Fispact II - Uncertainties, Pathways and all things nice

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Introduction

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- Nuclear data represents a major contributor to uncertainties in nuclear simulations
- Wherever a nuclear data file is used to provide access to the fundamental underlying physics, only one thing can be assumed - that these numbers are not correct
- The importance of uncertainty values depends on the final application - criticality, transmutation or high energy / accelerator
- CCFE being a fusion lab, transmutation is the key driver of our own self interest, nuclear data uncertainty dominates and analyses over the 1000’s of reaction channels presents a significant challenge

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Introduction

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

Pathways

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- Pathways are a very useful feature of Fispact-II - often having completed your inventory analysis you may have asked yourself the following questions (or been asked by a well meaning colleague)
  - How much of X comes from Y?
  - What if we isotopically tailored X?
  - Have you considered the case where ….
- All of these questions can be answered with **`UNCERTAINTY {UNCE}`** keyword which will provide a pathways analysis

```
UNCERTAINTY 3
```


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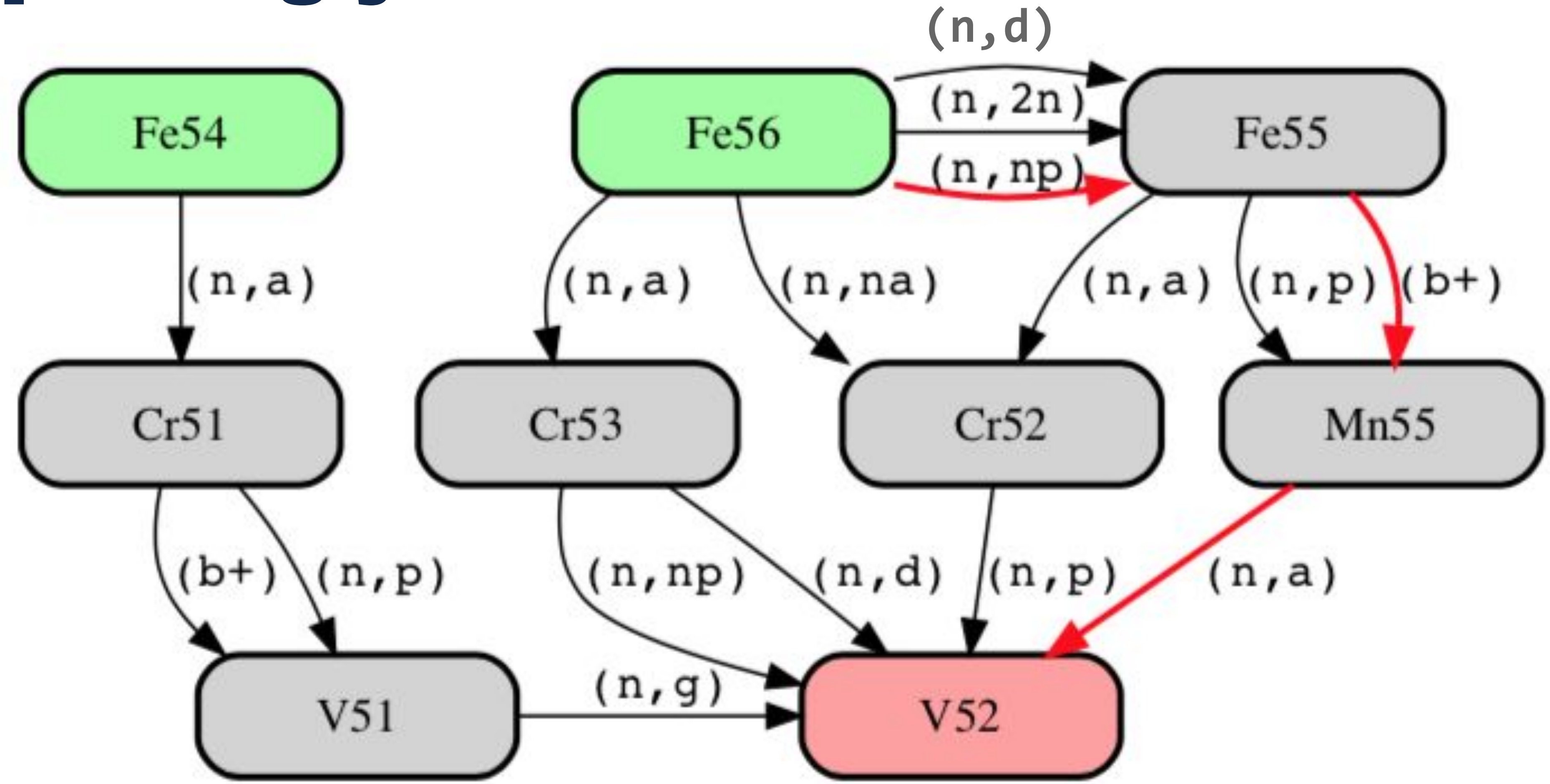
Pathways - Hmmm ^{52}V I wasnt expecting you

- Example, Irradation of Fe - where does all the ^{52}V come from

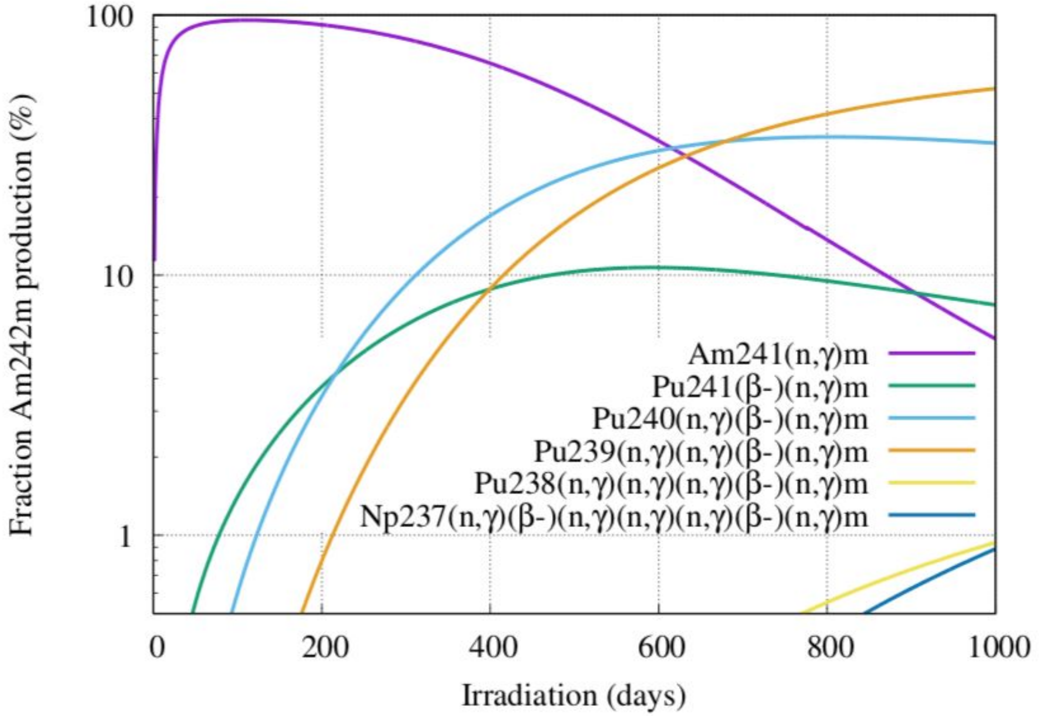
1. ^{54}Fe (n,α) ^{51}Cr (β+) ^{51}V (n,γ) ^{52}V (19.769%)
2. ^{54}Fe (n,α) ^{51}Cr (n,p) ^{51}V (n,γ) ^{52}V (0.416%)
3. ^{56}Fe (n,np) ^{55}Fe (β+) ^{55}Mn (n,α) ^{52}V (54.612%)
4. ^{56}Fe (n,d) ^{55}Fe (β+) ^{55}Mn (n,α) ^{52}V (5.947%)
5. ^{56}Fe (n,2n) ^{55}Fe (β+) ^{55}Mn (n,α) ^{52}V (5.817%)
6. ^{56}Fe (n,2n) ^{55}Fe (n,p) ^{55}Mn (n,α) ^{52}V (0.027%)
7. ^{56}Fe (n,α) ^{53}Cr (n,np) ^{52}V (2.766%)
8. ^{56}Fe (n,α) ^{53}Cr (n,d) ^{52}V (2.978%)
9. ^{56}Fe (n,nα) ^{52}Cr (n,p) ^{52}V (3.663%)
10. ^{56}Fe (n,2n) ^{55}Fe (n,α) ^{52}Cr (n,p) ^{52}V (3.056%)

Pathways - Hmmm ^{52}V I wasnt expecting you



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)
```

FISPACT-II Pathway Uncertainties

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TENDL-2015 contains upto 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:

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

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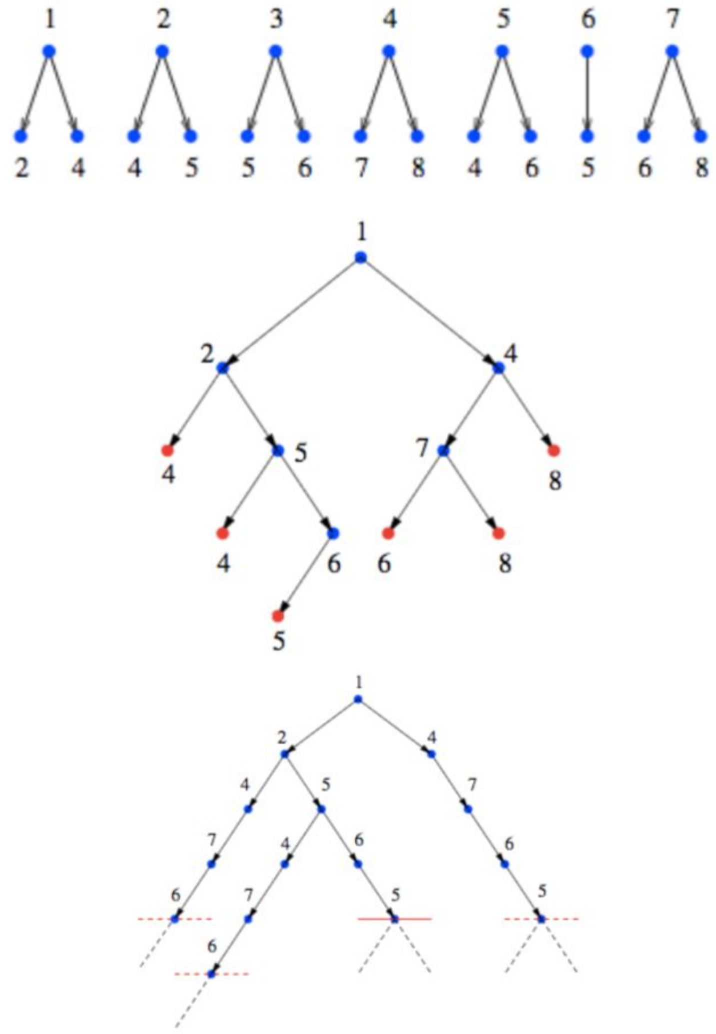
FISPACT-II Pathway Uncertainties

- 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



FISPACT-II Pathway Uncertainties

`UNCERTAINTY` iuncer {2} <path_floor {0.005} loop_floor {0.01} max_depth {10} iuncer >

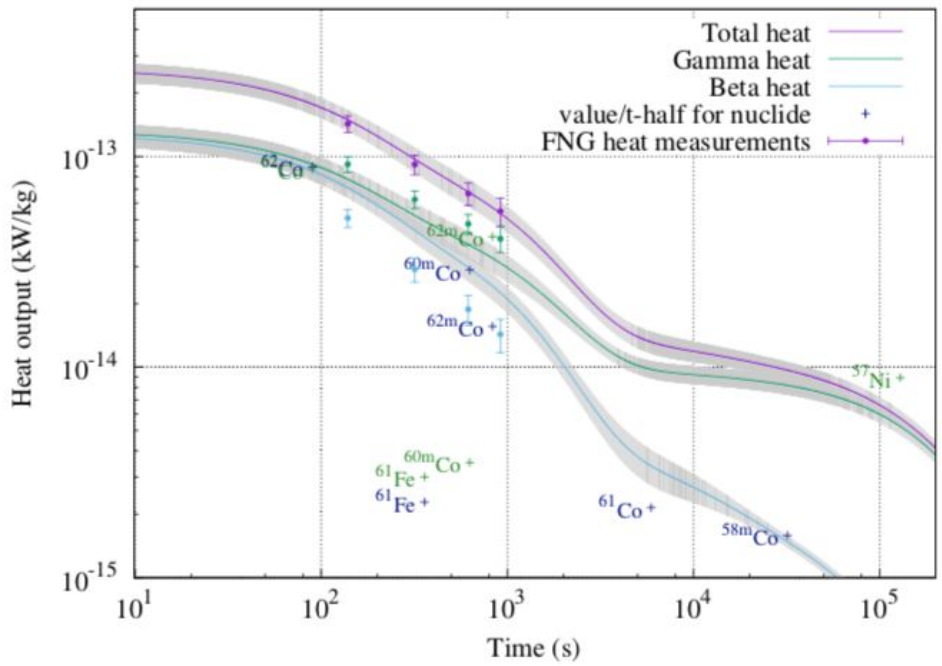
- Typically users take default parameters
- Standard use: UNCERTAINTY 2
  - path floor, can be lowered to take more contributions (below X%), loop floor for loops, max depth for length of chains
- In very complex, long irradiations paths greater than 10 in length can matter!
- NOTE: The inventory and pathways calculations are separately performed, with more strict TOLERANCE settings on the former - if you extend the UNCERTAINTY limits also revisit the TOLERANCE settings

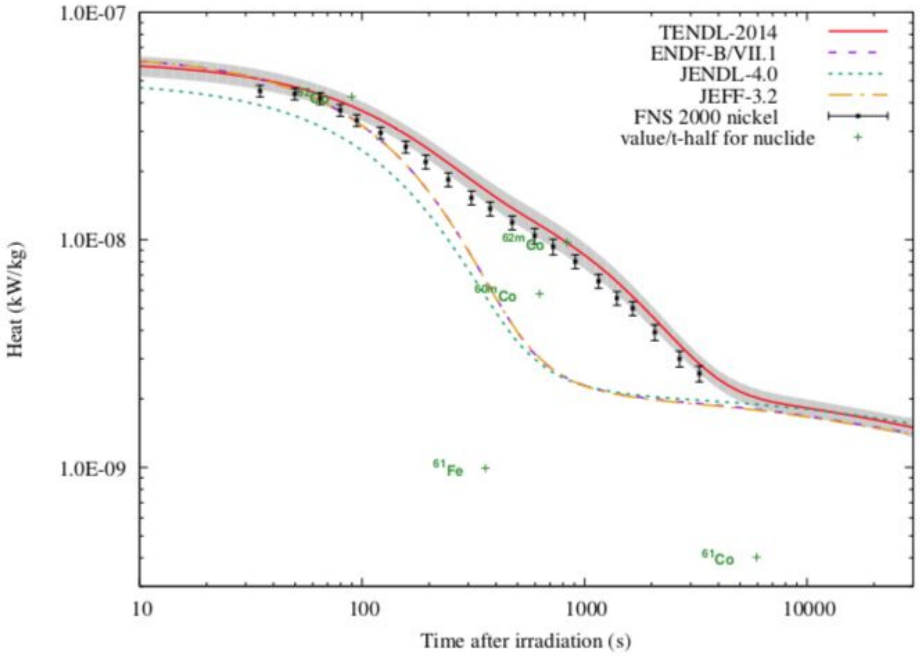
FISPACT-II Pathway Uncertainties

- 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 Pathway Uncertainties

- 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





Sensitivity-uncertainty analysis

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- 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. :

SIGMA/LAMBDA

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

Correlations

In this case, the sensitivity of the Sc48 inventory to the Ti48(n,p)Sc48 and Ti49(n,np+d)Sc48 reactions are used for Monte-Carlo sampling. 100 samples of each is used with a normal distribution between -2 and +2 standard deviations.

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Uncertainty Quantification

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- Given {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

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Uncertainty Quantification

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- 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

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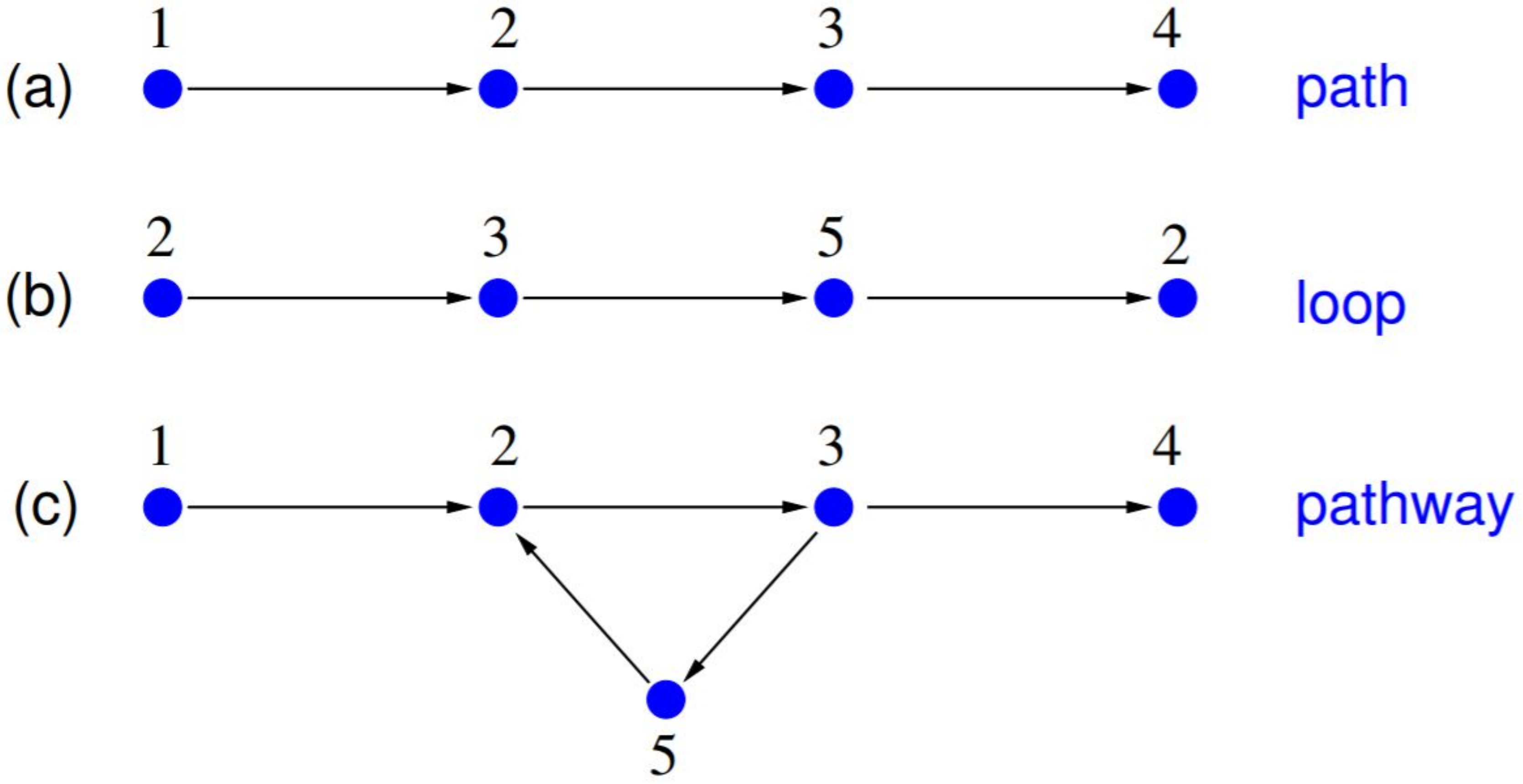
Uncertainty Quantification

- 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

<u>`UNCERTAINTY`</u> iuncer {2} <path_floor {0.005} loop_floor {0.01} max_depth {10}

iuncer >

Uncertainty Quantification



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

Uncertainty Quantification

```
                                   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)
```

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- The code uses the library data to compute collapsed covariance. Covariances are mapped by assuming that all isomeric daughters of a given pair of reactions have the same collapsed correlation function
  - 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 maybe 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.

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Uncertainty Quantification

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

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Uncertainty Quantification

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- 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`**

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Uncertainty Quantification

```
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

Questions

Are there any questions?