FISPACT-II

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

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Recap: FISPACT-II irradiation scenarios

- 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

Recap: What FISPACT-II does

- 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

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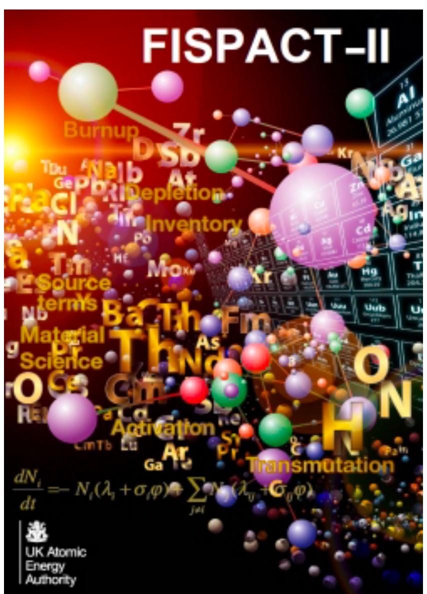
Recap: Simulation processes

- 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

- 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

Background

- 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

Extract and reduce library data

- Condense run extracts from decay files:
  - decay constant λ
  - decay constant uncertainty Δλ
- 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

Covariance collapse

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

1 TENDL, 3 EAF

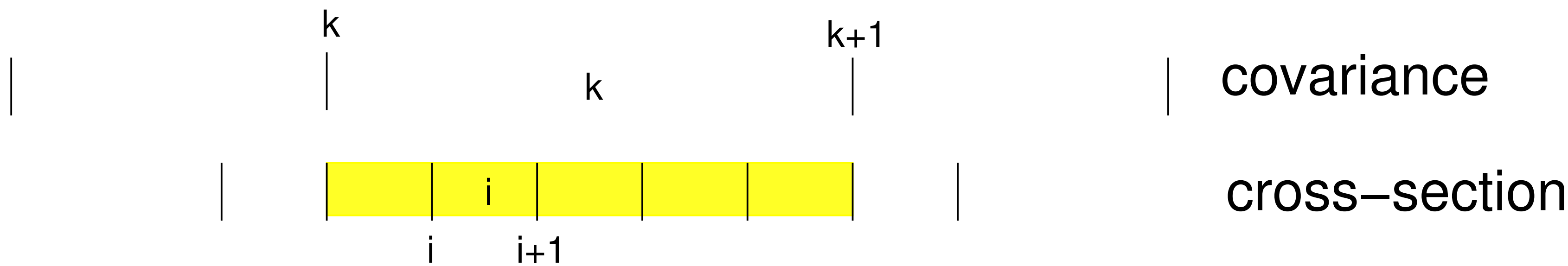
$$var = \sum_{i=1}^{N}\sum_{j=1}^{N} W_i W_j Cov(X_i, X_j); \qquad \Delta = \{1|3\}\sqrt{var}/\bar{X}$$

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

Covariance, variance

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

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



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

Covariance, variance

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

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

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

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

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

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

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

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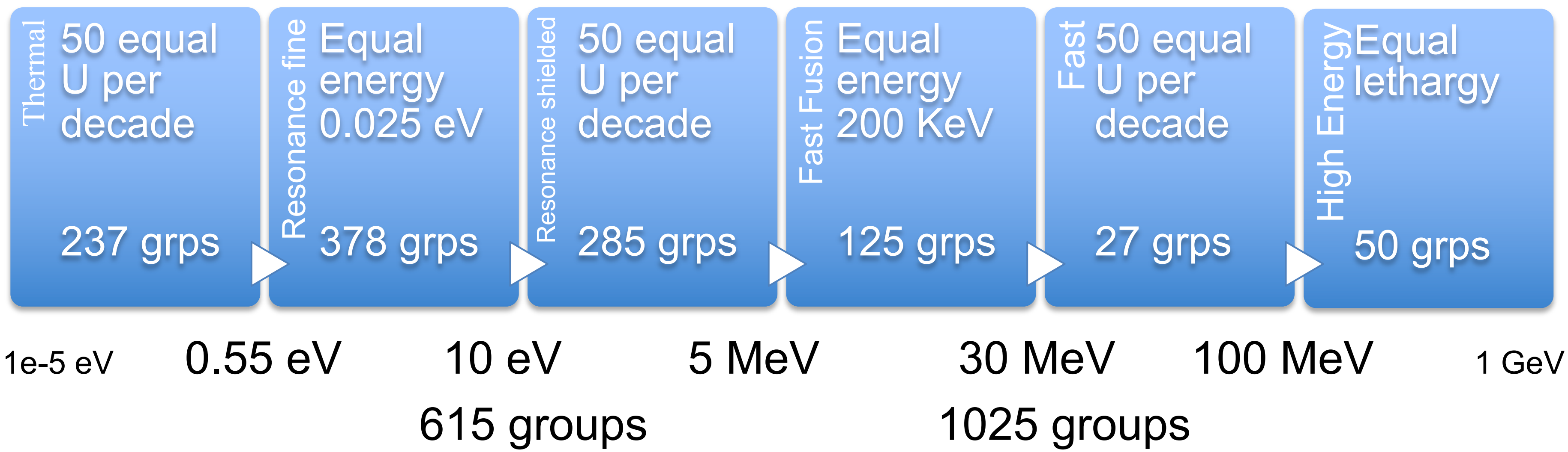
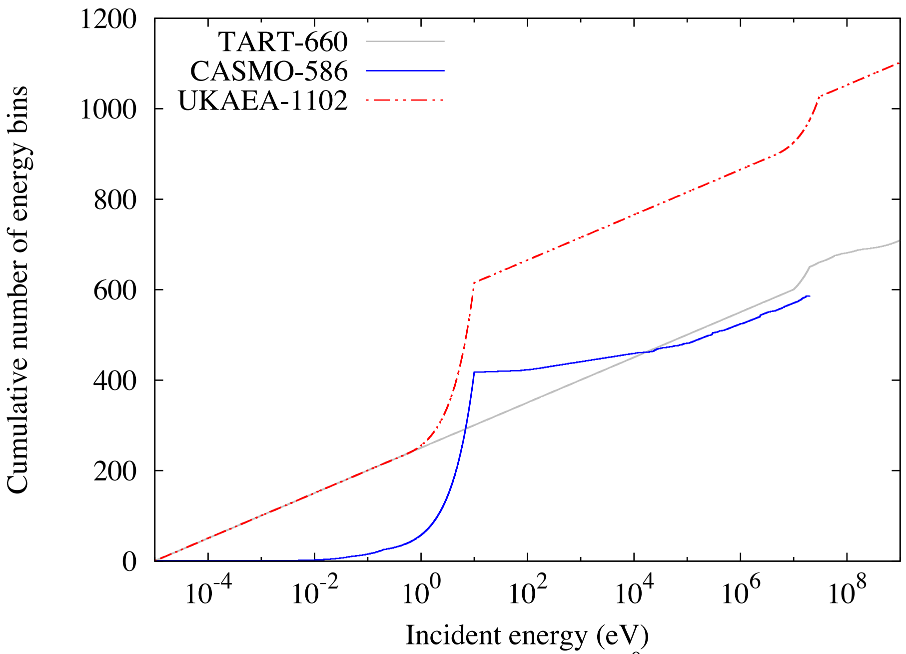
Group structures

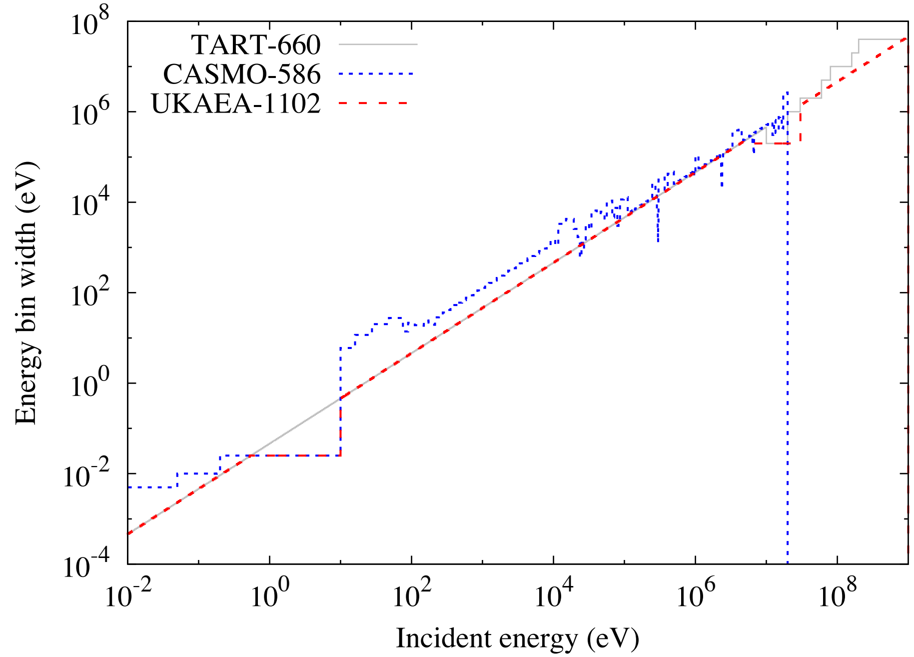
- For all 2813 TENDL target nuclides
- 1102 energy groups for all applications alike

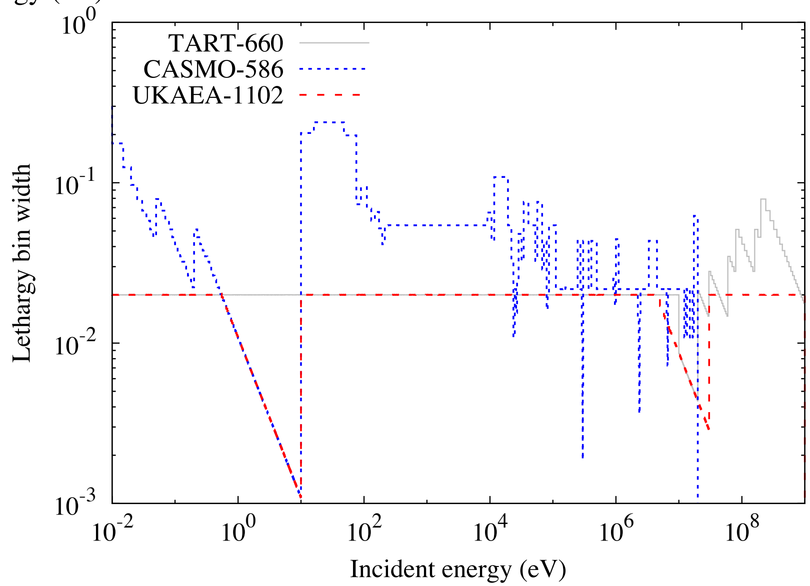


- 378 fine groups in the resonance range
- Resonance shielded data available in the RRR (0.1 eV) up to the end of the URR for all nuclide IDs
- Fast fine structure for accurate threshold reaction rate

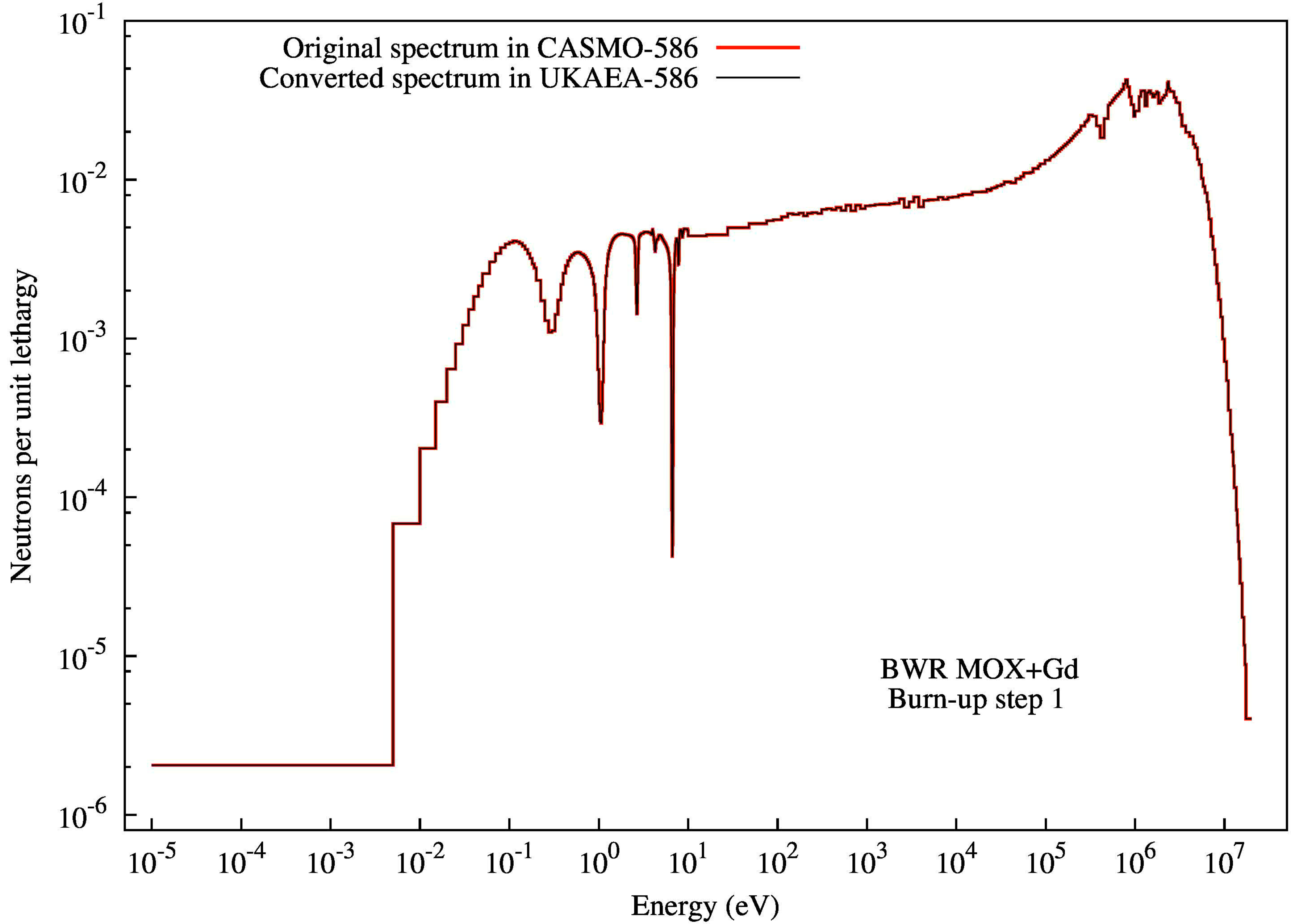
Group structures



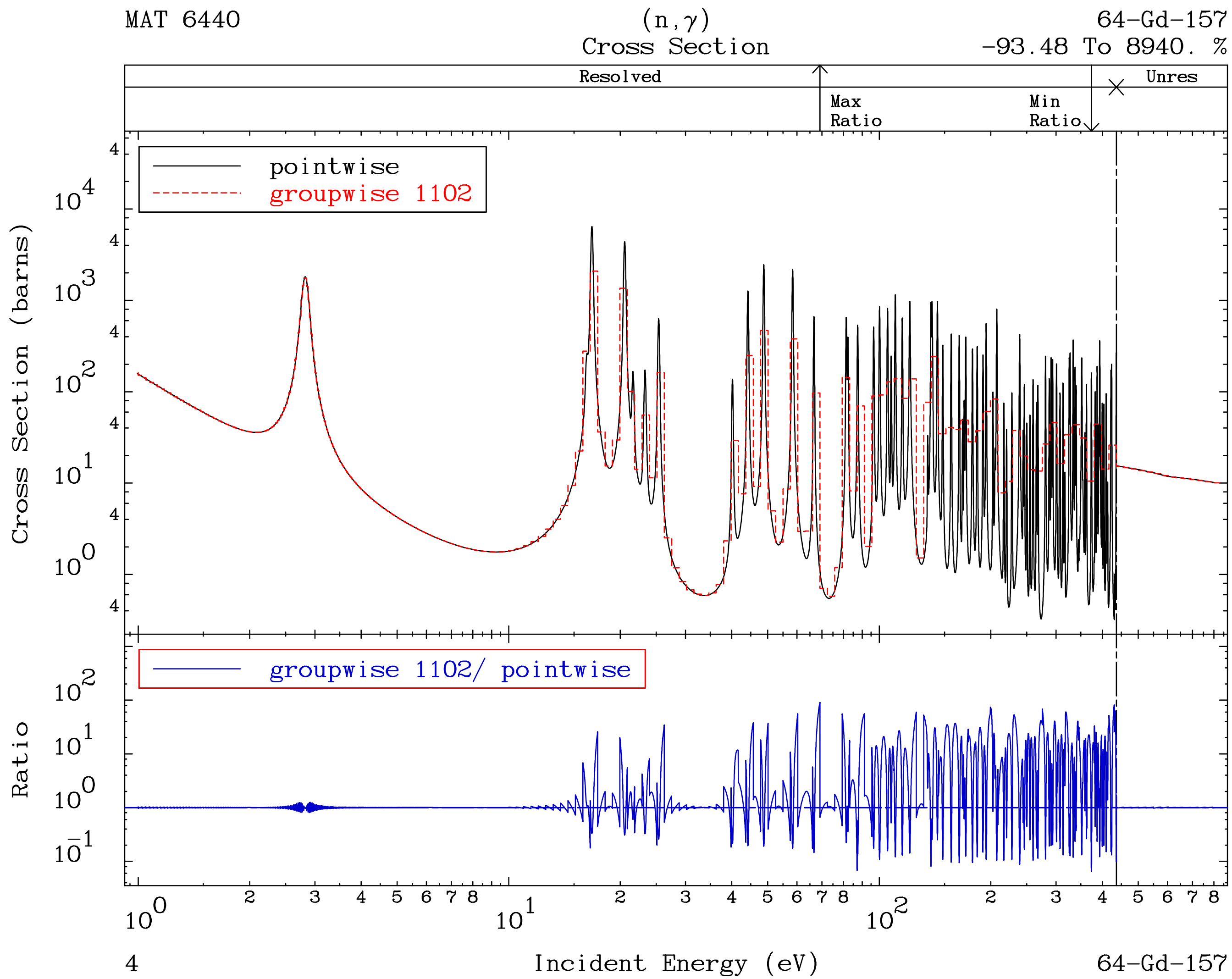




Time evolution of spectrum



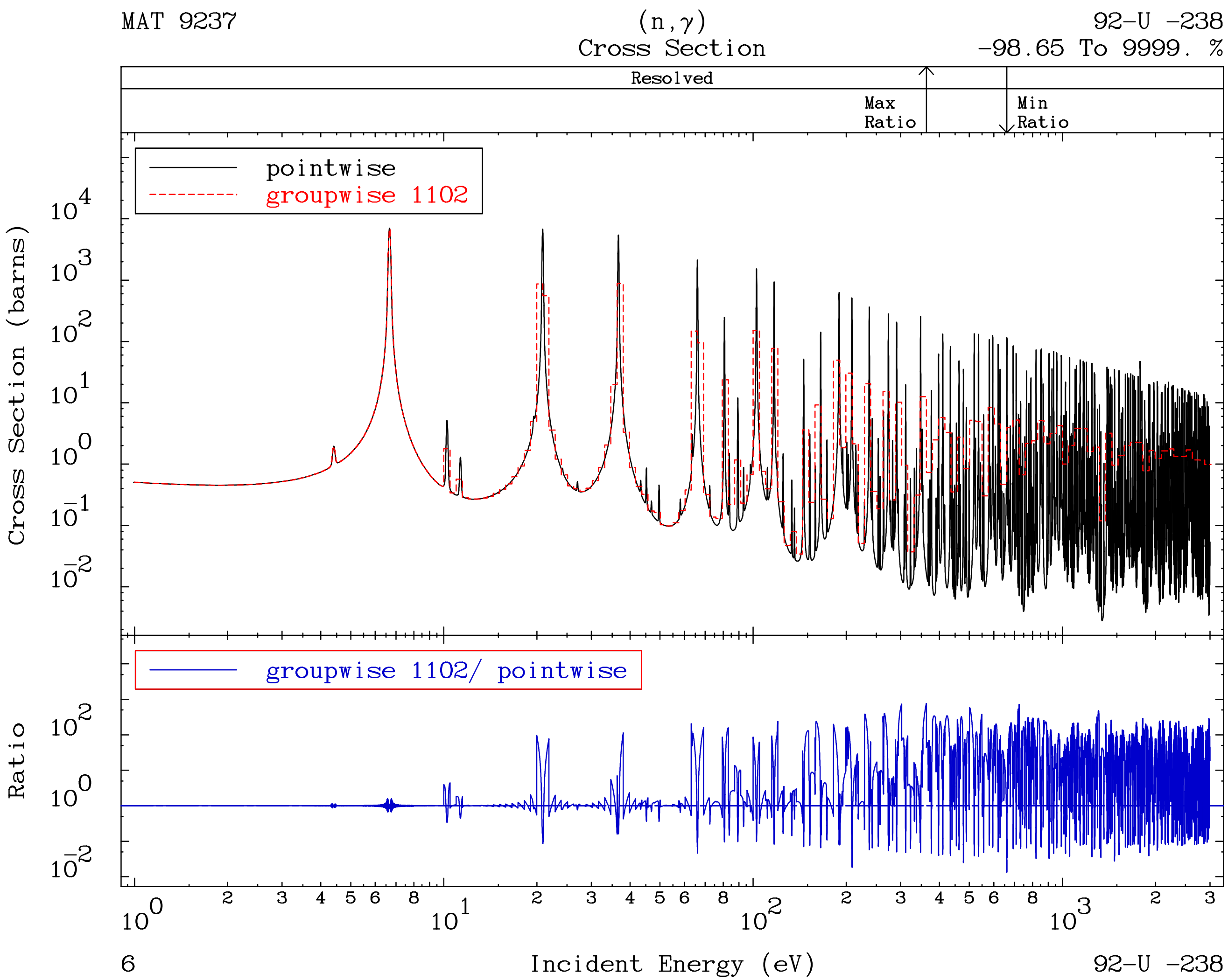
Group structure: 1102



Fine group to 10 eV

Resonance shielded to end of URR

Group structure: 1102



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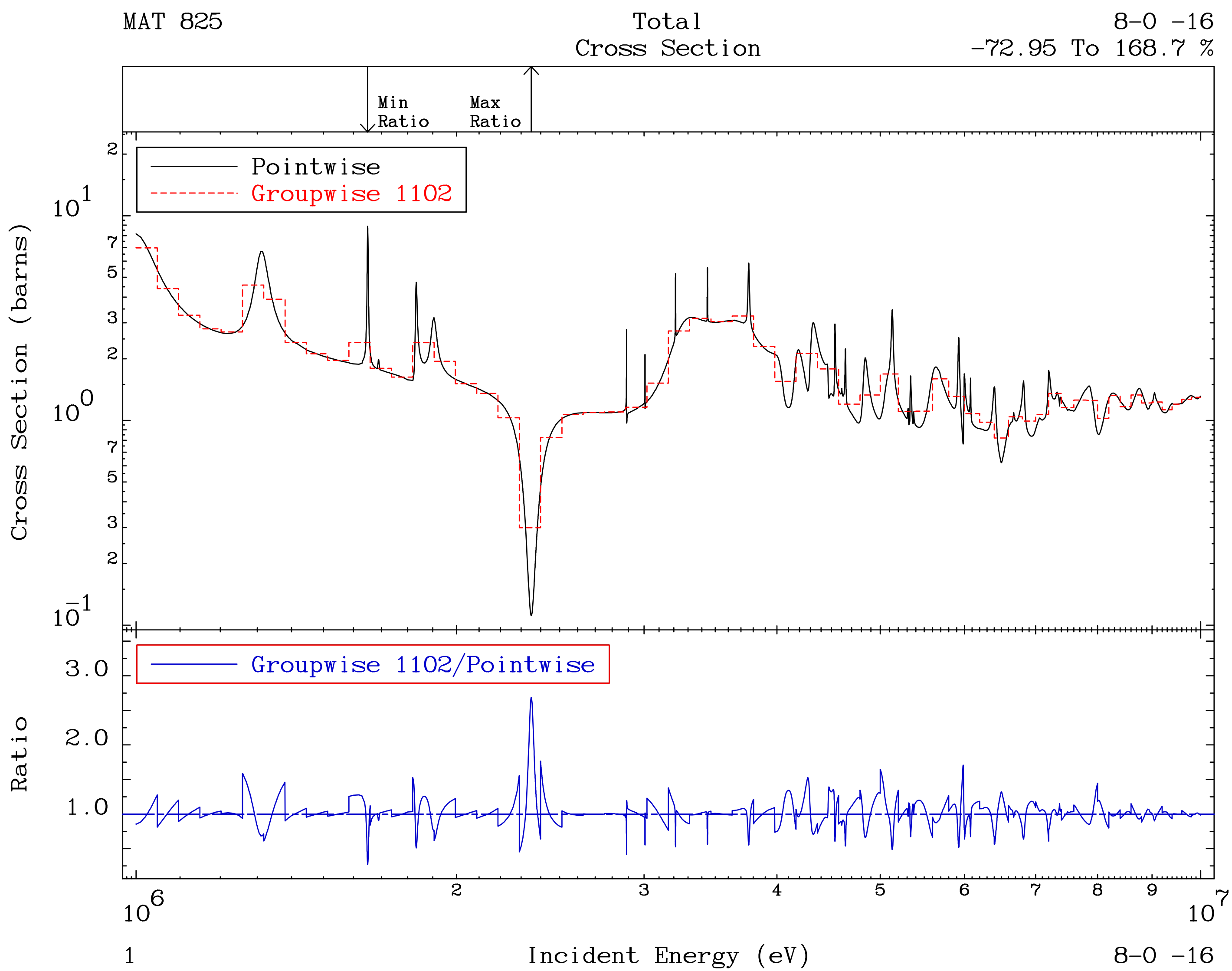


Peak and trough are well described

Uncertainty in FISPACT-II

- Given{ $\overline{XS}$, λ}
  - select irradiation scenario
  - solve for radiological quantities

- Use {ΔX, Δλ} to estimate uncertainties
  - method 1: pathways to dominant nuclides
  - method 2: Monte-Carlo sensitivity
  - method 3: reduced model Monte-Carlo sensitivity

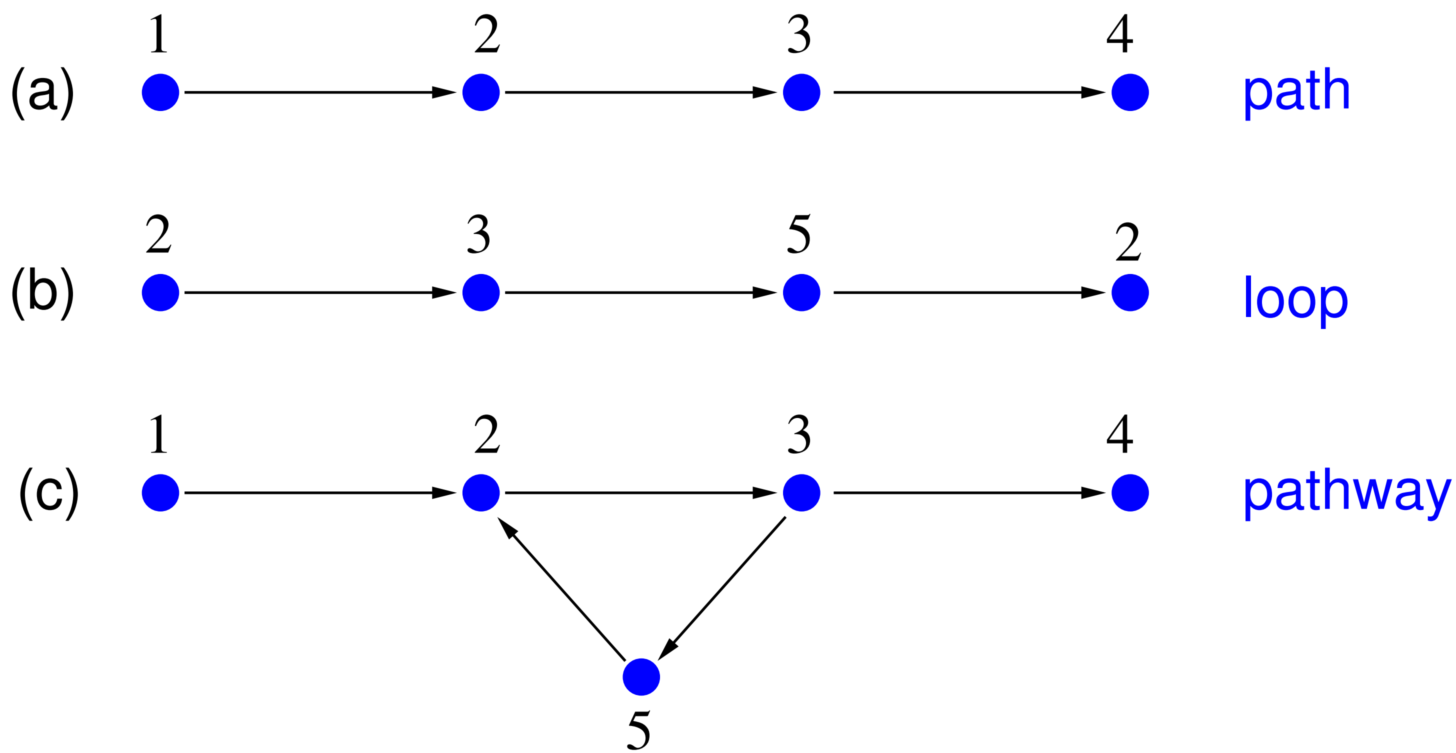
Uncertainty in FISPACT-II

- 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.

Uncertainty from pathways

- 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

Pathways



- keep pathways providing > `path_floor` of target inventory
- keep loop providing > `loop_floor` of pathway inventory

Error estimate

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

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

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

- 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)
...
```

Using LB = 6 data

- The TENDL library contains MF=33, LB=6 data for different reactions X_1, X_2, ... for a given parent, i.e., p(n, X_1)d_1, p(n, X_2)d_2, ...
- These covariance data cov(X_1,X_2) for X_1, X_2 are stored as fractional values f^{X1X2} and are tabulated in the same energy bins as used respectively for the LB=5 covariance data f^{X1X1}, f^{X2X2} 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

$$\left| \frac{f_{kl}^{X_1X_2}}{\sqrt{f_{kk}^{X_1X_1} f_{ll}^{X_2X_2}}} \right| > 1$$

Using LB = 6 data

- Then the code uses the corrected data to compute collapsed covariance 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, 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.

Uncertainty from sensitivity calculation

- reference run + S inventory calculations
- independent {X_i^s; i = 1,...,I; s = 1,...,S}
- dependent {Y_j^s; j = 1,...,J; s = 1,...,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

Monte Carlo approach to sensitivity analysis

- output mean and standard deviation

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

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

- 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`

Sample sensitivity output

```
Base cross section data
index        parent                     daughter                sigma      sigma_unc
   i   zai    nuc_no  name     i   zai    nuc_no  name            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

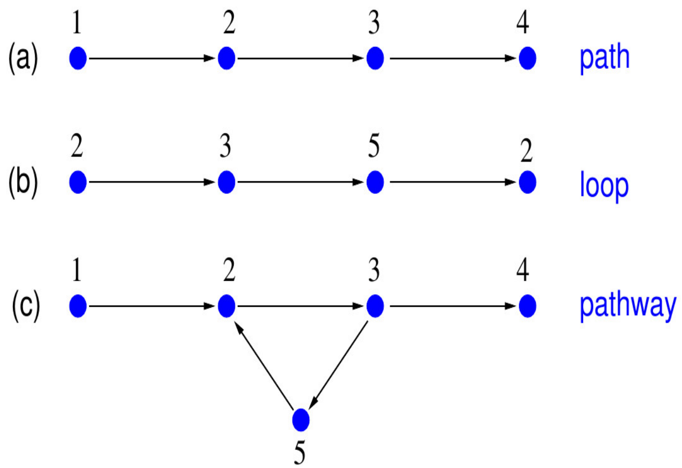
↑ output nuclides

Uncertainty from reduced models

- 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

Extended pathways search

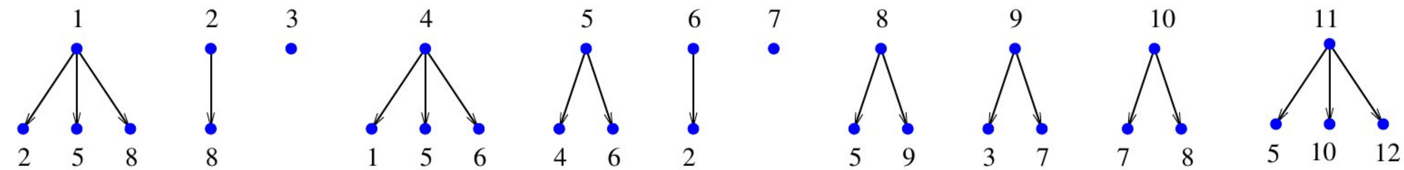
- Pathway = path + loop(s)
- Finds reaction/decay chains
- Identifies important
  - Nuclides
  - Reactions
  - Decays



- Used for uncertainty and sensitivity calculations

- Simple previous approach could fail through combinatorial explosion

Pathways – single visit tree

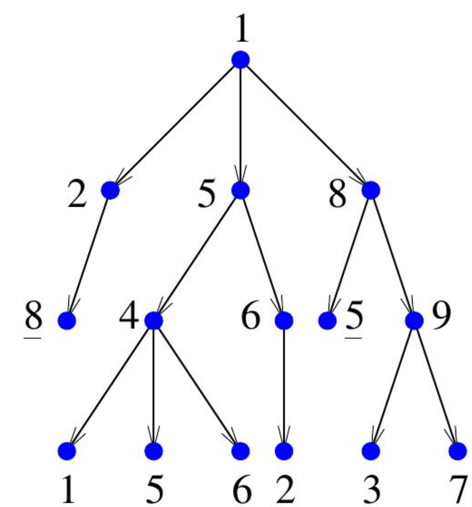


Adjacency lists

- 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

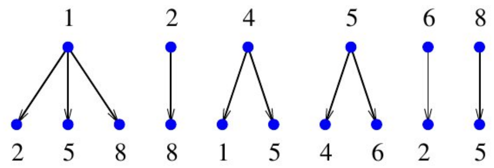
  typically < 50 p-d (parent-daughter)



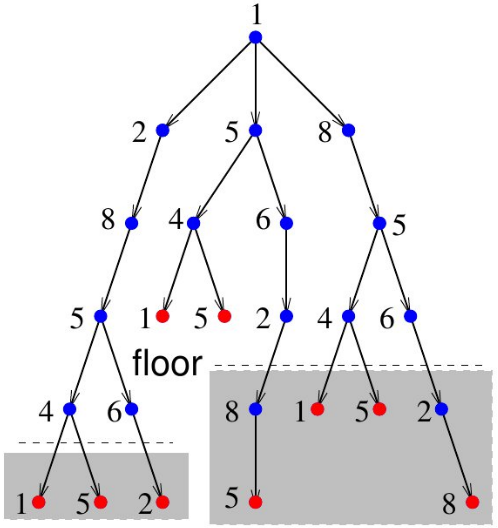
Single visit BFS tree for nuclide 1

Pathways

- 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

Standard pathways calculation

- 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)

Pathways with `LOOKAHEAD`

- `LOOKAHEAD` causes two-pass cooling:

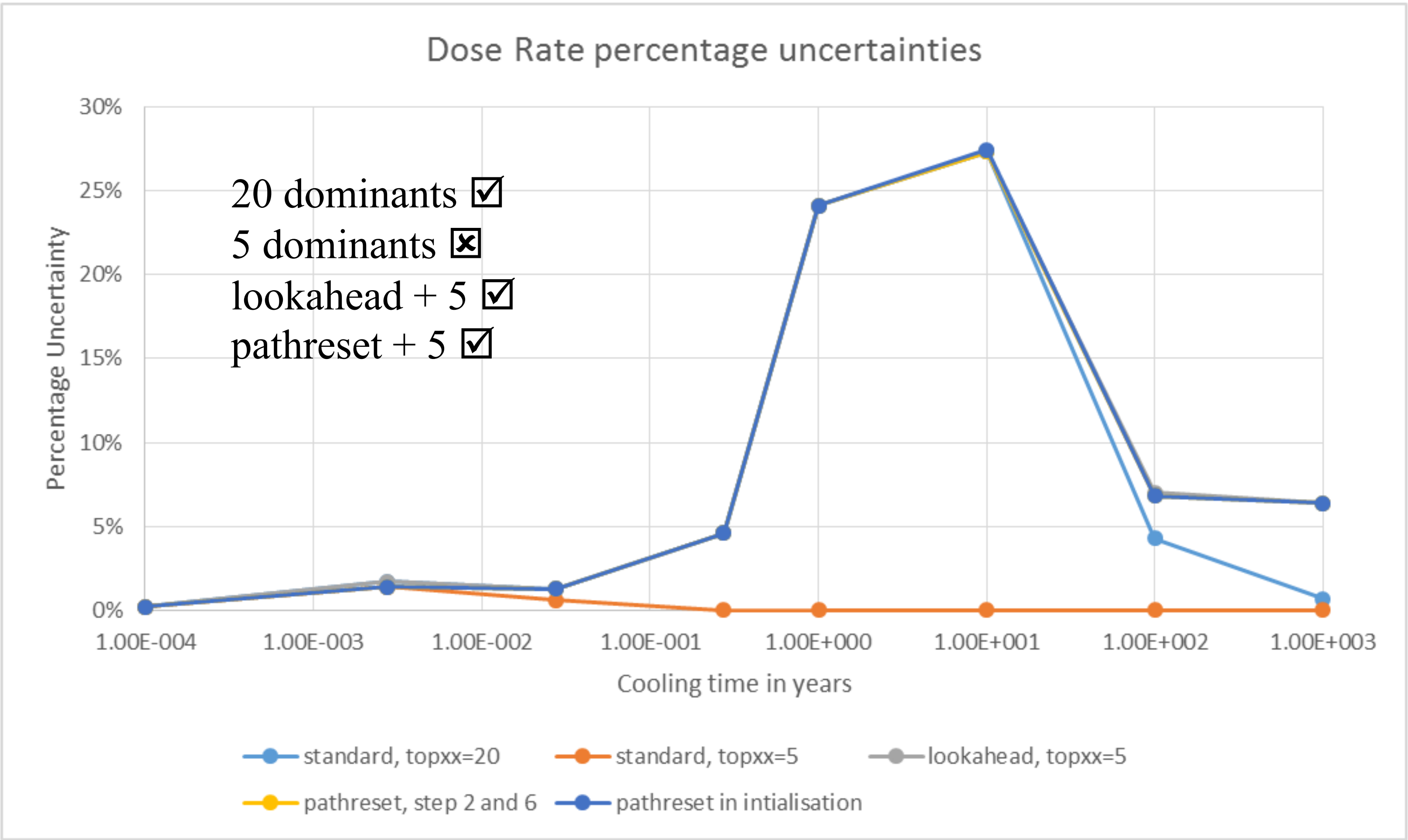
- at `ZERO`, integrate cooling steps to get late time dominant nuclides
- merge additional dominants with dominant list at `ZERO`
- use merged list in pathways calculation

Pathways with `PATHRESET`

- Save dominant list at `ZERO`, *ie* 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

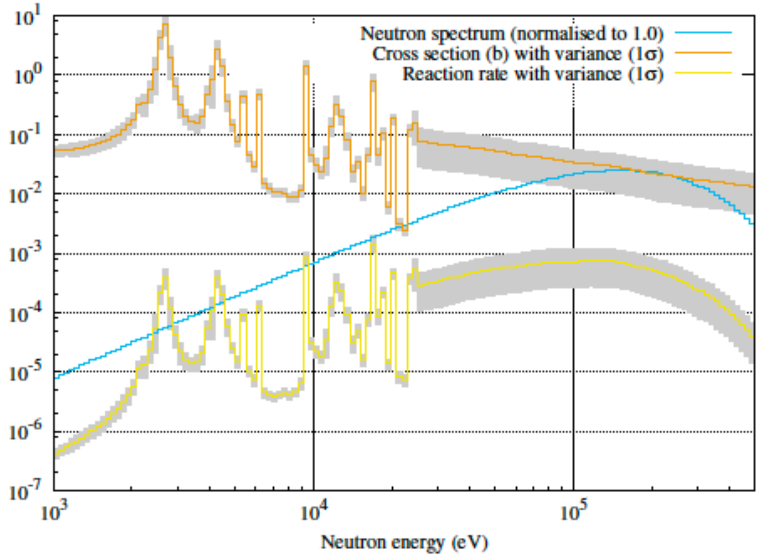
Example: dose rate for SS316

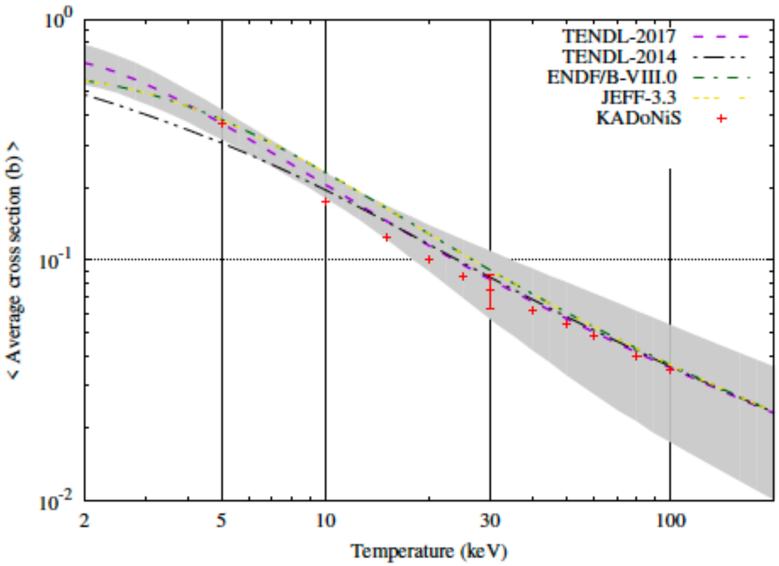
- standard cases show late cooling time underestimates uncertainty; 25% at 1-10 years cooling

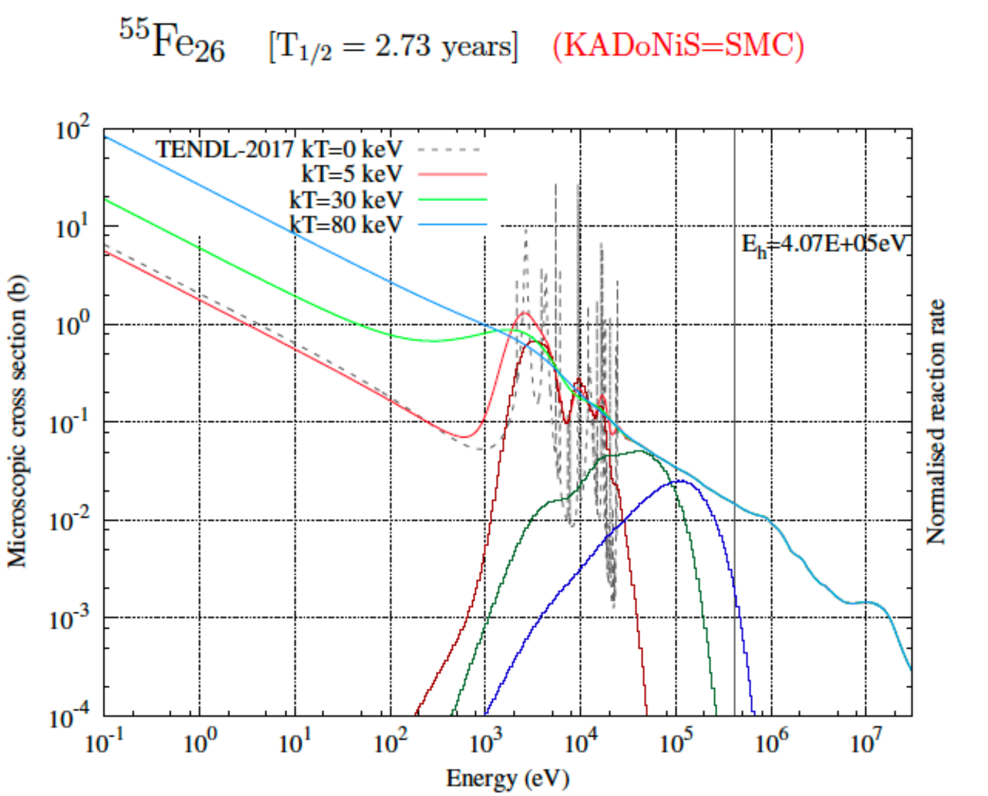


Cross section and reaction rates

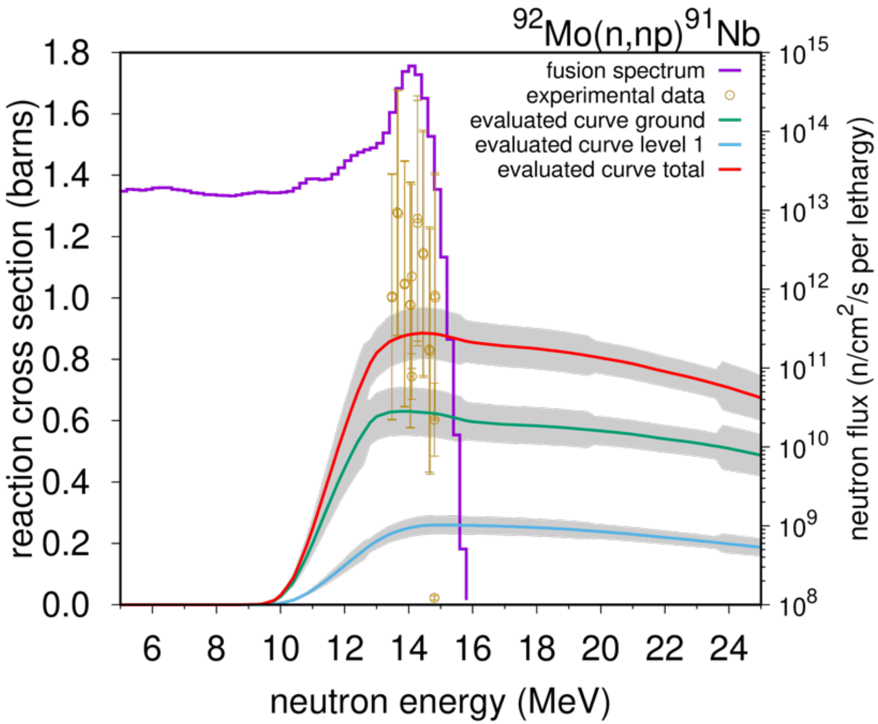
- Subtlility: cross section, reaction rate and variance

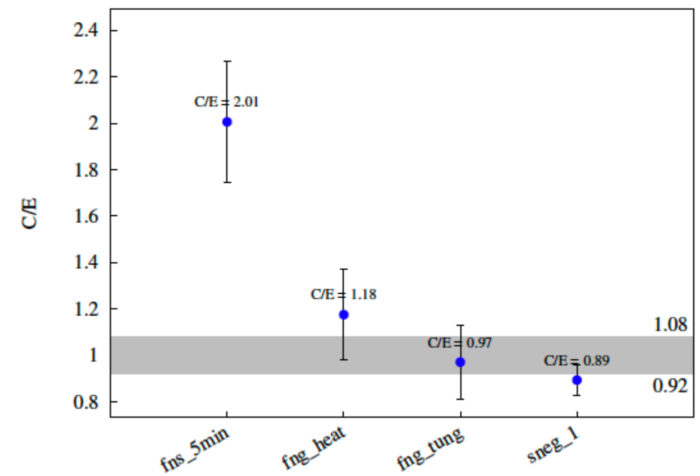


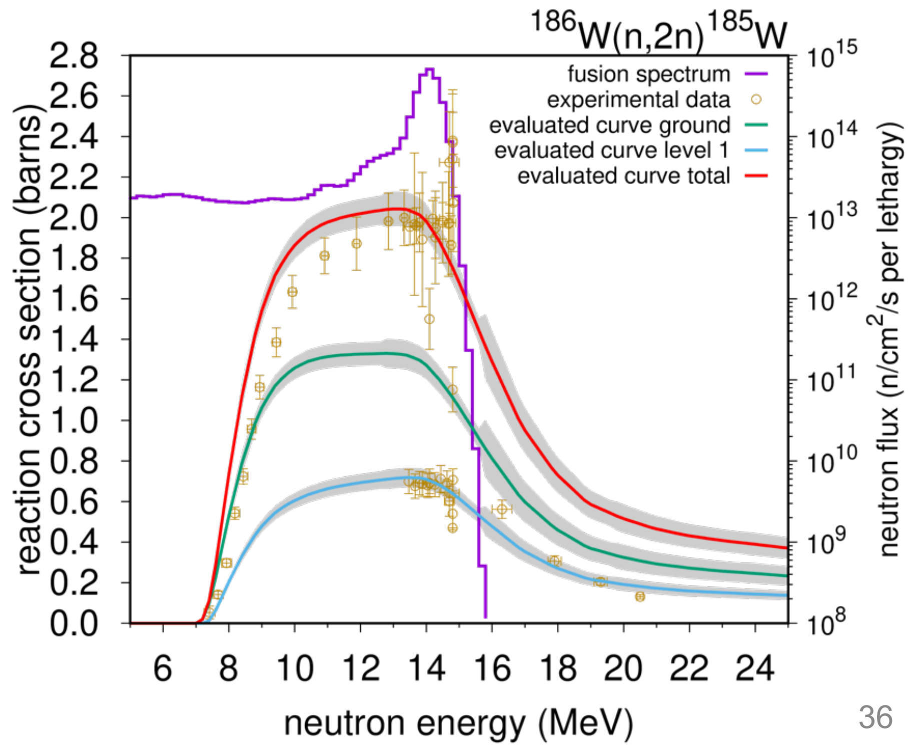




Threshold reaction uncertainty





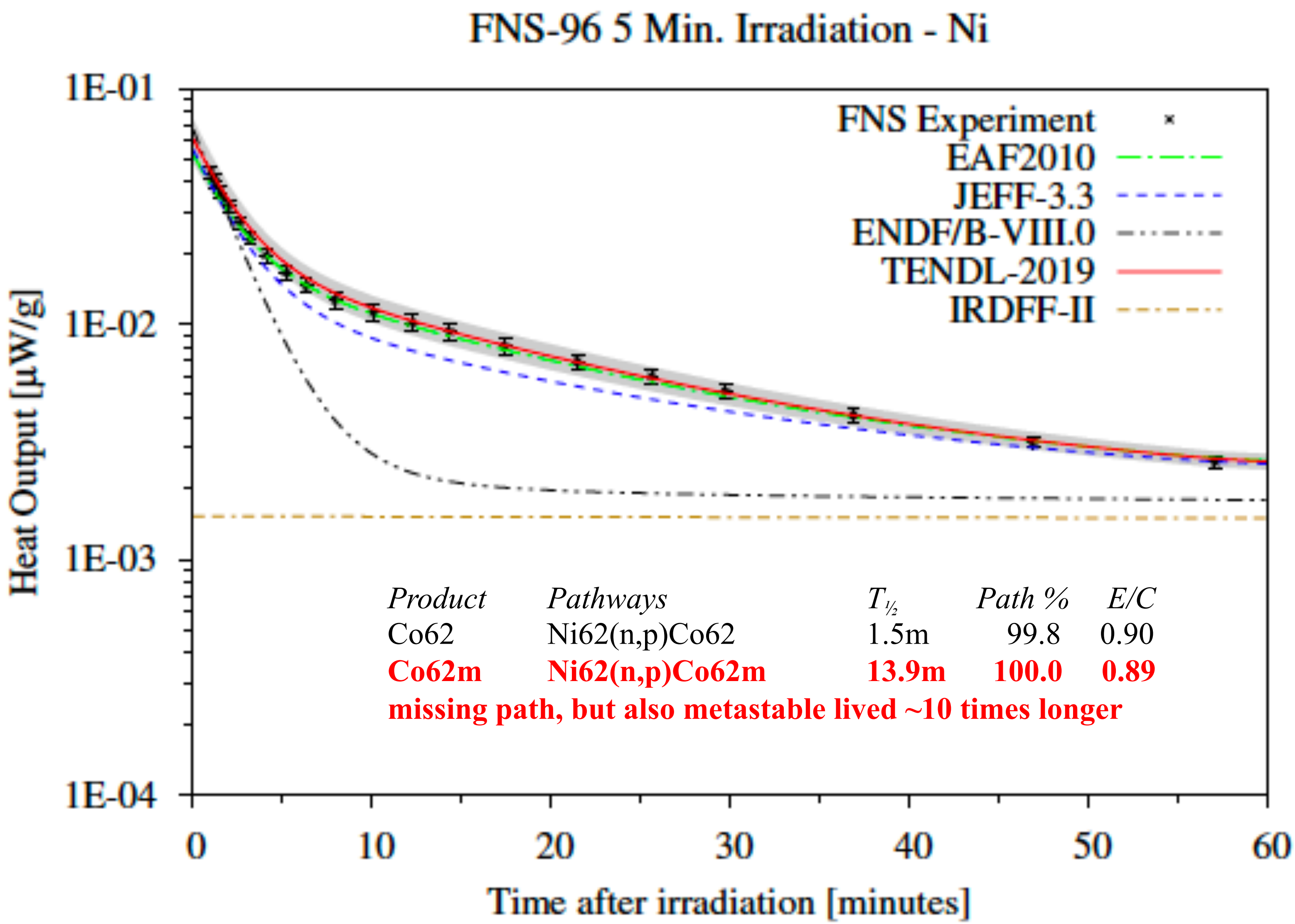


Not all integrals..
Not all differentials..

are as reliable, so the importance of the covariances

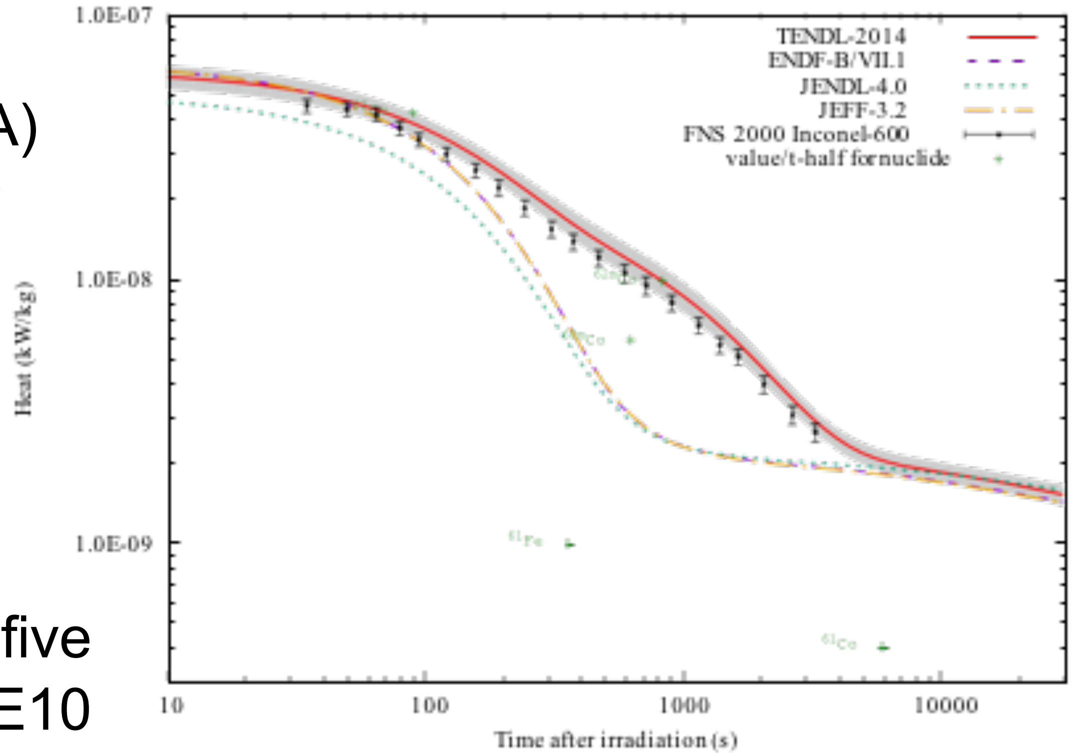
Ni FNS decay heat experiment

Random walk uncertainty



Inconel-600 decay heat

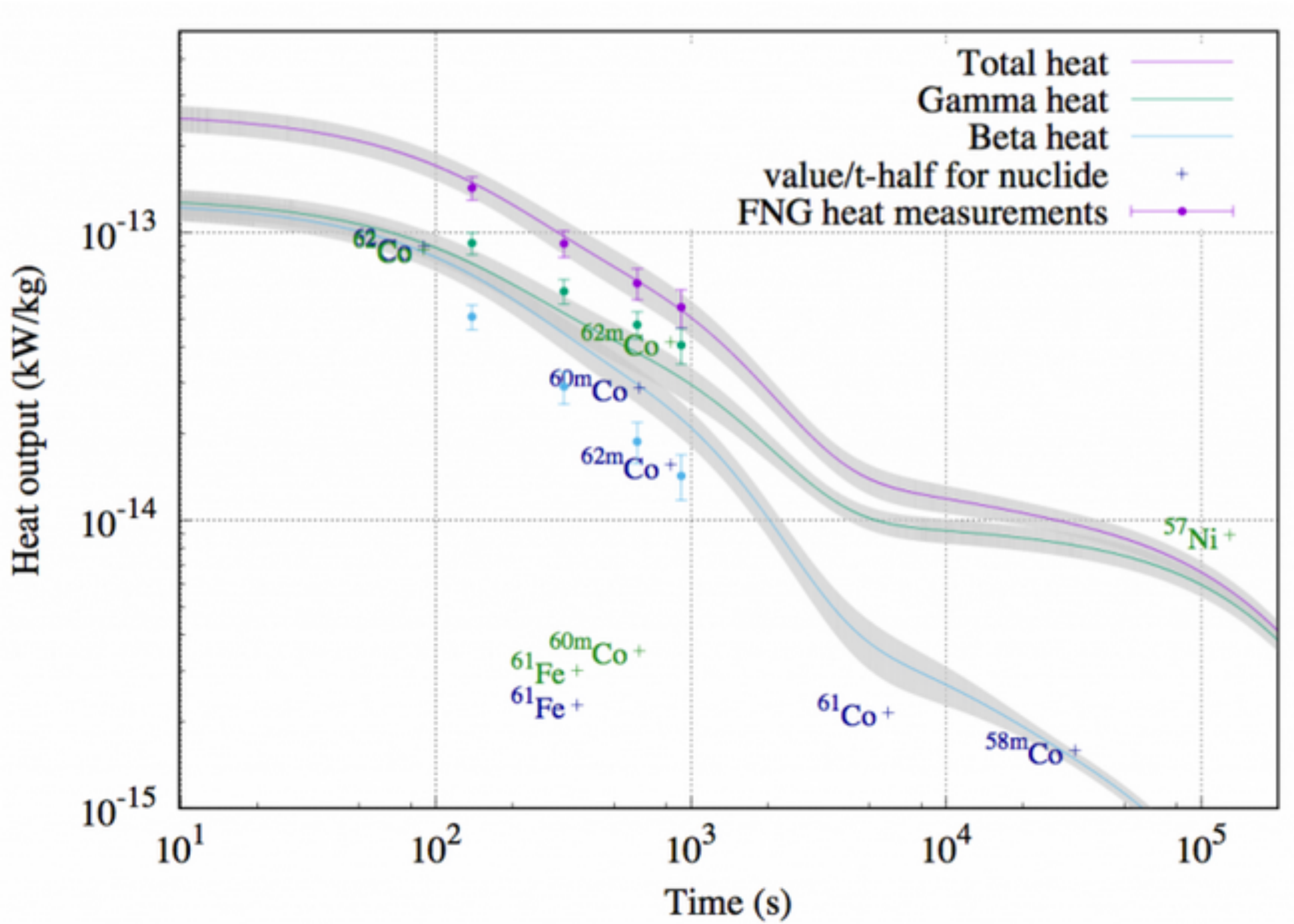
- FNS (JAEA) and FNG (ENEA) ^{2}H beam onto ^{3}H-Ti target for ~14 MeV source



- 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

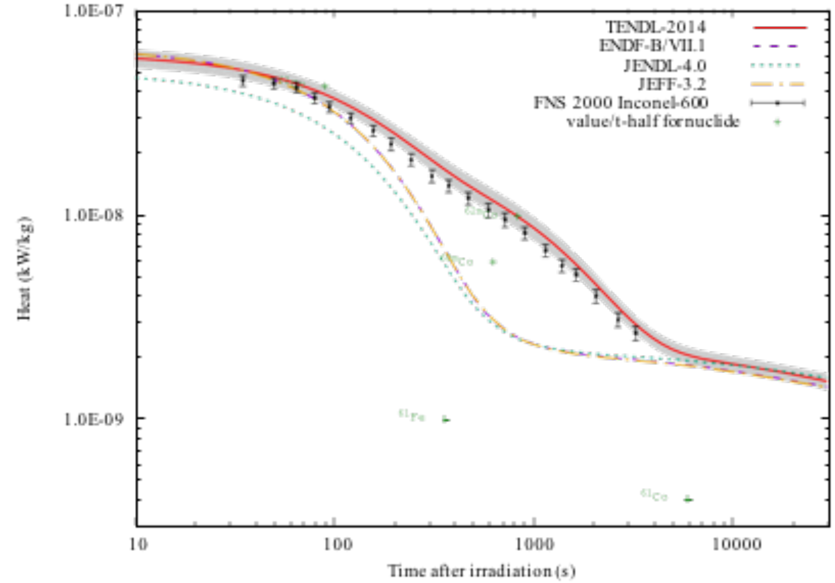


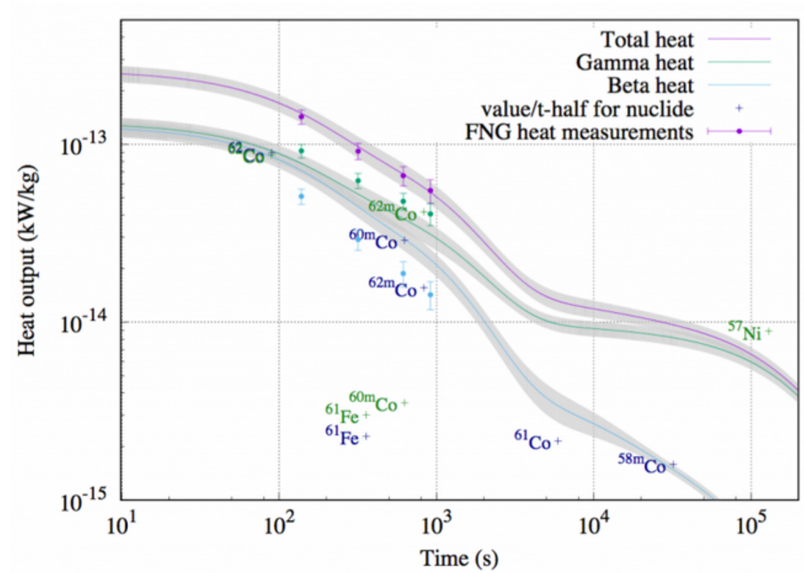
Total, beta and gamma heat apportionment

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



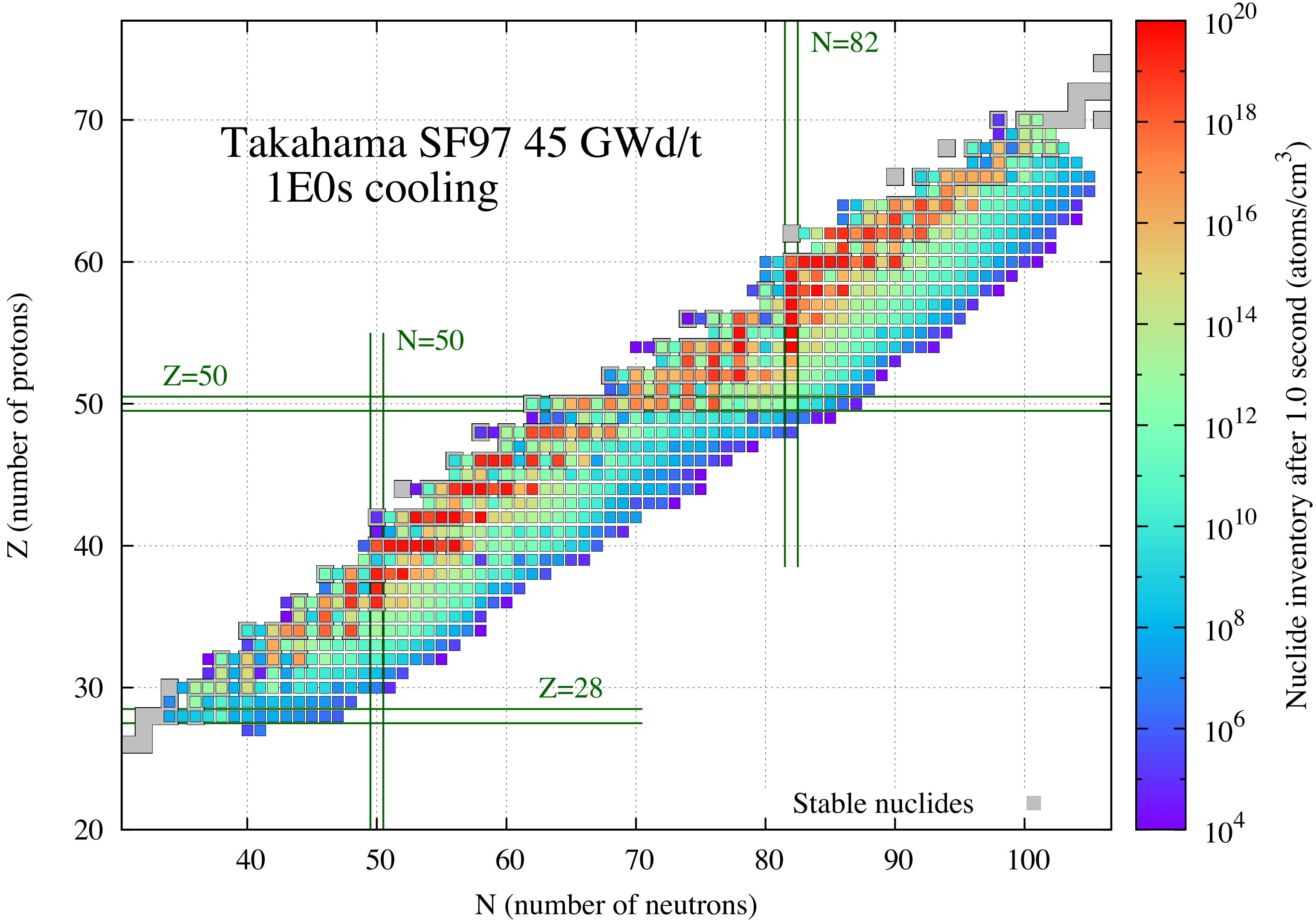


FISPACT-II fission yield uncertainty

- FISPACT-II makes use of Bayesian Monte-Carlo fission yields generated by:
  - Input parameter variation of GEF
  - $\chi 2$ 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

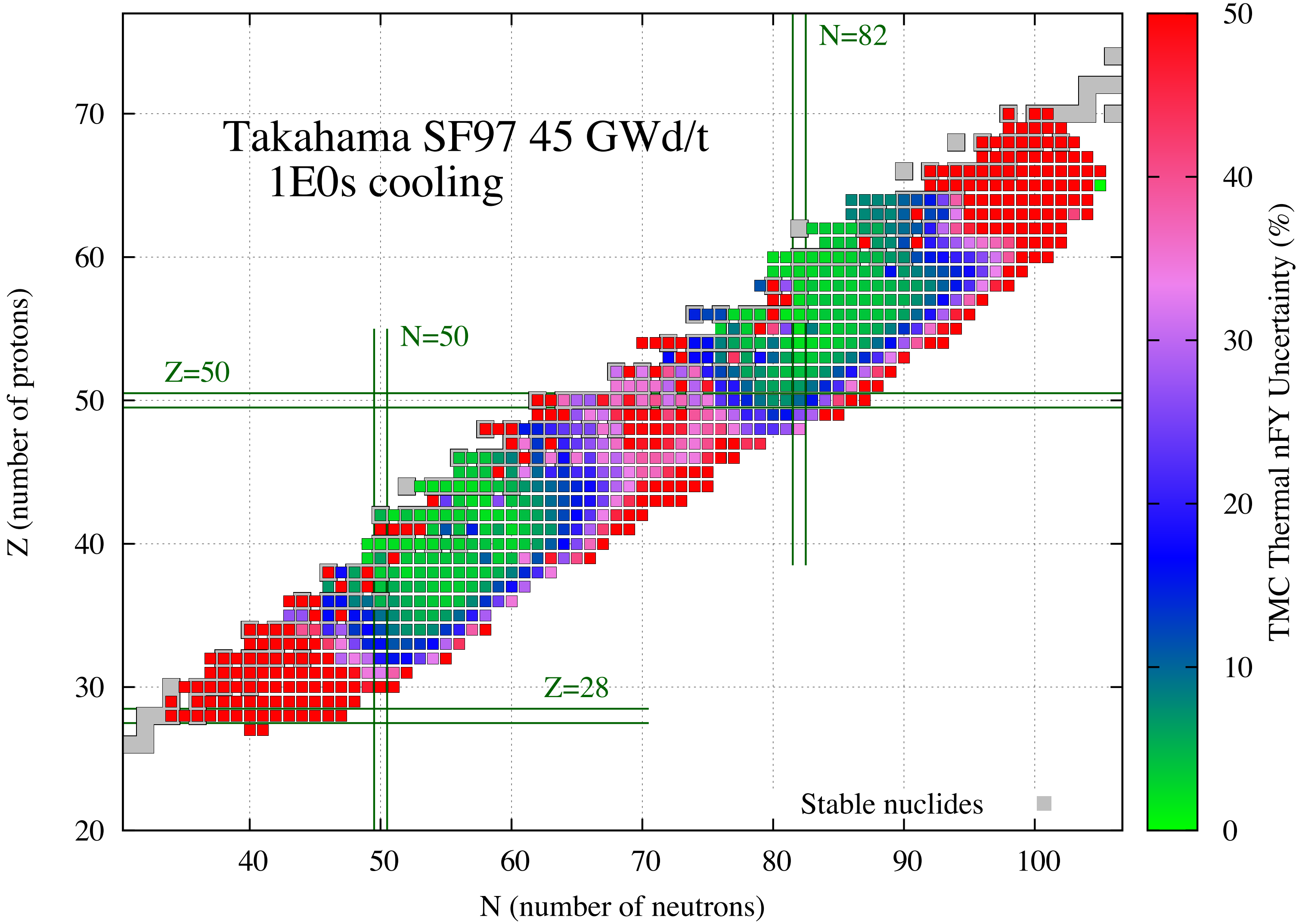
Not your typical LWR simulation

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

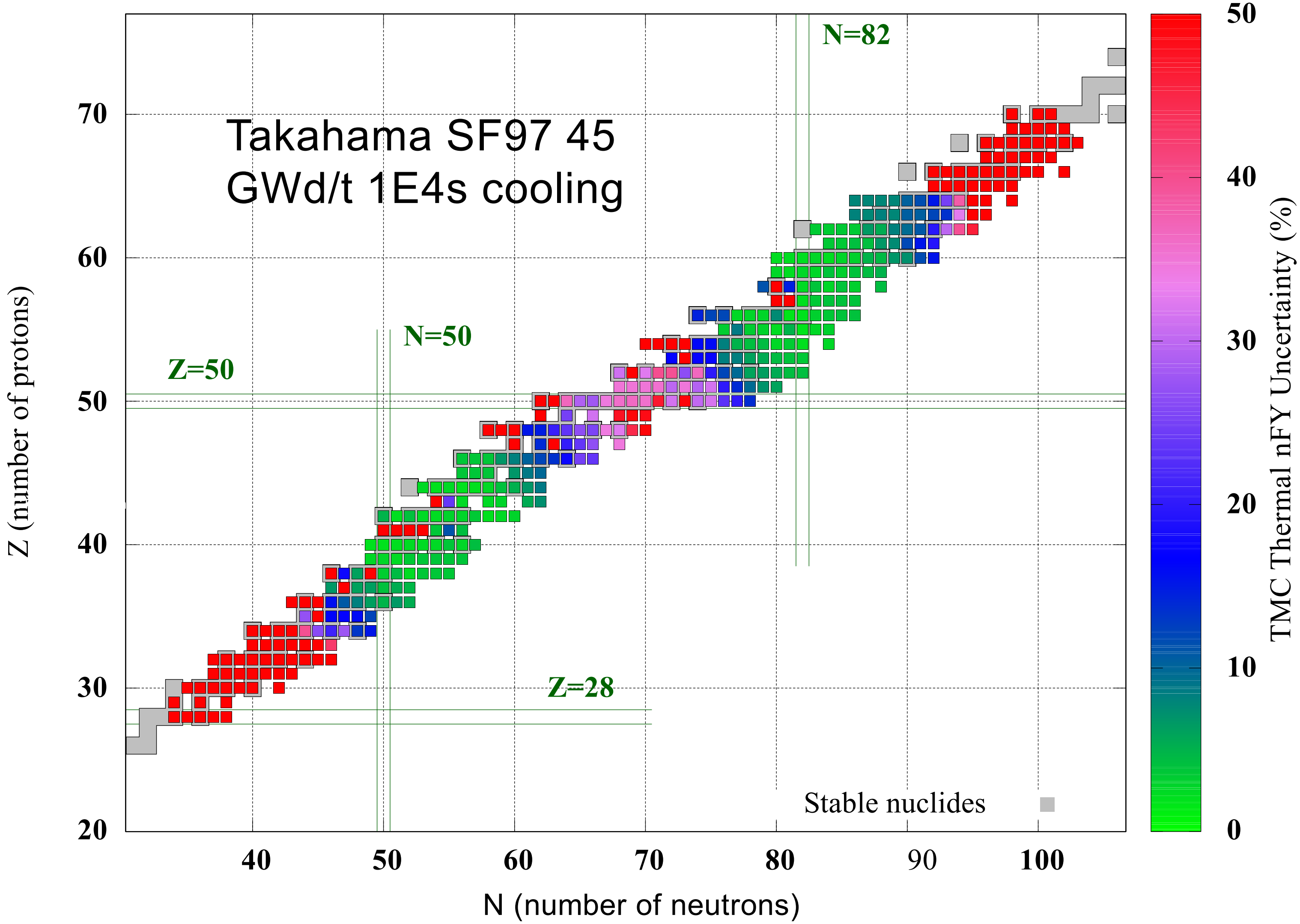


LWR assembly UQP

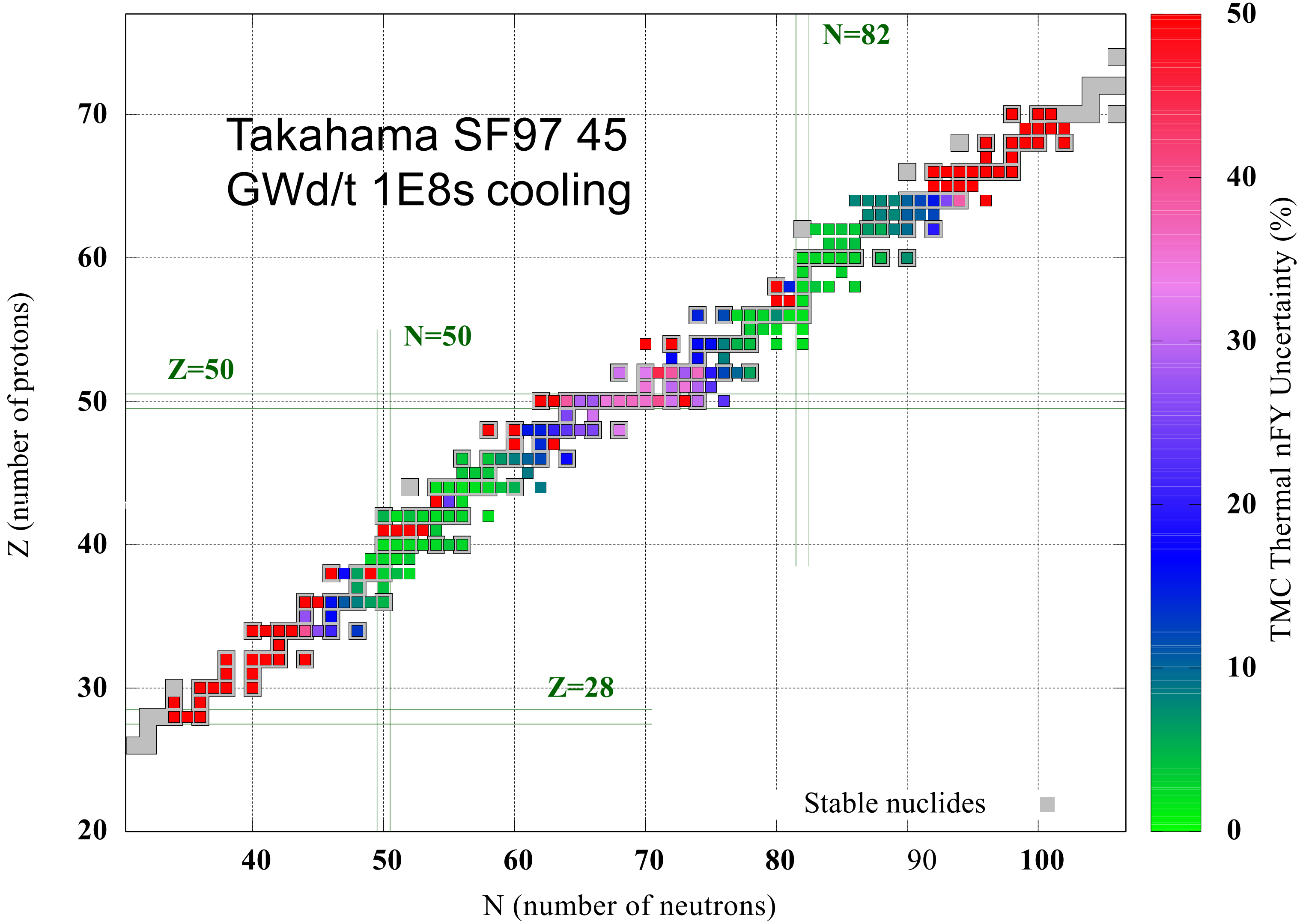
- Ability to handle technologically-generated TALYS & GEF(Y)



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

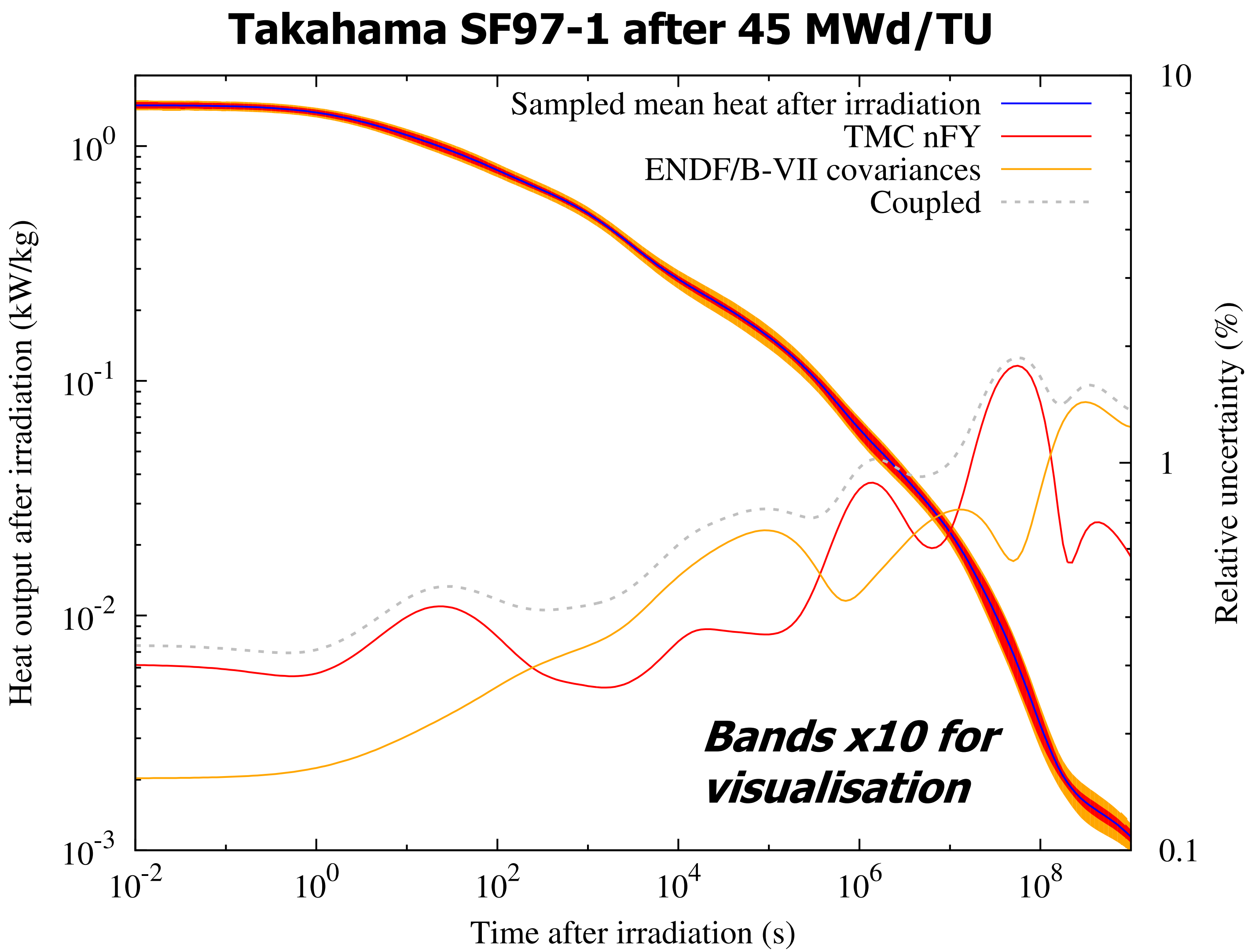


Example: Takahama-SF97 nFY uncertainties (10^8 s)



FISPACT-II RR + nFY UQP

- Coupling FISPACT-II 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.



Recap: FISPACT-II UQP

- 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