Nuclear data uncertainty quantification in Molten Salt Fast Reactors

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Framework and motivations

The robust design of a new reactor concept (like the MSFR) requires the quantification of the overall uncertainties

The uncertainty quantification is relevant also in view of the design safety assessment

MSFR has an intrisic multiphysics nature → simulations are fundamental for both design and safety assessment stages

NE

TH

Thermo-physical properties, closure relationships, and so on…

Multi-group neutronic models (diffusion, SP_N, …)

Monte Carlo code to homogenize and collapse nuclear data

Continuous-energy data (e.g. cross sections…) in libraries are affected by **statistical uncertainty**

Uncertainty propagation from the raw **nuclear data** to the main neutronic parameters in the frame of **stochastic transport**

Techniques for nuclear data UQ

- General UQ can be carried out basically in two ways:

Direct sampling (Monte Carlo)

CONs

1. It may be unaffordable
2. It is difficult to evaluate the contributions to the uncertainty

PROs

1. No need to modify the model (non-intrusive)
2. (Almost) independent on number of output parameters
3. Full statistical distribution of the output parameters can be estimated

Surrogate sampling

CONs

1. It may be intrusive
2. Often, only the first moments of the distribution can be estimated

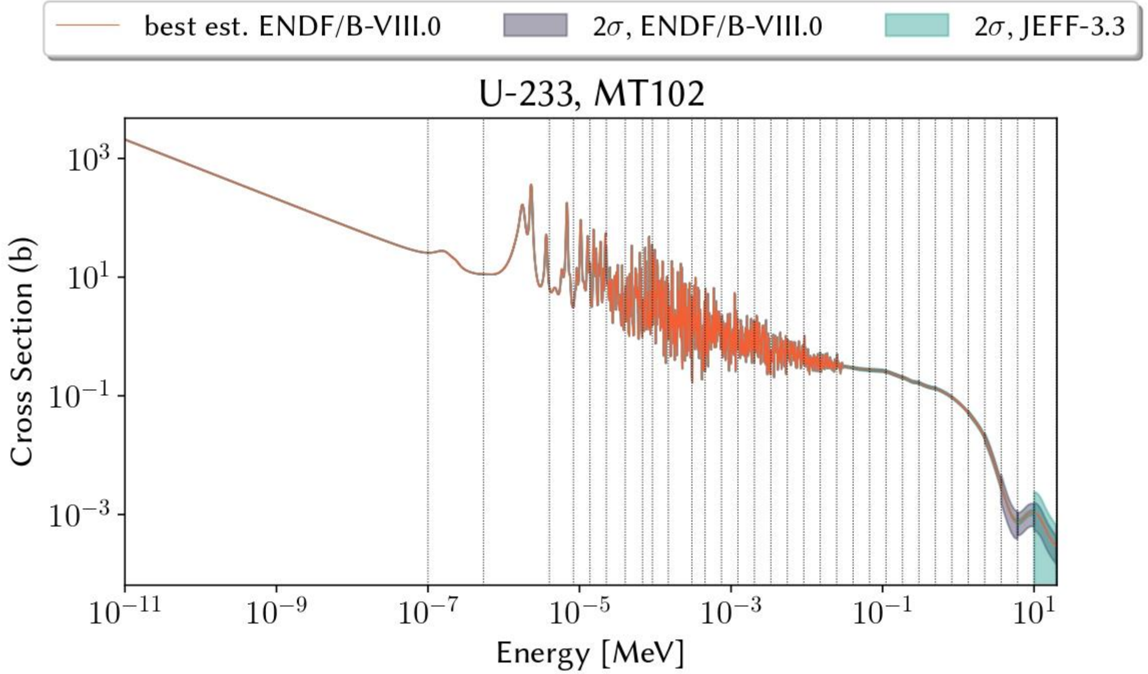
PROs

1. Flexible, adequate also for Sensitivity Analysis (SA)
2. Computationally cheaper than direct sampling

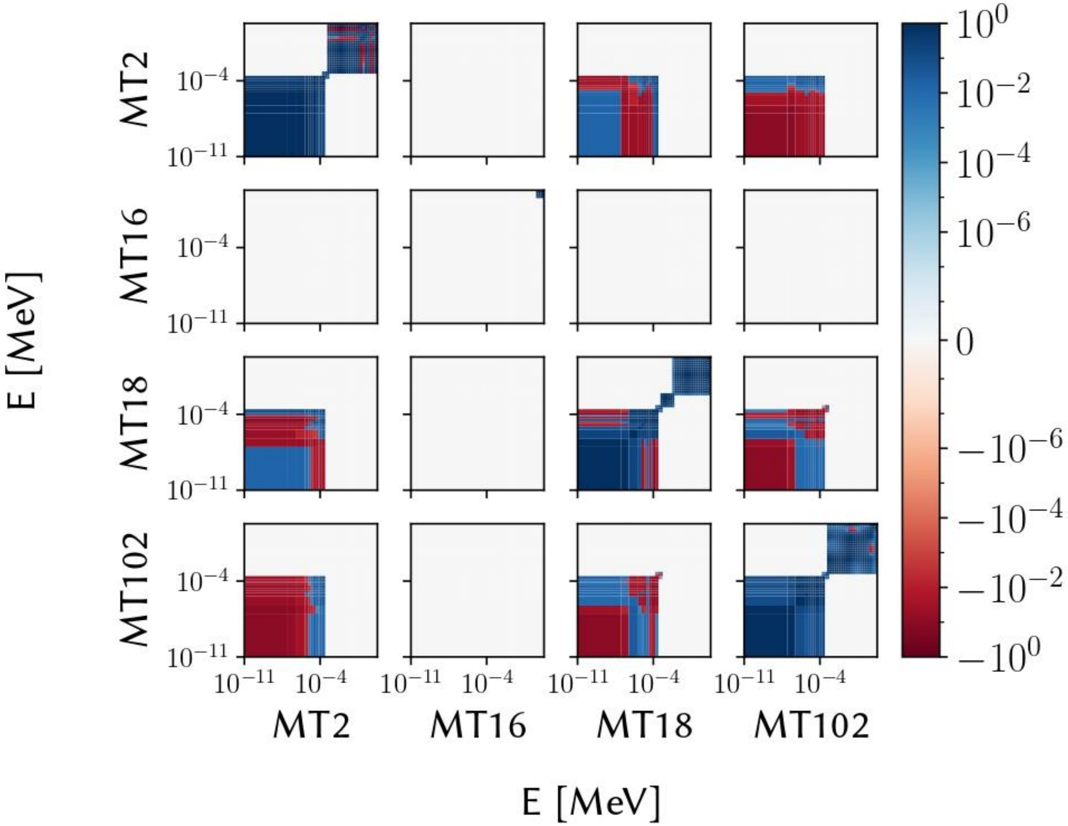
A few examples: Polynomial Chaos, Kriging, Adjoint-based methods…

Nuclear data UQ

- Nuclear data UQ has some peculiarities…



1. Complex, heterogeneous data (cross sections, energy-angular emission distributions, number of neutrons by fission, fission yields…)
2. They span 12 orders of magnitude
3. Variance/covariance depends on library evaluation, no statistical distribution is given



U-233 covariance matrix, processed on the ECCO-33 group structure

Techniques for nuclear data UQ

- Are general UQ techniques suitable for nuclear data UQ in Monte Carlo codes? Yes, a subset of them

Direct sampling (Monte Carlo)

D. Rochman et al., "Nuclear data uncertainty propagation: Perturbation vs. Monte Carlo" Annals of Nuclear Energy 38, 2011

Total Monte Carlo

Hybrid methods, e.g. Unscented Transform (UT)

Surrogate sampling

M. Aufiero et al., "A collision history-based approach to sensitivity/perturbation calculations in the continuous energy Monte Carlo code SERPENT" **Annals of Nuclear Energy 85, 2015**

Perturbation methods

$$\underbrace{\mathrm{var}[R]}_{\text{response variance}} = \overbrace{\vec{S}_b^{R}}^{\text{Sensitivity}} \underbrace{\mathrm{cov}[\hat{A}]}_{\text{input covariance}} \overbrace{\vec{S}_b^{R^T}}^{\text{Sensitivity}}$$

From nuclear data libraries

In Serpent?

Generalised Perturbation Theory (GPT)

eXtended Generalised Perturbation Theory (XGPT)

Generation of perturbed nuclear data files

T6

- ✔ **Continuous-energy perturbation of nuclear model parameters**
- ✘ **Issues for light and fissile nuclides**

SANDY

- ✔ **Multi-group perturbation of xs and fission multiplicities**
- ✘ **It assumes a multi-variate normal distribution for the data**

GPT vs. XGPT

N. Abrate et al., "Generalized perturbation techniques for uncertainty quantification in lead-cooled fast reactors" Annals of Nuclear Energy 164, 2021

$$\mathrm{var}[R] = \vec{S}_b^{R}\,\mathrm{cov}[\hat{A}]\,\vec{S}_b^{R^T}$$

GPT — Direct evaluation of the multi-group sensitivity

$$S^R_{P,g} = \int_{E_g}^{E_{g+1}} S^R_P(E)dE$$

CONs / PROs

CONs:

1. The energy resolution is limited by statistical convergence

PROs:

1. Sensitivities can be interpreted easily on a physical ground
2. Independent on the covariance information

Both are first-order techniques

Neutron transport is linear, but the relationship between XS and output may not

$$k_{\mathrm{eff}} = \frac{\nu\Sigma_f}{\Sigma_a + D^2B^2}$$

XGPT — Evaluation of sensitivity projections on continuous-energy basis functions

$$S^R_{P,b_k} = \int_{E_{\min}}^{E_{\max}} dE\ S^R_P(E)b_k(E)$$

CONs / PROs

CONs:

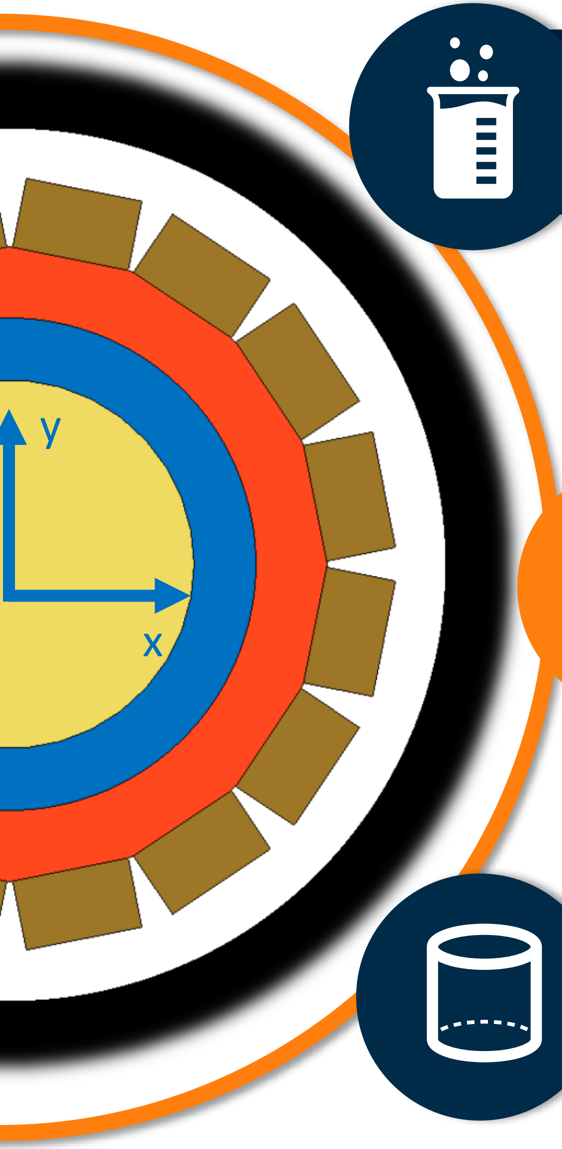
1. Dependent on the covariance information through the basis functions
2. No intuituve physical interpretation to the projected sensitivity

PROs:

1. Continuous-energy information on sensitivity can be conveyed
2. First-order Total Monte Carlo, provided that perturbed files are available → surrogate distributions

SANDY or T6 are needed to perturb nuclear data files!

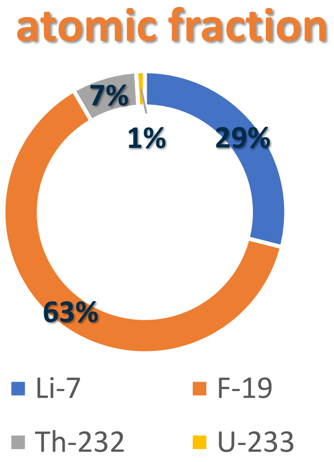
Molten Salt Fast Reactor simulation with Serpent

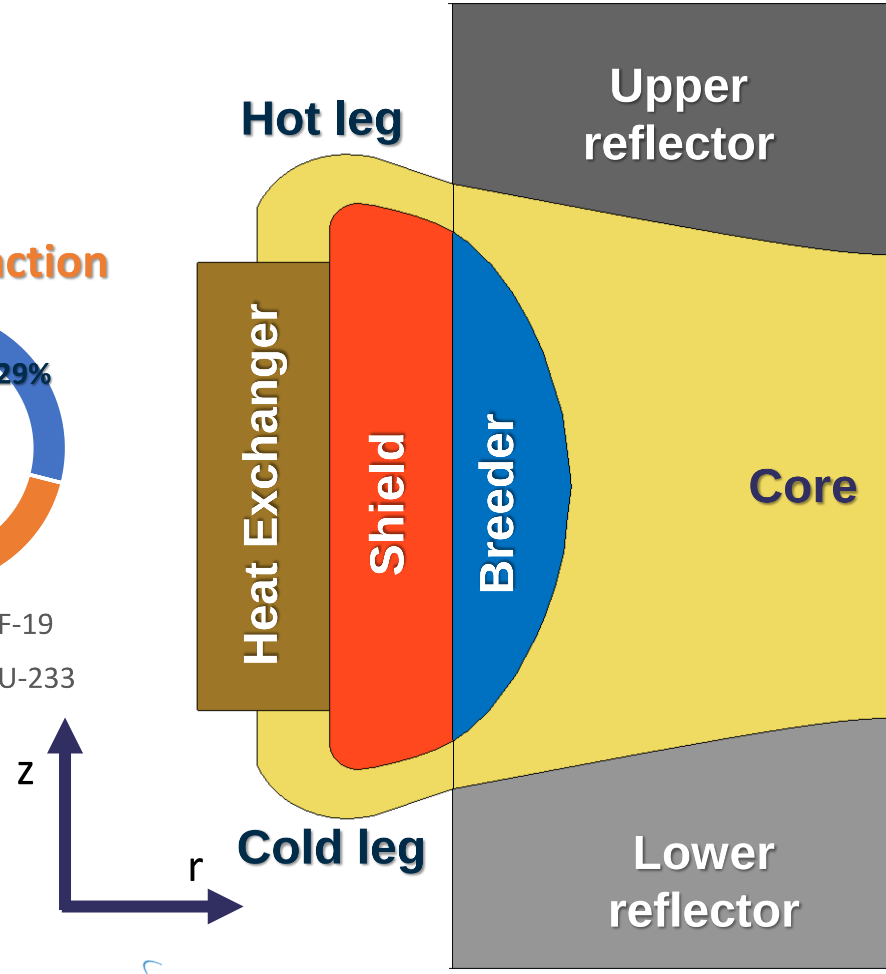


Equilibrium salt composition (n. moles):
2.63 ^{233}U, 19.87 ^{232}Th, 77.5 ^{7}Li, 167.5 ^{19}F …

Uniform temperature, 900 K

3D, CAD-based geometrical model





SAMOFAR

Model developed @ Politecnico di Milano in the framework of the SAMOFAR EU project

Preliminary results from SAMOFAR (2019)

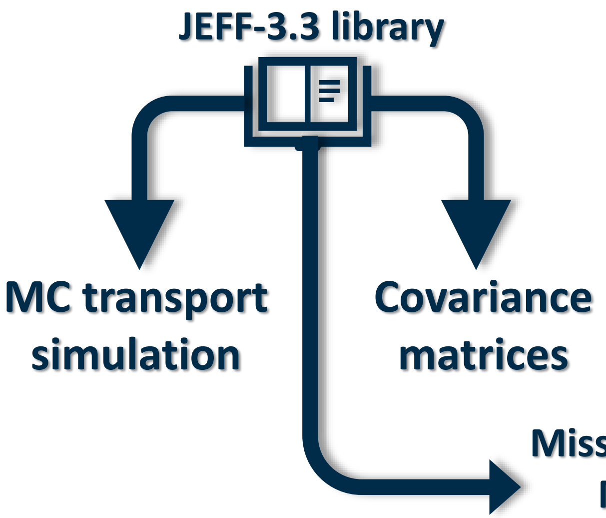
- Results obtained with preliminary calculations in the framework of the SAMOFAR EU project (2019)
- Serpent version 2.1.30

XGPT

- $5*10^5$ neutrons
- 500 active cycles
- 10 latent generations for IFP
- Covariance resolution: 5000 groups (uniform lethargy)

GPT

- $7.5*10^5$ neutrons
- 1000 active cycles
- 10 latent generations for IFP
- Covariance resolution: 500 groups (uniform lethargy)



rel. std. k_{eff} [pcm]	GPT	XGPT
MT2	178(3)	-
MT102	62.0(2)	-
Tot.	188(3)	-

F-19

rel. std. k_{eff} [pcm]	GPT	XGPT
MT2	95(1)	94(1)
MT18	20.32(5)	20.25(2)
MT102	1285.8(9)	1245.3(7)
Tot.	1289.5(8)	1249.0(7)

Th-232

Pretty huge uncertainties, huh?

rel. std. k_{eff} [pcm]	GPT	XGPT
MT2	122(2)	-
MT102	5.24(7)	-
Tot.	122(2)	-

Li-7

rel. std. k_{eff} [pcm]	GPT	XGPT
MT2	28(3)	15(3)
MT18	3877(2)	3864(2)
MT102	464.4(3)	466.5(2)
Tot.	3905(2)	3892(2)

U-233

Preliminary results from SAMOFAR (2019) - II

XGPT

- $5 \cdot 10^5$ neutrons
- 500 active cycles
- 10 latent generations for IFP
- Covariance resolution: 5000 groups (uniform lethargy)

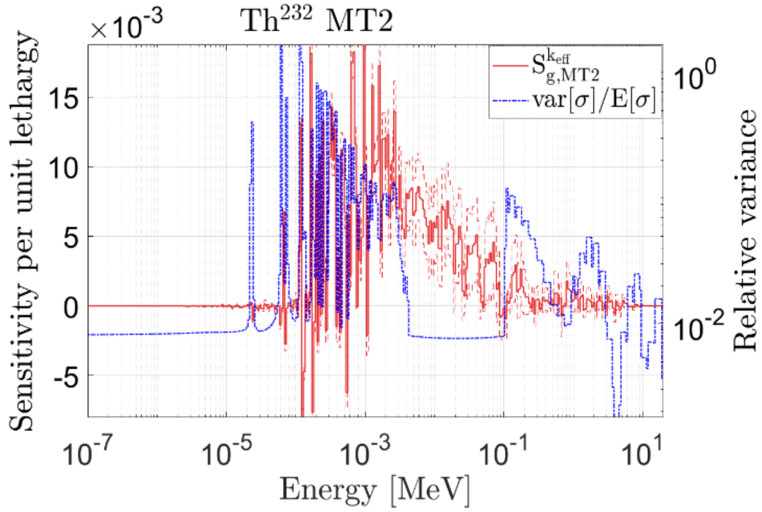
GPT

- $7.5 \cdot 10^5$ neutrons
- 1000 active cycles
- 10 latent generations for IFP
- Covariance resolution: 500 groups (uniform lethargy)

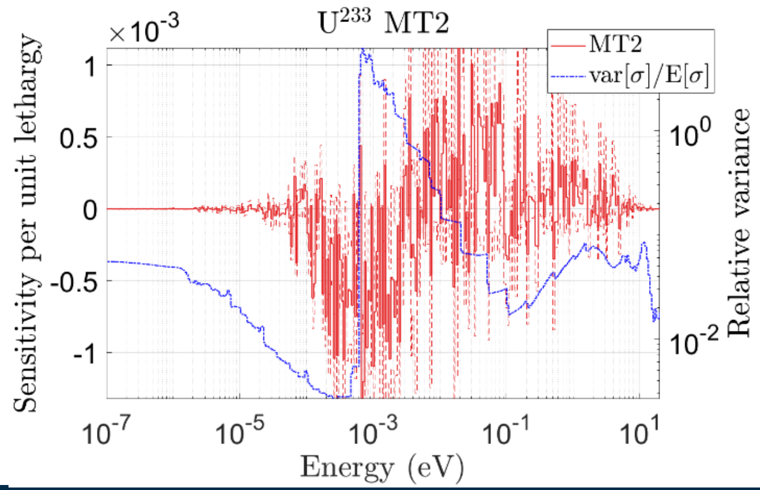
JEFF-3.3 library

MC transport simulation

Covariance matrices



MT2 affects the neutron leakages, which strongly affect the fission source distribution → more latent generations needed for accurate IFP calculations…



- **Satisfactory accuracy for MT102 and MT18 perturbations concerning k_{eff}**
- **Unsatisfactory accuracy for MT2 → better statistics and larger number of latent generations needed**
- **Unsatisfactory accuracy for all MT perturbations concerning bi-linear ratios (β_{eff}, Λ)**

What about getting good results with a less groups to reduce the statistical noise?

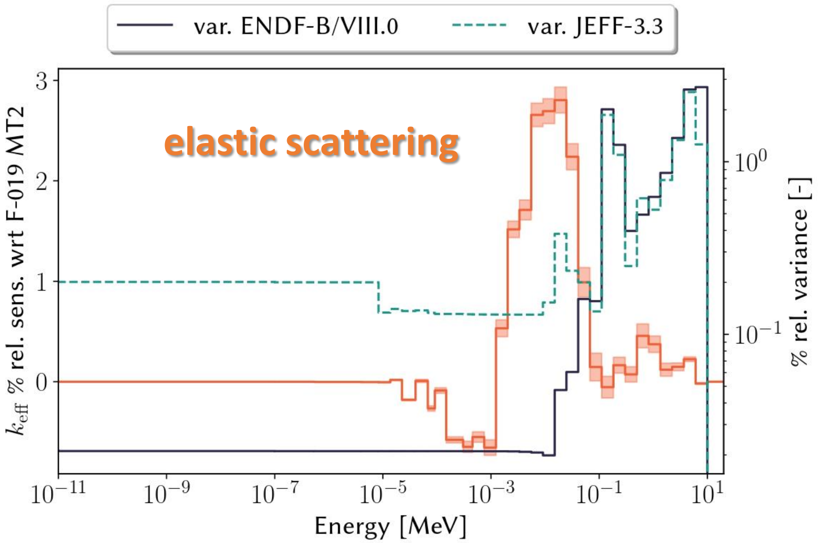
New GPT calculations (2022)

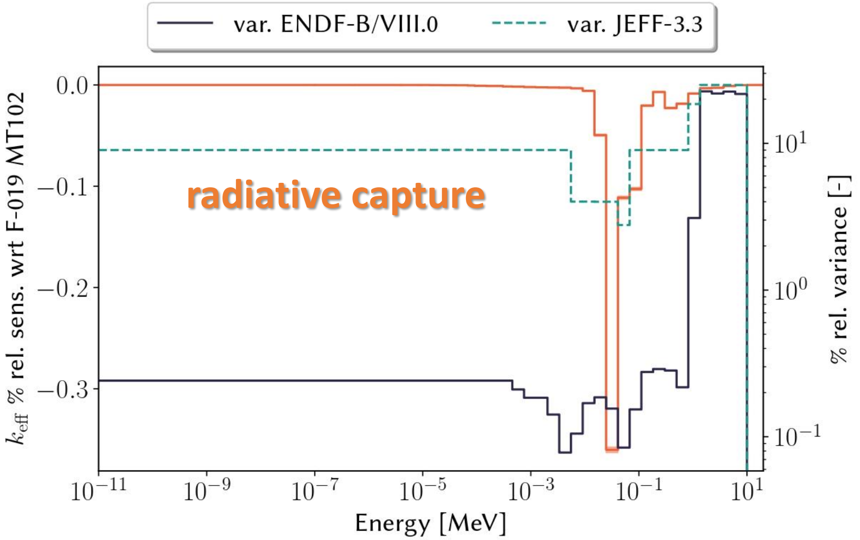
Year	2019	2022
Approach	GPT	GPT
Serpent version	2.1.30	2.1.32
# of neutrons per batch	$7.5*10^5$	10^6
active cycles	1000	1000
inactive cycles	100	200
# latent generations	10	15
group structure for sensitivity	500 group, uniform lethargy	ECCO-33
Perturbations	MT2, MT18, MT102 (U-233, Th-232, F-19, Li-7)	all MTs, ν, χ all nuclides
Output responses	k_{eff}	k_{eff}, β_{eff}, Λ

GPT – k_{eff} sensitivities

ENDF-B/VIII.0 and JEFF-3.3 have different covariance matrices

F-19

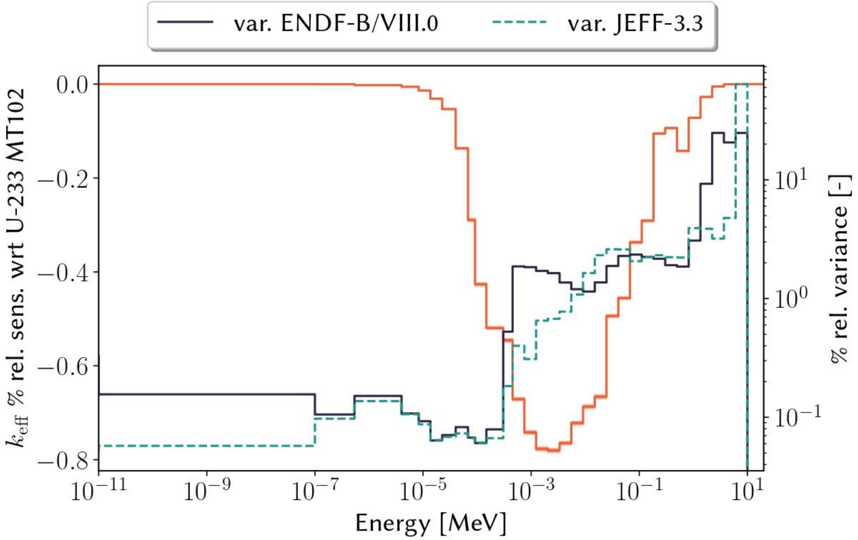


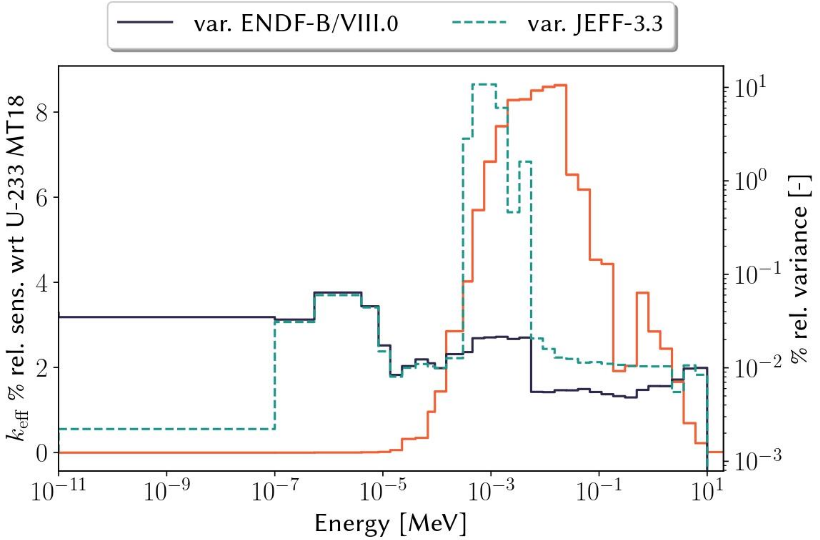


F-19

ENDF-B/VIII.0 data seems more accurate…What about forthcoming JEFF-3.4?

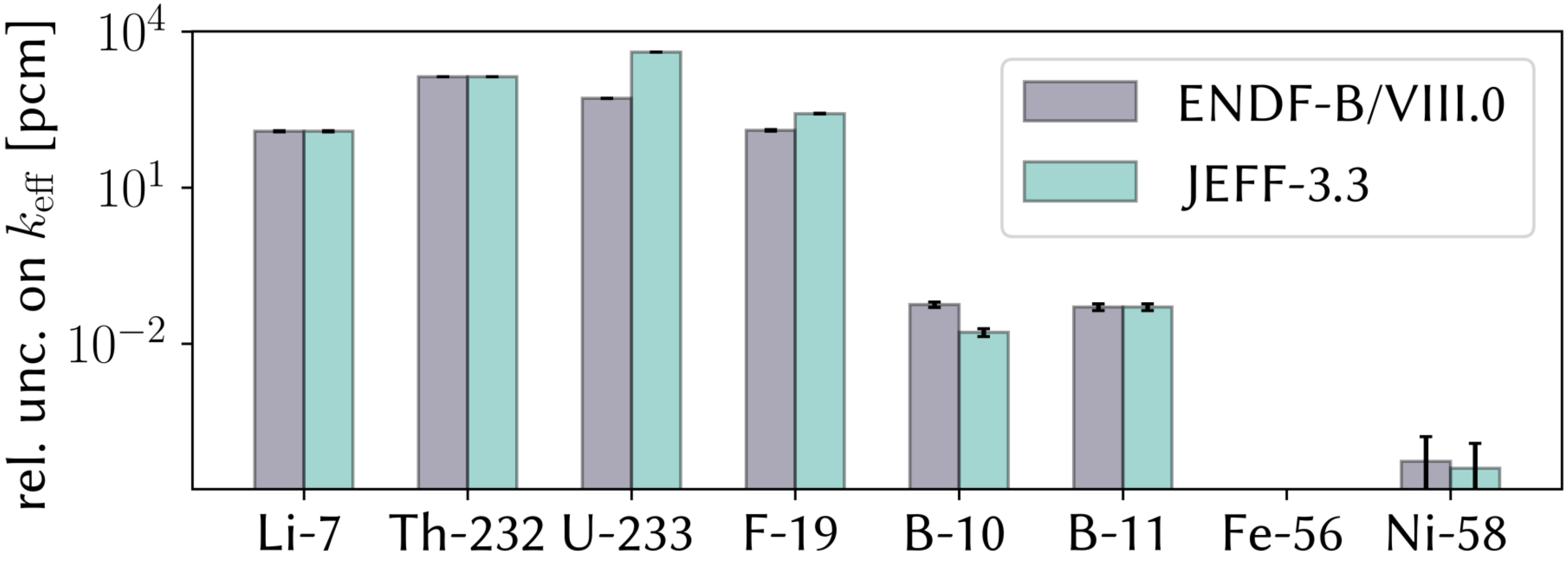
U-233

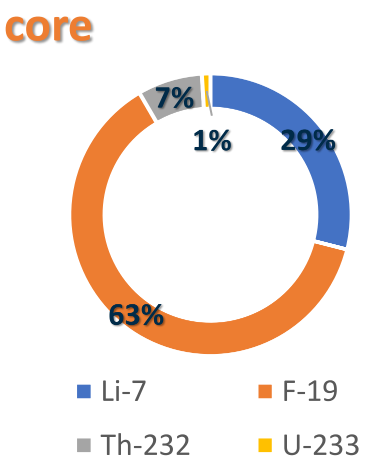


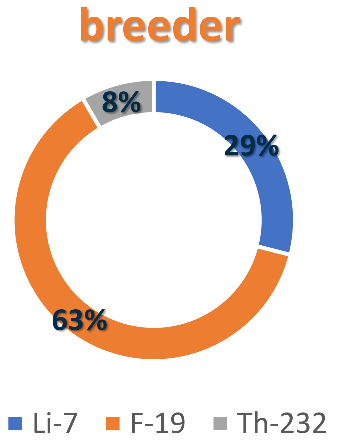


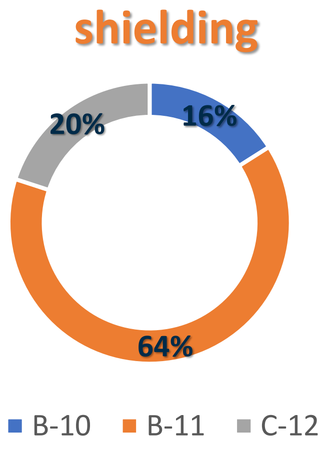
U-233

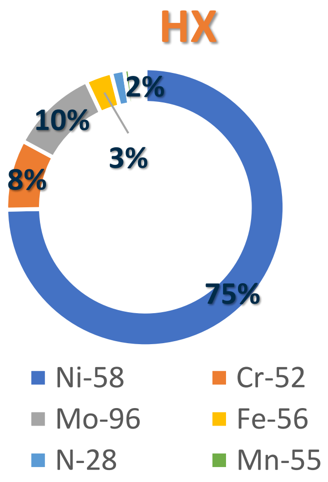
GPT – isotopic contributions to k_{eff} uncertainty

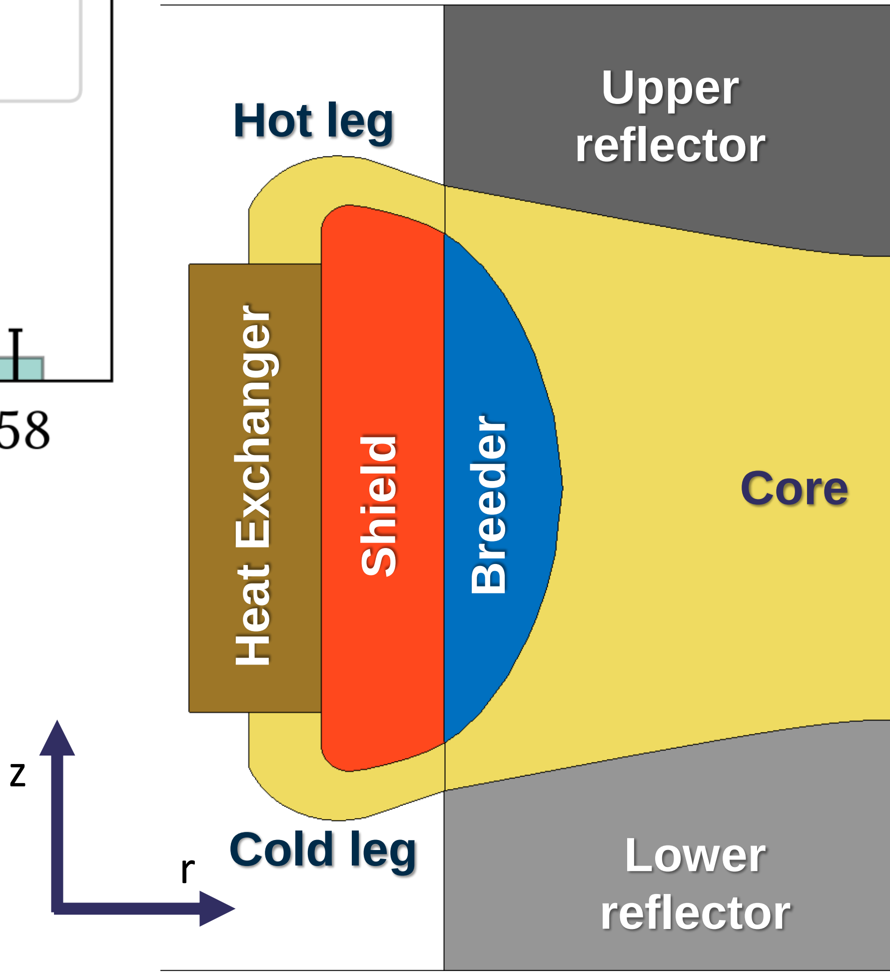




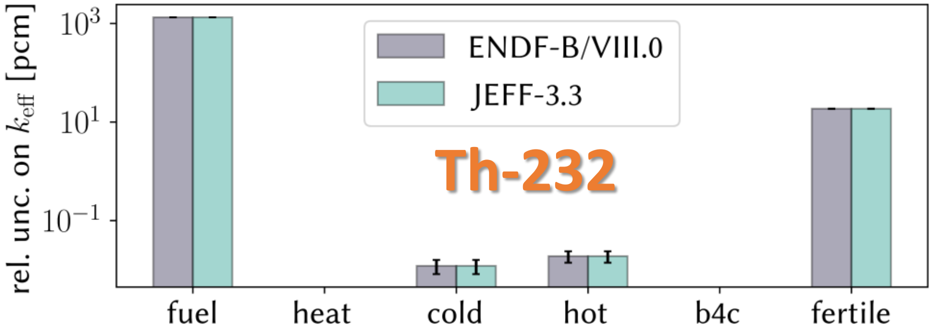


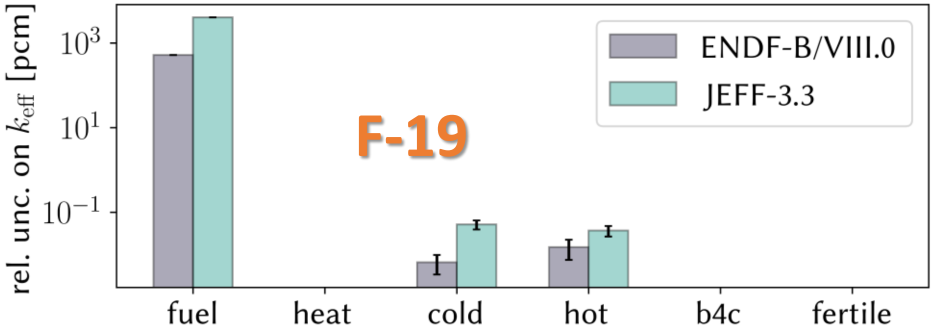


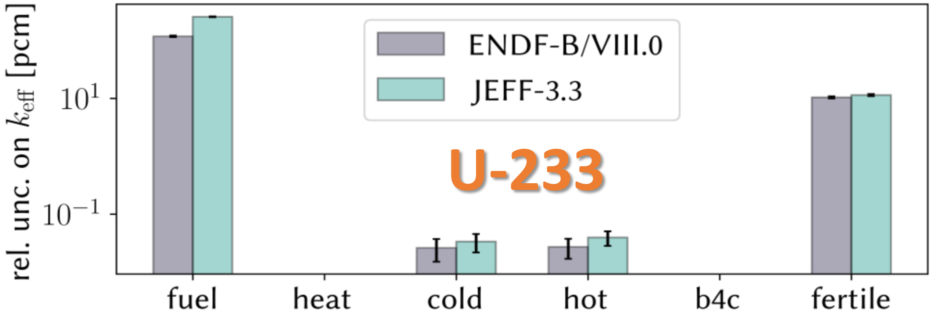


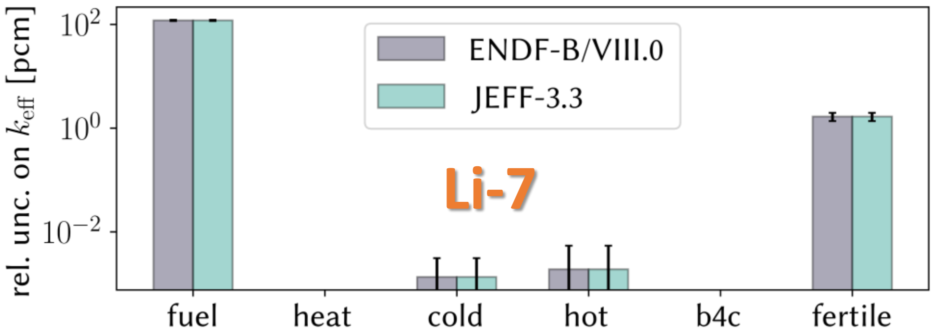


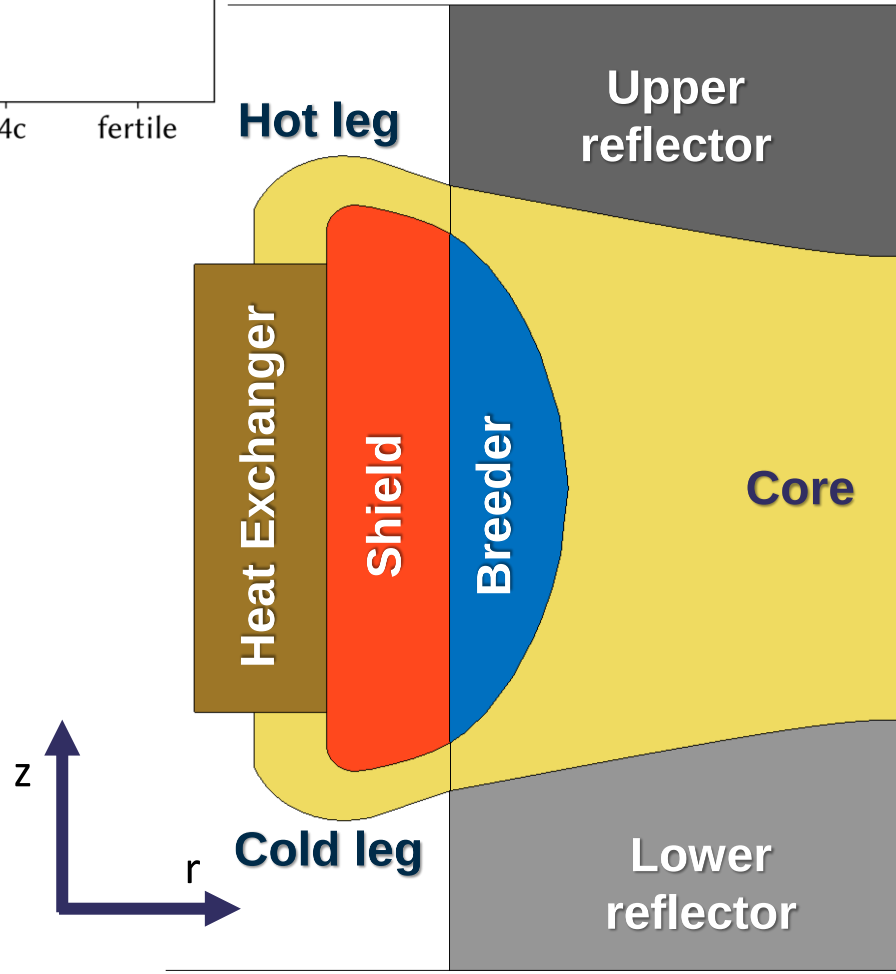
GPT – Reactor regions contributions to k_{eff} uncertainty



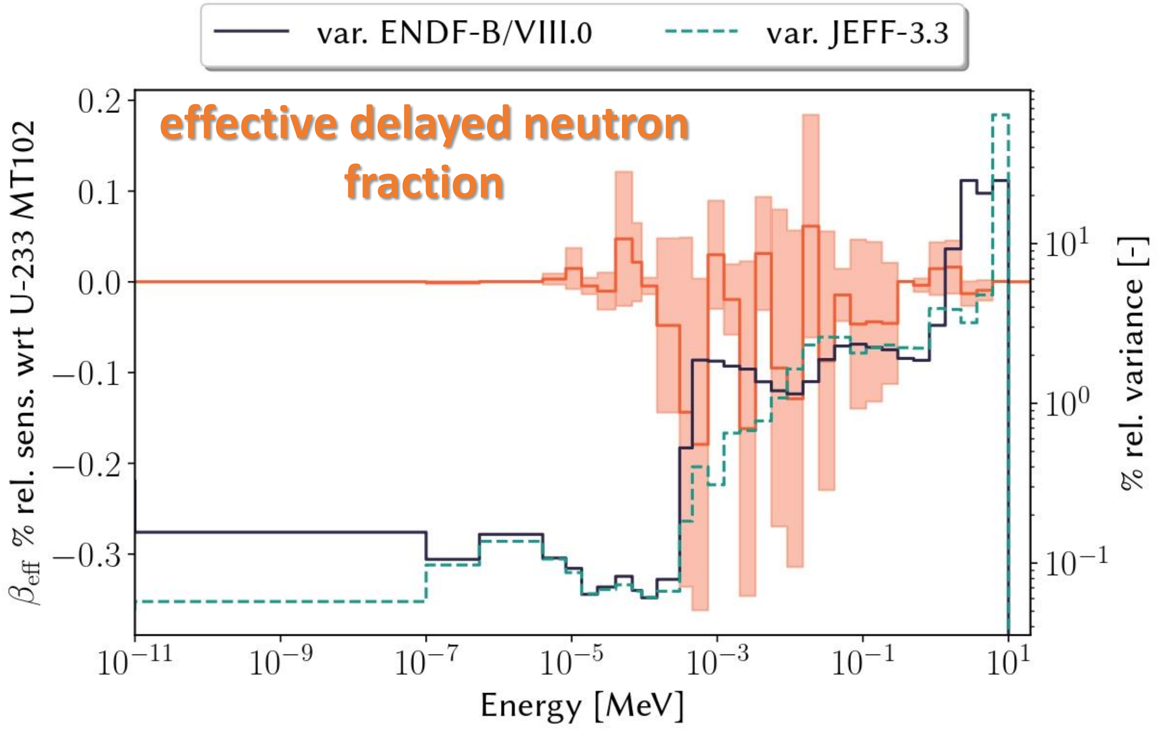


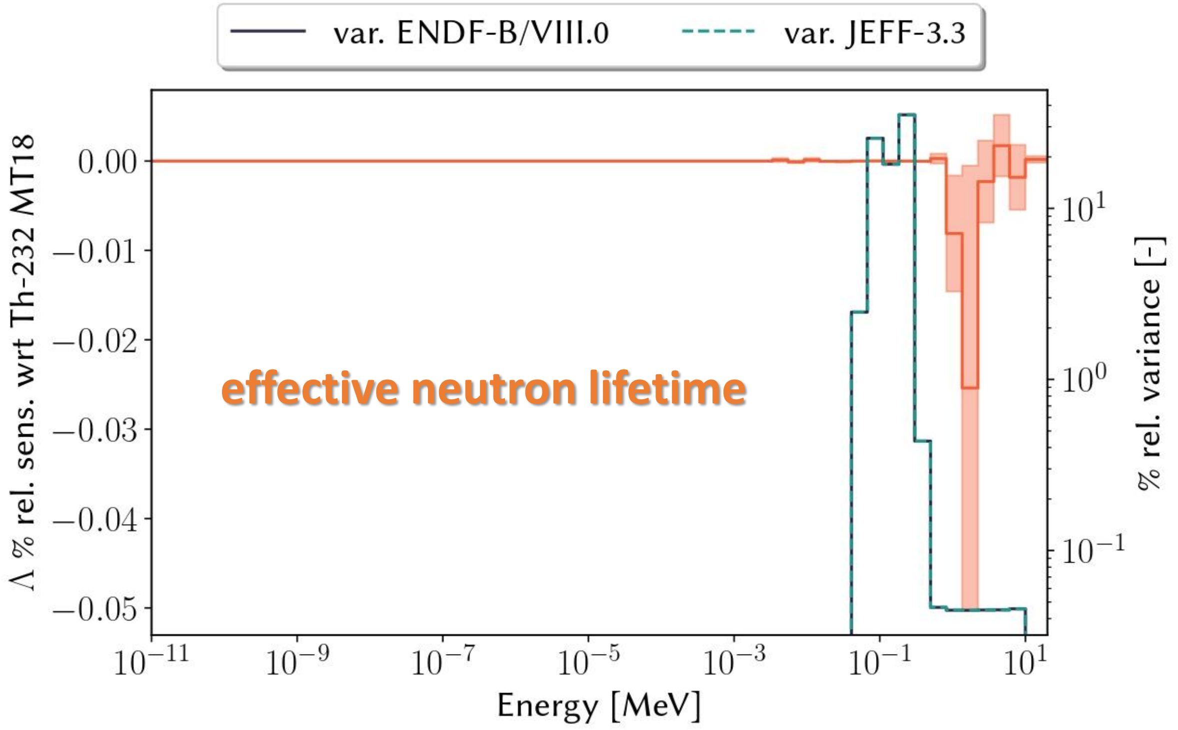






GPT – other sensitivities





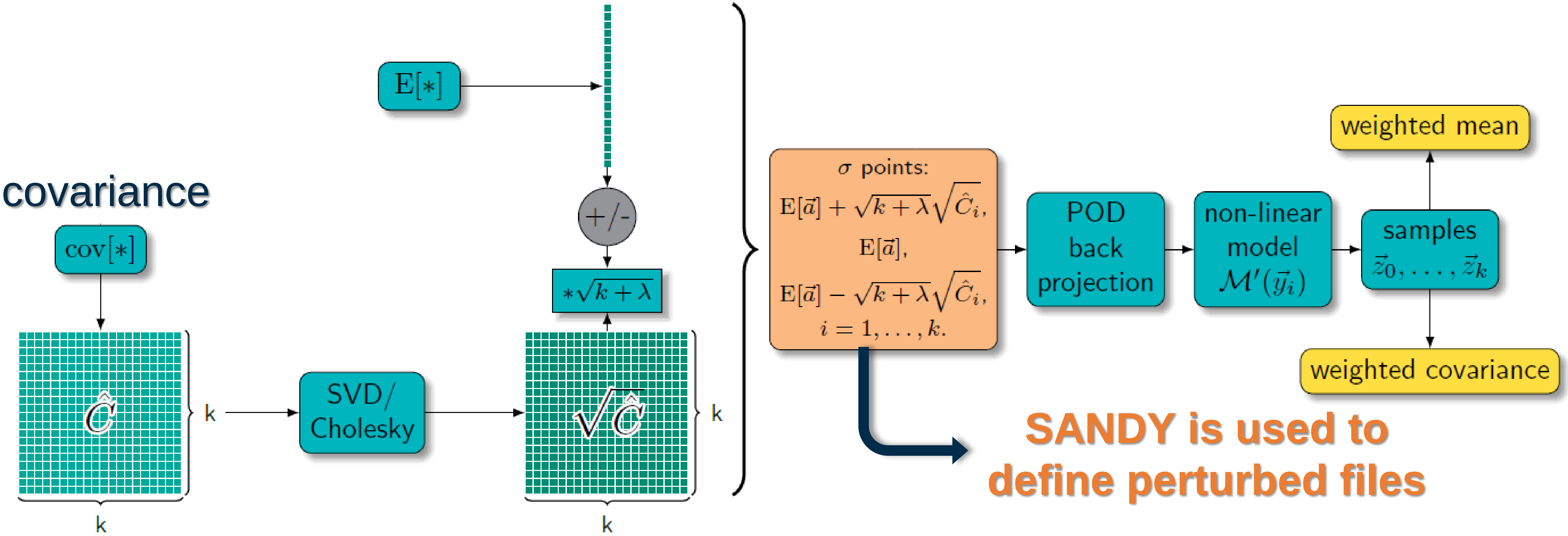
15 latent generations and 10^9 active histories apparently are not enough for accurate sensitivities…

Is there any cheaper and faster alternative?

Non-intrusive techniques, like the UT

Unscented Transform (UT) in a nutshell

Basic principle: it may be better to approximate the input distribution than approximating the model… → this is done taking selected samples, the so-called σ-points



- ✓ **Non-intrusive**
- ✓ **Computationally faster than TMC**
- ✓ **Independent on output responses**

- ✗ **Samples dependent on covariance**
- ✗ **One perturbation at a time**

UT preliminary results for Th-232 case

UT

- 10^6 neutrons
- 60 active cycles
- 20 inactive cycles (with pre-computed fission source)
- 226 samples generated according to UT-SVD → 226 runs (20' each)

	UT
k_{eff}	824.2 [pcm]
β_{eff}	1689.3 [pcm]
Λ	0.0124 $[s^{-1}]$
Conversion Ratio	1.69 %

Challenging responses for GPT/XGPT (linear and bi-linear ratios)

lower than ≈1290 pcm from GPT (linear)…

UT approximates the input distribution, the non-linear model is not approximated!

TMC is needed to get a reference, accurate estimate for both U-233 and Th-232

Conclusions and future perspectives

GPT and UT techniques used to estimate the uncertainties in some macroscopic neutronic parameters

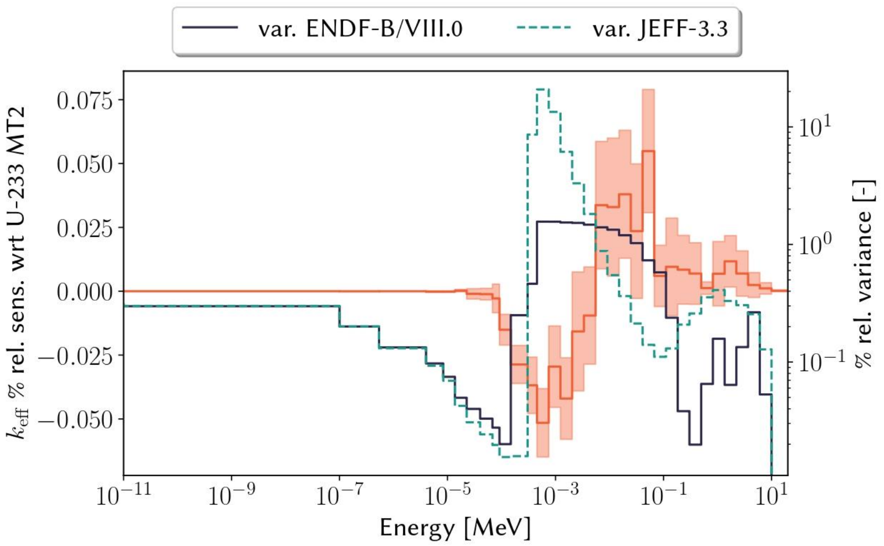
We need more accurate data evaluation if we want to use Th-U fuel cycle!

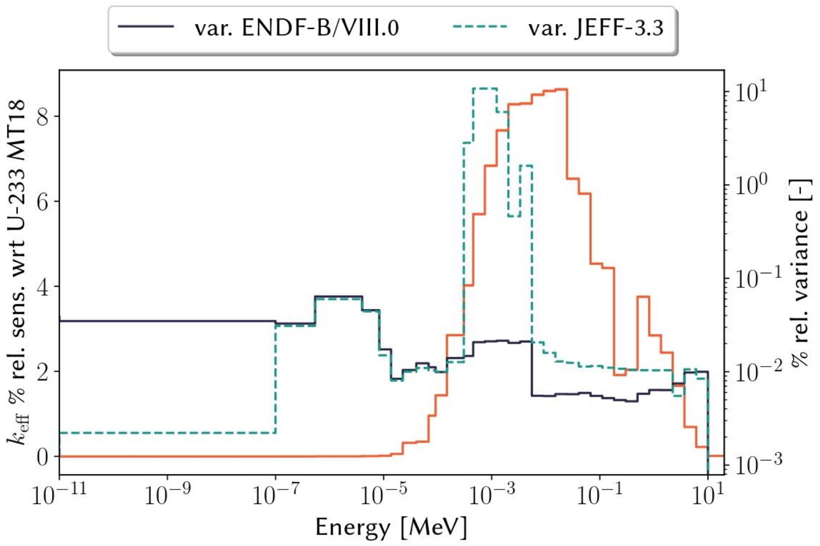
UQ for MSFR

UT results suggests that a TMC is worth for Th-232 and U-233

Thank you for
your kind attention.
Any questions?

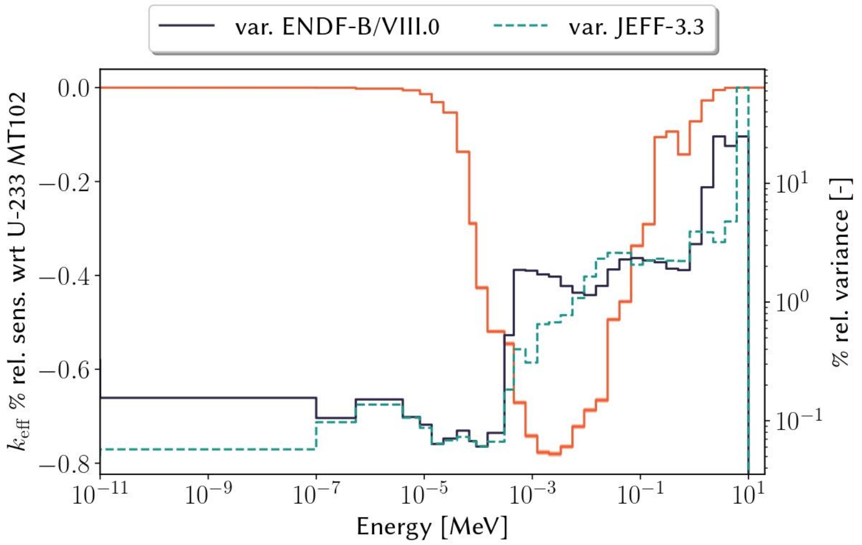
GPT – k_{eff} sensitivities, U-233



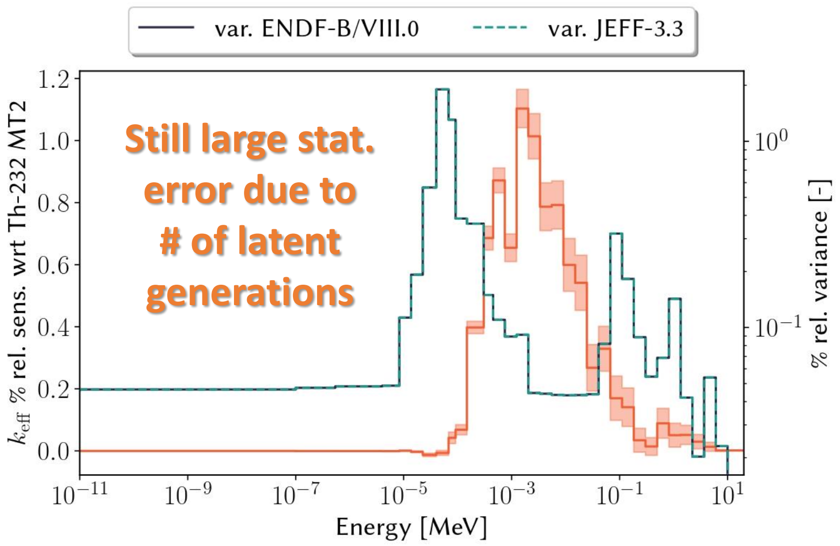


ENDF-B/VIII.0 and JEFF-3.3 have different covariance matrices

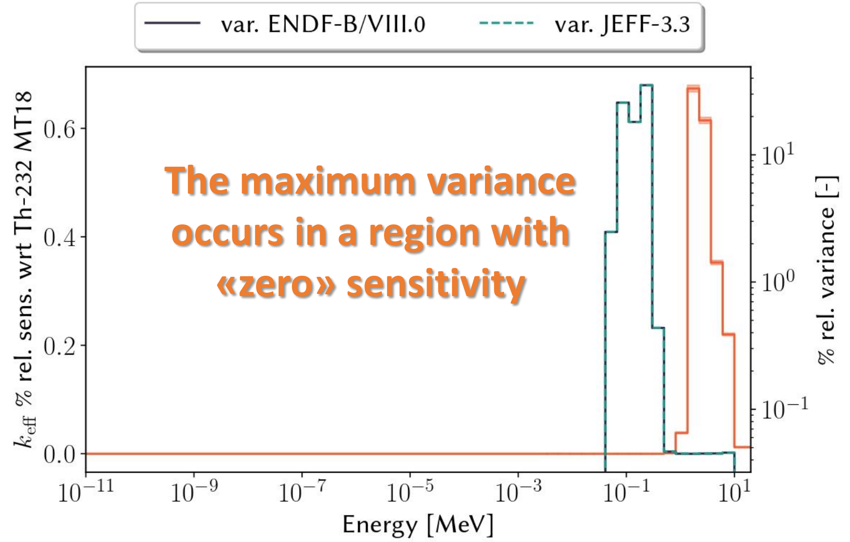
ENDF-B/VIII.0 data seems more accurate…What about forthcoming JEFF-3.4?



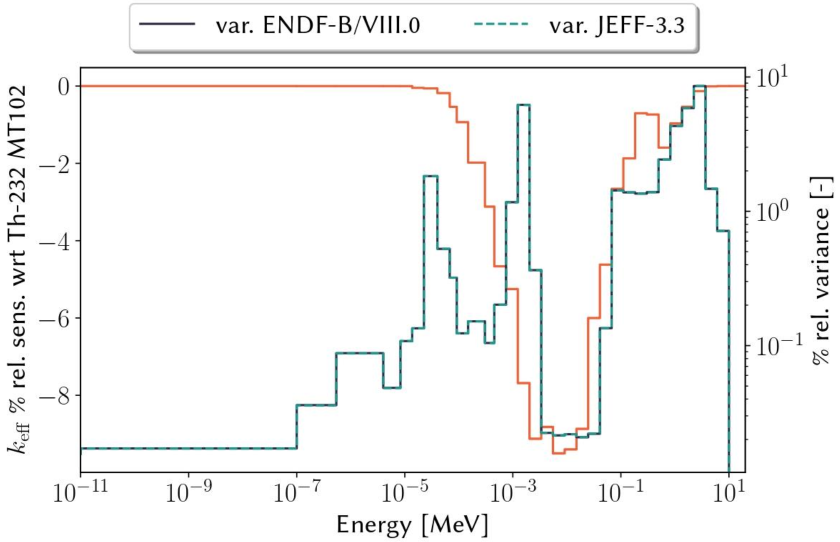
GPT – k_{eff} sensitivities, Th-232

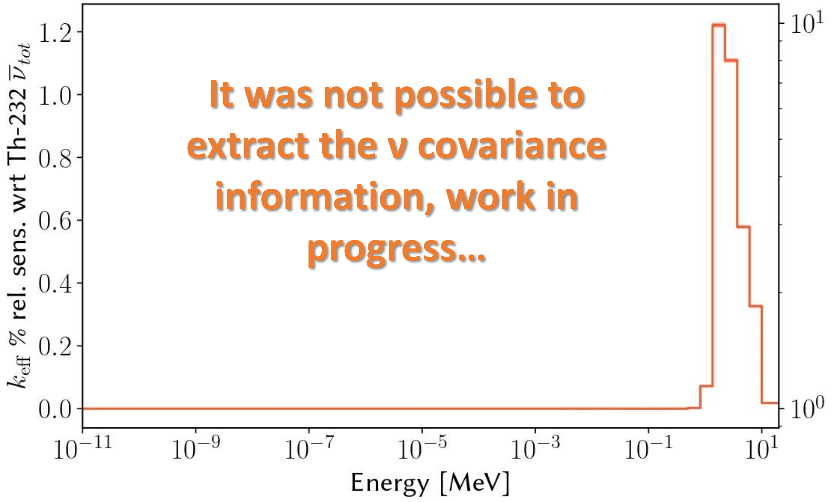


Still large stat. error due to # of latent generations



The maximum variance occurs in a region with «zero» sensitivity





It was not possible to extract the ν covariance information, work in progress…

GPT – k_{eff} sensitivities, Li-7