Serpent meeting 2016
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Nuclear data uncertainty quantification in SFR, LFR, and MSR via Monte Carlo perturbation theory.

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Nuclear Data S/U via Monte Carlo Perturbation

- Nuclear data represent the starting point of "any" neutronics calculation (*set acelib "...xsdata"* ...)
- Experimental uncertainties and model approximations affect our knowledge of nuclear data
- Interest in sensitivity and uncertainty analysis within the nuclear community is continuously increasing
- The implementation of Monte Carlo Perturbation Theory has been the focus of recent research activities
- Main goal: avoid any discretization for the solution of the adjoint problem (no mesh, no energy grid, no angular discretization)

Outline

- Monte Carlo Sensitivity/Perturbation in Serpent
  (short version!)
- Verification of Serpent sensitivity calculations against direct perturbation
- Analysis of the coolant void reactivity coefficient in LFR and SFR
- Results of the uncertainty quantification studies in ALFRED, ESFR, MSFR, MOSART, REBUS-3700

Generalized perturbation theory capabilities in Serpent

Generalized Perturbation Theory (GPT) allows calculating the effects of several different perturbations within a single run, usually in the form of sensitivity coefficients:

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

Sensitivity/perturbation capabilities were implemented in SERPENT for generalized response functions [*].

[*] M Aufiero, A Bidaud, M Hursin, J Leppänen, G Palmiotti 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).

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 (see Friday's presentation on Perturbation Theory for acceleration of multiphysics calculations)

Calculation of k_{eff} sensitivity to coolant density

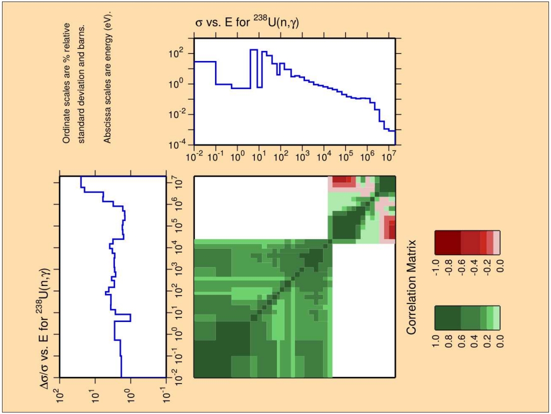
We can obtain space-dependent k_{eff} sensitivities to coolant density adopting the collision-history approach...

$$S_x^{k_{\text{eff}}} \equiv \frac{dk_{\text{eff}}/k_{\text{eff}}}{dx/x} = E\left[{}^{(-\gamma)}ACC_x - {}^{(-\gamma)}REJ_x\right] \qquad (1)$$

- **x** represents the coolant density in different zones
- ${}^{(-\gamma)}ACC_x$ and ${}^{(-\gamma)}REJ_x$ represent the accepted and rejected neutron collisions history of the particles
- γ is the number of latent generations adopted in the Iterated Fission Probability estimators for the convergence of the adjoint weighting.

First-order uncertainty propagation formula (sandwich rule)

$$Var[R] = \underline{S_x^R}\; Cov[\underline{x}]\; \left(\underline{S_x^R}\right)^T$$



Uncertainty propagation

First-order uncertainty propagation formula (sandwich rule)

$$Var\left[R\right] = \underline{S_x^R}\ Cov\left[\underline{x}\right]\ \left(\underline{S_x^R}\right)^T$$

COMMARA-2.0 Neutron Cross Section Covariance Library

(thanks to Pino Palmiotti @INL for precious suggestions!)

The coolant density reactivity coefficient in SFR & LFR

- The coolant density effect represents one of the main reactivity feedback in LFR and SFR
- Its accurate (space-dependent) calculation is important for a correct evaluation of the dynamics of these systems
- Monte Carlo neutron transport simulations are commonly adopted for the study of LFR and SFR [a,b]

[a] L. Buiron et al. "Evaluation of large 3600mwth sodium-cooled fast reactor neutronic oecd benchmarks." In: PHYSOR 2014, Kyoto, Japan, Sep. 28 - Oct. 3, 2014 (2014).
[b] G. Grasso et al. "The core design of ALFRED, a demonstrator for the european lead-cooled reactors." Nuclear Engineering and Design, 278: pp. 287–301 (2014).

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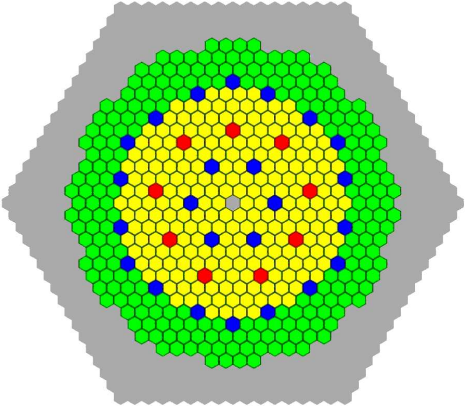
The coolant density reactivity coefficient in SFR & LFR

- Using MC, reactivity feedbacks are usually calculated via direct perturbations, i.e., comparing the effective multiplication factor of two separate Monte Carlo runs.
- This approach is inefficient and requires a separate calculation per each spatial zone
- Here we use sensitivity/perturbation calculations in Monte Carlo to analyze the coolant reactivity coefficient in SFR & LFR

Large sodium-cooled fast reactor
OECD/NEA SFR Benchmark Task Force



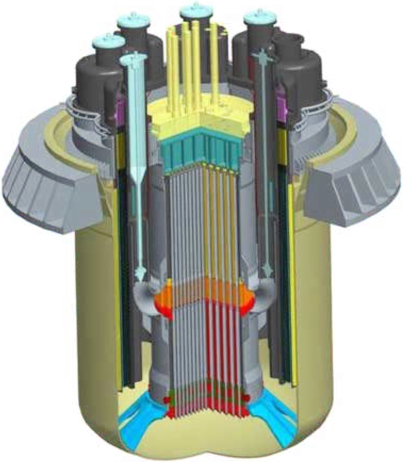
225 inner and 228 outer MOX FAs. Axially variable Pu content

2 radial $\times$ 5 axial zones considered for Na reactivity calculations

Advanced Lead Fast Reactor European Demonstrator

Developed within the European FP7 LEADER project

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



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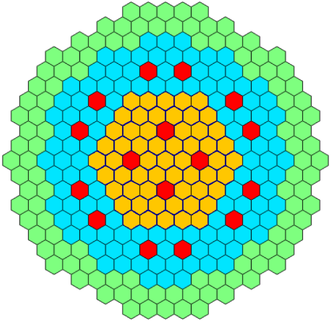
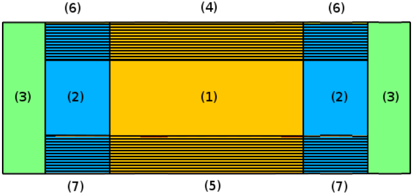
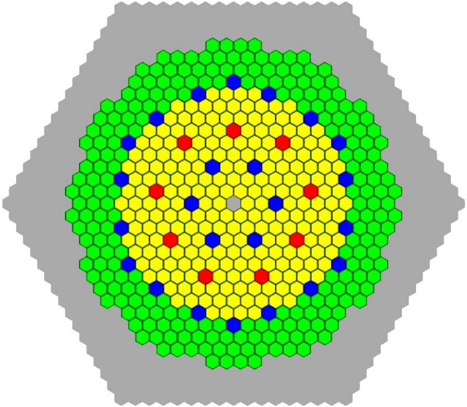




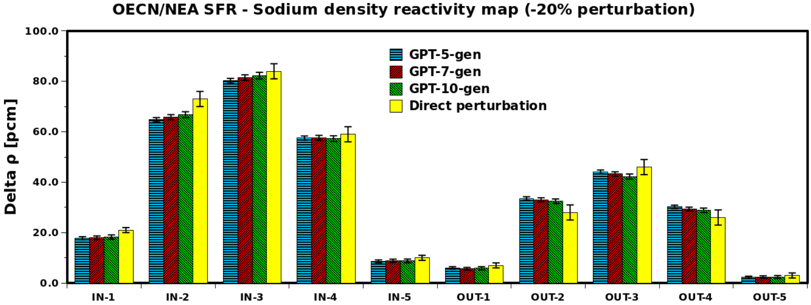
171 FAs are subdivided into two radial zones with different plutonium fractions

7 different zones were considered for the Pb density reactivity coefficient calculations

Verification of the perturbation calculations: SFR



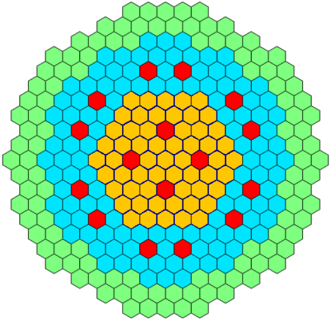
Verification of the perturbation calculations: SFR

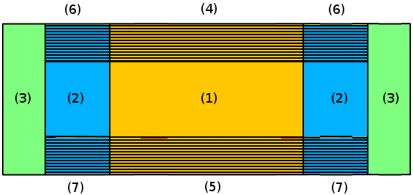


Positive void effect in all the zones:

Decreasing the sodium density in each of the 2×5 zones leads to a reactivity increase

Verification of the perturbation calculations: ALFRED





Verification of the perturbation calculations: ALFRED

Table: Lead density k_{eff} sensitivity coefficient in the considered ALFRED reactor core zones. Comparison between sensitivity/perturbation and direct perturbation Serpent results.

		k_{eff} lead density sensitivity coefficient*		
Fuel region	Axial zone	Direct Pert.#	Pert. Theory	Difference
Inner	Active	-7.54 ± 0.13	-7.75 ± 0.30	-0.21
Outer	Active	2.69 ± 0.13	2.68 ± 0.31	-0.01
Reflector	–	4.34 ± 0.13	4.34 ± 0.10	0.00
Inner	Lower plenum	4.86 ± 0.13	4.85 ± 0.10	-0.01
Outer	Lower plenum	7.20 ± 0.13	7.70 ± 0.08	**0.50**
Inner	Upper plenum	5.64 ± 0.13	5.55 ± 0.13	-0.09
Outer	Upper plenum	6.96 ± 0.13	6.79 ± 0.15	-0.17
Total	–	30.4 ± 0.13	29.6 ± 0.53	-0.8

* *pcm*/(% lead density) $\pm$ 1 sigma
\# Direct pert. with 10% lead density variation

All negative void reactivity except inner active region

Decomposition of the Pb density sensitivity coefficient

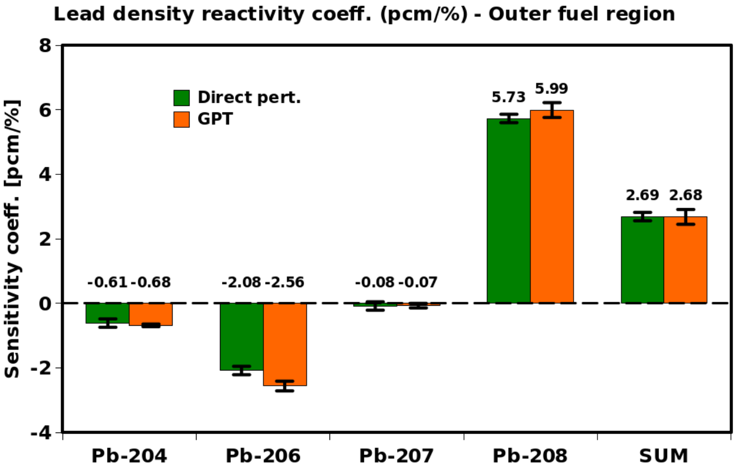
The lead density sensitivity coefficient is the result of the sum of different opposite effects.

For a better understanding of the phenomena involved, the outer fuel Pb density coefficient was analyzed via decomposition of the reactivity effect by:

- Isotope (^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb)
- Reaction (elastic, inelastic, capture)
- Energy group (33 groups ECCO structure)

Decomposition of the Pb density sensitivity coefficient

The lead density sensitivity coefficient is the result of the sum of different opposite effects.



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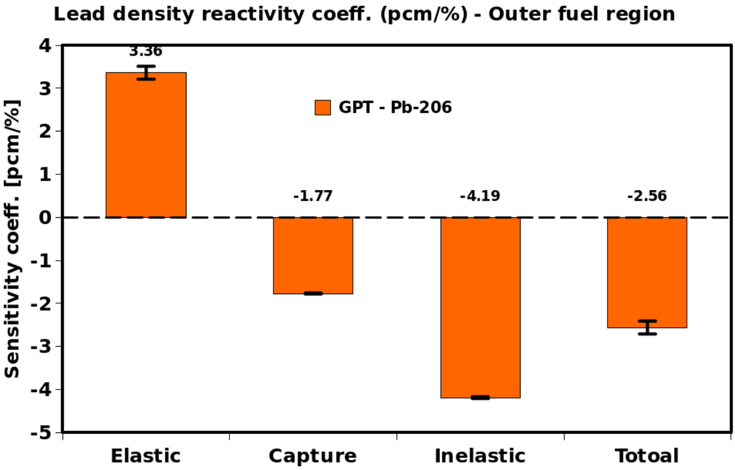


Decomposition of the Pb density sensitivity coefficient

The lead density sensitivity coefficient is the result of the sum of different opposite effects.

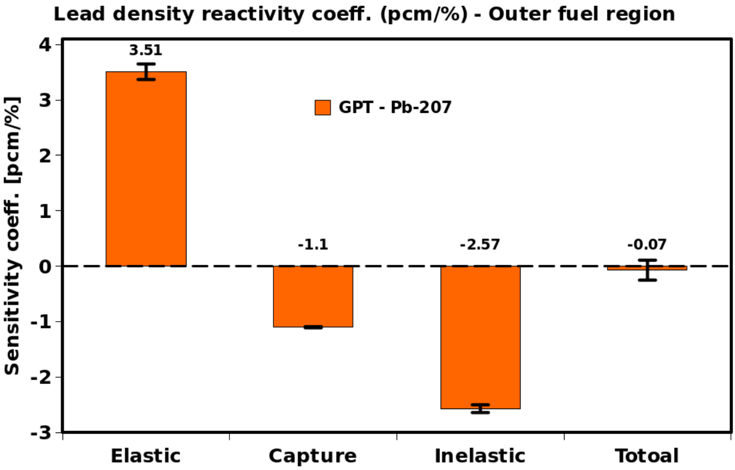
Elastic: main impact on leakage term, small spectral effect
slow IFP convergence due to modificiation of the fission source

Inelastic: negative spectral effect (reduces the average number of neutrons produced per absorption in the fuel)

Capture: direct negative impact on neutron balance

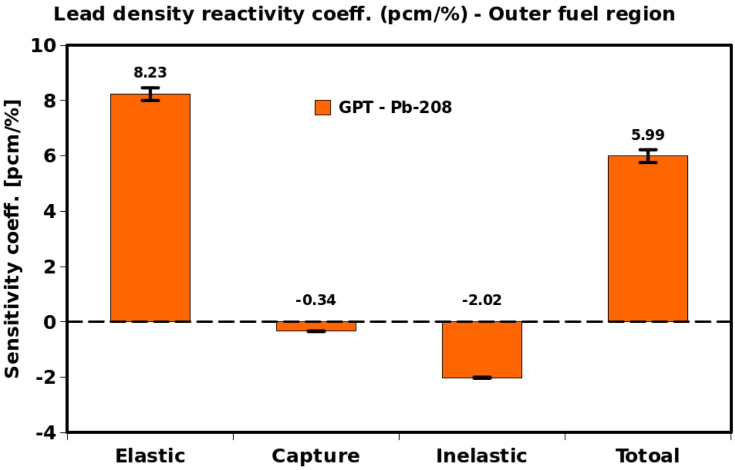
(n, xn): negligible effect

The lead density sensitivity coefficient is the result of the sum of different opposite effects.



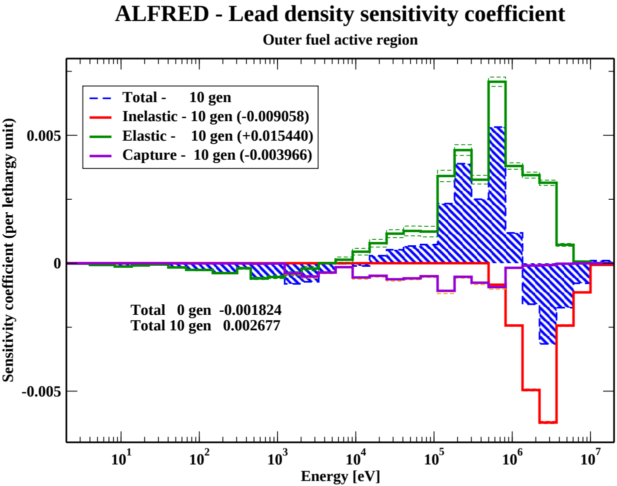
Decomposition of the Pb density sensitivity coeff. – Pb-208

The lead density sensitivity coefficient is the result of the sum of different opposite effects.



Decomposition of the Pb density sensitivity coefficient

The lead density sensitivity coefficient is the result of the sum of different opposite effects.



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Notes on coolant reactivity map via MC Pert. Thoery

- Serpent sensitivity calculations show good agreement against direct perturbation for both the SFR and LFR cases
- A single extended Serpent run to get the sensitivity coefficients for all the regions
- Negative void reactivity in ALFRED
  positive void reactivity in OECD/NEA SFR
- Coolant density reactivity coefficient is the result of the sum of different opposite effects.
- Energy-Isotope-Reaction decomposition can be obtained at no additional cost

Notes on coolant reactivity map via MC Pert. Thoery

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Uncertainty quantification is just a couple of matrix-vector products ahead...

$$Var\left[R\right] = \underline{S_x^R}\; Cov\left[\underline{x}\right]\; \left(\underline{S_x^R}\right)^T$$

Uncertainty quantification – ALFRED k_{eff}

Serpent GPT + ENDF/B-VII & COMMARA-2.0

Total k_{eff} uncertainty from nuclear data: 815 *pcm*

Major contributors (in *pcm*):

INELASTIC U238 INELASTIC U238
522.96
CAPTURE PU239 CAPTURE PU239
291.94
NU PU240 NU PU240
233.29
CAPTURE U238 CAPTURE U238
207.07
FISSION PU239 FISSION PU239
187.42
CAPTURE PU240 CAPTURE PU240
139.58
ELASTIC U238 INELASTIC U238
133.19
FISSION PU240 FISSION PU240
131.33
KHI PU239 KHI PU239
130.89

INELASTIC FE56 CAPTURE FE56
-3.5118
ELASTIC PU239 FISSION PU239
-5.6756
ELASTIC U238 CAPTURE U238
-12.622
FISSION PU239 CAPTURE PU239
-29.351

Total outer Pb density reactivity coeff. uncertainty: 25 % (1 sigma!!)

Major contributors (in %):

INELASTIC U238 INELASTIC U238
18.127
INELASTIC PB206 INELASTIC PB206
8.9843
INELASTIC PB207 INELASTIC PB207
7.3012
CAPTURE PU239 CAPTURE PU239
4.8552
CAPTURE U238 CAPTURE U238
3.8518
ELASTIC PB208 ELASTIC PB208
3.6351
CAPTURE PB207 CAPTURE PB207
3.5590
INELASTIC PB208 INELASTIC PB208
3.2379
CAPTURE PB208 CAPTURE PB208
3.1823

FISSION PU239 CAPTURE PU239
-0.37053
ELASTIC U238 CAPTURE U238
-0.37102
ELASTIC PU240 INELASTIC PU240
-0.69637
ELASTIC PU239 CAPTURE PU239
-0.82188

Total k_{eff} uncertainty from nuclear data: 1380 *pcm*

Major contributors (in *pcm*):

INELASTIC U238 INELASTIC U238
1205.0
CAPTURE U238 CAPTURE U238
279.55
NU PU240 NU PU240
228.43
CAPTURE PU239 CAPTURE PU239
219.43
KHI PU239 KHI PU239
208.23
FISSION PU239 FISSION PU239
193.16
ELASTIC U238 INELASTIC U238
175.63
NU U238 NU U238
154.15
INELASTIC FE56 INELASTIC FE56
138.99

ELASTIC NA23 CAPTURE NA23
-5.8231
INELASTIC FE56 CAPTURE FE56
-6.7224
ELASTIC U238 CAPTURE U238
-16.078
FISSION PU239 CAPTURE PU239
-25.984

Uncertainty in fast-spectrum Molten Salt Reactors

- REBUS-3700[a]
  - U-Pu cycle breeder: $NaCl - UCl_3 - PuCl_3$

[a] Mourogov, A., and P. M. Bokov. "Potentialities of the fast spectrum molten salt reactor concept: REBUS-3700." Energy conversion and management 47.17 (2006).

- Molten Salt Fast Reactor (MSFR)[b]
  - U-233 started: $LiF - ThF_4 - UF_4$
  - TRU started: $LiF - ThF_4 - [TRU]F_3$

[b] Merle-Lucotte, E., et al. "Launching the thorium fuel cycle with the Molten Salt Fast Reactor." (2011).

- MOSART[c]
  - TRU Burner: $NaF - LiF - BeF_2 - [TRU]F_3$

[c] F. Gabrielli, A. Rineiski, V. Ignatiev, O. Feinberg "Benchmark on MOlten Salt Advanced Reactor Transmuter (MOSART): Impact of Minor Actinide Nuclear Data Uncertainty on Integral Reactor Parameters" NEA/EGIEMAM-II.

Total k_{eff} uncertainty from nuclear data: 935 *pcm*

Major contributors (in *pcm*):

INELASTIC U238 INELASTIC U238
731.22
CAPTURE U238 CAPTURE U238
230.27
ELASTIC U238 INELASTIC U238
228.94
NU PU240 NU PU240
206.34
FISSION PU239 FISSION PU239
186.28
CAPTURE PU239 CAPTURE PU239
176.39
NU U238 NU U238
152.42
FISSION PU240 FISSION PU240
115.50
INELASTIC NA23 INELASTIC NA23
107.94

ELASTIC U238 CAPTURE U238
-5.6530
FISSION PU239 CAPTURE PU239
-6.2497
ELASTIC PU239 FISSION PU239
-7.0126
ELASTIC NA23 CAPTURE NA23
-8.4695

Total k_{eff} uncertainty from nuclear data: 1640 *pcm*

Major contributors (in *pcm*):

CAPTURE TH232 CAPTURE TH232
1220.5
FISSION U233 FISSION U233
899.06
CAPTURE U233 CAPTURE U233
455.88
NU U233 NU U233
376.06
ELASTIC LI7 ELASTIC LI7
125.17
ELASTIC F19 ELASTIC F19
92.890
ELASTIC TH232 ELASTIC TH232
79.712
CAPTURE F19 CAPTURE F19
72.669
INELASTIC F19 INELASTIC F19
69.498

ELASTIC U233 NxN U233
-0.27131
ELASTIC LI7 INELASTIC LI7
-1.7293
FISSION TH232 CAPTURE TH232
-21.180
ELASTIC TH232 CAPTURE TH232
-44.133

Total k_{eff} uncertainty from nuclear data: 1040 *pcm*

Major contributors (in *pcm*):

CAPTURE TH232 CAPTURE TH232
722.54
CAPTURE PU239 CAPTURE PU239
505.03
INELASTIC F19 INELASTIC F19
281.63
CAPTURE PU240 CAPTURE PU240
220.74
FISSION PU239 FISSION PU239
184.59
CAPTURE NP237 CAPTURE NP237
145.85
NU PU240 NU PU240
140.43
FISSION PU241 FISSION PU241
137.15
CAPTURE PU242 CAPTURE PU242
132.77

FISSION TH232 CAPTURE TH232
-16.362
ELASTIC TH232 CAPTURE TH232
-30.245
FISSION PU239 CAPTURE PU239
-69.163
ELASTIC F19 INELASTIC F19
-149.35

Uncertainty quantification – TRU-Burner MOSART k_{eff}

Serpent GPT + ENDF/B-VII & COMMARA-2.0

Total k_{eff} uncertainty from nuclear data: 945 *pcm*

Major contributors (in *pcm*):

FISSION PU239 FISSION PU239
518.57
CAPTURE PU240 CAPTURE PU240
445.94
FISSION PU241 FISSION PU241
439.50
CAPTURE PU242 CAPTURE PU242
265.71
CAPTURE PU239 CAPTURE PU239
229.02
CAPTURE PU238 CAPTURE PU238
158.77
ELASTIC NA23 ELASTIC NA23
144.47
ELASTIC F19 ELASTIC F19
111.84
ELASTIC PU240 ELASTIC PU240
110.99

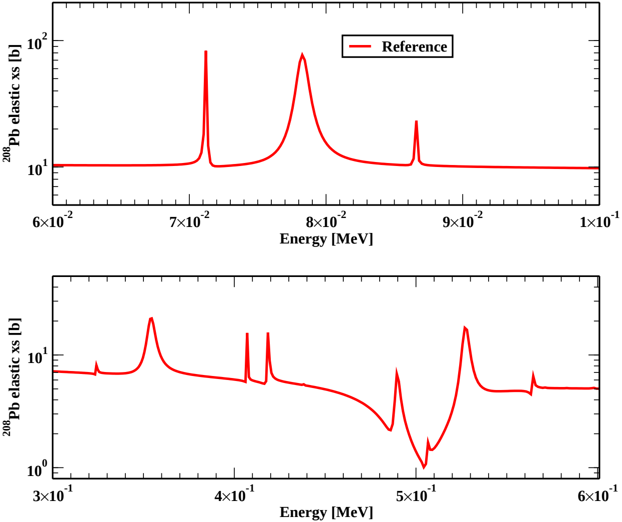
FISSION AM241 CAPTURE AM241
-1.2260
FISSION PU240 CAPTURE PU240
-11.078
ELASTIC AM241 CAPTURE AM241
-11.710
FISSION PU239 CAPTURE PU239
-176.83

Summary

- Monte Carlo Perturbation Theory has been implemented in Serpent for generalized response functions (GPT)
- This opens the possibility to perform reactor physics calculations in a more efficient way (e.g., see next two presentations by Eugene and Giorgio)
- Uncertainty quantification has been the territory of deterministic codes for decades... not anymore(?)
- The flexibility of Monte Carlo widens the legacy capabilities of Generalized Perturbation Theory towards continuous (in Energy and Space) sensitivity functions

- Monte Carlo eXtended Generalized Perturbation Theory (XGPT): building Reduced Order Models for continuous-energy XS uncertainty propagation
- Jacobian matrix approximation via eigenfunction perturbation theory: accelerating and stabilizing coupled Monte Carlo / CFD multiphysics calculations

Realistic representation of uncertainties: random XS



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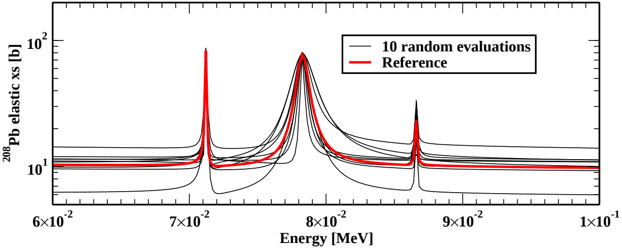
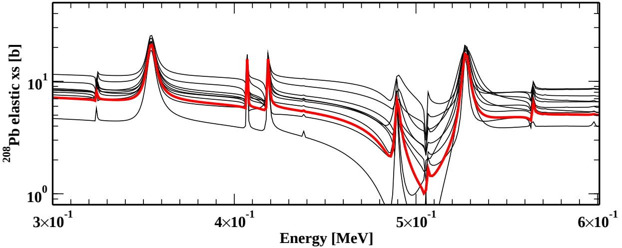
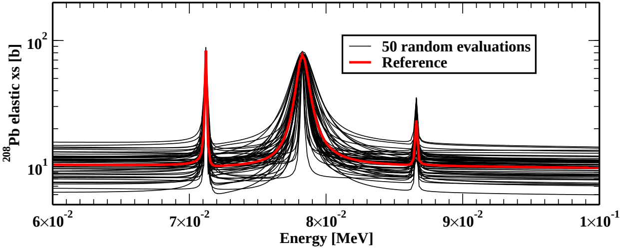
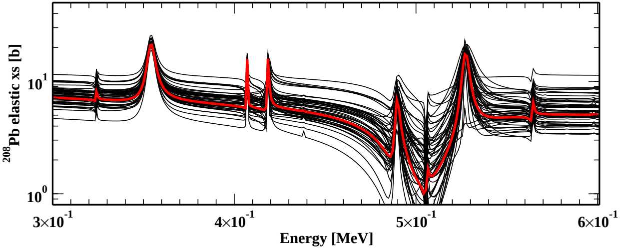
Realistic representation of uncertainties: random XS



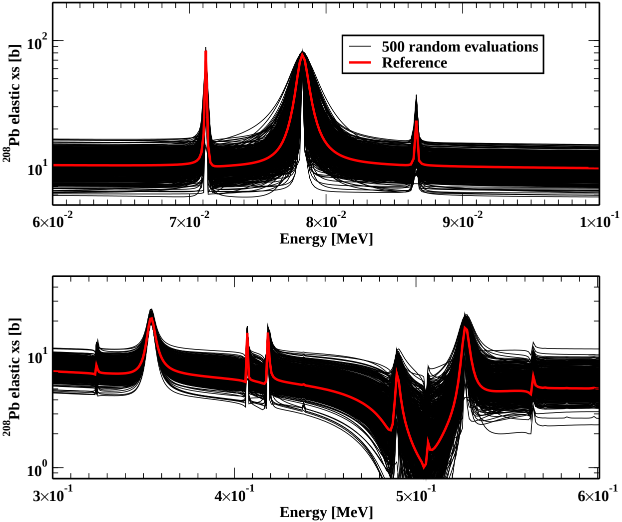


Realistic representation of uncertainties: random XS

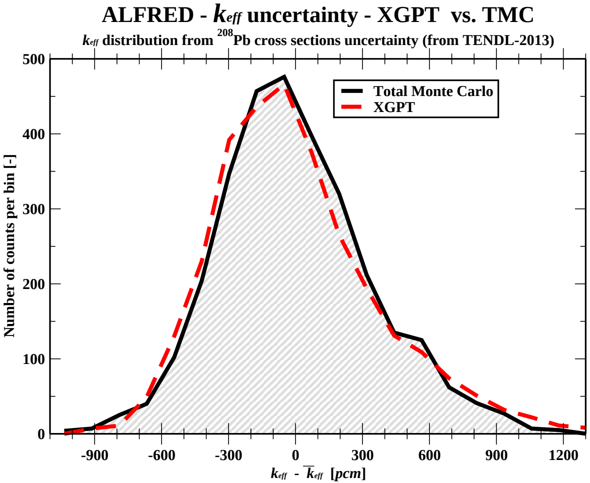




Realistic representation of uncertainties: random XS



ALFRED: ^{208}Pb uncertainty analysis via TMC & XGPT



Thank you for the attention!

Questions? Suggestions?