Nuclear data uncertainty quantification in Molten Salt Reactors with XGPT

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Introduction

- In the framework of Horizon 2020 Euratom research programme, SAMOFAR project aimed at demonstrating the Molten Salt Fast Reactor key safety features
- In this respect, uncertainty propagation is crucial in order to guarantee reliable output results of multiphysics calculations used in the design phase and safety assessment
- The purpose of this work is to **assess the influence of the nuclear data uncertainty on some relevant neutronic parameters**

SAMOFAR

Uncertainty quantification for MSFR

Adequate **safety assessment studies**
Require **multiphysics** simulations

Uncertainty quantification for MSFR

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Require **multiphysics** simulations

Neutronics

Thermal-hydraulics

Uncertainty quantification for MSFR

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

Uncertainty quantification for MSFR

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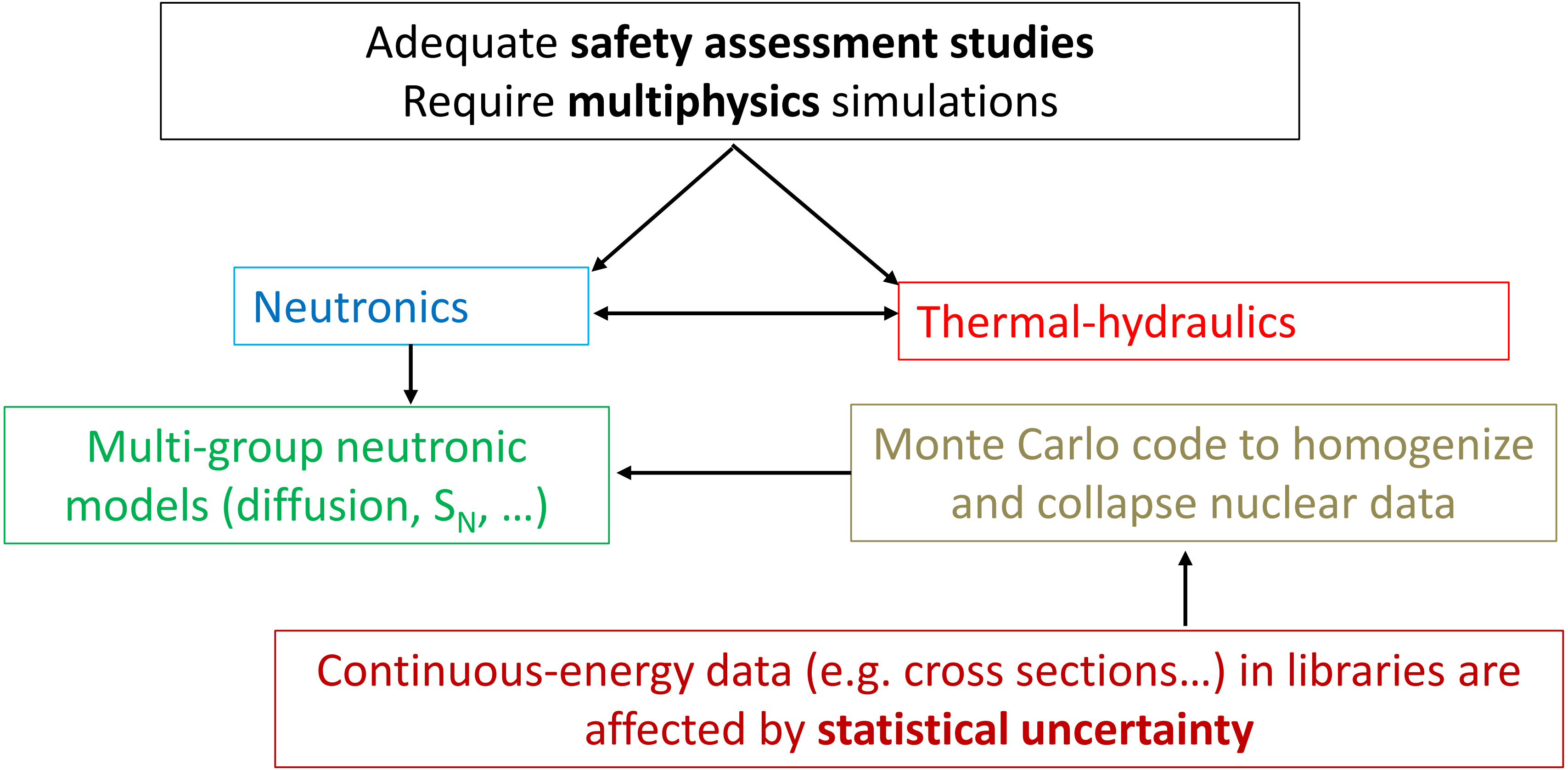
Neutronics

Thermal-hydraulics

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

Monte Carlo code to homogenize and collapse nuclear data

Uncertainty quantification for MSFR



UQ techniques

- Two possible approaches to quantify the uncertainty related to measured nuclear data can be adopted in Monte Carlo detailed calculations:

1. **Direct sampling** → *Total Monte Carlo (TMC)*
2. **Surrogate approach** → *Generalized Perturbation Theory (GPT) and eXtended GPT (XGPT)*

- Both approaches need nuclear data covariance matrices or, alternatively, already processed perturbed datasets according to the covariances (in *reasonable* large number)

UQ techniques

TMC

PROs	CONs
No curse of dimensionality, rich information	High computational burden
Non intrusive, no code modifications	Convergence $\propto {}^{1}/_{\sqrt{N}}$

nemo

UQ techniques

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GPT → Available in Serpent-2

PROs	CONs
Low computational burden	Limited amount of information retrieved
Widely adopted, both in stochastic and deterministic codes	Difficulty to capture non-linearities
	Statistical convergence limited by the number of energy group

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XGPT → Available in Serpent-2

PROs	CONs
Continuous-energy capabilities, flexibility	Difficulty to capture non-linearities
Richer amount of information than GPT (it can produce response distributions)	Higher computational burden than GPT

Surrogate approach

- XGPT and GPT are both based on sandwich rule,

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

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Variance of output response R

Sensitivity coefficients, computed via MC

Covariance matrix

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GPT: group-wise coefficients

XGPT: coefficients projected on continuous-energy basis functions

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- GPT: group-wise coefficients
- XGPT: coefficients projected on continuous-energy basis functions

Covariance matrix

Continuous-energy

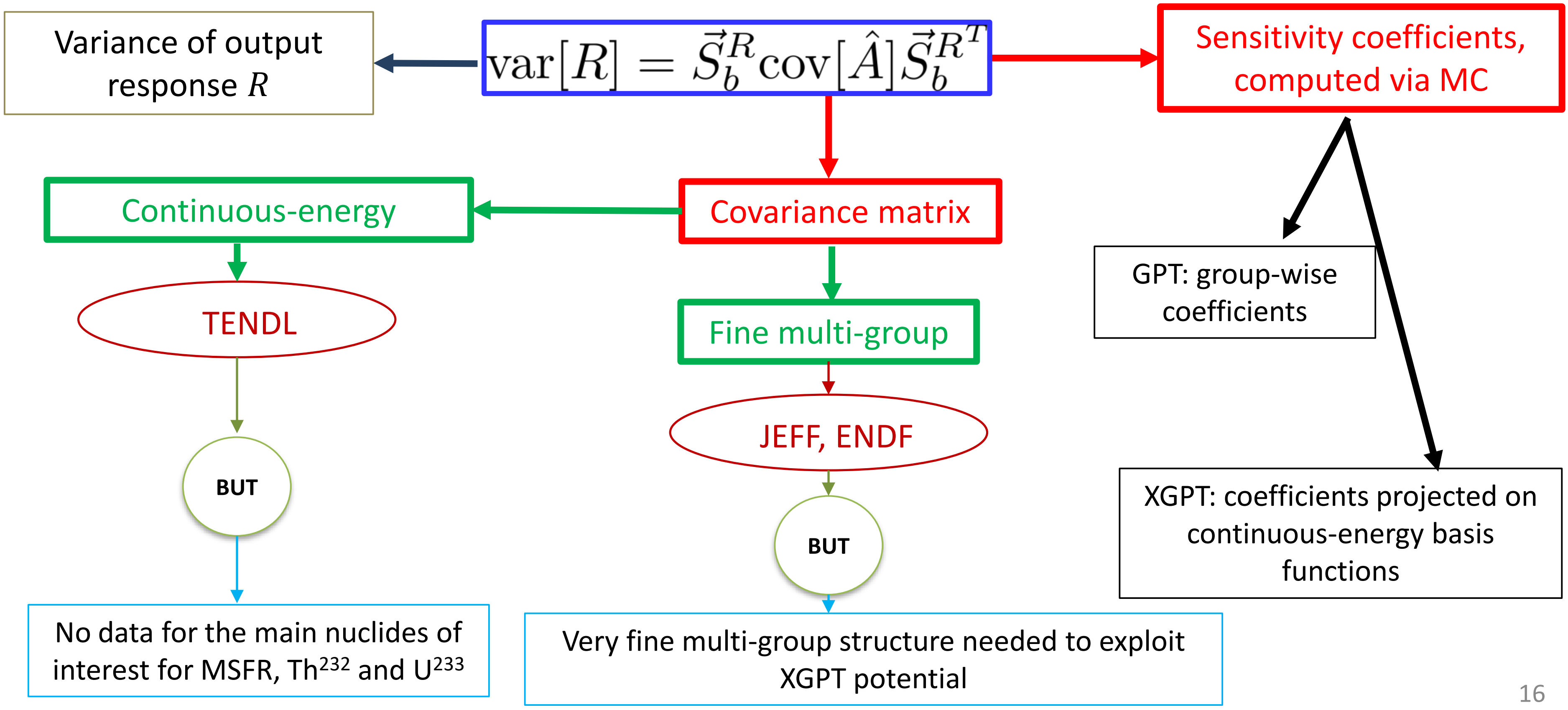
TENDL

BUT

No data for the main nuclides of interest for MSFR, Th^{232} and U^{233}

Surrogate approach

- XGPT and GPT are both based on sandwich rule,



XGPT: reduced order TMC

- XGPT can adopt two approaches to compute continuous-energy **basis functions**:

1. SVD (Singular Value Decomposition) of the covariance matrix to evaluate the sandwich formula
2. POD (Proper Orthogonal Decomposition) of a set of N perturbed nuclear data (as the output of a TMC calculations)

XGPT POD workflow

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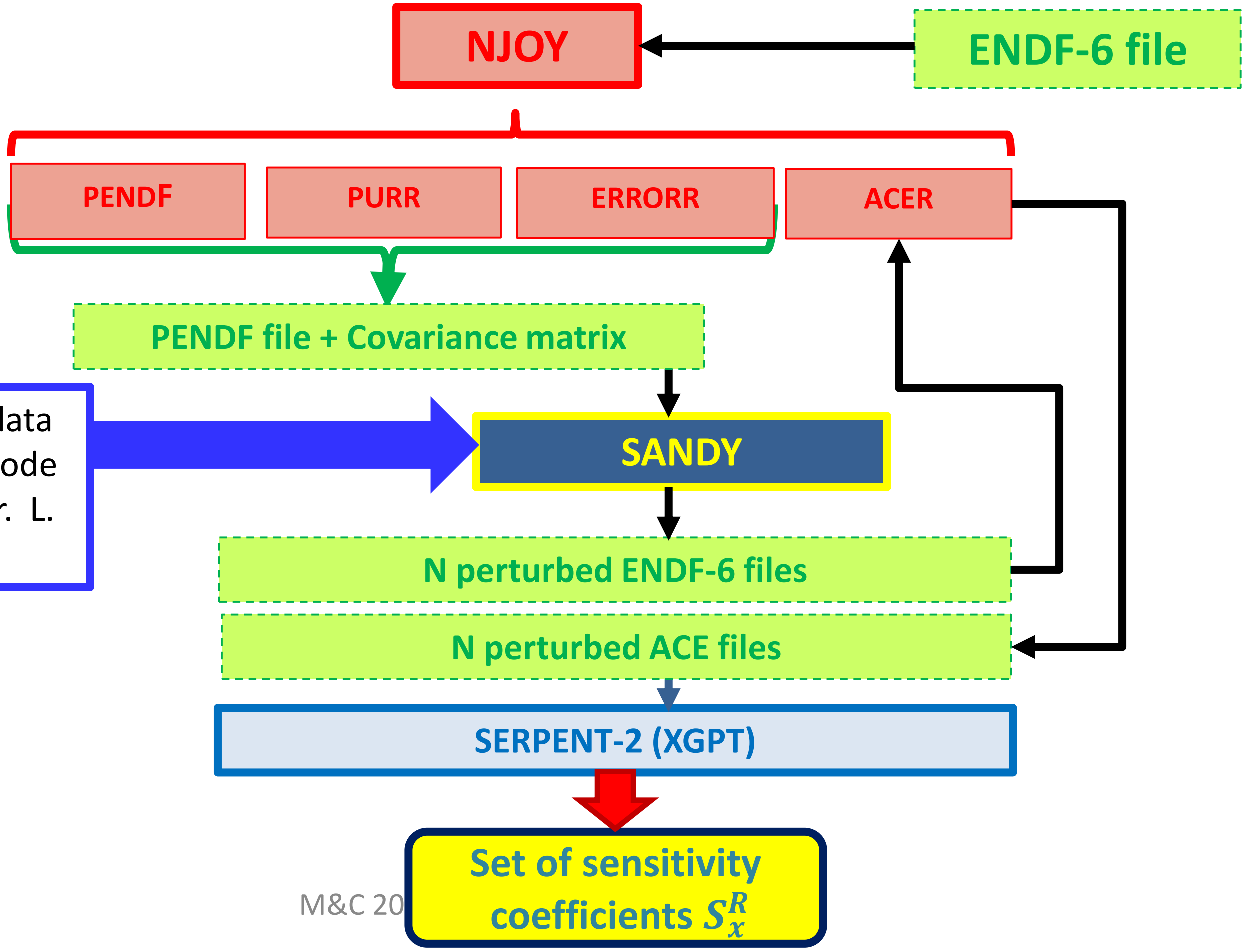
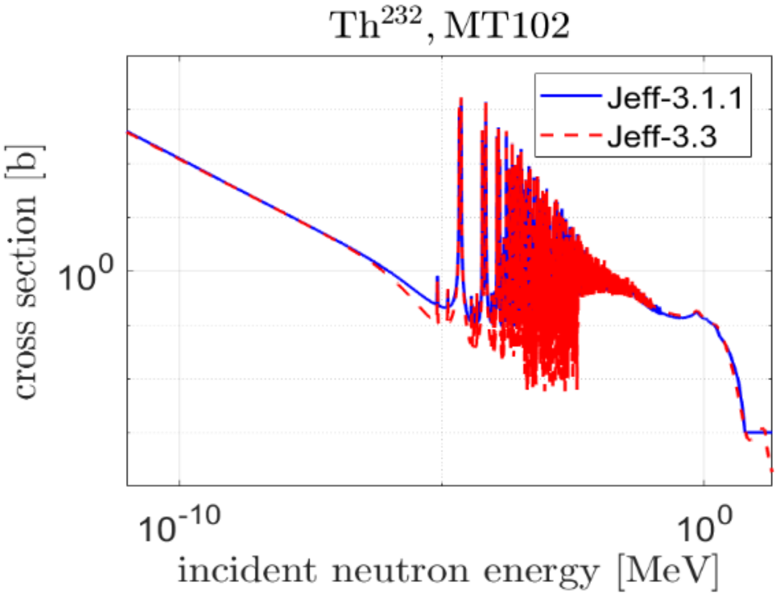
Approach N.2: «reduced» TMC

To perturb the nuclear data files, we employed the code SANDY (developed by Dr. L. Fiorito @ SCK-CEN)



UQ setup

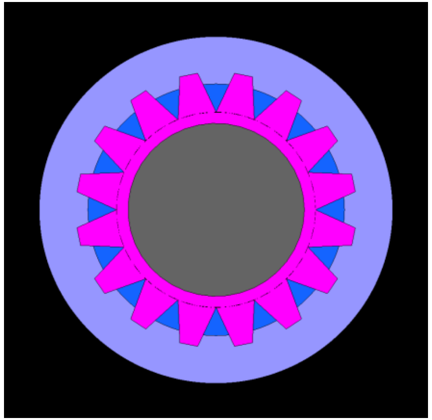
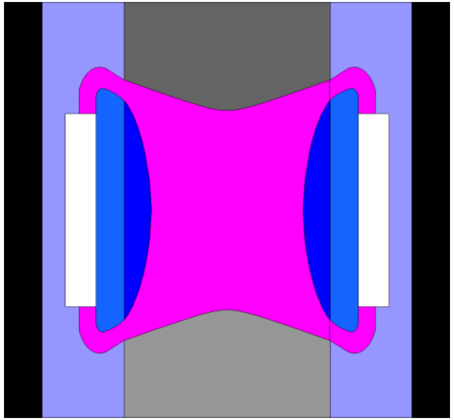
- **Library selection**: **Jeff-3.3** (more recent, complete covariance information for the main nuclides of interest for MSFR, Th^{232} and U^{233})



MT18, i.e. fission, is not present in Th-232 file of Jeff-3.1.1 library!

UQ setup

- **Library selection**: Jeff-3.3 (more recent, complete covariance information for the main nuclides of interest for MSFR, Th^{232} and U^{233})
- **MSFR model**: 3D, full-core simulation, uniform temperature of 900 K, equilibrium salt composition

UQ setup

- **Library selection**: Jeff-3.3 (more recent, complete covariance information for the main nuclides of interest for MSFR, Th^{232} and U^{233})
- **MSFR model**: 3D, full-core simulation, uniform temperature of 900 K, equilibrium salt composition
- **Responses**: due to the high computational burden and limited code development, homogenized cross sections were not perturbed. k_{eff} (and also β_{eff} and Λ, assuming perturbations of U^{233} only) were considered for the MSFR UQ activity

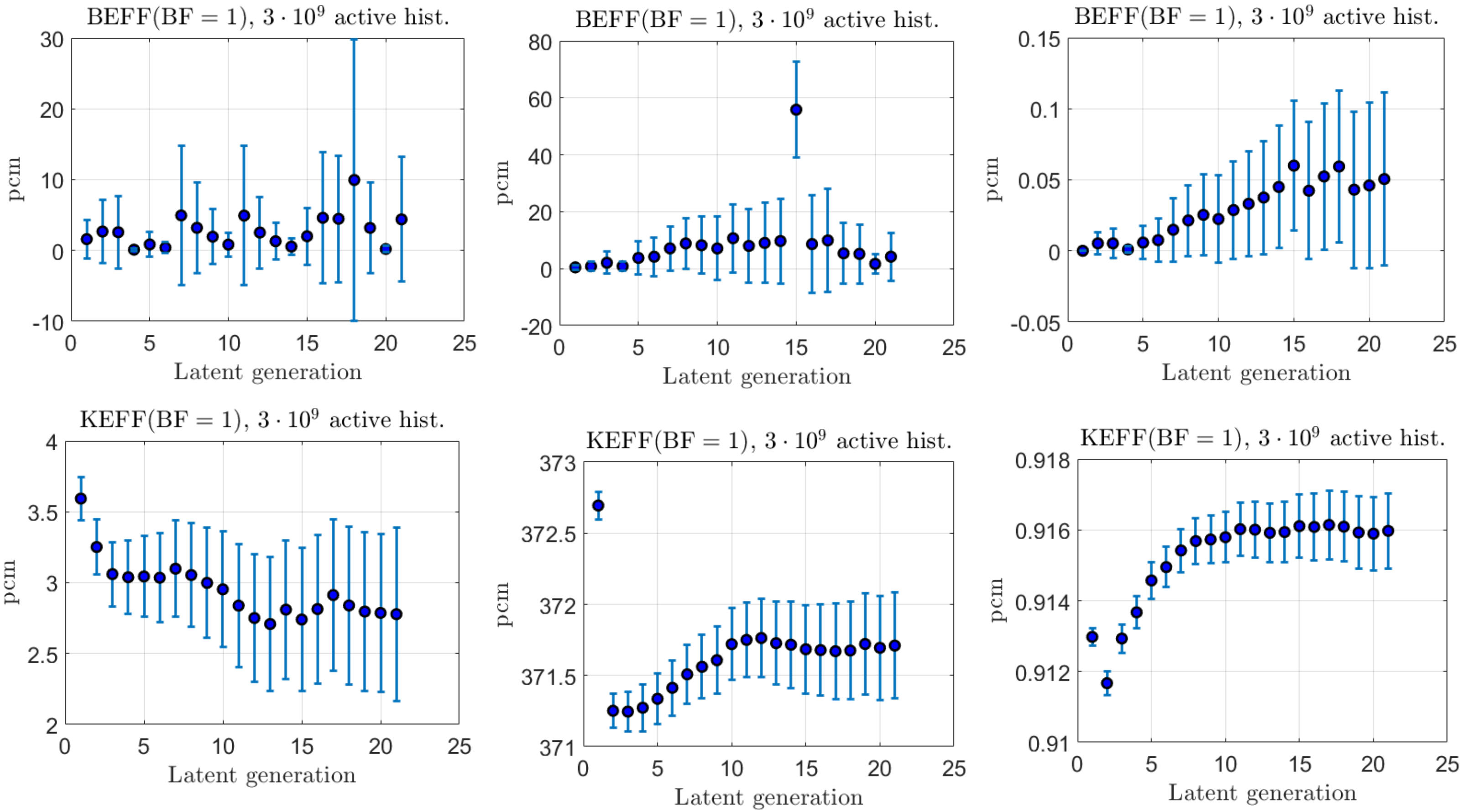
Latent generations issue

- Both linear and bi-linear ratios estimation with GPT and XGPT are based on a **collision-history** approach which follows neutrons for some generations (*latent generations*)
- The number of latent generations required for convergent results depends on the «**distance**» between reference and perturbed neutron distribution
- Bi-linear ratios like β_{eff} and Λ are more sensitive than k_{eff} to this parameter

Latent generation convergence

β_{eff}

k_{eff}



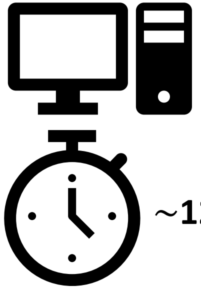
MT2 (elastic scattering)

MT18 (fission)

MT102 (rad. capture)

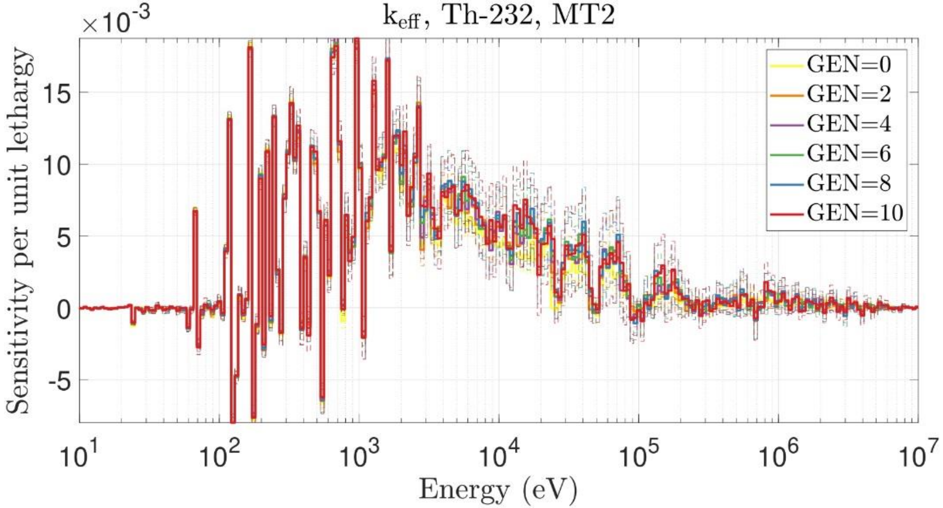
GPT output: Th^{232} , MT2

- 750000 neutrons
- 1000 active cycles
- 10 latent generations
- 500 groups



-Dell Precision Tower 7910 (Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40 GHz
-30 cores

~12 h



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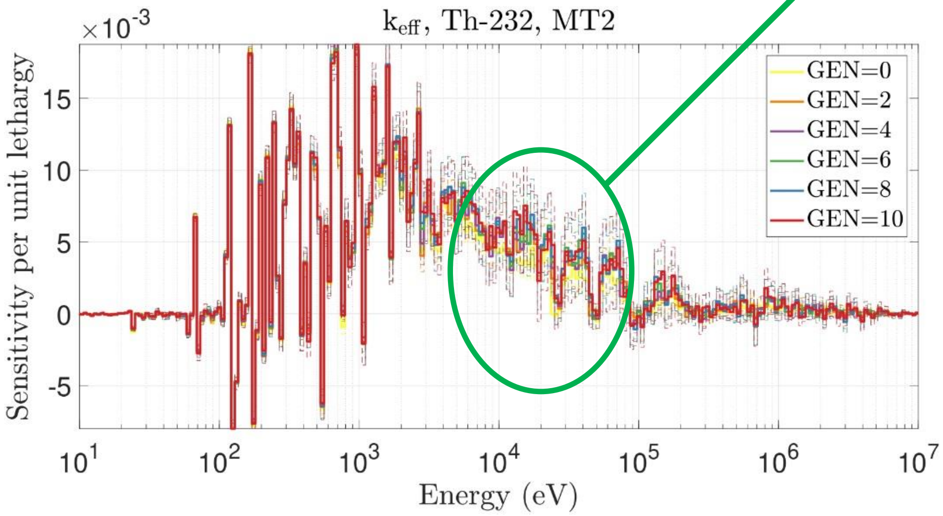
Poor statistics related to low number of latent generations for scattering

Scattering (MT2) perturbations strongly perturb the fission source



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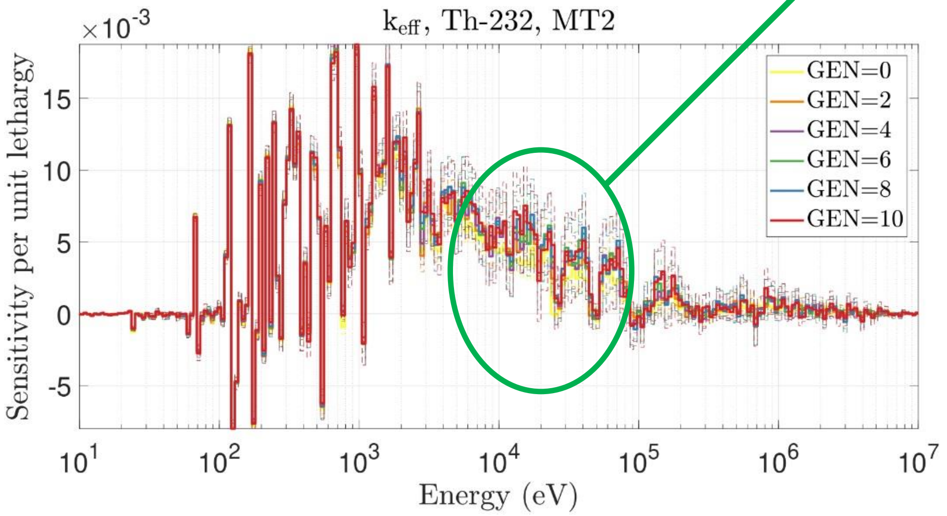
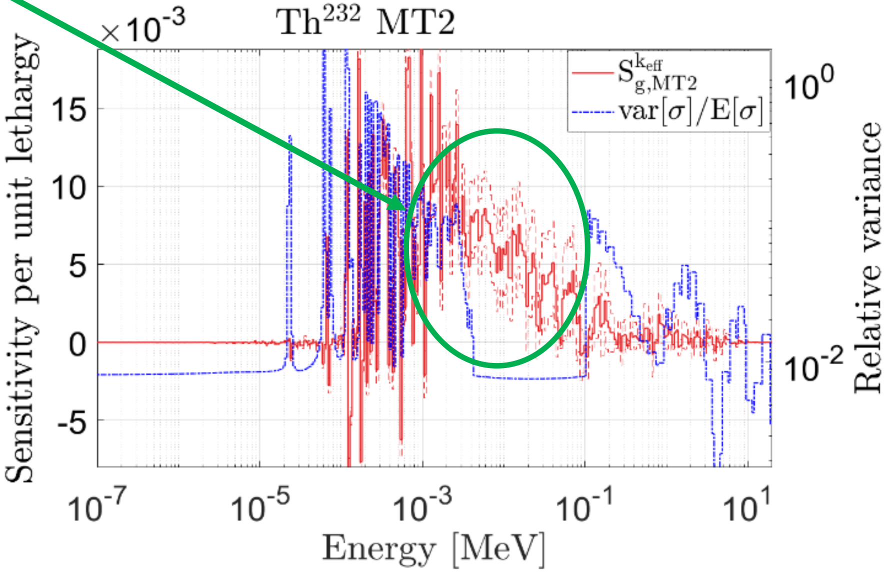
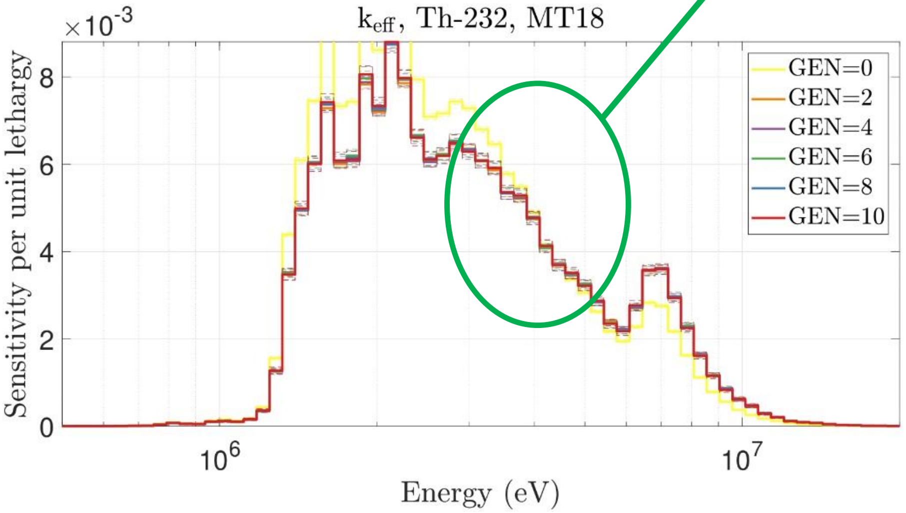


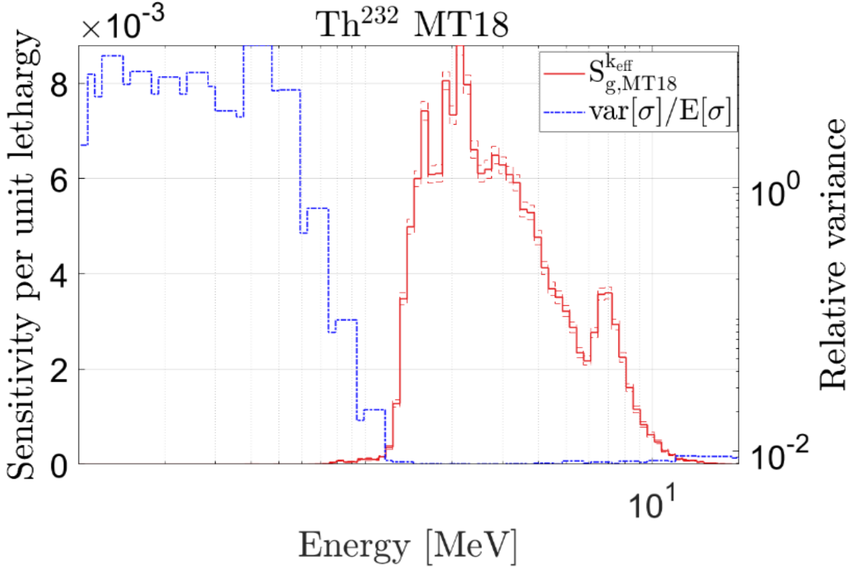


GPT output: Th^{232} , MT18

- 750000 neutrons
- 1000 active cycles
- 10 latent generations
- 500 groups

Good latent generation convergence for fission microscopic cross section





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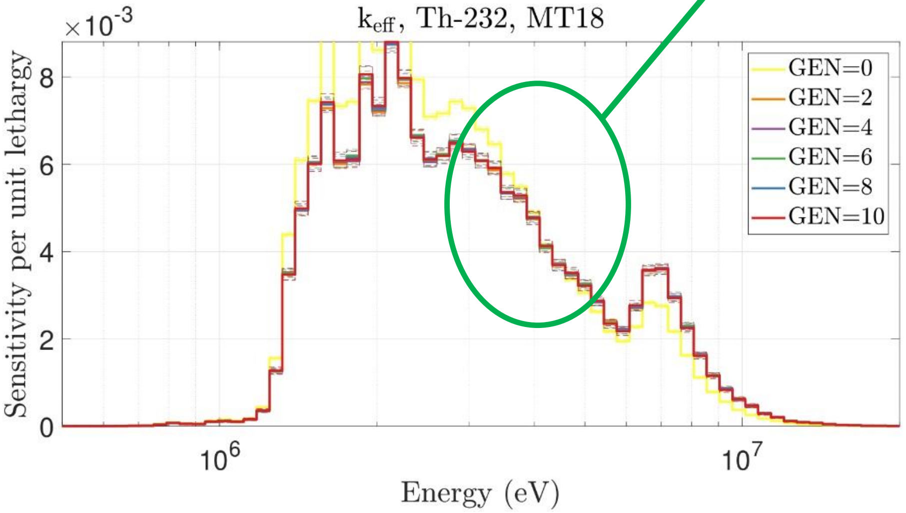
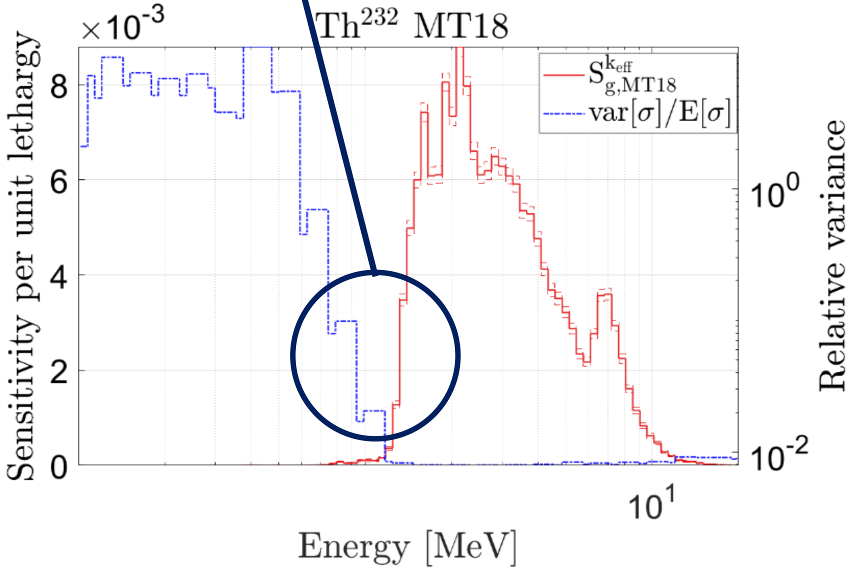
Sensitivity and variance do not superimpose





GPT output: Th^{232}, MT18

- 750000 neutrons
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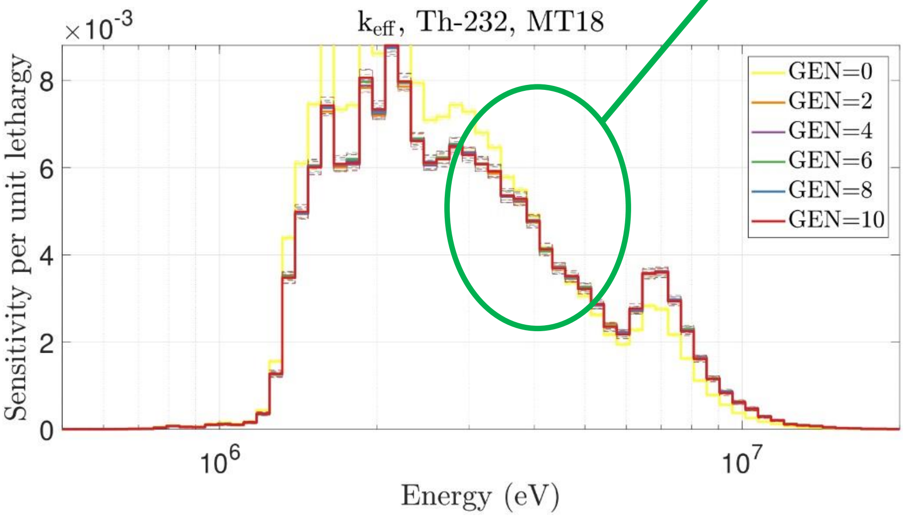
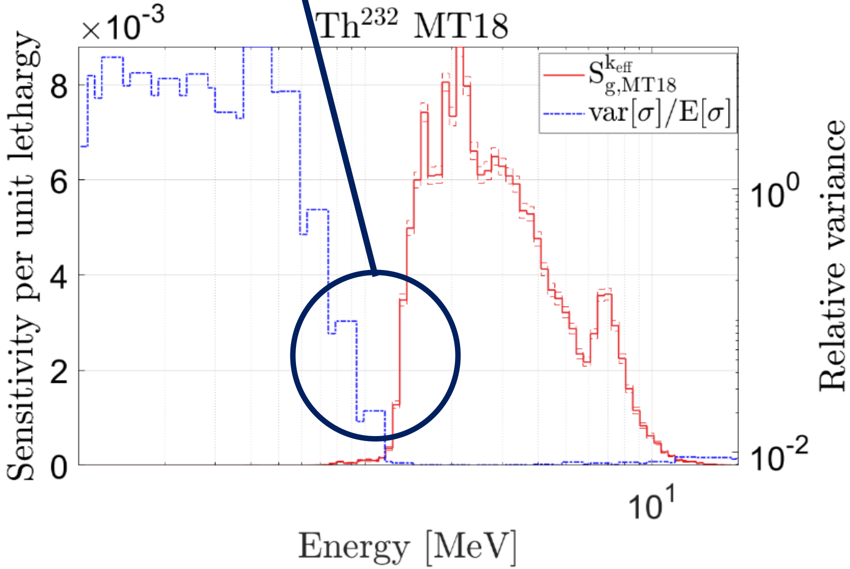
- 500 groups

Good latent generation convergence for fission microscopic cross section

Sensitivity and variance do not superimpose

Negligible response variance

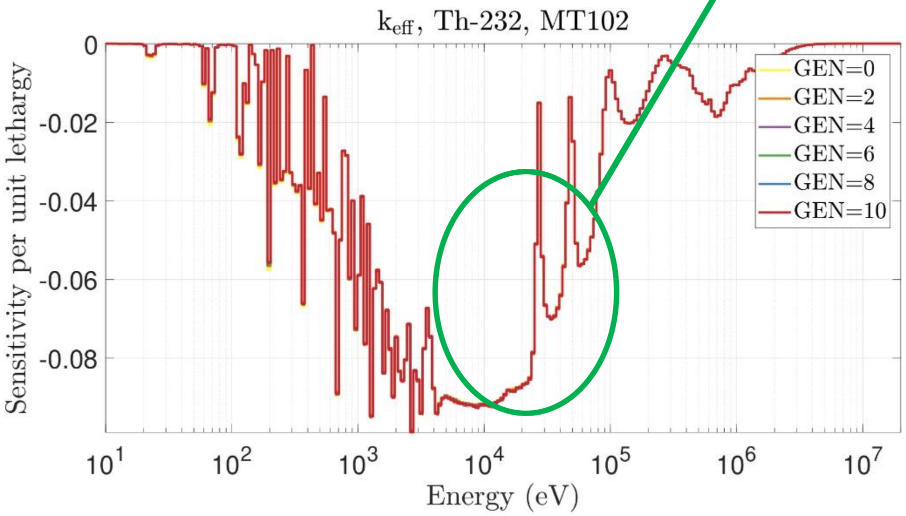


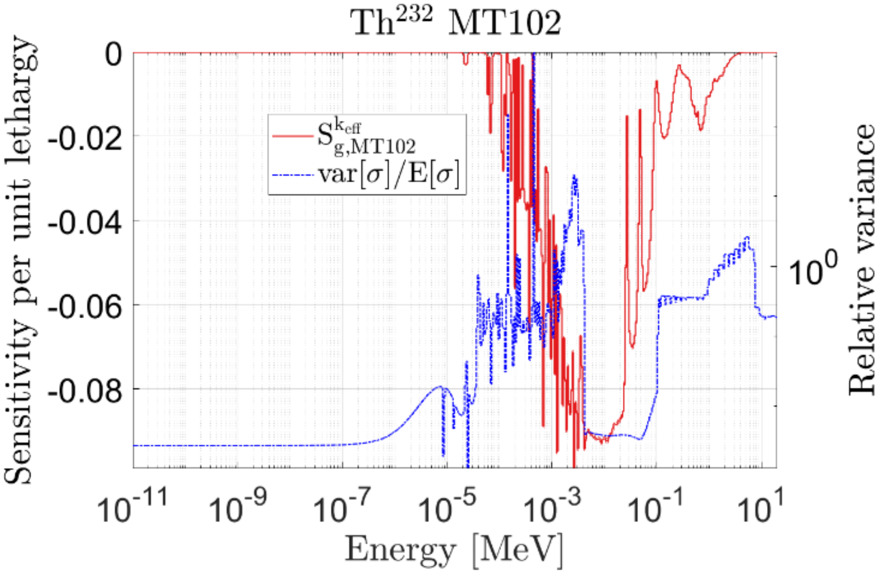


GPT output: Th^{232} , MT102

- 750000 neutrons
- 1000 active cycles
- 10 latent generations
- 500 groups

Good latent generation convergence for fission microscopic cross section





GPT output: Th^{232} , MT102

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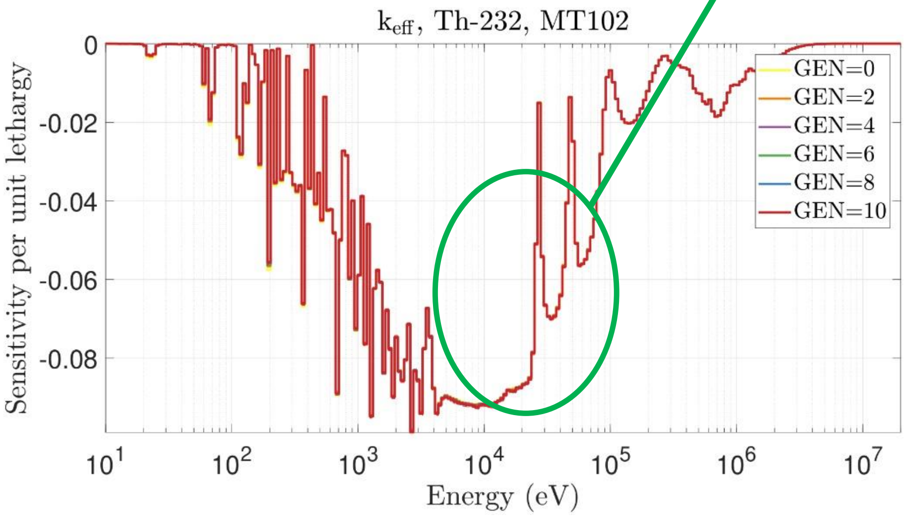
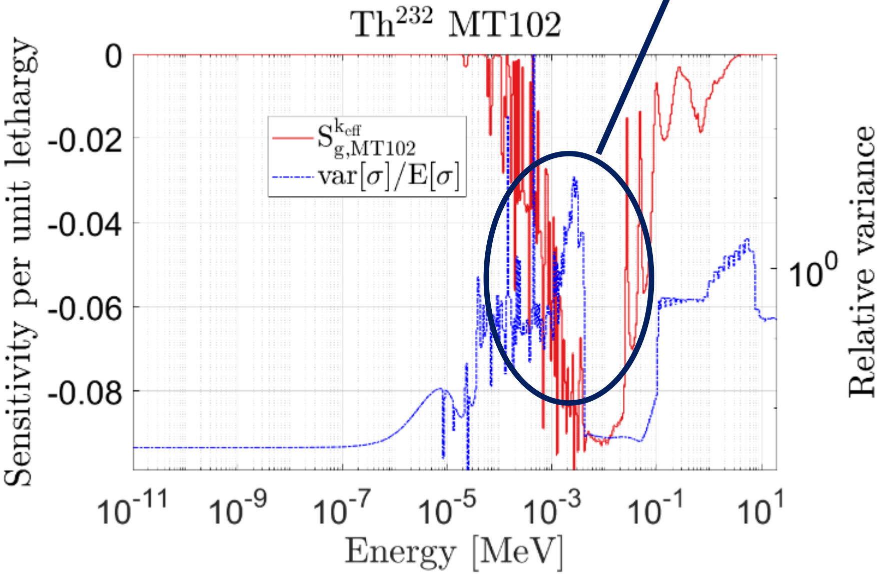
Sensitivity and variance superimpose





GPT output: Th^{232} , MT102

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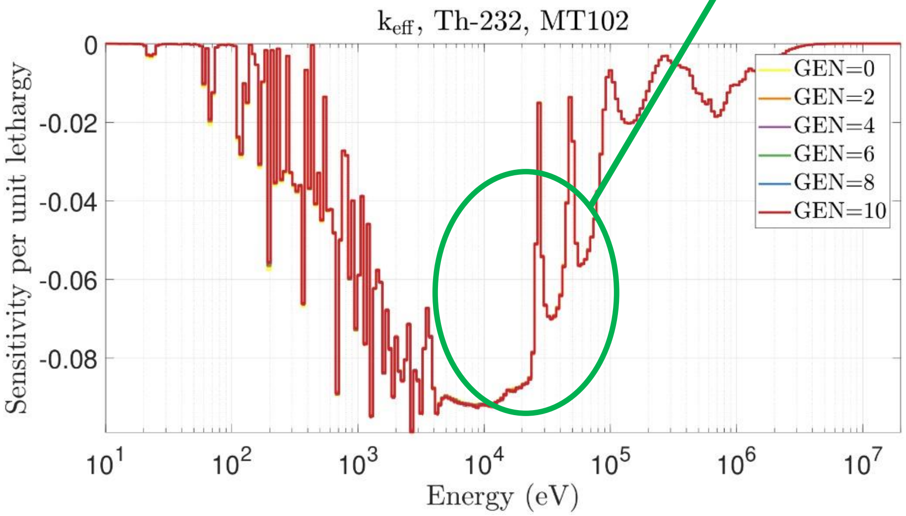
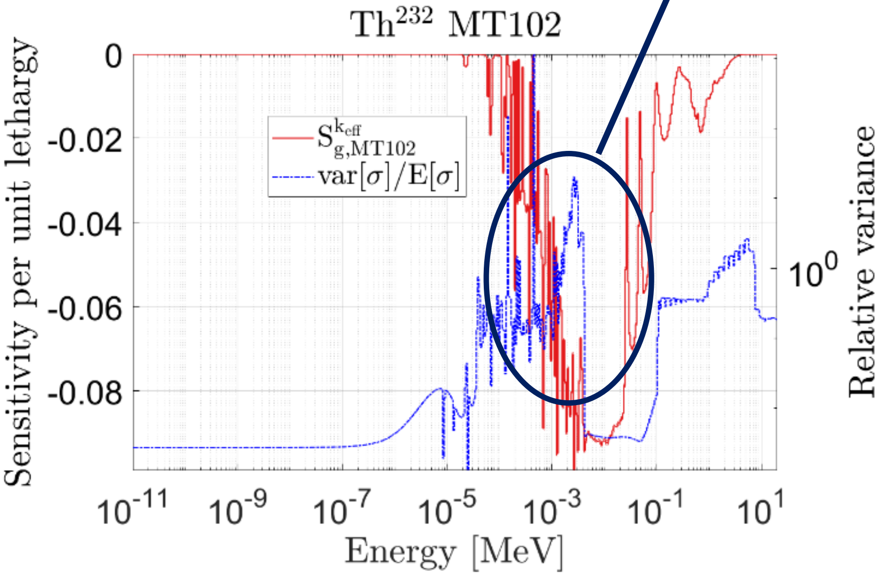
Good latent generation convergence for fission microscopic cross section

Sensitivity and variance superimpose

NON negligible response variance





Th^{232} results

Standard deviations are in pcm

GPT	LAT. GEN 0		LAT. GEN. 5		LAT. GEN. 10	
	std[k_{eff}]	MC stat. error	std[k_{eff}]	MC stat. error	std[k_{eff}]	MC stat. error
MT2	8.90519E+01	±5.58703E-01	9.37953E+01	±9.18935E-01	9.55651E+01	±1.24437E+00
MT18	2.01874E+01	±2.39076E-02	2.03064E+01	±3.95800E-02	2.03275E+01	±5.39219E-02
MT102	1.28074E+03	±4.05458E-01	1.28452E+03	±6.63389E-01	1.28582E+03	±8.93726E-01
TOT	1.28399E+03	±4.06283E-01	1.28810E+03	±6.64921E-01	1.28953E+03	±8.95916E-01

500 groups

Using covariance matrix from JEFF-3.3

XGPT SVD	LAT. GEN 0		LAT. GEN. 5		LAT. GEN. 10	
	std[k_{eff}]	MC stat. error	std[k_{eff}]	MC stat. error	std[k_{eff}]	MC stat. error
MT2	8.37917E+01	±3.68145E-01	9.18819E+01	±7.17697E-01	9.40103E+01	±1.06297E+00
MT18	2.19466E+01	±8.86200E-03	2.02225E+01	±1.73784E-02	2.02508E+01	±2.41705E-02
MT102	1.24230E+03	±2.66016E-01	1.24367E+03	±5.12886E-01	1.24537E+03	±7.26937E-01
TOT	1.24532E+03	±2.66525E-01	1.76276E+03	±6.30800E-01	1.24908E+03	±7.29182E-01

1000 groups

166 POD functions

Using perturbed files generated by SANDY

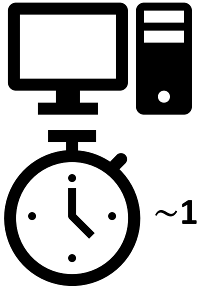
XGPT POD	LAT. GEN 0		LAT. GEN. 5		LAT. GEN. 10	
	std[k_{eff}]	MC stat. error	std[k_{eff}]	MC stat. error	std[k_{eff}]	MC stat. error
MT2	9.37622E+01	±3.27040E-01	1.03402E+02	±6.81124E-01	1.06978E+02	±1.01698E+00
MT18	2.14496E+01	±1.21912E-02	1.96887E+01	±2.32624E-02	1.97009E+01	±3.24118E-02
MT102	9.49968E+02	±2.55517E-01	9.51774E+02	±4.87198E-01	9.52989E+02	±6.91115E-01
TOT	9.54825E+02	±2.56238E-01	9.57577E+02	±4.89800E-01	9.59177E+02	±6.95962E-01

5000 groups

166 POD functions

GPT output: U^{233} , MT2

- 750000 neutrons
- 1000 active cycles
- 10 latent generations
- 500 groups



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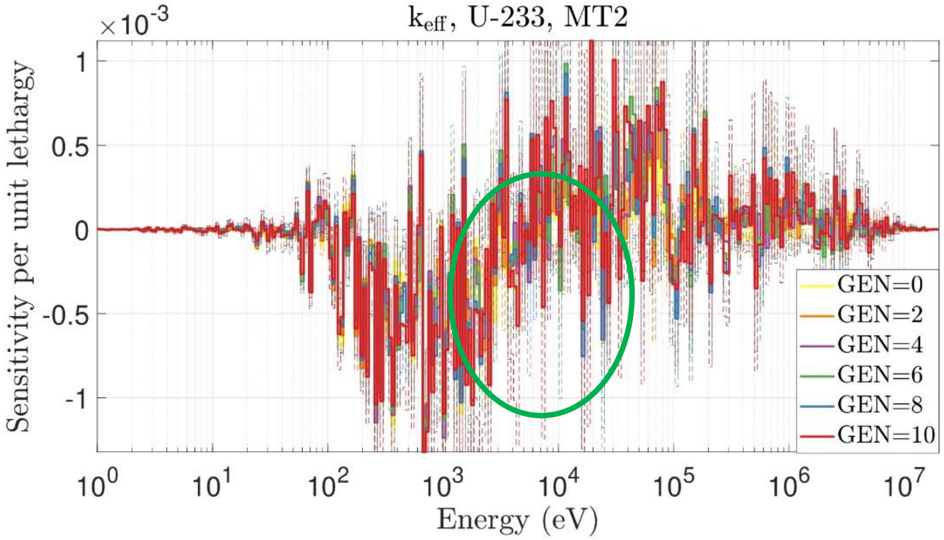

GPT output: U^{233} , MT2

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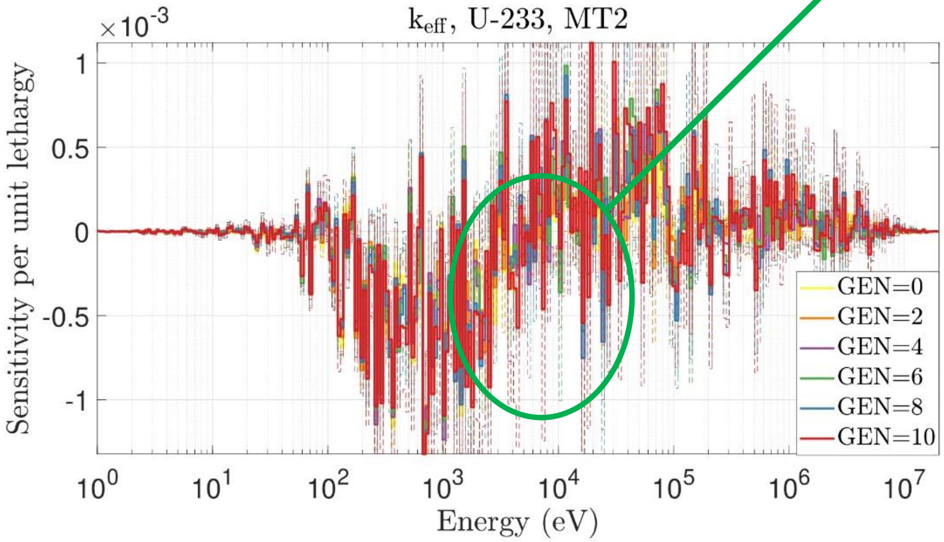
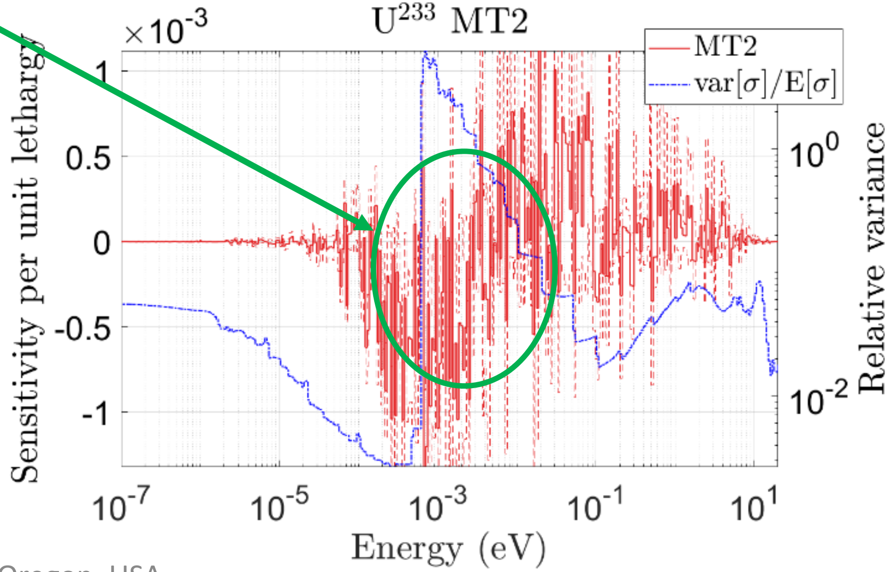
Poor statistics related to low number of latent generations for scattering

Scattering (MT2) perturbations strongly perturb the fission source





GPT output: U^{233} , MT18

- 750000 neutrons
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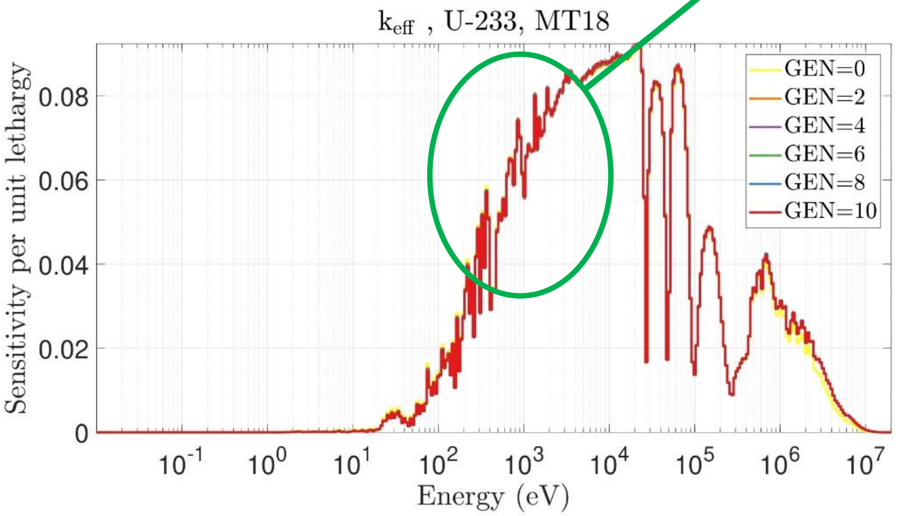
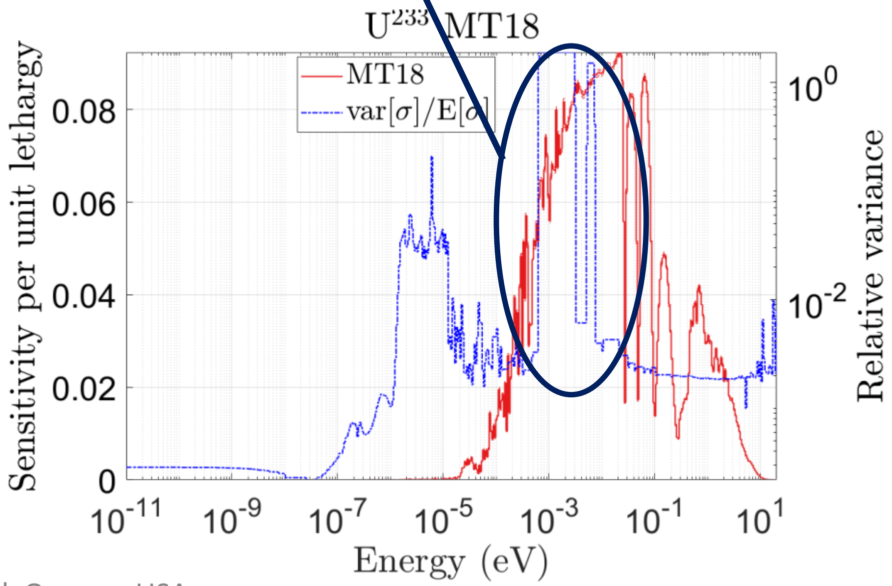
Good latent generation convergence for fission microscopic cross section

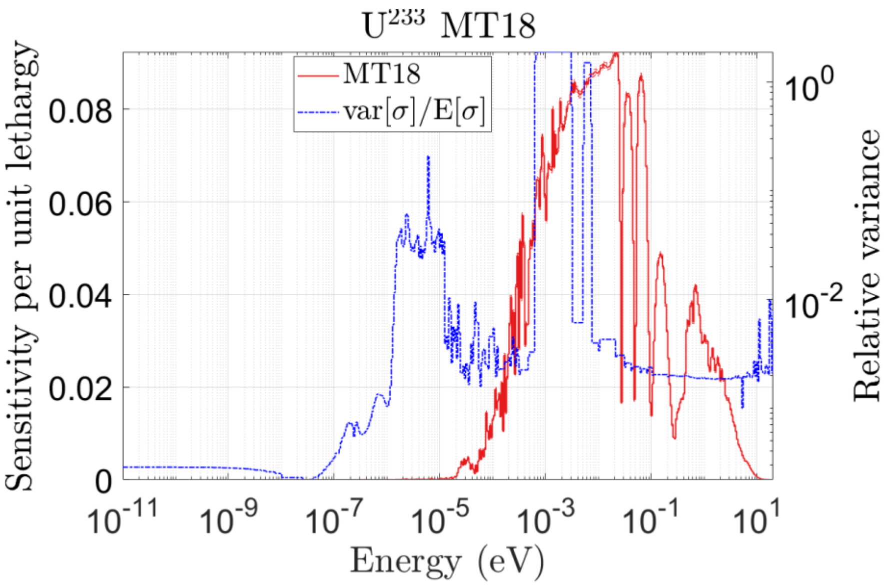
Sensitivity and variance superimpose

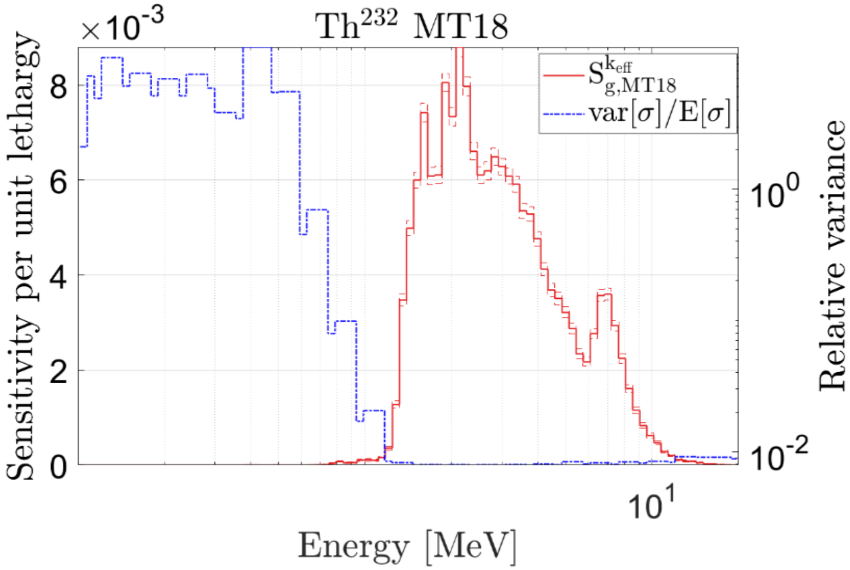
Big response variance



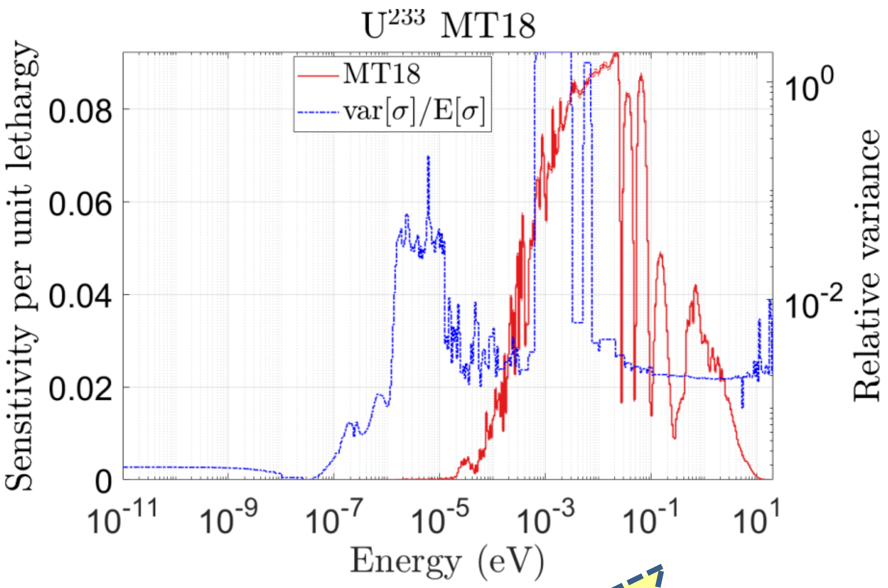


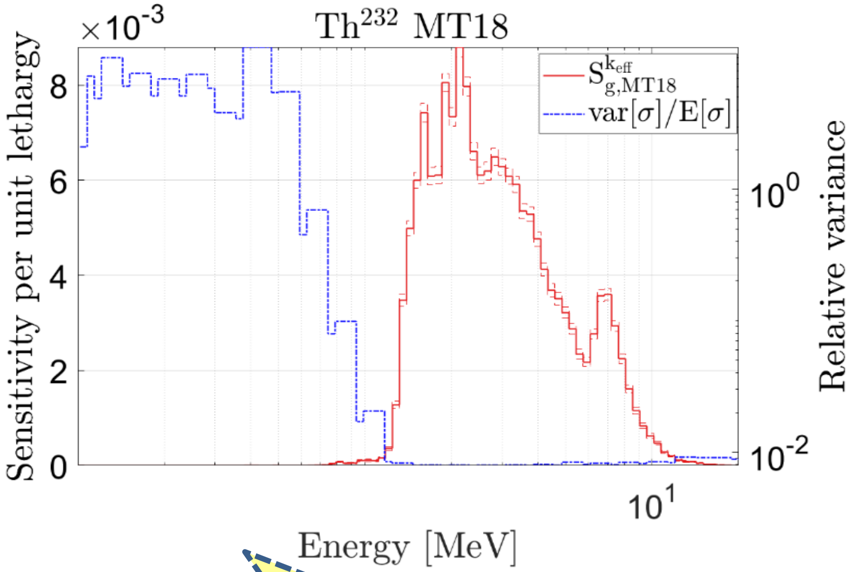
GPT output: U^{233} vs Th^{232} , MT18





GPT output: U^{233} vs Th^{232} , MT18

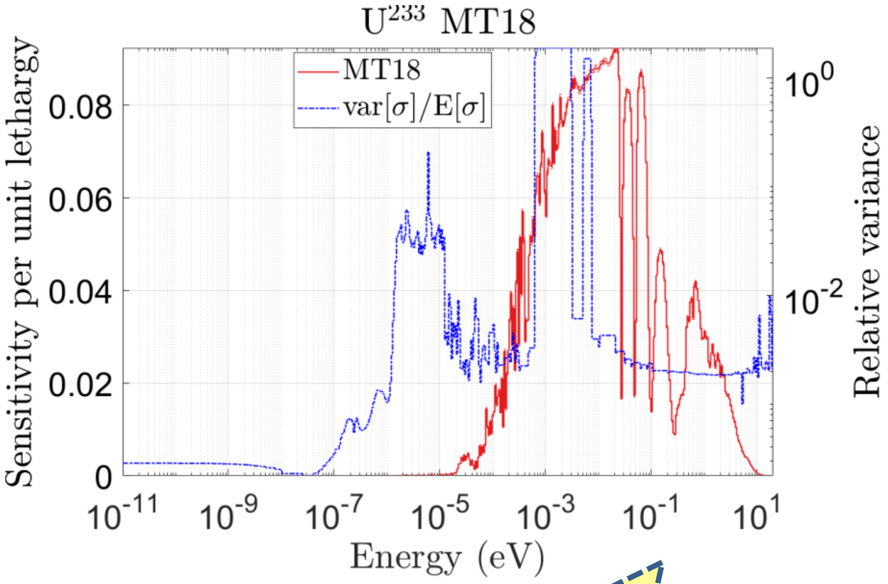


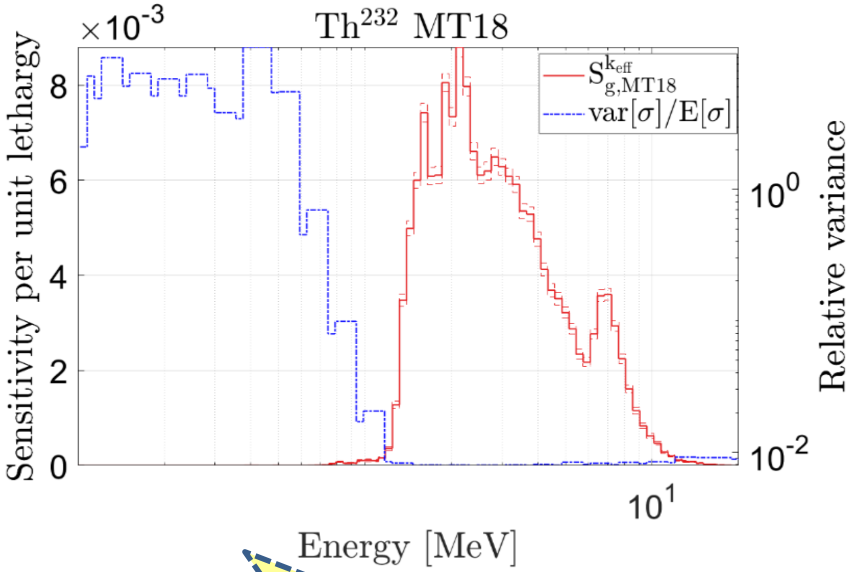


std[k_{eff}]
3.87730E+03

std[k_{eff}]
2.02508E+01

GPT output: U^{233} vs Th^{232}, MT18





std[k_{eff}]
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std[k_{eff}]
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GPT output: U^{233} , MT102

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- 10 latent generations
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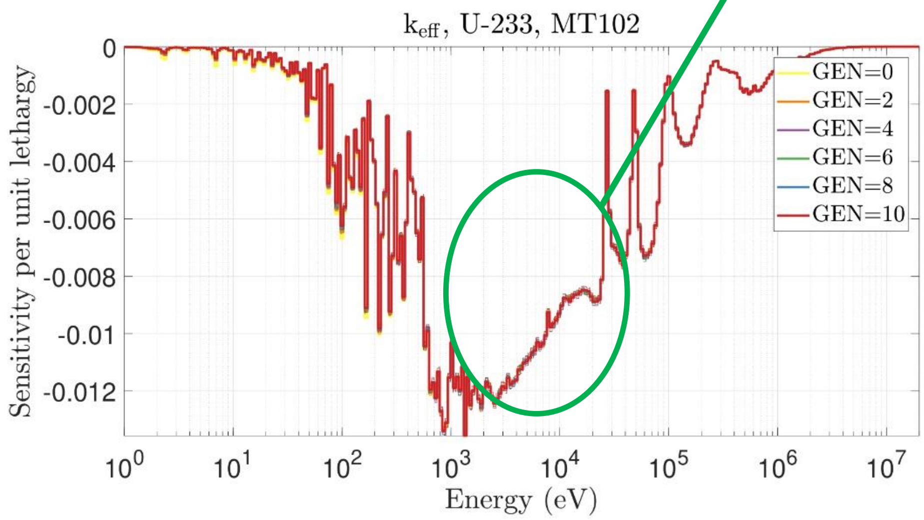
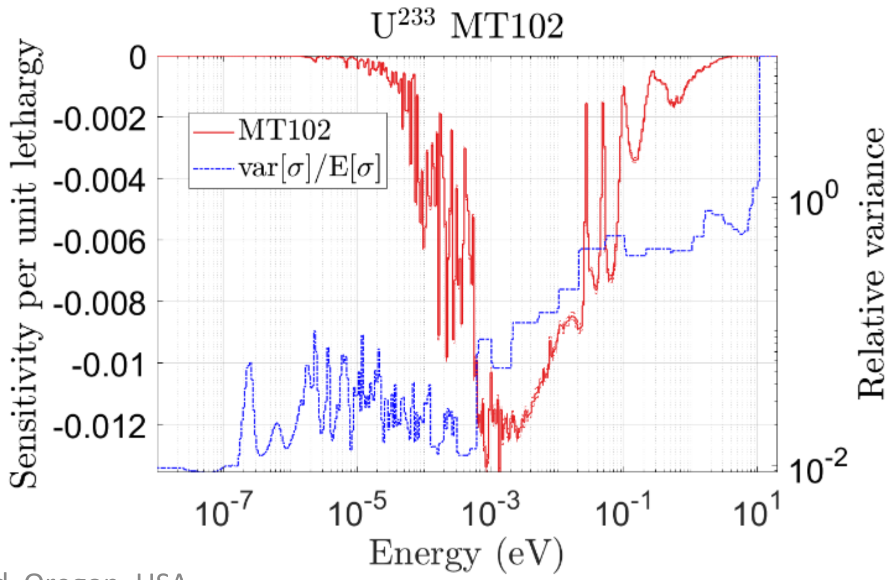
Good latent generation convergence for fission microscopic cross section





U^{233} results

- Standard deviations are in pcm

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MT18	3.87693E+03	±1.31891E+00	3.87730E+03	±2.15334E+00	3.87730E+03	±2.15334E+00
MT102	4.62307E+02	±1.61761E-01	4.64299E+02	±2.64860E-01	4.64394E+02	±3.59342E-01
TOT	3.90449E+03	±1.30978E+00	3.90509E+03	±2.13827E+00	3.90512E+03	±2.13855E+00

500 groups

Using covariance matrix from JEFF-3.3

XGPT SVD	LAT. GEN 0		LAT. GEN. 5		LAT. GEN. 10	
	$std[k_{eff}]$	MC stat. error	$std[k_{eff}]$	MC stat. error	$std[k_{eff}]$	MC stat. error
MT2	2.90274E+01	±1.17258E+00	2.45738E+01	±2.25777E+00	1.54131E+01	±3.31545E+00
MT18	3.87669E+03	±6.67481E-01	3.86337E+03	±1.32620E+00	3.86456E+03	±1.87811E+00
MT102	4.65186E+02	±8.68062E-02	4.66024E+02	±1.71673E-01	4.66497E+02	±2.48649E-01
TOT	3.90461E+03	±6.62846E-01	3.89145E+03	±1.31687E+00	3.89265E+03	±1.86484E+00

1000 groups

166 POD functions

Using perturbed files generated by SANDY

XGPT POD	LAT. GEN 0		LAT. GEN. 5		LAT. GEN. 10	
	$std[k_{eff}]$	MC stat. error	$std[k_{eff}]$	MC stat. error	$std[k_{eff}]$	MC stat. error
MT2	2.99851E+01	±1.87726E+00	2.66799E+01	±3.89855E+00	2.77825E+01	±5.62273E+00
MT18	3.78948E+03	±1.10233E+00	3.77694E+03	±2.14333E+00	3.78302E+03	±3.05290E+00
MT102	4.60241E+02	±1.51643E-01	4.61308E+02	±2.90474E-01	4.61437E+02	±4.16712E-01
TOT	3.81744E+03	±1.09450E+00	3.80510E+03	±2.12793E+00	3.81116E+03	±3.03106E+00

5000 groups

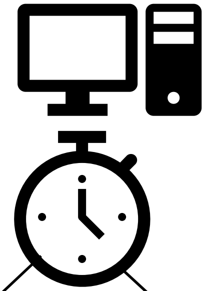
166 POD functions

NEMO

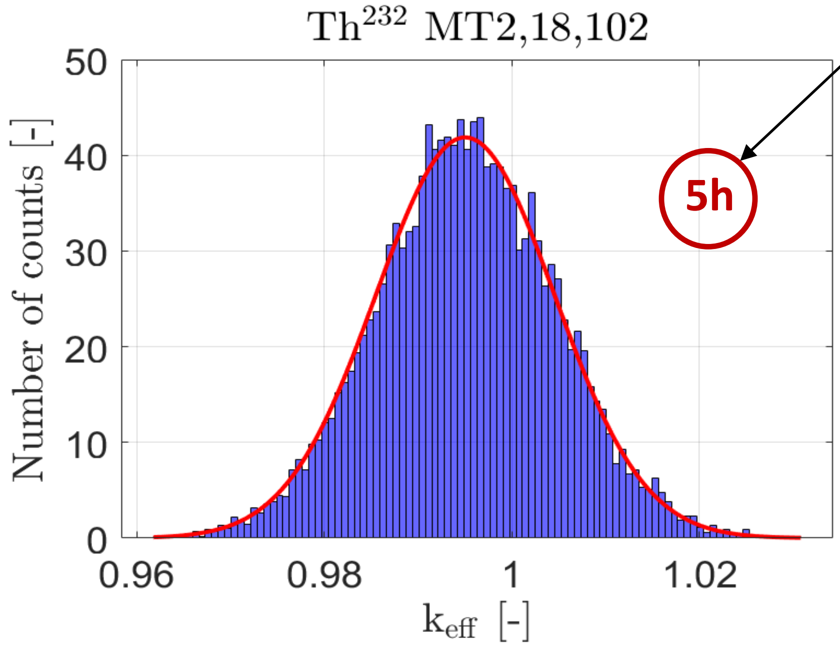
XGPT POD: U^{233} - Th^{232} , MT2,18,102

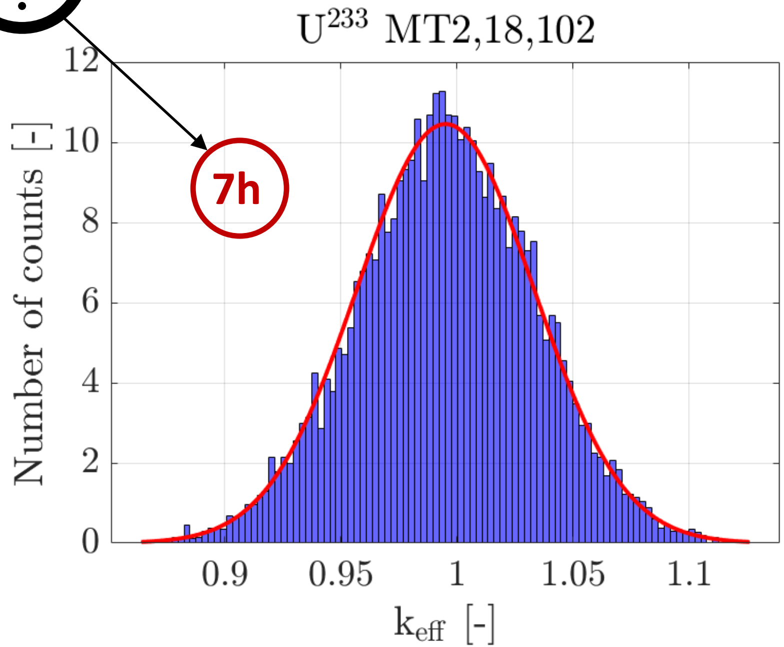
POLITECNICO DI TORINO

- 500000 neutrons
- 500 active cycles
- 10 latent generations
- 5000 groups



- -Dell Precision Tower 7910 (Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40 GHz
- -30 cores



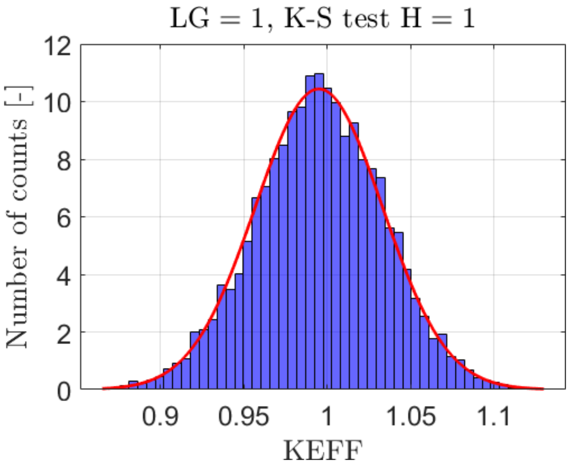


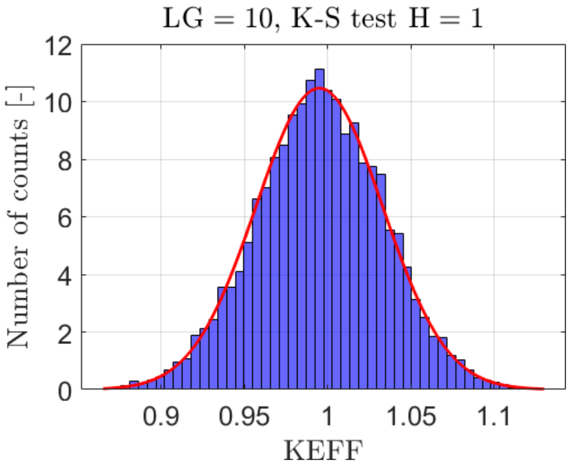
Improved statistics results: k_{eff}

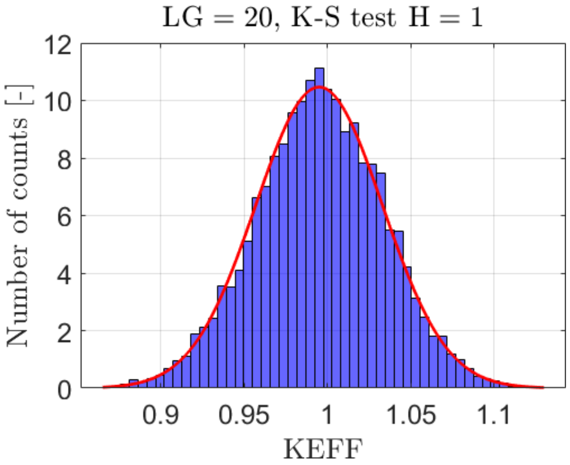
- 1000000 neutrons
- 1000 active cycles
- 20 latent generations
- 5000 groups
- According to Kolmogorov-Smirnov test, the distributions are not normal

-Dell Precision Tower 7910 (Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40 GHz
-30 cores

51h ($k_{\mathrm{eff}}, \beta_{\mathrm{eff}}$)





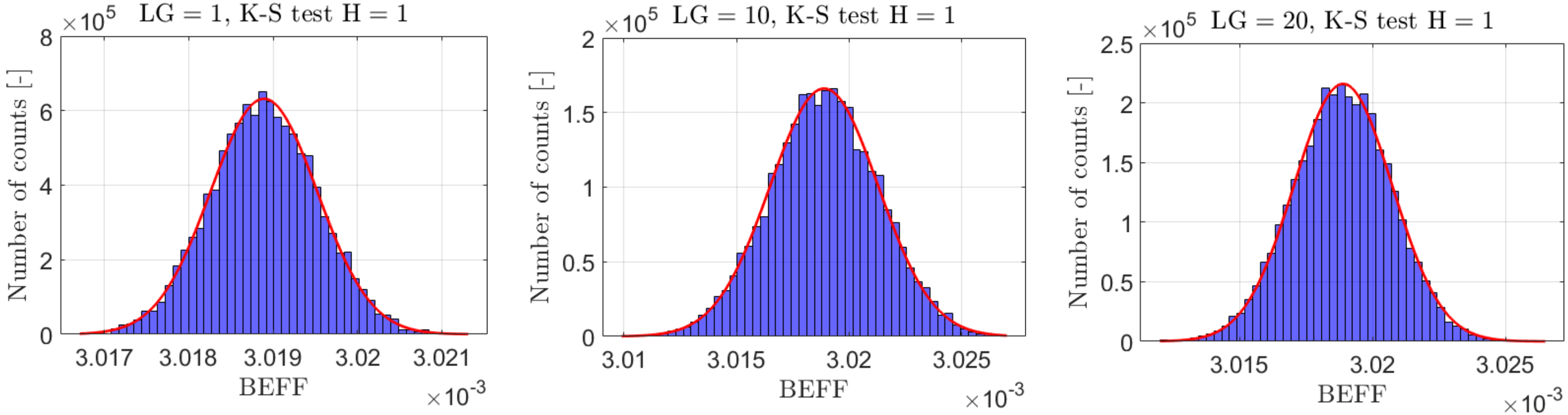


Improved statistics results: β_{eff}

- 1000000 neutrons
- 1000 active cycles
- 20 latent generations
- 5000 groups
- According to Kolmogorov-Smirnov test, the distributions are not normal

-Dell Precision Tower 7910 (Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40 GHz
-30 cores

51h ($k_{\mathrm{eff}}, \beta_{\mathrm{eff}}$)



Conclusions and perspectives

- SVD XGPT and GPT show good agreement
- Significant uncertainty on k_{eff} due to Th^{232} and U^{233} → > 1000 pcm

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- More accurate calculations needed to reduce the statistical error when the fission source is strongly perturbed

Conclusions and perspectives

- SVD XGPT and GPT show good agreement
- Significant uncertainty on k_{eff} due to Th^{232} and U^{233} → > 1000 pcm
- More investigations on kinetic integral parameters (maybe variance reduction techniques?)
- More accurate calculations needed to reduce the statistical error when the fission source is strongly perturbed
- Need for continuous-energy and finer multi-group covariances to improve results quality
- Exploiting the latest **Serpent-2 update**, UQ evaluation on multigroup homogenised cross sections (very computationally intensive)
- Adoption of **T6 package** (thanks to Dr. D. Rochman and Dr. A. Koning) to generate continuous-energy perturbations for cross sections for U-233 and Th-232.

Thank you for your attention!

Any questions?

NEMO

POLITECNICO DI TORINO

Backup

Improved statistics results: l_{eff}

POLITECNICO DI TORINO

- 1000000 neutrons
- 1000 active cycles
- 20 latent generations
- 5000 groups
- According to Kolmogorov-Smirnov test, the distributions are not normal

-Dell Precision Tower 7910 (Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40 GHz
-30 cores

51h (k_{eff}, β_{eff})