Adjusting GEF Model Parameters with Post Irradiation Examination Experiments

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Outline

- We want to do Data Assimilation on Fission Yields (FY)
- Evidence: PIE data from LWR-Proteus Phase II
- Posteriors:
  1. Improved nuclide compositions (biases and uncertainties)
  2. Adjusted FY data (means and covariances of model parameters)
- Recipe:
  1. GEF for FYs (sample model parameters)
  2. Simulations with CASMO-5 and GEF samples
  3. Marginal Likelihood Optimization: Inconsistent experimental data
  4. BFMC to fit model parameters to experimental data
  5. Rerun GEF with posterior model parameters
  6. Compare posterior FYs to prior, JEFF3.3, ENDFB/V-III.0
  7. Inspect posterior calculated nuclide concentrations

GEF Model Parameters

- Around 100 model parameters in GEF
- Parameters set once with benchmark experimental data
- 21 have uncertainties assigned to them
- Defined as normal and independent

Table: Means and standard deviations of GEF model parameters.

Input Parameter	Mean	Std.	Input Parameter	Mean	Std
Shell position for S_1 channel	-0.18	0.1	Shell curvature for S_1 channel	0.37	5%
Shell position for S_2 channel	-0.46	0.1	Shell curvature for S_2 channel	0.185	5%
Shell position for S_3 channel	-0.37	0.1	Shell curvature for S_3 channel	0.156	5%
Shell position at $Z \approx 42$	0.0	0.1	Shell curvature at $Z \approx 42$	0.035	5%
Shell effect for S_1 channel	-2.85	0.1	Weakening of the S_1 shell	0.31	0.1
Shell effect for S_2 channel	-4.4	0.1	$(\hbar\omega)_{eff}$ for tunneling of S_1 channel	0.32	0.1
Shell effect for S_3 channel	-6.4	0.2	$(\hbar\omega)_{eff}$ for tunneling of S_2 channel	0.31	0.1
Shell effect at $Z \approx 42$	-0.9	0.05	$(\hbar\omega)_{eff}$ for tunneling of S_3 channel	0.31	0.1
Rectangular contribution to S_2 channel width	12.5	5%	$(\hbar\omega)_{eff}$ for tunneling at $Z \approx 42$	0.31	0.1
Shell effect at mass symmetry	0	0.1	Width of fragment distribution in N/Z	1	10%
Charge Polarization	0.25	0.1			

PDF of Fission Product Concentration

- FYs have non-normal distributions
  - Max skewness = 1.3
  - Avg. skewness = 0.74 ± 0.08
- Coupled nature of equations creates non-linearity
- Some FPs have non-normal distributions
  - Max skewness = 1.6
  - Avg. skewness = 0.4 ± 1.12

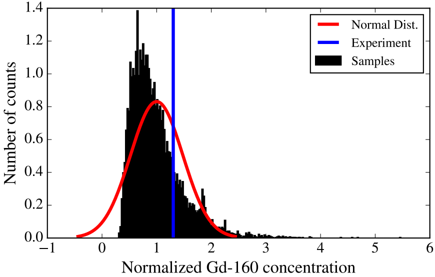


Figure: Histogram of Gd-160 concentration normalized to mean

BFMC: Bayesian Monte Carlo

- Stochastically searches for maximum likelihood
- No assumptions about prior distribution: can be non-normal!
- Each sample of nuclear data used in one calculation $\mathbf{C}_i(\boldsymbol{\sigma}_i)$
- Sample set of calculations used in likelihoods

$$L\left(\mathbf{E}\middle|\boldsymbol{\sigma}_i\right) \propto e^{-\chi_i^2/2} \tag{1}$$

$$\chi_i^2 = \left(\mathbf{E} - \mathbf{C}_i(\boldsymbol{\sigma}_i)\right)^T (\mathbf{M}_\mathbf{E})^{-1} \left(\mathbf{E} - \mathbf{C}_i(\boldsymbol{\sigma}_i)\right) \tag{2}$$

- Each χ_i^2 is used to calculate a weight, w_i

$$w_i = \chi_i^2 / \chi_{\text{min}}^2$$

Posteriors: Weighted Averages

$$\boldsymbol{\sigma}' = \frac{\sum_{i=1}^{N} w_i \times \boldsymbol{\sigma}_i}{\sum_{i=1}^{N} w_i}$$

$$\mathbf{M}'_{\sigma} = \frac{\sum_{i=1}^{N} w_i \times (\boldsymbol{\sigma}_i - \bar{\boldsymbol{\sigma}})(\boldsymbol{\sigma}_i - \bar{\boldsymbol{\sigma}})^T}{\sum_{i=1}^{N} w_i}$$

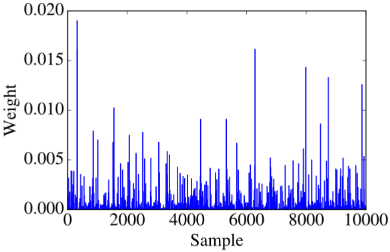


Figure: Weight distribution example.

BFMC Procedure

- Sample model parameters in GEF2017/1.2 to create samples of FYs
  - Thermal fission @ 0.0253 eV: U-235, Pu-239, Pu-241
  - Fast fission @ 0.5 MeV: U-238
- Do burnup calculation with sample set of FYs
- BFMC-update with burnup calculations and PIE data
  - Adjusted GEF model parameters
  - Reduced uncertainties
  - New correlations
- Re-run GEF with adjusted model parameters
  - Generate new FYs with GEF and adjusted model parameters
- Calculate new nuclide concentrations and their uncertainties

Application Case

- Test using PIE data from the Proteus experimental campaign
  - UO_2 fuel sample
  - Burnup of 38 MWd/kg
  - 33 fission products
  - Measured in the PSI hotlab with mass spectroscopy, gamma spectroscopy
- Simulate with CASMO-5
- 10,000 prior FY samples
- 500 posterior FY samples

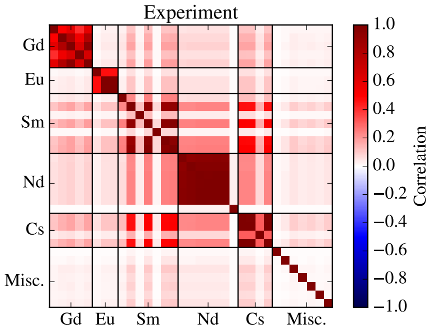


Figure: Experimental correlation matrix

Experimental Data

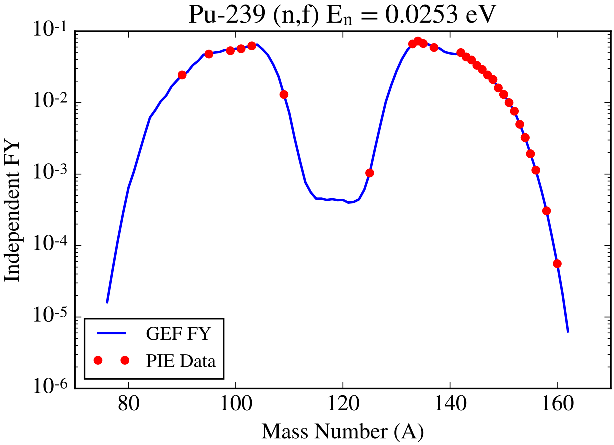
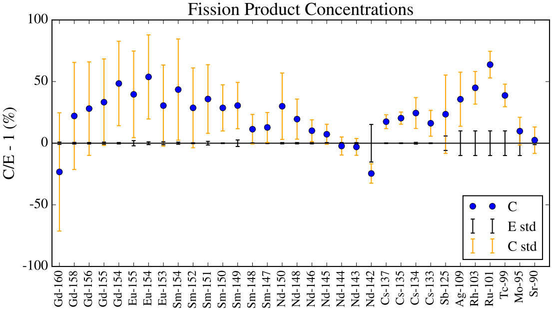


Figure: Experimental data part of LWR-PII on the Pu-239 FY spectrum

Inconsistent Data

- Certain nuclide compositions are *inconsistent*
  - Difference between C and E not explained by uncertainty
  - Model defect unaccounted for
  - Uncertainty underestimated
  - Correlations not taken into account
- Causes too large and unphysical adjustments to model parameters



Marginal Likelihood Optimization (MLO)

- We apply a technique called MLO for inconsistent data
  - Terranova et al., *Fission yield covariance matrices for the main neutron-induced fissioning systems contained inthe JEFF-3.1.1 library*, Annals of Nuclear Energy, **109**, 2017
- **Idea:** Account for biases or underestimated uncertainties with an extra uncertainty term, $\mathbf{M_{extra}}$
- Minimize the negative of the log-likelihood to estimate $\mathbf{M_{extra}}$

$$\chi^2 = (\mathbf{E} - \mathbf{C})^T (\mathbf{M_E} + \mathbf{M_C} + \mathbf{M_{extra}})^{-1} (\mathbf{E} - \mathbf{C}) \tag{3}$$

$$L = \frac{e^{-\chi^2/2}}{\sqrt{(2\pi)^N \det(\mathbf{M_E} + \mathbf{M_C} + \mathbf{M_{extra}})}} \tag{4}$$

$$\min\left[\frac{1}{2}\left(N * \log(2\pi) + \det(\mathbf{M_E} + \mathbf{M_C} + \mathbf{M_{extra}}) + \chi^2\right)\right] \tag{5}$$

MLO Results

- Before MLO $\chi^2/N = 23$
- After MLO $\chi^2/N = 0.7$

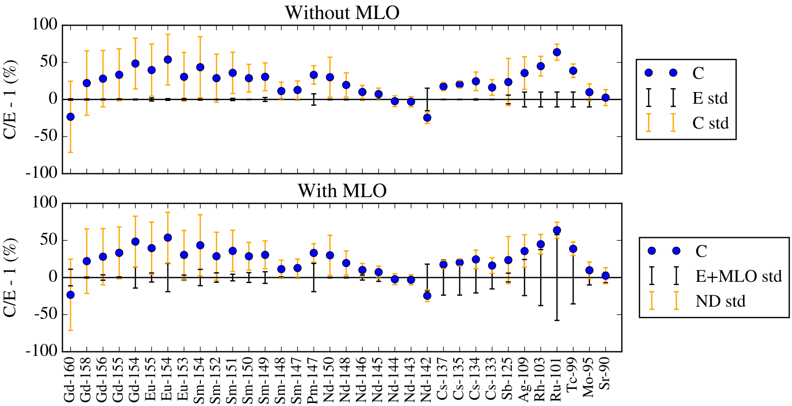
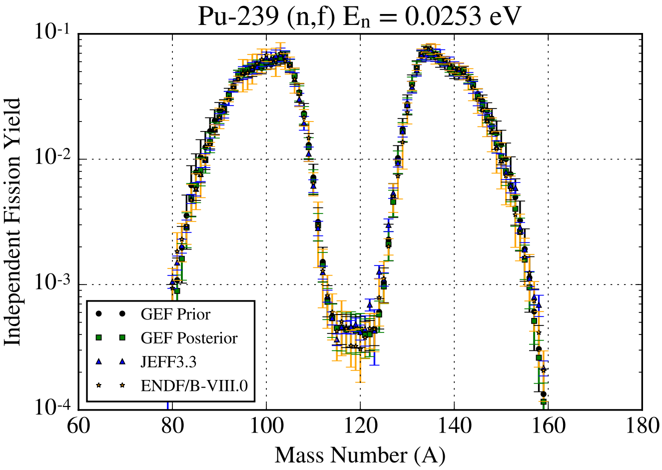
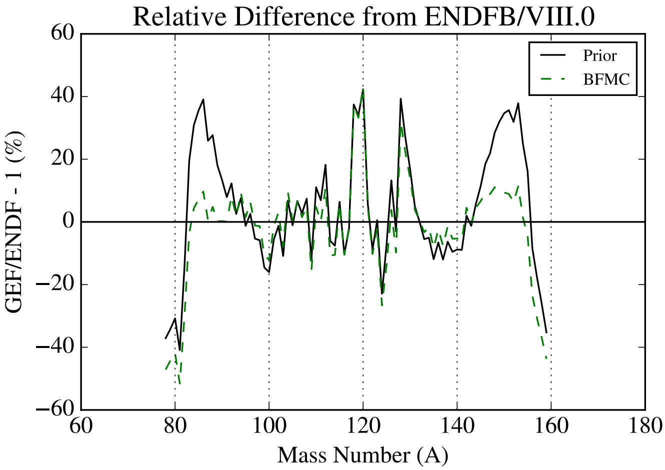


Figure: Biases before and after applying MLO to ensure consistency

Comparison to JEFF3.3 and ENDFB/V-III.0



Means: Relative Difference from ENDFB/V-III.0

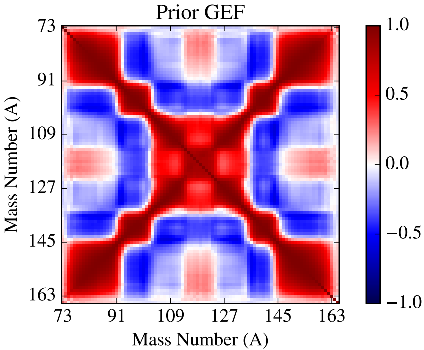


Comparison to ENDFB/VIII.0

Table: Average Relative Differences from ENDFB/VIII.0 (Absolute Values for Means)

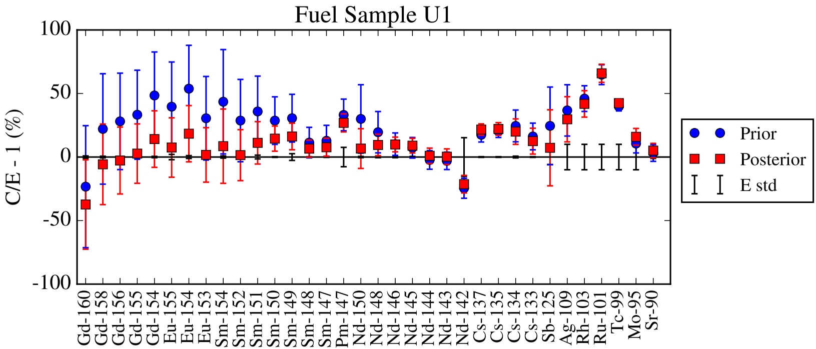
		Mean	Standard Deviation
Pu-239	Prior	15.8	15.9
	Posterior	11.4	-15.5
U-235	Prior	12.9	176.8
	Posterior	15.0	100.6
Pu-241	Prior	21.9	5.3
	Posterior	15.8	-27.7

Adjustments of Pu-239 FY Correlations



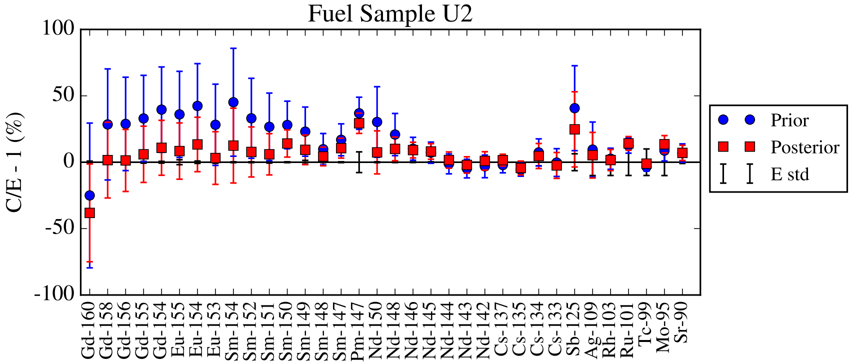
Posterior Calculated FP Concentrations

	Prior	Posterior
Average absolute bias	26.4%	15.4%
Average relative standard deviation	20.9%	8.83%



Applied to Another Fuel Sample

	Prior	Posterior
Average absolute bias	19.4%	8.71%
Average relative standard deviation	19.3%	13.5%



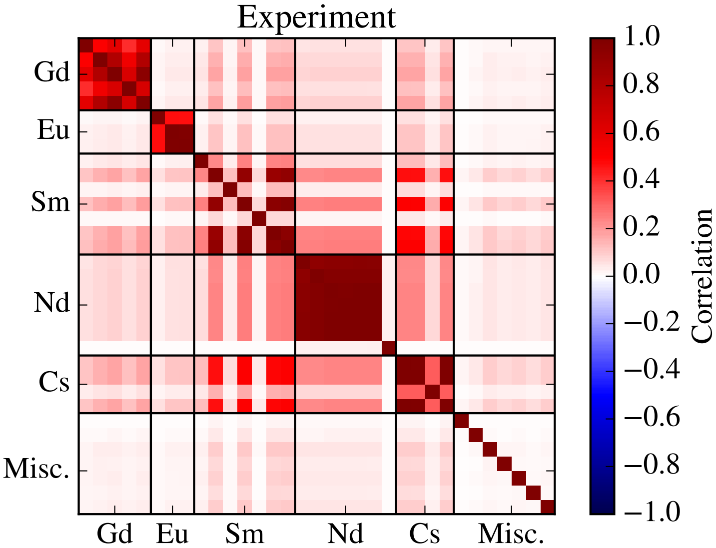
The End

- Showed an approach to incorporate PIE data into burnup simulations
- Improved biases and reduced uncertainties
- Improved agreement with ENDFB/VIII.0 FYs
- Weakened correlations between FYs
- Was an engineering application, how useful for nuclear data?
- More diverse PIE data would be better
- Cleaner experiments?

Questions?

Figure: Campus of EPFL in Lausanne, Switzerland

Experimental Correlations



Experimental Correlations

- Most nuclide concentrations measured with high-performance liquid chromatography (HPLC) and a multicollector inductively-coupled plasma mass spectrometer (MC-ICP-MS)
  - HPLC: to separate chemical elements
  - MC-ICP-MS: to measure the isotopic concentrations
- Only MC-ICP-MS for metallic fission products
  - No isobaric interference
  - Mo-95, Tc-99, Ru-101, Rh-103, and Ag-109
- Ru-106, Sb-125, Ce-144, and Cm-243 measured with gamma ray spectrometry
  - Present in very small concentrations

Experimental Correlations

- Experimental value: mass of isotope relative to the total mass of U (mg/g)

$$\epsilon_i = w_i \frac{\eta_j}{U_{\text{tot}}}$$

- Correlations arise from U_{tot} normalization, common element mass η_j
- Assume no correlations between w, U_{tot}, and η

$$\mathbf{V_{out}} = \mathbf{J}^T \mathbf{V_{in}} \mathbf{J}$$

$$\mathbf{J} = \begin{bmatrix} \frac{\delta\epsilon_1}{\delta U_{\text{tot}}} & \frac{\delta\epsilon_2}{\delta U_{\text{tot}}} & \dots & \frac{\delta\epsilon_n}{\delta U_{\text{tot}}} \\ \frac{\delta\epsilon_1}{\delta\eta_1} & \frac{\delta\epsilon_2}{\delta\eta_1} & \dots & \frac{\delta\epsilon_n}{\delta\eta_1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\delta\epsilon_1}{\delta\eta_n} & \frac{\delta\epsilon_2}{\delta\eta_n} & \dots & \frac{\delta\epsilon_n}{\delta\eta_n} \\ \frac{\delta\epsilon_1}{\delta w_1} & \frac{\delta\epsilon_2}{\delta w_1} & \dots & \frac{\delta\epsilon_n}{\delta w_1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\delta\epsilon_1}{\delta w_n} & \frac{\delta\epsilon_2}{\delta w_n} & \dots & \frac{\delta\epsilon_n}{\delta w_n} \end{bmatrix}$$

Model Adjustments: Means

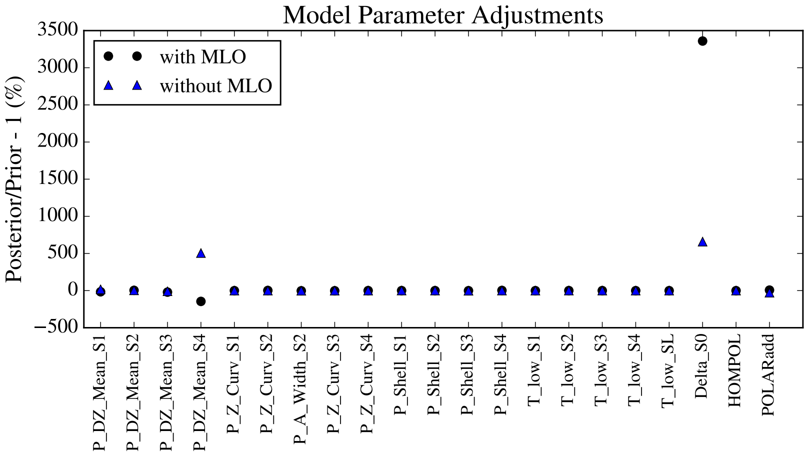


Figure: Adjustments to 21 model parameters, with and without MLO.

Model Adjustments: Means

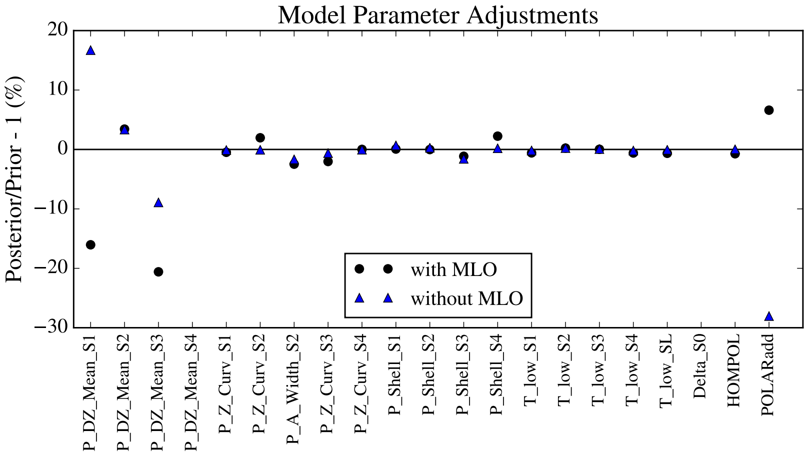


Figure: Adjustments to 21 model parameters, with and without MLO.

Model Adjustments: Standard Deviations

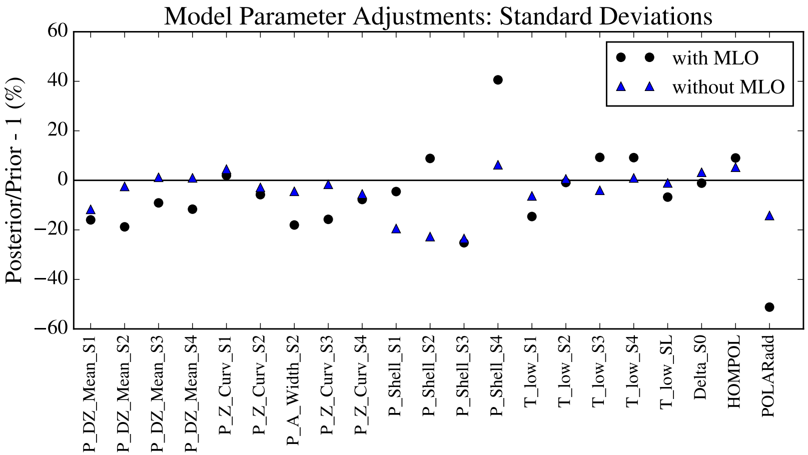


Figure: Adjustments to standard deviations of 21 model parameters, with and without MLO.

Development of Correlations Between Model Parameters

- Model parameters sampled from mulitvariate Gaussian distribution using these covariance matrices

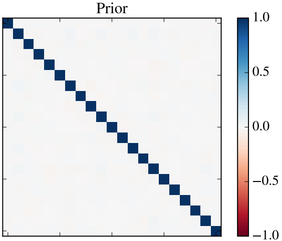


Figure: Prior

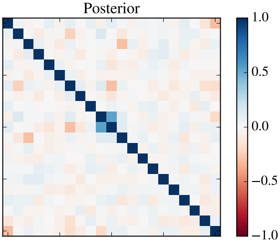


Figure: Without MLO

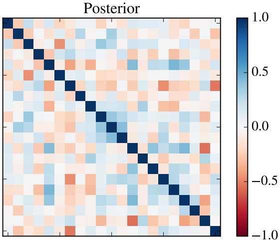
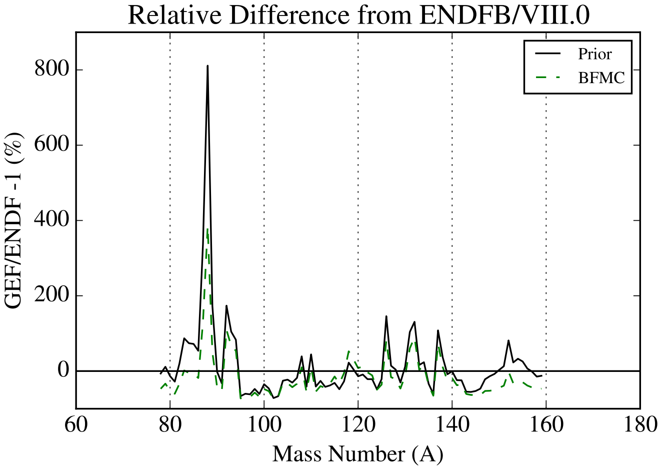
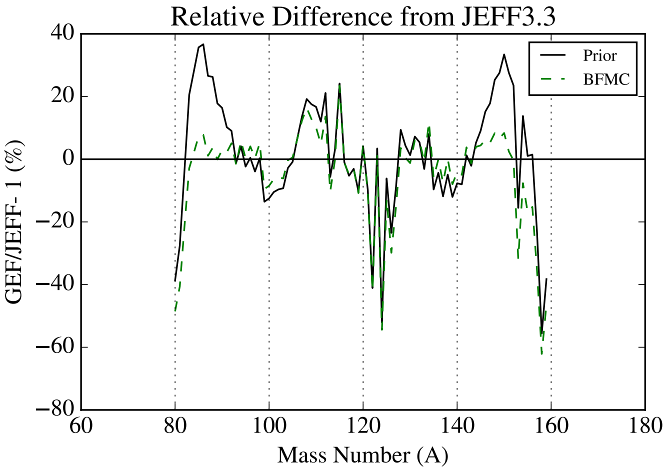


Figure: With MLO

Standard Deviations: Relative Difference from ENDFB/V-III.0



Means: Relative Difference from JEFF3.3



Standard Deviations: Relative Difference from JEFF3.3