n+^{239}Pu covariance evaluation at LLNL

mini-CSEWG, Livermore Valley Open Campus, April 2023

K. Kravvaris & K. Wendt

LLNL-PRES-848244

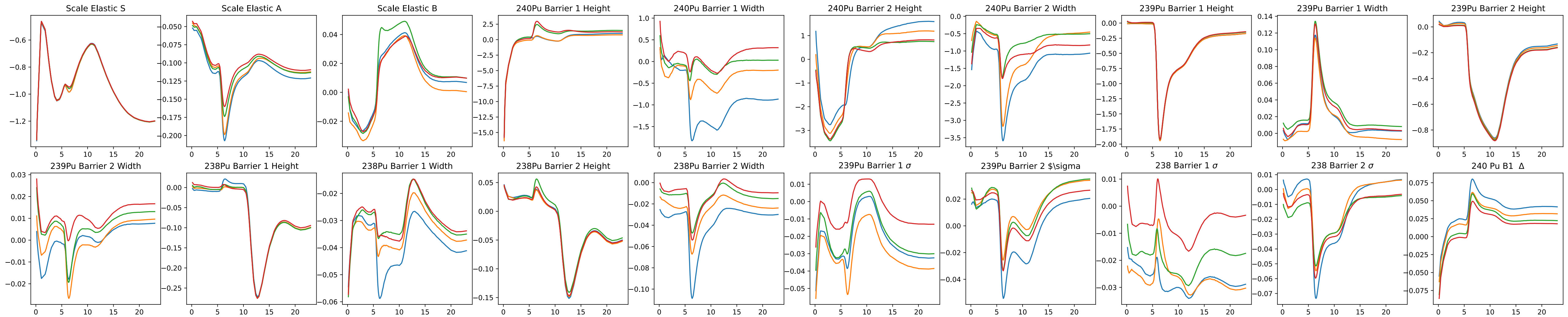
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Extracting covariances from model-driven evaluations.

- Calculations using LLNL-developed YAHFC (yet another Hauser-Feshbach code.)
- Multiple parameters can be varied and are thus fitted to experimental data.
- Ultimate goal is the Markov-chain Monte-Carlo evaluation of the model covariances.
- YAHFC runs take significant amount of time, developed parallel version (not discussed here.)
- Explore options for quick re-evaluation of covariances in the wake of new experimental data.

LLNL / Yet-Another-Hauser-Feshbach-Code Public

https://github.com/LLNL/Yet-Another-Hauser-Feshbach-Code



$$p_i$$

↓

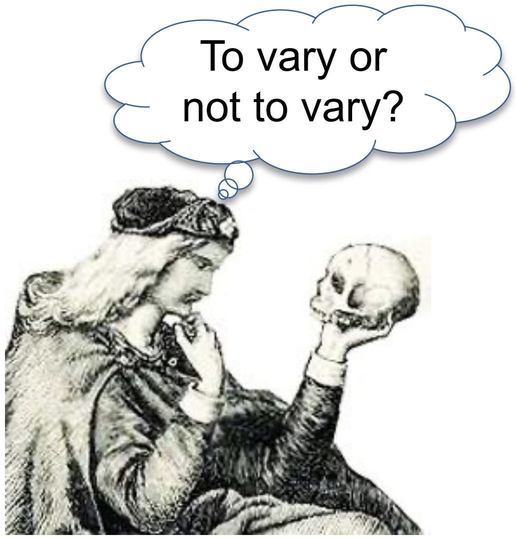
YAHFC

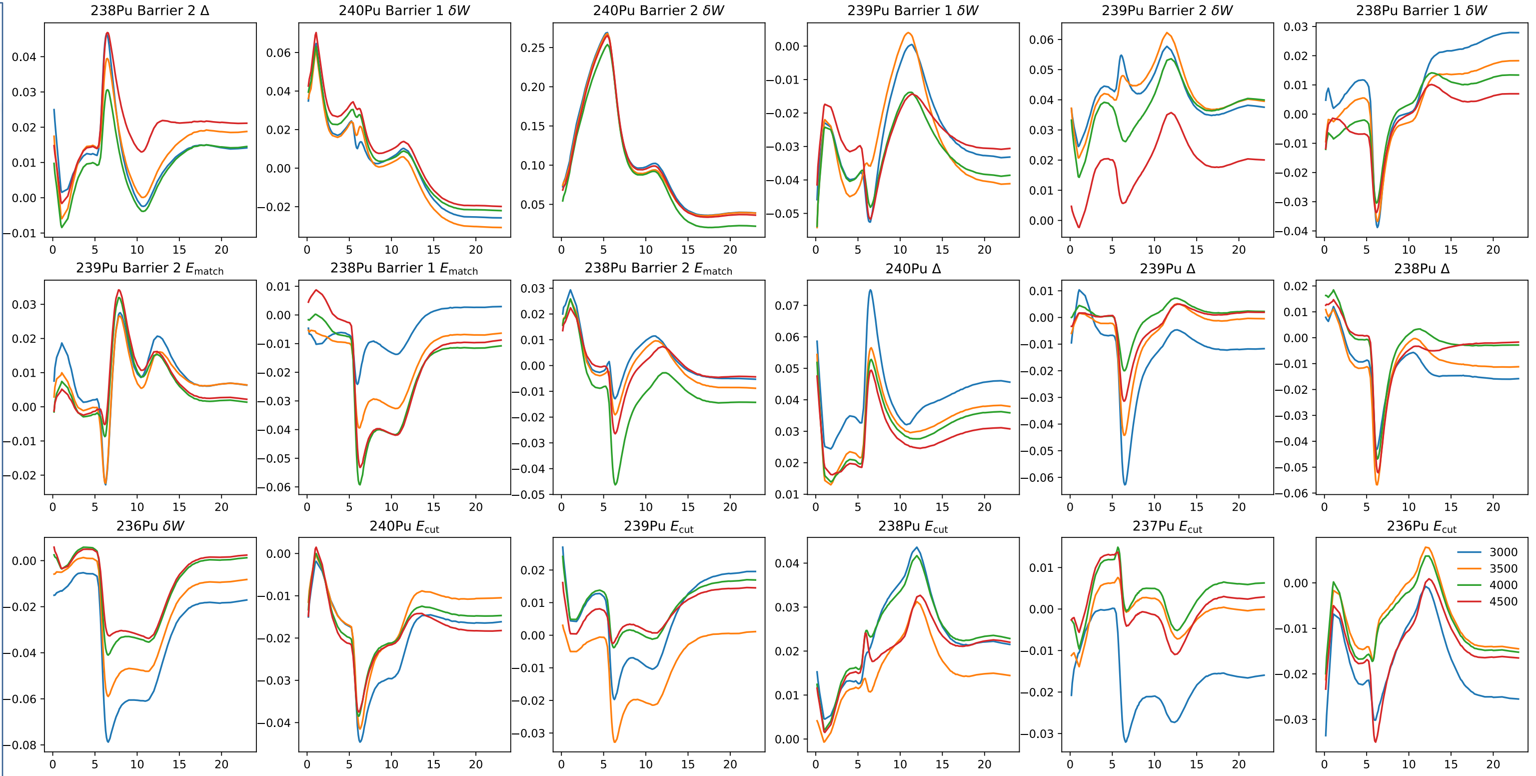
↓

$$\times k \qquad \sigma_j$$

Sensitivity

$$s_{ij} \sim \sum_k (p_i^k - \bar{p}_i)(\sigma_j - \bar{\sigma}_j)$$





Kalman filter (following NDS 109 (2008) 2752–2761)

Sensitivity Matrix

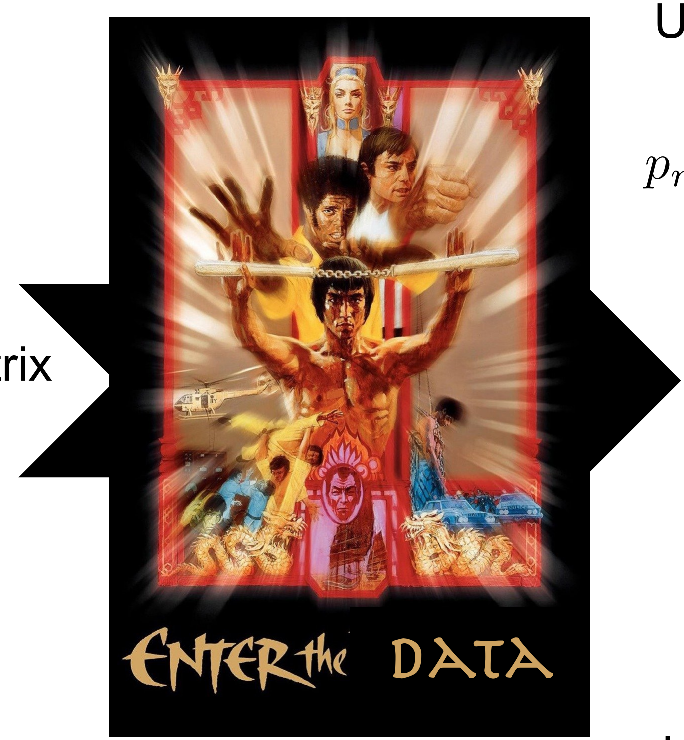
$$\sigma_i \equiv \sigma(E_i, \mathbf{p})$$

$$S_{ij} = \frac{\partial \sigma_i}{\partial p_j}$$

Parameter (p) covariance matrix
(Assumed diagonal)

Model covariance

$$C_0 = S P_0 S^T$$



Updated YAHFC parameter values

$$p_{n+1} = p_n + P_n S^T Q_{n+1}(\sigma^{\exp}_{n+1} - \sigma(\mathbf{p}_n))$$

$$P_{n+1} = P_n - P_n S^T Q_{n+1} S P_n$$

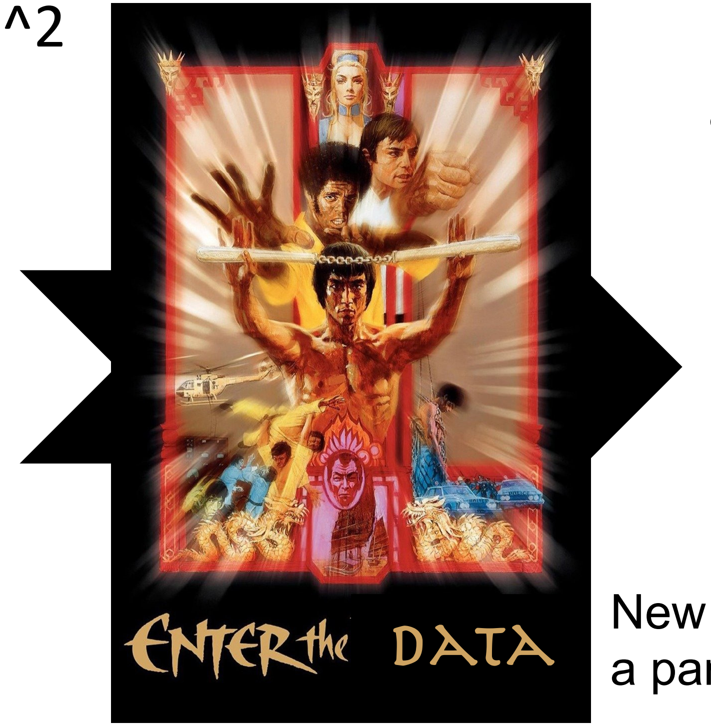
$$Q_{n+1} = (C_n + C^{\exp}_{n+1})$$

$$C_{n+1} = S P_{n+1} S^T$$

Updated covariances

Backwards-Forwards Monte Carlo.

- Start from some “guess” parametrization of YAHFC (eye^2 fit)
- Draw a bunch of samples that follow a “guess” covariance matrix



- Compute χ^2 for each parametrization
- New “mean” parametrization is the Bayesian model average of the parameters with weights

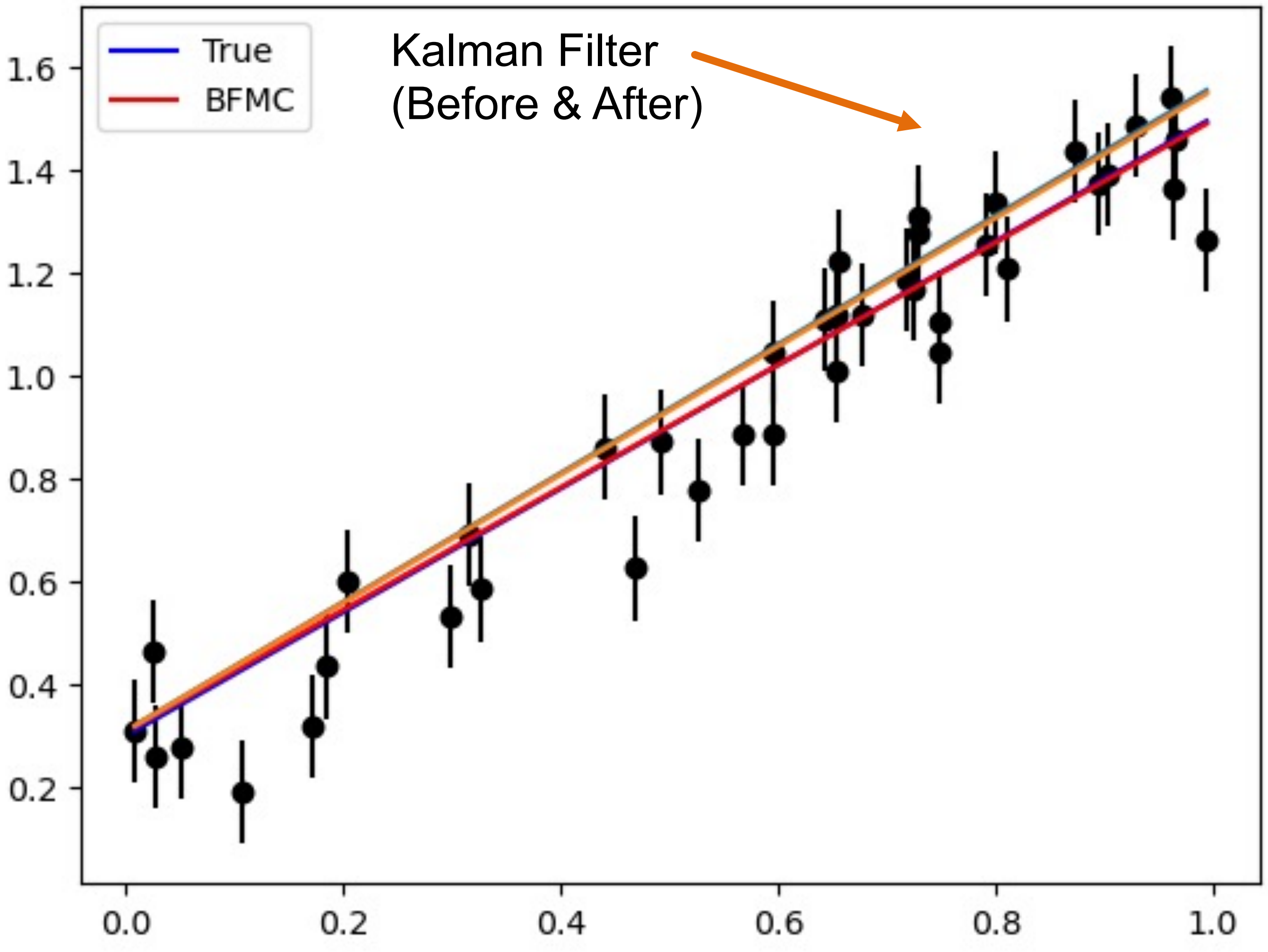
$$w_i = C\exp\left[-\left(\frac{\chi^2}{\chi^2_{\mathrm{min}}}\right)^2\right]$$

New probability for a parametrization: $P(\mathbf{p}) = \sqrt{P_1}G + p_1$

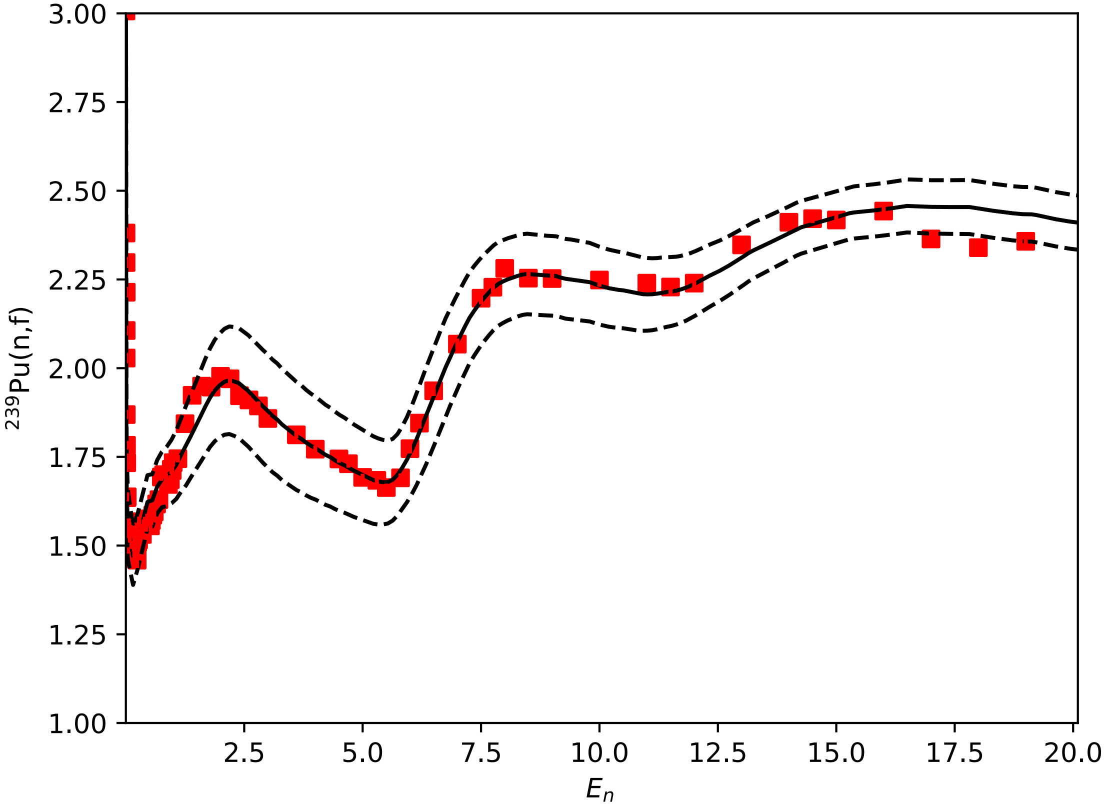
Gaussian with mean 0 and σ=1

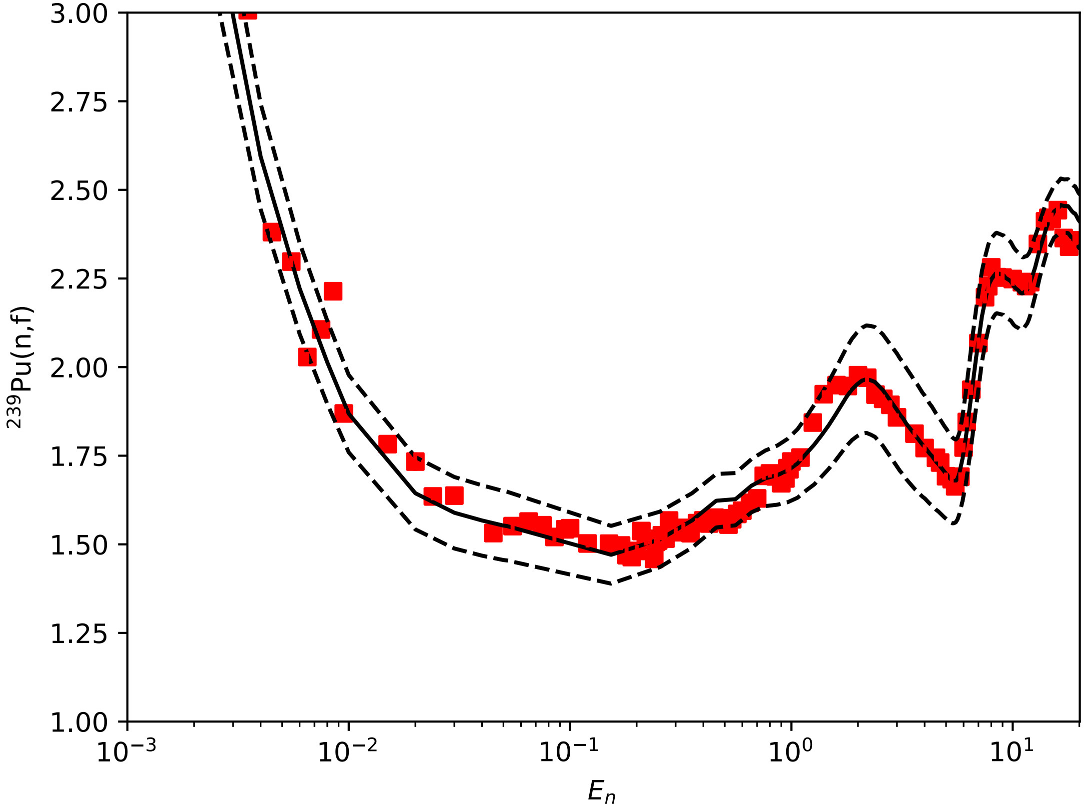
Which way to choose? BFMC seems to be performing better in toy problem.

- Fit line to data with random normal error.
- Both ways are responsive when it comes to introducing new data.
- Unscented Kalman filter could be next?

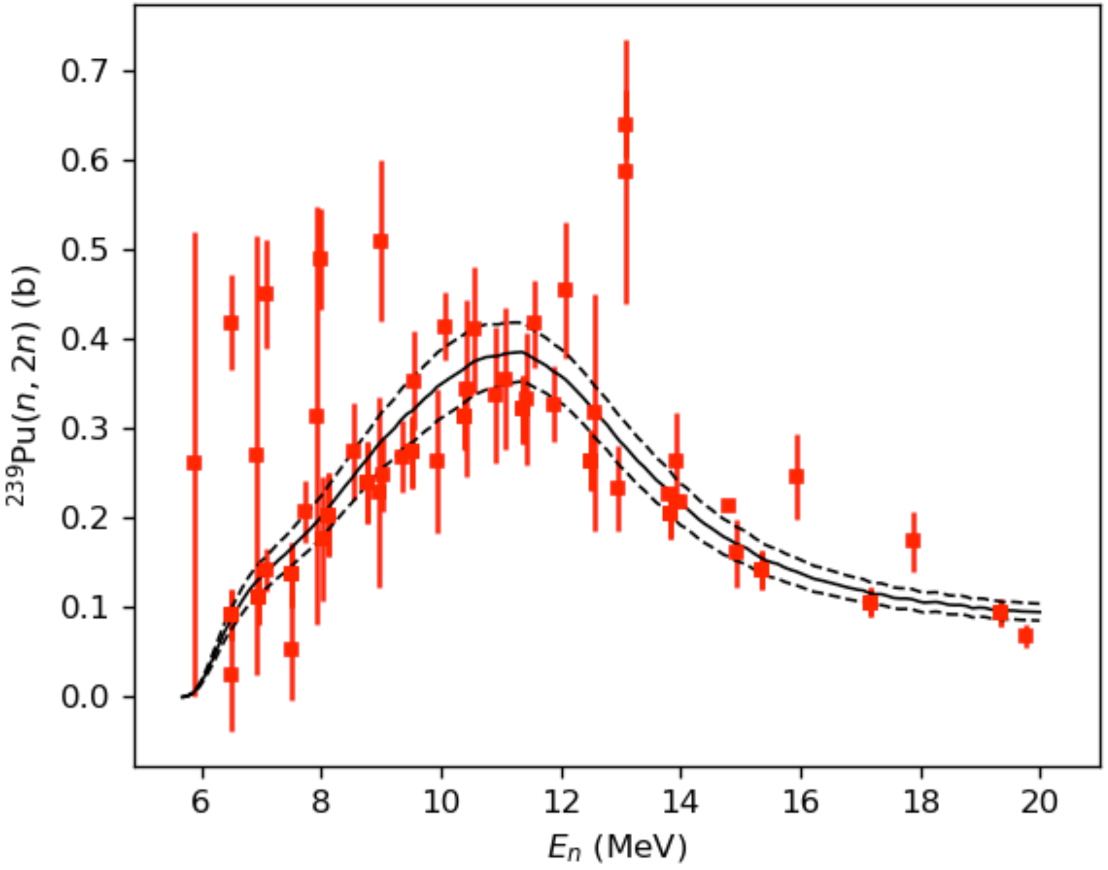


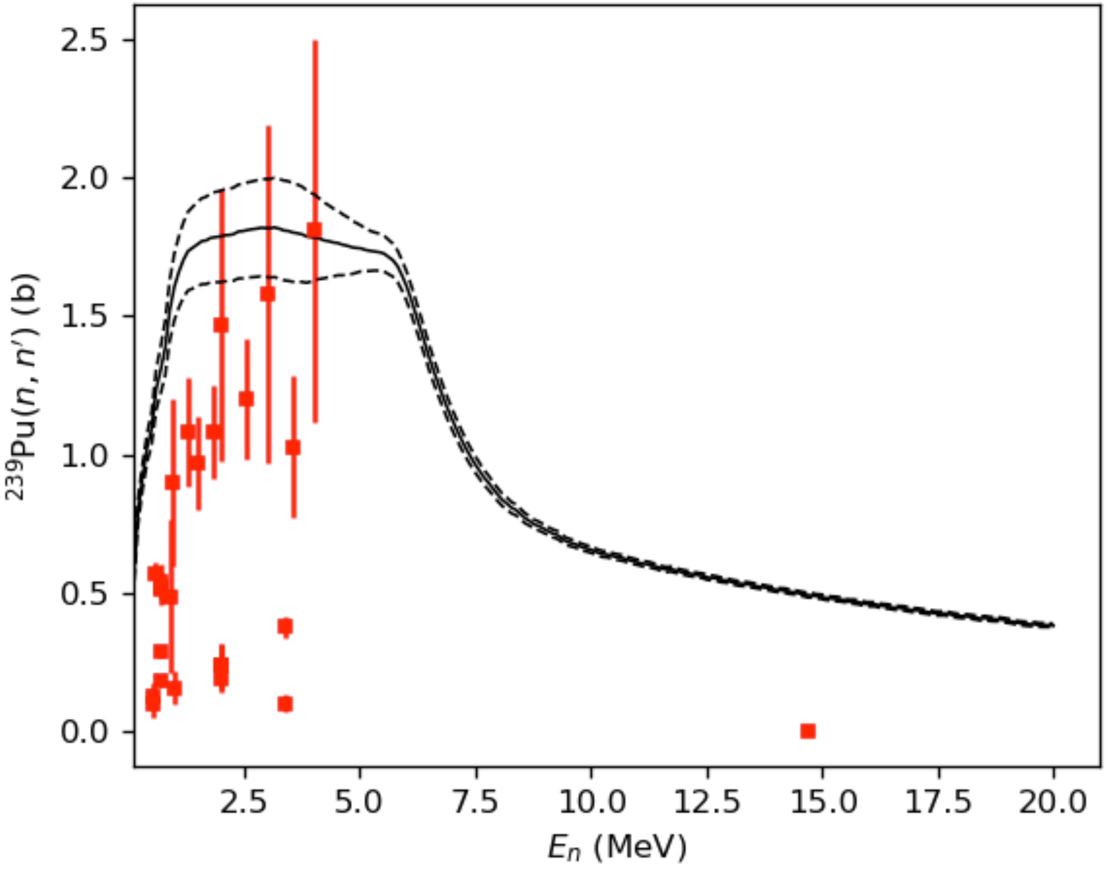
BFMC applied to the YAHFC n+P9 evaluation.



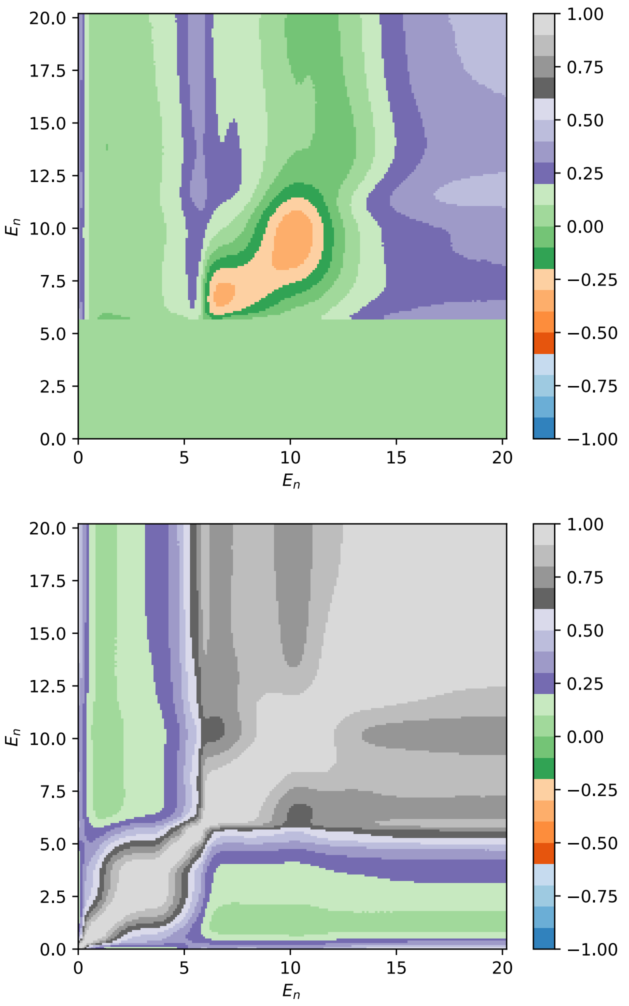


Other channels looking decent, uncertainty seems to be driven by fission barrier parameters.

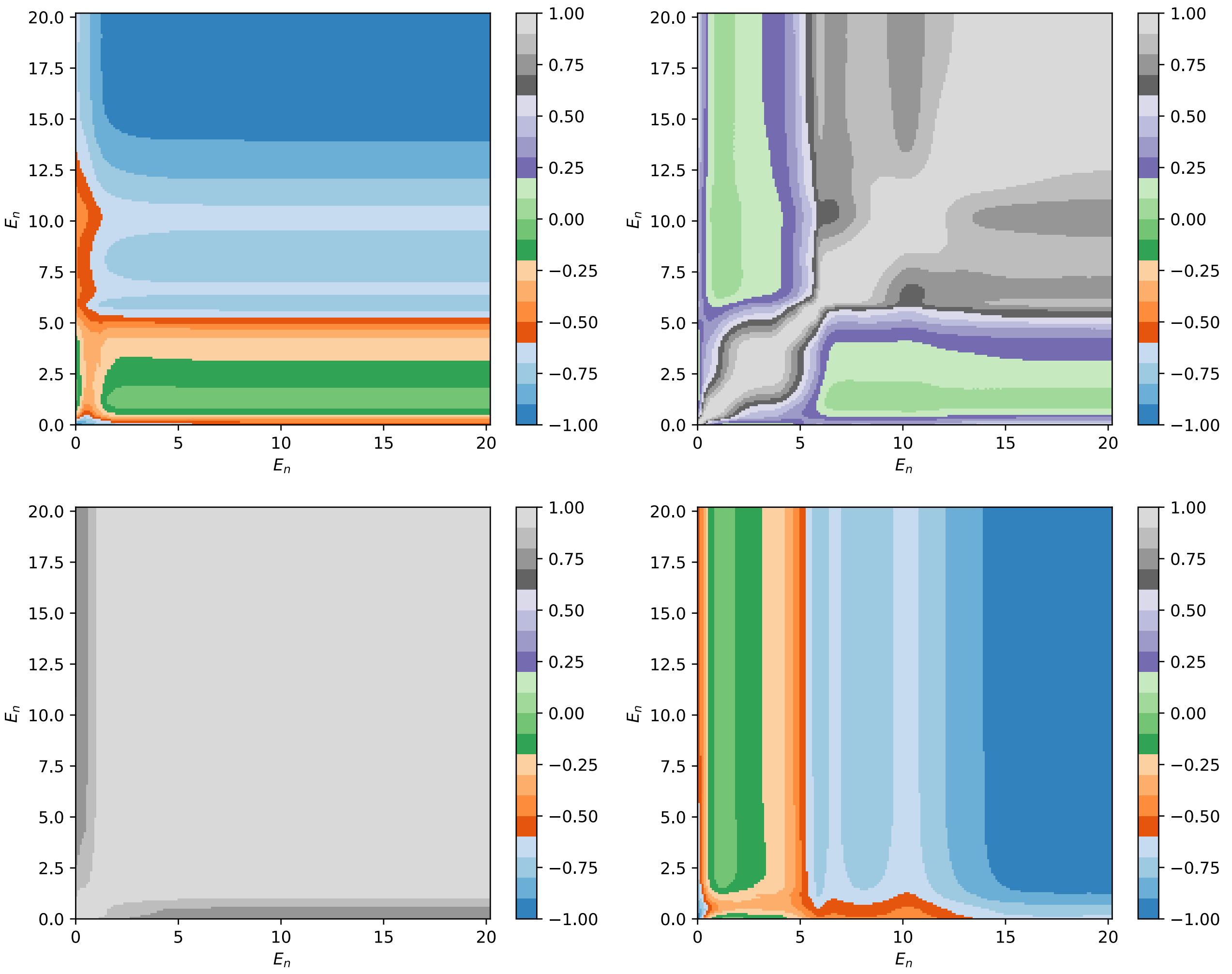




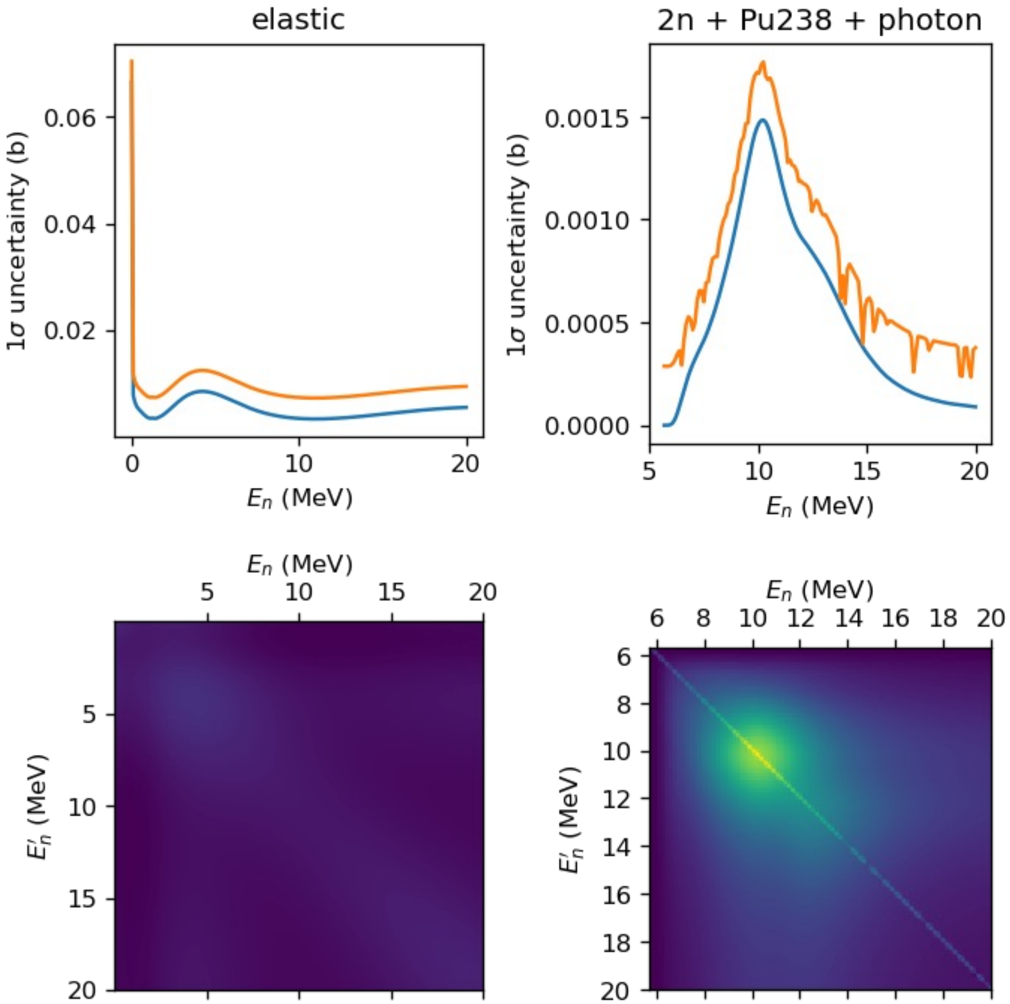
(n,f) vs (n,2n)



(n,el) vs (n,f)



Initial use of Gaussian Processes to soften model stiffness



- Model based (i.e. HF based) covariances can be stiff (small) due to stiffness and a lack of expressivity in the model.

- We want to extend the HF model to a super model
$$\sigma_\alpha(E) = \sigma_\alpha^{\mathrm{HF}}(E) + \delta\sigma_\alpha^{\mathrm{GPR}}(E)$$

- $\sigma_\alpha^{\mathrm{HF}}(E)$ is defined by mean and covariance of the HF model
$$\sigma_\alpha^{\mathrm{HF}}(E) \sim N\left(\mu_\alpha^{\mathrm{HF}}, \Sigma_{\alpha\beta}^{\mathrm{HF}}\right)$$

- $\delta\sigma_\alpha^{\mathrm{GPR}}(E)$ is from a Gaussian process, with mean zero and a data + model informed covariance
$$\delta\sigma_\alpha^{\mathrm{GPR}}(E) \sim GPR(0, \mathrm{K}_{\alpha\beta}(E, E'))$$

- We use a multi channel form for the kernel
$$K_{\alpha\beta}(E, E') = \left(w_\alpha w_\beta + \delta_{\alpha,\beta}\kappa_\alpha^2\right) e^{-\frac{(E-E')^2}{2 l_\alpha l_\beta}}$$

Conclusions & future work

- Quick evaluation of covariances relies on parallel Monte Carlo approach.
- Incorporating new experimental data is relatively painless in the BFMC approach.
- GPs allow for the evaluation of improved means and covariances by absorbing some of the model uncertainty.
- Estimation of sensitivity will lead to reduced number of dimensions for more efficient MCMC sampling.
- Improved covariances from MCMC will be topped with the same GP approach as described here.
- No optical model (σ_{tot}) UQ yet…