FISPACT-II Advanced Nuclear Data Uncertainty Quantification and Propagation Methods

United Kingdom Atomic Energy Authority

June 14, 2017

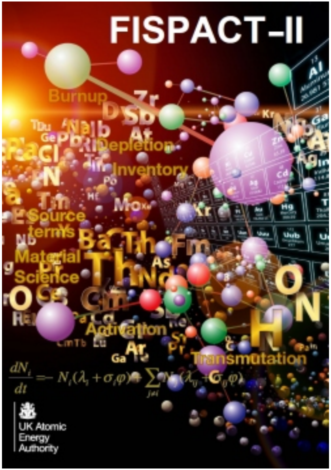
Introduction

Background

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

Simulation system

- 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



The FISPACT-II User Manual UKAEA-R(11)11 Issue 8 December 2016
Nuclear Data Sheets 139 (2017) 77-137
http://fispact.ukaea.uk

Uncertainties in different applications

For FISPACT-II, we encounter a few different scenarios:

- Inventories in lower-energy irradiations with few(er) target nuclides and reaction channels
  - These can be handled directly with Monte-Carlo sensitivity calculations by knowing the reaction channels of interest beforehand or by deducing them from the next method
- Multiple complex materials with high(er) energy incident particles and hundreds, thousands and more reaction channels
  - Dominant response nuclides are identified automatically and a combinatorial search for all reaction combinations leading to the product nuclide is used with reaction rate uncertainties
- Fission/spallation yields
  - These are highly correlated and at present the standard files do not contain the required information - we utilise the so-called Bayesian Monte-Carlo fission yields of D. Rochman, et al

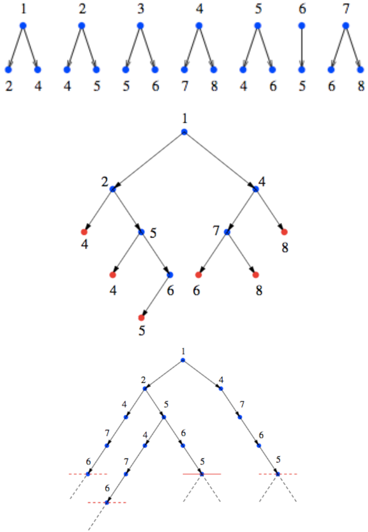
FISPACT-II pathways uncertainty (I)

- TENDL-2015 contains up to approximately 100 residual products per target nuclide
  - Important products are not generally known beforehand
  - Sampling reaction rates for a great many channels is not practical or desirable
  - Users typically want to know (1) how the radionuclide was produced and (2) how uncertain are the inventories and observables

- Four standard steps:
  - Identify dominant nuclides for activity, dose rates, decay heat (or user specified)
  - Create directed graph including these nuclides and prune unnecessary branches (adjustable parameters)
  - Combine paths and loops to form comprehensive pathway set
  - Read uncertainties on reaction rate edges to calculate inventory uncertainty

FISPACT-II pathways uncertainty (II)

- For a given system of nuclides (*right*: example of 8) the set of edges are found and all connections from parent to target (here 1 to 4) are found
- These are pruned by [1] combined RR weight below threshold [2] number of edges above threshold or [3] loops (handled separately)
- Thresholds and loop parameters can be specified by the user



Nuclear Data Sheets 123, 84-91, January 2015

UNCERTAINTY keyword

- `http://fispact.ukaea.uk/wiki/Keyword:UNCERTAINTY`
- Typically users take default parameters
- Standard use: `UNCERTAINTY 2`
- `path_floor`, can be lowered to take more contributions (below X%), `loop_floor` for loops, `max_depth` for length of chains
- In very complex, long irradiations paths greater than 10 in length can matter!
- NOTE: The inventory and pathways calculations are separately performed, with more strict `TOLERANCE` settings on the former - if you extend the `UNCERTAINTY` limits also revisit the `TOLERANCE` settings

FISPACT-II dominants and pathways

- FISPACT-II has been developed to handle the complex activation/transmutation uncertainty by considering the *cooling observables*
- Activity, decay heat, dose rate, etc, have their contributions ranked by most important radionuclides
- The top 20 are shown by default and `SORTDOMINANT` can be used to increase this number (see for example the pulse getting_started example)
- The uncertainty for each of these dominants is determined by considering all pathways for those nuclides

FISPACT-II pathways uncertainty (III)

- With the set of target nuclides of importance for observables, $N_t \in S_t$, we take the random walk approximation over all pathways p

$$\Delta N_t = \sqrt{\sum_p (\Delta N_{tp})^2}$$

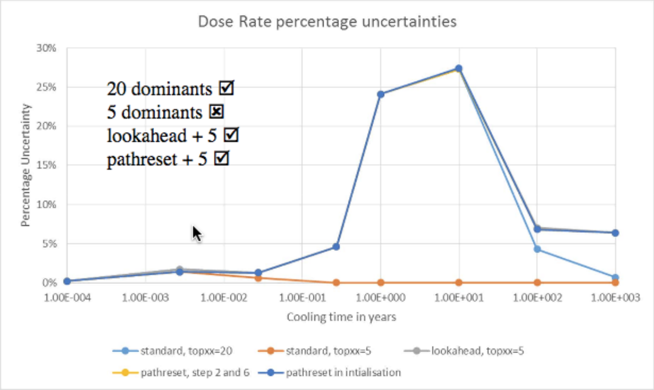
- While channel-channel covariances could be incorporated (see ref) using channel-channel similarity matrix, we use simply

$$\left(\frac{\Delta N_{tp}}{N_{tp}}\right)^2 = \sum_{e,r}\left(\frac{\Delta\sigma_r}{\sigma_e}\right)^2 + \sum_{e\in D_e}\left(\frac{\Delta\tau_e}{\tau_e}\right)^2,$$

where the edges e between any two nodes may contain multiple individual reaction channels r

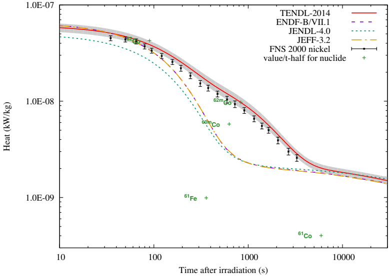
Pathway resets

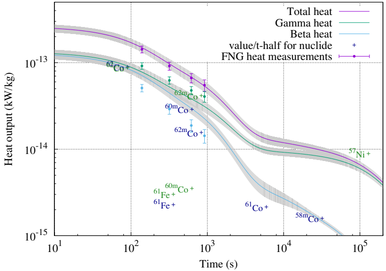
- The dominant nuclide list is populated at end of irradiation
- To recalculate the dominants, use `PATHRESET` or `LOOKAHEAD`



Pathways uncertainty with activation

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





CCFE-R(15)25 January 2015
CCFE-R(15)27 March 2015

Depletion addition (I)

- However, for coupled creation-destruction scenarios with uncertainty in the rate of destruction the pathways search only handles the paths to the target
- To add destruction with specific rate D and creation rate C, $dN/dt = -\mathrm{D}N + \mathrm{C}$, we take the simplified piece-wise constant approximation

$$N_{i+1} = \frac{\mathrm{C_i}}{\mathrm{D_i}} + \left(N_i - \frac{\mathrm{C_i}}{\mathrm{D_i}} \right) \exp\left(-\mathrm{D}_i \Delta t_i\right)$$

- The first order expansion for this approximation w.r.t. the creation and destruction uncertainties has been tested in the example

Depletion addition (II)

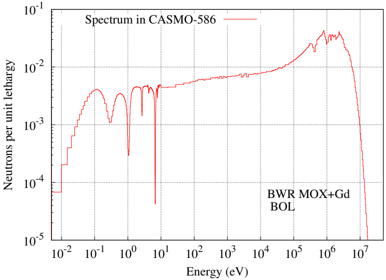
- A new keyword **DEPLETION** adds the depletion/destruction uncertainty into the output where, as with the pathway-based uncertainties,

$$var(R) = \sum_i \sum_j \phi_i \phi_j cov(\sigma_i, \sigma_j).$$

- Since depletion is the sum $\mathrm{D} = \lambda + \phi\sigma$, the variances of both are summed
- ϕ_i uncertainties may be considered (see paper) but at present are not implemented
- **DEPLETION** requires the user to specify the nuclide set, which may be in the initial inventory or otherwise

Example: Am242m in BWR MOX

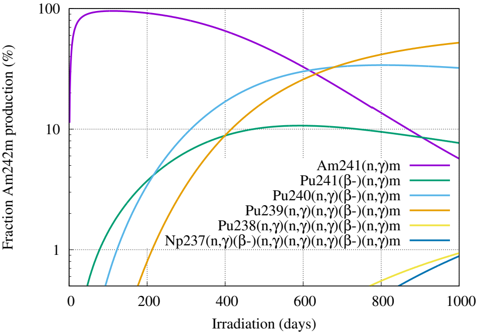
Using a 586-group spectrum for an indicative, assembly averaged neutron spectrum, we obtain a set of cross sections and uncertainties from the ENDF/B-VII.1 files.



Parent	Daughter	σ (b)	$\Delta\sigma$
Am242m	Fission	231.070	4.418%
Am242m	Am240	1.358E-07	0.000%
Am242m	Am241	2.189E-03	29.925%
Am242m	Am242	7.784	10.785%
Am242m	Am243	43.831	22.495%
Np237	Np238	22.750	4.100%
Pu238	Pu239	10.670	9.500%
Pu239	Pu240	20.886	1.093%
Pu240	Pu241	39.178	0.907%
Am241	Am242m	5.967	4.799%

Am242m Pathways

FISPACT-II calculates all of the paths as described above, determining the % composition of the total production over all of these pathways (*below*: 1000 day irradiation). These can be calculated for each irradiation period, as shown in the figure.



```
path  1   0.886% Np237 ---(R)--- Np238 ---(d)--- Pu238...
                   100.00%(n,g)    100.00%(b-)     100...
path  2   0.938% Pu238 ---(R)--- Pu239 ---(R)--- Pu240...
                   100.00%(n,g)    100.00%(n,g)    100...
path  3  52.162% Pu239 ---(R)--- Pu240 ---(R)--- Pu241...
                   100.00%(n,g)    100.00%(n,g)    100...
path  4  32.193% Pu240 ---(R)--- Pu241 ---(D)--- Am241...
                   100.00%(n,g)    100.00%(b-)     100...
path  5   7.683% Pu241 ---(D)--- Am241 ---(R)--- Am242m
                   100.00%(b-)     100.00%(n,g)
path  6   5.691% Am241 ---(R)--- Am242m
                   100.00%(n,g)
```

Sensitivity-uncertainty analysis

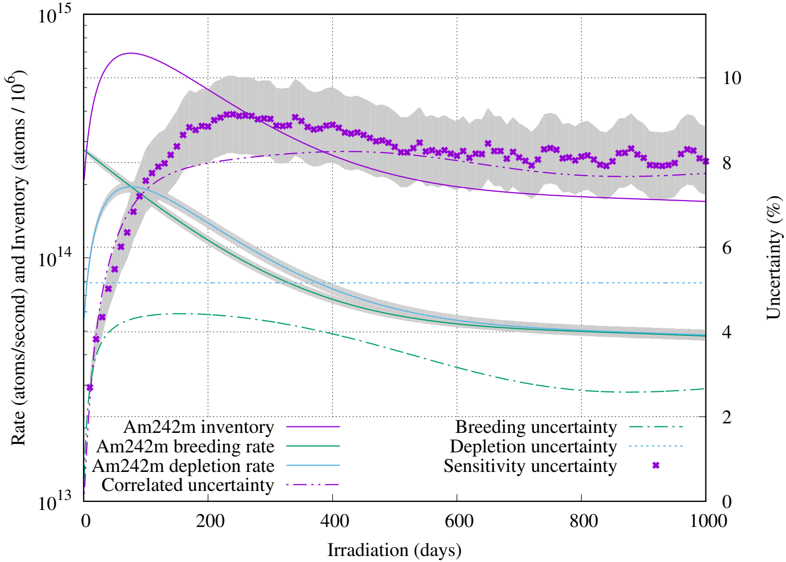
- With a knowledge of the reaction channels of importance (from previous work or pathways analysis) FISPACT-II can perform sampling of those cross sections using the full, collapsed covariance uncertainty
- The `SENSITIVITY` keyword is used for this purpose with the `MCSAMPLE` keyword for distribution selection, e.g. :

```
SENSITIVITY SIGMA 0.8 2 1
  Ti48 Sc48
  Ti49 Sc48
 Sc48
MCSAMPLE 2 100 -2.0 2.0
```

Depletion uncertainty and MC sampling

- In addition to the pathways determined in the previous slide and the uncertainties from that analysis, add the depletion
  - Rate proportional to inventory
  - Specific depletion rate constant in this simplified case with one spectrum - and therefore uncertainty % will be constant
- The combined uncertainty approximated from 1st order expansion on piece-wise constant solution, using time-dependent creation uncertainty values from above
- Compare with full MC sampling over 11 (pre-determined) channels, 500 samples per channel with 3σ bounds

Example: Am242m in BWR MOX (II)



Example: Am242m in BWR MOX (III)

Remarks

- Destruction uncertainty for many produced nuclides is **greater** than the uncertainty in the production, driving the overall uncertainty
    - Most important where the cross-section and/or uncertainty of the product's reactions are larger than the creation values
- Sampling the uncertainties from each reaction channel requires:
    - Knowledge and specification of all reaction channels
    - Many samples and demonstration of convergence of variance
- Pathways + depletion does not require knowledge of all channels, but informs the user of them!
- Uncertainty may drop as a function of irradiation time since:
    - Equilibrium inventory given by simple ratio C/D, a limit of the piece-wise constant approximation
    - As a result the uncertainty before (pseudo-)equilibrium may be greater

Example calculation (I)

- We pause the presentation now to perform some calculations
- First, complete the `getting_started` example calculations for solver tolerance, pulsed calculations (with fission) and the reactor normalisation example
- Then, navigate to

  `fispact.ukaea.uk/wiki/Reference_input_spectra`

  and select the spectra, 1102_PWR-UO2-Gd-0 (and 15 and 45)
- Create an input file that includes:
  - UNCERTAINTY 2
  - PRINTLIB 2
  - POWER normalisation to 300 W/cc
- Check effect of SSFs, re-normalisation of power, dominants list and tolerances
- `Tst_586fis` shows how to re-collapse multiple spectra

Example calculation (II)

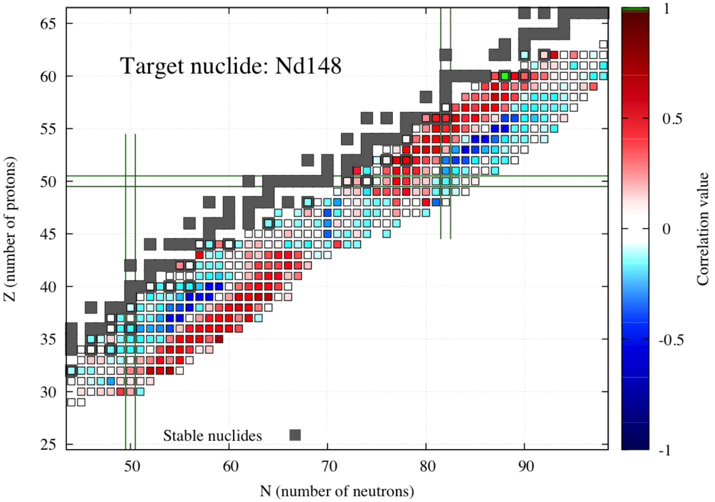
- Now check the `PRINTLIB` output and determine all of the reactions that *destroy* Pu239
- From the pathways analysis find all of the paths to Pu239 that include reactions
- Build a sensitivity-uncertainty calculation on these reactions using those reaction channels with `SENSITIVITY` and normal distributions of `MCSAMPLE`
    - Determine the number of samples required to converge your result
    - Compare with the depletion uncertainty and creation uncertainty values
    - Consider another minor actinide, activation product, etc. of interest to you

Fission yield uncertainties

- Fission yields are highly correlated
- Uncertainties from the standard ENDF-6 files have variances for each product, but no covariances - so uncertainty quantification cannot be done correctly
- Since FISPACT-II handles complete independent yields, technologically-generated GEF fission yields with parameter variation may be used for UQP
  - These are made with intelligently determined posterior distributions
  - System includes approximately 20 adjustable parameters so correlations are significant on a 1000+ nuclide system

Fission yield correlations

U5$_{th}$ Nd148 correlation *vector* from a matrix calculated by GEF



Nuclear Data Sheets 131 (2016) 107-221

http://www.khs-erzhausen.de/GEF.html

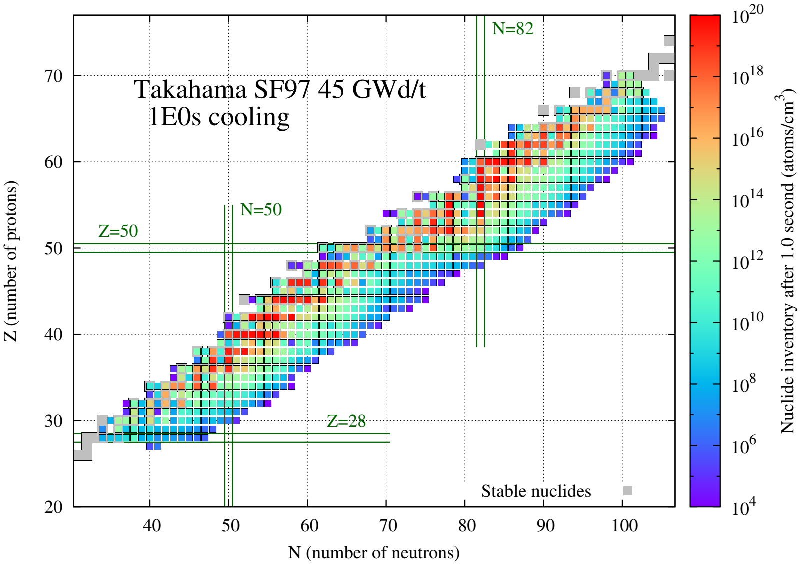
http://www.cenbg.in2p3.fr/-GEF,354-

FISPACT-II fission yield uncertainty

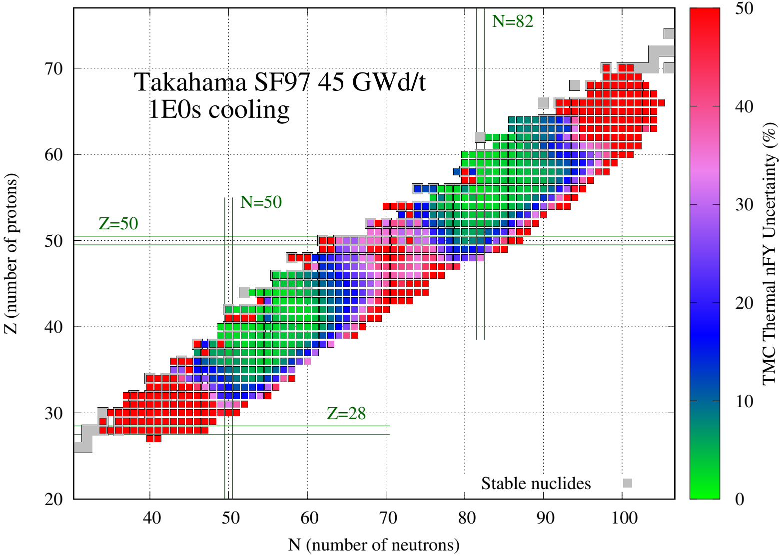
- FISPACT-II makes use of Bayesian Monte-Carlo fission yields generated by:
    - Input parameter variation of GEF
    - χ^2 calculation vs evaluated nuclear data files with their uncertainties
    - Weighting and updating to convergence
    - nb: values are highly sensitive to the evaluated file chosen!
- 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

Annals of Nuclear Energy 95 (2016) 125-134
Progress in Nuclear Energy 96 (2017) 76-96
Nuclear Data Sheets 139 (2017) 1-76

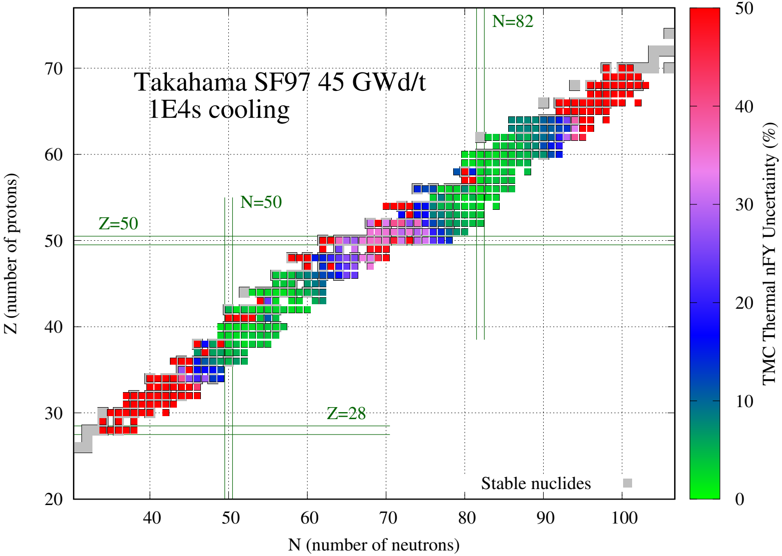
Example: Takahama-SF97 inventories



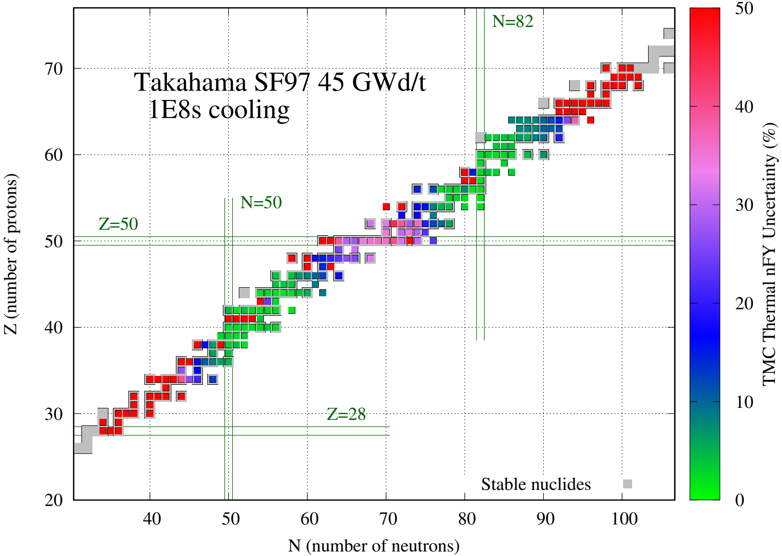
Example: Takahama-SF97 nFY uncertainties (1s)



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

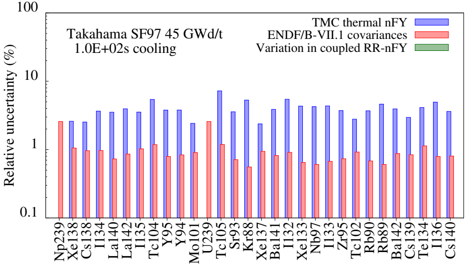


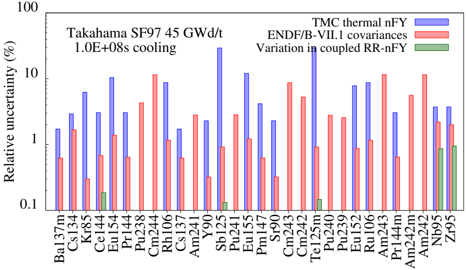
Example: Takahama-SF97 nFY uncertainties (10^8 s)



Addition of reaction uncertainties

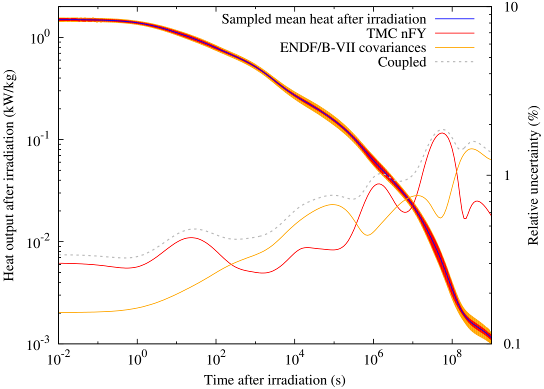
- Calculate the RR uncertainties in parallel
- The variations in fission yields will change the pathways-based uncertainties when two different fissioning nuclides produce similar quantities of the the same product
  - Seen in the variation of the PB-uncertainty
  - Longer cooling exposes these as the cumulative yields have more overlap





Integral Example: T-SF97 Decay Heat

- End of 45 GWd/t Takahama SF97 with UQP over all nuclides
- Incomplete MF=33 RRR data for some nuclides/channels
- Dominant nuclides have low uncertainty
  - Many nuclides still have large uncertainty, but do not affect integral quantities



Calculation with TMC/BMC random files

- Navigate to the random fission yield evaluations: `tendl.web.psi.ch/tendl_2015/randomYields.html`
- Select the Pu239 thermal fission yields (your choice which)
- Fill a folder of random evaluations and (with help) create a simple script (bash, python, etc.) to calculate with sampled fission yield files on the pulsed decay heat example. Suggestion:
  - 1. Perform only one collapse!
  - 2. Loop over condense and use an indexed folder for the fission yield
  - 3. Fission yield files must be named `U235` etc.
  - `grep ‘‘TOTAL BETA HEAT’’ grep ‘‘TOTAL GAMMA HEAT’’` are useful commands to parse outputs
  - Experimental results and uncertainties are provided in the `plot` folder of the `getting_started` example

```
#!/bin/bash
for ((i=0; i<100; i++)); do
mkdir -p sampled_nfy/${i}
mv /dir/with/nfy.${i} sampled_nfy/${i}/U235
cat>files<<EOF
fy_endf sampled_nfy/${i}
...
EOF
fispact condense
fispact inventory
mkdir -p outputs/${i}
mv inventory.out outputs/${i}/
done;
```