Uncertainty quantification of the optical model for fission fragment de-excitation

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Kyle Beyer[1] , Cole Pruitt[2], Brian Kiedrowski[1]

Department of Nuclear Engineering and Radiological Sciences, University of Michigan[1]

Lawrence Livermore National Laboratory[2]

Mission Relevance

Fission produces key observables for special nuclear material detection and quantification:

- Average neutron multiplicity $\bar{\nu}$

- neutron multiplicity distributions, $P(\nu)$, and factorial moments $E\left[\frac{\nu!}{(\nu-m)!}\right]$,

- neutron energy spectra; $\chi(E)$,

- correlations: neutron-photon multiplicity, energy, angle, …

… but it is complex and hard to model

Motivation: simulate event-by-event fission with uncertainty

- Tabulated evaluated data (ENDF, JENDL, JEFF, …):

    + uncertainty

    - no event-by-event correlations

- Model-based event generators (CGMF, Freya, …):

    - **no/limited uncertainty**

    - **computationally expensive**

    + event-by-event correlations

Goal: add uncertainty estimates to physics-based fission models

Physics based fission models use the optical model

Monte Carlo Hauser Fesbach fragment de-excitation:

- Start with post-scission fragment in some channel (J, π, E)
- Until stable, sample decay from current channel $a \to \{b, c, d, \dots\}$:

$$P(a \to b) \approx \frac{T_a \, T_b \, \rho(b)}{\sum_i |T_i|^2 \rho(i)}$$

Approximate transmission coefficients T_a using **the Optical Model**

The optical model is our best option, but it isn't perfect

- Optical model parameterizes mean-field nuclei-nucleon potential:
  - Microscopic: chiral effective field theory, …
  - Phenomenological: scattering experiments; local (single A,Z) or global
- Common choice: Koning-Delaroche global optical model
  - 5 terms
  - 36 parameters; fit to global neutron elastic scattering data

Fission fragments: too unstable for local phenomenological; too heavy for microscopic. How well do global models extrapolate?

Technical Approach to uncertainty quantification

Dr. Cole Pruitt:
Markov-chain Monte Carlo to determine distribution of Koning-Delaroche optical model parameters conditional on scattering data
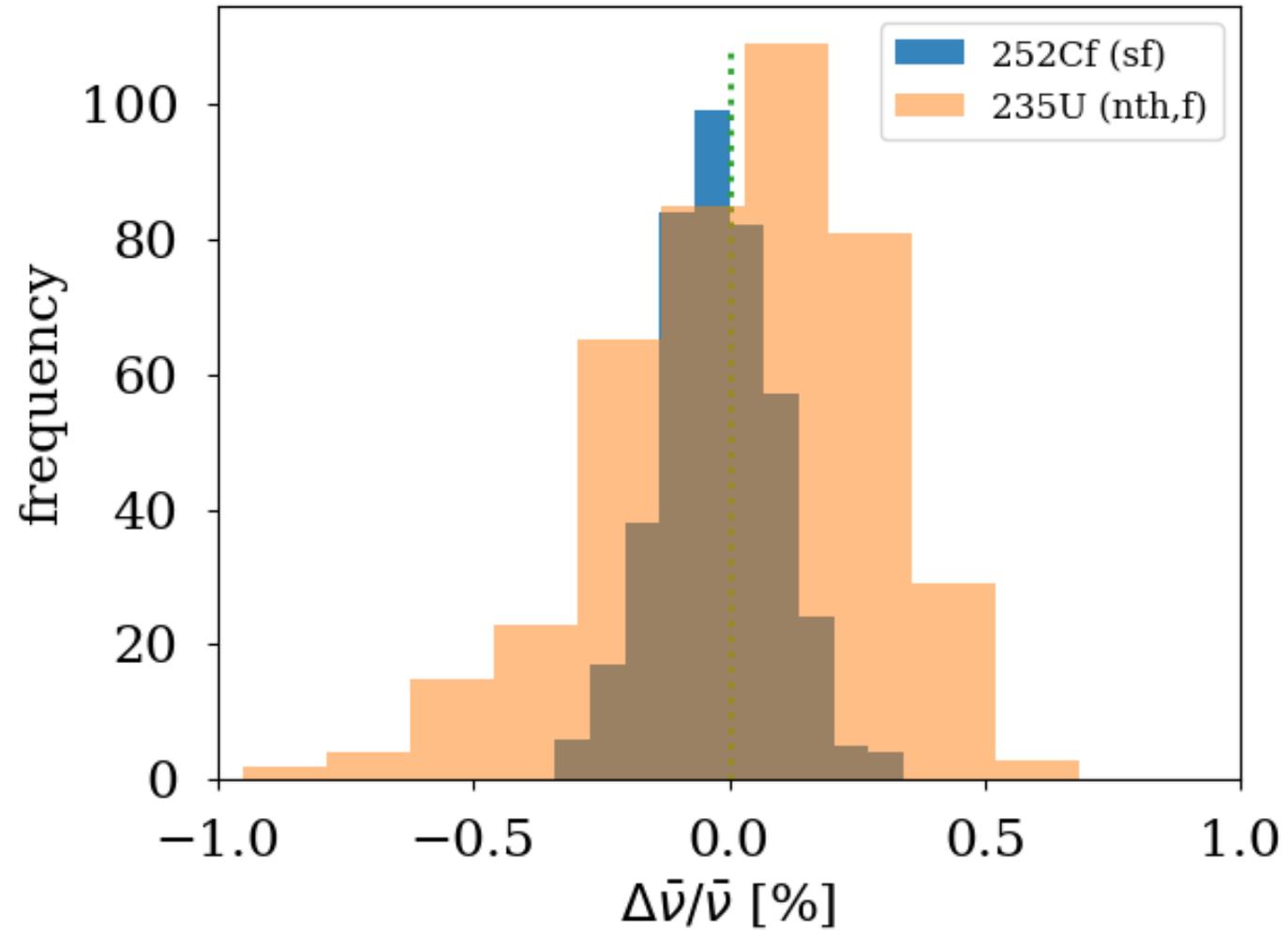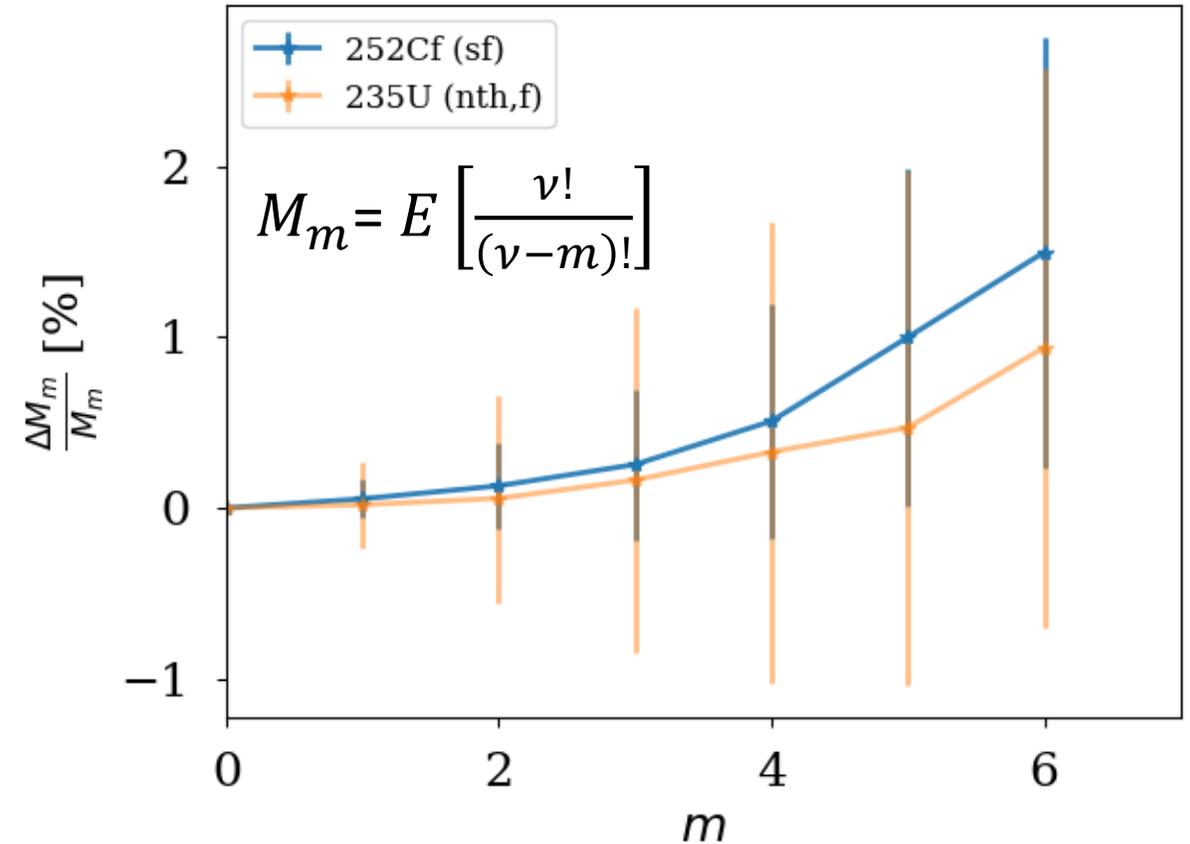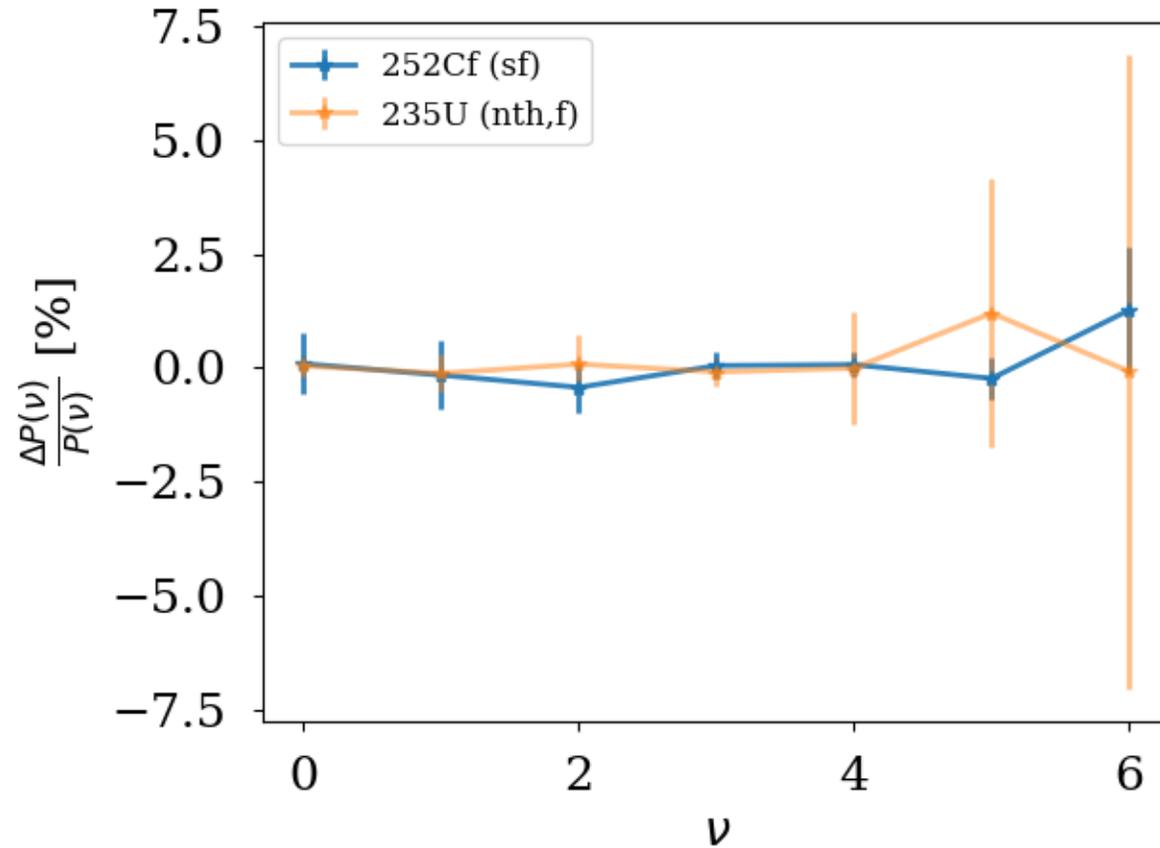
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This work:
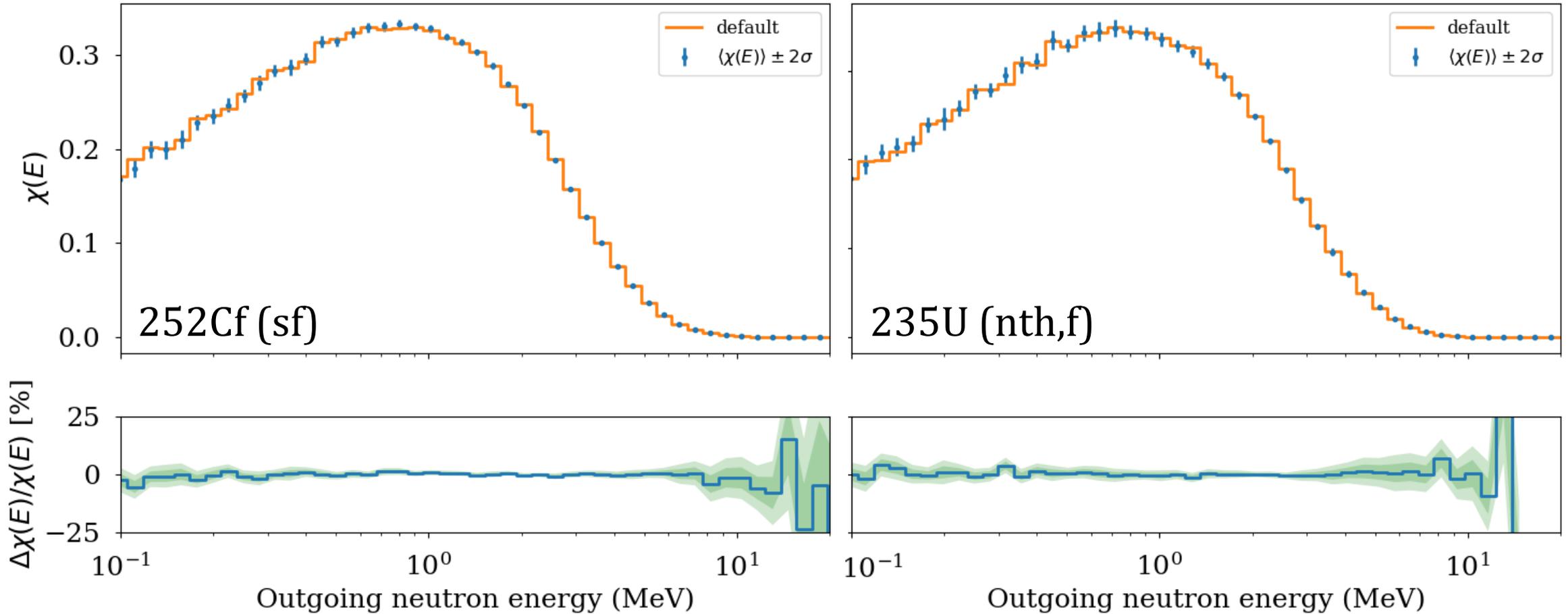Sample from optical model parameter distributions to calculate ensemble of fission observables in CGMF

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Uncertainty in $\bar{\nu}$: greater for 235U (nth,f)

Neutron multiplicity distributions and factorial moments
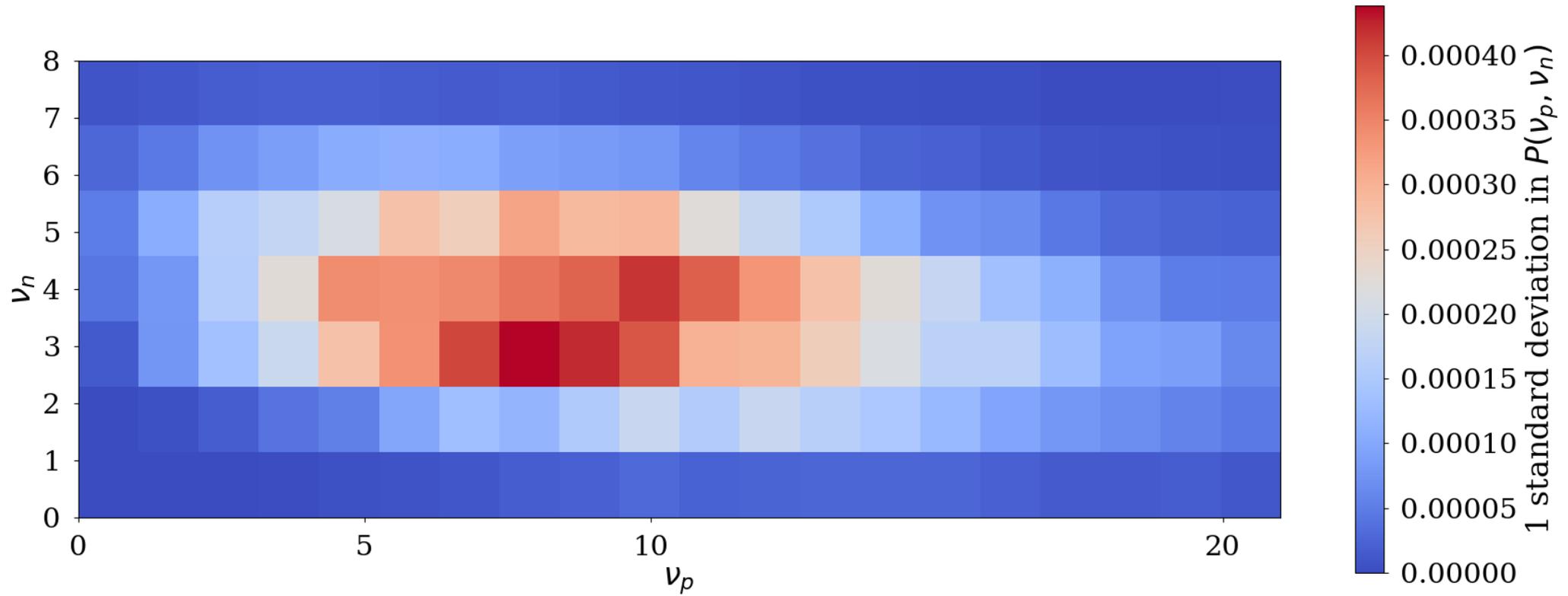

$$M_m = E\left[\frac{\nu!}{(\nu-m)!}\right]$$

Uncertainty in $\chi(E) \approx 5\%$ at low energy, 25% high energy

252Cf correlated n,p multiplicity
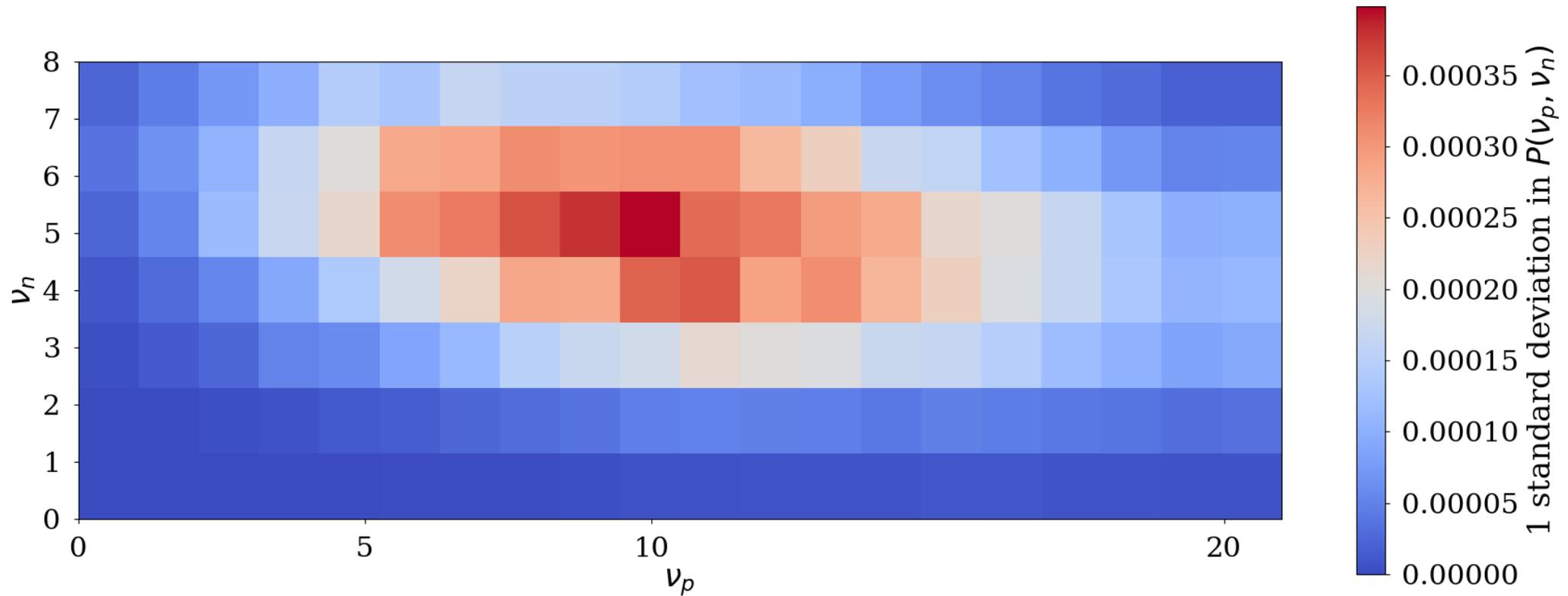
U235 correlated n,p multiplicity

Expected Impact

- **A step towards uncertainty in event-by-event fission models**
- Explore open questions in fission/fission modeling:
  - CGMF $\chi(E)$ high-energy tail smaller than experiment
  - How do fragments remove angular momentum?

MTV Impact

- Ongoing collaboration with Dr. Cole Pruitt at LLNL
  - Dr. Meghan McGarry connected Dr. Pruitt and I following discussion @UPR21
- Collaboration on global UQ/parameter optimization wrt fission observables with Dr. Amy Lovell at LANL

Conclusions

- Calculated covariances in fission observables due to model parameter uncertainty in the Koning-Delaroche global optical model
- Software developed is open source:
  - Optical model neutron-nuclei scattering code: github.com\beykyle\opxs
  - Modified version of CGMF for this work: github.com\beykyle\CGMF
  - UQ workflow: github.com\beykyle\omp-uq

Future work

- Explore model form uncertainty with other optical models, including microscopic (**add microscopic info -> improve extrapolation to fragments?**)
- Look at fragment specific observables, angular momentum, correlations

References

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