ANDES
NNL Progress
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Plan of talk

- Background/Goal
- Traditional justification of results and estimate of error
- "Total Monte Carlo approach" for decay heat pulse calculations using fission yield uncertainties
- Fission yield evaluation and uncertainties
- How to calculate fission product covariance
  - Radioactive decay data based branching summation Q matrix
  - Calculation of uncertainties and thus covariance terms
  - Extension to general case
- Future work

Background

- Spent fuel inventory / Activation calculations are used in a wide range of operational planning and safety cases

e.g. Reactor operation
Spent fuel storage and transport
Reprocessing/Recycling of actinides
Geological disposal, etc.

Depending on the case important parameters can be individual nuclide concentrations or integral parameters; e.g. decay heat, delayed neutron emission, radiative emission (neutron, photon, electron etc.). A knowledge of their uncertainties help determine safety margins and operating envelopes.

Goal

“To be able to produce inventory calculation results that will supply uncertainty information useful to engineering applications associated with design or operations”

Inventory calculations

Spent fuel compositions are calculated using the standard equations:

$$\frac{dN_i}{dt} = -\lambda_i N_i + \sum_j \lambda_j N_j B_{j,i}$$

$$+ \sum_k N_k \sigma_{f,k} \phi Y_{k,i} - \sum_l N_i \sigma_{i,l} \phi + \sum_m N_m \sigma_{m,i} \phi$$

Decay Heat, for example, can be calculated from the activities and energy release per decay of the radionuclides present in spent fuel.

$$\boxed{H = \sum Ni\ \lambda i\ Ei}$$

Historic Method 1- Justification of results

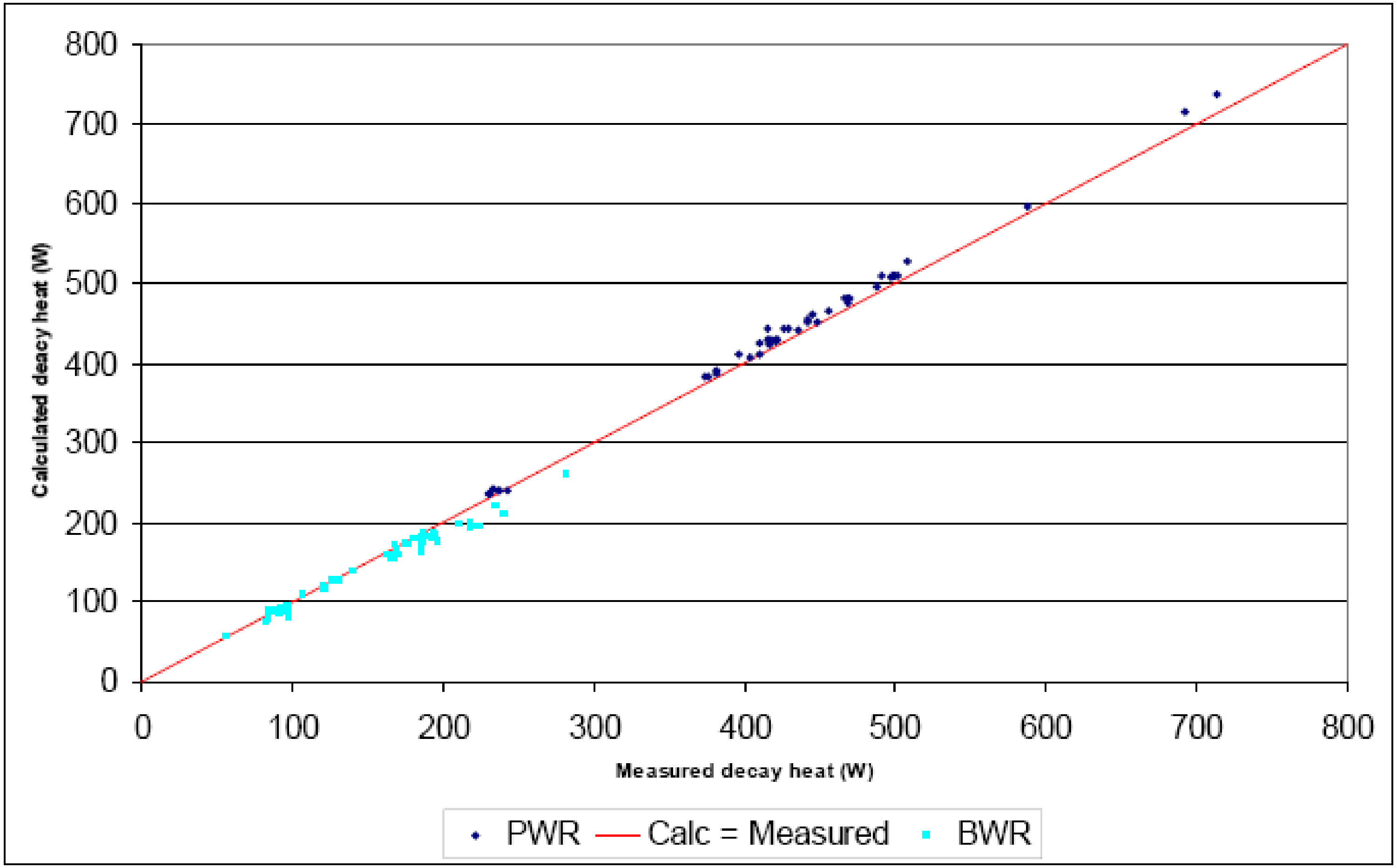
- Calculate with “best” nuclear data and then compare with post-irradiation examination analyses or other measurements

  e.g. ARIANE, SFCOMPO, SKB etc.

… but …

- Limited number of samples analyses
- Limited number of radionuclides measured
- Limited range of fuel parameters:
  - Enrichment
  - Irradiation/Burn-up
  - Cooling times

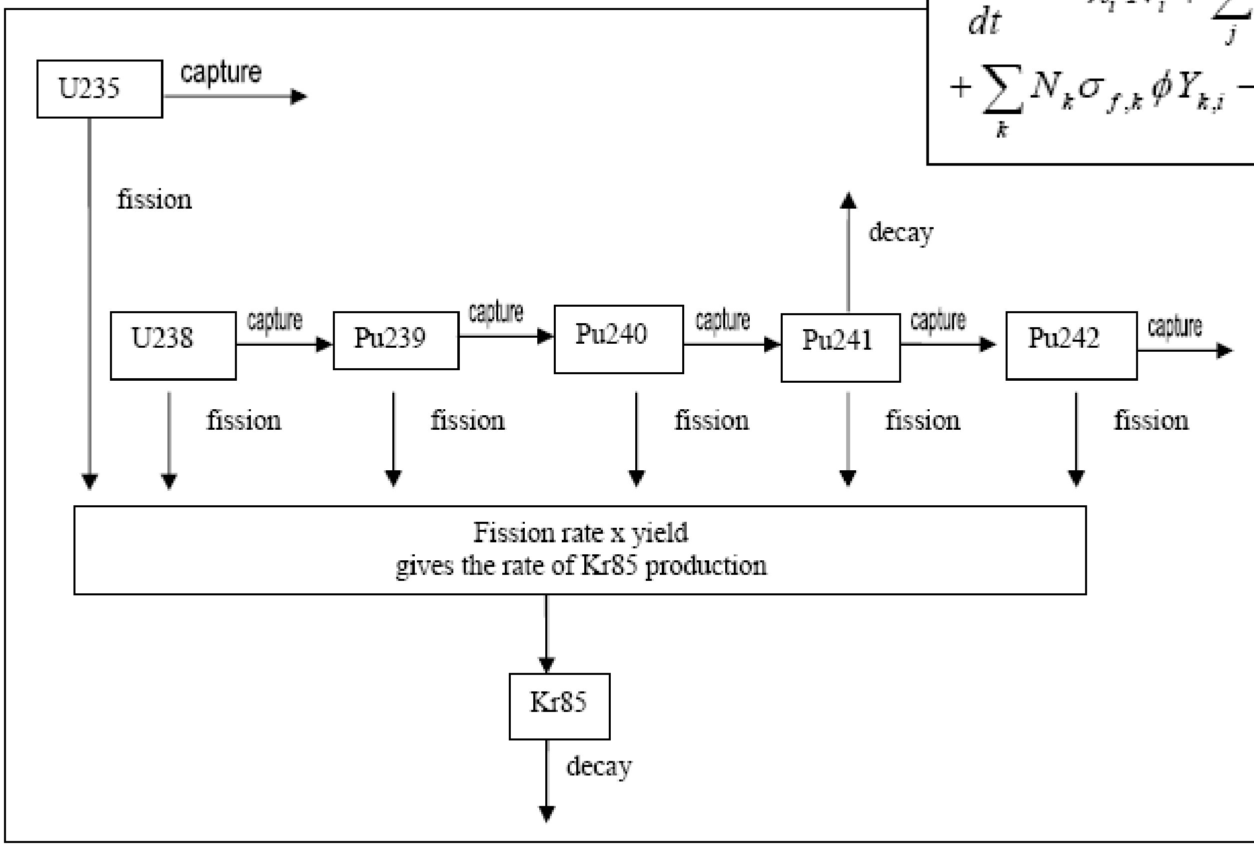
Decay Heat Calculated against Experimental



Historic Method 2- Simply case and propagate uncertainty

- **Reaction and decay paths considered in SIMFIS**

$$\frac{dN_i}{dt} = -\lambda_i N_i + \sum_j \lambda_j N_j B_{j,i} + \sum_k N_k \sigma_{f,k} \phi Y_{k,i} - \sum_l N_i \sigma_{i,l} \phi + \sum_m N_m \sigma_{m,i} \phi$$

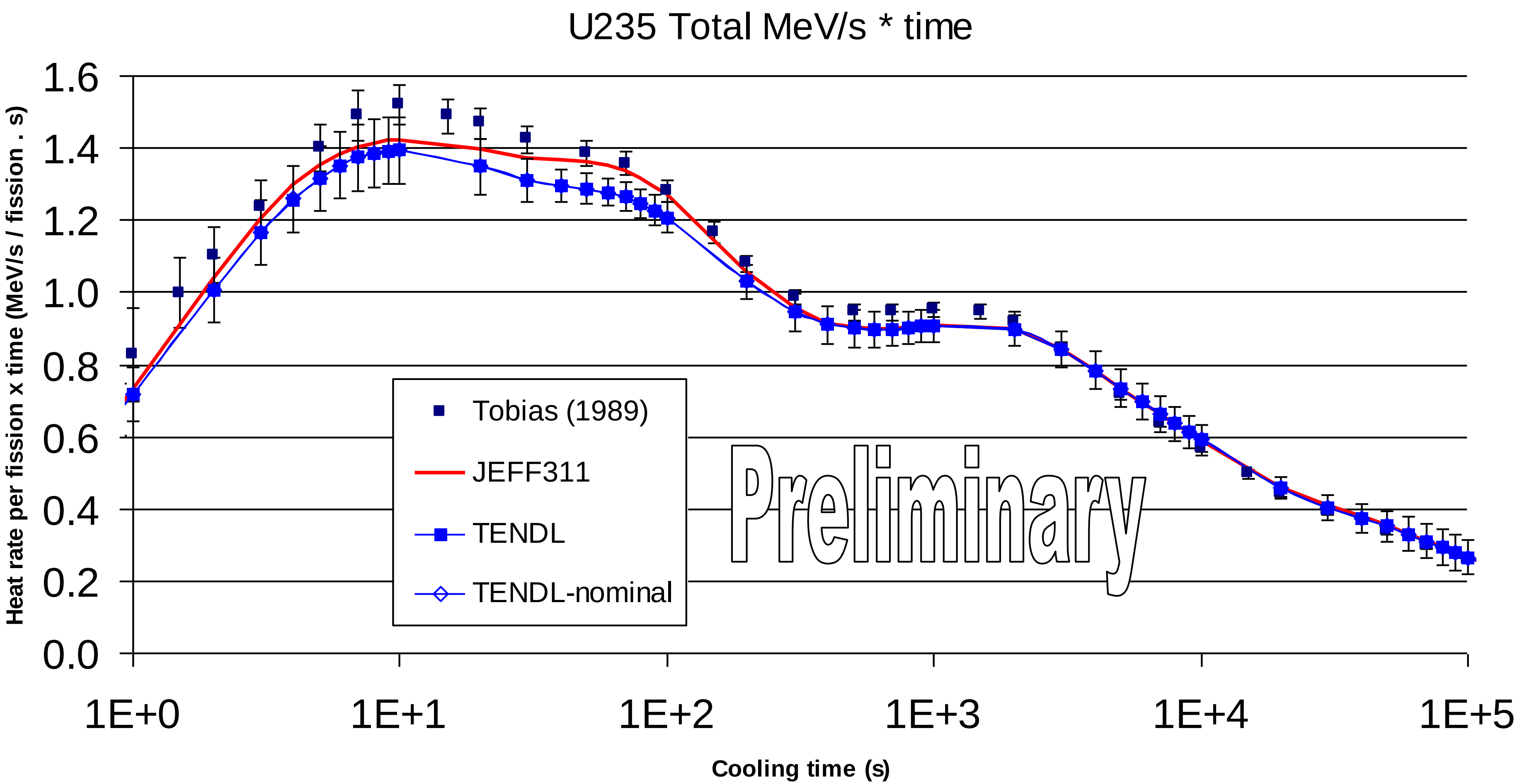


Problems of these methods

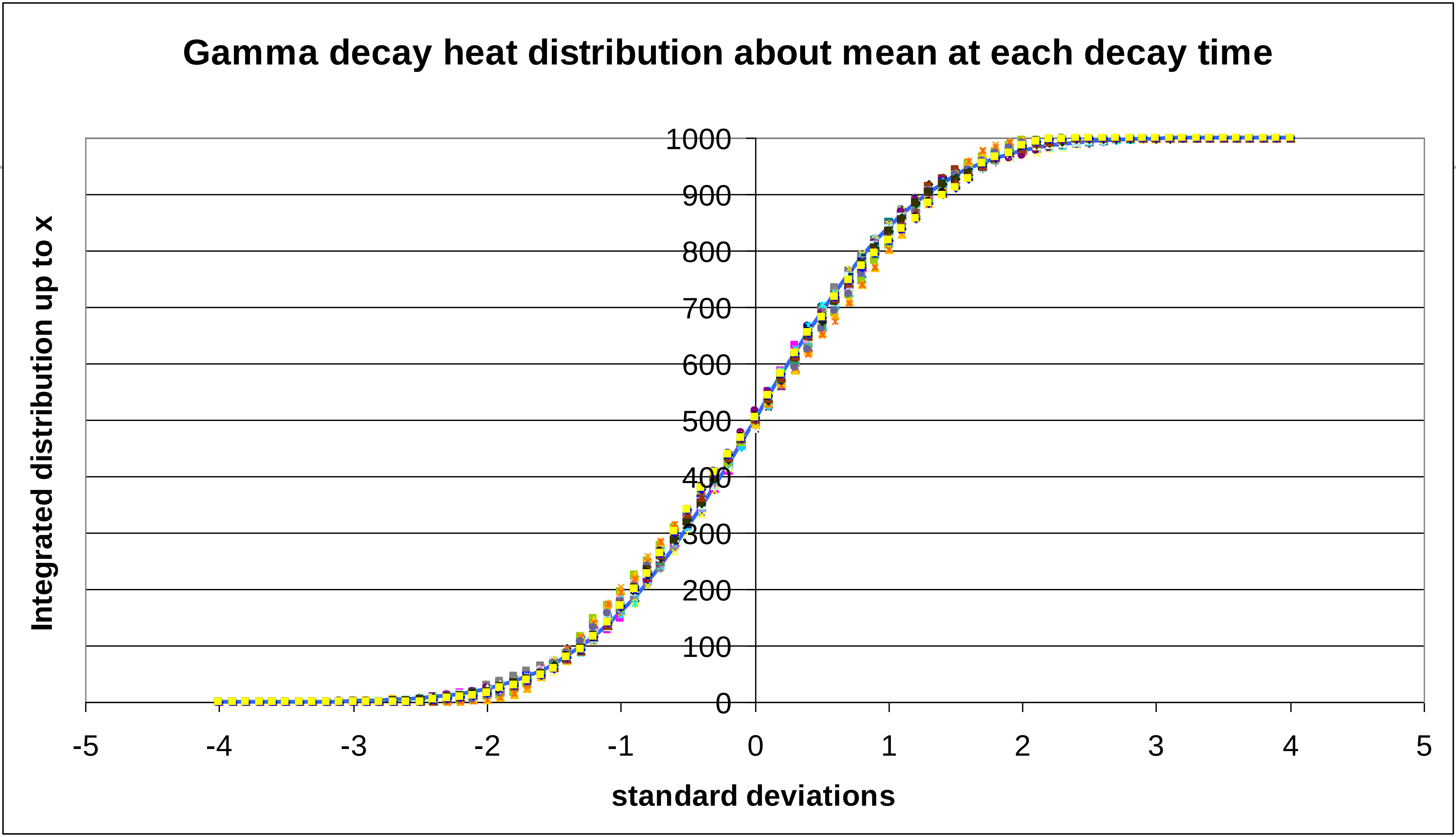
- The first method is highly dependent upon a few measurements for a few enrichments, burn-ups and cooling times. Second method is very simplistic.
- Ideally would want to propagate all initial uncertainties to all resultant parameters in a way to include physical constraints in process and data covariance so that these can be used to justify safety cases and new reactor/fuel cycle designs with less benchmarking.
- Nuclear data uncertainties
  - Cross-sections, decay data, fission yields.
- Input parameters uncertainties
  - Irradiation time, Power, Cooling time etc.

New method 1- Variance perturbation approach

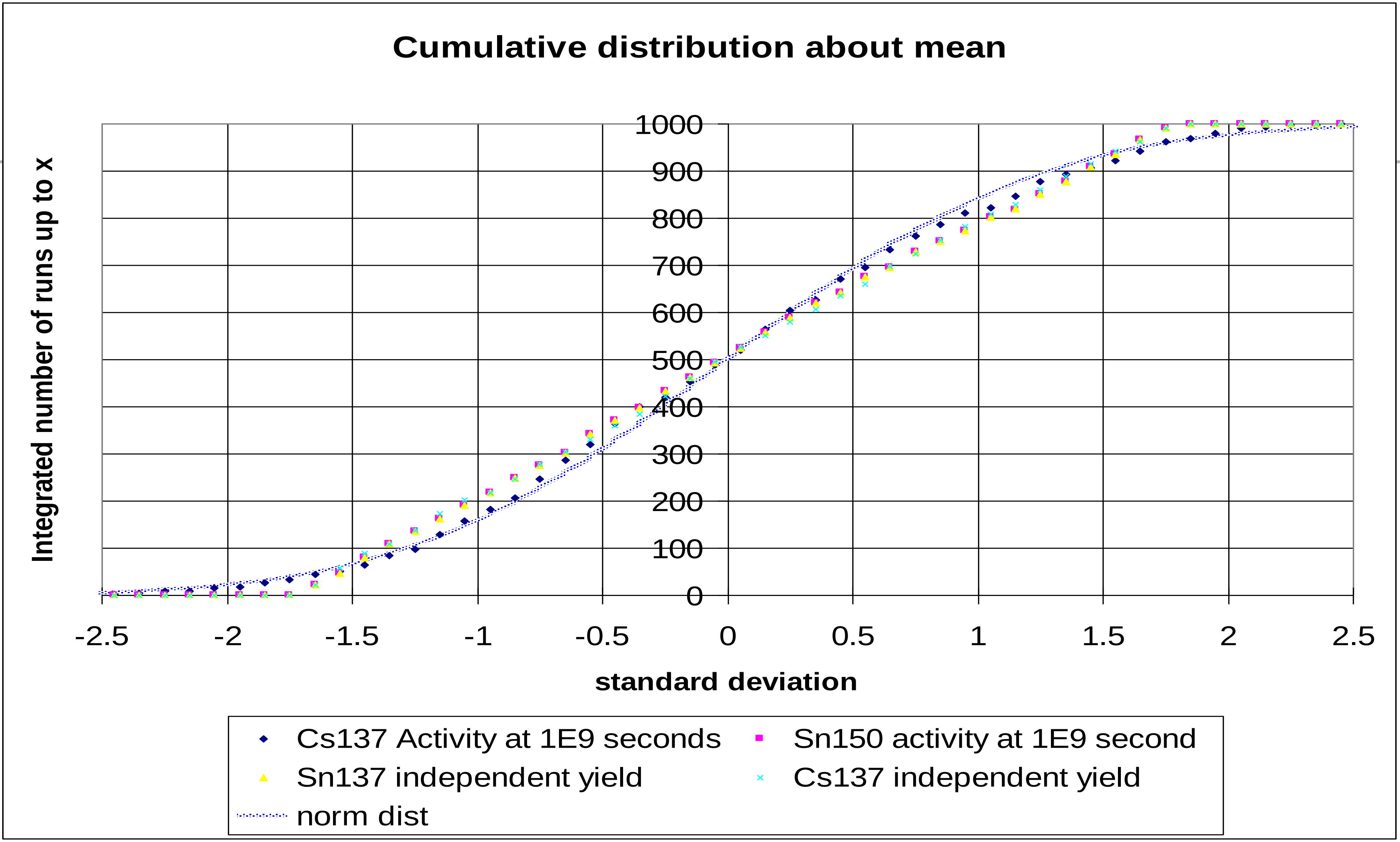
- An alternative to simple error propagation, is to run repeated inventory calculations with data values perturbed by their respective uncertainty. Then average the results and calculate standard deviation from distribution of results. (see Rochman et al, 2010 etc.)
  USES EXISTING CODES within perturbation framework
- FISPIN can read ENDF formatted radioactive decay and fission yield files for fission product calculations directly enabling fission pulse calculations to be modelled without considering heavy element and activation product decay data or cross-sections.
- The following shows TENDL nominal and perturbed library based results for U235 for 1000 perturbed files (square PDF).



U235 Total MeV/s * time
Heat rate per fission x time (MeV/s / fission . s)
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
1E+0
1E+1
1E+2
1E+3
1E+4
1E+5
Cooling time (s)
Tobias (1989)
JEFF311
TENDL
TENDL-nominal
Preliminary

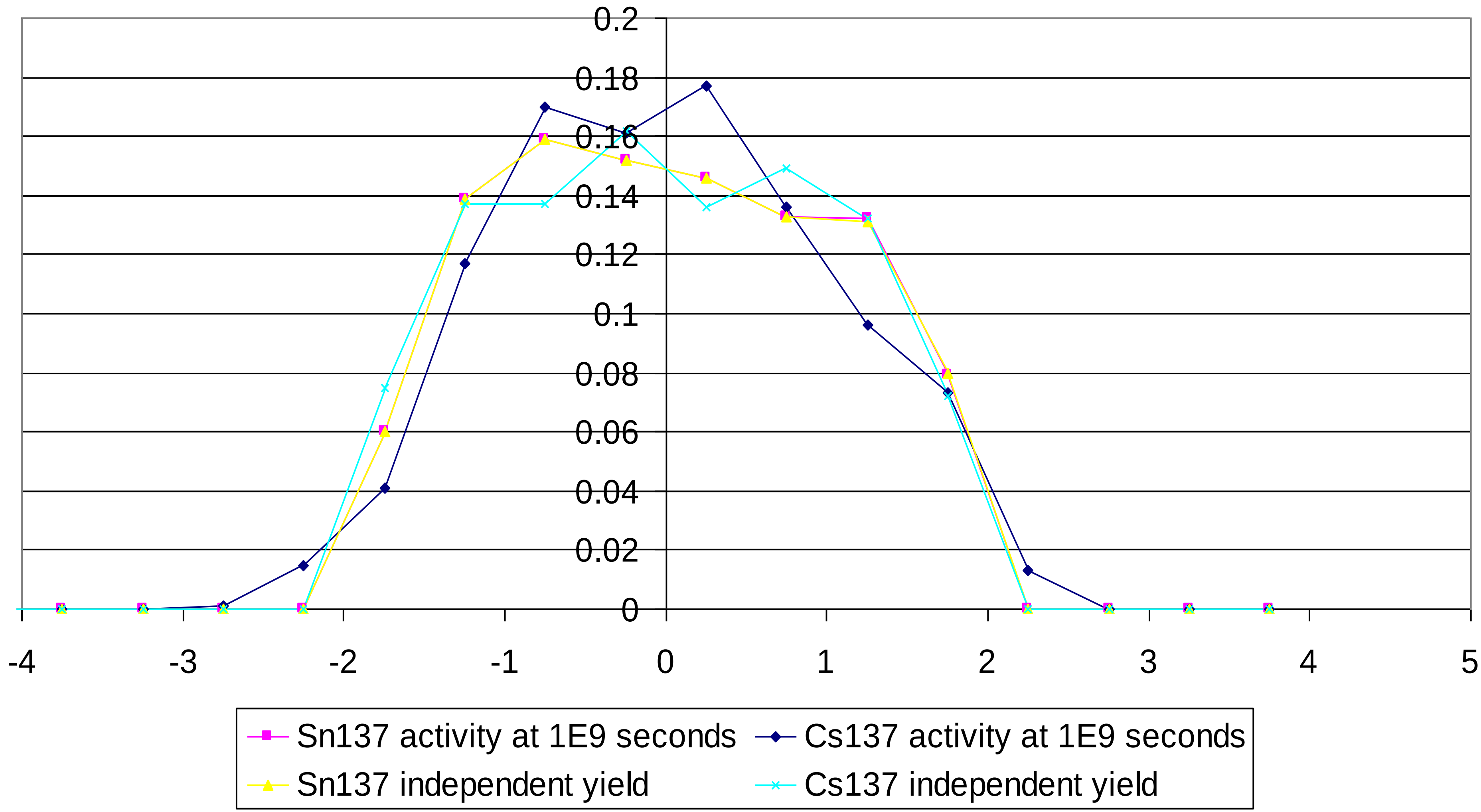


Blue line is integrated normal distibution



Blue line is integrated normal distibution

distribution about mean



Experimental/Evaluation co-variances

- The above method deals with error propagation not with the correlated uncertainties within the evaluated data.
- The JEFF-3.1.1 fission yields are based upon a database of >2000 papers, reports etc.
- 14710 measurements were analyzed to give “best estimates” of each measured yield and their uncertainties. MANY RELATIVE MEASUREMENTS.
- Most of these were cumulative yield measurement with few independent yield measurements.

New method 2- Error propagation using co-variance

- Sensitivity matrix approximation
- Used in ACAB (UPM)
- However needs covariance terms for nuclear data
  - Limited cross-section data covariance
  - None existing for decay data and fission yields

Note

- Much quicker that running 1000's of cases
- No issues with choosing PDF e.g. for values 0.05 ± 0.03
- Code needs to be changed to use new methods.

Fission Yield Definitions

The **independent yield** y(A,Z,I) is the number of atoms of (A,Z,I) produced directly from one fission, but after the emission of prompt neutrons (but before any radioactive decay and hence the emission of delayed neutrons). It can be written as the product of 3 factors:

$$y(A, Z, I) = Y(A) \times f(A, Z) \times R(A, Z, I)$$

where the **sum yield** or **mass yield** Y(A) is the total of the independent yields (before delayed neutron emission) of all fission products of mass number A; f(A,Z) is the **fractional independent yield** of all isomers of (A,Z); and R(A,Z,I), the **isomeric yield ratio**, is the fraction of (A,Z) produced directly as isomer I.

Fission Yield Definitions

The **cumulative yield** c(A,Z,I) of nuclide (A,Z,I) is the total number of atoms of that nuclide produced over all time after one fission. If the nuclide is stable the cumulative yield is the total number of atoms of that nuclide remaining per fission after all precursor decays (ignoring the effects of other nuclear reactions e.g. neutron capture). However, for a radioactive nuclide for which this is not the case, some atoms will have decayed before all have been produced.

An equivalent definition that is more useful is the following: immediately at the end of an "infinite" irradiation at the rate of 1 fission per second, c(A,Z,I) is the rate of decay of (A,Z,I) if that nuclide is radioactive, or its rate of production if it is stable.

The **chain yield** Ch(A) is equal to the sum of all stable or long-lived cumulative yields for a given mass chain. It should be noted that the chain yield, Ch(A), and the sum or mass yield, Y(A), for a mass chain A may differ by a few per cent because the former applies after, and the latter before, delayed neutron emission.

Fission Yield Evaluation

- For inventory calculations want independent yields – hard to measure, few measurements reported, many discrepancies and only approximate empirical models => large uncertainties
- Have large database of cumulative yields, more easily measured, can be fitted to good empirical models and can more easily identify discrepant data => small uncertainties
- Cumulative yields can be calculated from independent yields based upon decay branching
- In JEFF-3.1.1 both datasets combined to give self-consistent data including physical constraints.

Cumulative yields

- The cumulative yield can be calculated from the independent yields and the decay data branching fractions

$$c_i = y_i + \sum_j b_{j \to i} c_j$$

or in matrix form

$$c = y + \bar{b}c$$

which can be rearranged to give

$$c = Qy \text{ where } Q = (1 - \bar{b})^{-1}$$

ENDSF plot for mass chain 85

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Mass chain 85

- **Q matrix for mass chain (including part of mass 86)**

	TC 85	MO 85	NB 85	NB 85	ZR 85M	ZR 85	Y 85M	Y 85	SR 85M	SR 85	GA 85	GE 85	AS 85	GA 86	GE 86	AS 86	SE 85	BR 85	KR 85M	KR 85	RB 85
TC 85	1.00	0.50	0.50		0.50	0.46		0.50	0.50	0.43											0.50
MO 85		1.00	1.00		1.00	0.92		1.00	1.00	0.87											1.00
NB 85M			1.00		1.00	0.92		1.00	1.00	0.87											1.00
NB 85				1.00		1.00		1.00	1.00	0.87											1.00
ZR 85M					1.00	0.92		1.00	1.00	0.87											1.00
ZR 85						1.00		1.00	1.00	0.87											1.00
Y 85M							1.00	0.00	0.11	0.99											1.00
Y 85								1.00	1.00	0.87											1.00
SR 85M									1.00	0.87											1.00
SR 85										1.00											1.00
GA 85											1.00	1.00	0.86				0.67	0.67	0.67	0.14	0.67
GE 85												1.00	0.86				0.67	0.67	0.67	0.14	0.67
AS 85													1.00				0.78	0.78	0.78	0.17	0.78
GA 86														1.00	1.00	1.00	0.33	0.33	0.33	0.07	0.33
GE 86															1.00	1.00	0.33	0.33	0.33	0.07	0.33
AS 86																1.00	0.33	0.33	0.33	0.07	0.33
SE 85																	1.00	1.00	1.00	0.22	1.00
BR 85																		1.00	1.00	0.22	1.00
KR 85M																			1.00	0.21	1.00
KR 85																				1.00	1.00
RB 85																					1.00

Mass chain 85

- **Q matrix subset for fission products in JEFF-3.1.1**

	GA 85	GE 85	AS 85	GA 86	GE 86	AS 86	SE 85	BR 85	KR 85M	KR 85	RB 85
GA 85	1.00	1.00	0.86				0.67	0.67	0.67	0.14	0.67
GE 85		1.00	0.86				0.67	0.67	0.67	0.14	0.67
AS 85			1.00				0.78	0.78	0.78	0.17	0.78
GA 86				1.00	1.00	1.00	0.33	0.33	0.33	0.07	0.33
GE 86					1.00	1.00	0.33	0.33	0.33	0.07	0.33
AS 86						1.00	0.33	0.33	0.33	0.07	0.33
SE 85							1.00	1.00	1.00	0.22	1.00
BR 85								1.00	1.00	0.22	1.00
KR 85M									1.00	0.21	1.00
KR 85										1.00	1.00
RB 85											1.00

Mass chain 85

- **JEFF-3.1.1 yields for U235 thermal fission**

Nuclide	Independent yld	uncertainty	%	Cumulative yld	uncertainty	%
SR 85	1.1013E-12	4.1127E-13	37.34	1.3218E-12	4.1961E-13	31.75
GA 85	8.0472E-09	3.0052E-09	37.34	8.0472E-09	3.0061E-09	37.36
GE 85	0.000024374	9.0771E-06	37.24	0.000024382	9.0631E-06	37.17
AS 85	0.0014083	0.00046884	33.29	0.0014293	0.0004186	29.29
GA 86	1.8249E-10	6.654E-11	36.46	1.8249E-10	6.6565E-11	36.48
GE 86	2.8497E-06	1.0388E-06	36.45	2.8499E-06	0.000001039	36.46
AS 86	0.00044233	0.00015891	35.93	0.00044518	0.00015537	34.90
SE 85	0.009583	0.00094717	9.88	0.010845	0.00020989	1.94
BR 85	0.002192	0.00071417	32.58	0.013037	0.00011935	0.92
KR 85M	0.000011222	4.1776E-06	37.23	0.013027	0.00011943	0.92
KR 85	0.000048531	0.000018067	37.23	0.0028575	0.00021036	7.36
RB 85	3.2958E-08	1.2308E-08	37.34	0.013097	0.00011861	0.91

Mass chain 85

- **Statistics**

Weighted sum of variables

The scaling property and the Bienaymé formula, along with this property from the covariance page: Cov(*aX*, *bY*) = *ab* Cov(*X*, *Y*) jointly imply that

$$\mathrm{Var}(aX+bY)=a^2\,\mathrm{Var}(X)+b^2\,\mathrm{Var}(Y)+2ab\,\mathrm{Cov}(X,Y).$$

This implies that in a weighted sum of variables, the variable with the largest weight will have a disproportionally large weight in the variance of the total. For example, if *X* and *Y* are uncorrelated and the weight of *X* is two times the weight of *Y*, then the weight of the variance of *X* will be four times the weight of the variance of *Y*.

The expression above can be extended to a weighted sum of multiple variables:

$$\mathrm{Var}\left(\sum_i a_i X_i\right)=\sum_i a_i^2\,\mathrm{Var}(X_i)+2\sum_i\sum_{j>i}a_i a_j\,\mathrm{Cov}(X_i,X_j)$$

$$\boxed{\text{cf. } C_j = \textstyle\sum_i Q_{i,j}\, I_i}$$

- Wikipedia – "variance" section 5.4 (2011)

Mass chain 85

- **Calculation of uncertainties**

	GA 85	GE 85	AS 85	GA 86	GE 86	AS 86	SE 85	BR 85	KR 85M	KR 85	RB 85
calc cum	8.05E-09	2.44E-05	0.001429	1.82E-10	2.85E-06	0.000445	0.010845	0.013037	0.013027	0.002857	0.013097
cum in file	8.05E-09	2.44E-05	0.001429	1.82E-10	2.85E-06	0.000445	0.010845	0.013037	0.013027	0.002858	0.013097
ratio	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
cum sd in file	3.01E-09	9.06E-06	0.000419	6.66E-11	1.04E-06	0.000155	0.00021	0.000119	0.000119	0.00021	0.000119
cum 1 sd	3.01E-09	9.08E-06	0.000469	6.65E-11	1.04E-06	0.000159	0.001017	0.001242	0.00124	0.000268	0.001243
ratio	1.00	1.00	1.12	1.00	1.00	1.02	4.84	10.41	10.39	1.27	10.48
%error in file	37.35585	37.17127	29.28706	36.47597	36.45742	34.90049	1.935362	0.915471	0.916788	7.36168	0.905627
%error from calc	37.34467	37.2287	32.80662	36.46227	36.4504	35.69644	9.374701	9.530208	9.522069	9.381771	9.487607
Difference	-0.01	0.06	3.52	-0.01	-0.01	0.80	7.44	8.61	8.61	2.02	8.58

- Given the above the covariance terms can be calculated

How the covariance could be used

- Given the independent yields and their uncertainties, the Q matrix and the covariance terms the cumulative yields can be calculated.
- Now if we had an inventory calculation in which the fission product number densities are available, the total production from fission of each direct fission product and the fraction of that which currently exists as a specific nuclide (cf. Q matrix) then we can generalize the above to calculate the uncertainty of the fission product including the covariance term.
- PARTIAL SOLUTION- cross-sections, half lives?

Future work (1)

- Milestone 2.4. New computational method for the use of covariance information of reaction, decay and fission yield data in an inventory calculation (**31 April 2012**)
  - Delayed, expect by end of June.
- Developing a code called GRENDL to perturb fission yield and radioactive decay data in ENDF files using different PDFs

NB yields with large errors, must still be +ve
ie. $0<Y<1.0$, what to do with 0.05 +/- 0.05 !

Testing a solution whilst keeping mean and SD same.

Future work (2)

- Need to extend code to include Q matrix calculation (from existing MkQ code) and calculate covariance matrix terms from independent and cumulative yields sets (as above).
- Need to develop perturbation for other data types and input operational parameters within a FISPIN "harness" to allow uncertainties on all FISPIN output values.
- D2.5. Report with transmutation calculations for advanced reactors (M36)
- Propose to release GRENDL via NEA DataBank

Acknowledgements

THANK YOU FOR YOUR ATTENTION

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