DE LA RECHERCHE À L'INDUSTRIE



Comparisons between a priori Uncertainty Quantification and Calculation/Measurement Discrepancies Applied to the MERCI UO2 Fuel Rod Decay Heat Experiment.

Sébastien LAHAYE, Tan Dat HUYNH, Aimé TSILANIZARA, Jean-Charles JABOULAY, Stéphane BOURGANEL

Commissariat à l'Énergie Atomique et aux Énergies Alternatives

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Results on Concentrations

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MERCI experiment

In 2008, an UO_2 fuel rod was irradiated up to $\sim 3.5 GWd/t_{HL}$ in the CEA/Saclay research reactor OSIRIS through the MERCI experiment. Some rod's pellets were analysed.
Experimental results were obtained:

- fuel rod decay heat measurement by calorimetry (cooling times from 27 minutes to 42 days),
- evaluation of the amounts of some nuclei (U, Pu, Cs, Nd...) by isotopic dilution mass spectrometry,
- nuclide activities.

Experiment goals:

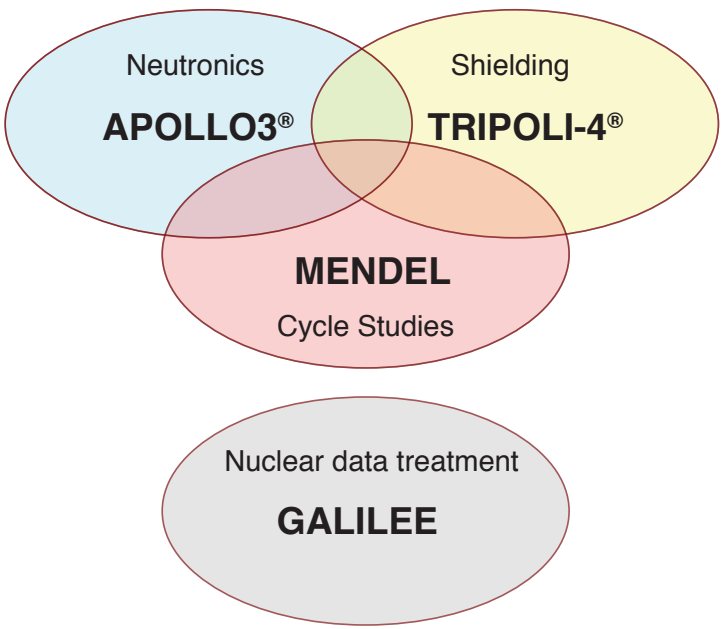
- CEA Fuel Cycle code systems validation
  - short decay times
  - small burnups
- Validation of the uncertainty propagation

CEA Fuel Cycle Code Systems

DARWIN/PEPIN2 [1] is the current industrial code system used by CEA, EDF and AREVA.

DARWIN/PEPIN2 & MENDEL

- Fuel Cycle,
- Dismantling,
- Criticity,
- Waste Management...



MENDEL [2, 3] is the successor of DARWIN/PEPIN2. Its Bateman equation solver is directly used by three CEA new generation codes: APOLLO3® [4], TRIPOLI-4® [5] and MENDEL itself.

CEA Fuel Cycle Code Systems

DARWIN/PEPIN2 is a stand alone code system. Neutron flux and cross sections inputs from APOLLO2 [6], TRIPOLI-4®, ECCO/ERANOS [7] or GENDF files.

MENDEL is either:

- a stand alone code for fuel cycle. Same scope as DARWIN/PEPIN-2. Neutron flux and cross sections inputs from APOLLO2, APOLLO3®, TRIPOLI-4®, ECCO/ERANOS or GENDF files
- a Bateman equation solver given to APOLLO3® and TRIPOLI-4®

Here, we use the stand-alone versions.

CEA Fuel Cycle Code Systems

DARWIN/PEPIN2 and MENDEL compute:

- **isotopic concentrations**,
- **activities**,
- **masses**,
- **decay heat**,
- decay particle sources (α, β, γ, n),
- radiotoxicity...

Those quantities can be observed at any time.

Nuclear data uncertainties can be propagated to physical quantities in bold letters.

MERCI Validation: Input data

In current study (validation on MERCI experiment measurements), DARWIN/PEPIN2.4 and MENDEL use the same input data:

- multigroup flux from an APOLLO2 calculation, equivalent to previous validation work [8],
- self-shielded multigroup cross sections from APOLLO2, completed by a GENDF library from JEFF-3.1.1 evaluation,
- DARWIN and MENDEL depletion chain for fuel application, with 2631 nuclei [2],
- decay data from JEFF-3.1.1.

Nuclear Data

Nuclear data can be used from any post treated evaluation.
JEFF-3.1.1 [9] is the current default evaluation, but ENDF/B-VII.1 [10] and JENDL2011 [11] decay data files have also been used [2, 12].

Uncertainty quantification [3] can be done propagating uncertainties due to the following nuclear data:

- independent fission yields (assuming correlations),
- radioactive decay periods (no correlations),
- radioactive decay energies (generally no correlations),
- radioactive decay branching ratios (sum=1),
- multigroup microscopic cross sections.

Uncertainties on Nuclear Data: correlations

In this study, we assume that there is no correlation between two different physical quantities.
Furthermore:

- **radioactive decay periods** and **radioactive decay energies** are two by two independant,
- **radioactive decay branching ratios** are correlated in such a way that the sum of branching ratios from a same father is equal to 1 without uncertainty,
- **multigroup cross sections** correlations are taken from COMAC data base [13],
- **independent fission yields** are chosen with:
  - sum equal to a constant (normalization)
  - taking into account the mass yields constraints.

Uncertainties on Nuclear Data: correlations

Example for radioactive decay branching ratios from one father isotope i to N daughter isotopes j:

$$\sum_{j=1}^{N} b_{j,i} = 1$$

Assuming the sum constant:

$$\mathrm{Var}\left(\sum_{j=1}^{N} b_{j,i}\right) = 0$$

Which leads to:

$$r_{jk} = \mathrm{const} = -\frac{\sum_{j=1}^{N} \mathrm{Var}(\mathrm{b_{j,i}})}{2\sum_{1\leq j<k\leq N}\sqrt{\mathrm{Var}(b_{j,i})\mathrm{Var}(b_{k,i})}}$$

Uncertainties on Nuclear Data

JEFF-3.1.1	Total of data	with uncertainties
decay periods	3626	3205
decay branching ratios	3052	525
α decay energies	1328	320
β decay energies	3170	1461
γ decay energies	3217	1418
independent fission yields	32752	32752
total	47145	39680

Table: Total number of nuclear data (mean values) and number of associated uncertainty data in JEFF-3.1.1 evaluation.

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- CEA Fuel Cycle Code Systems
- Nuclear Data Uncertainties

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UQ methods in DARWIN/PEPIN2.4 and MENDEL

CEA/DEN has developed two different approaches to propagate nuclear data uncertainties DARWIN/PEPIN2.4 and MENDEL outputs.

Deterministic approach in DARWIN/PEPIN2.4:

- creation of sensitivity profiles,
- direct forward first order perturbation method,
- launched through the INCERD module.

Stochastic approach in MENDEL:

- correlated samples created by URANIE [14],
- launched directly through MENDEL,
- creation of stochastic distributions.

DARWIN/PEPIN2.4 perturbation method

Deterministic perturbation propagation:

- first order forward perturbation,
- no adjoint calculation,
- **linearity hypothesis** or **small perturbation hypothesis**

The uncertainty propagation in DARWIN/PEPIN2.4 involves the supervisor module INCERD. INCERD gathers all user's data and uncertainties data of physical parameters and launches depletion calculating in parallel mode (using MPICH2/OPENMPI) to determine the sensitivity coefficient values ($S_{Y/X}$). Then, INCERD performs the uncertainty propagation as described through equation:

$$\mathrm{Cov}(Y) = S_{Y/X}\mathrm{Cov}(X)S_{Y/X}^{T}$$

DARWIN/PEPIN2.4 perturbation method

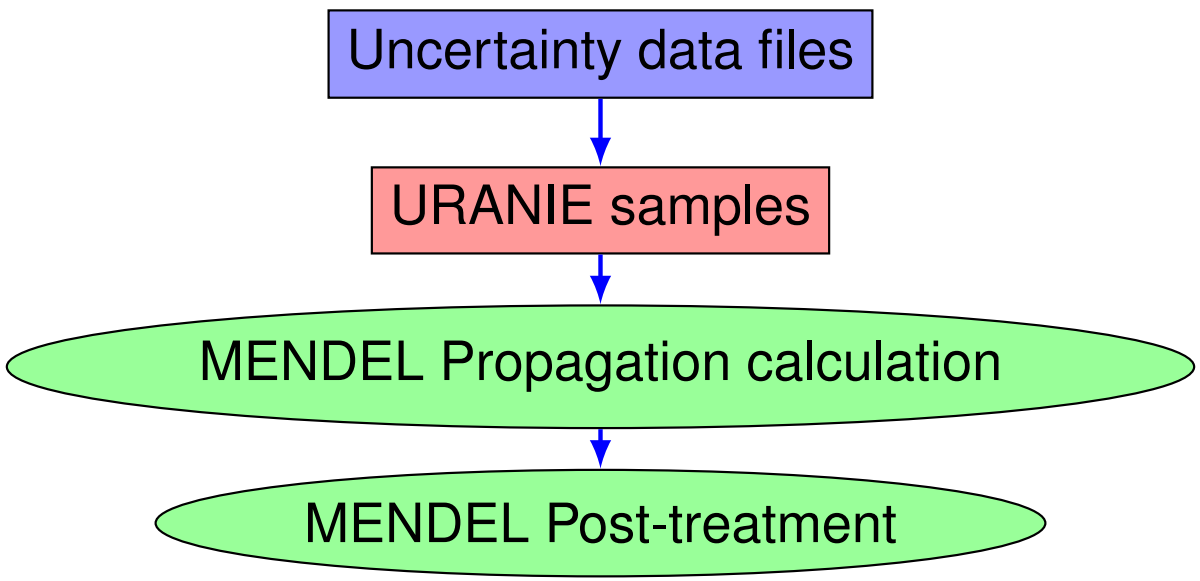
Equivalent to a One At a Time approach $\Rightarrow$ One computation needed per uncertain parameter.

Sensitivity is automatically achieved as a part of the method.

MENDEL method

Stochastic Monte Carlo sampling propagation method.

- sampling done through URANIE (CEA/DEN uncertainty platform),
- **Hypothesises on uncertainty laws**.
- all results shown here result from a use of 2000 realisations.



MENDEL method

Multigroup cross sections, **radioactive decay periods**, **radioactive decay branching ratios** and **radioactive decay energies** law:

- positively truncated Gaussian distribution if relative uncertainty is less than 50%,
- Log-Normal distribution if relative uncertainty is more than 50%,

Independent fission yields law:

- Log-Normal distribution.

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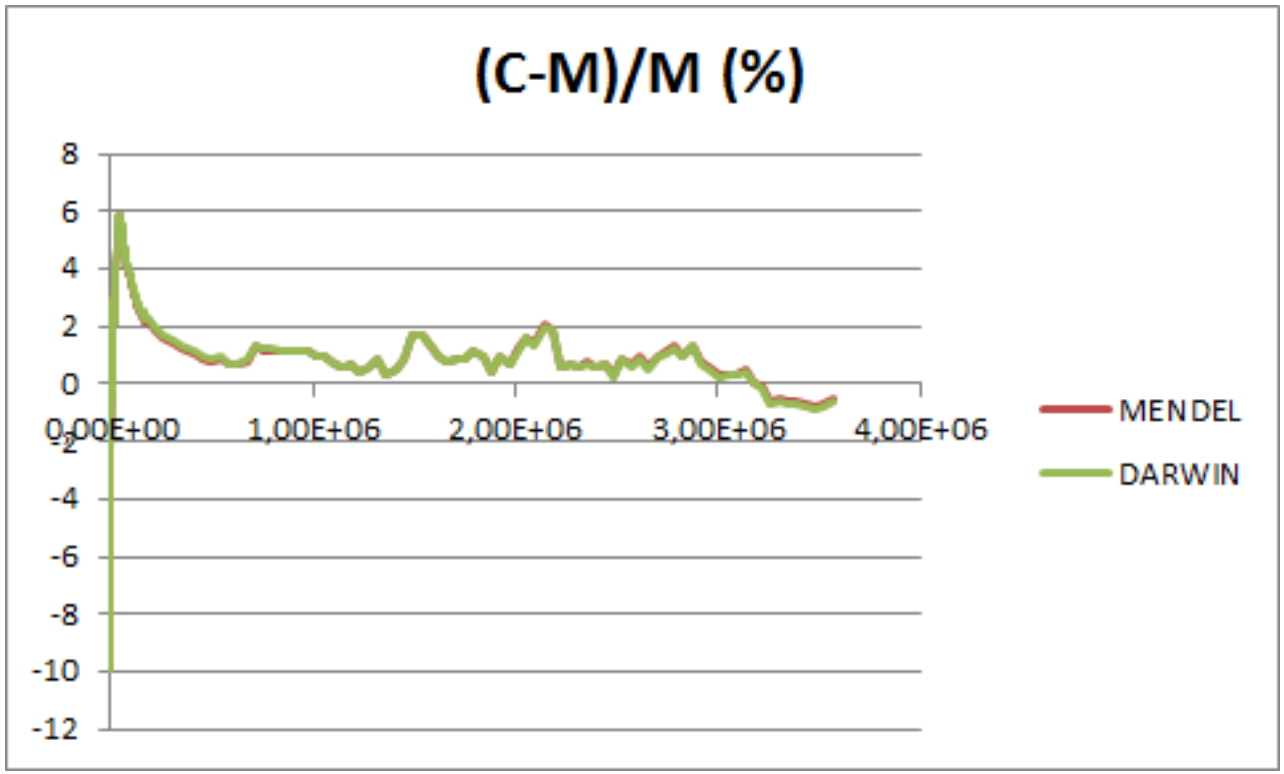
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Decay Heat computation validation

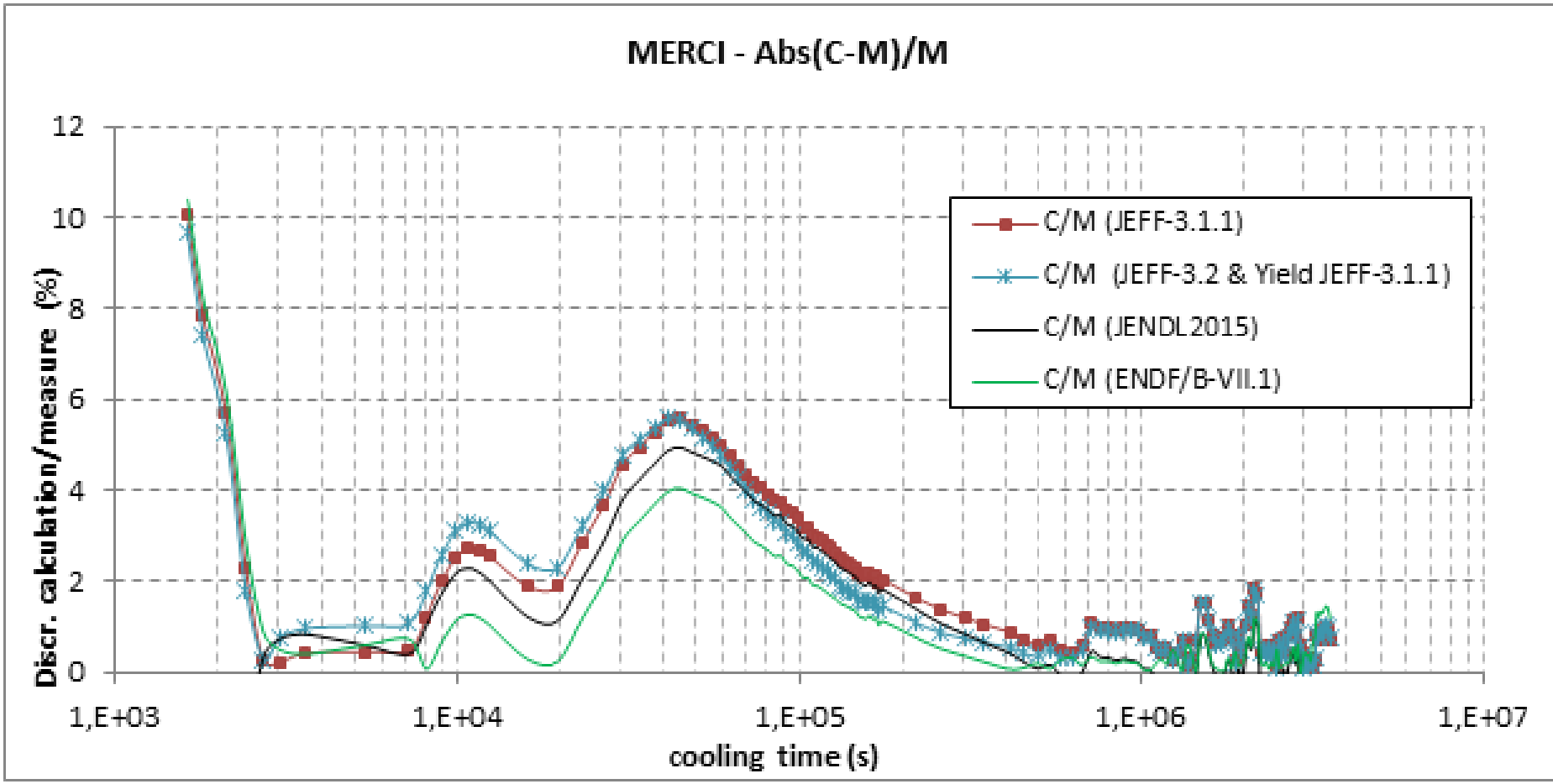


Decay Heat computation validation

We observe a relatively good agreement between calculation (C) and measurement (M).
Discrepancy observed for:

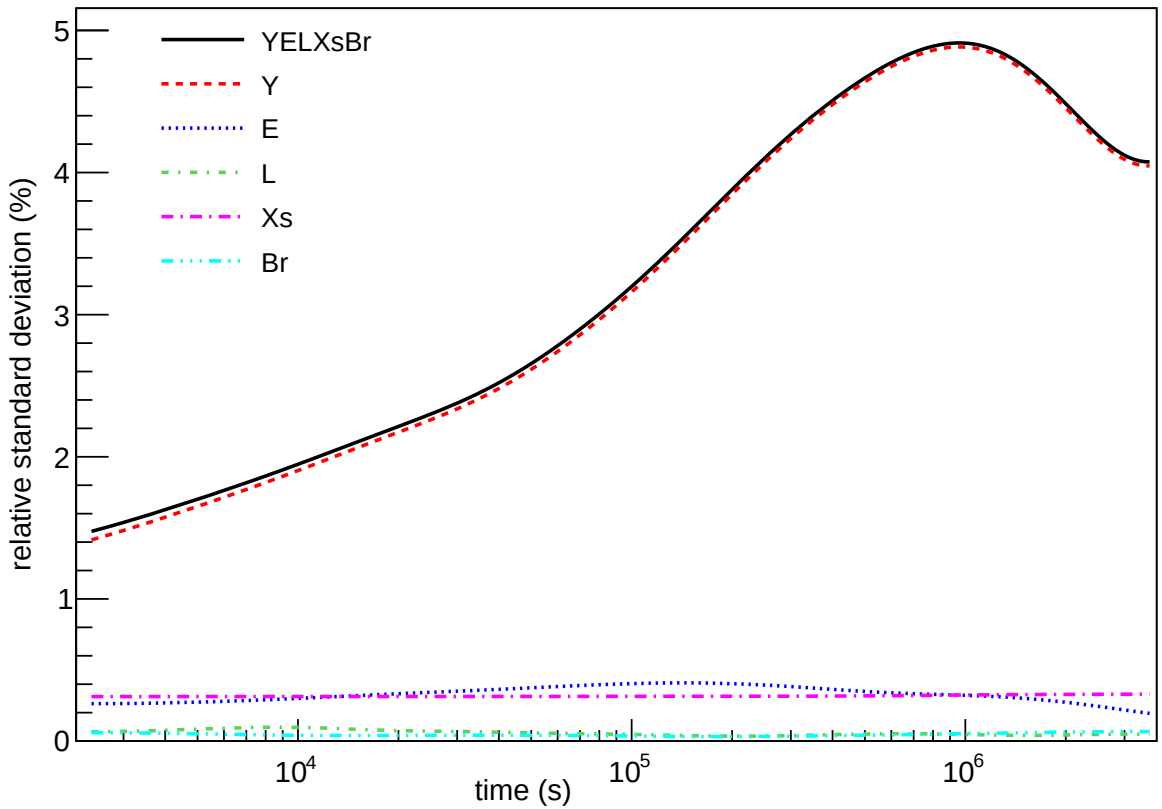
- Very short time, discrepancy attains 10%: due to an overheat during the first minutes of the measurement in the MOSAIC calorimeter $\rightarrow$ measures before 45 minutes are not to be considered.
- Around 12h30, we find the 6% discrepancy already found in the 2009 study. One idea at this time was a problem in JEF-2 library. Not solved by any modern evaluations, as shown in next slide.

Decay Heat computation validation



▸ contributors

Uncertainty Quantification on DH: sensitivity to parameters



Decay Heat uncertainty is mainly due to U235 thermal fission yields.

Hypothesis on fission yield correlations: sum constant.

UQ on DH vs Discrepancy to Measurement

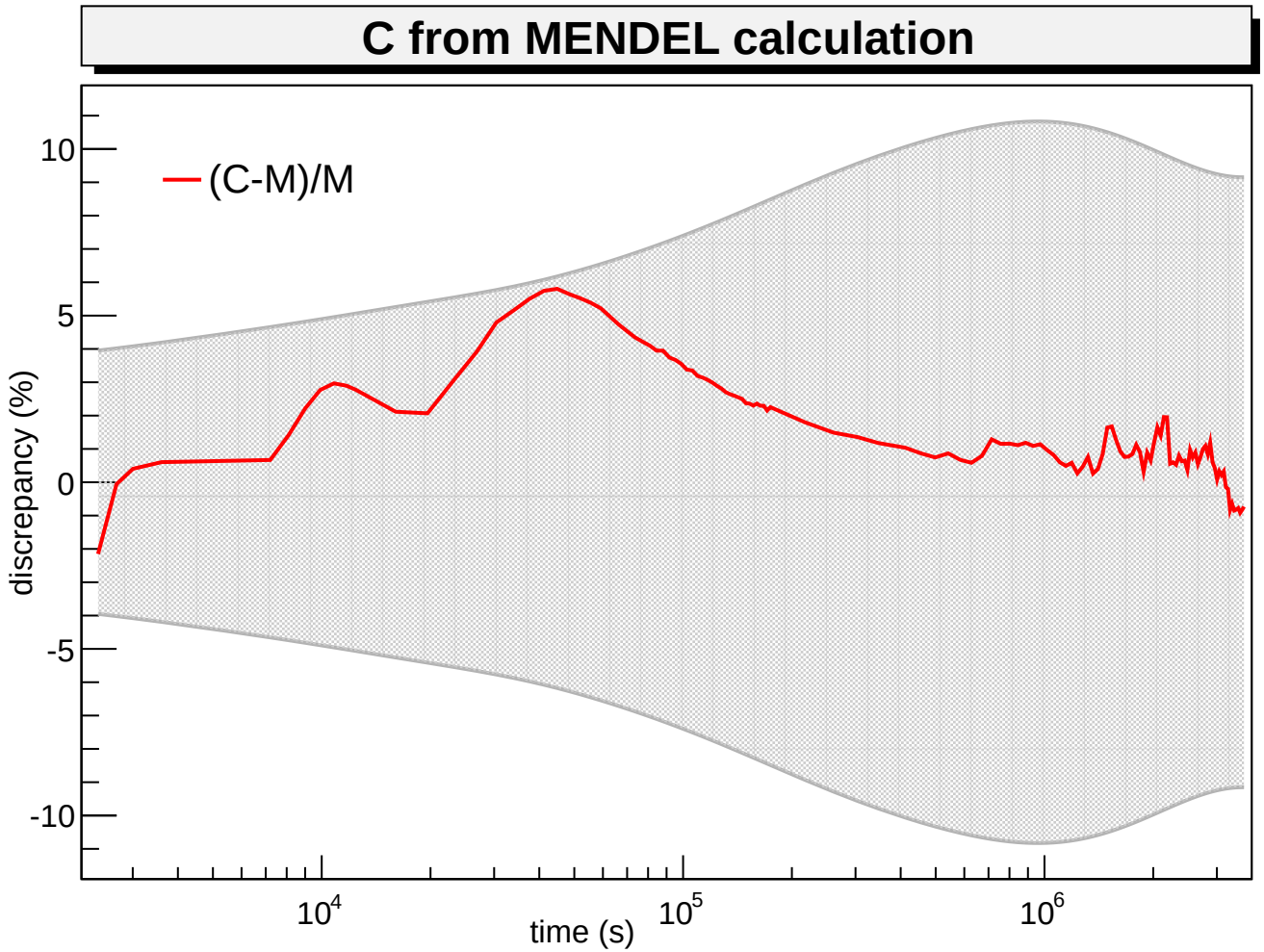
In next two slides:

- red curve corresponds to the relative discrepancy between computation and measurement,
- gray domain corresponds to the two standard deviation zone taking into account:
  - nuclear data uncertainty propagation
  - measurement uncertainty

If we consider Decay Heat as a Gaussian distribution, the grey domain is the 95% likelihood domain.

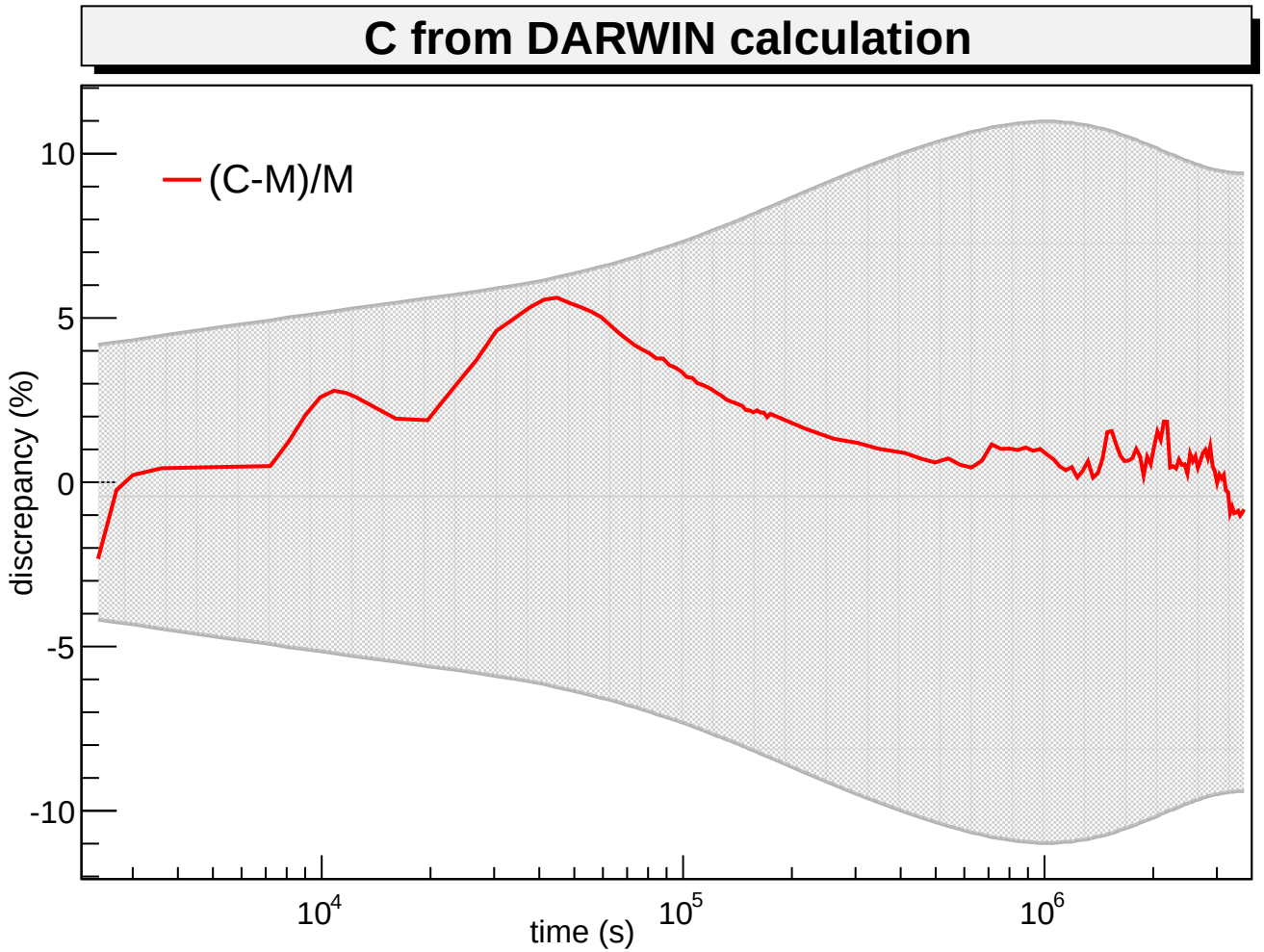
UQ on DH vs Discrepancy to Measurement

MENDEL

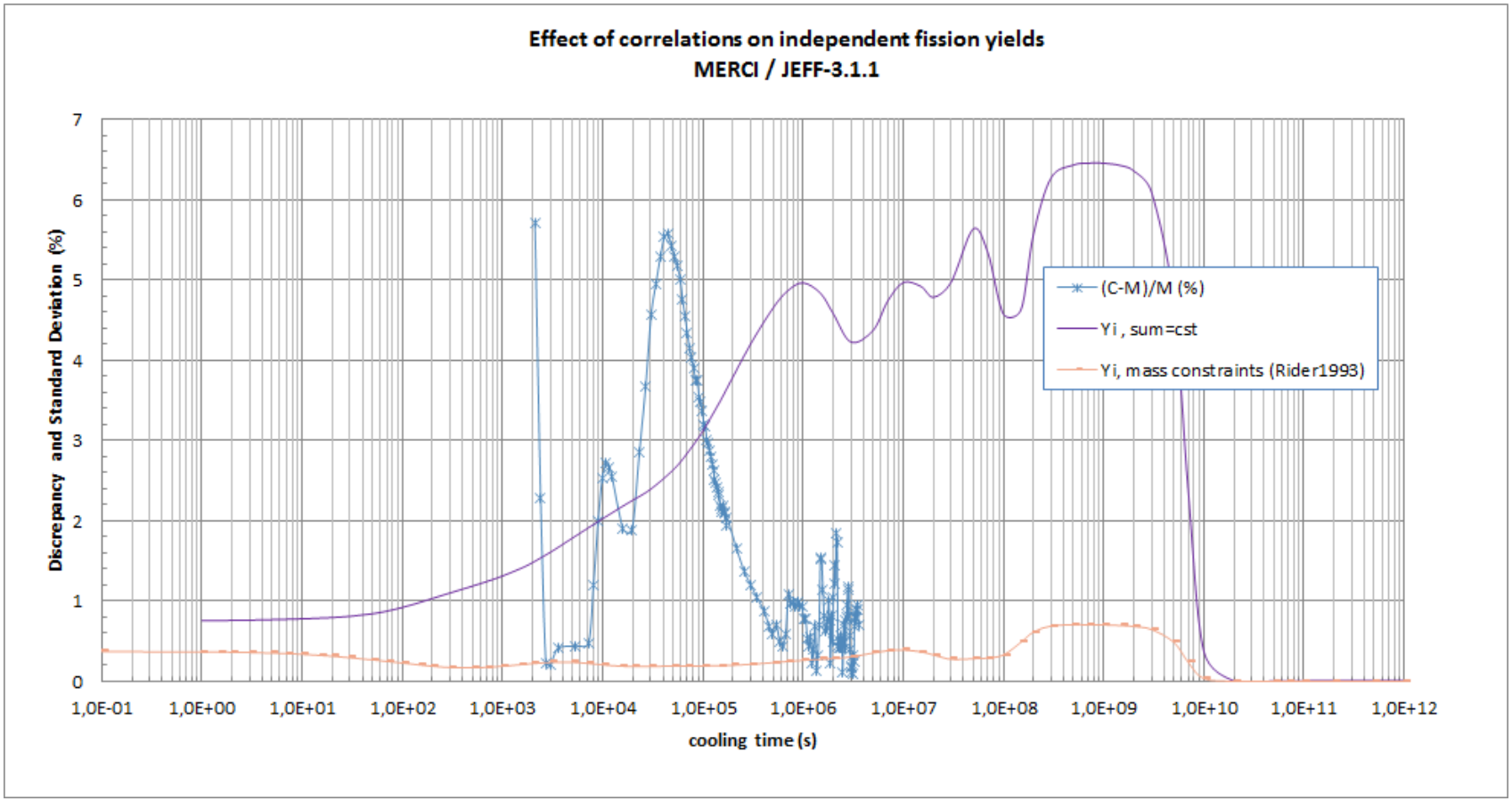


UQ on DH vs Discrepancy to Measurement

DARWIN



UQ on DH vs Discrepancy to Measurement



Important reduction of propagated uncertainty when taking into account mass constraints on fission yields $\Rightarrow$ (C-M)/M discrepancy is non longer in the two standard deviation (95% likelihood).

Isotopic concentration measurements

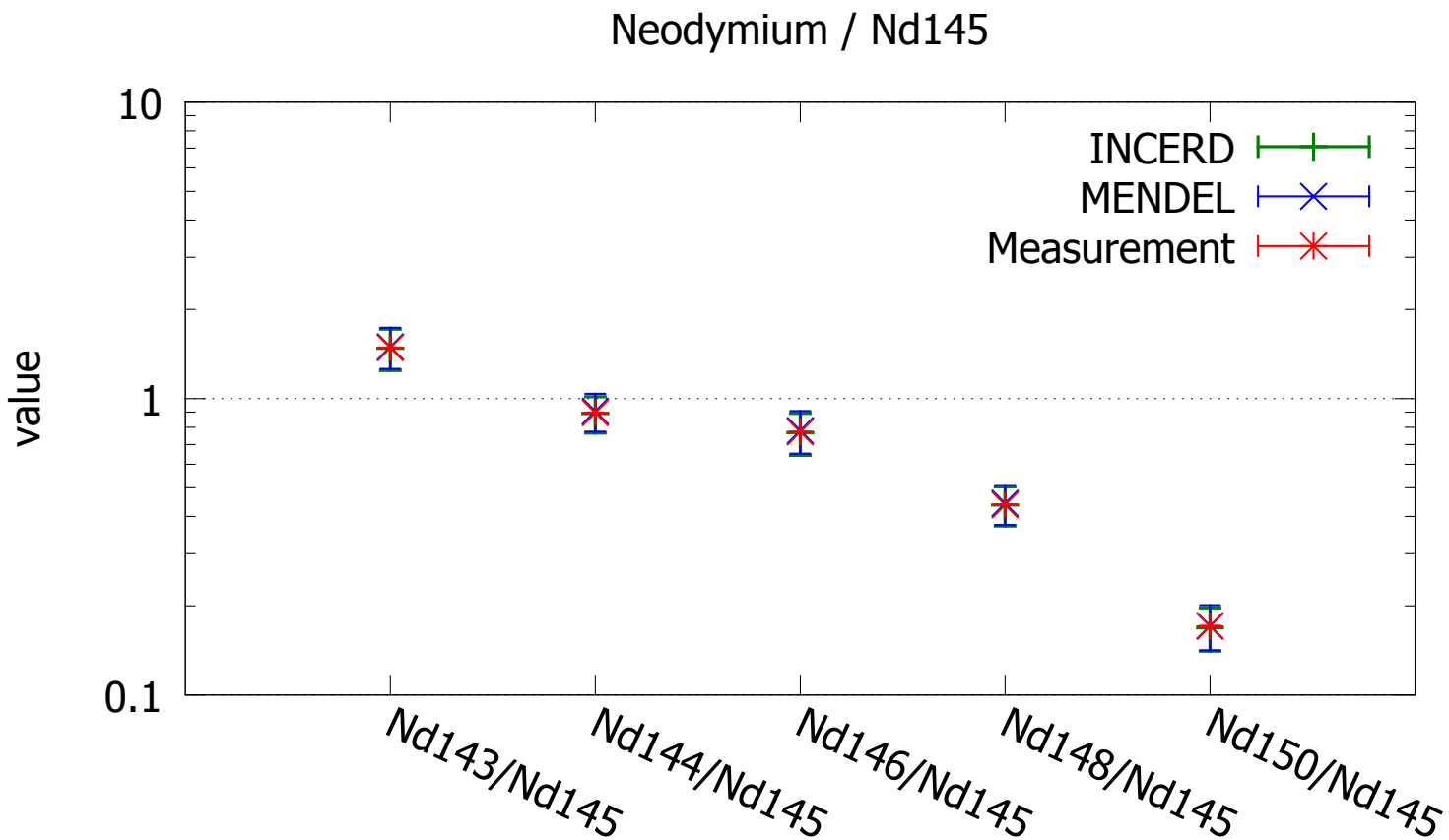
Fuel rod was dissolved and analysed at CEA.

Both heavy nuclides (U, Pu) and fission products (Cs, Nd) concentration ratios were measured.

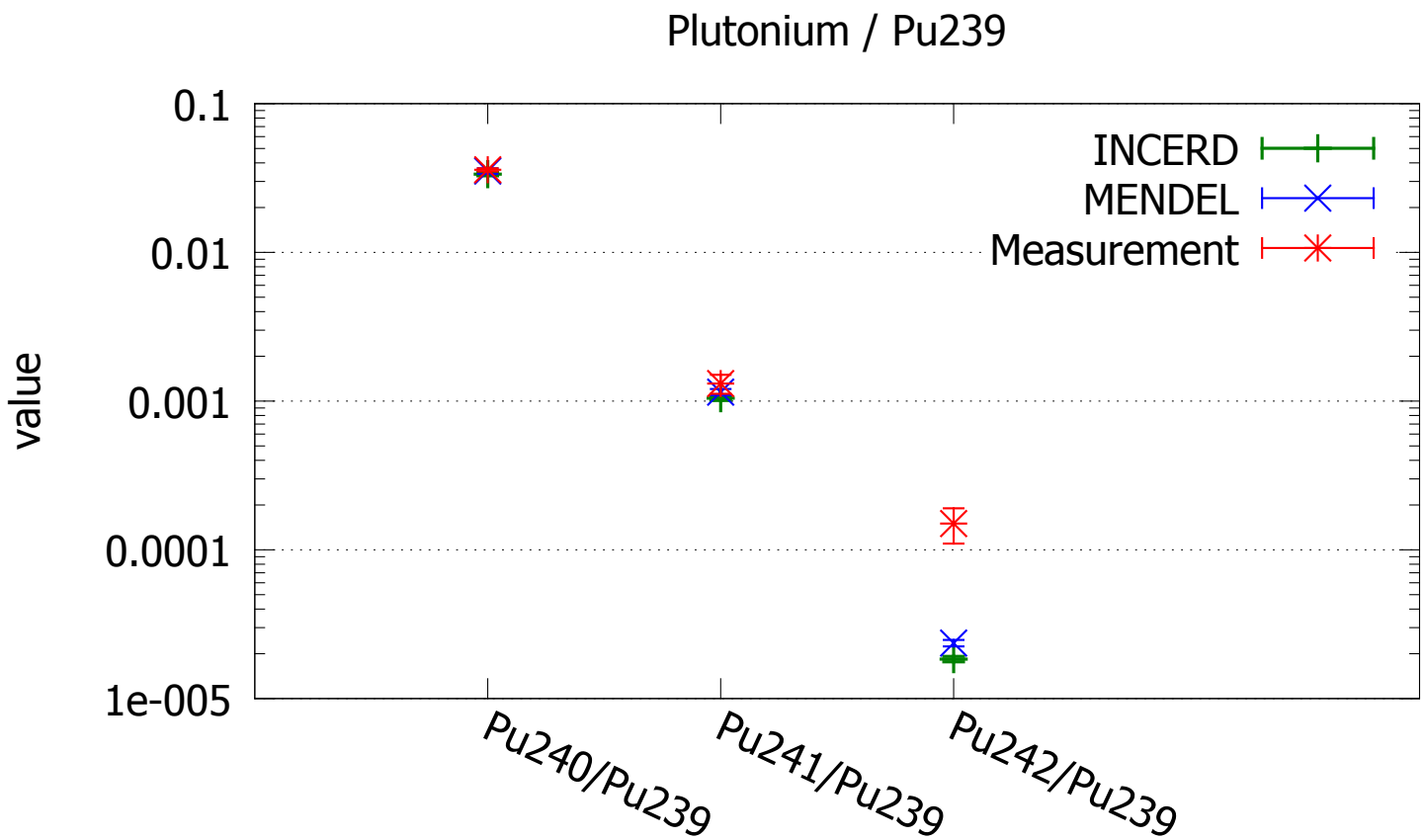
By using those data, we verify both the actual burnup and validate the uncertainty propagation to isotopic ratios for DARWIN/PEPIN2.4 and MENDEL.

We obtain good agreement for all ratios but Pu242/Pu239, certainly due to the very few amount of Pu242 in the pellet.

Isotopic concentration ratios: Neodymium



Isotopic concentration ratios: Plutonium



▸ others

Conclusion

Very good agreement between the two codes, and globally good agreement when comparing to MERCI experimental data.
This work is a new contribution to CEA fuel code system validation for uncertainty quantification.
Lack of data for correlation on independent fission yields.

Appendix

Decay Heat computation validation

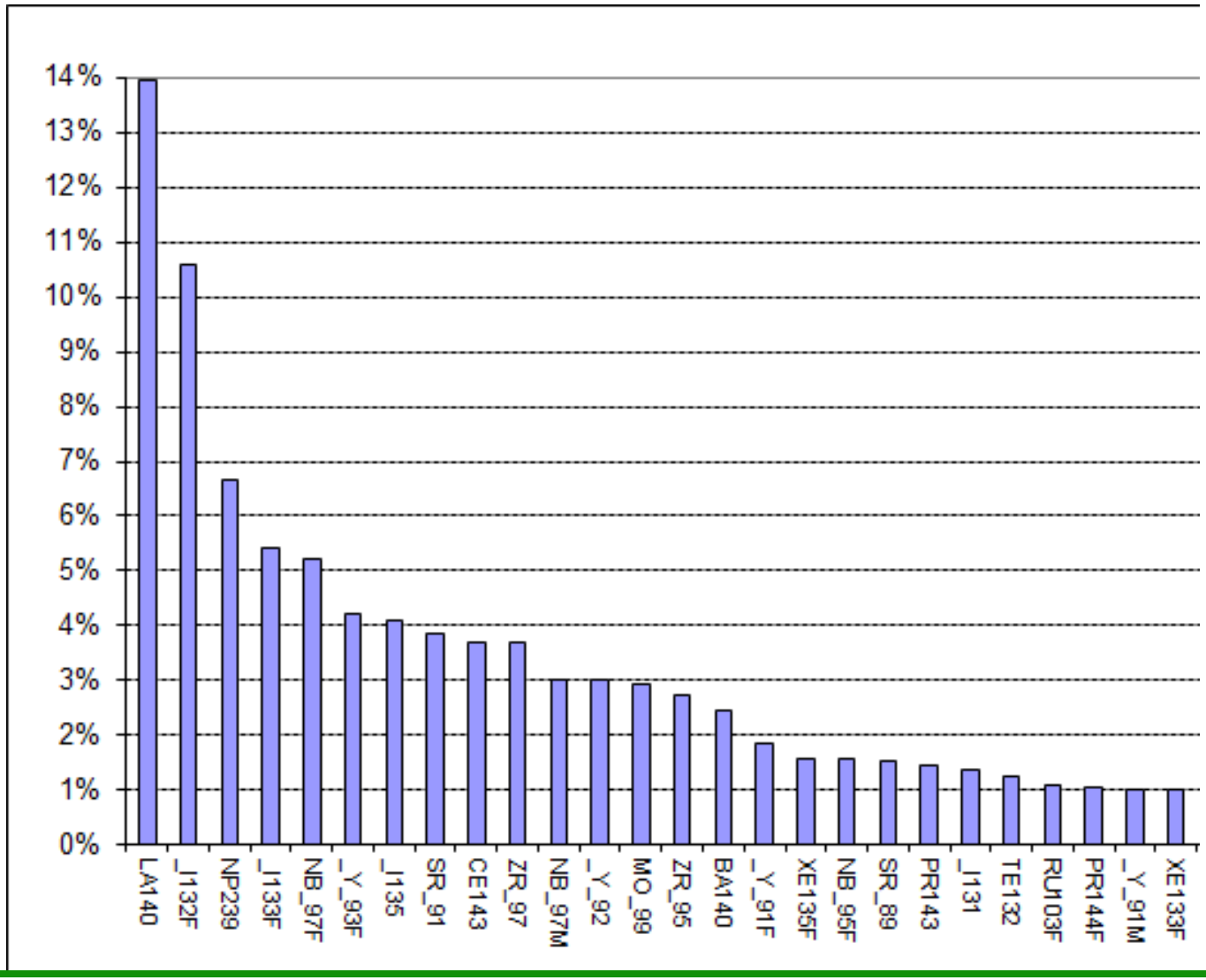
At 12h30, main contributors are:

13.97%	La140
10.58%	I132
6.66%	Np239
5.43%	I133
5.21%	Nb97
4.23%	Y93
4.09%	I135
3.86%	Sr91
3.68%	Ce143
3.68%	Zr97

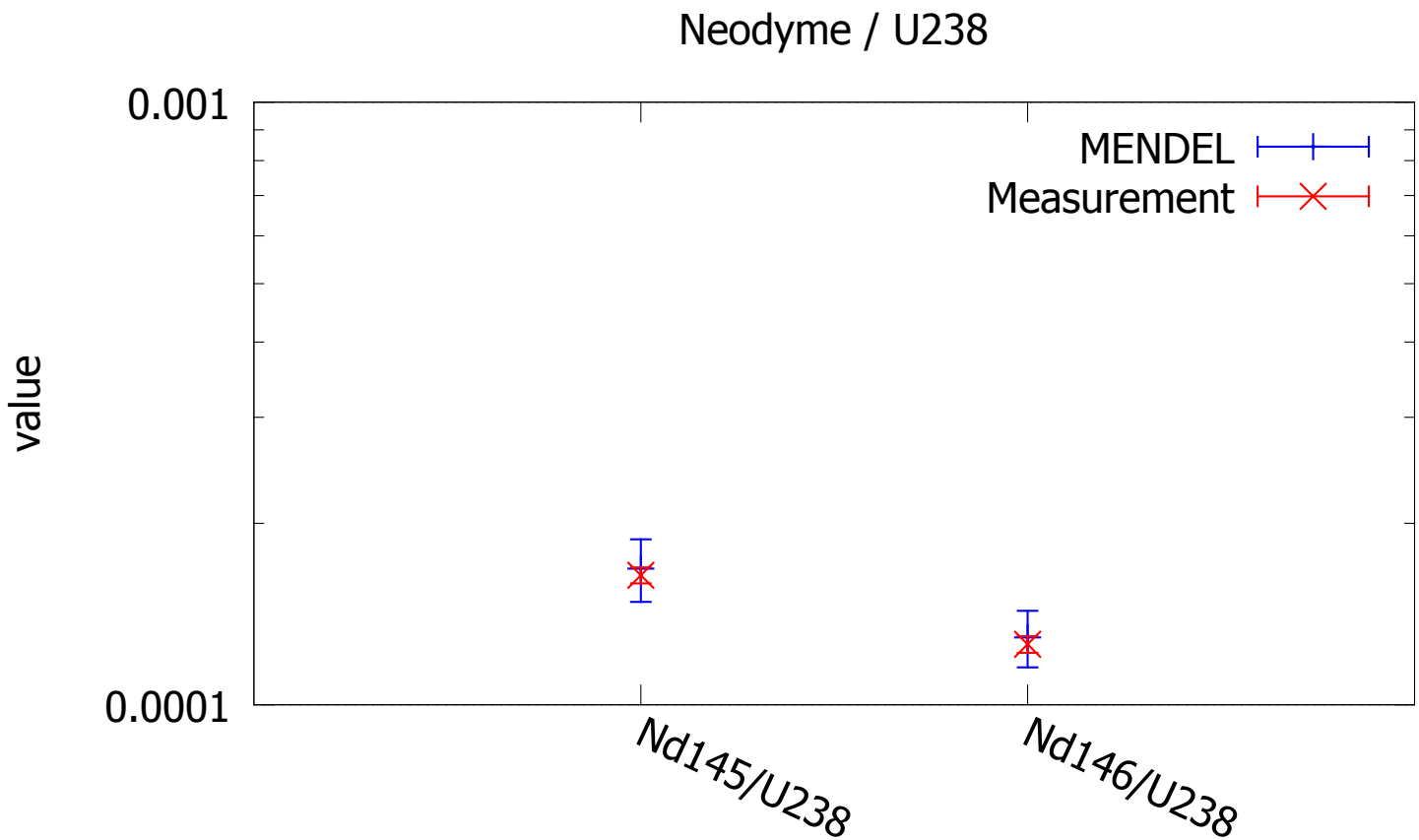
Decay Heat computation validation

At 12h30

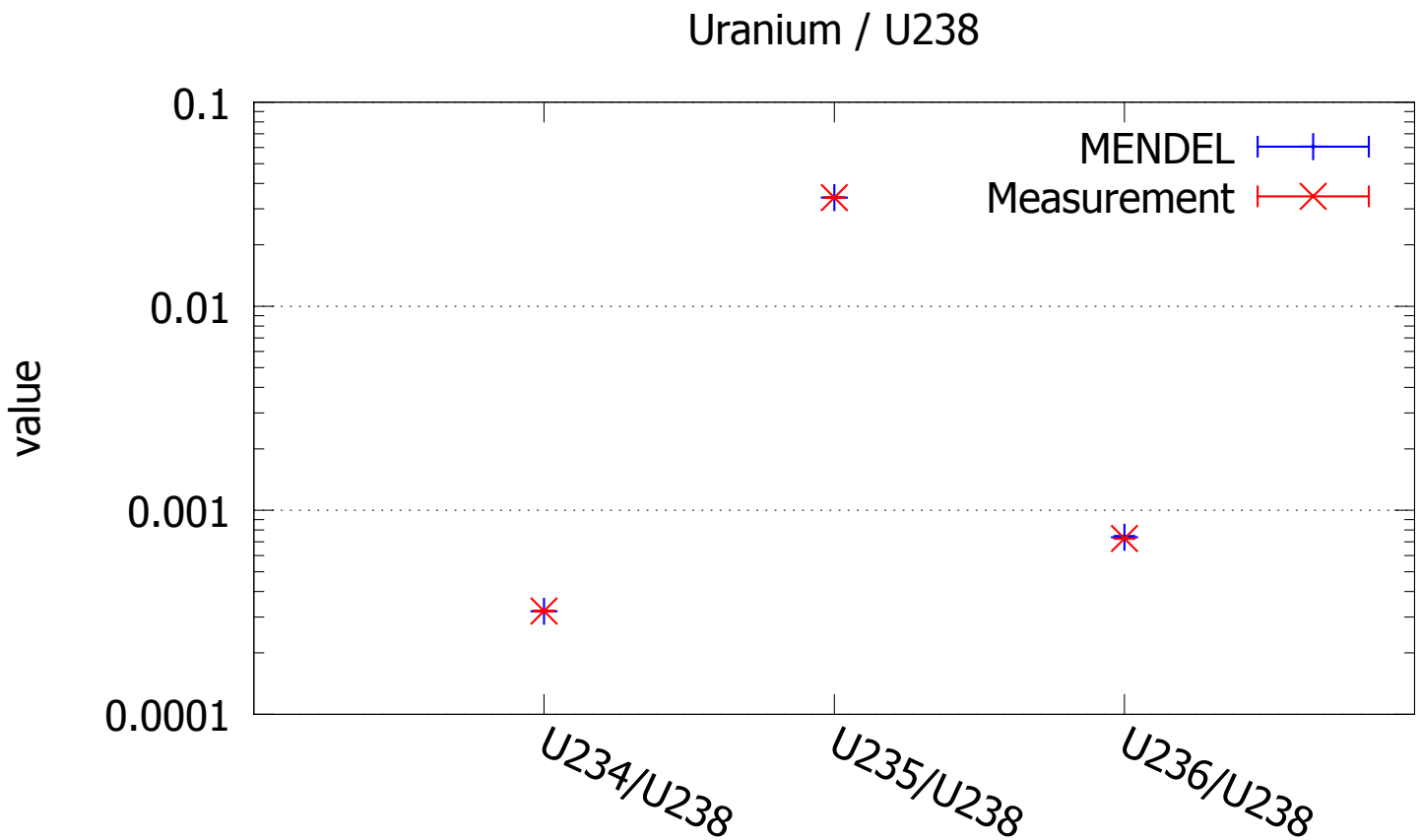
return



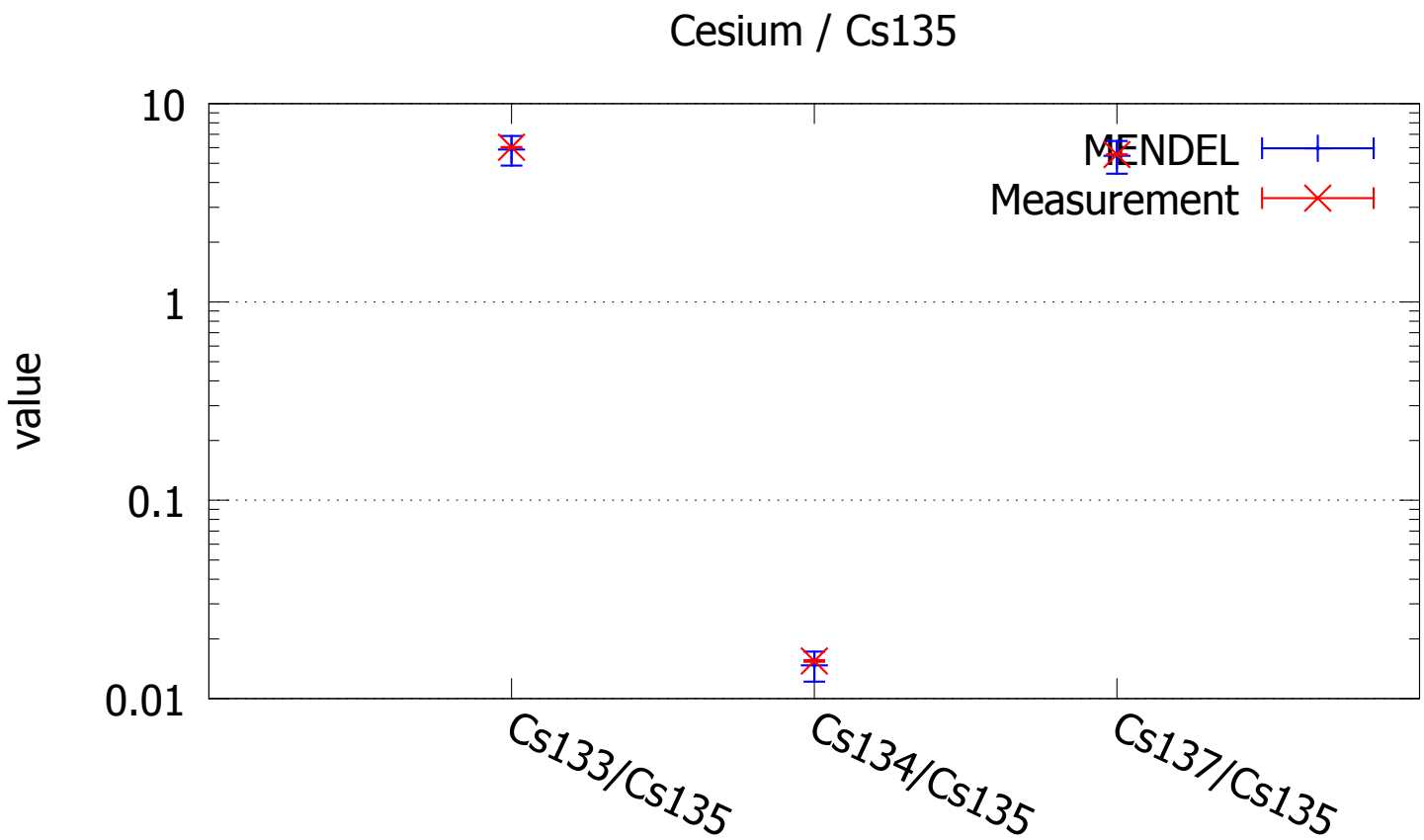
Isotopic concentration ratios: Neodymium vs U238



Isotopic concentration ratios: Uranium



Isotopic concentration ratios: Cesium



return

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