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Chapter 5: Applications
Fission simulations

Using fission in FISPACT-II

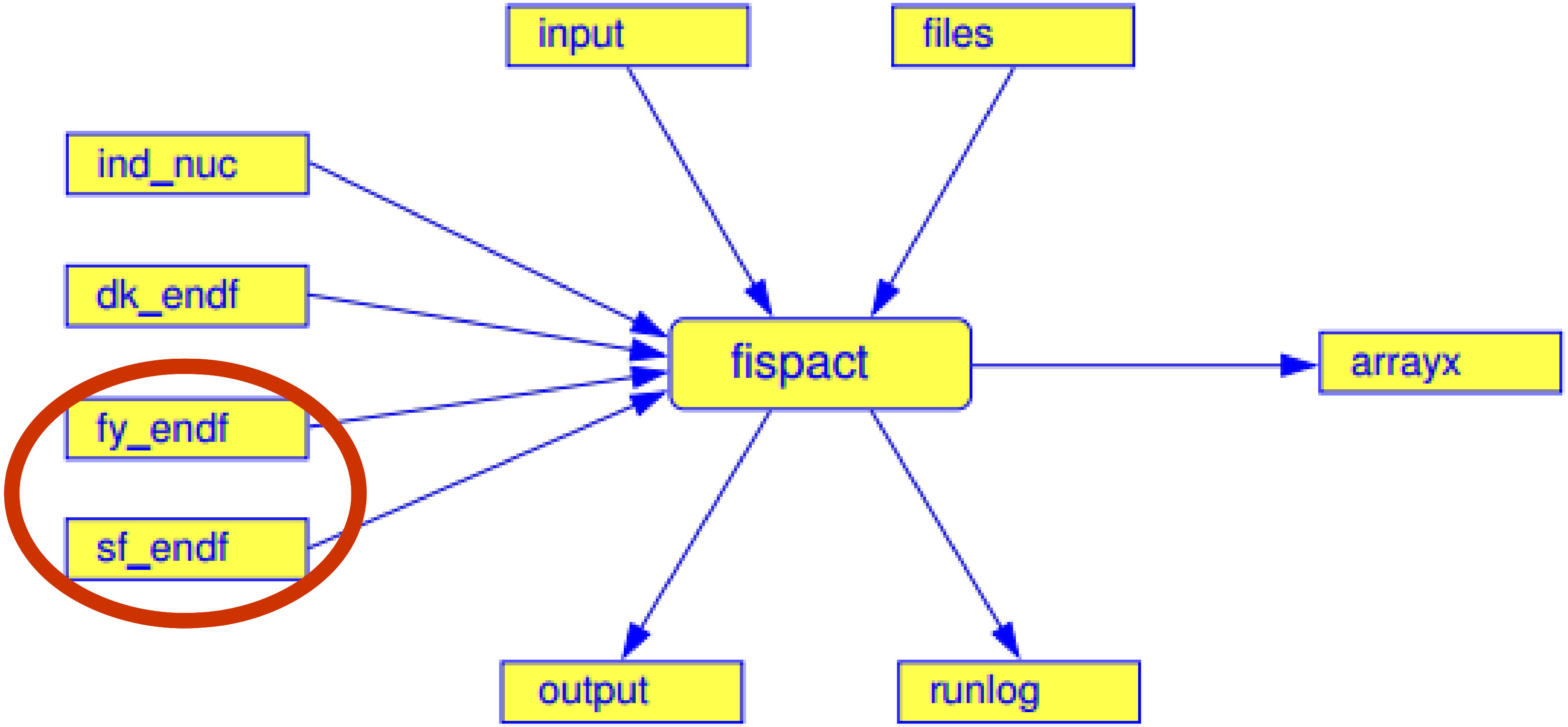
- FISPACT-II is distributed with a variety of fission yields and decay data, just as incident particle cross sections, etc.

- Fission is **by default turned off** and must be included with the following keywords:
  - `USFISSION` – turns on fission
  - `FISYIELD` – selects the fission yield files to read
  - `FISCHOOSE` – turns on fission for the given nuclides

- The default fission yields are read from mt=454, the independent fission yields. To use the cumulative mt=459 add the keyword: `CUMFYLD`

Fission within FISPACT-II

- Fission (*fy_endf* and *sf_endf*) are handled within the ARRAYX processing process with decay
- Note that (n,f) reactions will populate without the full ARRAYX data, but not produce the yields



Fission yields for simulation

- The standard modern fission yields are all distributed with FISPACT-II, including ENDF/B, JEFF, JENDL
  - These have at most three incident energies: thermal (0.0253 eV), fast (~400-500 keV) and 14 MeV
  - Fission yields are very sensitive to incident energy, particularly at higher energies – also note multi-chance
  - For thermal reactors, this may be fine, but not for many others
- Simulation of fission yields has become much more sophisticated in past 10 years, particularly with codes such as GEF and FREYA

GEF

- The GEF code has been developed (and much of the physics within it!) by several physicists
- We cite those below (and their collaborators), from which we take the following material
- It is a fast, freely available code with surprisingly complex capabilities

Karl-Heinz Schmidt,
Beatriz Jurado,
Christelle Schmitt

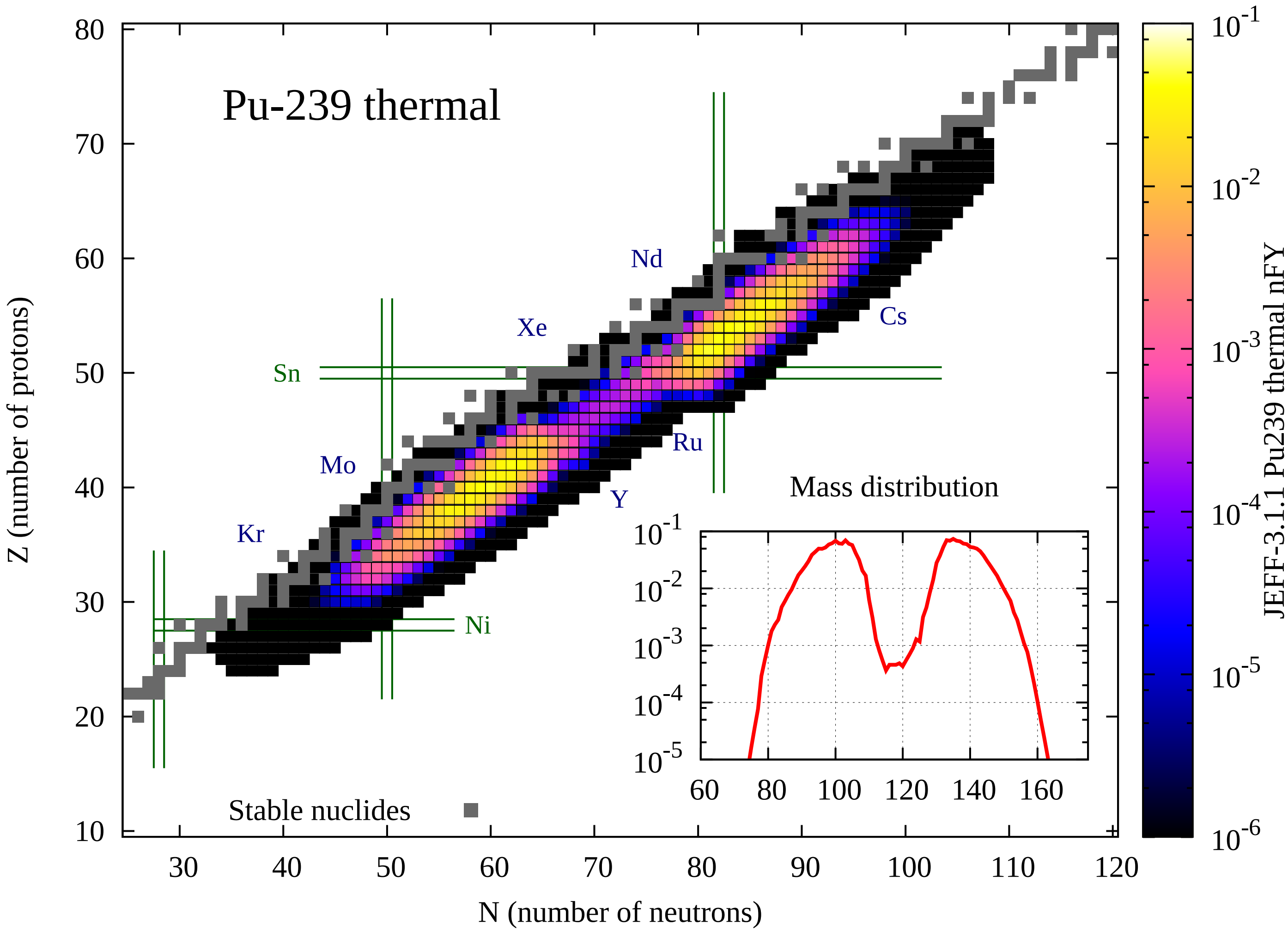
Nucl. Data Sheets 131 (2016) 107

There is also considerable added theory in the model! And the semi-empirical parameters are fit to experimental data

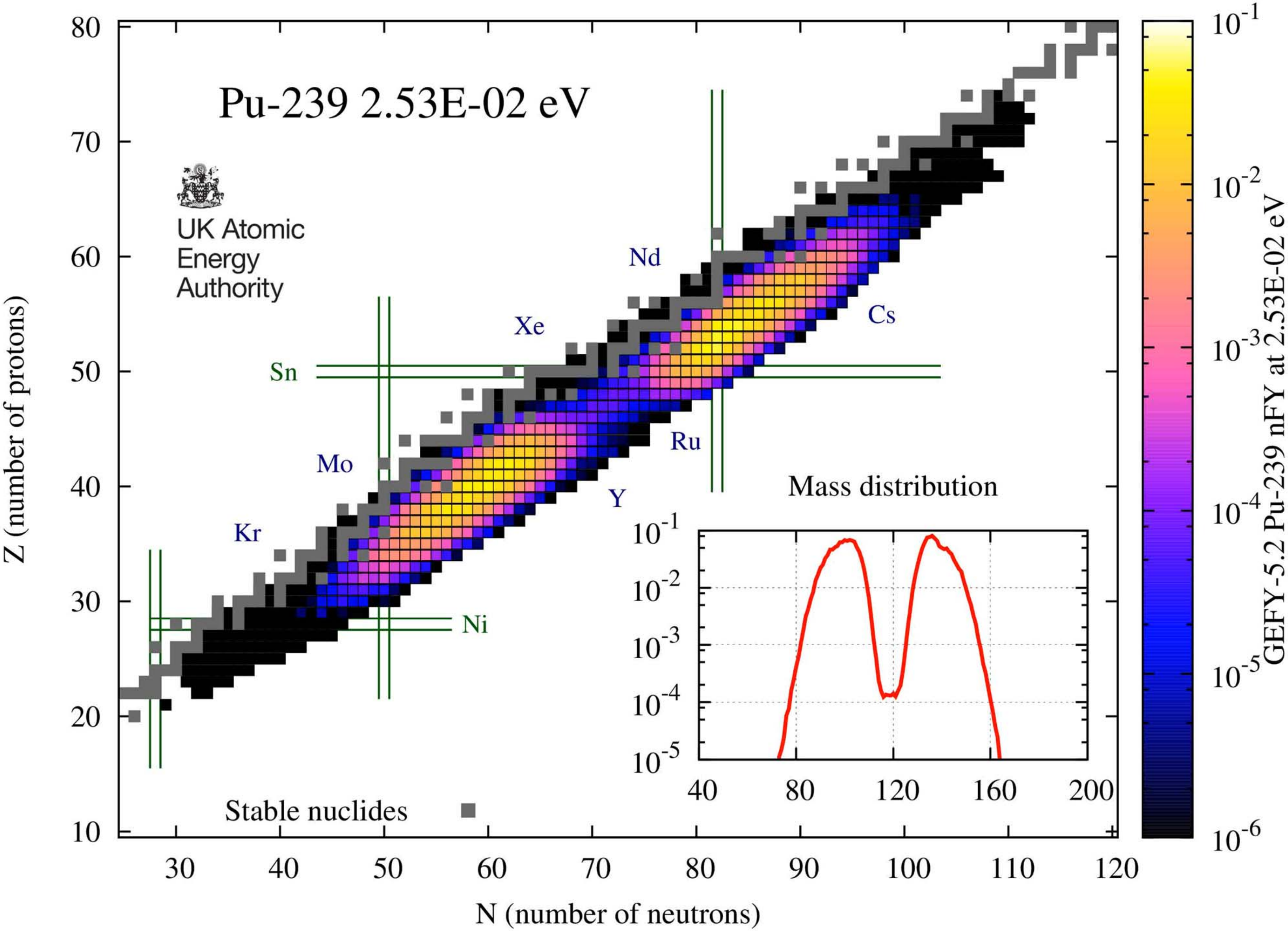
- "Assessment of saddle-point-mass predictions for astrophysical applications", A Kelic, K.-H. Schmidt, Phys. Lett. B 634 (2006) 362
- "On the topographical properties of fission barriers", A. V. Karpov, A. Kelic, K.-H. Schmidt, J. Phys. G: Nucl. Part. Phys. 35 (2008) 035104
- "Experimental evidence for the separability of compound-nucleus and fragment properties in fission", K.-H. Schmidt, A. Kelic, M. V. Ricciardi, Europh. Lett. 83 (2008) 32001
- "Entropy-driven excitation-energy sorting in superfluid fission dynamics", K.-H. Schmidt, B. Jurado, Phys. Rev. Lett. 104 (2010) 212501
- "Thermodynamics of nuclei in thermal contact", K.-H. Schmidt, B. Jurado, Phys. Rev. C 83 (2011) 014607
- "Final excitation energy of fission fragments", K.-H. Schmidt, B. Jurado, Phys. Rev. C 83 (2011) 061601(R)
- "Inconsistencies in the description of pairing effects in nuclear level densities", K.-H. Schmidt, B. Jurado, Phys. Rev. C 86 (2012) 044322
- "General laws of quantum and statistical mechanics governing fission", K.-H. Schmidt, B. Jurado, FIAS Interdisciplinary Science Series (2014) 121
- "Influence of complete energy sorting on the characteristics of the odd-even effect in fission-fragment element distributions", B. Jurado, K.-H. Schmidt, J. Phys. G 42 (2015) 055101
- "Revealing hidden regularities with a general approach to fission", K.-H. Schmidt, B. Jurado, Eur. Phys. J. A 51 (2015) 176

Example fission yield

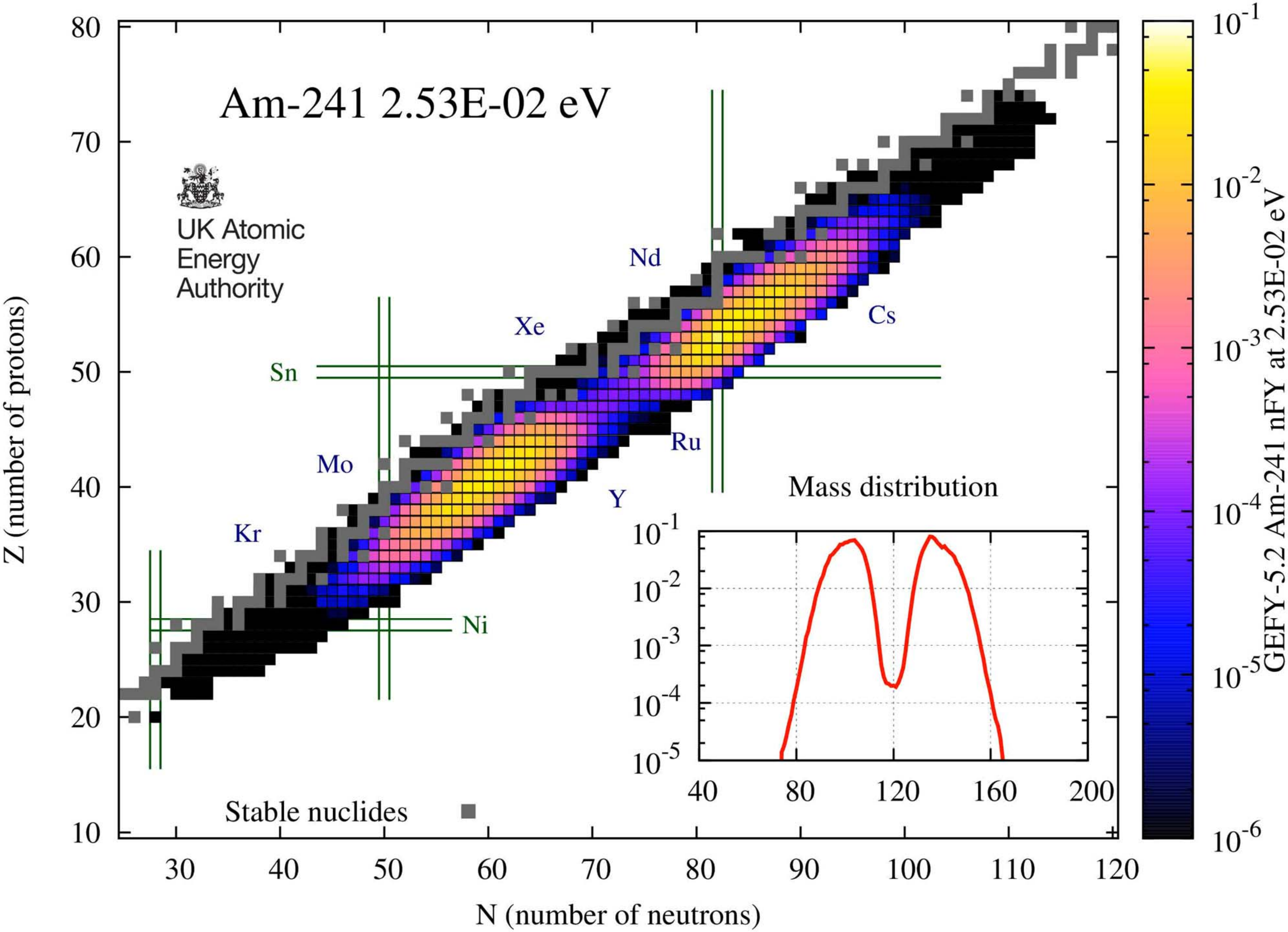
- The JEFF-3.1.1 thermal Pu239 is shown below, there is also a 400 keV file but nothing more



The GEFY-5.2 Pu239 file

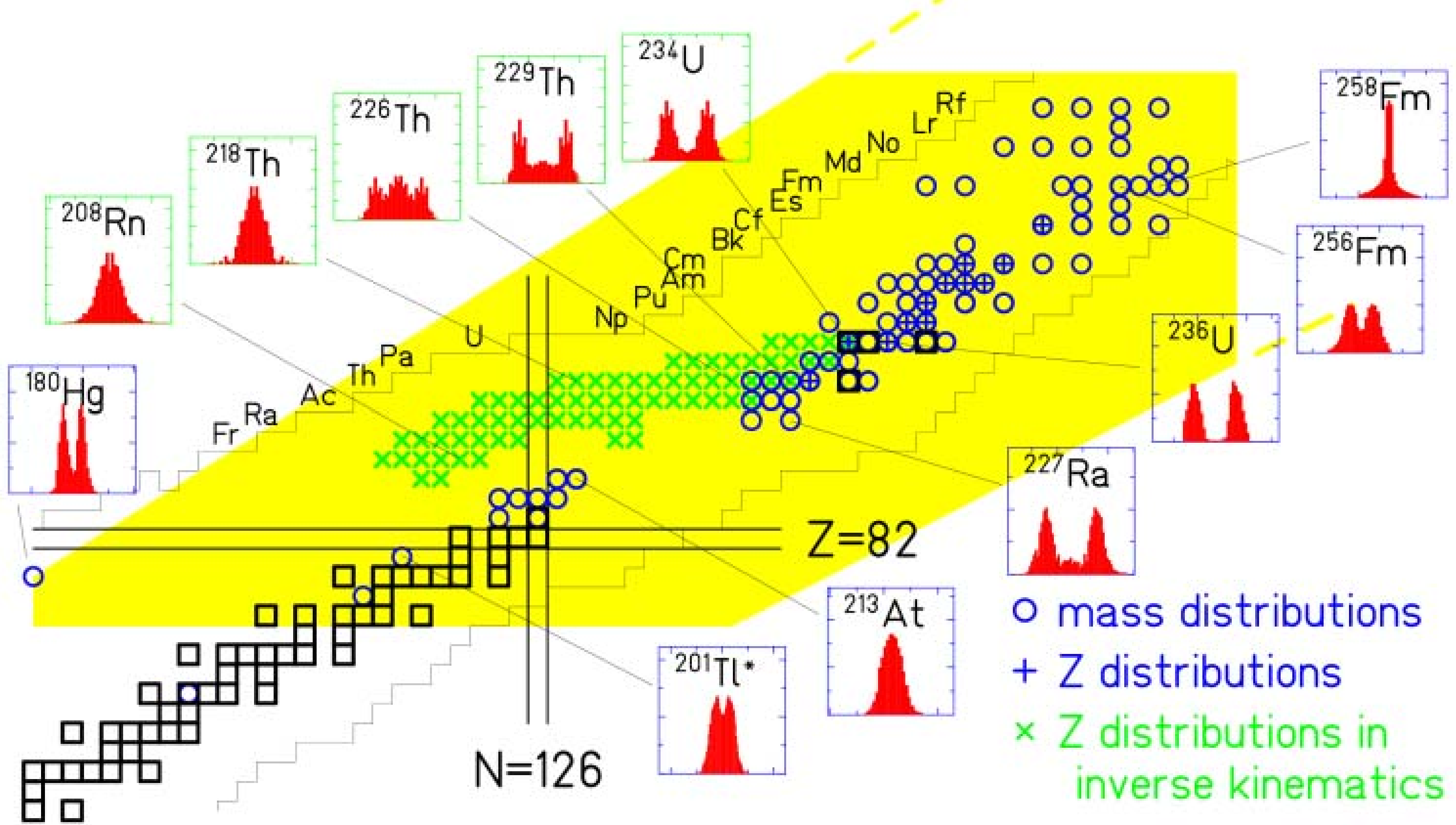


GEFY-5.2 Am241 file



GEF Application range

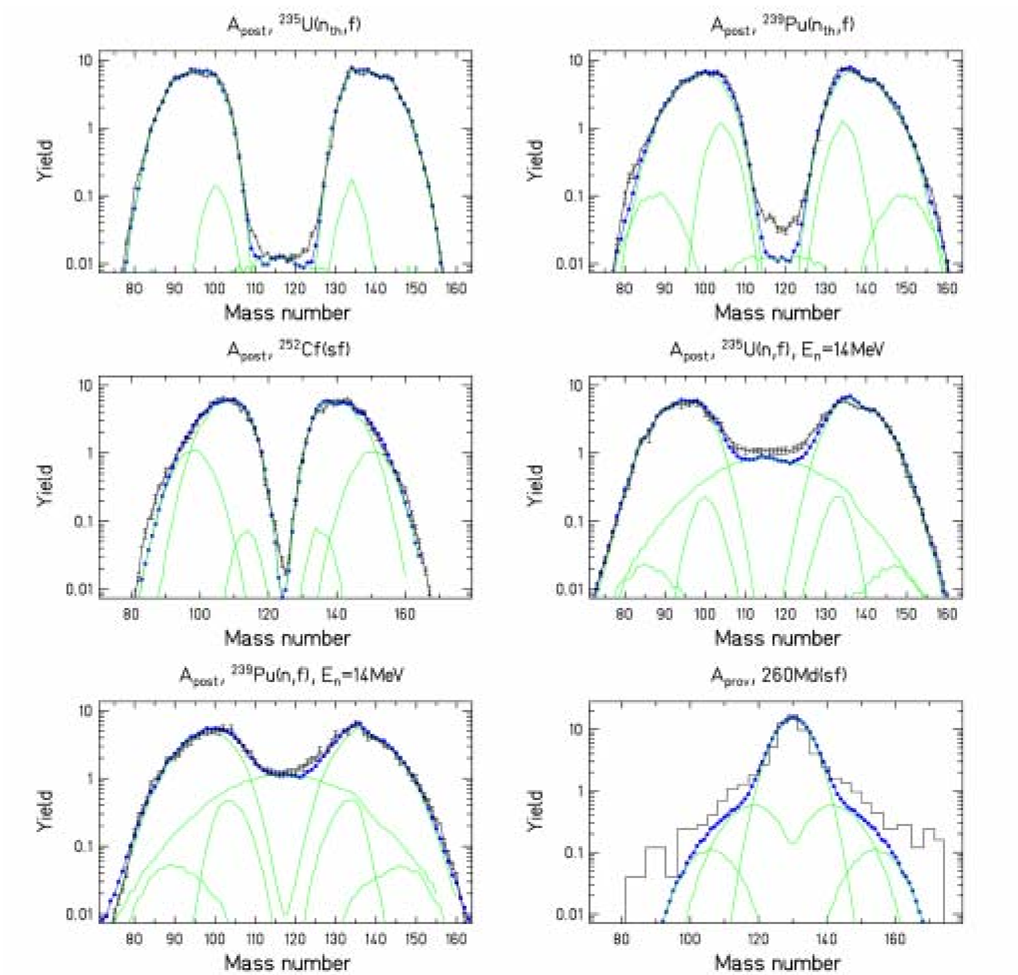
- Taken from https://www-nds.iaea.org/index-meeting-crp/TM-Fission-Yields/docs/Schmidt_slides.pdf



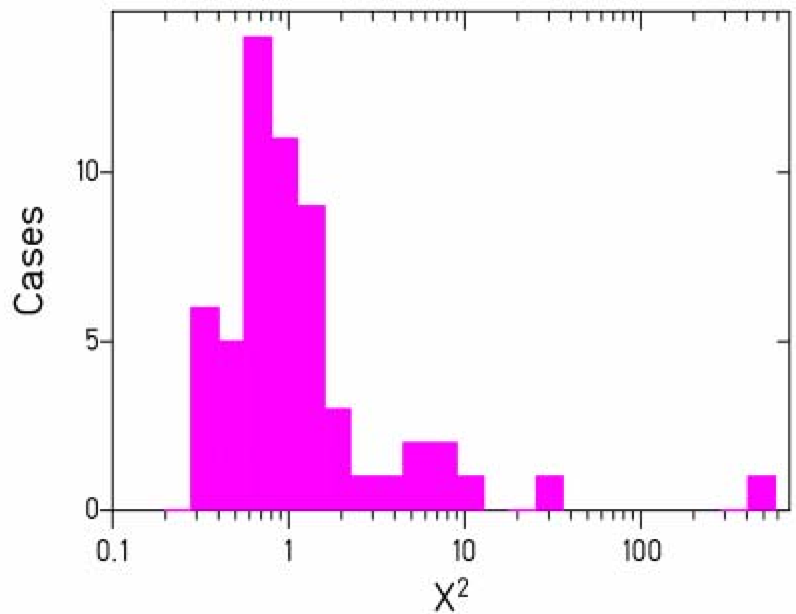
In many cases outside this ‘application range’, GEF remains *at least* one of the best simulation codes

GEF testing (by K-H Schmidt et al)

- Extensive chi-squared analysis against mass yields and evaluated files have demonstrated power of the system



Chi-squared deviations per system

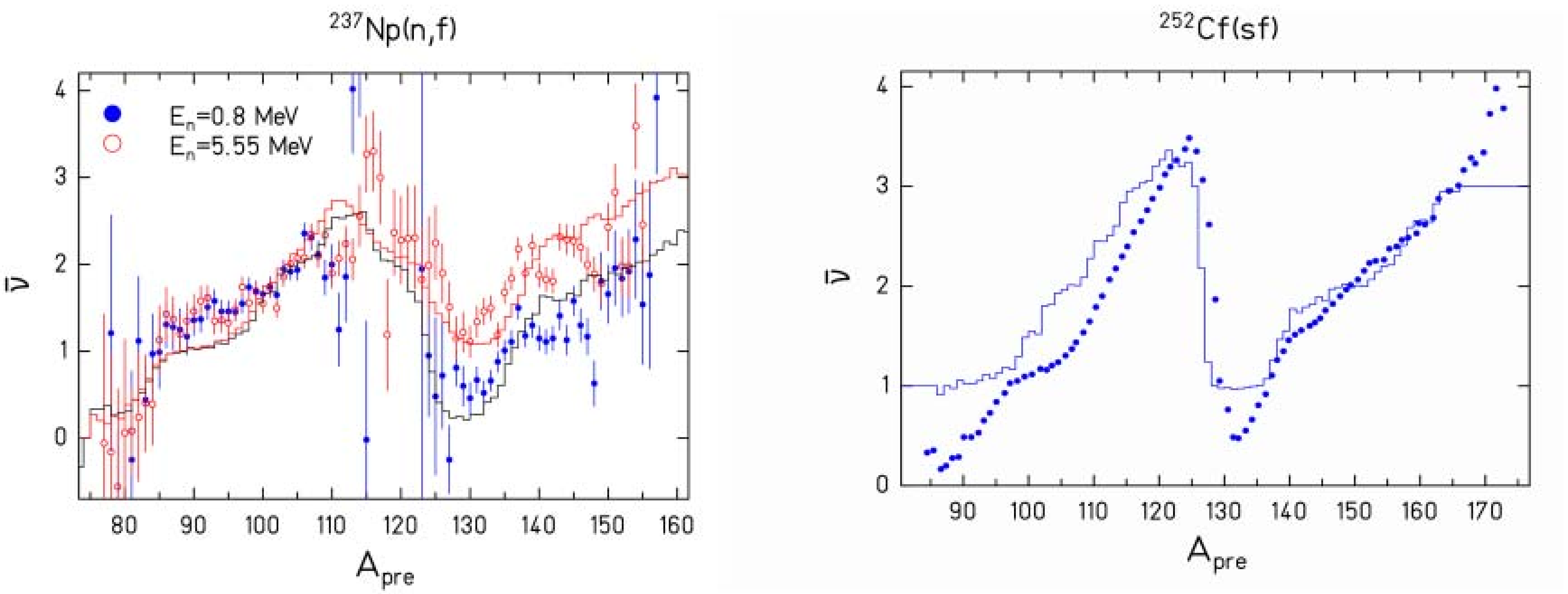


Excerpt from K.-H. Schmidt et al., Nucl. Data Sheets 131 (2016) 107

Advanced GEF applications

- GEF possesses many advanced features, such as A-dependent nu-bar, TKEs, covariances etc. Not currently employed since no standardised format – watch this space!

Prompt neutron emission



https://www-nds.iaea.org/index-meeting-crp/TM-Fission-Yields/docs/Schmidt_slides.pdf

FISPACT-II with fission yields

- FISPACT-II condenses the fission yields as a function of energy with the incident particle spectrum, producing effective yields which account for full multi-chance (when using GEF)

- A full decay library is required and FISPACT-II will issue warnings for missing decays

- *BEWARE: missing data is a common issue for legacy libraries – employing independent yields without checking the decays will leave nuclides ‘in the sink’*

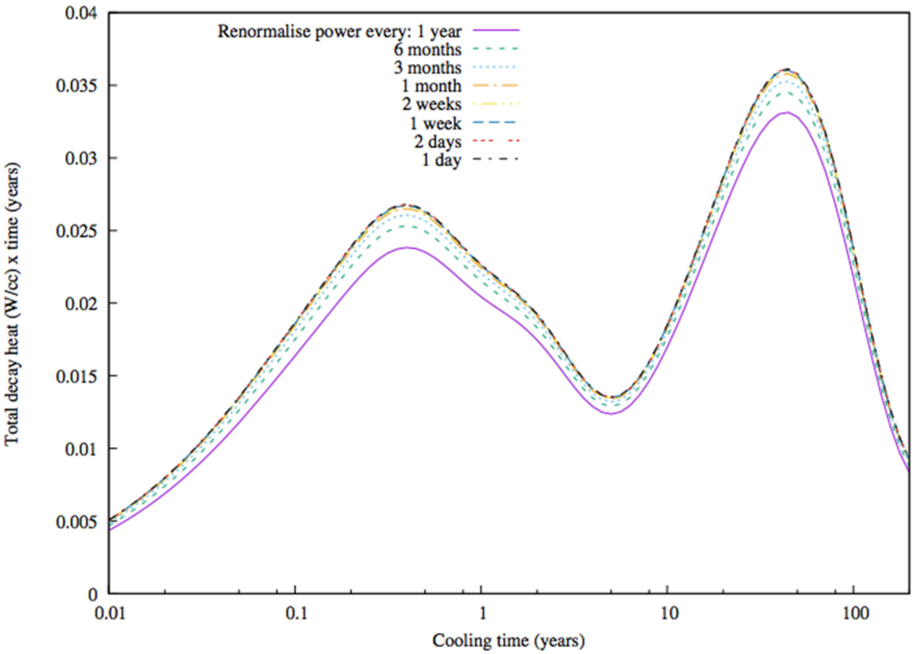
```
00009: Warning: nuclide_m:read_decay_new: 1:
       decay data for parent Os199   NOT found
       filename= Os199
00010: Warning: nuclide_m:read_decay_new: 1:
       decay data for parent Os200   NOT found
       filename= Os200
00011: Warning: nuclide_m:read_decay_new: 1:
       decay data for parent Os201   NOT found
       filename= Os201
00012: Warning: nuclide_m:read_decay_new: 1:
       decay data for parent Ir200   NOT found
       filename= Ir200
00013: Warning: nuclide_m:read_decay_new: 1:
       decay data for parent Ir201   NOT found
       filename= Ir201
00014: Warning: nuclide_m:read_decay_new: 1:
       decay data for parent Ir202   NOT found
       filename= Ir202
00015: Warning: nuclide_m:read_decay_new: 1:
       decay data for parent Pt203   NOT found
       filename= Pt203
```

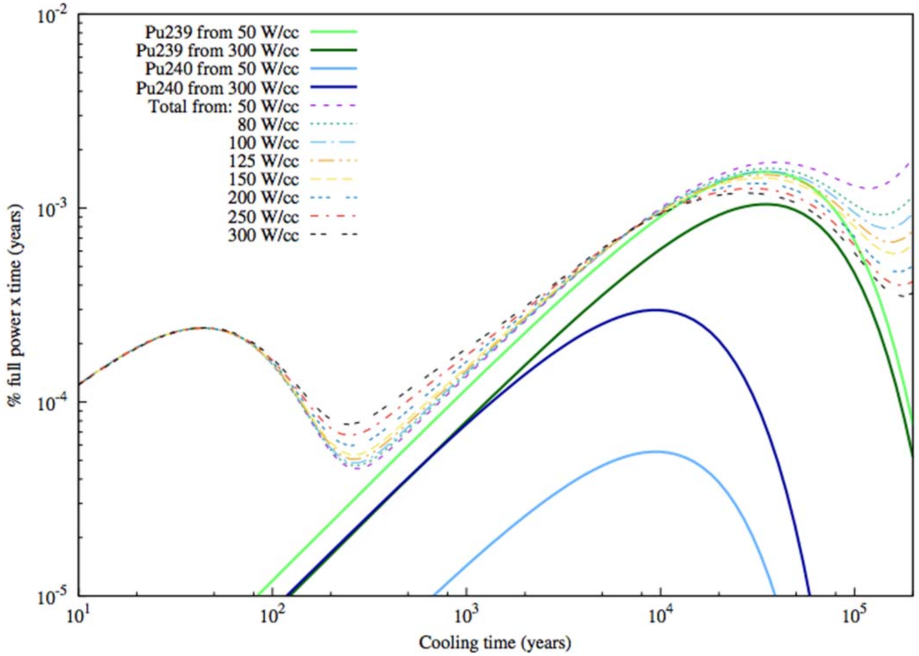
Normalisation choices

- FISPACT-II can employ normalisation through two methods:
  - `FLUX` – given in standard incident particles per cm^2 per second
  - `POWER` – normalise flux to match a power output in W/cm^3. The power per incident particle is given by the full collapse of KERMA based on user-supplied reactions (total, only fission, fission plus specific channels, etc)
- Note that as the nuclide inventory changes, the energy release per kg of target will change (for example with depletion of U235)
  - Correct for changes in nuclide inventory with repeated use of the `POWER` keyword

Example: In-Cycle Fission Reactor

- Examples of % reactor power after shut-down following:
  - Left – LWR fuel with frequency of power renormalisation ranging over 2/year to 1/day
  - Right – Variation over burn-up, showing effect on Pu239/240 isotopic inventory ratios

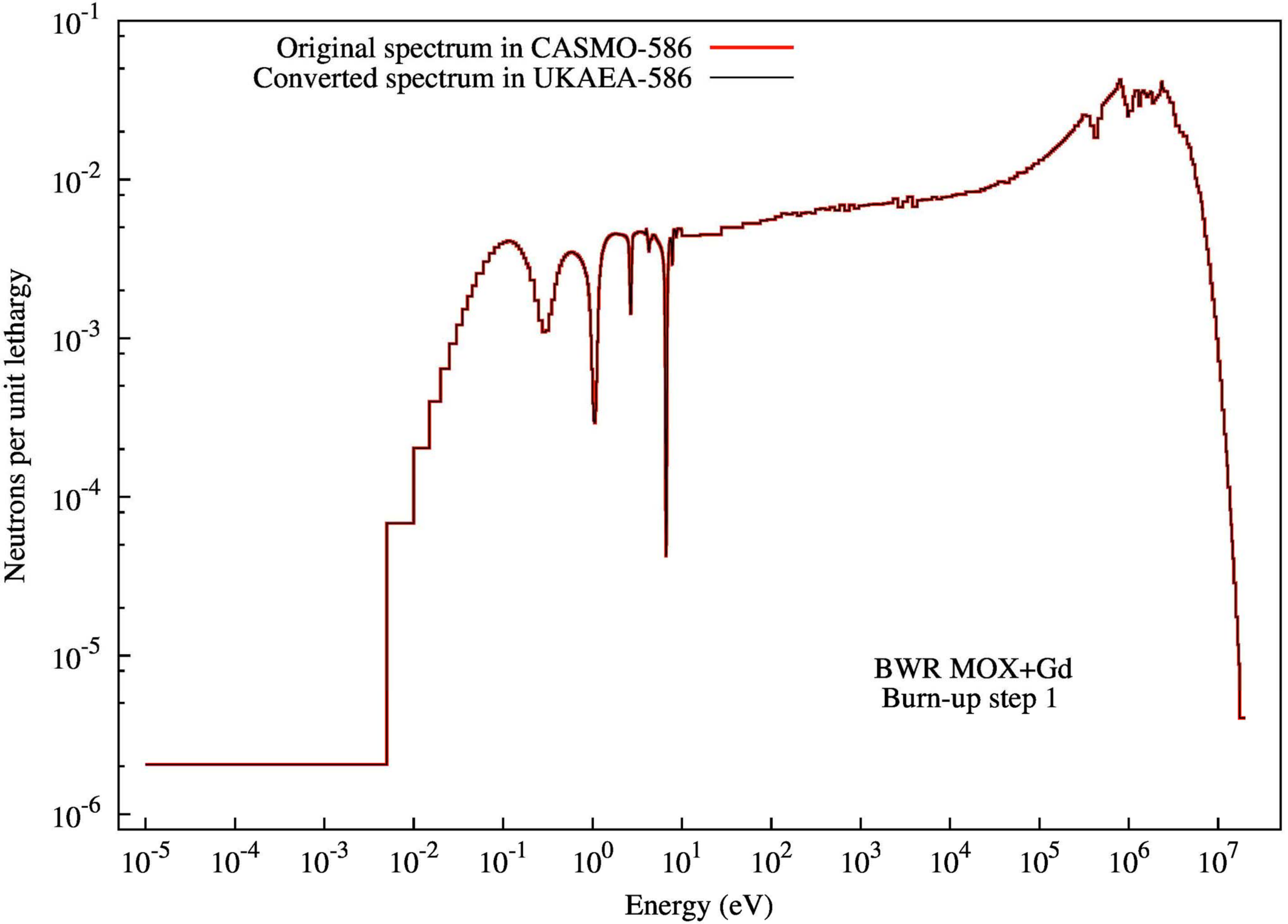




Multi-collapse simulation

- In realistic simulations, renormalisation and spectral modification are necessary, so multiple `POWER` uses must be combined with new `GETXS`
- `GETDECAY` is typically not required since the decays and fissions are unaffected, unless the proportion of fissions as a function of energy are significantly changed
  - This would require massive spectral shift – not partial fuel burn
- In addition, re-self-shielding is typically required, particularly as fuel composition and/or poison inventories change

Time evolution of spectrum



Multiple collapse

- FISPACT-II accommodates multiple collapses using multiple spectra with the FILES file

- xs_endf and prob_tab must be re-specified for each – potentially with updates if desired

```
# condensed decay and fission data (in and out)
arrayx  ARRAYX

# collapsed cross section 1
fluxes flux_data/ave/1/fluxes
xs_endf /Volumes/F7908-Td8/Code/EASY-II-Release-3-00-00/ENDFdata/ENDFB71data/endfb71-n/gxs-586-600
prob_tab  /Volumes/F7908-Td8/Code/EASY-II-Release-3-00-00/ENDFdata/ENDFB71data/endfb71-n/tp-586-600
collapxi  collapx_ave/COLLAPX.1
collapxo  collapx_ave/COLLAPX.1
# collapsed cross section 2
fluxes flux_data/ave/2/fluxes
xs_endf /Volumes/F7908-Td8/Code/EASY-II-Release-3-00-00/ENDFdata/ENDFB71data/endfb71-n/gxs-586-600
prob_tab  /Volumes/F7908-Td8/Code/EASY-II-Release-3-00-00/ENDFdata/ENDFB71data/endfb71-n/tp-586-600
collapxi  collapx_ave/COLLAPX.2
collapxo  collapx_ave/COLLAPX.2
# collapsed cross section 3
fluxes flux_data/ave/3/fluxes
xs_endf /Volumes/F7908-Td8/Code/EASY-II-Release-3-00-00/ENDFdata/ENDFB71data/endfb71-n/gxs-586-600
prob_tab  /Volumes/F7908-Td8/Code/EASY-II-Release-3-00-00/ENDFdata/ENDFB71data/endfb71-n/tp-586-600
collapxi  collapx_ave/COLLAPX.3
collapxo  collapx_ave/COLLAPX.3
# collapsed cross section 4
```

Input specification and self-shielding

- Self-shielding and collapses can be run in multiple ways, depending on user input, for example:
  - Users may specify for each and run individual collapses – followed by one simulation which reads each
  - Users with all spectra can include multiple collapses during a single simulation
  - Directly coupled Boltzmann-Bateman can be done for each step with new inputs
- Power normalisation can be set constant to re-calculate flux given inventory and kerma values

Charged incident particles, high-energy and residuals

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Projectile choice

- FISPACT-II can handle the incident nuclear data for five particles, which are selected using the `PROJECTILE` keyword

  - `PROJECTILE 1` neutrons (default if not stated)
  - `PROJECTILE 2` deuterons
  - `PROJECTILE 3` protons
  - `PROJECTILE 4` alphas
  - `PROJECTILE 5` gammas

- For neutrons, the 709 group data are used (and 1102, 586 in development versions)

- For charged particles, the 162 group is used instead
  - Note that `GETXS 1 162` must be used as well

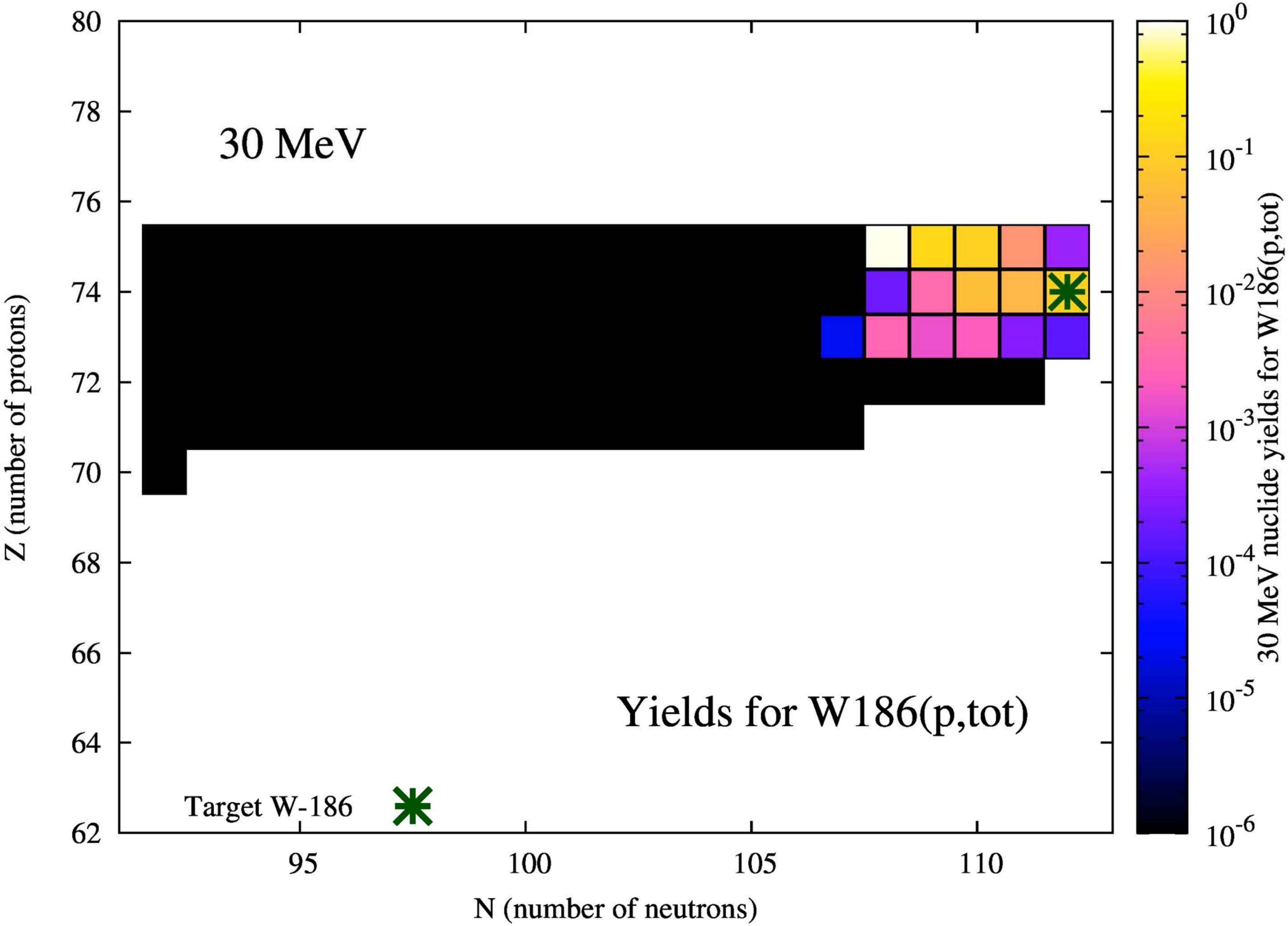
TENDL residual nuclide production

- Above 30 MeV, reaction channel uniqueness breaks down as a functional description within ENDF6
  - Too many reactions for < 200 mt values
  - Many reactions give equivalent products
  - Only total residual production tends to have experimental data

- At 30 MeV TENDL changes from specific-mt descriptions to mt=5 mf=10 yield data

- These include summation over all reaction channels and condense the data into yield x cross-section for production of each residual nuclide

W-186 proton irradiation



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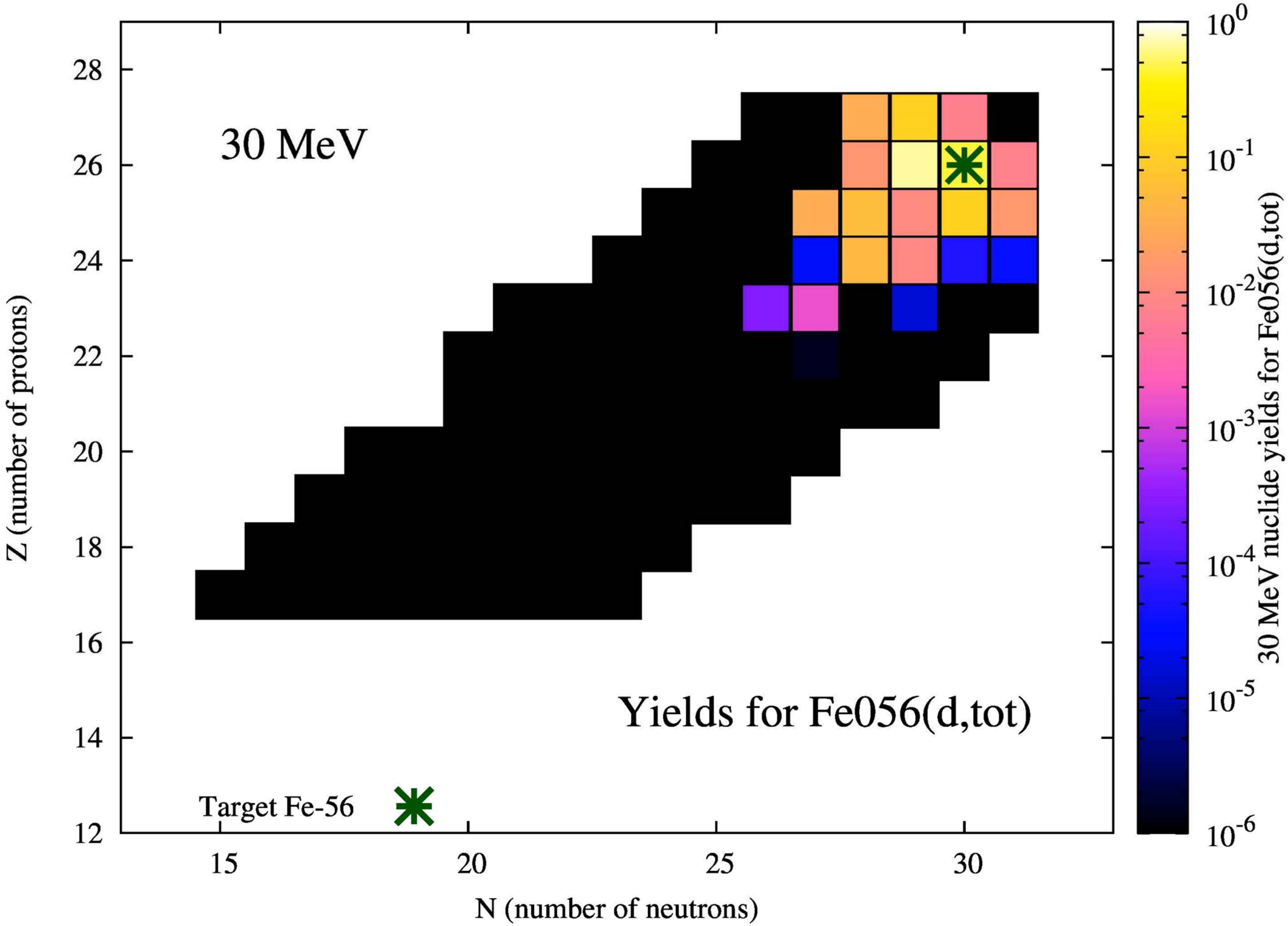
F-56 deuteron irradiation



Fission addition

- TENDL contains additional knowledge of fission cross sections which are stored and read by FISPACT-II above 30 MeV
- These exist for neutron-induced reactions as well as proton, deuteron, alpha, gamma…
- The remaining data required for these are fission yields. While these are not supplied in the standard FISPACT-II distribution, approximate files can be generated by any suitable code (*eg* GEF)
  - FISPACT-II can read these (in ENDF6 format) within the same *fy_endf* directory irrespective of incident particle

Total Monte-Carlo

Total Monte-Carlo

- FISPACT-II has a powerful pathway-based uncertainty method which allows UQP for target nuclides produced through reactions.

- Depletion uncertainty of fuels also can be determined from full covariance treatment with the code

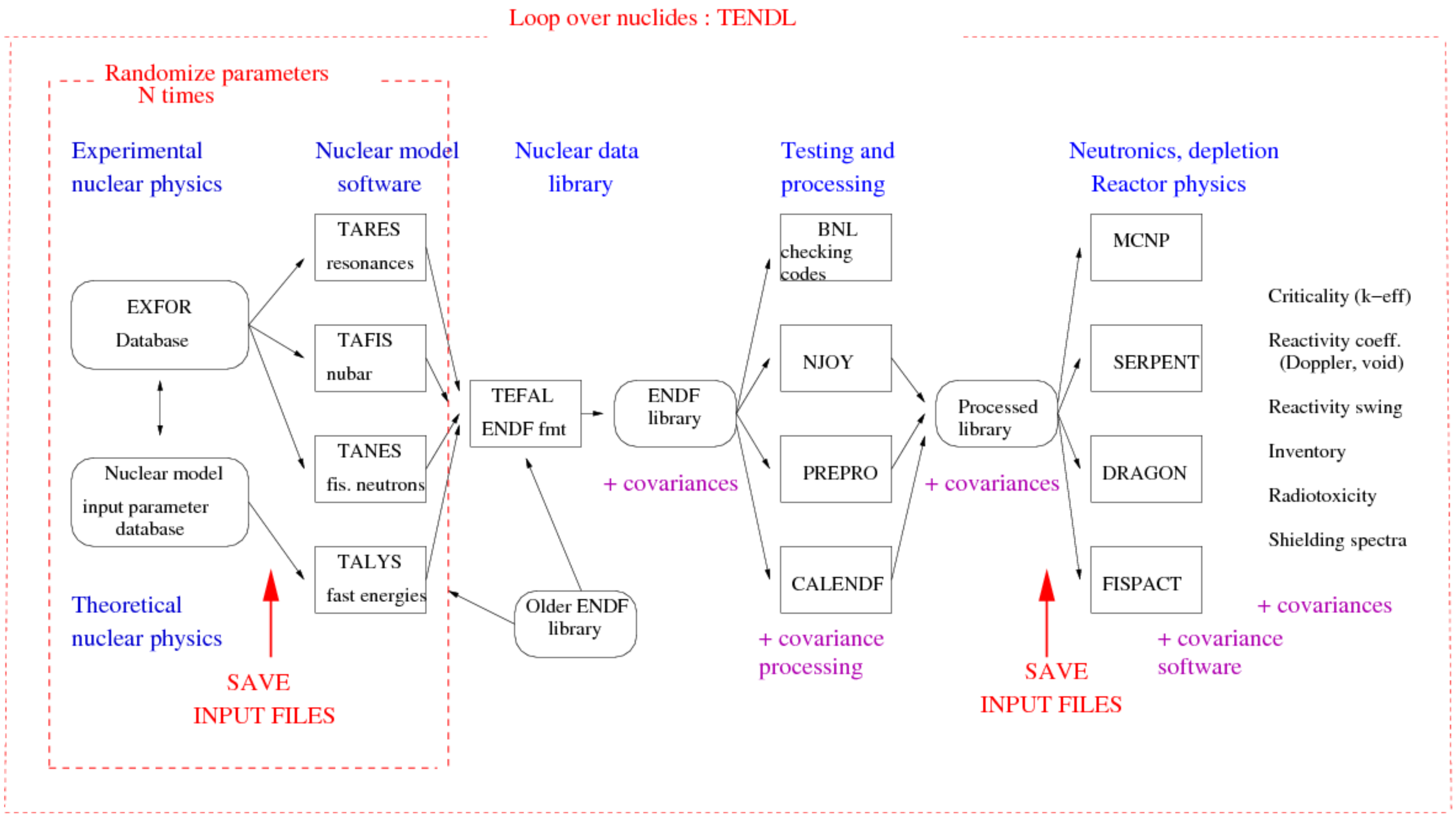
- An alternative, powerful method for uncertainty quantification is the Total Monte-Carlo, based on semi-empirical model parameter variation in the nuclear data generation

- Multiple ‘random’ (not random, but based on random parameter sampling) files are used for simulation and observables are statistically collapsed

Sampled nuclear data

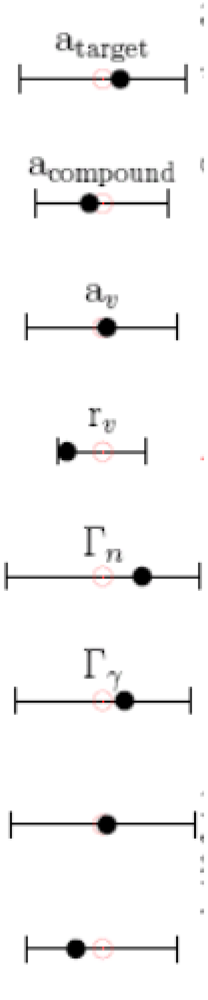
- The key ingredient is a set of nuclear data files which reflect sampling of input parameters and nuclear data uncertainty
- These may include reaction data, fission yields, decays, etc.
- For reactions, the TMC method has been extensively developed by the TENDL/TALYS/T6 project
- For fission yields, GEF has been used for UQP, particularly using semi-Bayesian methods

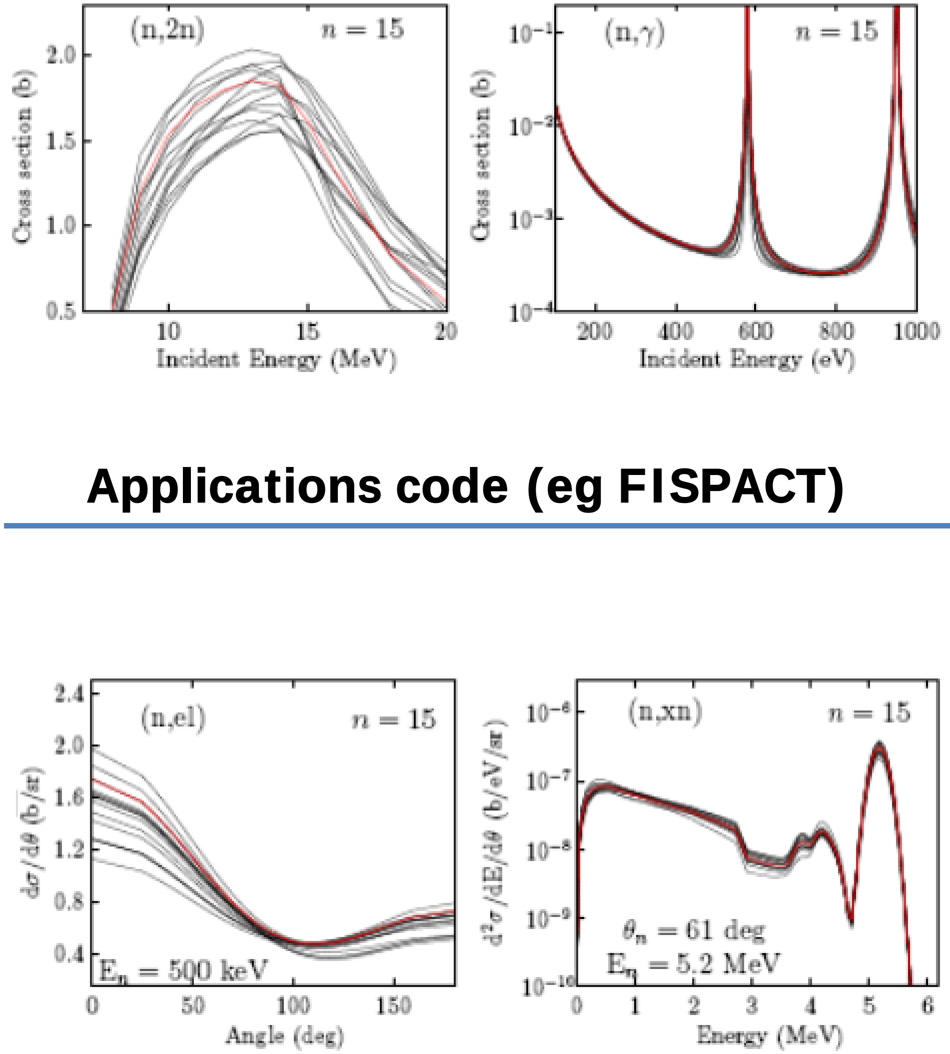
TENDL Nuclear data methodology = T6



A.J. Koning and D. Rochman ,"Modern nuclear data evaluation with the TALYS code system“, Nuclear Data Sheets 113, 2841 (2012).

NRG





Applications code (eg FISPACT) →

UQP

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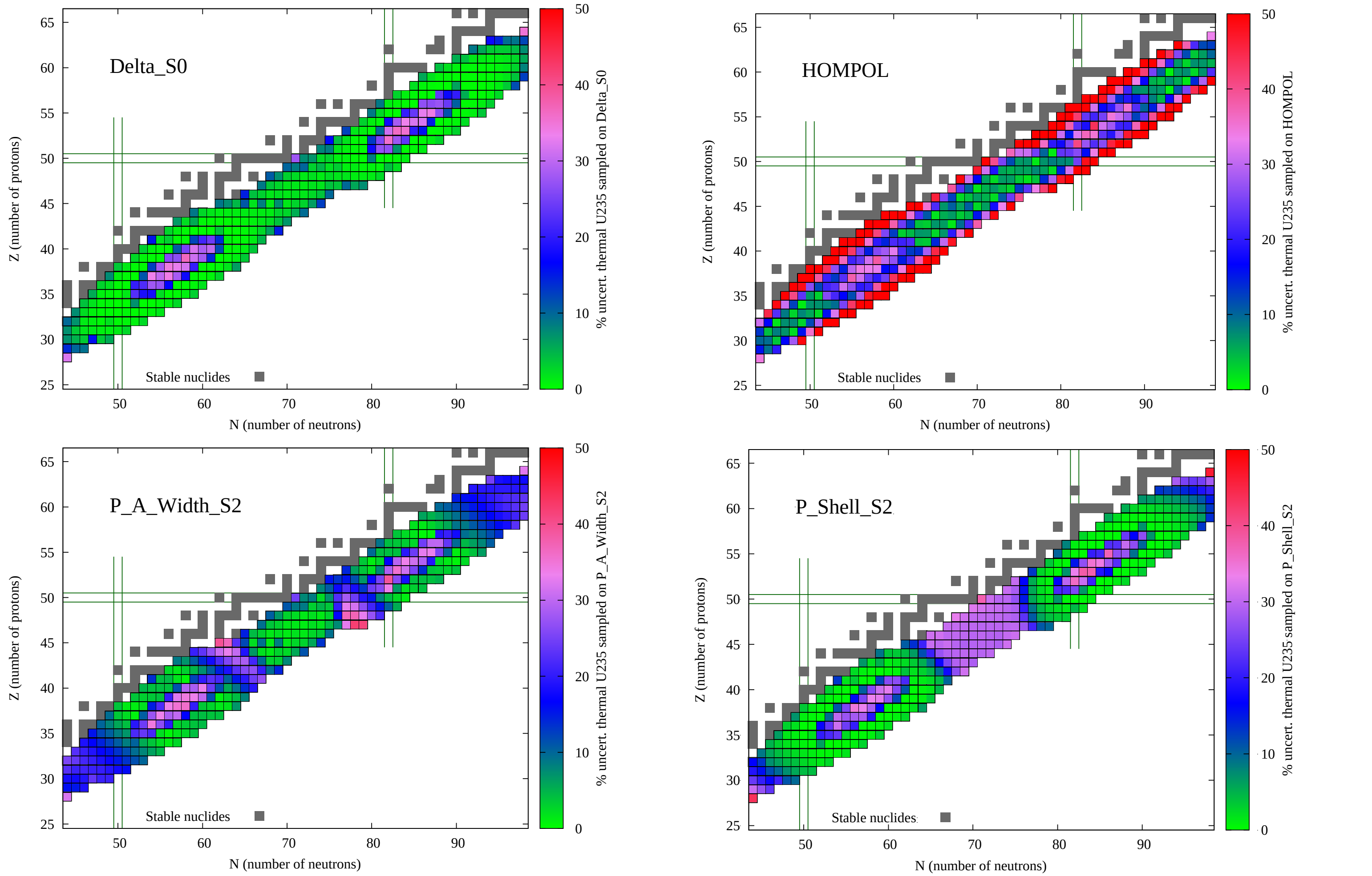
Yield sensitivities

- The fission yields are sensitive to various input parameters which have some uncertainty – this is translated to yield uncertainties



Some random files available

- TENDL-2015 (and several earlier distributions) contain sampled files, eg:

https://tendl.web.psi.ch/tendl_2015/neutron_html/Sn/NeutronSn120.html

Random Evaluated formatted data (gzipped)

ACE 1	Random ENDF 1	TALYS input 1	xsdir 1	ACE 2	Random ENDF 2	TALYS input 2	xsdir 2
ACE 3	Random ENDF 3	TALYS input 3	xsdir 3	ACE 4	Random ENDF 4	TALYS input 4	xsdir 4
ACE 5	Random ENDF 5	TALYS input 5	xsdir 5	ACE 6	Random ENDF 6	TALYS input 6	xsdir 6
ACE 7	Random ENDF 7	TALYS input 7	xsdir 7	ACE 8	Random ENDF 8	TALYS input 8	xsdir 8
ACE 9	Random ENDF 9	TALYS input 9	xsdir 9	ACE 10	Random ENDF 10	TALYS input 10	xsdir 10
ACE 11	Random ENDF 11	TALYS input 11	xsdir 11	ACE 12	Random ENDF 12	TALYS input 12	xsdir 12

- These come with full parameter information for complete reproducibility and statistical tests

Other random files

- For fission yields
  https://tendl.web.psi.ch/tendl_2015/randomYields.html

- For thermal scattering
  https://tendl.web.psi.ch/tendl_2015/randomThermalScattering.html

List of isotopes

• Z=90, ^{229}Th	(16/10/2015)	0.0253 eV, 500 ENDF files (11 Mb)
• Z=90, ^{232}Th	(21/08/2015)	spontaneous fission, 2 ENDF files (40 kb)
• Z=92, ^{233}U	(16/10/2015)	0.0253 eV, 500 ENDF files (12 Mb)
• Z=92, ^{234}U	(19/05/2016)	spontaneous fission, 2 ENDF files (40 kb)
• Z=92, ^{235}U	(21/08/2015)	spontaneous fission, 2 ENDF files (40 kb)
• Z=92, ^{235}U	(14/09/2015)	0.0253 eV, original GEF parameters: 6000 ENDF files (132 Mb)
• Z=92, ^{235}U	(14/09/2015)	0.0253 eV, updated GEF parameters: 2500 ENDF files (55 Mb)
• Z=92, ^{238}U	(21/08/2015)	spontaneous fission, 2 ENDF files (40 kb)
• Z=92, ^{238}U	(01/10/2015)	500 keV, original GEF parameters: 1100 ENDF files (44 Mb)
• Z=92, ^{238}U	(01/10/2015)	500 keV, updated GEF parameters: 2500 ENDF files (55 Mb)

FISPACT-II use

- The ability to fully read any of these files allows repeat simulation and collapse – particularly unique for full TENDL

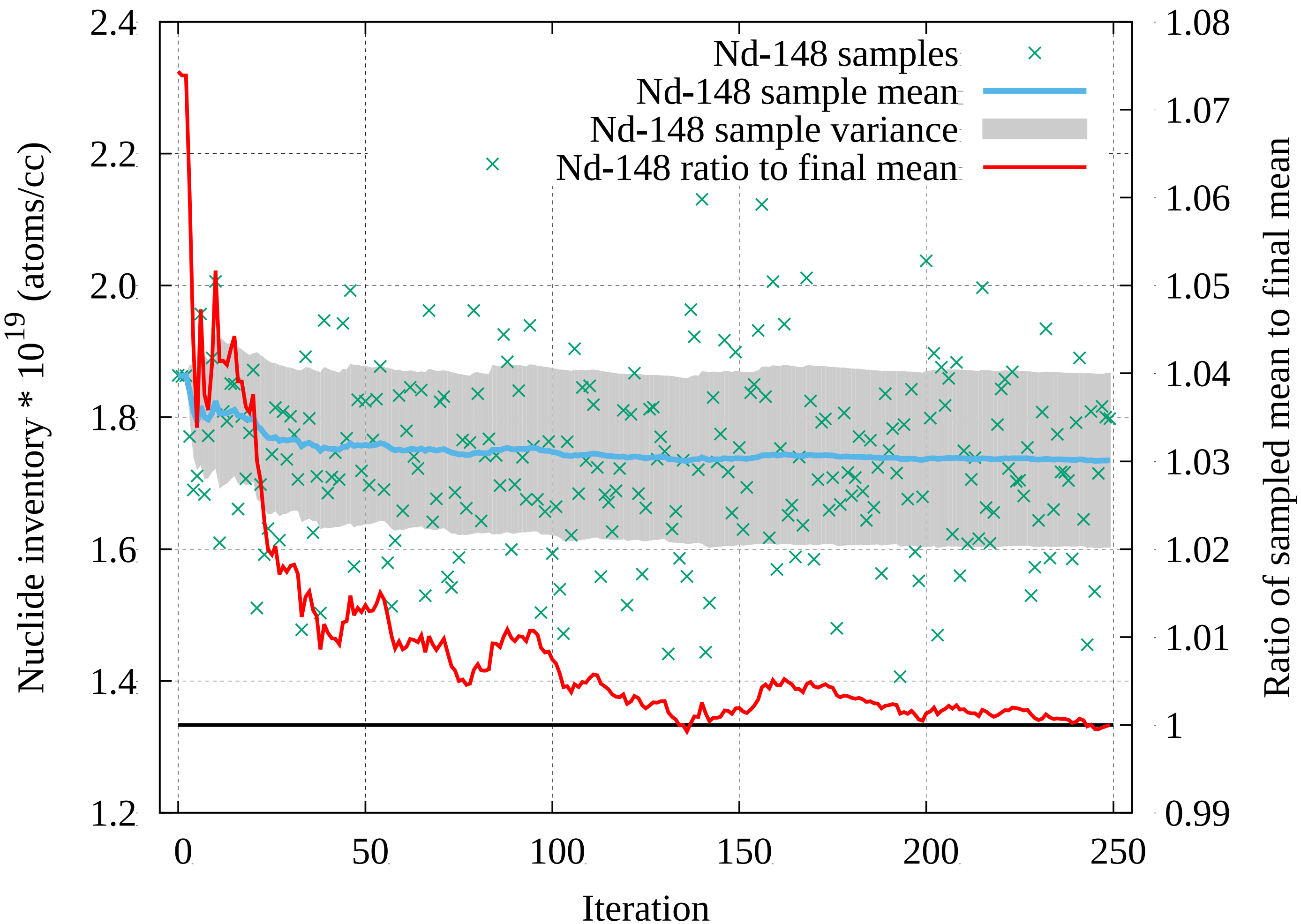
- Simply point to different directories for sampled files within the FILES file

```
# collapsed cross section ${i}
fluxes fluxes
xs_endf ${fisp_folder}ENDFdata/TENDL2015data/tal2015-n/gxs-586-600_sample_${i}
prob_tab  ${fisp_folder}ENDFdata/TENDL2015data/tal2015-n/tp-586-600_sample_${i}
collapxi  COLLAPX.${i}
collapxo  COLLAPX.${i}
```

- Alternatively use the covariance data provided within TENDL (and processed by FISPACT-II), which is based on the same parameter variation

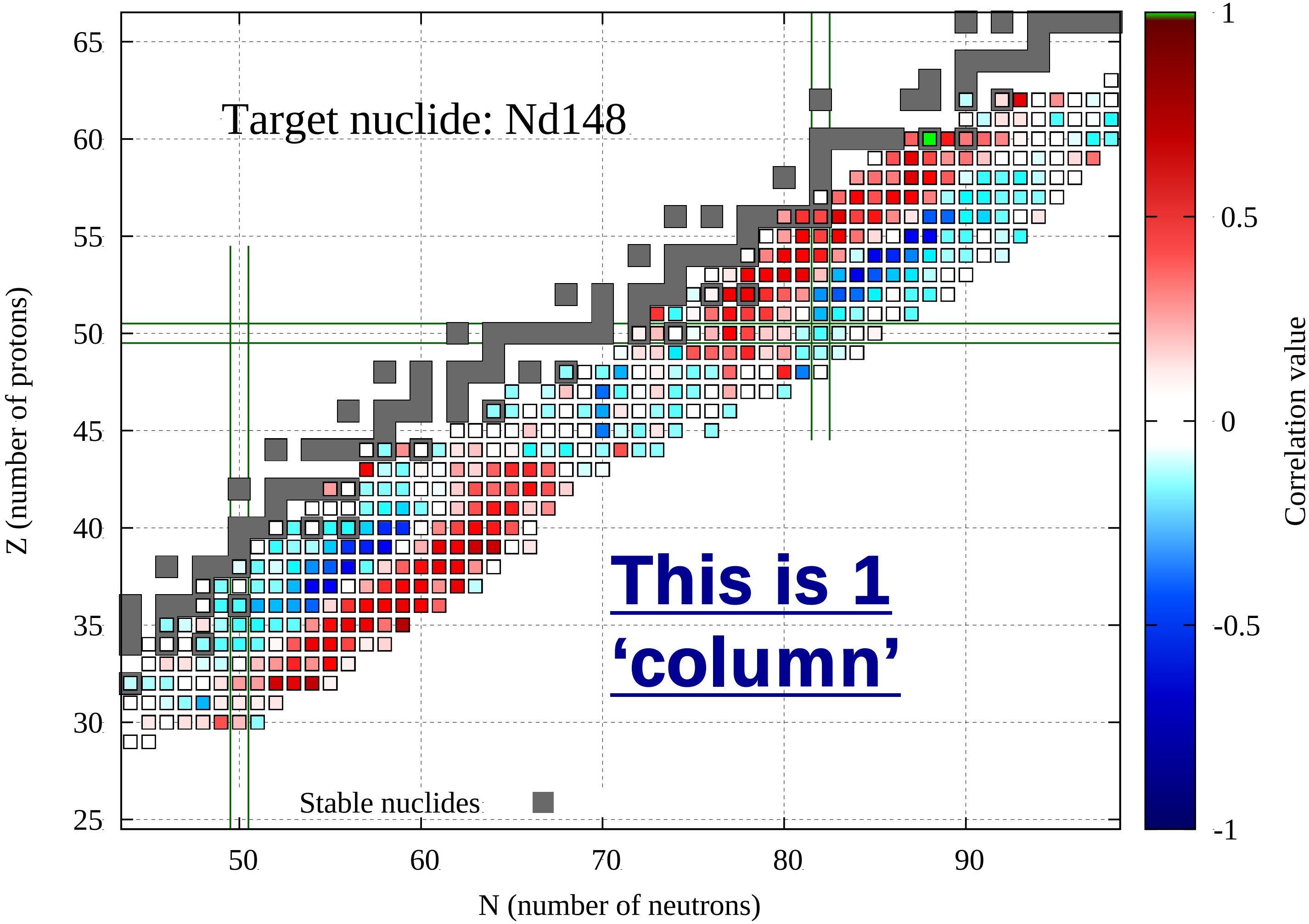
Convergence with TMC

Sampling of the files and repeated simulation results in different simulated quantities, such as this Nd148 inventory after 40 GWd/tn burn-up in a BWR-MOX assembly. Statistics on these results gives the full TMC uncertainty



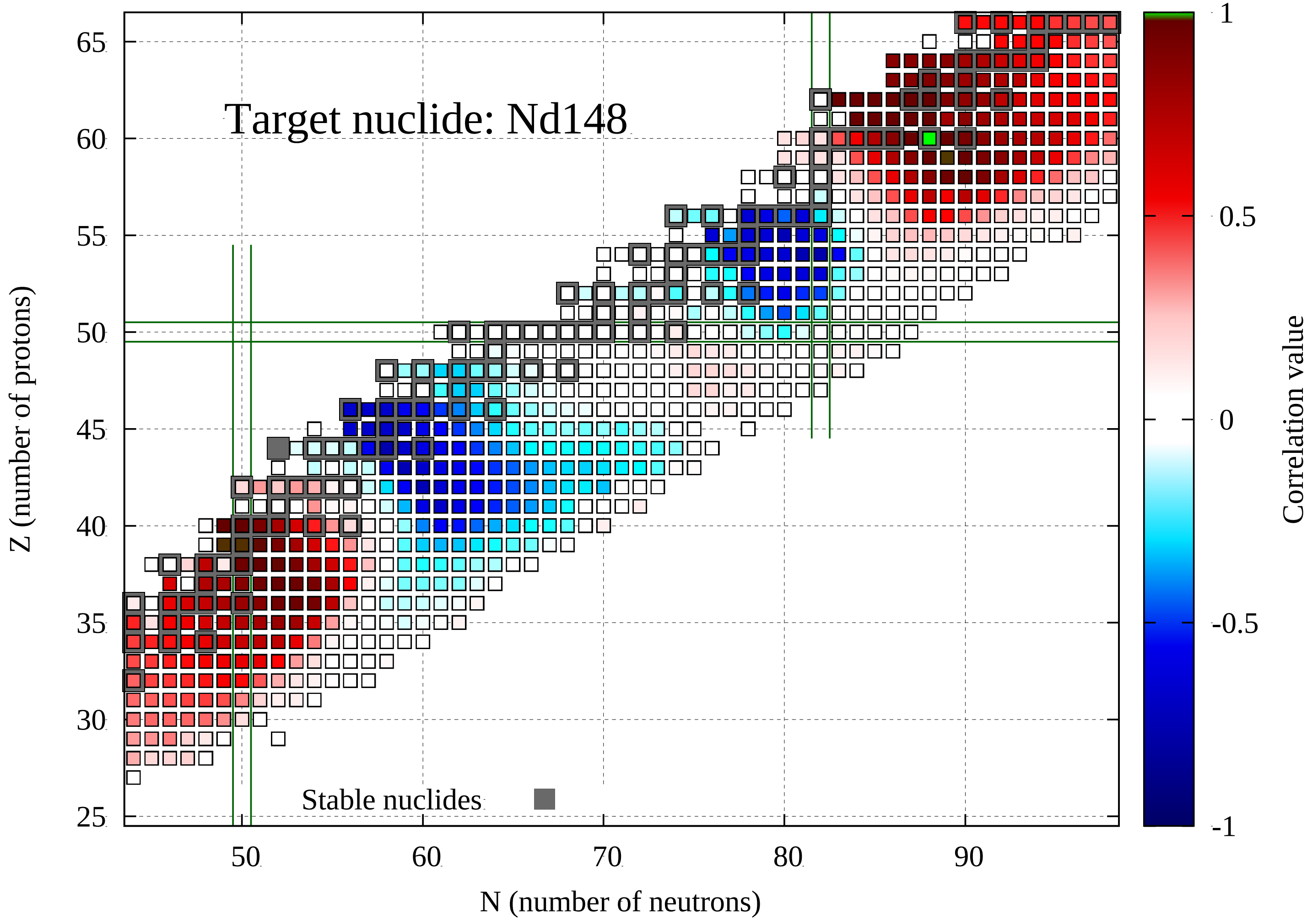
Comments on covariances

- Independent covariances intuitive based on simulation of fission events (independent correlation chart for Nd148 GEFY-5.3 U5_th)



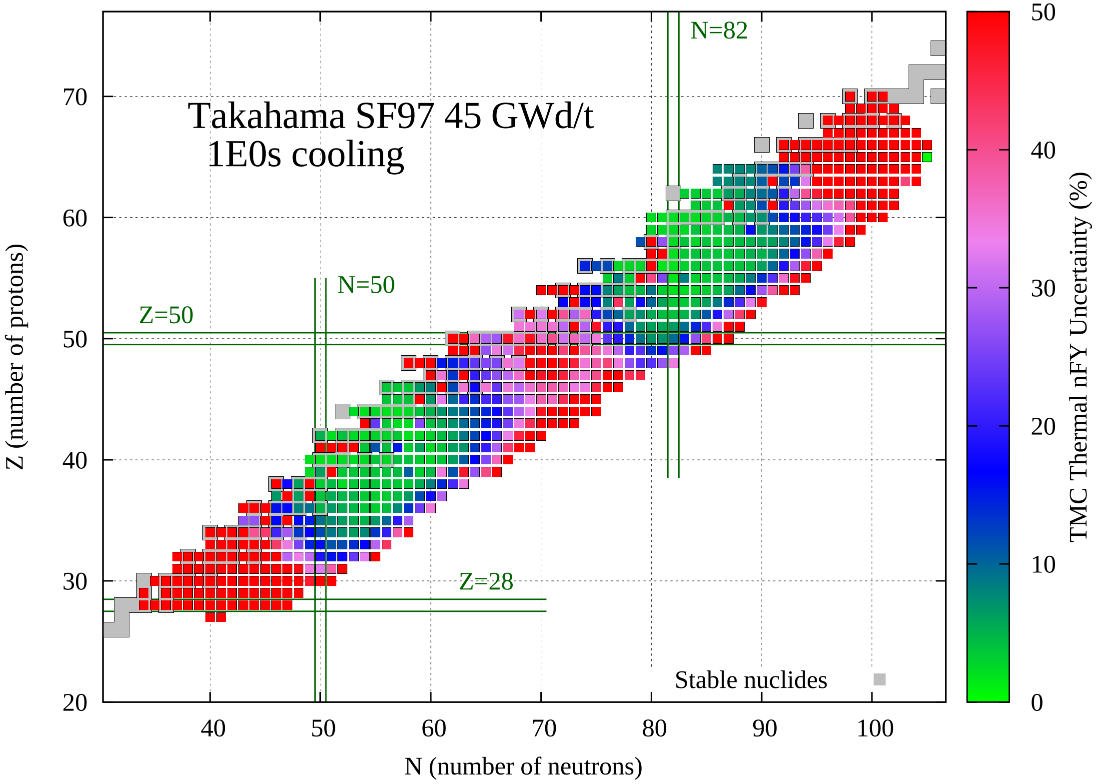
Comments on covariances

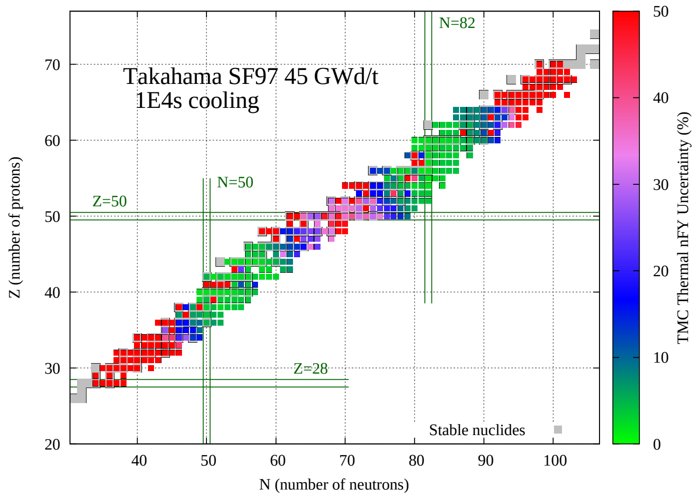
- Cumulative covariances and covariances from full irradiation scenarios show completely different trends (assembly 40 GWd/tn)

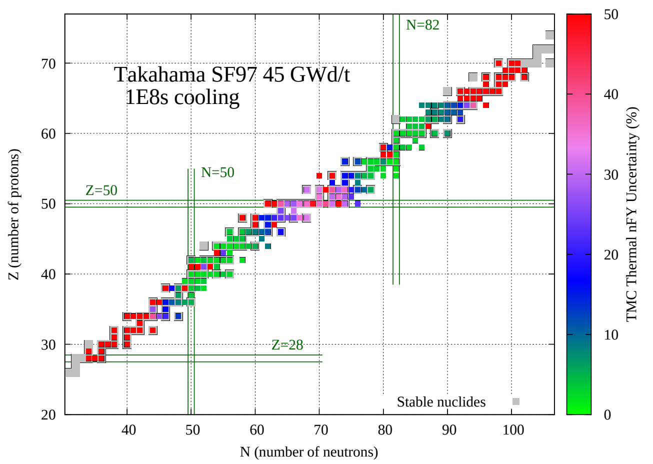


FISPACT-II and nFY TMC

- FISPACT-II can be used to fully sample random independent (or cumulative) yield files with any decay library, propagating uncertainties through full fuel life-cycle*

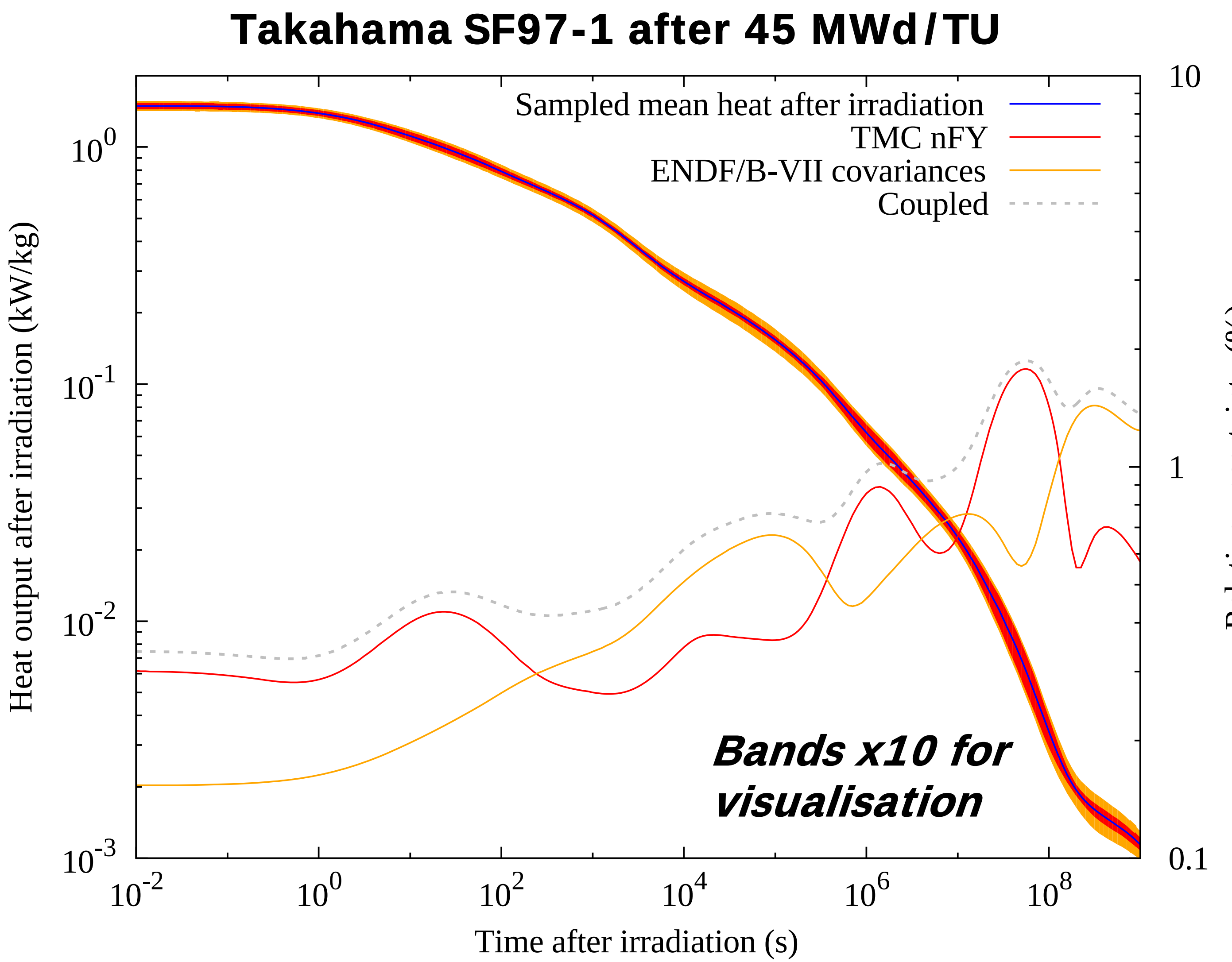






FISPACT-II RR + nFY UQP

- 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.



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Verifications and Validations

- Since TENDL-2012 the NRG libraries have entered the secluded world of criticality benchmarking – also superseding the terminated EAF libraries (last EAF-2010)
- TENDL uniquely contains covariance information
- TENDL provides for all applications: transport, burn-up, inventory, transmutation, dosimetry, astrophysics,…
- TENDL-2015 has fully benefited from TENDL-2008, -09 (EAF), -10, -11, -12, -13, -14, V&V and the T6 technological construction framework
- n-TENDL-2015 nuclear data libraries already outwit in many aspects the regional majors: ENDF/B, JENDL, JEFF,..
- However, low z isotopes still will need to come from R-matrix theory and the actinides from carefully nurtured TALYS model

TENDL-2015: reliable, V&V libraries for all applications

Conclusions

FISPACT-II:

- A powerful predictive activation-transmutation-burnup, radiation source term prediction tool
- Identifies and quantifies important reactions and decays
- Uses full TENDL-2015 covariance data
- Uncertainty estimates:
  - pathways to dominant nuclides
  - Monte-Carlo sensitivity
  - reduced model + Monte-Carlo sensitivity
- Uncertainty on all responses: number density, activity, decay heat, dose rate, inhalation and ingestion indices, ….

http://www.ccfe.ac.uk/fispact.aspx