WPEC 2016 meetings
OECD/NEA Paris,
10–11 May 2016

Continuous energy adjustments: a potential breakthrough(?)

Manuele Aufiero & Massimiliano Fratoni

“dreaming” about continuous-energy cross sections adjustment
thanks to:

G. Palmiotti and M. Salvatores

eXtended Generalized Perturbation Theory (XGPT)
Sensitivity analysis and uncertainty quantification adopting continuous-energy functions.

First results of XS adjustment via XGPT
Is it possible to produce adjusted continuous energy XS?

Generalized Perturbation Theory capabilities

Effect of a perturbation of the parameter x on the response R :

$$S_x^R \equiv \frac{dR/R}{dx/x}$$

Considered response functions:

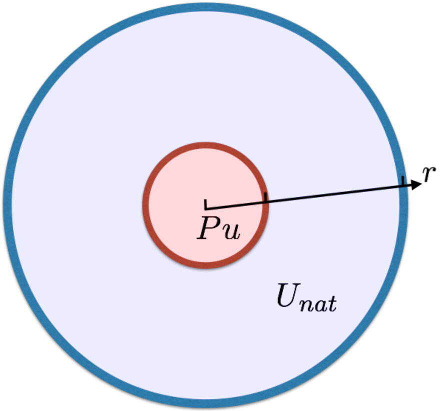
$R = k_{\mathrm{eff}}$ Effective multiplication factor

$R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle}$ Reaction rate ratios

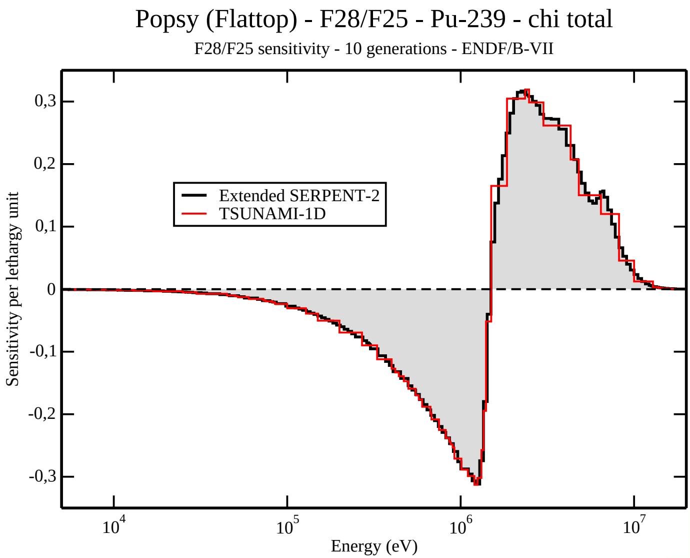
$R = \frac{\langle \phi^\dagger, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle}$ Bilinear ratios (Adjoint-weighted quantities)

$R = \frac{E[e_1]}{E[e_2]}$ Something else

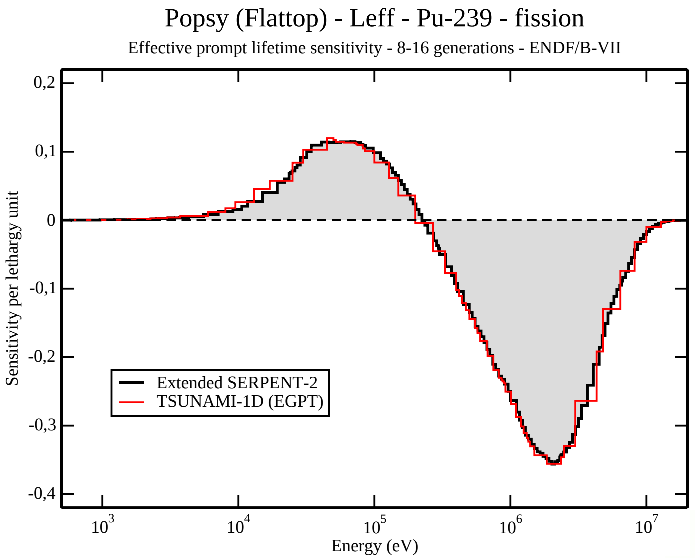
Flattop-Pu



Generalized sensitivities: a couple of examples



Generalized sensitivities: a couple of examples



Generalized sensitivities: a couple of examples

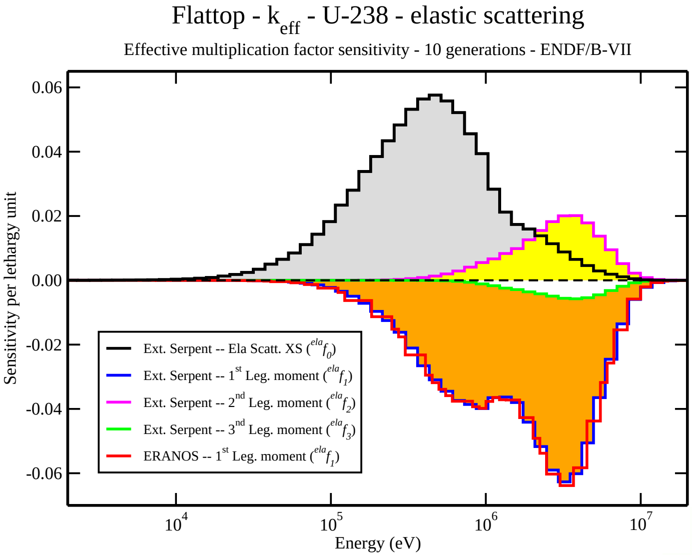
No bi-linear ratio sensitivity available in Scale (?)...
Adopting EGPT for comparison against Serpent

$$S_x^{\ell_{\text{eff}}} = \frac{\partial \left(\dfrac{\partial k_{\text{eff}} / k_{\text{eff}}}{\partial a_{1/v}} \right)}{\partial x / x} \Bigg/ \frac{\partial k_{\text{eff}} / k_{\text{eff}}}{\partial a_{1/v}}$$

$$S_x^{\ell_{\text{eff}}} = \frac{\partial \left(\dfrac{\partial k_{\text{eff}} / k_{\text{eff}}}{\partial x / x} \right)}{\partial a_{1/v}} \Bigg/ \frac{\partial k_{\text{eff}} / k_{\text{eff}}}{\partial a_{1/v}} = \frac{\dfrac{\partial S_x^{k_{\text{eff}}}}{\partial a_{1/v}}}{\dfrac{\partial k_{\text{eff}} / k_{\text{eff}}}{\partial a_{1/v}}}$$

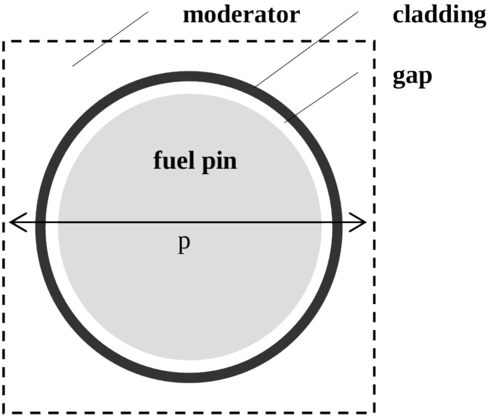
$$S_x^{\ell_{\text{eff}}} \simeq \frac{{}^*S_x^{k_{\text{eff}}} - S_x^{k_{\text{eff}}}}{\dfrac{{}^*k_{\text{eff}} - k_{\text{eff}}}{k_{\text{eff}}}}$$

Generalized sensitivities: a couple of examples



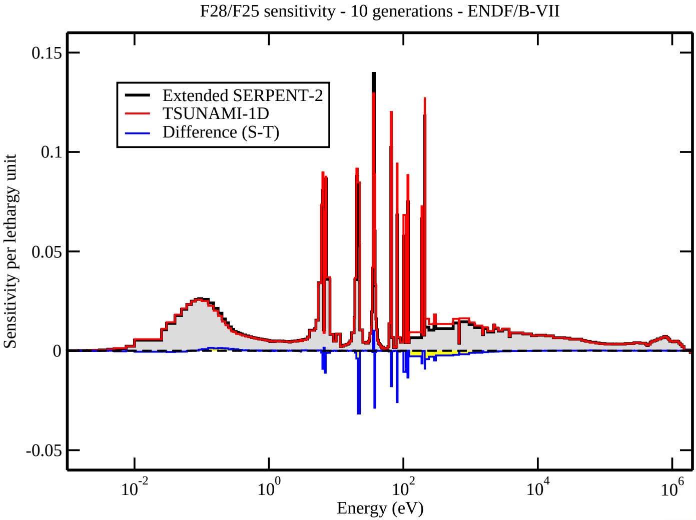
Berkeley UNIVERSITY OF CALIFORNIA

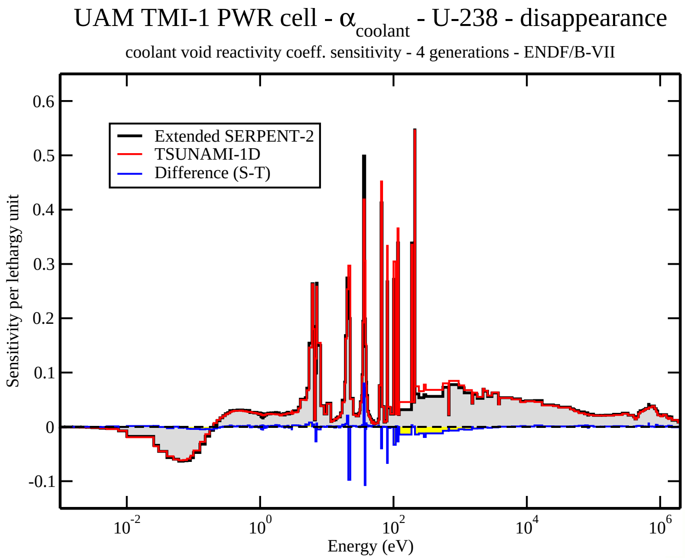
PWR pin cell



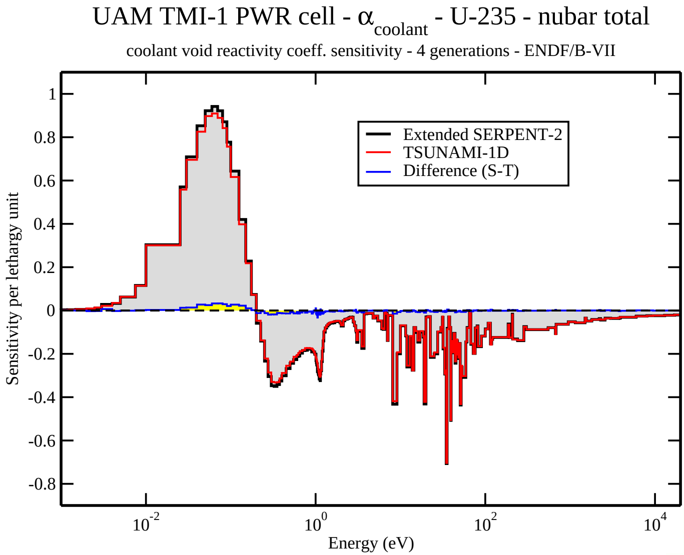
Generalized sensitivities: a couple of examples

UAM TMI-1 PWR cell - F28/F25 - U-238 - disappearance

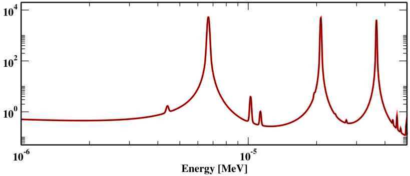


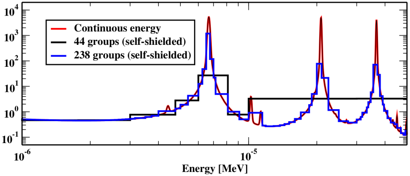

UAM TMI-1 PWR cell - $\alpha_{coolant}$ - U-238 - disappearance
coolant void reactivity coeff. sensitivity - 4 generations - ENDF/B-VII
Extended SERPENT-2
TSUNAMI-1D
Difference (S-T)
Sensitivity per lethargy unit
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
Energy (eV)

Generalized sensitivities: a couple of examples

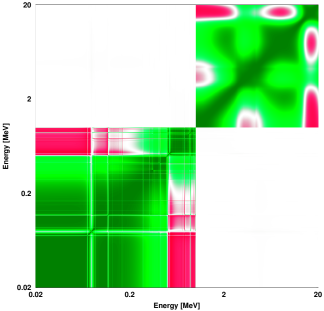


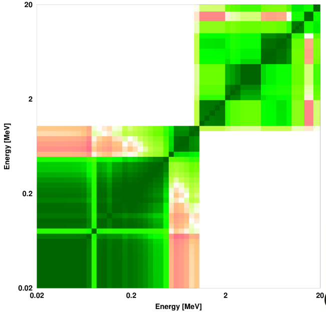
Cross sections





Covariance matrices





Continuous-energy function sensitivity approach

Continuous energy uncertainty propagation formula:

$$Var\left[R\right] = \int_{E_{min}}^{E_{max}} \int_{E_{min}}^{E_{max}} S_{\Sigma}^{R}\left(E\right) \cdot COV\left[\Sigma(E), \Sigma(E')\right] \cdot S_{\Sigma}^{R}\left(E'\right)\, dE\, dE'$$

It is hard to solve double integrals with Monte Carlo transport.

- Legacy approach: multi-group discretization
  + sum over **bin-averaged** sensitivities
- New approach: eigenvalue expansion
  + sum over **continuous-energy** integrated sensitivities

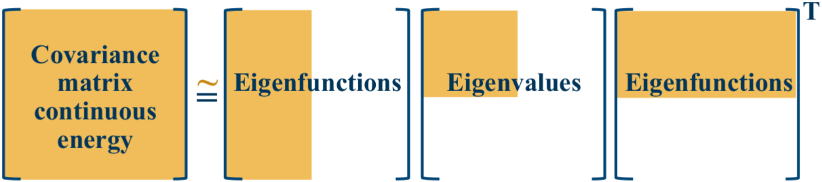
Eigenvalue decomposition of the covariance matrix

$$COV\left[\Sigma(E)\,,\Sigma(E')\right] = \sum_{j=1}^{\infty} U_j(E) \cdot V^j \cdot U_j(E')$$

$$\begin{bmatrix} \textbf{Covariance matrix continuous energy} \end{bmatrix} = \begin{bmatrix} \textbf{Eigenfunctions} \end{bmatrix} \begin{bmatrix} \textbf{Eigenvalues} \end{bmatrix} \begin{bmatrix} \textbf{Eigenfunctions} \end{bmatrix}^{\mathbf{T}}$$

Eigenvalue decomposition of the covariance matrix

$$COV\left[\Sigma(E)\,,\Sigma(E')\right] \sim \sum_{j=1}^{n} U_j(E)\cdot V^j \cdot U_j(E')$$



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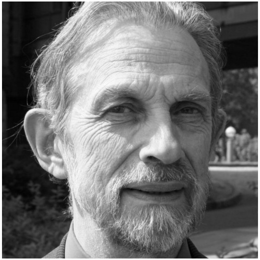
$$Var\left[R\right] = \int_{E_{min}}^{E_{max}} \int_{E_{min}}^{E_{max}} S_{\Sigma}^{R}\left(E\right) \cdot COV\left[\Sigma(E)\,,\Sigma(E')\right] \cdot S_{\Sigma}^{R}\left(E'\right)\, dE\, dE'$$

$$COV\left[\Sigma(E)\,,\Sigma(E')\right] \sim \sum_{j=1}^{n} U_j(E) \cdot V^j \cdot U_j(E')$$

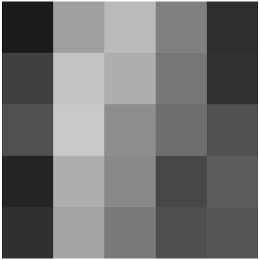
$$Var\left[R\right] \sim \sum_{j=1}^{n} V^j \cdot \left(\int_{E_{min}}^{E_{max}} U_j\left(E\right) \cdot S_{\Sigma}^{R}\left(E\right)\, dE \right)^2$$

$$Var\left[R\right] \sim \sum_{j=1}^{n} V^j \cdot \left(S_{U_j}^{R}\right)^2$$



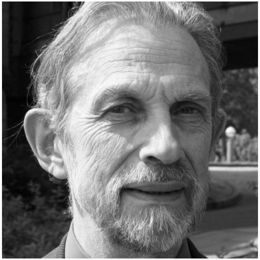
Original
image

SVD/POD
5 basis functions



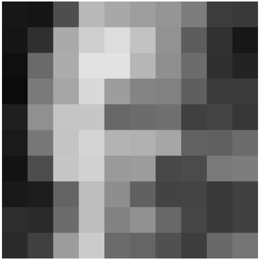
Multi-group
5 energy groups

```
A=imread("massimo.png"); [A, map]=gray2ind(A,255);
[U, S, V]=svd(A);
A_SVD_5 = U(:,1:5) * S(1:5,1:i) * V(:,1:5)';
imwrite(A_SVD_5, gray(255), "massimo_5.png");
```



Original
image

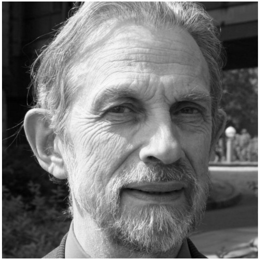
SVD/POD
10 basis functions



Multi-group
10 energy groups

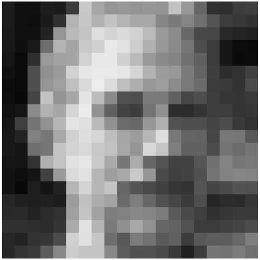
```
A=imread("massimo.png"); [A, map]=gray2ind(A,255);
[U, S, V]=svd(A);
A_SVD_10 = U(:,1:10) * S(1:10,1:i) * V(:,1:10)';
imwrite(A_SVD_10, gray(255), "massimo_10.png");
```

Singular Value Decomposition



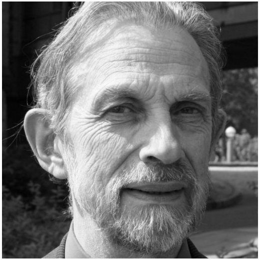
Original image

SVD/POD
20 basis functions

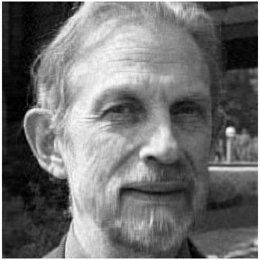


Multi-group
20 energy groups

```
A=imread("massimo.png"); [A, map]=gray2ind(A,255);
[U, S, V]=svd(A);
A_SVD_20 = U(:,1:20) * S(1:20,1:i) * V(:,1:20)';
imwrite(A_SVD_20, gray(255), "massimo_20.png");
```



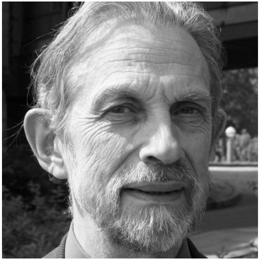
Original
image



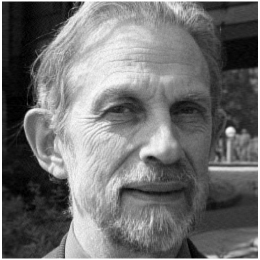
SVD/POD
40 basis functions

Multi-group
40 energy groups

```
A=imread("massimo.png"); [A, map]=gray2ind(A,255);
[U, S, V]=svd(A);
A_SVD_40 = U(:,1:40) * S(1:40,1:i) * V(:,1:40)′;
imwrite(A_SVD_40, gray(255), "massimo_40.png");
```



Original
image



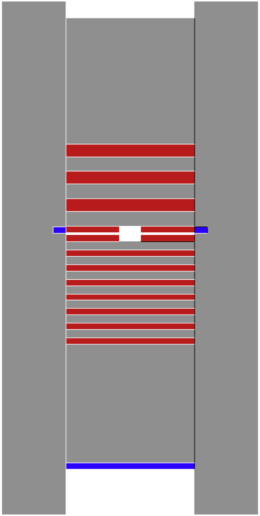
SVD/POD
80 basis functions

Multi-group
80 energy groups

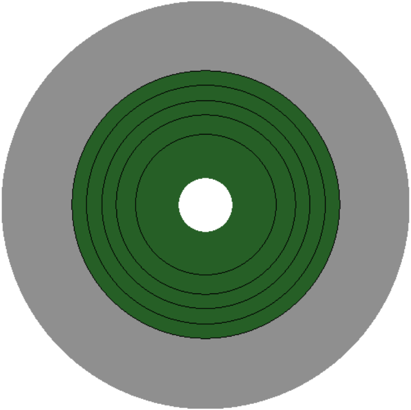
```
A=imread("massimo.png"); [A, map]=gray2ind(A,255);
[U, S, V]=svd(A);
A_SVD_80 = U(:,1:80) * S(1:80,1:i) * V(:,1:80)′;
imwrite(A_SVD_80, gray(255), "massimo_80.png");
```

Two simple case studies

HMF-64



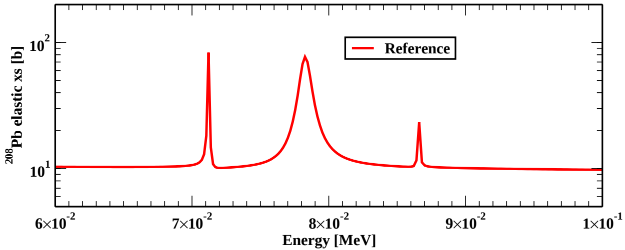
PMF-35

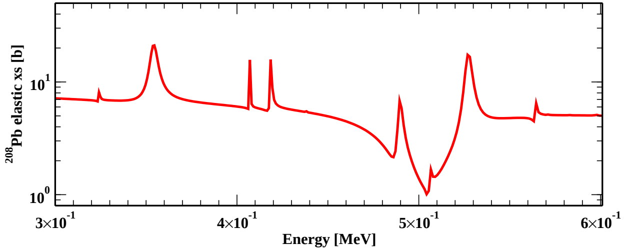


Random cross sections

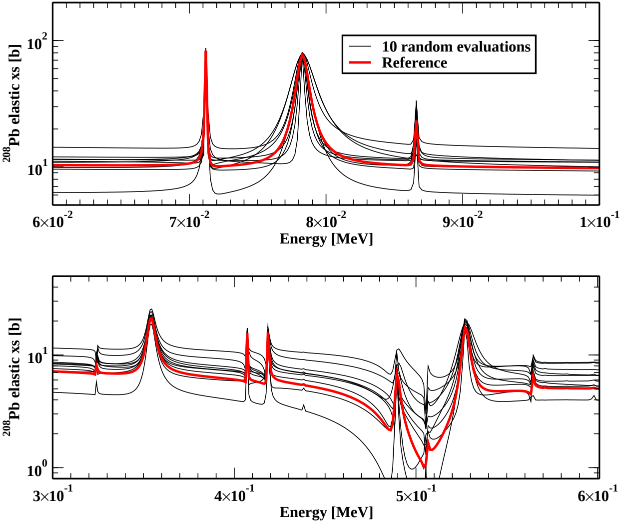
- 3000 different ^{208}Pb ENDF files from TENDL-2013
- Random MF2-MT151 (resonances), MF3-MT1, MF3-MT2 (elastic), MF3-MT51-58,91 (inelastic), and MF3-MT102 (n, γ) processed with NJOY
- 3000 ACE files with random cross sections
- The random continuous energy XS reflect the **UNCERTAINTIES** and their **CORRELATIONS** (according to TENDL-2013)
- Continuous-energy covariances reconstructed from random XS

Random cross sections

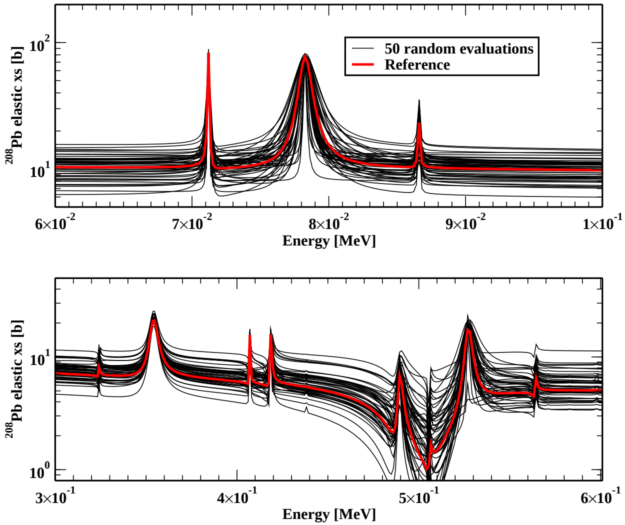




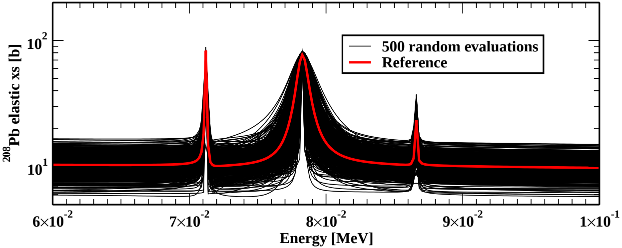
Random cross sections

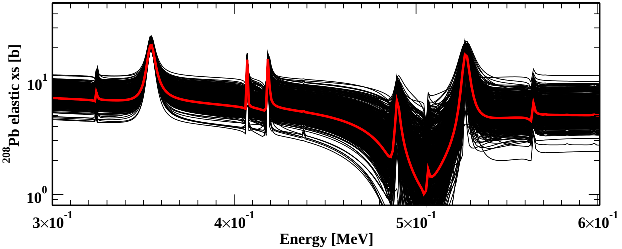


Random cross sections



Random cross sections

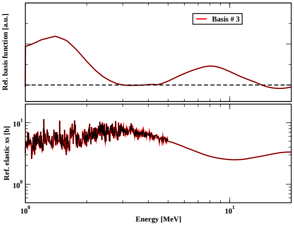




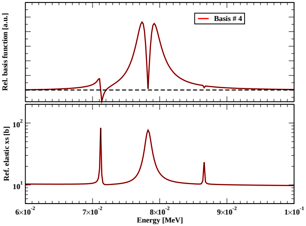
We want a set of orthogonal basis functions $\boldsymbol{b_{\Sigma,j}}$ so that:

$$\widetilde{\Sigma}_i(E) = \Sigma_0(E) \cdot \left(1 + \sum_{j=1}^{n} \alpha_i^j \cdot b_{\Sigma,j}(E)\right)$$

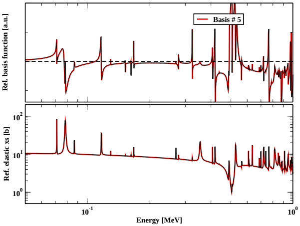
3 basis functions from the POD of ^{208}Pb (n, ela)



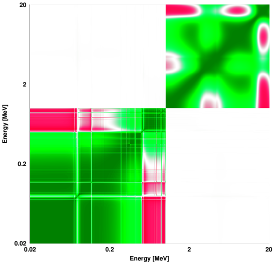
Basis # 3



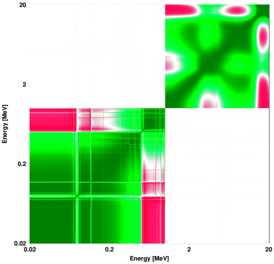
Basis # 4



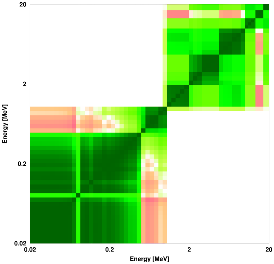
Basis # 5



Continuous Energy



SVD/POD
20 basis functions



Multi-group
>100 ene g.

We need to calculate the effect on the response $\boldsymbol{R}$ due to a perturbation on $\boldsymbol{\Sigma}$ equal to $\boldsymbol{b_{\Sigma,j}}$

$$S^R_{b_{\Sigma,j}} = \frac{dR/R}{d\,b_{\Sigma,j}} = \int_{E_{min}}^{E_{max}} b_{\Sigma,j}(E) \cdot S^R_{\Sigma}(E)\, dE$$

The calculation of $S^R_{b_{\Sigma,j}}$ is the main innovation of XGPT (implemented in Serpent).

XGPT+POD: uncertainty propagation

From the Proper Orthogonal Decomposition of Nuclear data...

$$\Sigma_i\left(E\right) \simeq \widetilde{\Sigma}_i\left(E\right) = \Sigma_0\left(E\right) \cdot \left(1 + \sum_{j=1}^{n} \alpha_i^j \cdot b_{\Sigma,j}\left(E\right)\right)$$

...and the basis functions sensitivity coefficients $\boldsymbol{S^R_{b_{\Sigma,j}}}$, we can approximate the response function $\boldsymbol{R_{\Sigma_i}}$ for each random XS $\boldsymbol{\Sigma_i}$

$$R_{\Sigma_i} \simeq \widetilde{R_{\Sigma_i}} = R_{\Sigma_0} \cdot \left(1 + \sum_{j=1}^{n} \alpha_i^j \cdot S^R_{b_{\Sigma,j}}\right)$$

XGPT+POD: uncertainty propagation

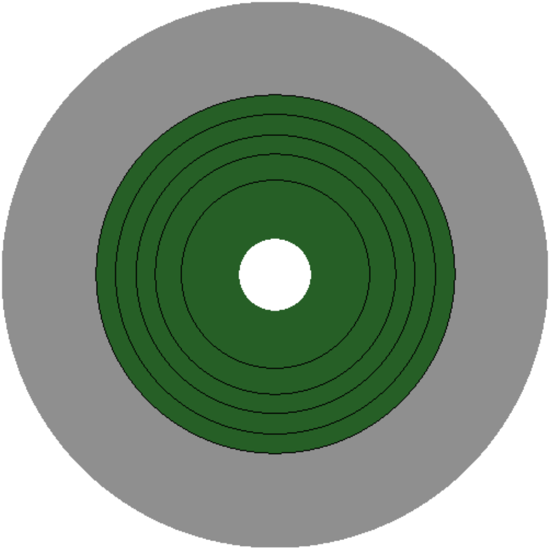
Estimating the k_{eff} distribution in the simple case study

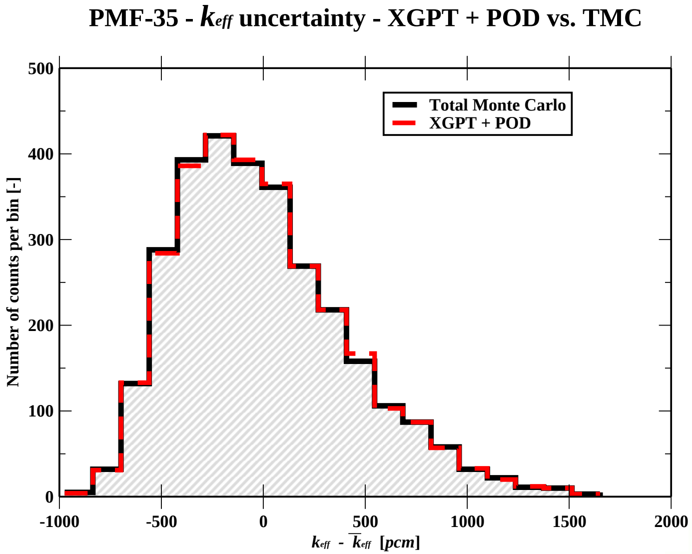
$$k_{\text{eff}\,\Sigma_i} \simeq \widetilde{k_{\text{eff}}}_{\Sigma_i} = k_{\text{eff}\,\Sigma_0} \cdot \left(1 + \sum_{j=1}^{n} \alpha_i^j \cdot S_{b_{\Sigma,j}}^{k_{\text{eff}}}\right)$$

The k_{eff} for all the N (3000) random XS Σ_i were calculated in a single Serpent run (ACE file for Σ_0) with $n = 50$ bases

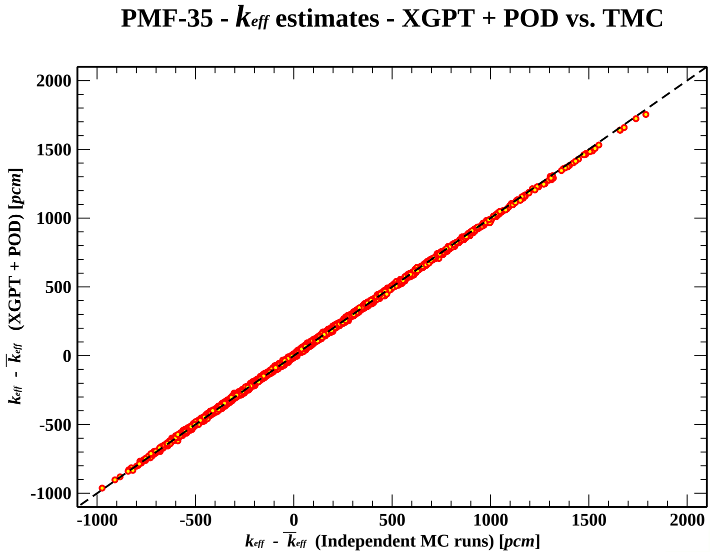
The XGPT+POD results are compared to TMC results (3000 separate Serpent runs)

PMF-35



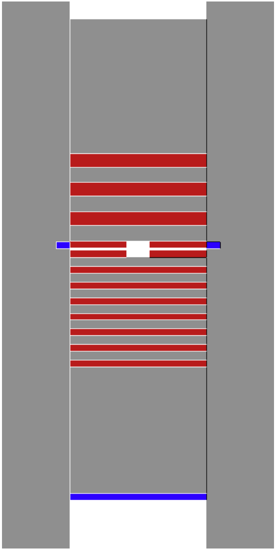

PMF-35 - keff uncertainty - XGPT + POD vs. TMC
Total Monte Carlo
XGPT + POD
Number of counts per bin [-]
0
100
200
300
400
500
-1000
-500
0
500
1000
1500
2000
keff - keff [pcm]

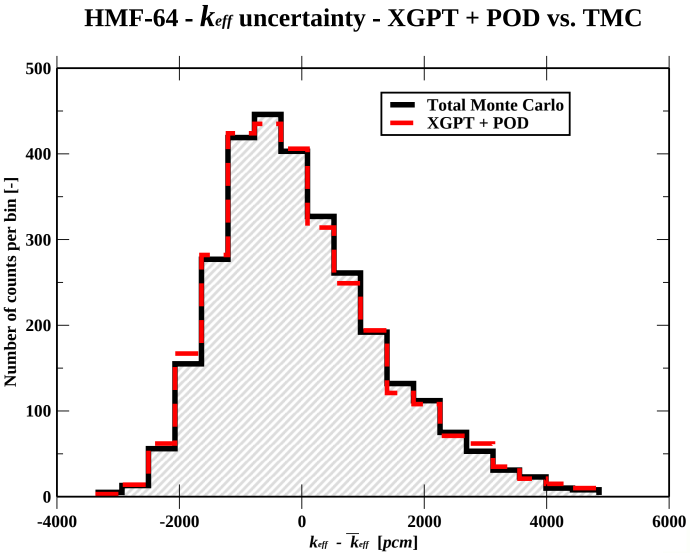
XGPT+POD: uncertainty propagation in PMF-35 – k_{eff}



XGPT+POD: uncertainty propagation in **HMF-64**

PMF-35




HMF-64 - keff uncertainty - XGPT + POD vs. TMC
Total Monte Carlo
XGPT + POD
Number of counts per bin [-]
500
400
300
200
100
0
-4000
-2000
0
2000
4000
6000
keff - keff [pcm]

XGPT+POD: uncertainty in **PMF-35 & HMF-64**

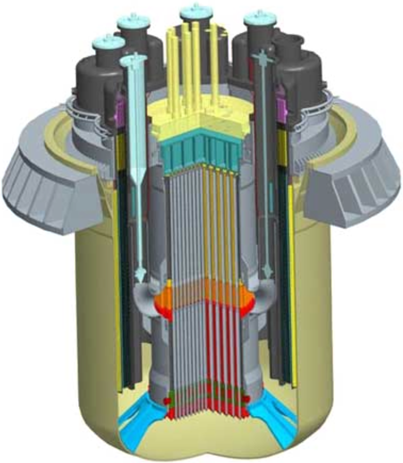
Table: Standard deviation, skewness and kurtosis of the *PMF-35* k_{eff} distribution from TENDL-2013 ^{208}Pb cross section data.

Methos	Standard deviation	skewness	kurtosis
TMC	426 *pcm*	0.81	3.62
XGPT	423 *pcm*	0.80	3.58

Table: Standard deviation, skewness and kurtosis of the *HMF-64* k_{eff} distribution from TENDL-2013 ^{208}Pb cross section data.

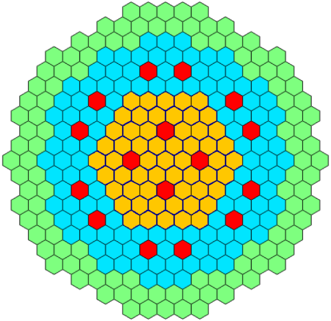
	Standard deviation	skewness	kurtosis
TMC	1326 *pcm*	0.74	3.49
XGPT	1371 *pcm*	0.81	3.65

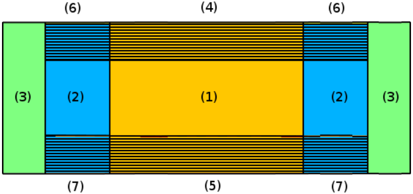
ALFRED, is a small-size (300MWth) pool-type LFR.



Advanced Lead Fast Reactor European Demonstrator

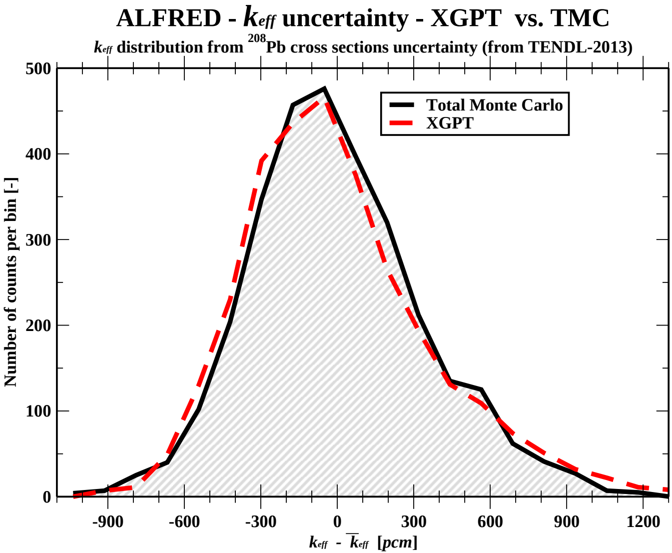
Developed within the European FP7 LEADER project





171 FAs are subdivided into two radial zones with different plutonium fractions

k_{eff} uncertainty in ALFRED



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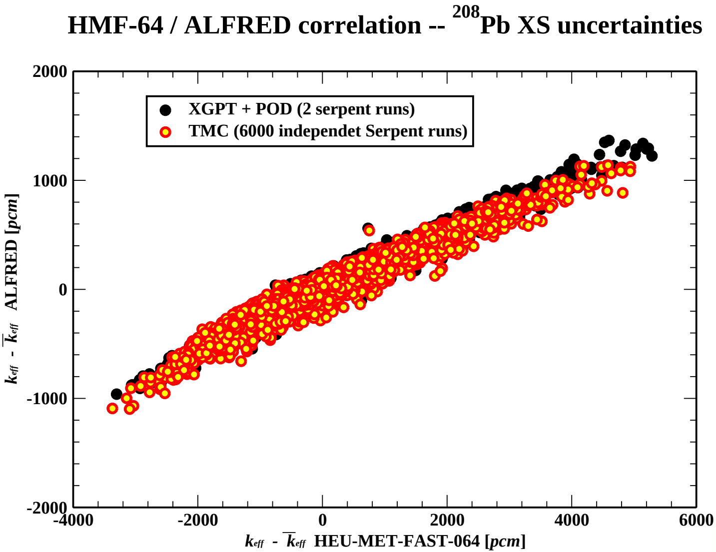
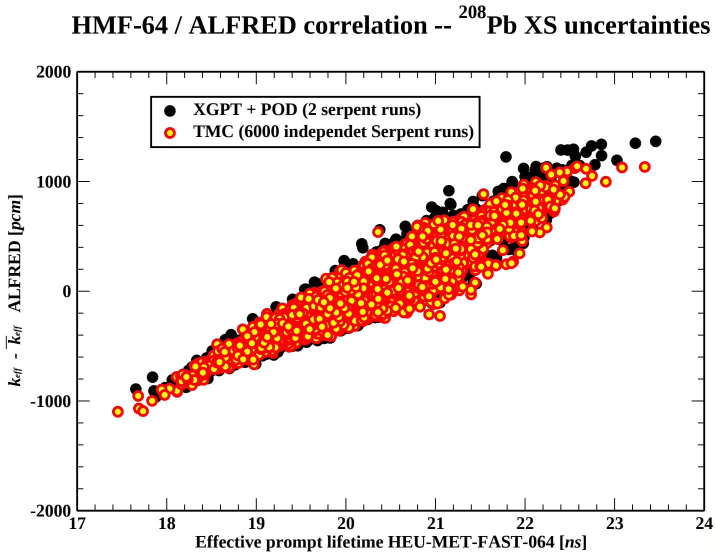
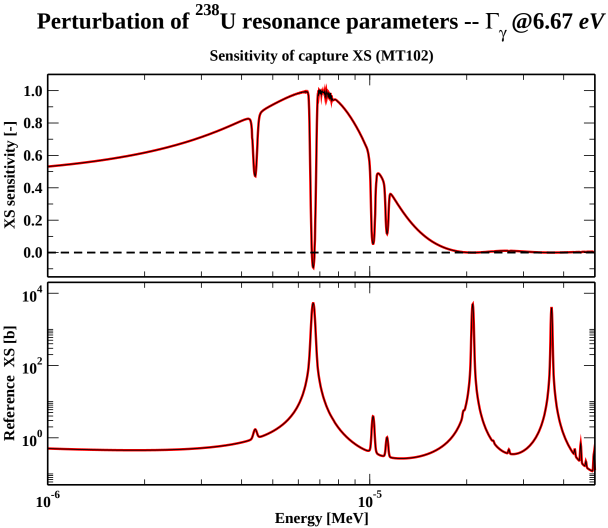
Representativity study ALFRED vs. HMF-64



Representativity study ALFRED vs. HMF-64



Cross section sensitivity to resonance parameters
Cross sections derivatives are calculated numerically via NJOY



Cross section sensitivity to resonance parameters

Definition of sensitivity coefficient: $S_x^R \equiv \frac{dR/R}{dx/x}$

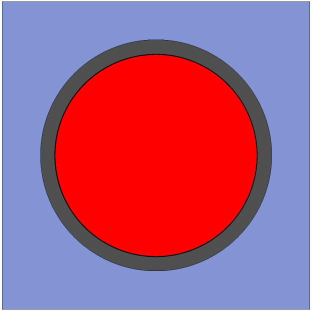
$$S_{\Gamma_\gamma}^{k_{\text{eff}}} = \int S_{\sigma_{capture}}^{k_{\text{eff}}}(E) \cdot S_{\Gamma_\gamma}^{\sigma_{capture}}(E) \cdot dE + \int S_{\sigma_{elastic}}^{k_{\text{eff}}}(E) \cdot S_{\Gamma_\gamma}^{\sigma_{elastic}}(E) \cdot dE + \ldots$$

Multi-group discretization is usually introduced here...

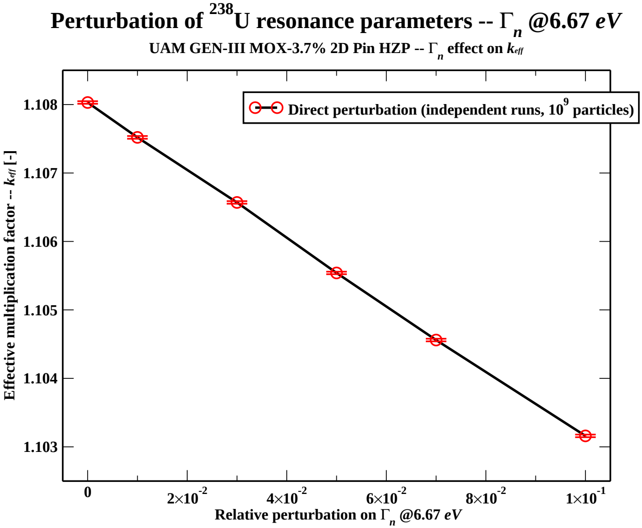
The new method avoids any discretization

Material compositions and geometry specifications from:
Benchmarks for uncertainty analysis in modelling (UAM) for the design, operation and safety analysis of LWRs

Case: GEN-III PWR MOX 2D pin cell
Pu content in fuel 3.7%



Verification against direct perturbation: ^{238}U



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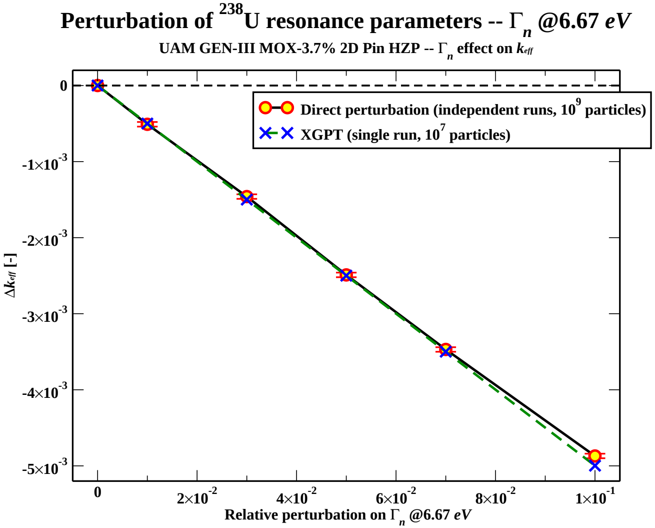
Verification against direct perturbation: ^{238}U

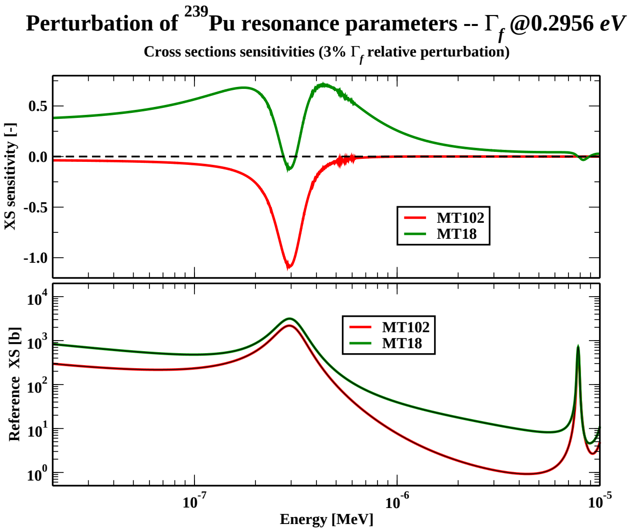


Verification against direct perturbation: ^{238}U

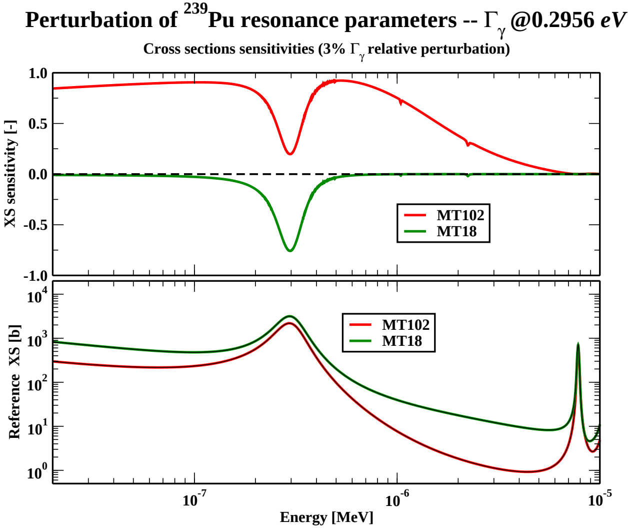
^{238}U @6.67eV	Direct perturbation	GPT
$S^{k_{\mathrm{eff}}}_{\Gamma_\gamma}$	-4.603×10^{-2} $\pm 9.9 \times 10^{-4}$	-4.469×10^{-2} $\pm 1.4 \times 10^{-4}$
$S^{k_{\mathrm{eff}}}_{\Gamma_n}$	-4.392×10^{-2} $\pm 9.9 \times 10^{-4}$	-4.512×10^{-2} $\pm 1.6 \times 10^{-4}$

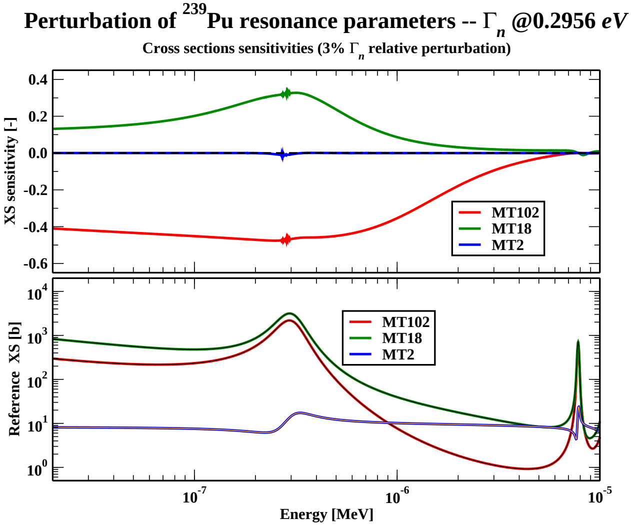
- Sensitivities are very large
- GPT is more efficient: 10^7 vs 10^9 particles, smaller err.
- All GPT sensitivities calculated in a single run

Verification against direct perturbation: ^{239}Pu

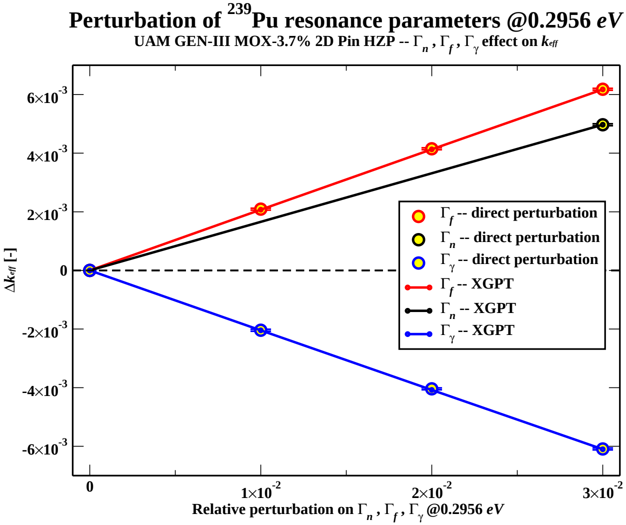


Verification against direct perturbation: ^{239}Pu




Perturbation of 239Pu resonance parameters -- Γn @0.2956 eV
Cross sections sensitivities (3% Γn relative perturbation)
XS sensitivity [-]
0.4
0.2
0.0
-0.2
-0.4
-0.6
MT102
MT18
MT2
Reference XS [b]
10^4
10^3
10^2
10^1
10^0
MT102
MT18
MT2
10^-7
10^-6
10^-5
Energy [MeV]

Verification against direct perturbation: ^{239}Pu



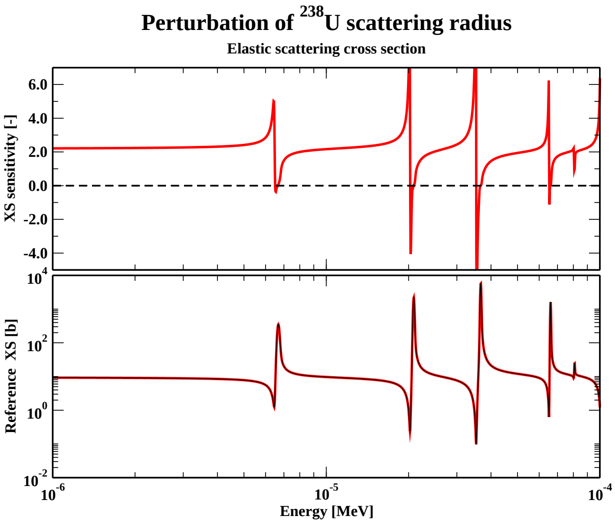
Verification against direct perturbation: ^{239}Pu

^{239}Pu @0.295eV

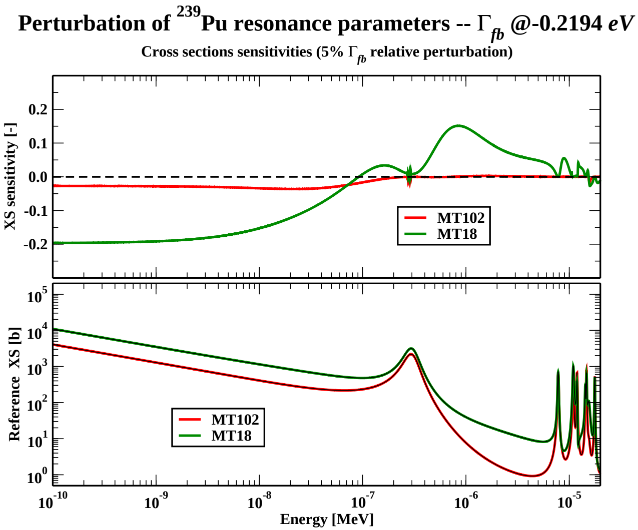
	Direct perturbation	GPT
$S^{k_{\text{eff}}}_{\Gamma_\gamma}$	-1.832×10^{-2} $\pm 9.9 \times 10^{-4}$	-1.835×10^{-2} $\pm 3.8 \times 10^{-4}$
$S^{k_{\text{eff}}}_{\Gamma_n}$	1.495×10^{-2} $\pm 9.9 \times 10^{-4}$	1.495×10^{-2} $\pm 1.6 \times 10^{-4}$
$S^{k_{\text{eff}}}_{\Gamma_f}$	1.859×10^{-2} $\pm 9.9 \times 10^{-4}$	1.857×10^{-2} $\pm 4.1 \times 10^{-4}$

- Sensitivities are very large
- GPT is more efficient: 10^7 vs 10^9 particles, smaller err.
- All GPT sensitivities calculated in a single run

Fancy sensitivities (scattering radius)



Fancy sensitivities (negative energy resonances)



Continuous energy adjustment

1. Generate continuous-energy basis functions
   - SVD of the continuous-energy covariance matrices
   - XS derivatives for resonance parameters, scatt. radius & co.
   - Sensitivity to nuclear model parameters?

2. Project the uncertainties on these bases (MF-32, MF-33, etc.)

3. Run Serpent-XGPT once for each system
   - Get the uncertainty for each response function

$$Var\left[R\right] \sim \sum_{j=1}^{n} V^{j} \cdot \left(S_{U_j}^{R}\right)^{2}$$

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4 Get C/E, $Var[R]$, V^j, and $S^R_{U_j}$

5 Solve the GLLS problem to get:
$^{adjusted}COV[\underline{\mathbf{V}}, \underline{\mathbf{V}}]$, $\Delta\alpha^j_U$

6 Reconstruct the adjusted Σ

$$^{adj}\Sigma(E) \simeq {}^{prior}\Sigma(E) \cdot \left(1 + \sum_{j=1}^{n} \Delta\alpha^j_U \cdot U_j(E)\right)$$

7 Reconstruct the adjusted $COV\left[\Sigma\, , \Sigma\right]$

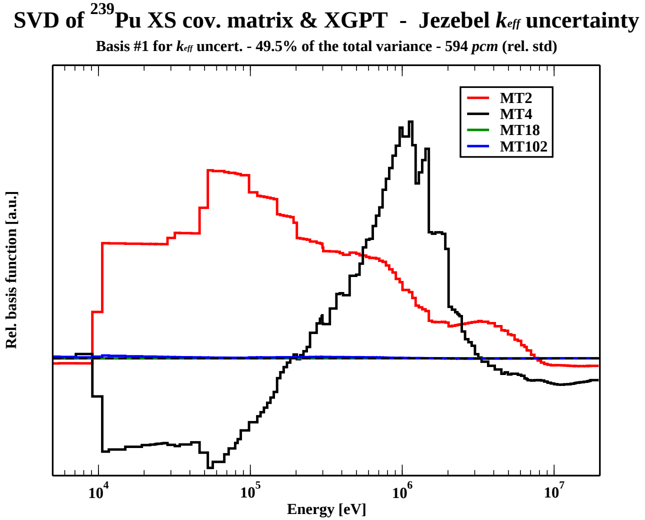
- $^{prior}COV\left[\Sigma(E)\, , \Sigma(E')\right] \sim \sum_{j=1}^{n} U_j(E) \cdot V^j \cdot U_j(E')$
- $^{adj}COV\left[\Sigma(E)\, , \Sigma(E')\right] \sim \underline{\mathbf{U}}\; ^{adj}COV\left[\underline{\mathbf{V}}\, , \underline{\mathbf{V}}\right] \underline{\mathbf{U}}^T$

$$= \begin{bmatrix} U_1(E) & U_2(E) & \dots \end{bmatrix} \; ^{adj}COV\left[\underline{\mathbf{V}}\, , \underline{\mathbf{V}}\right] \begin{bmatrix} U_1(E) \\ U_2(E) \\ U_3(E) \\ \vdots \end{bmatrix}$$

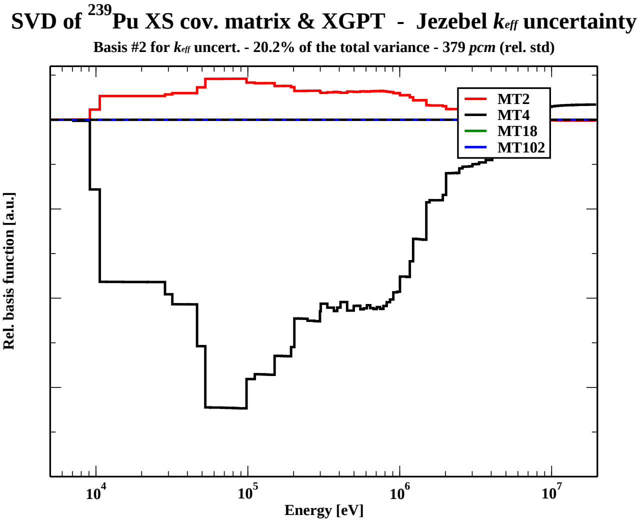
Very simple case study

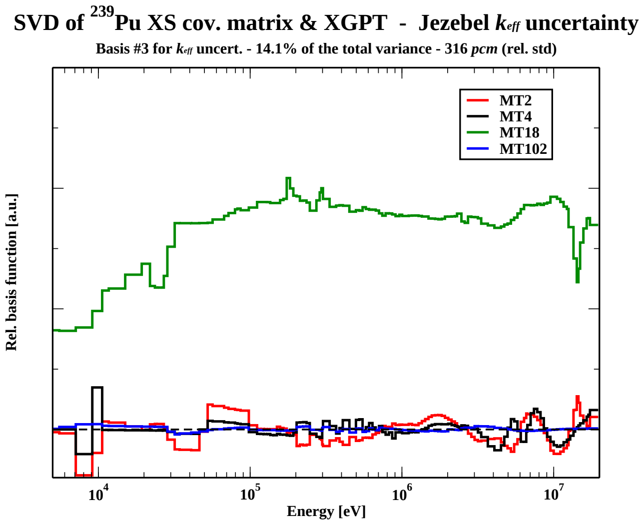
- Only one system: Jezebel
- Only one response function: k_{eff}
- Only one isotope: ^{239}Pu
- Covariances from ENDF/B-VII.0 (multigroup!)

Adjustment via XGPT

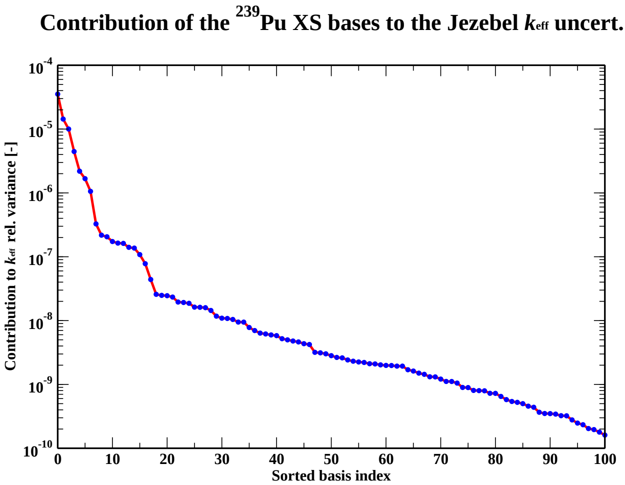


Adjustment via XGPT




SVD of 239Pu XS cov. matrix & XGPT - Jezebel keff uncertainty
Basis #3 for keff uncert. - 14.1% of the total variance - 316 pcm (rel. std)
MT2
MT4
MT18
MT102
Rel. basis function [a.u.]
10^4
10^5
10^6
10^7
Energy [eV]

Adjustment via XGPT



Adjustment via XGPT (SQUADRA output)

(E-C)/C (%) BEFORE AND AFTER ADJUSTM.

#	EXPERIMENT	BEFORE	AFTER	CHANGE
1	JEZEBEL KEFF	0.014	0.001	-0.013

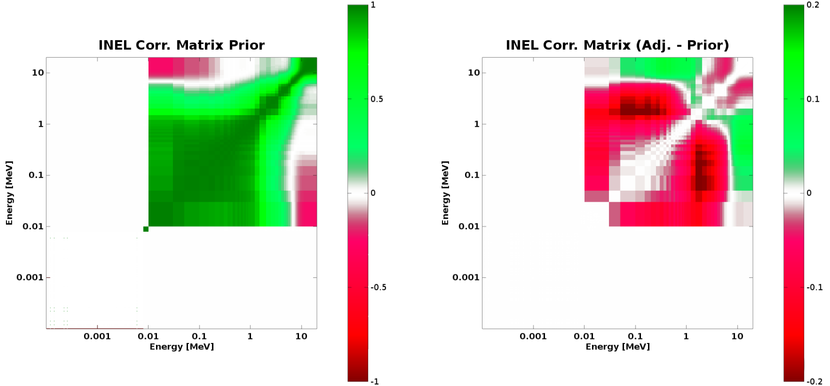
EXPERIMENT UNCERT. (%) BEFORE AND AFTER ADJUSTM.

#	EXPERIMENT	BEFORE	AFTER	CHANGE
1	JEZEBEL KEFF	0.950	0.196	-0.754

NUCL. DATA UNCERT. BEFORE AND AFTER ADJUSTM.

NUCLEAR DATA		NUC. DATA CHANGE	BEFORE	AFTER	CHANGE
EIGENV_INEL	1	-14.1	1274.8	820.4	-454.4
EIGENV_INEL	2	-2.5	463.0	429.4	-33.6
EIGENV_KHI	1	-2.1	600.3	583.0	-17.3
EIGENV_INEL	4	-0.9	342.4	336.3	-6.1
EIGENV_INEL	5	-0.5	218.7	215.7	-3.0
EIGENV_KHI	2	-0.4	247.4	246.2	-1.2
EIGENV_CAPT	1	0.5	884.6	883.9	-0.7
EIGENV_KHI	3	0.2	115.4	114.9	-0.5

Strong negative correlation in the inelastic covariance



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Adjustment via XGPT

PROBLEMS/OPEN ISSUES:

- Continuous-energy cov. matrices are not available
- Covariances with unphysical negative eigenvalues
- Few cross-terms in the covariances
- Inelastic: MT4 versus MT51-91
- Resonances: MF32 or MF33
- Angular distributions: P_n or $\Sigma(\mu, E)$
- Ongoing: sensitivity for $S(\alpha, \beta)$ and URR

Adjustment via XGPT

MAIN GOAL:

Simplify (and reduce) the steps between:

the data (XS and covariances)...

...and their use (SA/UQ and adjustment).

Acknowledgments

Thanks to:
A. Bidaud (LPSC Grenoble)
D. Rochman (PSI)
A. Sartori (SISSA Trieste)

Jaakko & Serpent developers team

THANK YOU FOR THE ATTENTION

QUESTIONS? SUGGESTIONS? IDEAS?

The bay area from the Berkeley hills (multi-group version).

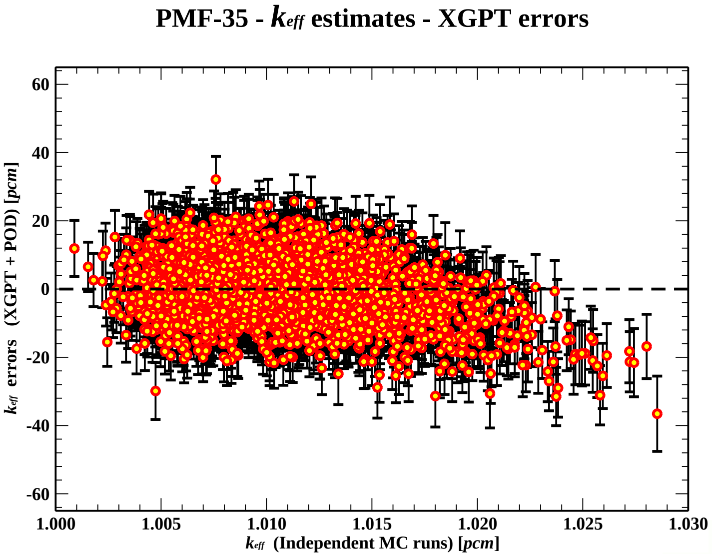
Off-line steps

- Generate the optimal bases via POD (from random XS):
  - Load N random ACE files for the selected isotope
  - Score the rel. diff. of the XS on the unionized e-grid
  - Build the (weighted) correlation matrix $K \in \mathbb{R}^{N \times N}$
  - Solve `[S, V] = EIG(K)` for the first n eigenvalues
  - Reconstruct the bases and store them in a cache-friendly way
- Generate the optimal bases via SVD (from cov. matrices):

  Should you already have the relative covariance matrices, the bases can be obtained directly via SVD:
  Solve `[U, S, V] = SVD(COV)` for the first n eigenvalues
- The off-line steps need to be done just once

CPU-time & memory

	TMC	GPT + COV	XGPT + POD
CPU-time	$\propto \boldsymbol{N}$	small $\propto$ # of coll.	small $\propto \boldsymbol{n}$
Memory	–	$\propto$ # of coll. $\times\ \boldsymbol{\lambda} \times$ pop	$\propto \boldsymbol{n} \times \boldsymbol{\lambda} \times$ pop


PMF-35 - keff estimates - XGPT errors
60
40
20
0
-20
-40
-60
keff errors (XGPT + POD) [pcm]
1.000
1.005
1.010
1.015
1.020
1.025
1.030
keff (Independent MC runs) [pcm]

XGPT+POD: uncertainty propagation in PMF-35