_{\mathrm{n}})}}\chi_{\mathrm{n}}^{m}\right]\right\}. \quad (6.39)$$

Finally we obtain for the space components

$$\langle p|\,\mathbf{V}(0)+\mathbf{A}(0)\,|n\rangle = \sqrt{\frac{(W_{\mathrm{n}}+M_{\mathrm{n}})}{2W_{\mathrm{n}}}}\sqrt{\frac{(W_{\mathrm{p}}+M_{\mathrm{p}})}{2W_{\mathrm{p}}}}$$
$$\times\left\{\left[\frac{\mathbf{p}_{\mathrm{p}}}{W_{\mathrm{p}}+M_{\mathrm{p}}}+\frac{\mathbf{p}_{\mathrm{n}}}{W_{\mathrm{n}}+M_{\mathrm{n}}}\right](\chi_{\mathrm{p}}^{m'})^{+}\chi_{\mathrm{n}}^{m}+(\chi_{\mathrm{p}}^{m'})^{+}\right.$$
$$\times\left[\frac{\mathrm{i}(\boldsymbol{\sigma}\times\mathbf{p}_{\mathrm{p}})}{W_{\mathrm{p}}+M_{\mathrm{p}}}-\frac{\mathrm{i}(\boldsymbol{\sigma}\times\mathbf{p}_{\mathrm{n}})}{W_{\mathrm{n}}+M_{\mathrm{n}}}\right]\chi_{\mathrm{p}}^{m}-\lambda(\chi_{\mathrm{p}}^{m'})^{+}\boldsymbol{\sigma}\chi_{\mathrm{n}}^{m}$$
$$+\lambda\frac{\mathbf{p}_{\mathrm{p}}\mathbf{p}_{\mathrm{n}}}{(W_{\mathrm{p}}+M_{\mathrm{p}})(W_{\mathrm{n}}+M_{\mathrm{n}})}\{(\chi_{\mathrm{p}}^{m'})^{+}\boldsymbol{\sigma}\chi_{\mathrm{n}}^{m}\}+\lambda\frac{\mathrm{i}(\mathbf{p}_{\mathrm{p}}\times\mathbf{p}_{\mathrm{n}})}{(W_{\mathrm{p}}+M_{\mathrm{p}})(W_{\mathrm{n}}+M_{\mathrm{n}})}$$
$$\left.\times(\chi_{\mathrm{p}}^{m'})^{+}\chi_{\mathrm{n}}^{m}-\lambda\left[(\chi_{\mathrm{p}}^{m'})^{+}\frac{(\boldsymbol{\sigma}\mathbf{p}_{\mathrm{p}})\mathbf{p}_{\mathrm{n}}+\mathbf{p}_{\mathrm{p}}(\boldsymbol{\sigma}\mathbf{p}_{\mathrm{n}})}{(W_{\mathrm{p}}+M_{\mathrm{p}})(W_{\mathrm{n}}+M_{\mathrm{n}})}\chi_{\mathrm{n}}^{m}\right]\right\}. \quad (6.40)$$

$$-\frac{\mathrm{i}}{2M_{\mathrm{A}}}F_{\mathrm{M}}(q^2)(\mathbf{P}\times\mathbf{q})\boldsymbol{\sigma}-F_{\mathrm{S}}(q^2)q_0+\frac{1}{4(2M_{\mathrm{A}})^2}F_{\mathrm{S}}(q^2)q_0(\mathbf{P}^2-\mathbf{q}^2)$$
$$\left.-\frac{\mathrm{i}}{2}\frac{1}{(2M_{\mathrm{A}})^2}F_{\mathrm{S}}(q^2)q_0(\mathbf{P}\times\mathbf{q})\boldsymbol{\sigma}\right\}\chi^{M_i} \quad (9.15)$$

$$\langle\phi_f(p_f)|\,A_0(0)\,|\phi_i(p_i)\rangle = N(\chi^{M_f})^{+}\left\{-\frac{1}{2M_{\mathrm{A}}}F_{\mathrm{A}}(q^2)(\mathbf{P}\boldsymbol{\sigma})\right.$$
$$-\frac{q_0}{2M_{\mathrm{A}}}F_{\mathrm{P}}(q^2)(\mathbf{q}\boldsymbol{\sigma})-F_{\mathrm{T}}(q^2)(\mathbf{q}\boldsymbol{\sigma})+\frac{1}{4}\frac{1}{(2M_{\mathrm{A}})^2}F_{\mathrm{T}}(q^2)$$
$$\left.\times[(\mathbf{P}\mathbf{q})(\boldsymbol{\sigma}\mathbf{P}+\boldsymbol{\sigma}\mathbf{q})-(\boldsymbol{\sigma}\mathbf{q})(\mathbf{P}^2-\mathbf{q}^2)]\right\}\chi^{M_i} \quad (9.16)$$

$$\langle\phi_f(p_f)|\,\mathbf{V}(0)\,|\phi_i(p_i)\rangle = N(\chi^{M_f})^{+}\left\{\frac{1}{2M_{\mathrm{A}}}F_{\mathrm{V}}(q^2)\mathbf{P}+\frac{\mathrm{i}}{2M_{\mathrm{A}}}F_{\mathrm{V}}(q^2)(\boldsymbol{\sigma}\times\mathbf{q})\right.$$
$$+\mathrm{i}F_{\mathrm{M}}(q^2)(\boldsymbol{\sigma}\times\mathbf{q})-\frac{1}{2M_{\mathrm{A}}}F_{\mathrm{M}}(q^2)q_0\mathbf{q}-\frac{\mathrm{i}}{4M_{\mathrm{A}}}F_{\mathrm{M}}(q^2)q_0(\boldsymbol{\sigma}\times\mathbf{P})$$
$$-F_{\mathrm{S}}(q^2)\mathbf{q}+\frac{1}{4(2M_{\mathrm{A}})^2}F_{\mathrm{S}}(q^2)\mathbf{q}(\mathbf{P}^2-\mathbf{q}^2)-\frac{\mathrm{i}}{2(2M_{\mathrm{A}})^2}F_{\mathrm{S}}(q^2)\mathbf{q}$$
$$\times((\mathbf{P}\times\mathbf{q})\boldsymbol{\sigma})-\frac{\mathrm{i}}{2(2M_{\mathrm{A}})^2}F_{\mathrm{M}}(q^2)\mathbf{P}((\mathbf{P}\times\mathbf{q})\boldsymbol{\sigma})-\frac{\mathrm{i}}{4(2M_{\mathrm{A}})^2}$$
$$\left.\times F_{\mathrm{M}}(q^2)(\mathbf{P}^2+\mathbf{q}^2)(\boldsymbol{\sigma}\times\mathbf{q})+\frac{\mathrm{i}}{2(2M_{\mathrm{A}})^2}F_{\mathrm{M}}(q^2)(\mathbf{P}\mathbf{q})(\boldsymbol{\sigma}\times\mathbf{P})\right\}\chi^{M_i} \quad (9.17)$$

$$\langle\phi_f(p_f)|\,\mathbf{A}(0)\,|\phi_i(p_i)\rangle = N(\chi^{M_f})^{+}\left\{-F_{\mathrm{A}}(q^2)\boldsymbol{\sigma}+\frac{1}{2(2M_{\mathrm{A}})^2}\right.$$
$$\times F_{\mathrm{A}}(q^2)\mathbf{P}^2\boldsymbol{\sigma}-\frac{1}{4(2M_{\mathrm{A}})^2}F_{\mathrm{A}}(q^2)(\mathbf{P}^2+\mathbf{q}^2)\boldsymbol{\sigma}-\frac{i}{2(2M_{\mathrm{A}})^2}$$
$$\times F_{\mathrm{A}}(q^2)(\mathbf{P}\times\mathbf{q})-\frac{1}{2(2M_{\mathrm{A}})^2}F_{\mathrm{A}}(q^2)[(\boldsymbol{\sigma}\mathbf{P})\mathbf{P}-(\boldsymbol{\sigma}\mathbf{q})\mathbf{q}]$$
$$+\frac{1}{2M_{\mathrm{A}}}F_{\mathrm{T}}(q^2)[(\mathbf{P}\mathbf{p})\boldsymbol{\sigma}-\mathbf{q}(\boldsymbol{\sigma}\mathbf{P})]-F_{\mathrm{T}}(q^2)q_0\boldsymbol{\sigma}$$
$$+\frac{1}{2(2M_{\mathrm{A}})^2}F_{\mathrm{T}}(q^2)q_0\mathbf{P}^2\boldsymbol{\sigma}-\frac{1}{4(2M_{\mathrm{A}})^2}F_{\mathrm{T}}(q^2)q_0(\mathbf{P}^2+\mathbf{q}^2)\boldsymbol{\sigma}$$
$$-\frac{\mathrm{i}}{2(2M_{\mathrm{A}})^2}F_{\mathrm{T}}(q^2)q_0(\mathbf{P}\times\mathbf{q})-\frac{1}{2(2M_{\mathrm{A}})^2}F_{\mathrm{T}}(q^2)q_0[(\boldsymbol{\sigma}\mathbf{P})\mathbf{P}$$
$$\left.-(\boldsymbol{\sigma}\mathbf{q})\mathbf{q}]-\frac{1}{2M_{\mathrm{A}}}F_{\mathrm{P}}(q^2)(\boldsymbol{\sigma}\mathbf{q})\mathbf{q}\right\}\chi^{M_i}. \quad (9.18)$$

454 SPECIAL FORMULAE

$$\left.+\sqrt{\tfrac{2}{3}}\left(\int rI'(r)\beta\gamma_5 T_{121}\right)\right\}$$
$$\mp\frac{f_{\mathrm{P}}}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{D}}\mathfrak{N}_{110}^{(0)}(1,1,1,1) \quad (14.101)$$

$${}^{\mathrm{A}}F_{121}^{(0)}=\mp\lambda\,{}^{\mathrm{A}}\mathfrak{M}_{121}^{(0)}-\frac{f_{\mathrm{T}}}{R}\left[\frac{5}{\sqrt{3}}\,{}^{\mathrm{C}}\mathfrak{N}_{111}^{(0)}-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{A}}\mathfrak{M}_{121}^{(0)}\right]\mp\frac{f_{\mathrm{P}}}{R}5\sqrt{\tfrac{2}{3}}\,{}^{\mathrm{D}}\mathfrak{N}_{110}^{(0)} \quad (14.102)$$

$${}^{\mathrm{A}}F_{121}^{(0)}(1,1,1,1)=\mp\lambda\,{}^{\mathrm{A}}\mathfrak{M}_{121}^{(0)}(1,1,1,1)$$
$$-\frac{f_{\mathrm{T}}}{R}\left\{\sqrt{\tfrac{1}{3}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta T_{111}\right)\right.$$
$$\left.-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{A}}\mathfrak{M}_{121}^{(0)}(1,1,1,1)\right\}$$
$$\mp\frac{f_{\mathrm{P}}}{R}\sqrt{\tfrac{2}{3}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta\gamma_5 T_{110}\right) \quad (14.103)$$

$${}^{\mathrm{V}}F_{211}^{(0)}=-{}^{\mathrm{V}}\mathfrak{M}_{211}^{(0)}-\frac{f_{\mathrm{M}}}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{C}}\mathfrak{N}_{211}^{(0)} \quad (14.104)$$

$${}^{\mathrm{V}}F_{220}^{(0)}={}^{\mathrm{V}}\mathfrak{M}_{220}^{(0)}+\frac{f_{\mathrm{M}}}{R}\sqrt{(10)}\,{}^{\mathrm{C}}\mathfrak{N}_{211}^{(0)}\pm\frac{f_{\mathrm{S}}}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{V}}\mathfrak{M}_{220}^{(0)} \quad (14.105)$$

$${}^{\mathrm{V}}F_{220}^{(0)}(1,1,1,1)={}^{\mathrm{V}}\mathfrak{M}_{220}^{(0)}(1,1,1,1)$$
$$+\frac{f_{\mathrm{M}}}{R}\left\{\sqrt{\tfrac{2}{5}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta T_{211}\right)\right.$$
$$\left.+\sqrt{\tfrac{3}{5}}\left(\int\left(\frac{r}{R}\right)rI'(r)\beta T_{231}\right)\right\}$$
$$\pm\frac{f_{\mathrm{S}}}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{V}}\mathfrak{M}_{220}^{(0)}(1,1,1,1) \quad (14.106)$$

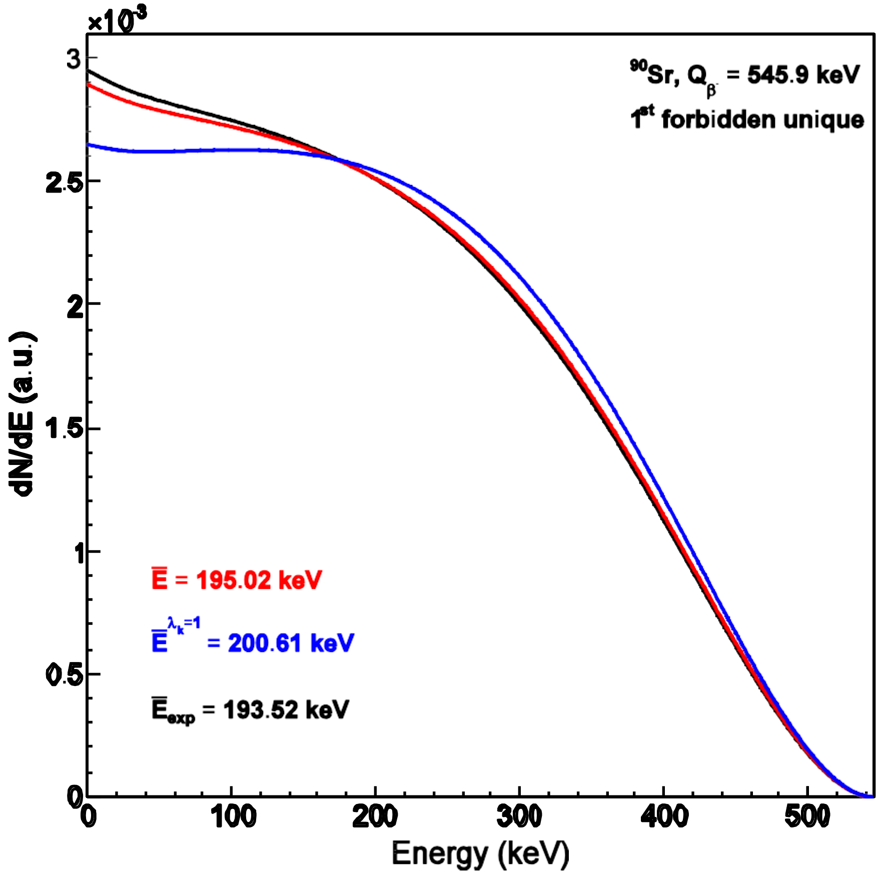
$${}^{\mathrm{A}}F_{221}^{(0)}=\pm\lambda\,{}^{\mathrm{A}}\mathfrak{M}_{221}^{(0)}+\frac{f_{\mathrm{T}}}{R}[\sqrt{(15)}\,{}^{\mathrm{C}}\mathfrak{N}_{211}^{(0)}-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{A}}\mathfrak{M}_{221}^{(0)}] \quad (14.107)$$

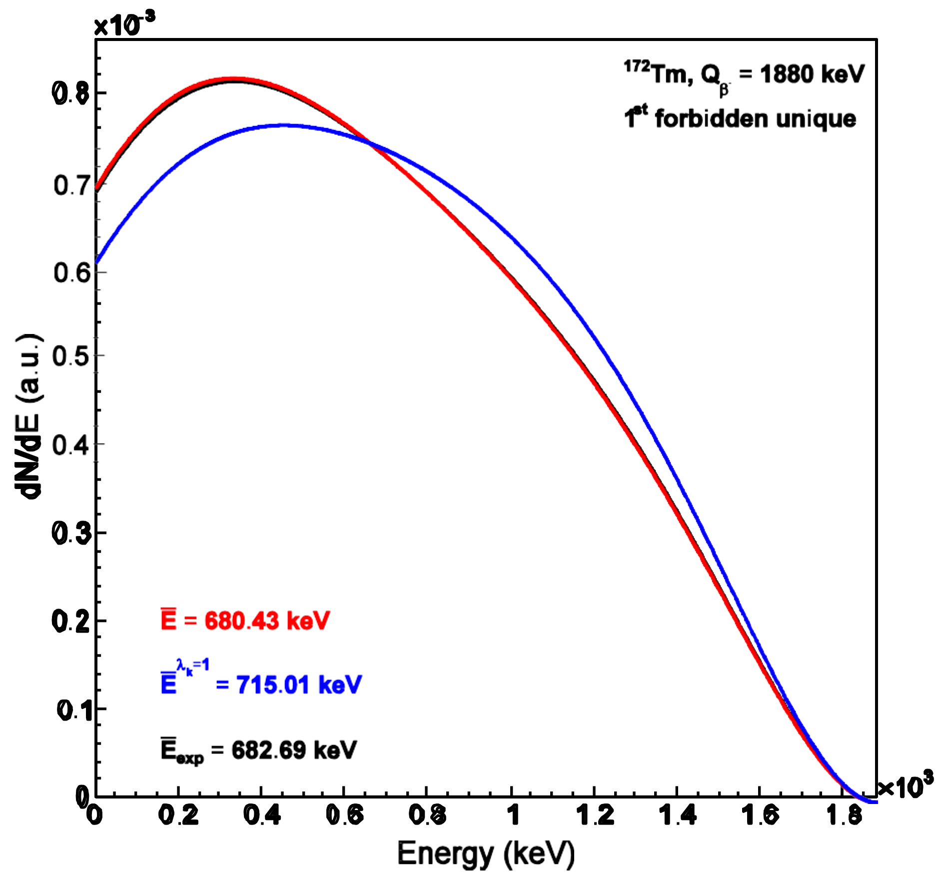
$${}^{\mathrm{A}}F_{221}^{(0)}(1,1,1,1)=\pm\lambda\,{}^{\mathrm{A}}\mathfrak{M}_{221}^{(0)}(1,1,1,1)$$
$$+\frac{f_{\mathrm{T}}}{R}\left\{\sqrt{\tfrac{3}{5}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta T_{211}\right)\right.$$
$$-\sqrt{\tfrac{2}{5}}\left(\int\left(\frac{r}{R}\right)rI'(r)\beta T_{231}\right)$$
$$\left.-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{\mathrm{A}}\mathfrak{M}_{221}^{(0)}(1,1,1,1)\right\} \quad (14.108)$$

H. Behrens, W. Bühring, *Electron Radial Wave functions and Nuclear Beta Decay*, Oxford Science Publications (1982)

More than 600 pages !!

BetaShape (analytical), systematic comparison





Mean energy disagrees by **3.6 %**

High influence at low energy

Mean energy disagrees by **4.6 %**

High influence at low energy and on the overall shape of the spectrum

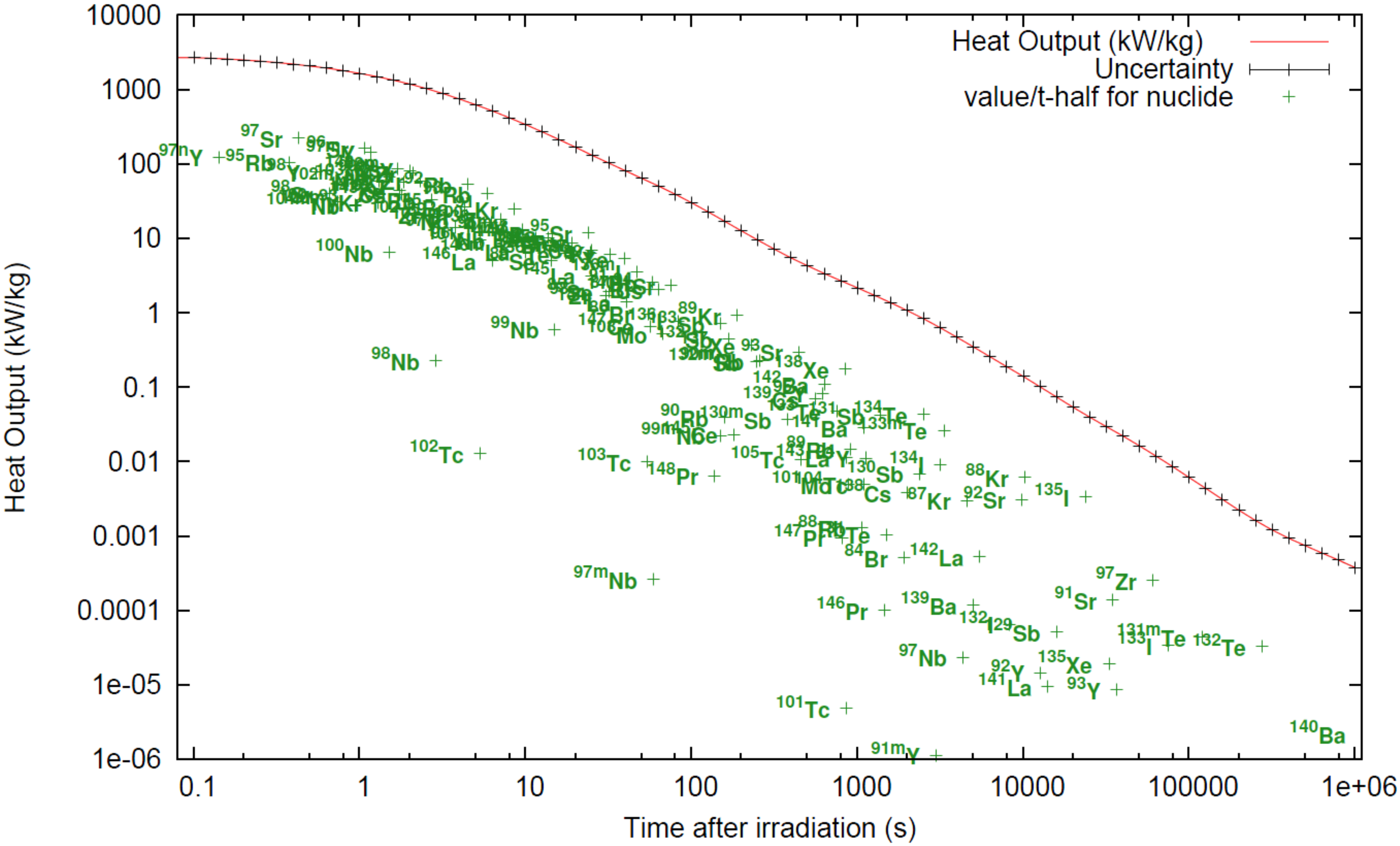
$\lambda_k = 1$ approximation, usually **bad approximation** !!

ξ **approximation** is correct **only** for ~ 50 % of the **1st forbidden non-unique**

Fission products

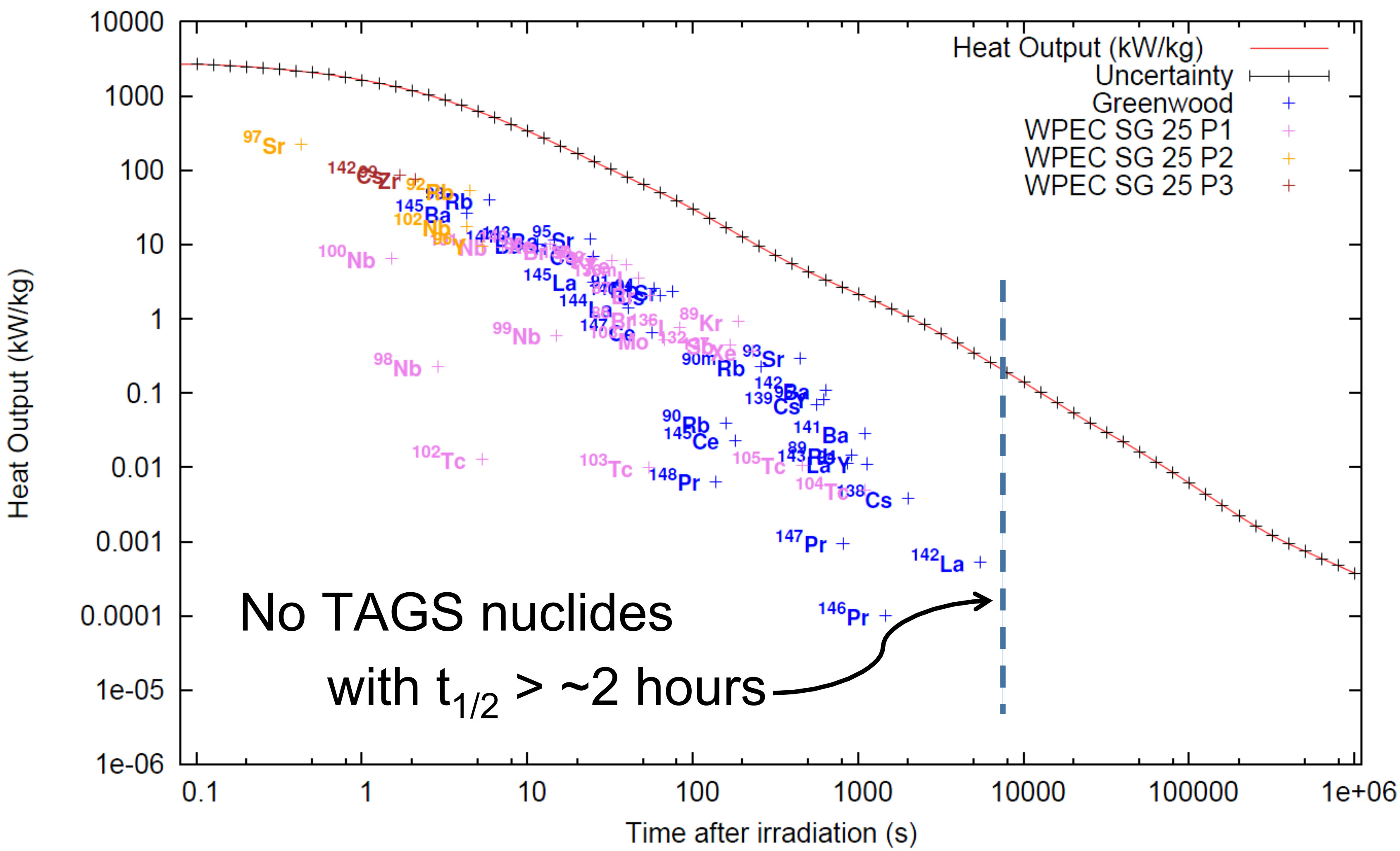
Thermal ^{235}U pulse generates a large inventory...

Each nuclide at $(x,y)=(t_{1/2},heat(t_{1/2}))$



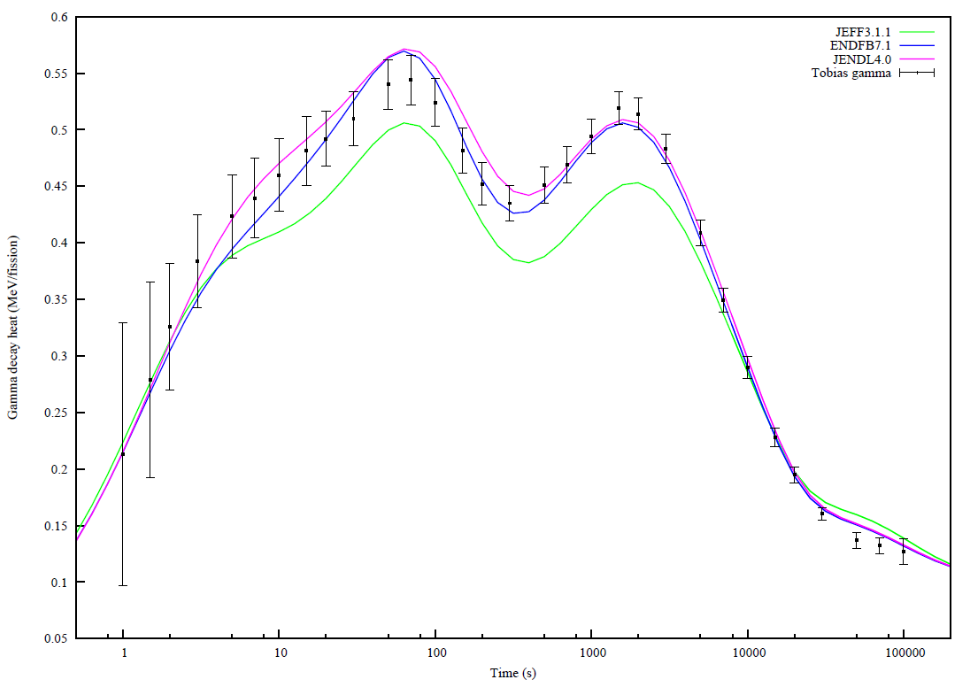
Fission products

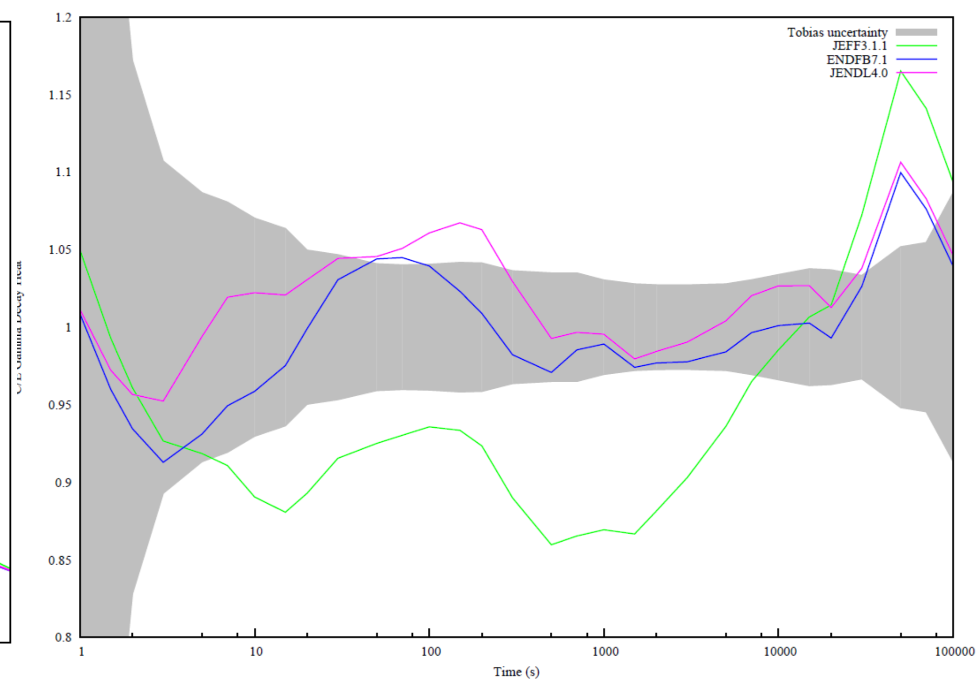
Blue = Greenwood nuclides and WPEC SG 25 P1, P2, P3 are priority 1, 2, 3 nuclides with requested TAGS by subgroup 25



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

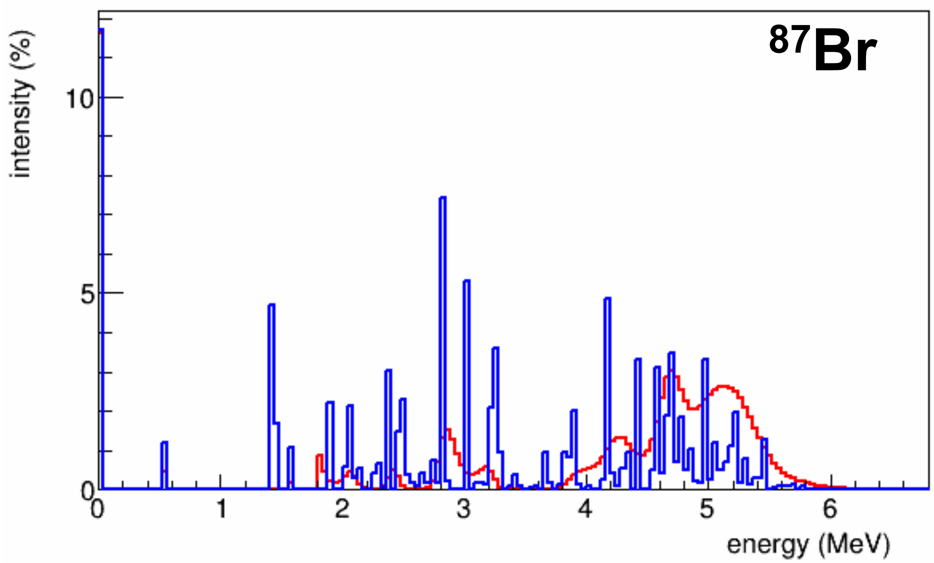
Dominant nuclide heat production for $^{239}Pu_{th}$

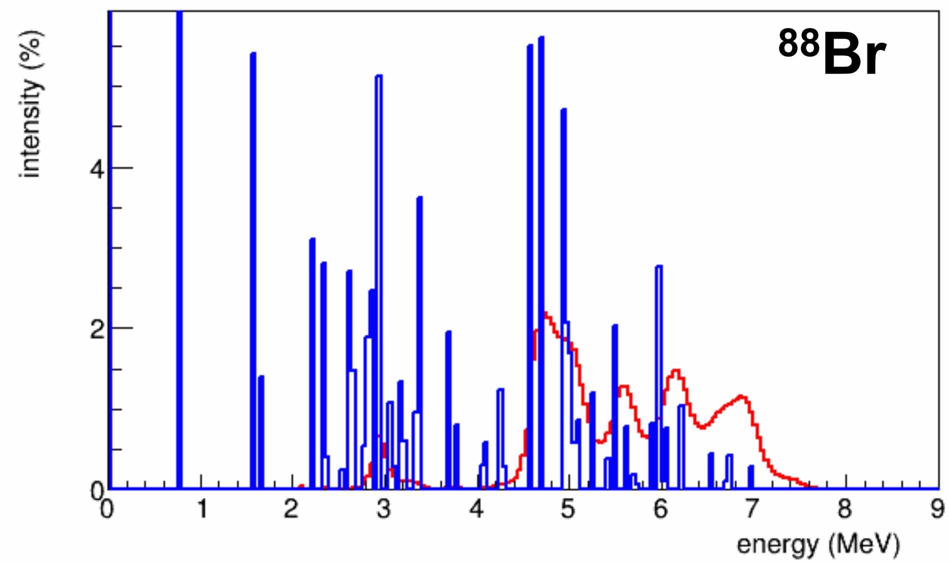
- Below are the dominant nuclides and their ***gamma*** heat contribution at 800s after pulse for $^{239}Pu_{th}$ in kW
- Again Tc 104/5 different feeding for JEFF-3.1.1
- Sr93 jumps by 30% between ENDF and JENDL

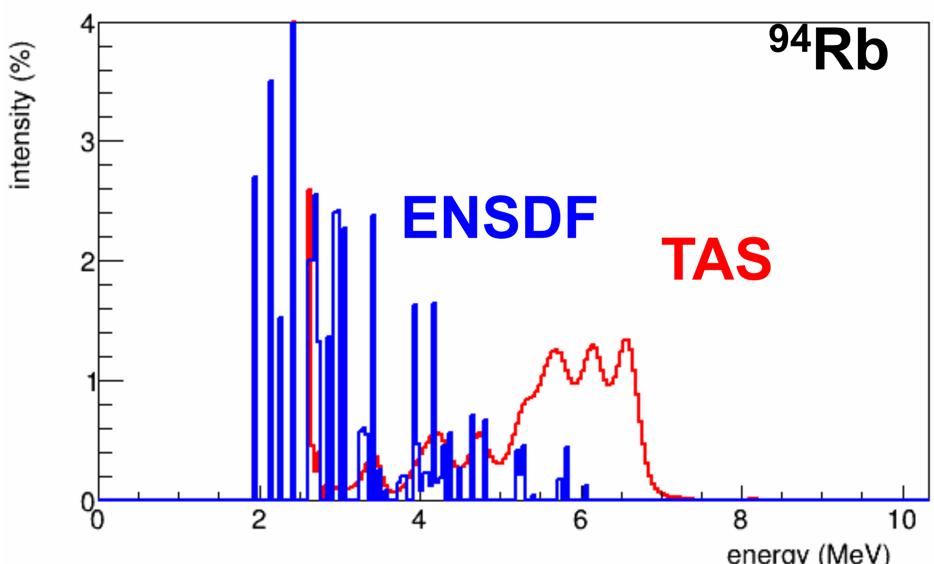
Nuclide	ENDF/B-VII.1	Nuclide	JENDL-4.0	Nuclide	JEFF3.2/3.1.1
Tc104	**93.8**	**Tc104**	**93.8**	**Tc104**	**54.9**
Tc105	**59.5**	**Tc105**	**59.6**	**Sr93**	**44.6**
Mo101	44.5	Mo101	45.9	Mo101	44.5
Sr93	**53.6**	**Sr93**	**40.6**	Y95	29.5
Y95	33.1	Y95	30.0	Xe138	28.7
Xe138	28.8	Xe138	28.8	Cs138	26.9
Cs138	27.0	Cs138	27.0	Ba142	26.7
Ba142	26.7	Ba142	26.5	**Tc105**	**21.8**

Different nuclear data # results on dominants ??

Comparison of high resolution (ENSDF) with TAS β-intensity







- In all three cases TAS reveals considerable *Pandemonium* effect

Isotope	<Eγ> ENSDF	<Eγ> TAS
87Br	3057 keV	3945 keV
88Br	2861 keV	4591 keV
94Rb	1729 keV	4060 keV

- Impact on reactor decay heat and anti-neutrino spectrum summation calculations

Issue(s), challenges

- Certainly not the result of neutrino oscillations but rather a sign that researchers need to know, simulate better the processes that produce antineutrinos:
  - ^{239}Pu versus ^{235}U
  - figure out how the beta decay of each fission product that contributes to the antineutrino spectrum (exchange and screening effects have been demonstrated to have a great influence on the spectrum shape at low energy; better approximation, new measurements, theory for the forbidden non-unique transitions,..)
  - Cumulative FYs and consistent FP decay schemes data

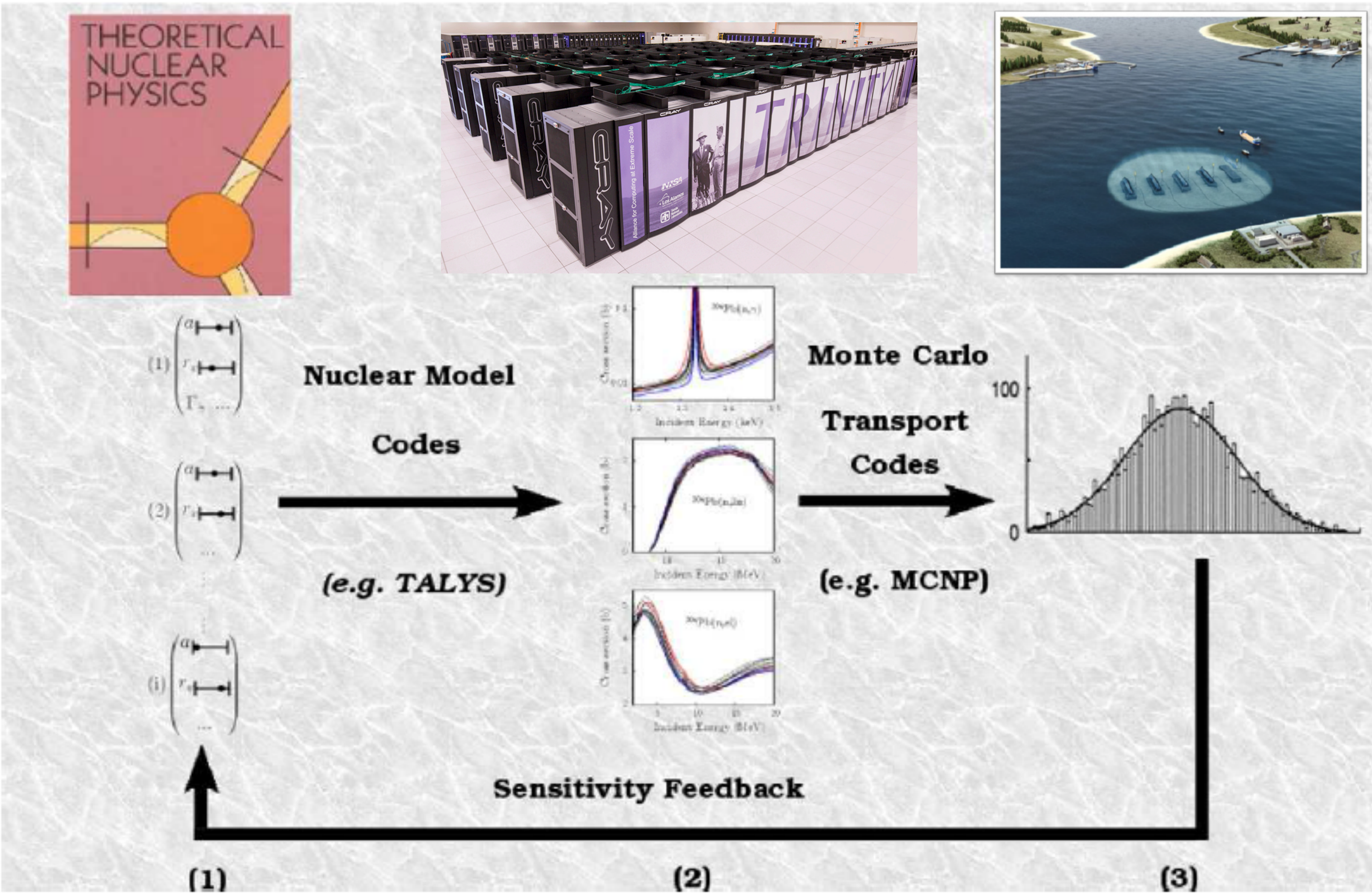
- Why? such predictions could be used in efforts to detect nuclear reactor misuse, as the antineutrino flux and energy depend on the reactor fuel composition

Yesterday and tomorrow trends

- Generation III+ EPR 1650 Mwe, build on site

- Small modular reactor, SMR < 300 Mwe, factory build

Today – Tomorrow reactor physics ??



Reactor physics future

Engineers value short turnaround times

Waiting…..
Waiting…..
Waiting…..
Waiting…..
Waiting…..
Waiting……..

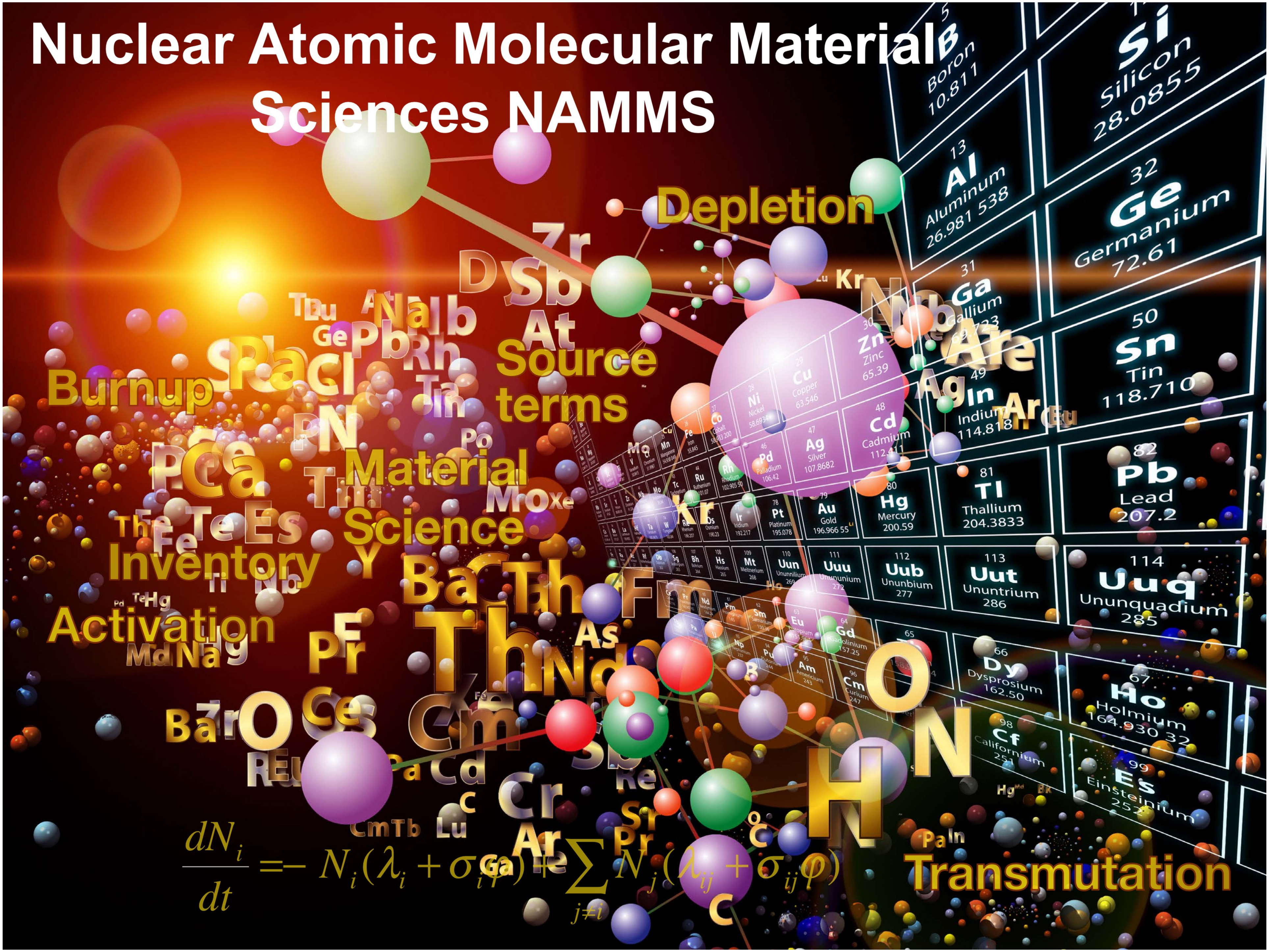
- "Hero runs" are rare: design, analysis, and testing require fast turnaround times
- Real engineering projects require simultaneous execution of many jobs
- Mid-range HPC machines often provide "best" turnaround today
- Most HPC machine queues need to dramatically improve many-user performance

Acknowledgements

The author would like to acknowledge the influence of the following colleagues in the making of this talk.

Kord Smith (MIT), Muriel Fallot (Mines Nantes), David Lhuillier, Xavier Mougeot, Benjamin Morillon, Pascal Romain, Helder Duarte (CEA), Mark Gilbert, Michael Fleming (UKAEA), Dimitri Rochman (PSI), Arjan Koning (IAEA), Alejandro Sonzogni (BNL), Jose Luis Tain, Alejandro Algora (IFIC), Cyriel Wagemans (JRC), Vladimir Maslov (JINER), Dermott Cullen (LLNL),…

In no particular order


Nuclear Atomic Molecular Material Sciences NAMMS
Depletion
Burnup
Source terms
Material Science
Inventory
Activation
Transmutation
$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i\varphi) + \sum_{j\neq i} N_j(\lambda_{ij} + \sigma_{ij}\varphi)$