Total Monte Carlo acceleration for the PETALE experimental programme in the CROCUS reactor

Axel Laureau¹
Vincent Lamirand²
Dimitri Rochman²
Andreas Pautz¹,³

¹: LRS/EPFL*
²: LRT/PSI
³: NES/PSI

*Ecole Polytechnique Fédérale de Lausanne

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Summary

I - Introduction

- Context: BMC for integral experiment
- PETALE exp & specific requirements

II - TMC-CS

- Correlated Sampling principle
- Correlated Sampling on Nuclear Data

III - Validation

- Reference and comparison
- $k_{\text{eff}}$ uncertainty propagation
- Flux / dosimetry application
- Inter-dosimeter correlation
**Bayesian Monte Carlo**

**Principle**

- Step 1: generation of random cross sections (XS) in agreement with the experimental knowledge
  - sampling on nuclear model parameters - TENDL
  - sampling from covariance matrices
- Step 2: Total Monte Carlo (TMC) uncertainty propagation
  - prior “C” value for each set of cross sections
- Step 3: Comparison to experimental “E” results and XS-weighting in the BMC process
  - reduced posterior uncertainty using $w_x = \exp \left( -\frac{\chi^2}{2} \right)$

*(some of the) Advantages*

- No first order approximation
- Applicable to many kinds of observables…

*(some of the) Drawbacks*

- Requires one calculation per set of cross sections
- … requires observables with a large dispersion

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PETALE experiment & specific requirements

Principle

- Heavy reflector near to the CROCUS reactor at EPFL
  ➔ all details in V. Lamirand’s presentation!

- Regular spacing of dosimeters in the reflector
  ➔ ~ cm radius and ~ 0.1 mm thickness

- Apply a BMC (and other) nuclear data assimilation processes on
  the dosimeter activation
  ➔ progressive evolution of the reaction rate between the
dosimeters
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Challenges

- Monte Carlo modeling
  Low flux (statistics) / streaming effect / dosimeter self-shielding

- Difficult classic TMC uncertainty propagation on reaction rates: \( \sigma_{\text{Nuclear Data}} \sim \sigma_{\text{MC statistics}} \)
  and \( \sigma_{\text{ND}} \) estimated via \( \Delta \) Monte Carlo with independent neutron histories...

- Classic CROCUS calculation: days
  ➔ one calculation required per random cross section!

Additional objective of this work

- Use the TMC technics to optimise the experimental setup / organise the experimental programme
  ➔ several configurations have to be studied
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Correlated Sampling technics?

Principle

- Objective: replace 2 “close” calculations by a single one
  - calculation speed-up - only 1 run
  - variance reduction - same neutron path
  - no first order assumption

- Neutron weight modification
  - ratio of probabilities between the two systems

- Different application fields
  - surface displacement
  - element concentration / density modification
  - Doppler effect
  - ... nuclear data uncertainty

\[
\text{Ratio of probability for a distance } d \text{ sampling: } \frac{\Sigma_{\text{tot}} \exp(-d \cdot \Sigma_{\text{tot}})}{\Sigma_{\text{tot}} \exp(-d \cdot \Sigma_{\text{tot}})}
\]

\[
\text{Ratio of probability for the reaction sampling: } \frac{\Sigma_{\text{n,r}} \cdot \Sigma_{\text{pert}}}{\Sigma_{\text{tot}} \cdot \Sigma_{\text{pert}}}
\]
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\[
\Sigma = 1.1 \Sigma
\]

Ratio of probability for a distance \(d\) sampling:

\[
\frac{\Sigma_{\text{tot}}^{\text{pert}} \exp(-d \cdot \Sigma_{\text{tot}}^{\text{pert}})}{\Sigma_{\text{tot}} \exp(-d \cdot \Sigma_{\text{tot}}^{\text{pert}})}
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[Diagram of neutron path and fission distribution]
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Drawbacks

- Needs probabilities different from zero and infinity
  - can not make isotope appears from scratch
- If the systems are too different the neutron weight is too different
  - bad convergence

\[ \Sigma = \frac{\Sigma \text{pert} \exp(-d \cdot \Sigma \text{tot})}{\Sigma \text{tot} \exp(-d \cdot \Sigma \text{tot})} \]

\[ \frac{\Sigma_{n,r} \cdot \Sigma \text{pert}}{\Sigma \text{tot} \cdot \Sigma_{n,r}} \]
Correlated Sampling with multiple Cross Sections: TMC-CS

Principle

- Each set of cross sections corresponds to a different system  
  \( \rightarrow \) different probabilities during the transport
- Neutron weight modification for each XS set
- Multiple “isotopes” and “mt” all together  
  \( \rightarrow \) ratio of probabilities between the two systems

Nuclear Data cross sections

- “Classic” TENDL cross section  
  \( \rightarrow \) sampling on the nuclear data parameters
- “Extended” TENDL - EUROfusion (“to fill the gap”)  
  \( \rightarrow \) sampling on the nuclear models themselves (more challenging)
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- discontinuities
- non linearity?
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TMC-Ref
- Classic Total Monte Carlo uncertainty propagation (reference)
- $N$ calculations for $N$ cross section sets

TMC-CS
- Uncertainty propagation using the correlated sampling technics
- $N / (\sim 64)$ calculations for $N$ cross section sets
  \textit{memory limitation}

TMC-sensi
- Uncertainty propagation using the sensitivities (Serpent code)
- XS % variation between ACE files $#x$ and $#0$
  \rightarrow \text{uncertainty propagation for each XS file}

Sensi
- Uncertainty propagation using the sensitivities (Serpent code)
- Covariance matrix from all the random XS files
  \rightarrow \text{one uncertainty propagation value}
Validation

$k_{eff}$ uncertainty propagation

HMI-001: $^{56}\text{Fe}$

- Large uncertainty ~1000 pcm
- Same global distributions
- Good file to file agreement
- TMC-CS: difference appears after 2000 pcm
- TMC-sensi: good linearity with a comma trend

$^{235}\text{U}(93\%)$ / Iron cylinder reflected by stainless steel

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$\mu$ and $\sigma$ values for each method:
- TMC-Ref: $\mu = 1.00236$, $\sigma = 1046$ pcm
- TMC-CS: $\mu = 1.00315$, $\sigma = 970$ pcm
- TMC-sensi: $\mu = 1.00342$, $\sigma = 949$ pcm
Validation

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**HMI-001: $^{56}$Fe & extended TENDL**
- Large uncertainty ~1000 pcm
- Same global distribution
- Good file to file agreement
- Non linearity appears on the sensitivity approach
Validation

$k_{eff}$ uncertainty propagation

CROCUS: $^{56}$Fe

- Small uncertainty ~3pcm
- TMC-CS / TMC-sensi: good agreement! …
- … no TMC-Ref

$\sigma_{MC \ stat} \sim \sigma_{ND}$
Validation

$k_{\text{eff}}$ uncertainty propagation

CROCUS: $^{56}\text{Fe}$
- Small uncertainty ~3pcm
- TMC-CS / TMC-sensi: good agreement! …
- … no TMC-Ref
  $\sigma_{\text{MC stat}} \sim \sigma_{\text{ND}}$

- Neutron flux / reaction rate in the dosimeters can be compared to TMC-Ref!
- But requires neutron biasing
Introduction

Principle

- On the fly learning of the “minimal number of displacements” required to reach the target
  ➞ *Neutron splitting*

- Geometric X Energy grid (no angular grid yet)
Introduction

PETALE exp & specific requirements

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Thermal neutron with a weight of 1

Thermal neutron with a weight of 0.5

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PETALE exp & specific requirements

On the fly learning ➔ automatic bias on the actual neutron path

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Weight field

Thermal neutrons

Fast neutrons
Introduction

PETALE exp & specific requirements

Weight field

Raw flux

Weighted flux (real flux)

Thermal neutrons

Fast neutrons
Introduction

PETALE exp & specific requirements

Weight field

Raw flux

Weighted flux (real flux)

Thermal neutrons

Fast neutrons

Acceleration factor (FOM)
- ~10 in the fast range
- ~50 in the thermal range
CROCUS dosimetry: neutron flux
- Flux calculated in all the dosimeters

- Each flux is declined according to each TENDL cross section
  → all Fe isotopes, all mt reactions

- Spectrum distribution different according to the XS

Observation:
- Impact of ND uncertainty directly visible on the flux in the dosimeters
- Very close trend line between TMC-Ref and TMC-CS
- Reduced statistical uncertainty with TMC-CS
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CROCUS dosimetry: reaction rate

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- Very good prediction of the reaction rates difference between the TENDL cross sections (useful for BMC)
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Separation power

- Multiple dosimeters… all independant?
- Rhodium-Indium inelastic threshold reactions: similar ordering
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Dosimeter correlation matrix

\[ \begin{array}{ccc}
\text{Reaction} & \text{Dosimeter number} \\
\hline
\text{In} & \text{In} \\
\text{In} & \text{Rh} \\
\text{Rh} & \text{In} \\
\end{array} \]

\begin{align*}
\Delta R_{\text{N}} & \text{ [\%]} \\
\hline
1.7 \text{ eV} & 3 \text{ MeV} \\
1.2 \text{ eV} & 2.0 \text{ MeV} \\
\end{align*}

\[ \text{Volume number} \]

same ordering!
Validation

Separation power
- Multiple dosimeters… all independant?
- Rhodium-Indium inelastic threshold reactions: similar ordering

Dosimeter correlation matrix

- Method generic for many dosimeters
- Important for dosimeter choice!
  ➞ see V. Lamirand presentation
Conclusion

Methodology

- The correlated sampling is nuclear data uncertainty propagation friendly

Results

- Approach usable for different systems HMI-001, CROCUS, ...
- Helpful for observables with a small dispersion

Perspectives

- Apply BMC assimilation using TMC-CS
- Add $\nu$, $\chi$ in the CS for fissionable isotopes & angular sampling
- Consider the angular dependance for the automatic biasing
Thank you for your attention!

Do you have some questions?