



FISPACT-II

Reaction rate & uncertainty quantification
and propagation, variance-covariance &
Pathways

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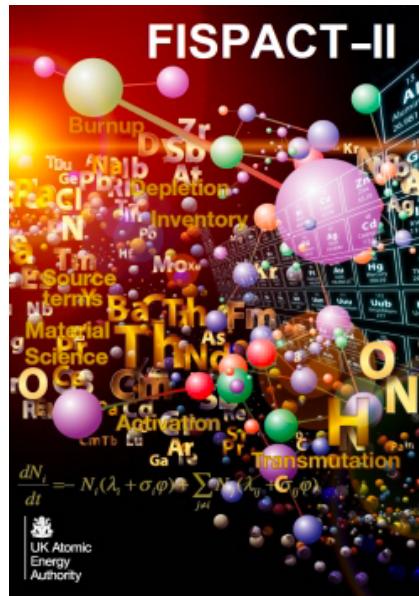
- Single irradiation pulse followed by cooling
- Multiple irradiation pulses
 - changing flux amplitude
 - cooling
- Multi-step
 - changing flux amplitude and spectrum
 - changing cross-section (e.g., temperature dependence)
 - cooling
- Pathways and sensitivity for all cases



- Extracts and reduces nuclear and radiological data
- Solves rate equations for time evolution of inventory
- Computes and outputs derived radiological quantities
- Identifies and quantifies key reactions and decay processes:
 - dominant nuclides
 - pathways and uncertainty
 - Monte-Carlo sensitivity and uncertainty
 - reduced model calculations
- Uncertainty calculation
 - input cross-section and decay uncertainties
 - output uncertainties for all radiological quantities

Recap: Simulation processes

- FISPACT-II is an inventory code that accommodates all modern ENDF-6 particle-induced reaction data (TENDL, ENDF/B, JEFF, JENDL, CENDL, GEFY), including the full MF=33 covariance files (where provided)
- The energy-dependent data is collapsed with user-provided multi-group particle fluxes to calculate one-group cross-section values with uncertainties (+- column)
- FISPACT-II printlib.out



Al 27 (n,Xp)	3.891E-01+-0.0E+00
Al 27 (n,Xd)	2.557E-02+-0.0E+00
Al 27 (n,Xt)	8.848E-04+-0.0E+00
Al 27 (n,Xa)	1.264E-01+-0.0E+00
Al 27 (n,total)	1.908E+00+-3.1E+00
Al 27 (n,na) Na 23	2.535E-02+-1.2E+01
Al 27 (n,a) Na 24	1.010E-01+-8.2E+00
Al 27 (n,t) Mg 25	8.848E-04+-5.1E+01
Al 27 (n,np) Mg 26	3.240E-01+-2.1E+01
Al 27 (n,d) Mg 26	2.557E-02+-3.6E+01
Al 27 (n,p) Mg 27	6.510E-02+-1.3E+01
Al 27 (n,2n) Al 26	3.160E-02+-2.0E+01
Al 27 (n,2n) Al 26m	1.055E-03+-3.7E+01
Al 27 (n,E) Al 27	9.750E-01+-2.6E+00
Al 27 (n,n) Al 27	3.581E-01+-1.3E+01
Al 27 (n,g) Al 28	3.321E-04+-1.1E+02



- Nuclear data often represents a major contributor to uncertainties in nuclear simulations, they are not the only ones !!
- Wherever you use a nuclear data file to provide the various fundamental physics (cross-sections, nu-bars, decay data, fission yields, etc.) there is only one sure truth: **the numbers are not unique**
- The nature and importance of uncertainty values changes, evolves by application - e.g. criticality, activation/transmutation, high-energy, dosimetry, etc.
- As a fusion laboratory ourselves, activation-transmutation with neutron fields up to 14 MeV (not more) are of particular importance, nuclear data uncertainties are very significant and uncertainty analyses over thousands of reaction channels presents a challenge



- Condense run extracts from decay files:
 - decay constant λ
 - decay constant uncertainty $\Delta\lambda$
- Collapse constructs flux spectrum weighted averages:

➤ Library input

- cross-section vs energy
- covariances vs energy
- flux spectrum vs energy

$$W_i = \frac{\phi_i}{\sum_{i=1}^N \Phi_i}$$

$$\overline{XS} = \sum_{i=1}^n W_i X_i$$

- Data used in code
- collapsed cross-section \overline{XS}
 - collapsed uncertainty Δ



- reactions X and Y
- energy bins i and j $\in [1, N]$ with N = 1102
- uses $\text{Cov}(X_i, Y_j)$ for $X \neq Y$ only in Monte-Carlo
- collapse $\text{Cov}(X_i, X_j)$ to get uncertainty Δ for \bar{X}

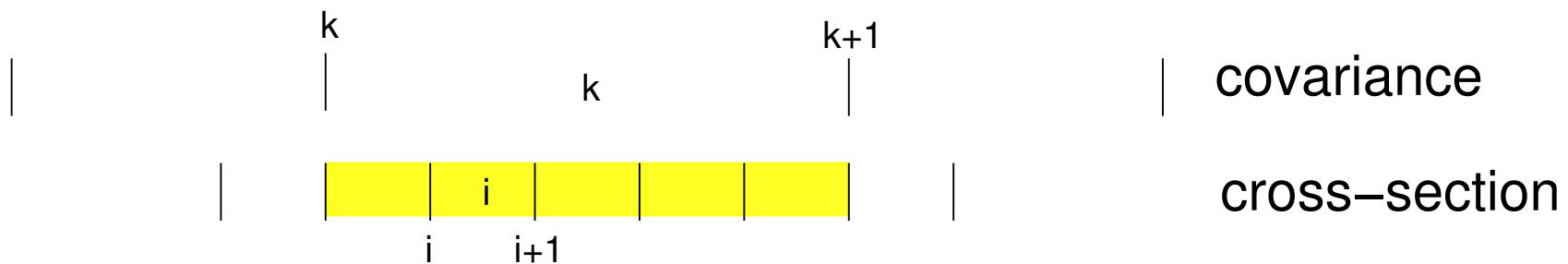
$$\text{var} = \sum_{i=1}^N \sum_{j=1}^N W_i W_j \text{Cov}(X_i, X_j); \quad \Delta = \{1|3\} \sqrt{\text{var}} / \bar{X}$$

1 TENDL, 3 EAF

- Collapse $\text{Cov}(X_i, Y_j)$ to get $\text{Cov}(\bar{X}, \bar{Y})$ for $X \neq Y$
- Cov data in ENDF file 33 & 40, NI type LB=1, 5, 6
- Cov data in wider energy bins k $\in [1, M]$, M \sim 40

The projection operator S_i^k maps cross-section energy bins to covariance energy bins

$$S_i^k = \begin{cases} 1 & \text{bin } i \text{ in bin } k \\ 0 & \text{otherwise} \end{cases}$$



The ENDF style covariance data forms, different LB's are read directly without the need of pre-processing



Using S_i^k , the formula to construct estimates of the covariance matrix are as follows:

$$LB = 1 : \quad Cov(X_i, X_j) = \sum_{k=1}^M S_i^k S_j^k F_k X_i X_j$$

$$\Rightarrow LB = 5 : \quad Cov(X_i, Y_j) = \sum_{k=1}^M \sum_{k'=1}^M S_i^k S_j^{k'} F_{kk'} X_i Y_j$$

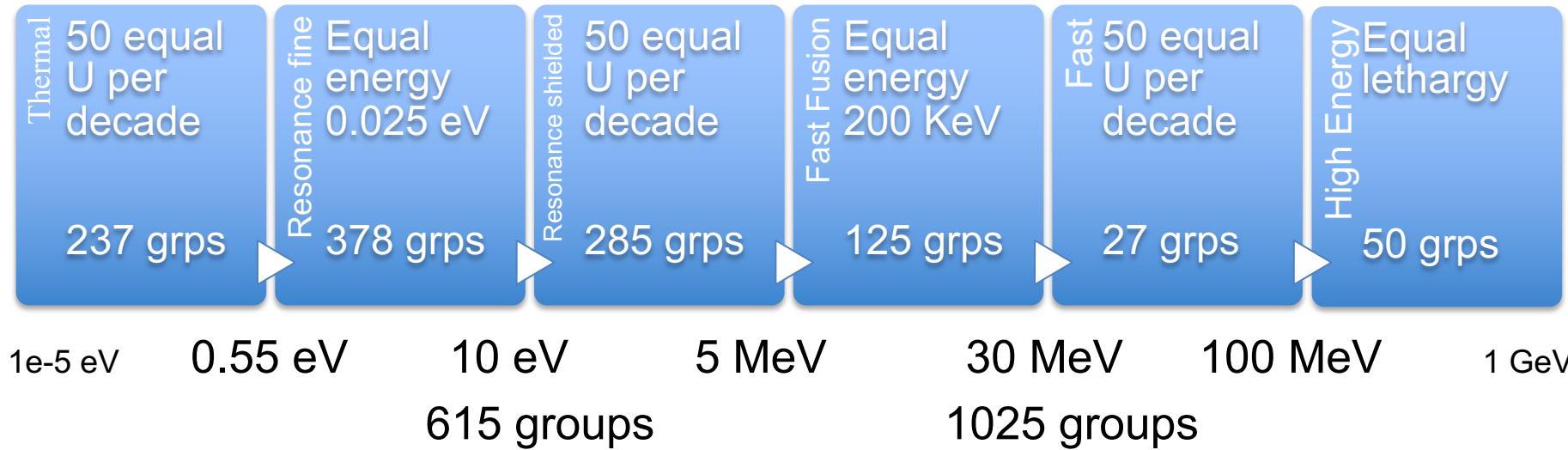
$$\Rightarrow LB = 6 : \quad Cov(X_i, Y_j) = \sum_{k=1}^M \sum_{k'=1}^{M'} S_i^k S_j^{k'} F_{kk'} X_i Y_j$$

$$LB = 8 : \quad Cov(X_i, X_j) = \sum_{k=1}^M S_i^k S_j^k 1000 F_k \quad (Koning)$$

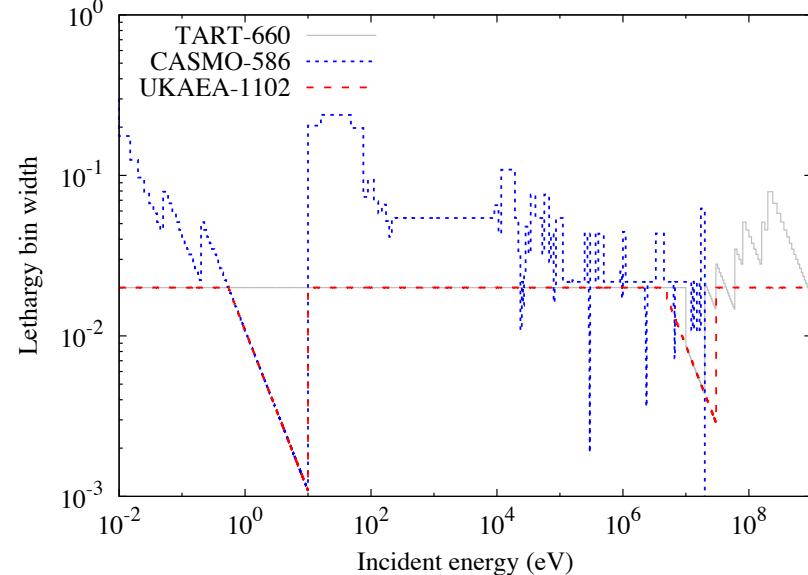
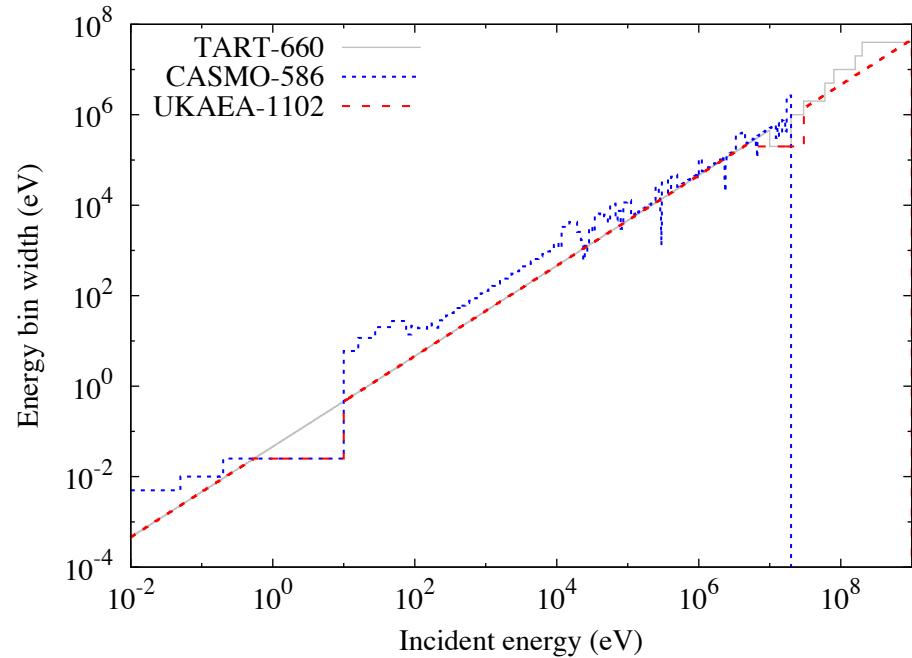
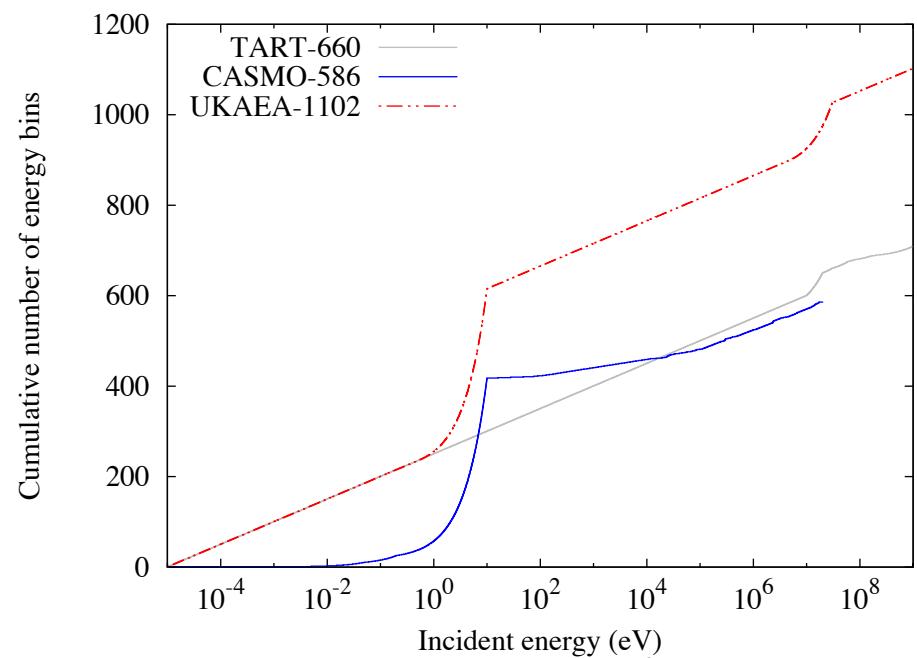
$$(or \quad = \sum_{k=1}^M S_i^k \delta_{ij} 1000 F_k)$$

The LB=1 case is the one that was applied to the computation of Δ for the EAF's libraries

- For all 2813 TENDL target nuclides
- 1102 energy groups for all applications alike

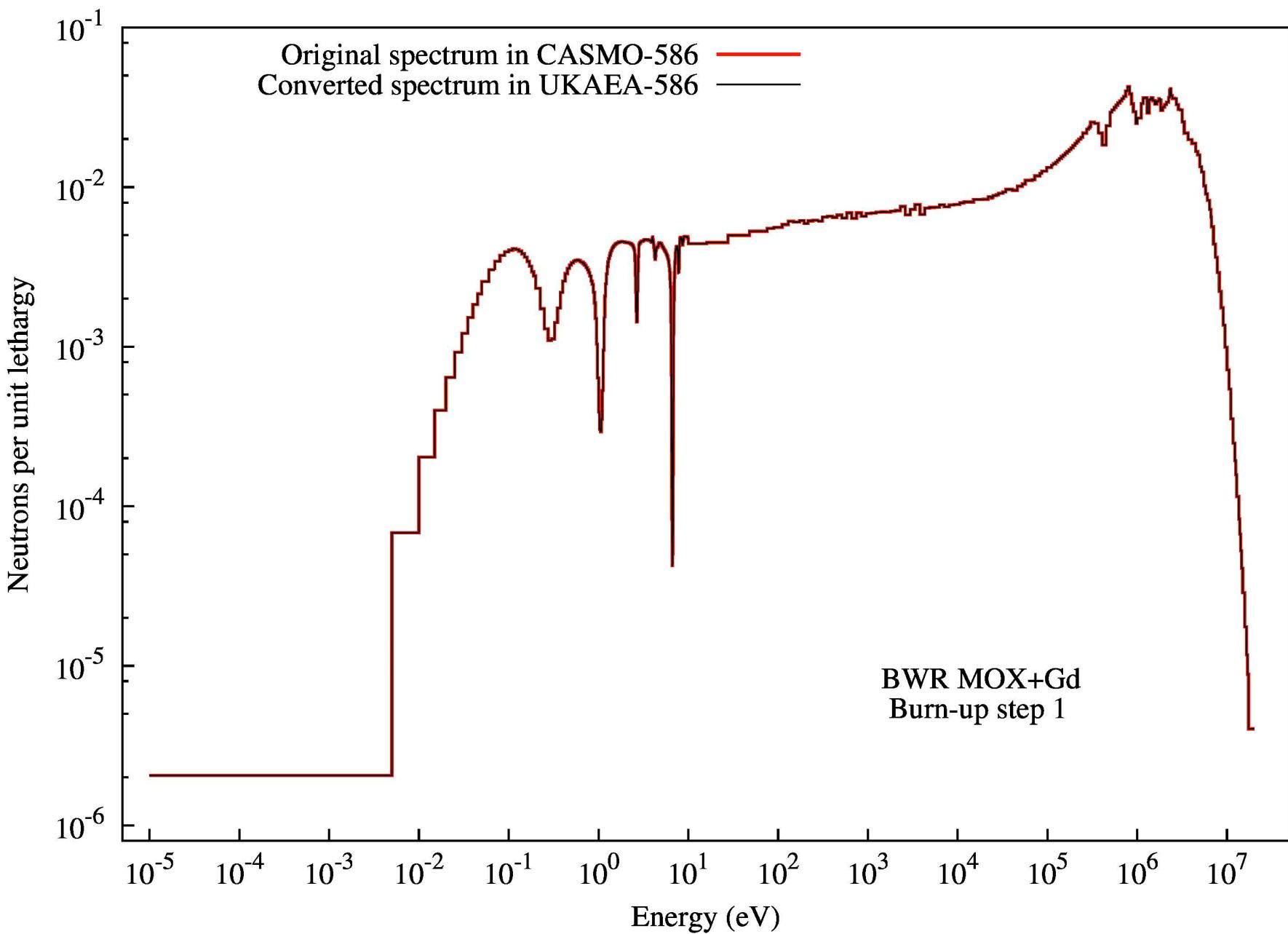


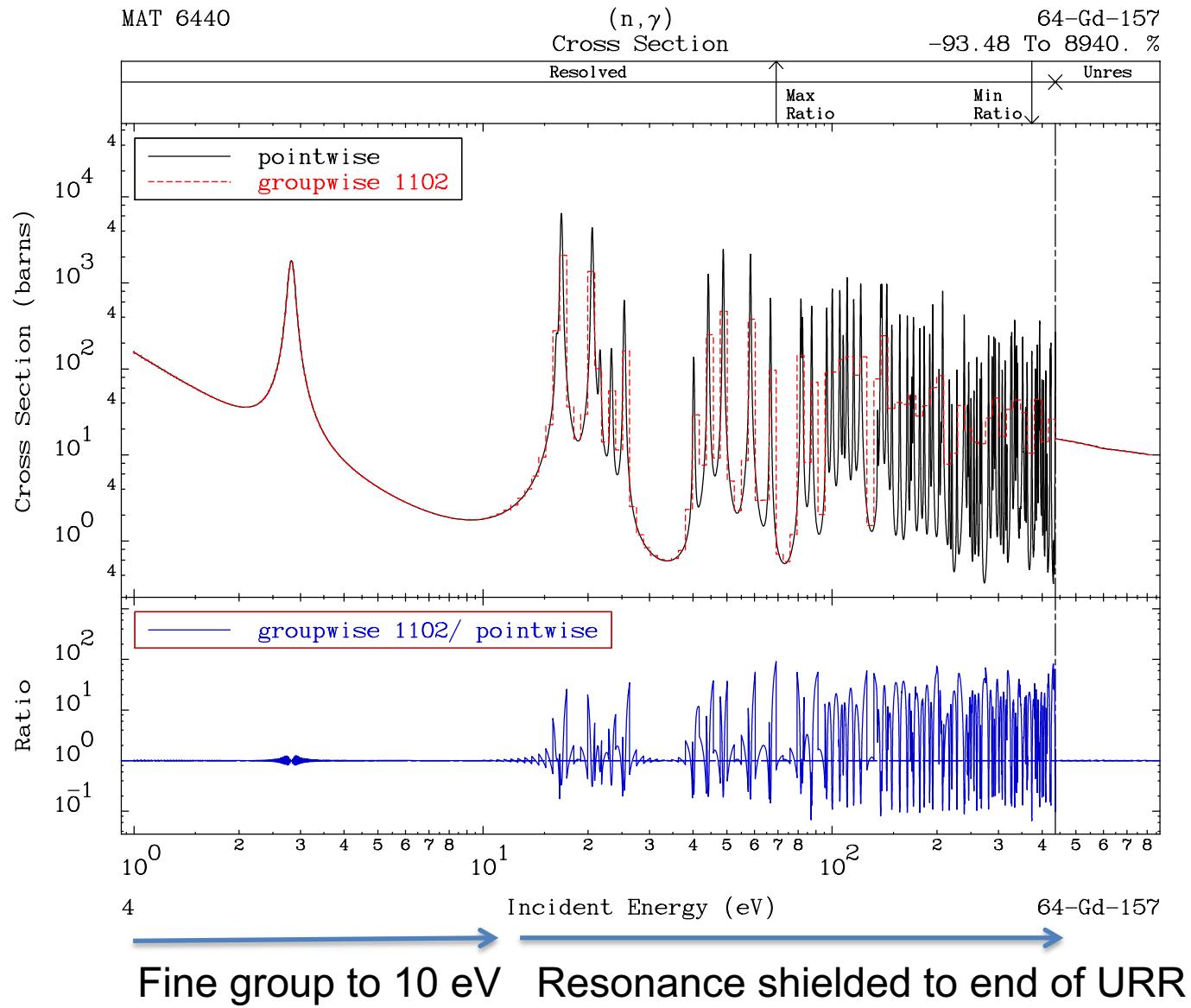
- 378 fine groups in the resonance range
- Resonance shielded data available in the RRR (0.1 eV) up to the end of the URR for all nuclide IDs
- Fast fine structure for accurate threshold reaction rate

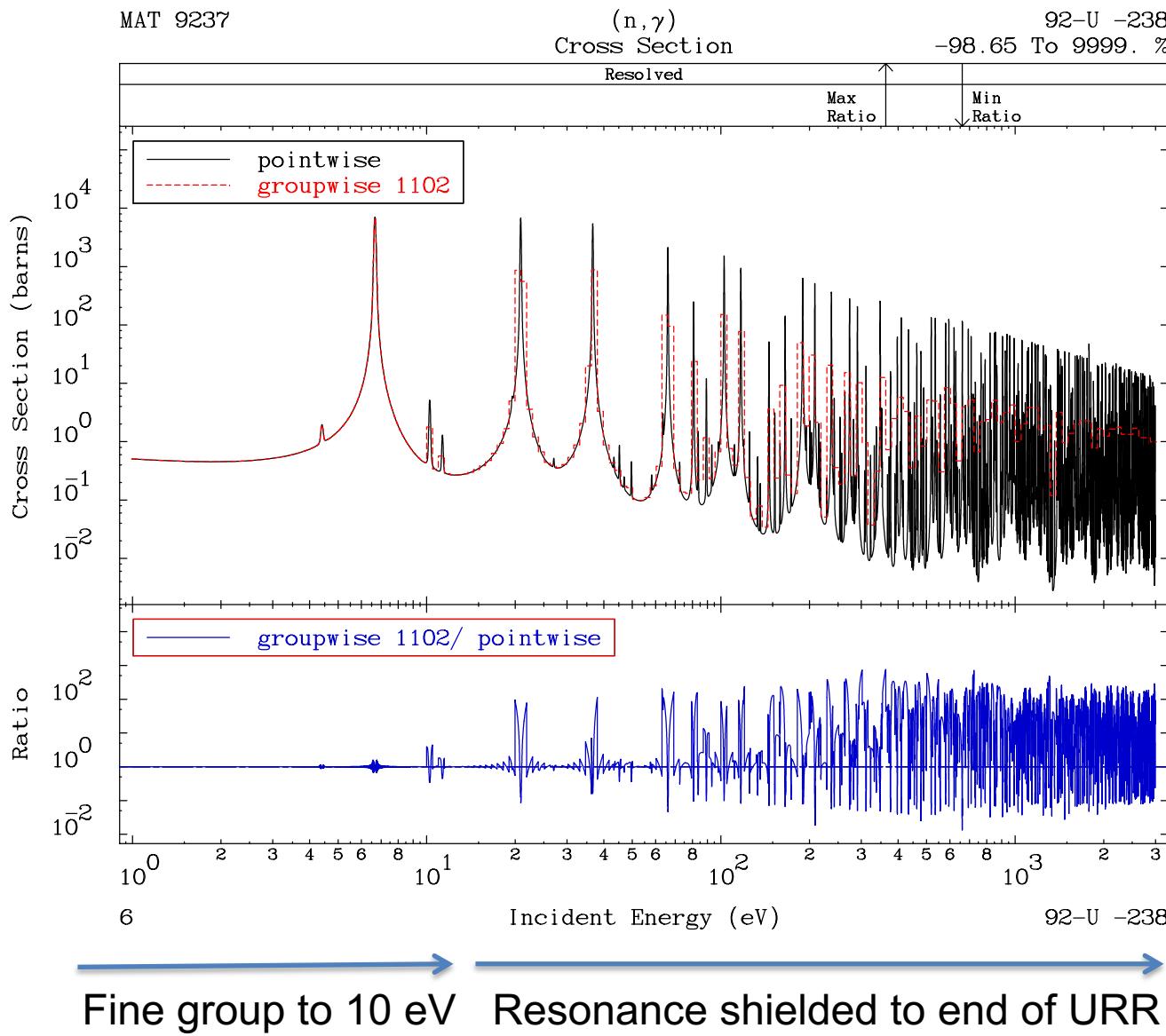


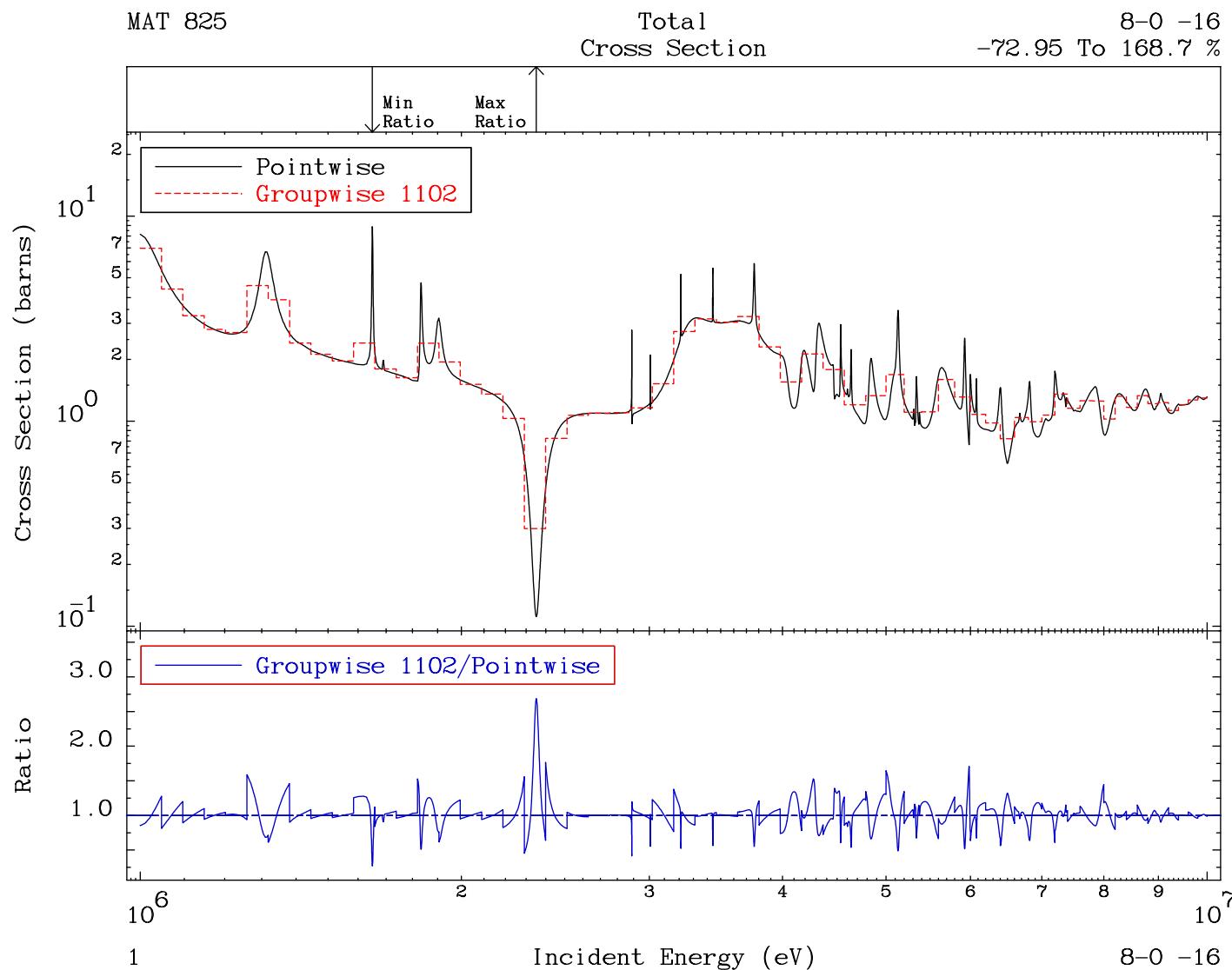


Time evolution of spectrum









Peak and trough are well described



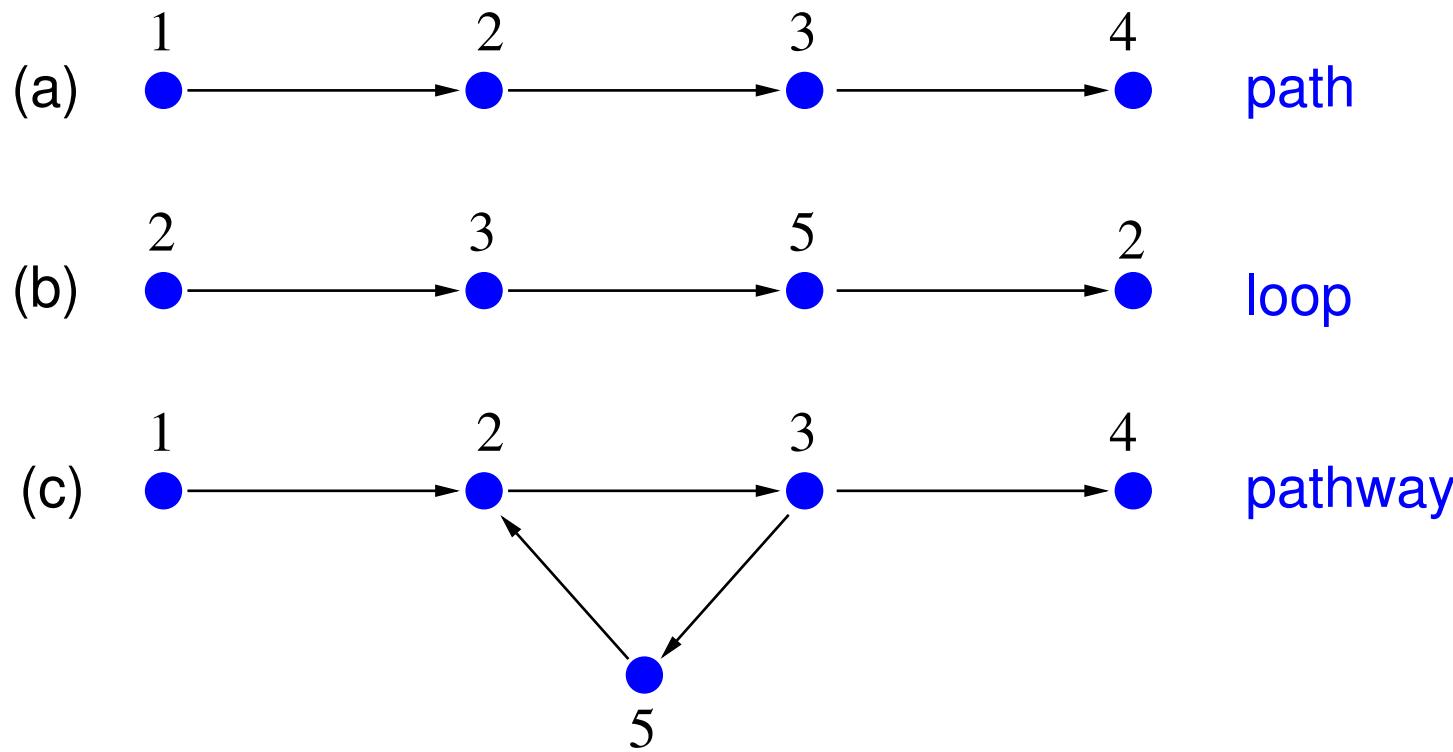
- Given{ \overline{XS} , λ }
 - select irradiation scenario
 - solve for radiological quantities
- Use { ΔX , $\Delta \lambda$ } to estimate uncertainties
 - method 1: pathways to dominant nuclides
 - method 2: Monte-Carlo sensitivity
 - method 3: reduced model Monte-Carlo sensitivity



- Pathways are used to identify the dominant contributors to the activation products for the specific irradiation scenario under consideration.
- This makes the calculation of uncertainties more practicable for all methods (random-walk approximation and Monte-Carlo).
- The standard uncertainty output uses a random-walk approximation to estimate error bounds.
- This estimate is much quicker than Monte-Carlo but is likely to give larger bounds since it ignores many possible correlations.



- given initial inventory and irradiation scenario
- sort dominant nuclides at end of irradiation phase
 - `topxx` (=20) controls number
 - 8 categories - activity, heat production, dose, etc.
- construct pathways from initial to dominant nuclides
 - `path_floor` (=0.005) and `loop_floor` (=0.01)
 - iterate on single-visit breadth-first search tree
- compute inventory contributions of pathways
- construct error estimate



- keep pathways providing $> \text{path_floor}$ of target inventory
- keep loop providing $> \text{loop_floor}$ of pathway inventory



$$Q = \sum_{t \in S_t} q_t; \quad (\Delta Q)^2 = \sum_{t \in S_t} \left(\frac{\Delta N_t}{N_t} \right)^2 q_t^2$$

$$(\Delta N_t)^2 = \sum_{p \in S_o} \Delta_{tp}^2 N_{tp}^2 + \sum_{a \in S_{sa}} \left(\sum_{p \in S_a} |\Delta_{tp}| N_{tp} \right)^2$$

$$\Delta_{tp}^2 = \sum_{e \in S_e} \sum_{r \in S_r} \left[\frac{R_r \Delta_r}{R_e} \right]^2 + \sum_{e \in D_e} \left[\frac{\Delta \lambda_e}{\lambda_e} \right]^2$$

- N_t (atoms) and q_t (radiological quantity) from rate equation
- Δ_{tp} , N_{tp} , ΔN_t from pathways
- R_r and R_e pulse averaged reaction rates
- reactions uncorrelated, fission correlated



Pathways and uncertainty output example

UNCERTAINTY ESTIMATES (cross sections only)

Uncertainty estimates are based on pathway analysis for the irradiation phase

Total Activity is 1.25070E+14 +/- 8.52E+11 Bq. Error is 6.81E-01 % of the total.

Total Heat Production is 3.60059E-02 +/- 3.09E-04 kW. Error is 8.60E-01 % of the total.

Total Gamma Dose Rate is 5.63098E+04 +/- 5.04E+02 Sv/hr. Error is 8.95E-01 % of the total.

Total Ingestion Dose is 1.38528E+05 +/- 1.17E+03 Sv. Error is 8.45E-01 % of the total.

...

Target nuclide Sc 44 99.557% of inventory given by 8 paths

path 1 20.048% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44 ---(S)---
98.16%(n,np) 100.00%(n,2n)
1.84%(n,d)

path 2 12.567% Ti 46 ---(R)--- Sc 45 ---(R)--- Sc 44m---(b)--- Sc 44 ---(S)---
98.16%(n,np) 100.00%(n,2n) 100.00%(IT)
1.84%(n,d) 0.00%(n,n)

path 3 11.143% Ti 46 ---(R)--- Sc 45m---(d)--- Sc 45 ---(R)--- Sc 44 ---(S)---
96.62%(n,np) 100.00%(IT) 100.00%(n,2n)
3.38%(n,d)

...

- The TENDL library contains MF=33, LB=6 data for different reactions X_1, X_2, \dots for a given parent, i.e., $p(n, X_1)d_1, p(n, X_2)d_2, \dots$
- These covariance data $\text{cov}(X_1, X_2)$ for X_1, X_2 are stored as fractional values $f^{X_1 X_2}$ and are tabulated in the same energy bins as used respectively for the LB=5 covariance data $f^{X_1 X_1}, f^{X_2 X_2}$ for reactions X_1, X_2
- If the COVARIANCE keyword is used, FISPACT-II reads these data for all energy bins k and l and corrects for any instances where

$$\left| \frac{f_{kl}^{X_1 X_2}}{\sqrt{f_{kk}^{X_1 X_1} f_{ll}^{X_2 X_2}}} \right| > 1$$

- Then the code uses the corrected data to compute collapsed covariance $\text{cov}(X_1, X_2)$. Covariances are mapped to MF=10 by assuming that all isomeric daughters of a given pair of reactions with rates X_1, X_2 have the same collapsed correlation function, $\text{corr}(X_1, X_2)$.
- Tables of all reactions which have covariance data and their collapsed covariances and correlations are printed by the collapse run. Inspection of these data will show those cases where the assumption of zero correlation between reactions of a given parent is not good.
- The effect of non-negligible correlations on uncertainties may be introduced into Monte-Carlo sensitivity calculations by choosing distributions of sample cross-sections to have the same variances and covariances as given by the TENDL data.



- reference run + S inventory calculations
- independent $\{X_i^s; i = 1, \dots, I; s = 1, \dots, S\}$
- dependent $\{Y_j^s; j = 1, \dots, J; s = 1, \dots, S\}$
- independent variables selected using random numbers
 - normal, log-normal, uniform, log-uniform
 - means $\langle X_i \rangle$ and standard deviations $\langle \Delta X_i \rangle$
- compute summary results:
 - means
 - standard deviations
 - Pearson correlation coefficients
- output full data for post-processing



- output mean and standard deviation

$$\bar{X}_i = \frac{1}{S} \sum_{s=1}^S X_i^s$$

$$\Delta X_i = \sqrt{\frac{1}{S-1} \sum_{s=1}^S [(X_i^s)^2 - \bar{X}_i^2]}$$

$$\bar{Y}_j = \frac{1}{S} \sum_{s=1}^S Y_j^s$$

$$\Delta Y_j = \sqrt{\frac{1}{S-1} \sum_{s=1}^S [(Y_j^s)^2 - \bar{Y}_j^2]}$$

- Pearson correlation coefficient

$$r_{ij} = \frac{\sum_s X_i^s Y_j^s - S \bar{X}_i \bar{Y}_j}{\Delta X_i \Delta Y_j}$$

- controlled by keywords **SENSITIVITY**, **MCSAMPLE**, **MCSEED**, **COVARIANCE**



Base cross section data

index	parent			daughter			sigma	sigma_unc	
i	zai	nuc_no	name	i	zai	nuc_no	name	cm**2	cm**2
1	220460	233	Ti 46	210460	219	Sc 46	0.39039E-25	0.35942E-01	
2	220460	233	Ti 46	210461	220	Sc 46m	0.10142E-25	0.35942E-01	
3	220480	235	Ti 48	210480	222	Sc 48	0.11049E-25	0.87272E-02	

...

Output nuclides

j	zai	nuc_no	name
1	210460	219	Sc 46
2	210470	221	Sc 47
3	210480	222	Sc 48

...

Normal, x cutoff = [-3.0000 , 3.0000] std dev ↪ Normal random sampling

j	atoms_base	atoms_mean	atoms_unc
1	2.50290E+20	2.49955E+20	2.46164E-02
2	7.99801E+18	7.99665E+18	1.68690E-03
3	9.91006E+18	9.90588E+18	8.55649E-03

...

Correlation coefficients

j\i	1	2	3	4
1	9.66468E-01	- - - -	- - - -	- - - -
2	- - - -	- - - -	- - - -	9.99810E-01
3	- - - -	- - - -	1.00000E+00	- - - -
4	- - - -	- - - -	9.99993E-01	- - - -
5	- - - -	- - - -	- - - -	-9.99911E-01
6	- - - -	- - - -	-9.60898E-01	- - - -
7	-9.66478E-01	- - - -	- - - -	- - - -

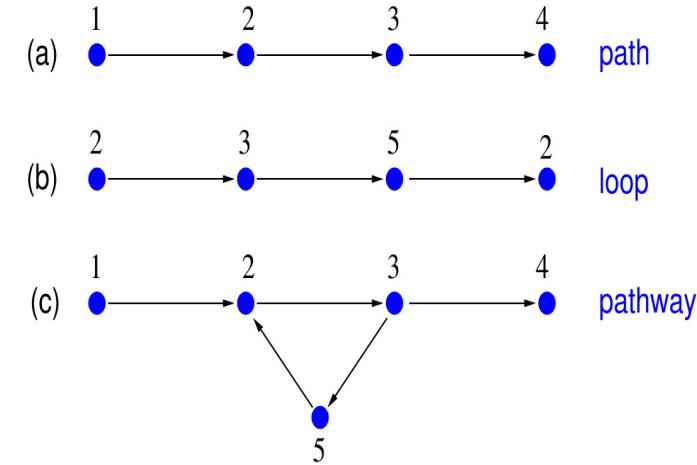
↪ reactions

↑ output nuclides

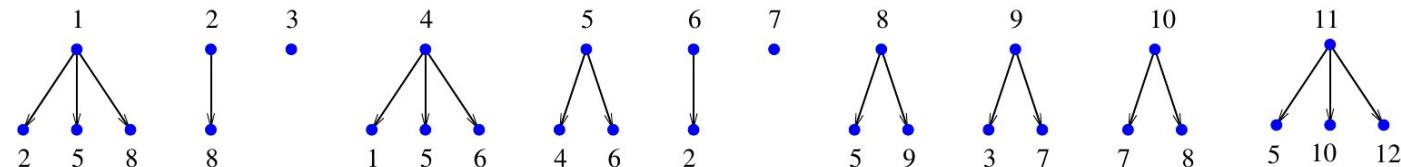


- UKDD-2012 decay - 3873 nuclides
- calculation includes all nuclides in master index
- INDEXPATH generates reduced master index from pathways
 - typically few 10s of nuclides
 - number adjustable by pathway parameters
- reduced master index run versus full run to validate discards
- Monte-Carlo sensitivity for reduced master index runs
 - faster + comparable answers

- Pathway = path + loop(s)
- Finds reaction/decay chains
- Identifies important
 - Nuclides
 - Reactions
 - Decays
- Used for uncertainty and sensitivity calculations
- Simple previous approach could fail through combinatorial explosion

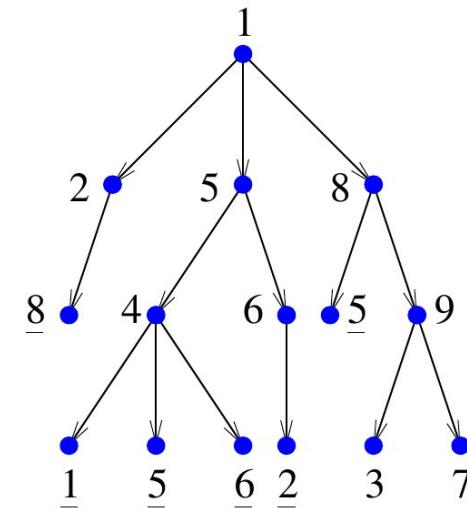


Pathways – single visit tree



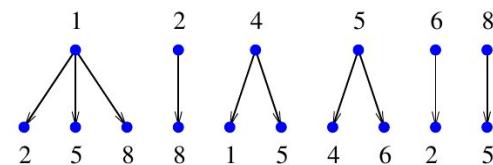
Adjacency lists

- tree search gives reduced p-d set
- pruning controlled using
 - path_floor
 - loop_floor
 - max_depth
- TENDL library
 - 3873 nuclides, ~240000 reactions
 - ~160,000 p-d pairs (57/nuclide)
 - single visit breadth-first search BFS typically < 50 p-d (parent-daughter)

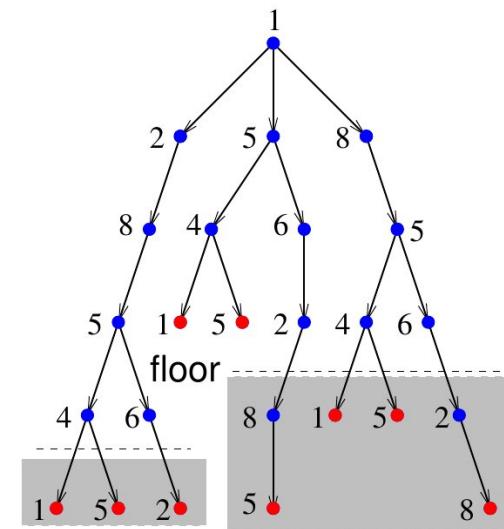


Single visit BFS tree for nuclide 1

- build full tree for reduced p-d set
 - leaf node if
 - repeat nuclide (loop)
 - path inventory below path floor
 - path depth greater than max depth
 - combine paths and loops
 - control keywords
 - UNCERTAINTY (path_floor, loop_floor, max_depth)
 - SORTDOMINANT (topxx)
 - TOLERANCE (absolutetol_path, relativetol_path)
 - ZERO
 - LOOKAHEAD
 - PATHRESET



nuclide 1 to 4 path edges



full tree with pruning

paths: 154 1854 12854

loops: 1541 545



- Initiated by `ZERO` keyword
- Combined `topxx` from dominant lists
- May miss late cooling time dominant nuclides
- Some typical ‘fixes’ to increase the depth of the simulation for more demanding simulations:
 - Reduce `path_floor` (prune fewer pathways)
 - Increase `topxx` (more dominant nuclides)
 - Use `LOOKAHEAD` (finds dominant nuclides at late times)
 - Use `PATHRESET` (re-calculates pathways at requested time)



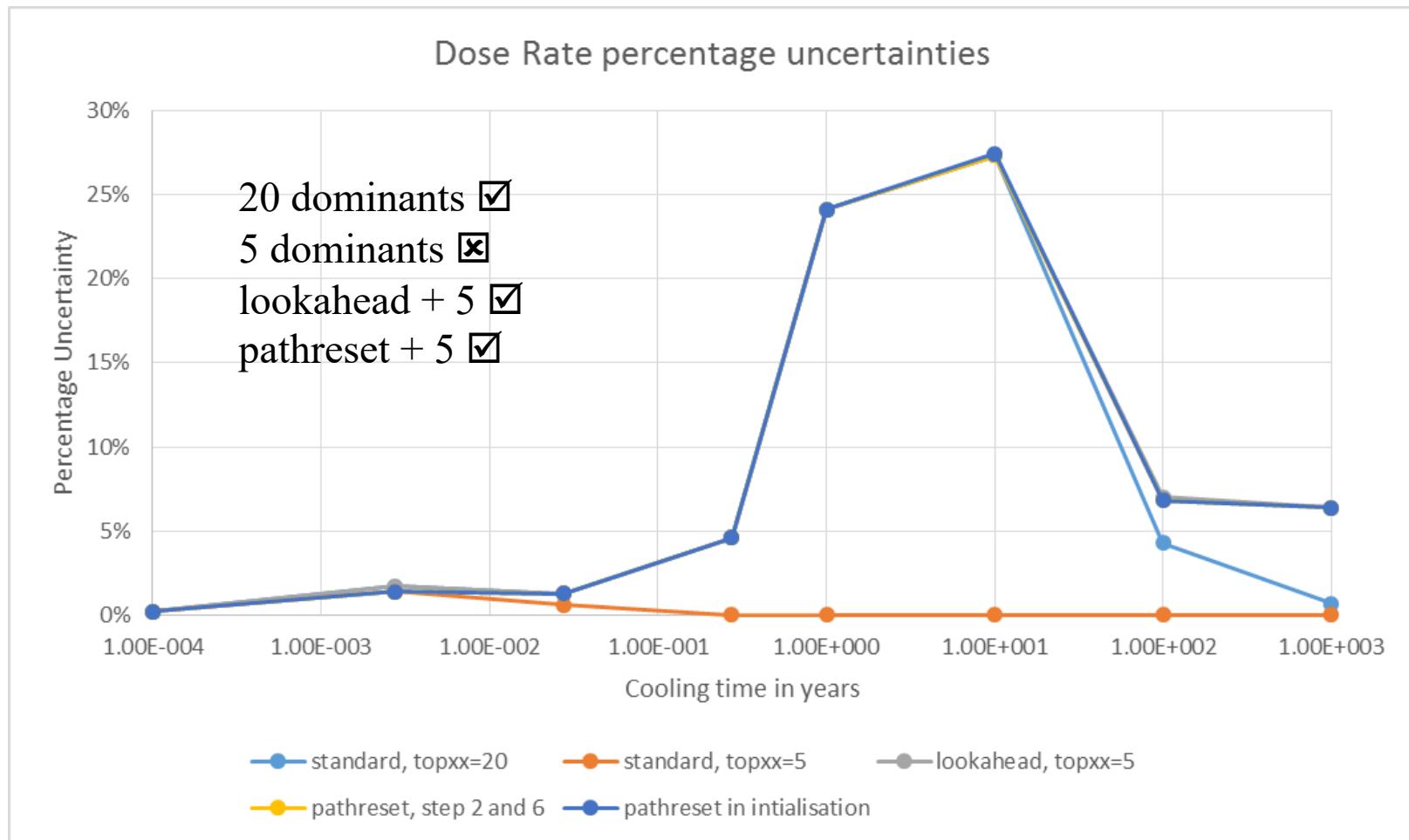
- LOOKAHEAD causes two-pass cooling:
- at ZERO, integrate cooling steps to get late time dominant nuclides
- merge additional dominants with dominant list at ZERO
- use merged list in pathways calculation



- Save dominant list at ZERO, *i.e.* the end of irradiation
- PATHRESET in cooling phase:
 - At PATHRESET keyword, check for new dominant nuclides
 - If no new dominant nuclides, do nothing
 - If found, redo pathways calculation with current dominant list
- PATHRESET in initialisation phase
 - Same as PATHRESET at all cooling steps

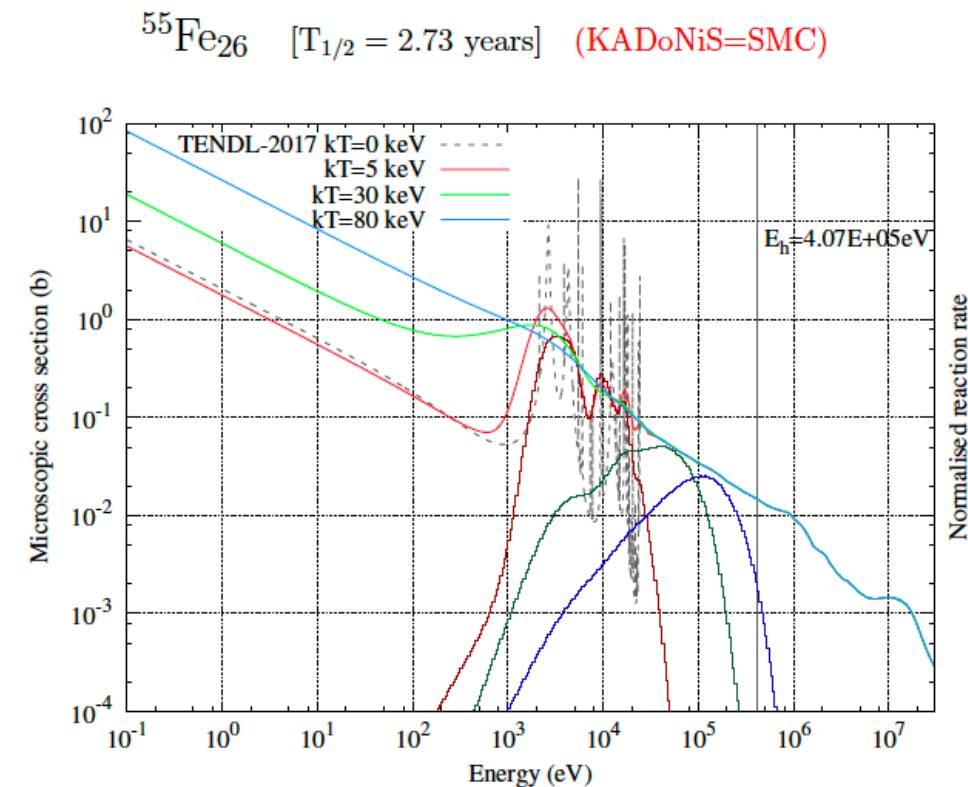
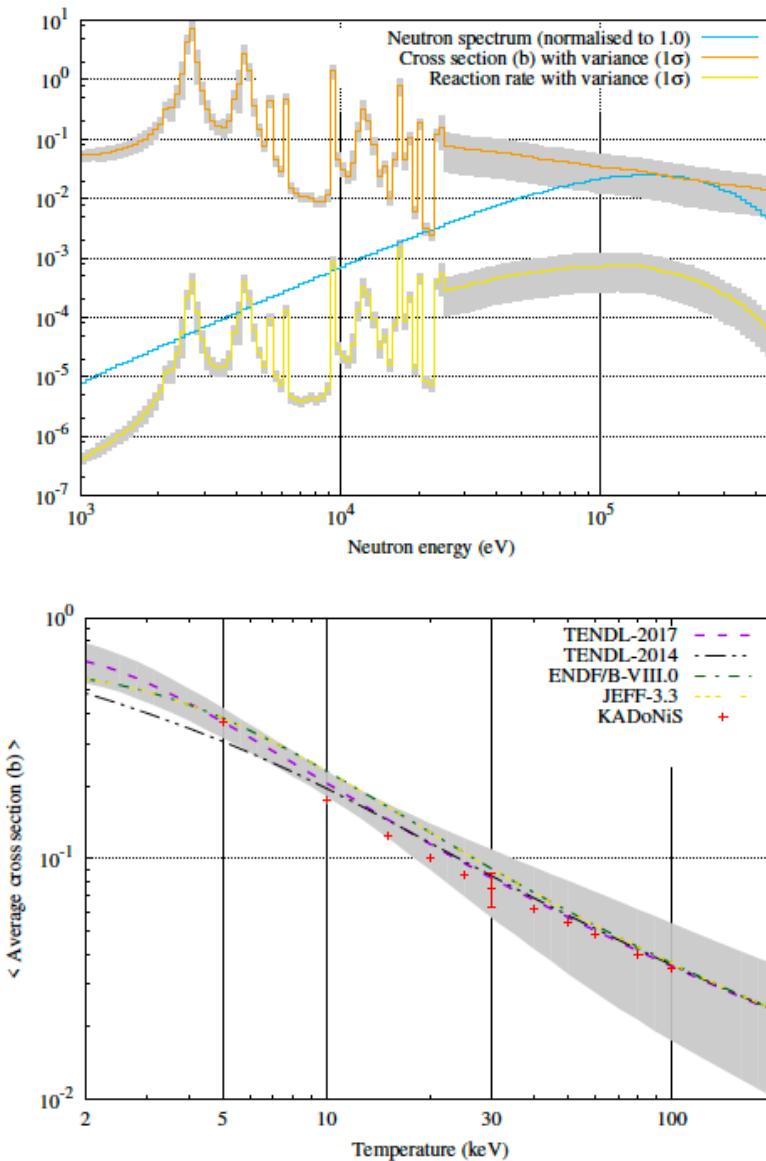
Example: dose rate for SS316

- standard cases show late cooling time underestimates uncertainty; 25% at 1-10 years cooling

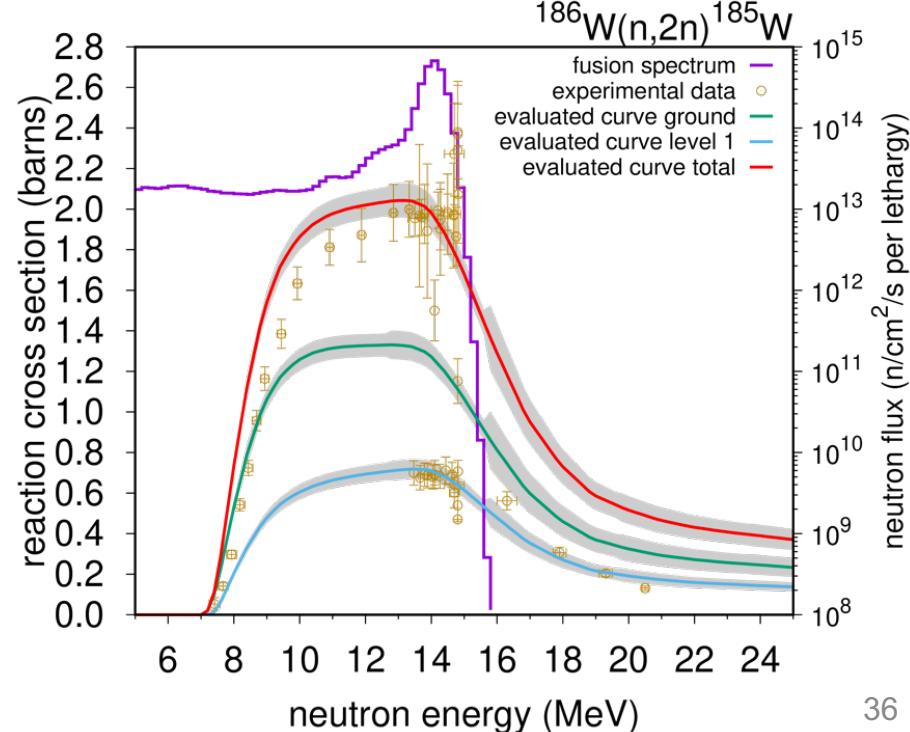
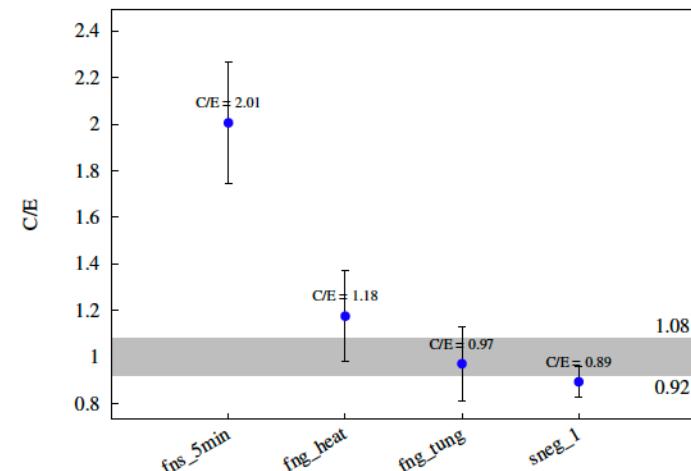
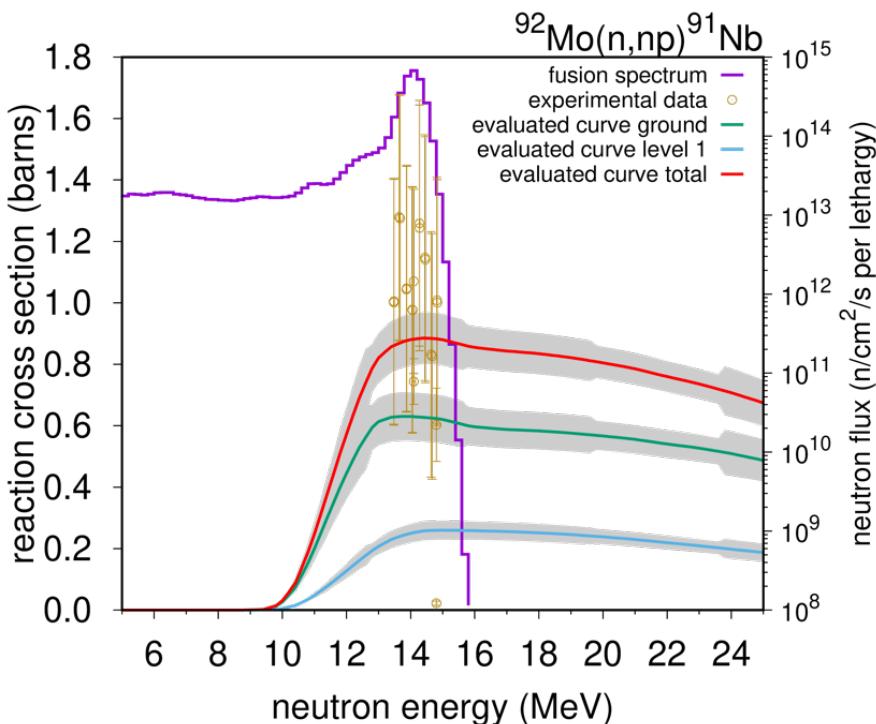


Cross section and reaction rates

- Subtility: cross section, reaction rate and variance



Threshold reaction uncertainty



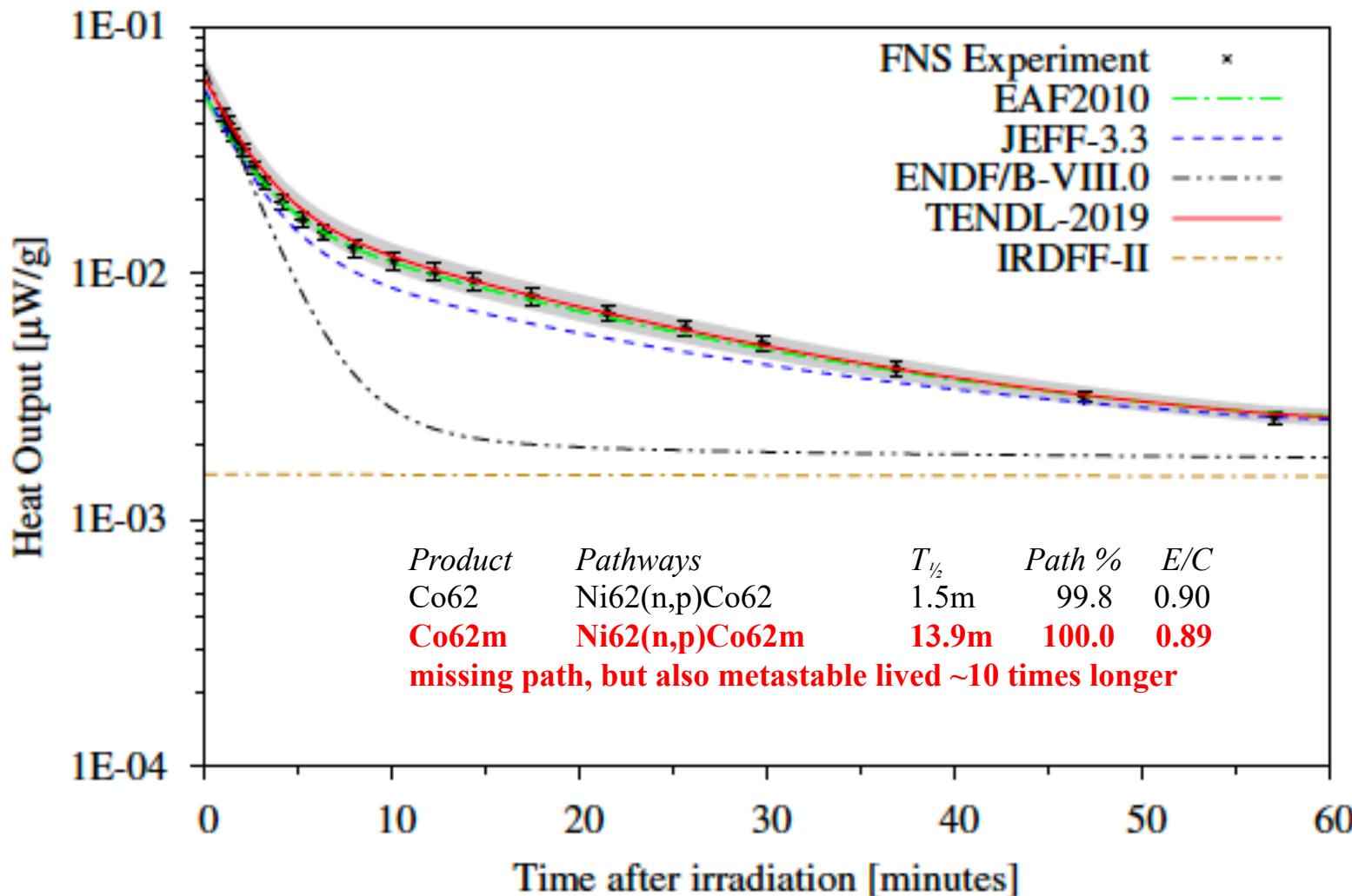
Not all integrals..
Not all differentials..

are as reliable, so the
importance of the
covariances

Ni FNS decay heat experiment

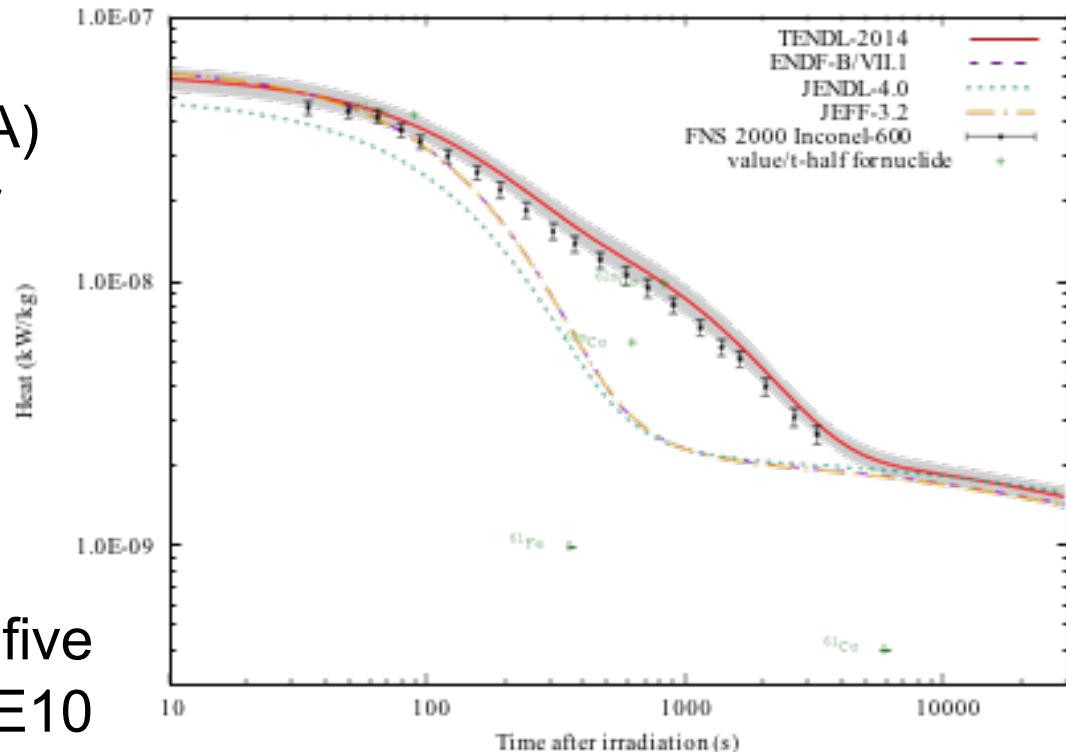
Random walk uncertainty

FNS-96 5 Min. Irradiation - Ni



Inconel-600 decay heat

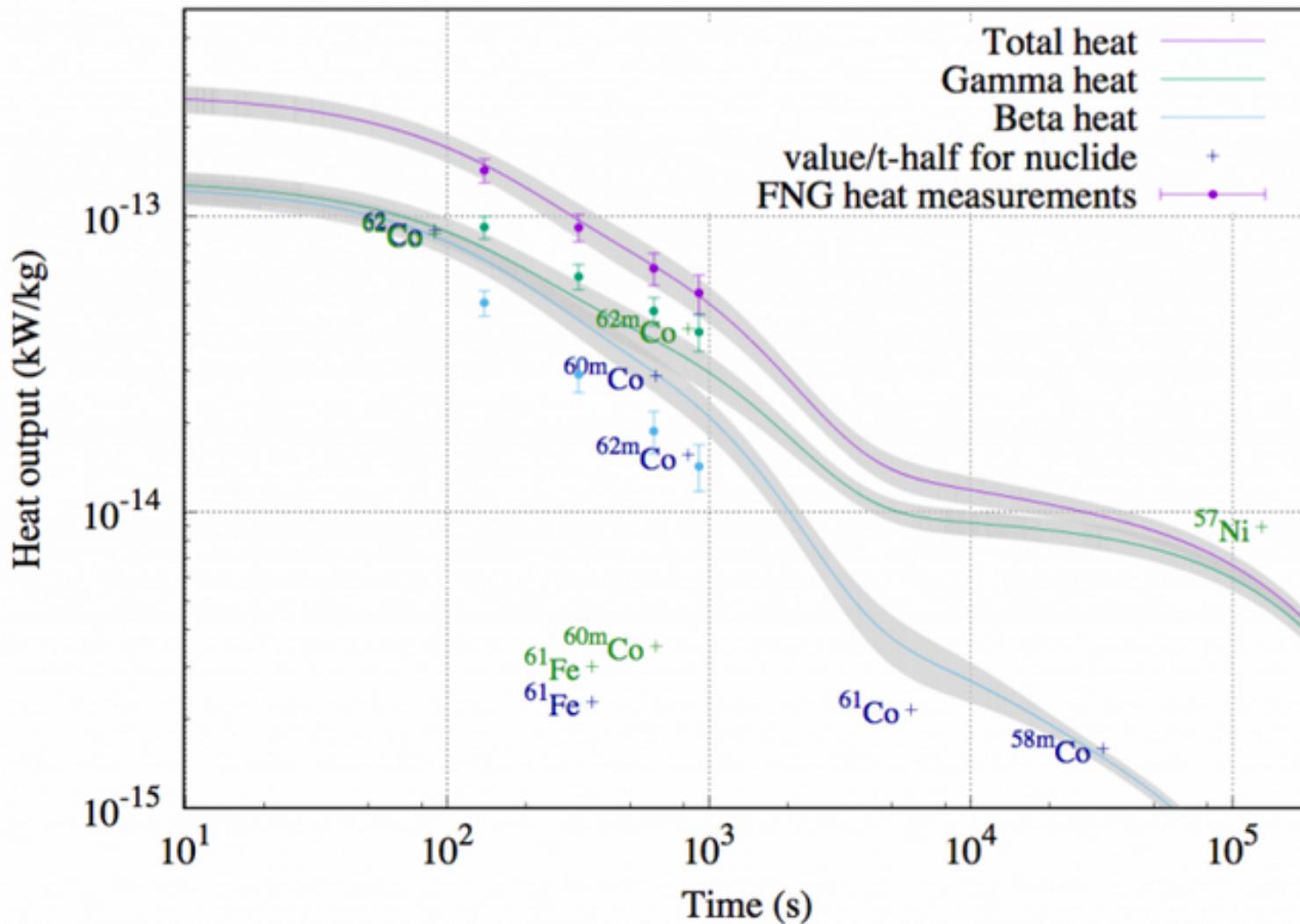
- FNS (JAEA) and FNG (ENEA)
 ^2H beam onto ^3H -Ti target for
~14 MeV source



- Right: total decay heat from five minute irradiation of Ni at ~1E10 n/s on target
 - Only TENDL has ^{62m}Co isomer which dominates heat at 100-3000 s (~1min - 1hour)
 - Only TENDL has complete covariance data for all channels

Isomeric states play a major roles

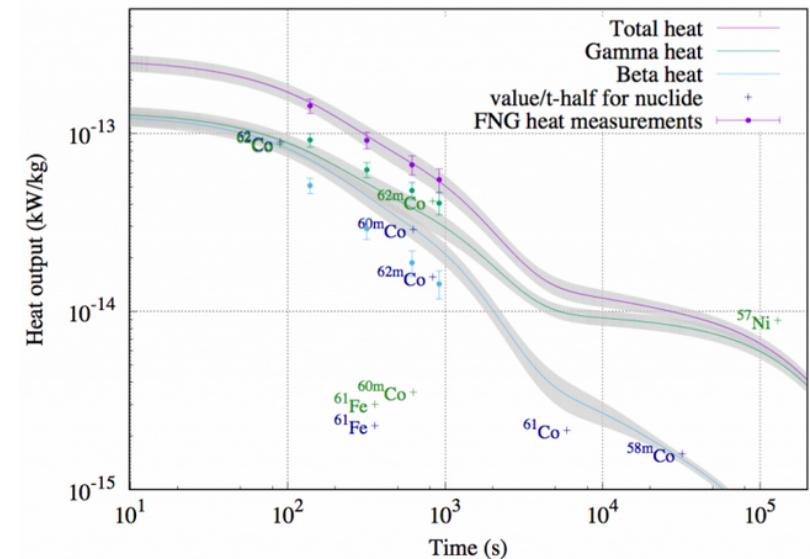
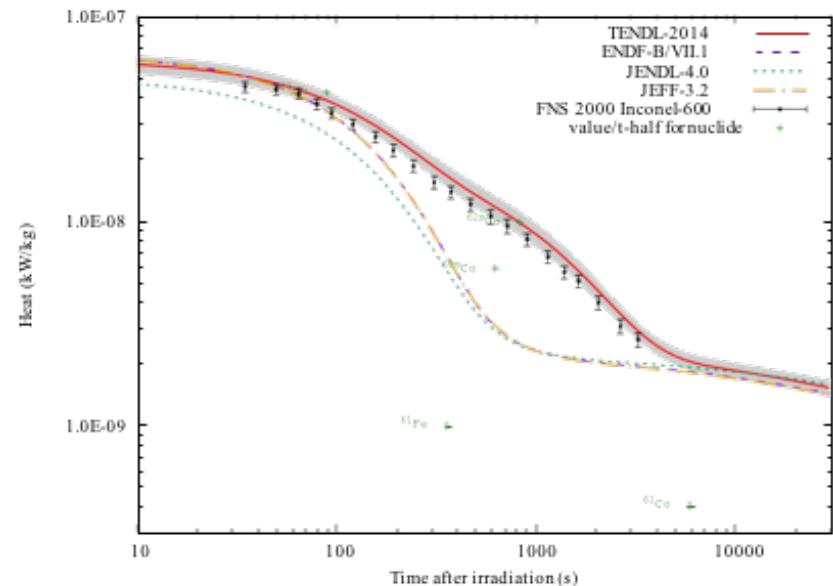
FNG decay heat experiment



Total, beta and gamma heat apportionment

Pathways uncertainty with activation

- The pathways-based uncertainty has been extensively validated in pure activations scenarios, where production of a nuclide occurs with loss of that same product
- Default uncertainty treatment for FISPACT-II, used in all fusion and integral V&V reports



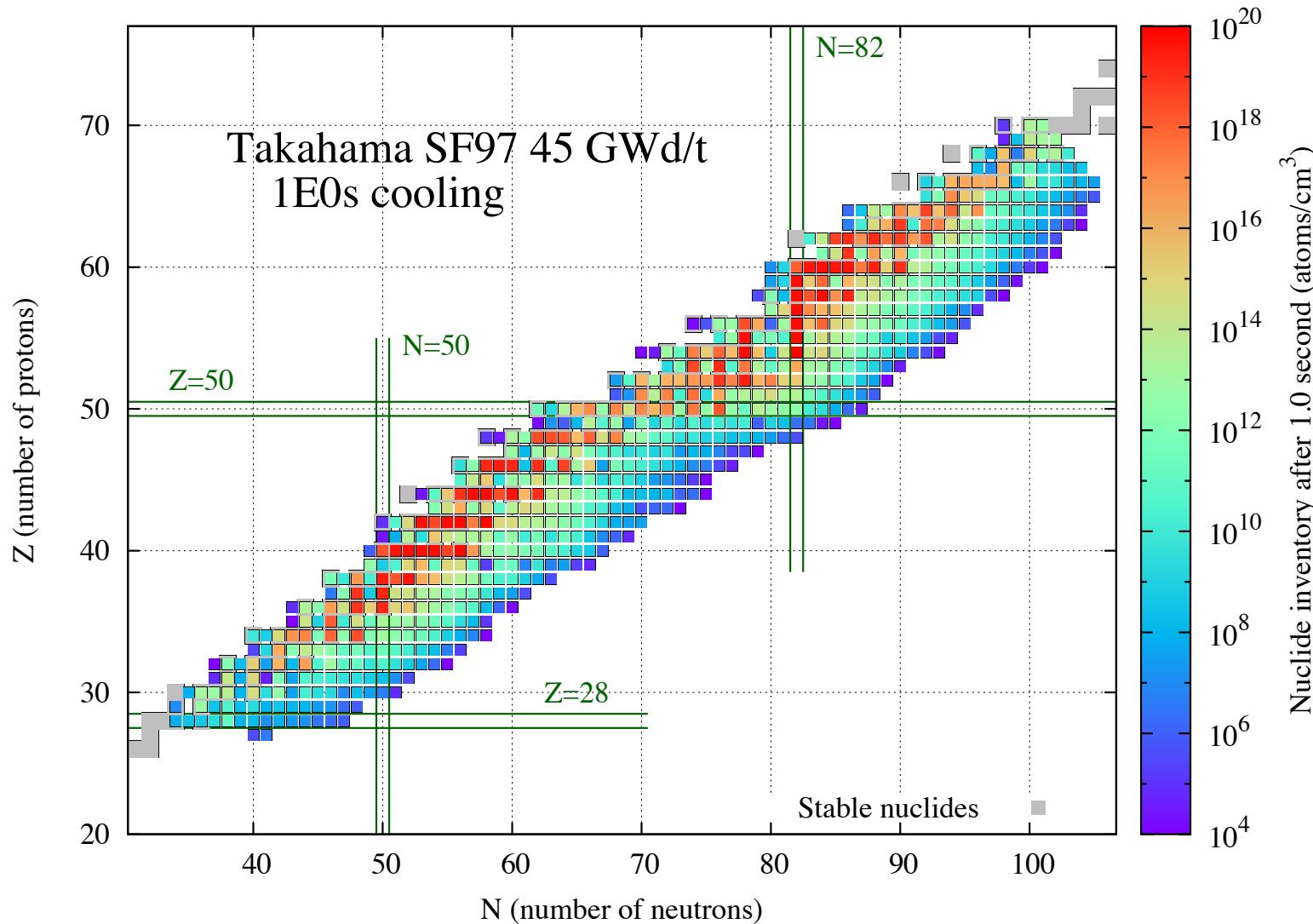


FISPACT-II fission yield uncertainty

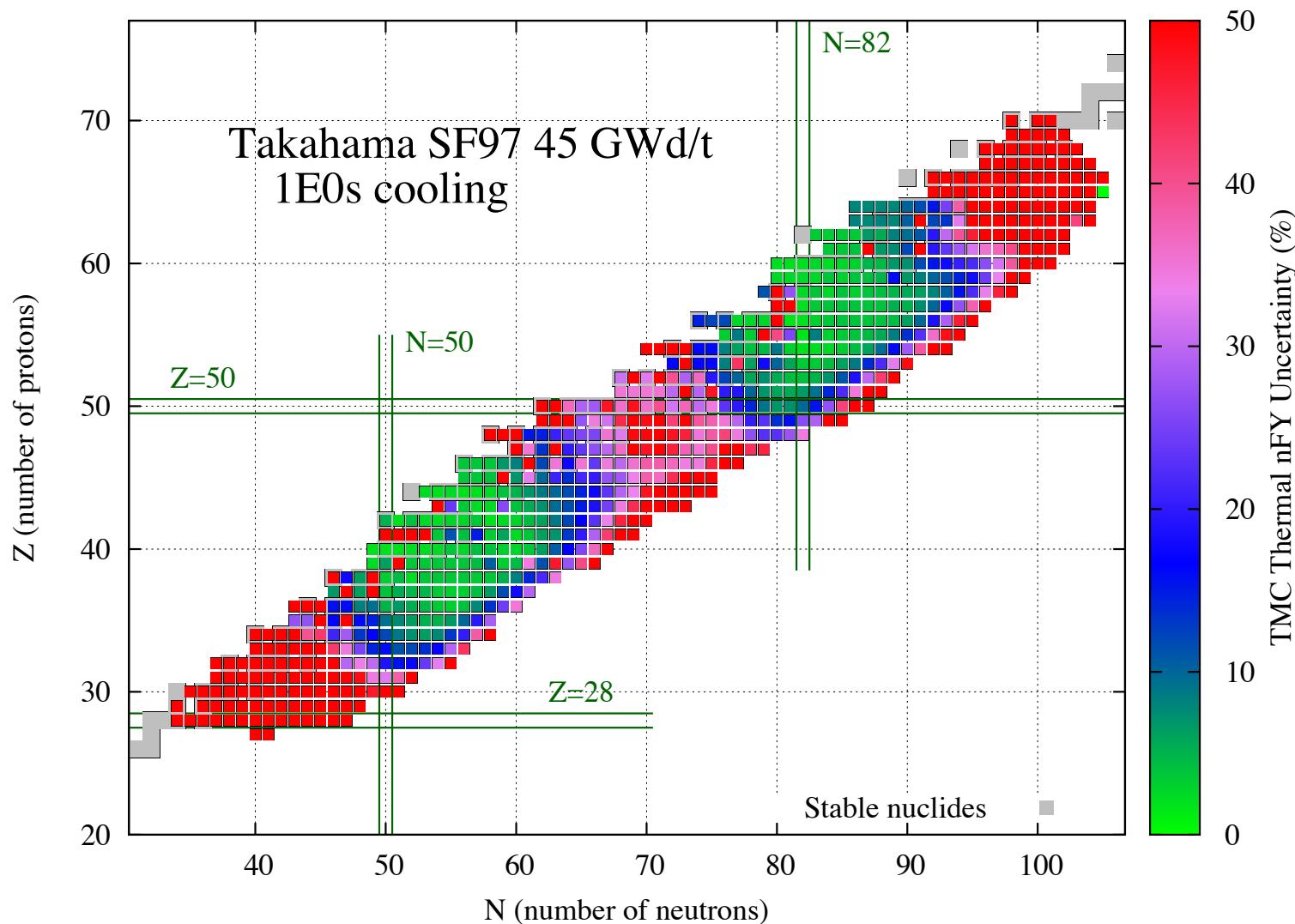
- FISPACT-II makes use of Bayesian Monte-Carlo fission yields generated by:
 - Input parameter variation of GEF
 - χ^2 calculation vs evaluated nuclear data files with their uncertainties
 - Weighting and updating to convergence
 - nb: values are highly sensitive to the evaluated file chosen!
- These files may be sampled by FISPACT-II to perform parallel simulations with complete and consistent fission yield files, incorporating all yield correlations implicitly
- Application of this method has been performed for a variety of assemblies with coupling to CASMO-5 calculations
- FISPACT-II follows all independent yields, accommodating all of the yields and correlations

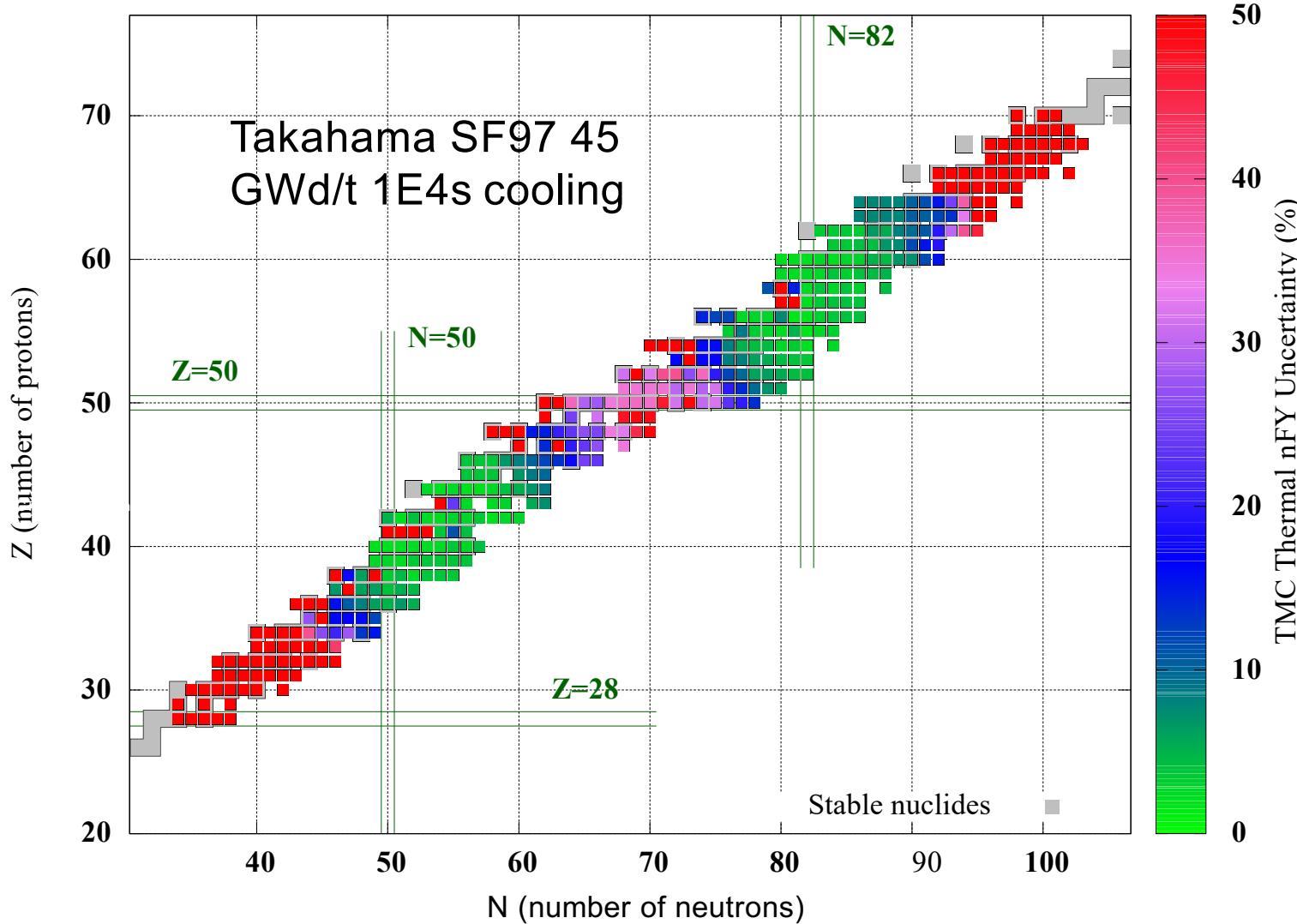
Not your typical LWR simulation

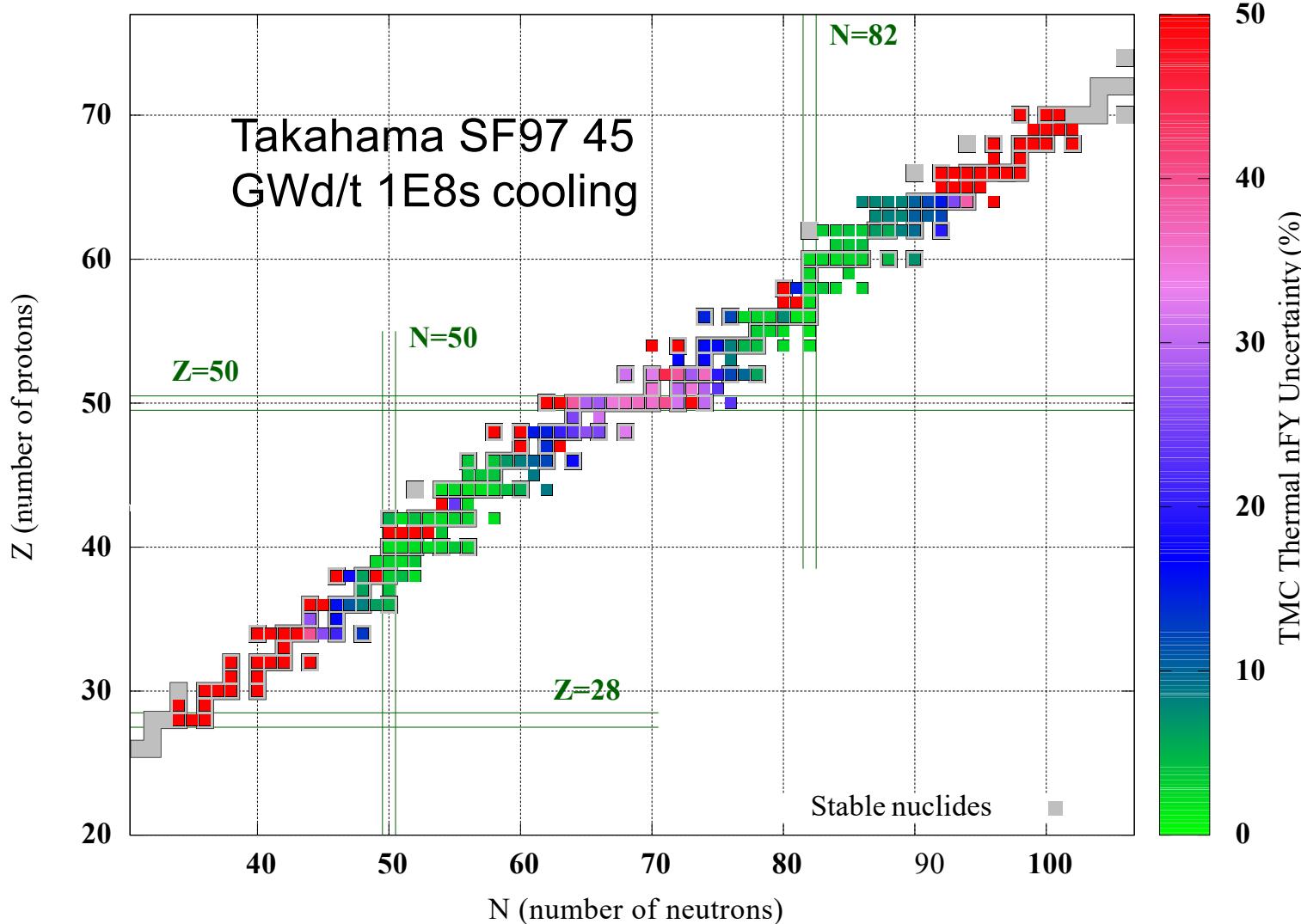
- Unlike legacy codes, FISPACT-II uses all independent yields and decays to follow every nuclide



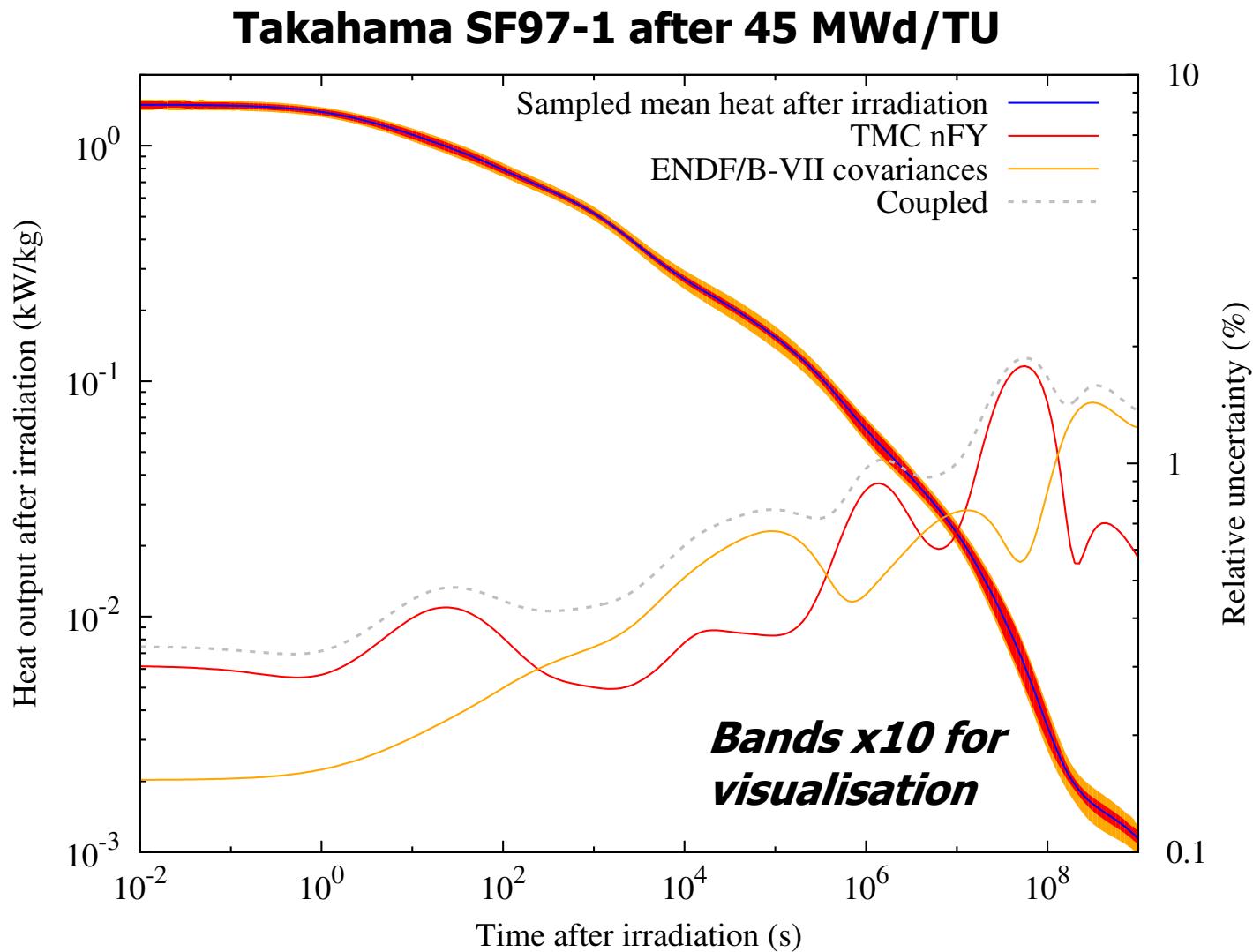
- Ability to handle technologically-generated TALYS & GEF(Y)



Example: Takahama-SF97 nFY uncertainties (10^4 s)

Example: Takahama-SF97 nFY uncertainties (10^8 s)

- Coupling FISPACT-I covariance UQP for reaction rates with TMC we can provide coupled uncertainties:
 - From unc. of fissions and production of fissionable nuclides
 - From unc. in fission yields
 - And the coupled nFY + RR unc.





- FISPACT-II provides predictions of inventory, radiological quantities and their uncertainties using nuclear data covariance information.
- Central to the method is a novel fast pathways search algorithm using directed graphs. The pathways output provides (1) an aid to identifying important reactions, (2) fast estimates of uncertainties, (3) reduced models that retain important nuclides and reactions for use in the code's Monte-Carlo sensitivity analysis module
- The nuclear data files are read directly by FISPACT-II without any further intermediate processing. Variance and covariance data are processed and used by FISPACT-II to compute uncertainties in collapsed cross-sections, and these are in turn used to predict uncertainties in inventories and all derived radiological data

J. W. Eastwood, J. G. Morgan, J.-Ch. Sublet. Inventory Uncertainty Quantification using TENDL Covariance Data in FISPACT-II. [Nuclear Data Sheets 123, 84-91, January 2015](#)