VTT

Nuclear Data Uncertainty Propagation in Total Monte-Carlo Method

26/08/2022 VTT – beyond the obvious

On Todays Menu

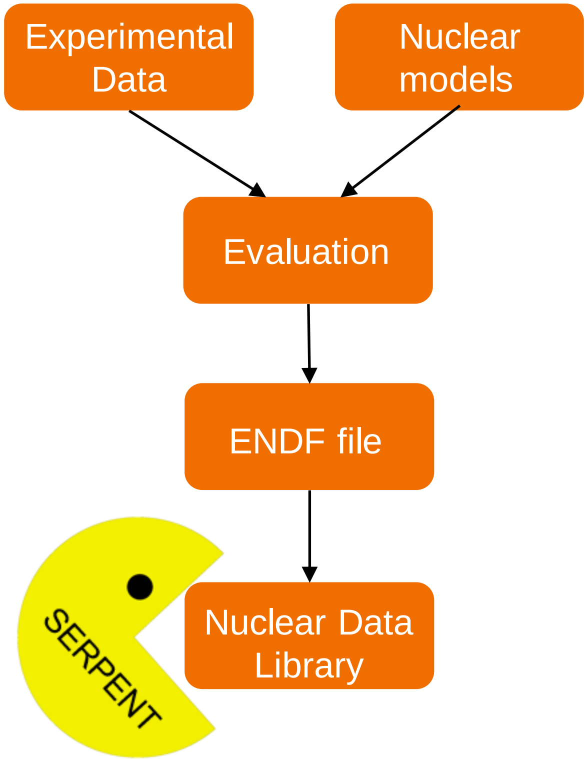
1. General overview of nuclear data & its uncertainties
2. Total Monte-Carlo method & T6 software package
3. Description of the calculation routine for perturbed files
4. Description of the performed calculations
5. Results

Nuclear data for particle transport

- Serpent relies on nuclear data to realistically simulate neutron transport in a modelled geometry.
- Nuclear data for many reaction channels is significantly uncertain
- This means that the output of Serpent is uncertain as well!
- How could we quantify this uncertainty?

Nuclear data: Sources of Uncertainty

- Nuclear data evaluations are based on experimental measurements and utilization of nuclear model codes.
- Different evaluations are based on different model codes, evaluators and reference data, which has resulted in significant inconsistencies between the major library projects.
- Sources of error in experimental measures:
  - Detector calibration
  - Correction of multiple scattering
  - Statistical error
  - Impurities



Nuclear data: Sources of uncertainty

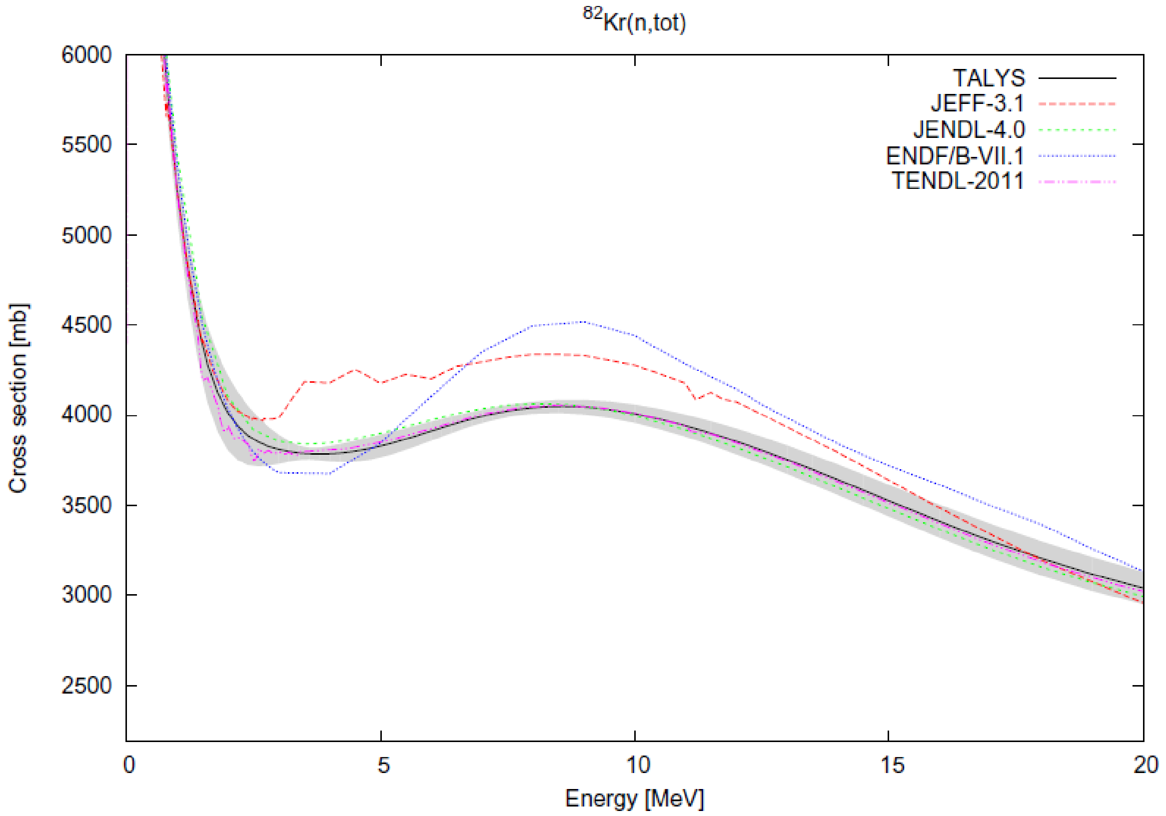
- Experimental approach can be infeasible for many nuclides.
  - The nuclide in question may not be easily producible
  - The nuclide may have a short half-life
  - Difficulties differentiating between reaction channels

- Exhaustive, high quality experimental data sets are only available for relatively few reaction channels.
  - Most nuclides rely solely on default model calculations
  - Quality of the data for these nuclides is questionable at best

Nuclear Data: Sources of Uncertainty

- Nuclear model parameters are calibrated by attempting to reproduce the experimental data of a given data set.
  - Experimental data is uncertain → model parameters are uncertain too.
- Nuclear models are also subject to many shortcomings.
  - No exact description of the strong interaction
  - No exact solution to the many-body problem

Which Library Has It ”Most Right”?



Nuclear data: Sources of uncertainty

- Problem: It is currently not well known how much of an impact the nuclear data uncertainties can have on the output of Serpent.
  - If there just was a way to realistically perturb nuclear data files within their respective error margins...
  - This would allow us to capture the nuclear data uncertainties in the variance of the results of Serpent…
- Fortunately this process has been outlined and there is a software package designed for producing random nuclear data files.

Total Monte-Carlo

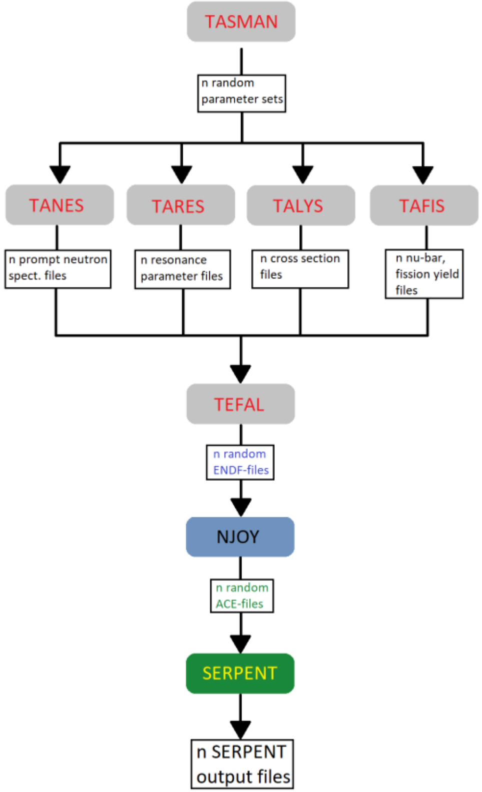
- The idea behind the Total Monte-Carlo method is rather simple:
  - Produce hundreds of perturbed nuclear data files for key nuclides
  - Assign a random combination of files for a particle transport simulation
  - Repeat this hundreds of times, and collect results.
  - The variance in the output of the particle transport simulation contains contribution from two sources: the Monte-Carlo variance and the additional variance arising from the perturbed nuclear data. Differentiate between these.
  - Quantify uncertainty in some output quantity with an appropriate statistic.
- The perturbed nuclear data files are produced with a software package called T6.

T6 Software Package

- A set of nuclear codes designed for the evaluation of nuclear data
  - Main set of codes: TALYS, TANES, TARES, TEFAL, TASMAN, TAFIS
- TENDL-libraries are produced with these
- The package also contains plenty of other well known nuclear physics codes…
  - Physics validations, format validations, data processing
- … and a massive compilation of nuclear data from existing libraries (EXFOR, ENDF/B-VII.0,…)
- Currently under development: Only available from the developers
  - Plenty of bugs and incompatibilities ☹

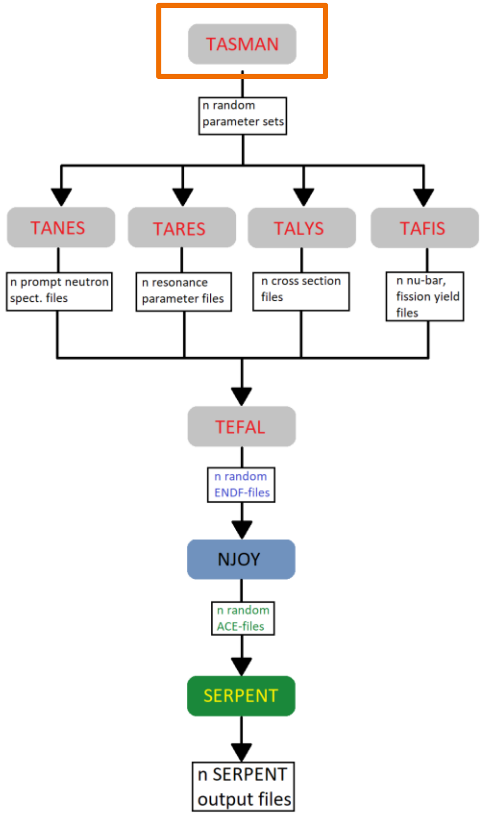
Production of random nuclear data

- The process of producing random nuclear data differs between nuclides and reaction channels significantly.
  - Variations in nuclear model parameters
  - Uncertainties from experimental data
  - Model calculations, normalization to experimental data
  - Adoption of data from ENDF/B-VII.0 (Light nuclides)
- Correlations between the nuclear model parameters are taken into account with a binary accept/reject method
  - Only if all model-predicted values fall within the uncertainty ranges of experimental data, is the produced file accepted.



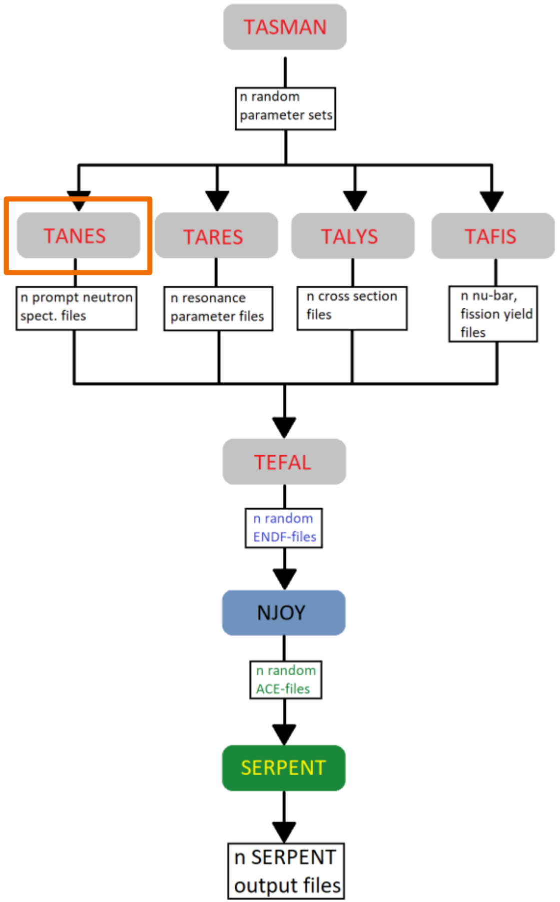
TASMAN

- Randomizes inputs for TALYS, TANES, TARES, TEFAL.
- Rejects produced data file if experimental error margins are not respected.
  - Normalization to experimental data is performed for some reaction channels.
- Calculates covariance data
  - Included in the random ENDF-files



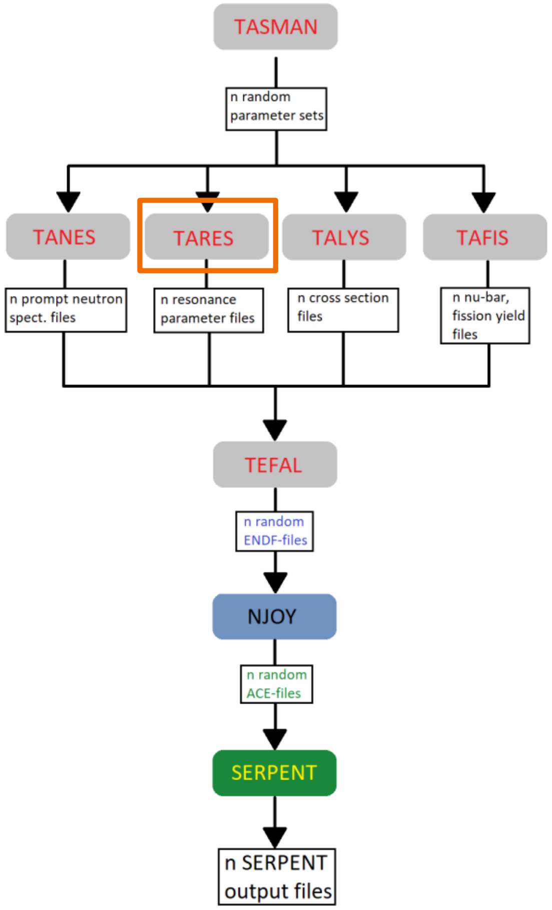
TANES

- Responsible for producing data for neutron energy spectra from fission
- Los Alamos model with random sampling in
  - Total released energy
  - Total released kinetic energy
  - Multi-chance fission probabilities



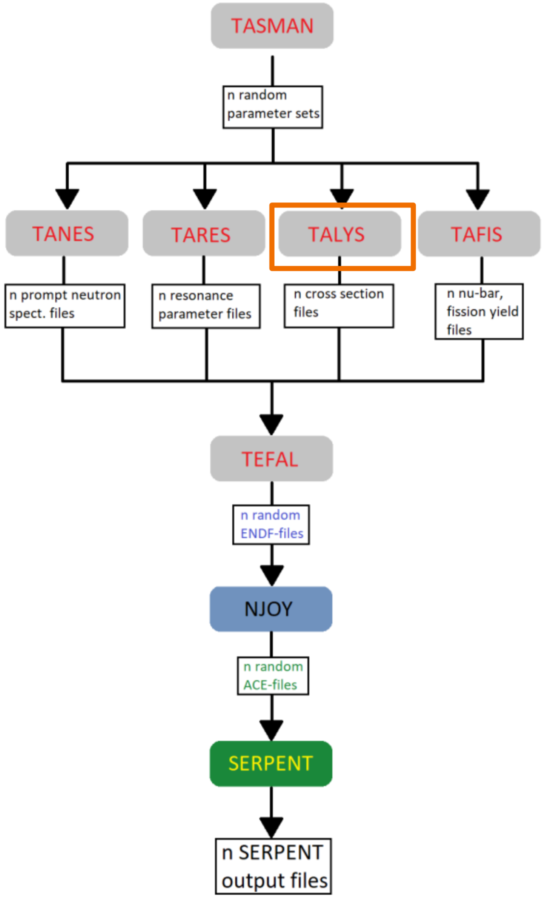
TARES

- Responsible for producing resonance parameters.
  - These are of importance in cross section reconstruction performed with NJOY.
- Resonance parameters can not be predicted from theory.
- If experimental data is available:
  - Adopts data from existing libraries and assigns variations from within error margins.
- If experimental data is not available:
  - Guesses the resonance parameters.



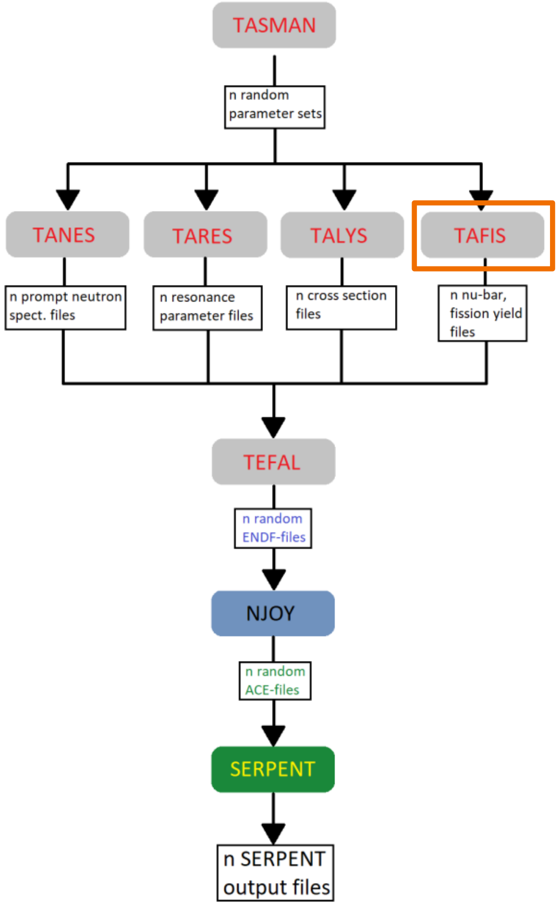
TALYS

- Responsible for predicting cross sections in the 1eV – 200 MeV energy range.
  - Optical model for direct reactions (etc. elastic scattering)
  - Compound nucleus model for absorption reactions
- Can not simulate nuclides with mass number less than 12.
  - Automatically adopts data from ENDF/B-VII.0
- Uncertainties from nuclear model parameter variations.
  - Pre-specified variances for each parameter.
  - Supports uniform and normal distributions.



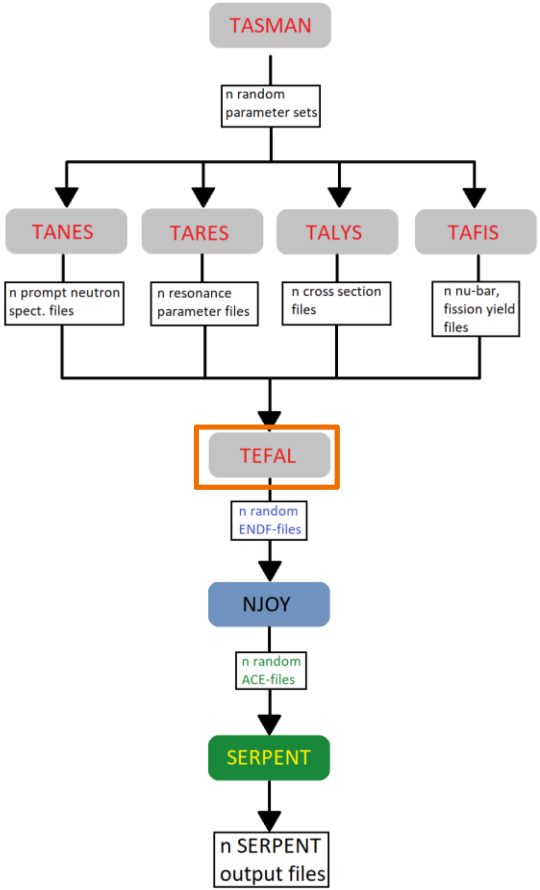
TAFIS

- Responsible for calculating Nubar data for prompts neutrons
  - Based on Wahl's systematics
- Currently not capable of generating Nubar data for delayed neutrons
  - This data is adopted from existing libraries
- Also capable of producing fission yield data
  - However this feature has been disabled due to bad performance.
  - Meaning that random fission yield files are currently out of reach.



TEFAL

- Responsible for converting the output from TALYS, TANES, TARES, TAFIS into ENDF-format
- This is a necessary step in the data processing routine for the correct input for NJOY

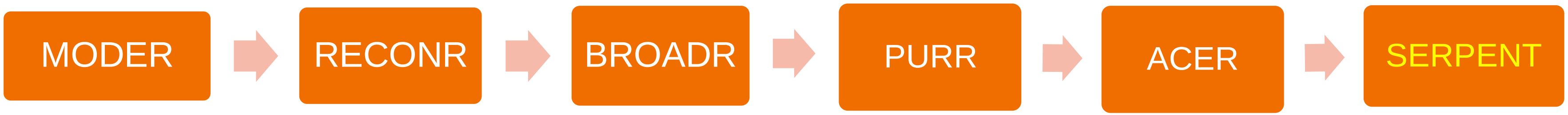


Processing ENDF into ACE

- The produced ENDF files contain randomized data in:
  - Cross sections (MF3), Angular distributions (MF4), Nubar and energy released per fission (MF1), Resonance parameters (MF2), fission neutron spectrum (MF5), double differential data (MF6), isomeric data (MF8-10) and gamma production data (MF12-15)
- The ENDF formatted cross section data can not be applied directly to Serpent
  - The data processing is automatically initiated after TEFAL (and a few other programs) have finished.
  - Manual use of NJOY is also a must, since we usually wish to have cross section files in multiple temperatures.

Processing ENDF into ACE

- Njoy consists of different modules
- The essential modules are
  - MODER (Blocked binary conversion)
  - RECONR (Resonance reconstruction)
  - BROADR (Doppler broadening)
  - ACER (Data conversion, correction check)
- PURR module should be enabled for major actinides
  - Generates probability tables which are used to treat self-shielding in the unresolved resonance range



T6 in practice

- The data production process can be initiated by calling a shell script AUTOTALYS
- The input follows a typical key – value format

```
[lovlauri@espnr130 ~]$ autotalys -element Am -mass 242 -ntalys 200 -Liso 1 -Ltarget 1
-noplot -seed 15179176  -binsrand 60 -low -noclean  -noresbase -nonubarbase -nofnsbase
.
```

  - 200 random files for the first excited state of Am-242 with 60 energy bins…
- Calculation time varies significantly between nuclides
  - 200 replications can take between 24 hours and 4 weeks.
  - Random files for U-235, U-238 and Pu-239 were taken from web due to long production times.

So what was done?

- 200 random cross section files were produced for 43 nuclides:
  - Transuraniums (Np, Pu, Am, Cm isotopes)
  - Structural materials (Iron, Nickel, Zirconium, Tin…)
  - Important fission products
  - O-16
- 500 random files were adopted from TALYS-website for:
  - U-235
  - U-238
  - Pu-239
- The adopted files were processed with the same NJOY settings as used by the T6.

So what was done?

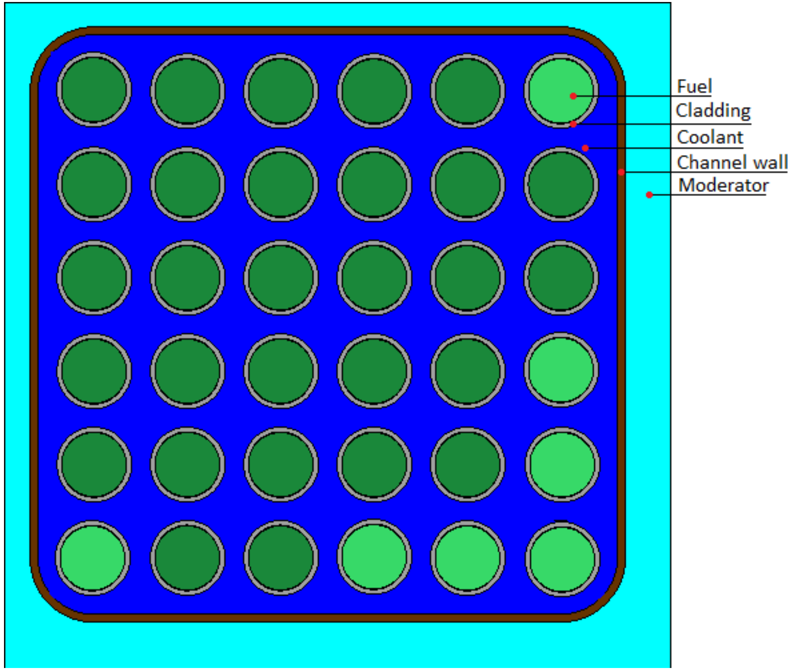
- A reference database of nuclear data was set up for a reference calculation set.
  - To estimate the Monte-Carlo variance.
- The most natural approach was to use the newest TENDL-library.
  - These files have been produced with the codes in T6.
  - 72 nuclides were chosen, these included the set of randomized nuclides, as well as other necessary nuclides for the construction of the model.

So what was done?

- In total 5 calculation sets were calculated.
  - A reference calculation set (500 reps) with the TENDL-library.
  - An ”all varied” calculation set where the data was varied for the 43 nuclides (200 reps).
  - 3 calculation sets where U-235/U-238/Pu-239 were varied individually (500 reps each).
- The varied files were placed on top of the TENDL-library.

The Serpent model

- A 6x6 fuel assembly of a decommisioned BWR-reactor Gudremming A.
- Accompanied with three reactor shutdowns at 5.8, 12.0 and 17.5 MWd/kgU.
- Burnup steps were extended to 80 MWd/kgU.
- A decay calculation was initiated from 50 MWd/kgU.



Dark green depicts 2.53 % U-235 enrichment. Light green 1.87 %.

What was studied?

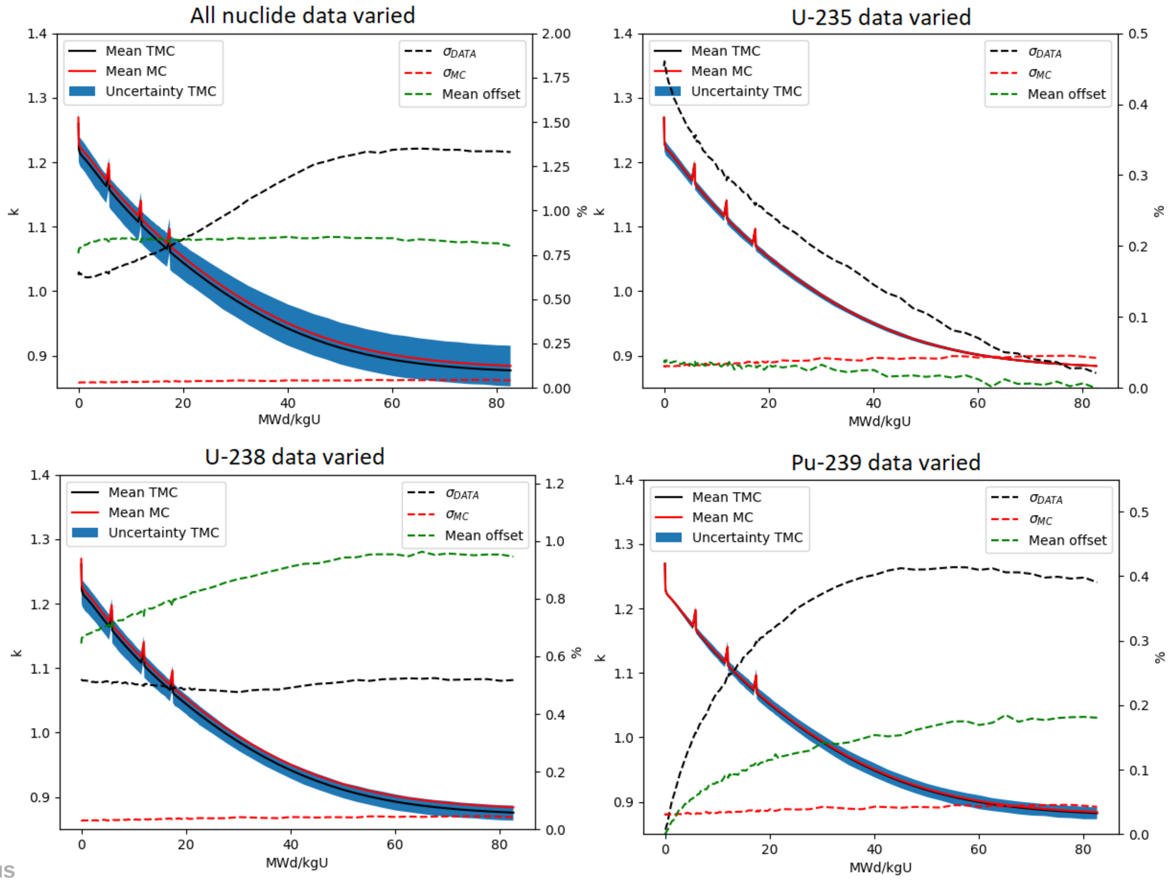
- The analysis was focused on multiplication factor and decay heat.
  - Motivated by reactor safety and the storing of nuclear waste.
- The variance in the studied output quantity has contribution from two sources:
  - Monte-Carlo variance
  - Varied nuclear data
- Monte-Carlo variance was estimated with the reference calculation set. The ”total” variance was estimated with calculation sets where data was varied.
  - The contribution from data can be obtained by substracting latter from the former.
- Measure of uncertainty: Relative standard deviation

$$\sigma^2_{TOT} = \sigma^2_{DATA} + \sigma^2_{MC}$$

$$\sigma_{DATA} = \sqrt{\sigma^2_{TOT} - \sigma^2_{MC}}$$

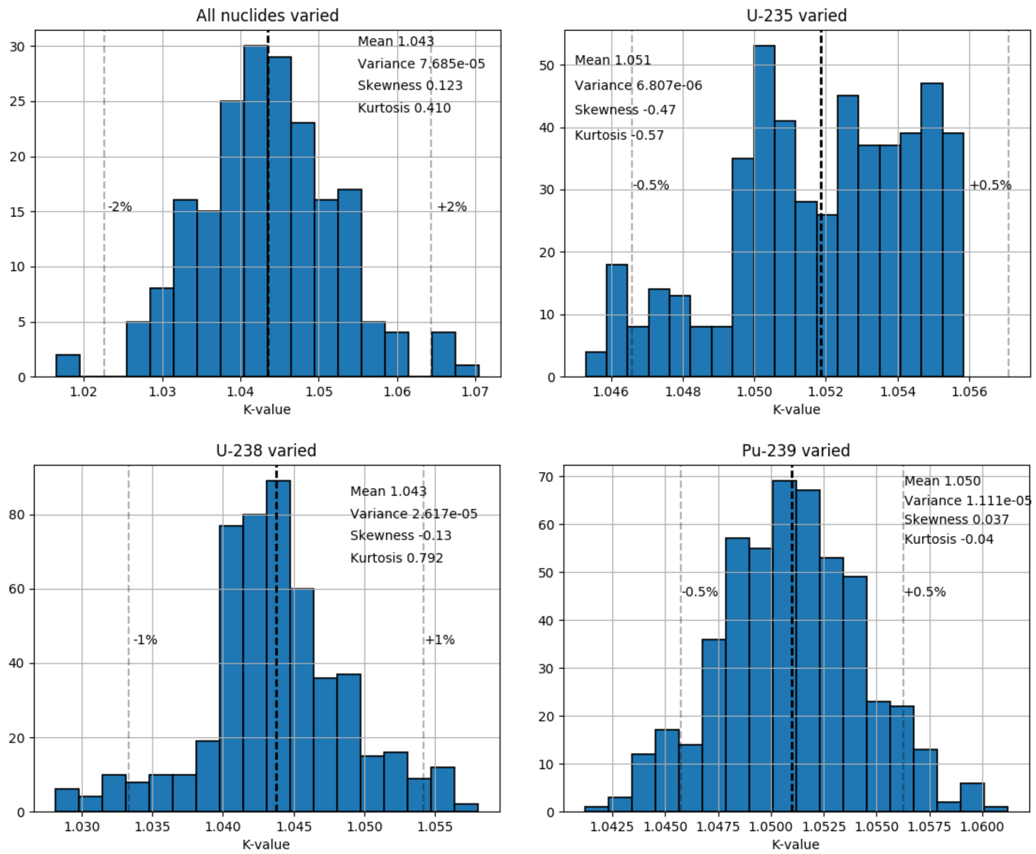
Results: K-value

- Data variance dominated over Monte-Carlo variance
- Significant spread when all of the data was varied simultaneously
- Reactor shutdown are visible as spikes in the plots



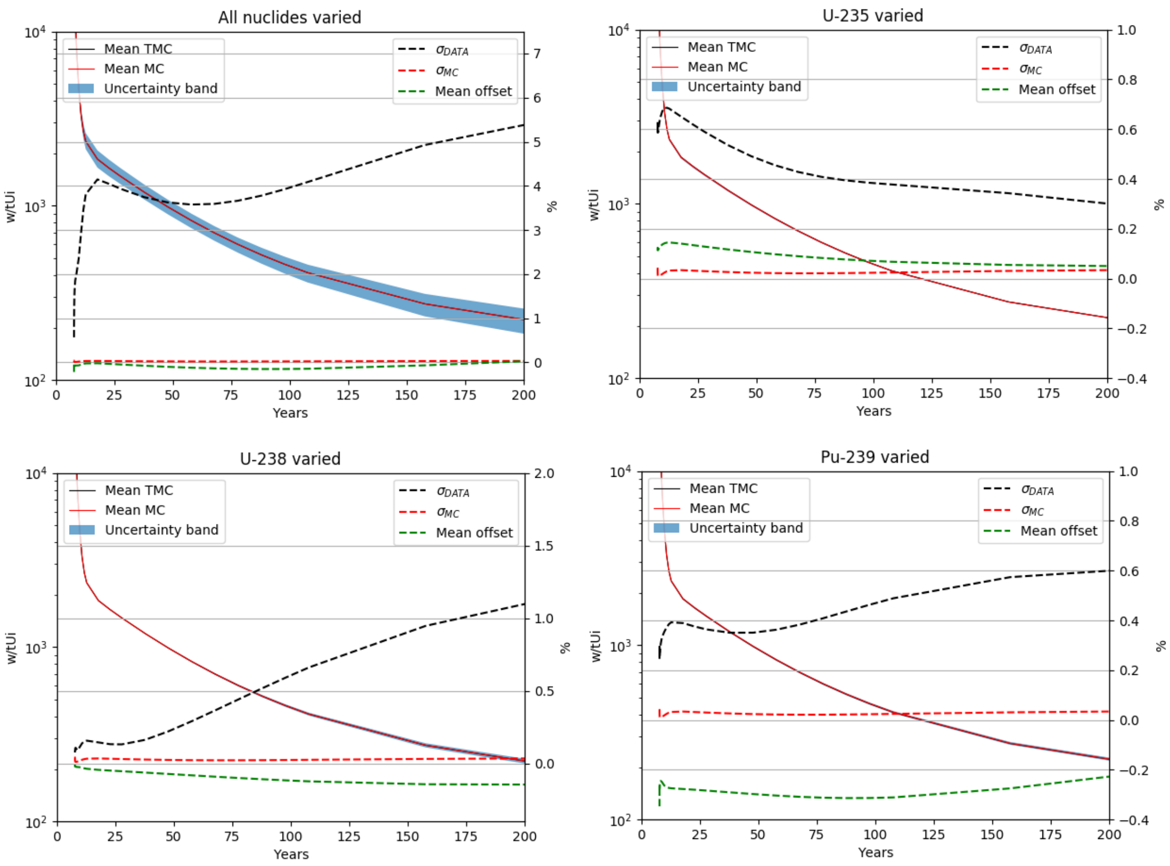
Results: K_{eff}

- Snapshots of the k_{eff} -distributions at 20 MWd/kgU
- Surprisingly different shapes for the distributions
- U-238 varied set exhibited most outliers

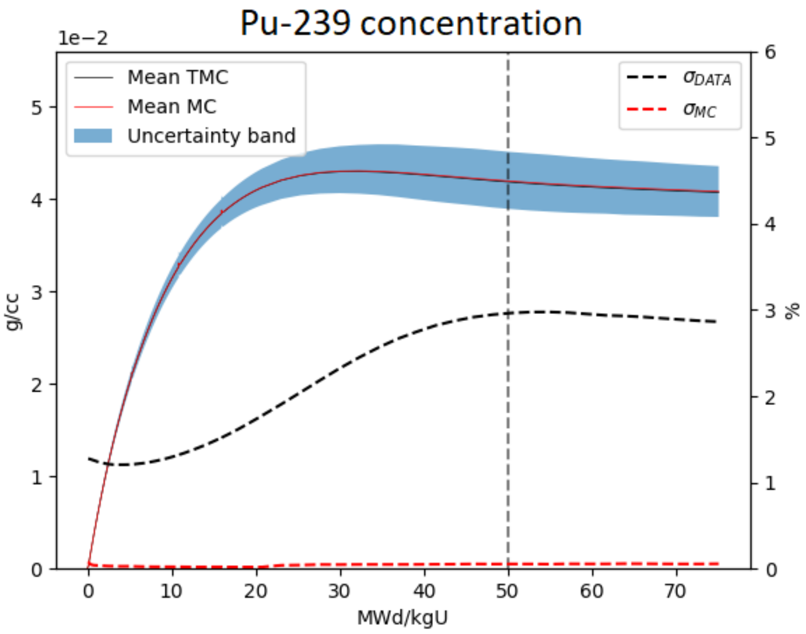


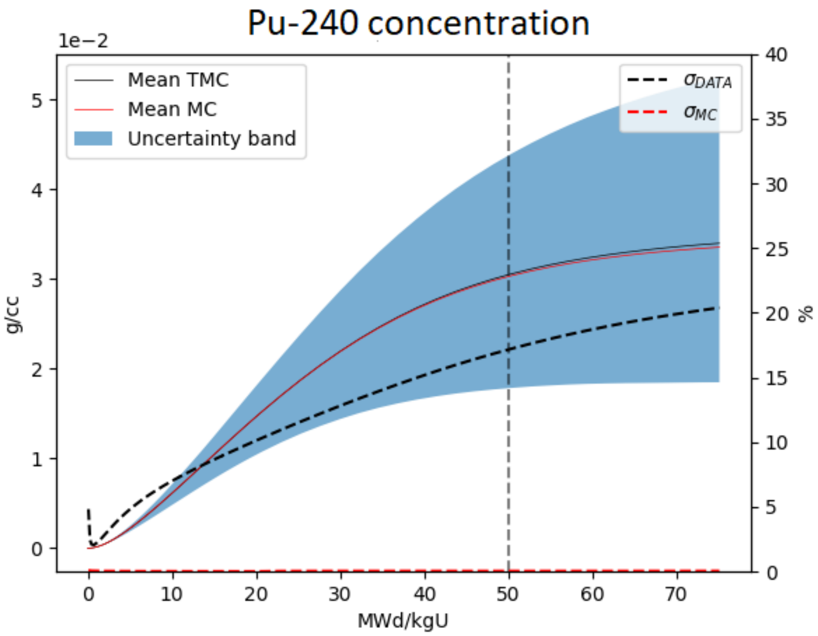
Results: Decay heat

- Early decay times may be off since fission yield uncertainties were not considered in this project
- Significant uncertainties were found for transuranium concentrations post Pu-239
- These mostly explain the spread of Am-241 and Pu-240 concentration at 50 MWd/kgU.



Pu-239 & Pu-240 concentrations



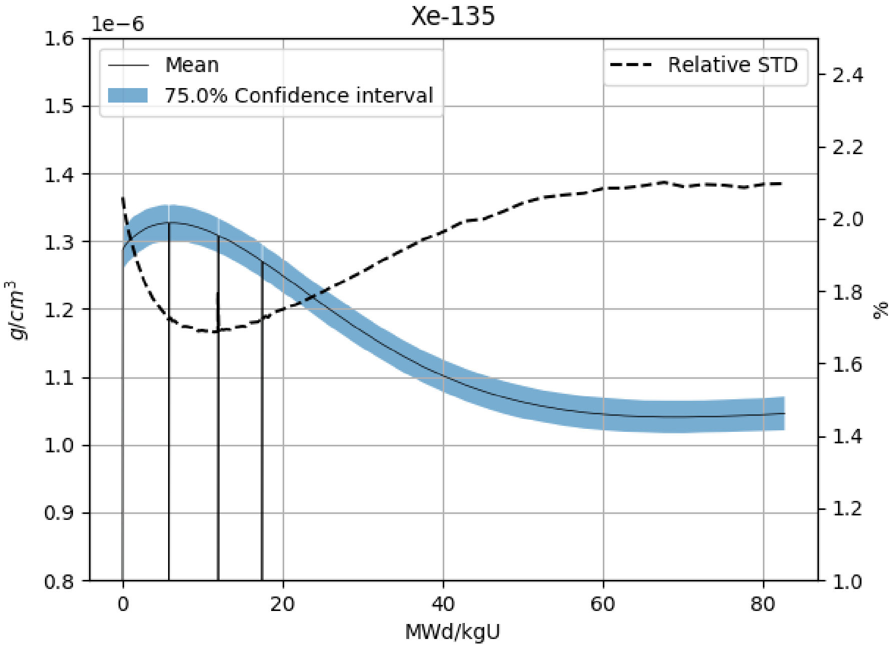


Key findings

- Nuclear data uncertainties pose significant uncertainty to the output of Serpent
- Pu-240 cross section data produced with T6 is subject to significant variations.
- Relative std for K-value peaked at: ~1.2%.
- Relative std for decay heat peaked at ~5.2%

How is the project continued?

- The study is extended to cover fission yield uncertainties.
- Random fission yield files available on the TALYS-website (produced with the GEF-code)
- Preliminary results have been obtained



Xe-135 concentration and uncertainty from 500 calculation with FY-variations in U-235, U-238, Pu-239 and Pu-241.

beyond the obvious

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