Development and Application of Data Assimilation Methods in Reactor Physics

Ph.D. Defence

Lausanne, Switzerland

Daniel J. Siefman

Swiss Federal Institute of Technology in Lausanne

EPFL

August 16, 2019

Goals

- **Scientific goals**:
  1. Review, analyze, improve, and propose new methods for DA in neutronics
- **Project aims**:
  1. Integrate data assimilation into SHARK-X system at PSI
  2. Create data assimilation tools for continuous-energy Monte Carlo
  3. Use Proteus experimental data

Outline

1. Theoretical overview of methods
   - Provide first case study
   - DAN: tools for continuous energy Monte Carlo
2. eXtendend Generalized Linear Least Squares[1](not presented)
   - New method for neutronics
   - How do statistically uncertain sensitivities affect adjustments?
3. New ways to data assimilation and new methodological framework
   - Use LWR-Phase II Proteus experiments
   - Develop tools for PSI's SHARK-X
   - Assimilate reactivity experiments (not presented)
   - Adjust nuclear fission model parameters with post-irradiation examination data

[2]Siefman *et al.*, Annals of Nuclear Energy, 135 (2019)

Bayes' Theory

- Key components of Bayes' theory
  - Prior: Nuclear data ($\boldsymbol{\sigma}$)
  - Likelihood: Agreement between $C(\boldsymbol{\sigma})$ and E
  - Posterior: Updated $\boldsymbol{\sigma}$ after assimilating E

$$p(\boldsymbol{\sigma}') \propto L(\mathbf{E}|\boldsymbol{\sigma})p(\boldsymbol{\sigma}) \tag{1}$$

- Different methods to find $p(\boldsymbol{\sigma}')$

Data Assimilation Methods

Deterministic (1960s-present)

- GLLS:
  - First-order perturbation theory
  - Gaussian PDFs
  - Sensitivity coefficients

Stochastic (2015-present)

- MOCABA:
  - Non-linear $C(\boldsymbol{\sigma})$
  - Gaussian PDFs
- BMC:
  - Non-linear $C(\boldsymbol{\sigma})$
  - Any PDF
- BFMC:
  - Weight normalization
  - Non-linear $C(\boldsymbol{\sigma})$
  - Any PDF

Experiment Consistency Filtering

- Fundamental assumption: $C(\boldsymbol{\sigma}) = E$ with their uncertainties
- If not true, integral parameter is *inconsistent*
- May cause adjustments that
  - Do not respect nuclear physics models
  - Do not respect differential data
- Traditionally remove inconsistent experiments from the adjustment
- Marginal Likelihood Optimization (MLO):
  - Data-driven approach
  - Add uncertainty to integral parameters
  - Decrease their influence on the adjustment

Marginalized Likelihood Optimization (MLO)

- **Idea:** Account for biases or underestimated uncertainties with an extra uncertainty term, $\mathbf{M_{extra}}$
- Minimize the negative of the log-likelihood to estimate $\mathbf{M_{extra}}$

$$\chi^2 = \left(\mathbf{E} - \mathbf{C}\right)^T \left(\mathbf{M_E} + \mathbf{M_C} + \mathbf{M_{extra}}\right)^{-1} \left(\mathbf{E} - \mathbf{C}\right) \tag{2}$$

$$L = \frac{e^{-\chi^2/2}}{\sqrt{(2\pi)^N \det\left(\mathbf{M_E} + \mathbf{M_C} + \mathbf{M_{extra}}\right)}} \tag{3}$$

$$\min\left[\frac{1}{2}\left(N * \log(2\pi) + \log\left(\det\left(\mathbf{M_E} + \mathbf{M_C} + \mathbf{M_{extra}}\right)\right) + \chi^2\right)\right] \tag{4}$$

Test Case

- Want to compare GLLS, MOCABA, BMC, BFMC
- What happens with identical input conditions?
- Test case using Serpent2.1.29
- Jezebel-Pu239: k_{eff}, F28/F25, F49/F25, F37/F25
  - Highly linear
- 10,000 nuclear data samples with NUSS tool
  - Sample from Gaussian distributions

Nuclear Data Adjustments: Elastic & Inelastic

- Agree within confidence intervals
- Confidence intervals larger with BMC/BFMC

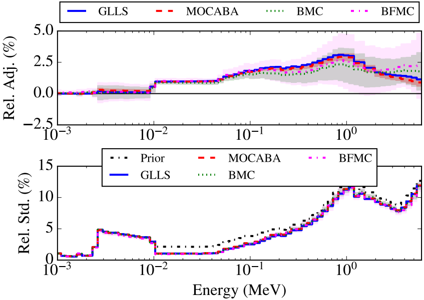


Figure: Pu-239 Elastic Scattering

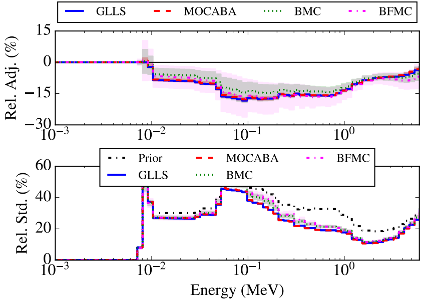
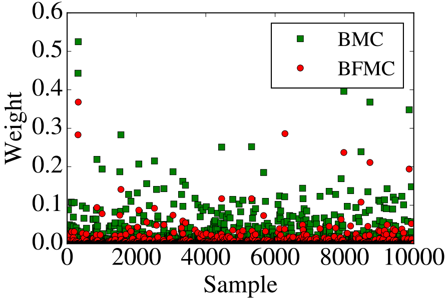


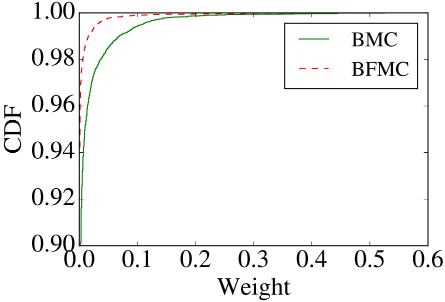
Figure: Pu-239 Inelastic Scattering

Weights from BMC/BFMC

Table: Weight definitions

BMC	BFMC
$w_i = e^{-\chi_i^2/2}$	$w_i = e^{-\chi_i^2/\chi_{\min}^2}$





Toy Problem

- Linear toy problem had known solution (GLLS)
- **BMC**:
  - Large χ^2 causes weight degeneracy
  - Many samples to converge
  - Upper χ^2 where all $w_i = 0$
- **BFMC**:
  - $\chi_i^2/\chi^2_{\text{min}}$ biases posteriors
  - **Low χ^2**: weight degeneracy
  - **High χ^2**: posterior $\rightarrow$ prior
  - **At $\chi^2_{\text{min}} = 2$**: BMC = BFMC

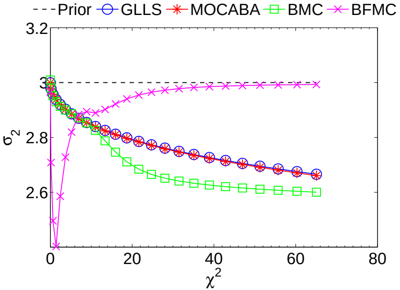


Figure: Posterior $\boldsymbol{\sigma}$ vs. χ^2

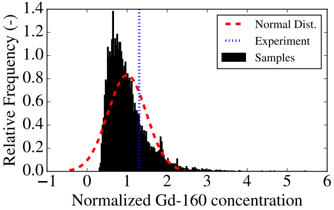
Conclusions

- Case study shows good agreement between methods[2]
- BMC/BFMC has larger confidence intervals than MOCABA
  - Weight degeneracy needs to be carefully monitored
  - Needs more samples to have same accuracy
- Linear & Gaussian toy problem:
  - BFMC gives mathematically biased estimate
  - Biased estimate **safer for large χ^2**
- Application regime:
  - $\chi^2_{\text{min}} < 2 \rightarrow$ BMC
  - $\chi^2_{\text{min}} > 2 \rightarrow$ BFMC

[3] **Siefman, D** *et al.*, European Physics Journal Plus, 133 (2018)

Post-Irradiation Examination (PIE) Data

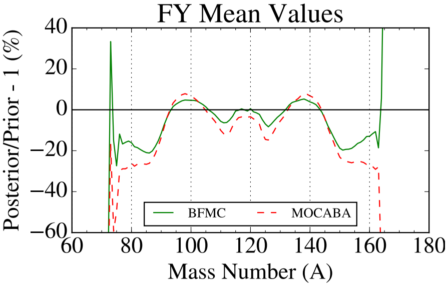
- Predicted spent fuel composition
  - Biases up to 64%
  - Uncertainties up to 56%
  - Fission yields (FYs) important
- **New framework:** DA + PIE + FYs
- Considerations:
  - GEF creates non-Gaussian FYs
  - Non-linear Boltzman/Bateman
  - Sensitivities between GEF/CASMO
- Data are inconsistent (large χ^2)
  - BMC $\rightarrow$ weight degeneracy
  - Need BFMC
  - Effect of MLO?

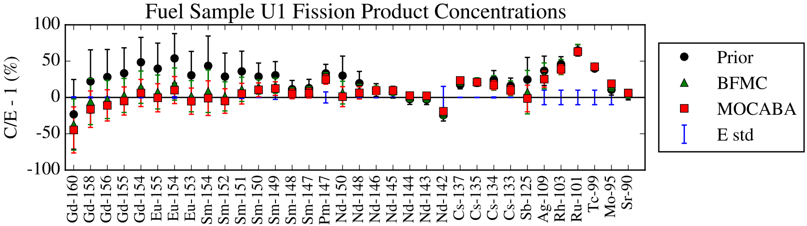


Approach

- **Prior** $p(\boldsymbol{\sigma})$:
  - GEF2017 model parameters $\rightarrow$ fission yields
- **Likelihood** $L(\mathbf{E}|\boldsymbol{\sigma})$:
  - LWR-Phase II experimental PIE data
  - Simulations with CASMO-5/SHARK-X
- **Posteriors** $p(\boldsymbol{\sigma}')$:
  - Adjusted model parameters $\rightarrow$ adjusted fission yields
- **Approach**:
  1. Sample GEF's model parameters 10,000 times
  2. Run CASMO-5 with GEF's fission yields
  3. Use MLO for inconsistency
  4. Data assimilation with MOCABA and BFMC
  5. Re-run CASMO-5 with adjusted fission yields

Posterior Fission Yields



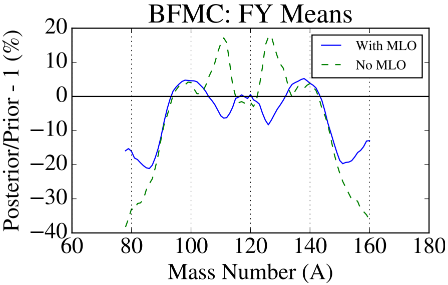


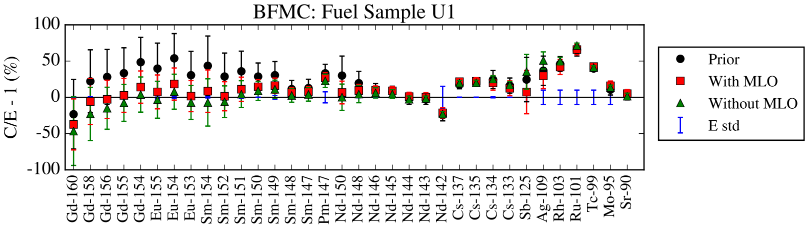
Comparison to ENDF/B-VIII.0

Table: Comparing GEF Independent FYs to ENDF/B-VIII.0

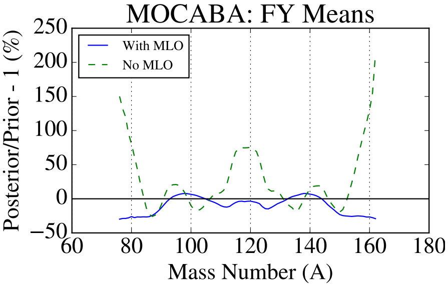
		Avg. Abs. Rel. Diff. (%)	Avg. Std. Rel. Diff. (%)
Pu-239	Prior	16	16
	BFMC	11	-16
	MOCABA	12	-38

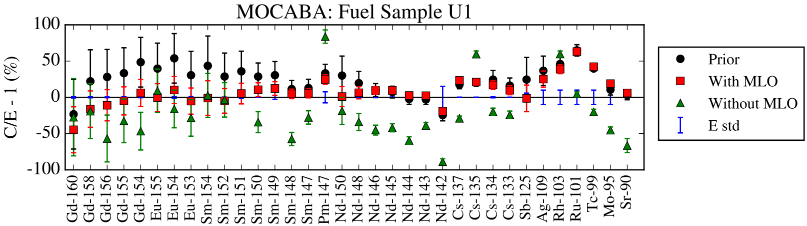
BFMC Without MLO





MOCABA Without MLO





Conclusions

- Proposed and tested new data assimilation framework
- MOCABA highly effected by MLO:
  - Over-fitting due to inconsistency
- BFMC not highly effected by MLO:
  - Slightly improved posteriors
  - Non-normality always accounted for
  - Weight definition accounts for inconsistency globally
  - MLO accounts for inconsistency locally
- Future work: separate effects with different PIE data
  - Highly Gaussian & inconsistent
  - Non-Gaussian & consistent

Ph.D. Outcomes

- Compared and characterized deterministic and stochastic methods
- Expanded GLLS equations for statistically uncertain sensitivities
- Applied data assimilation to LWR-Proteus Phase II
- Developed new framework for burnup simulations and fission yields
- Future: how far can we go?
  - Fuel cycle analysis?
  - Reactor kinetics?
  - Thermal hydraulics?
  - Fuel performance?
  - ...

Questions & Discussion

Figure: Campus of EPFL in Lausanne, Switzerland