Reconstructing SCRaP Benchmark Experiment Multiplicity Distributions From MCNP Generated Moments

MTV Workshop, 2022

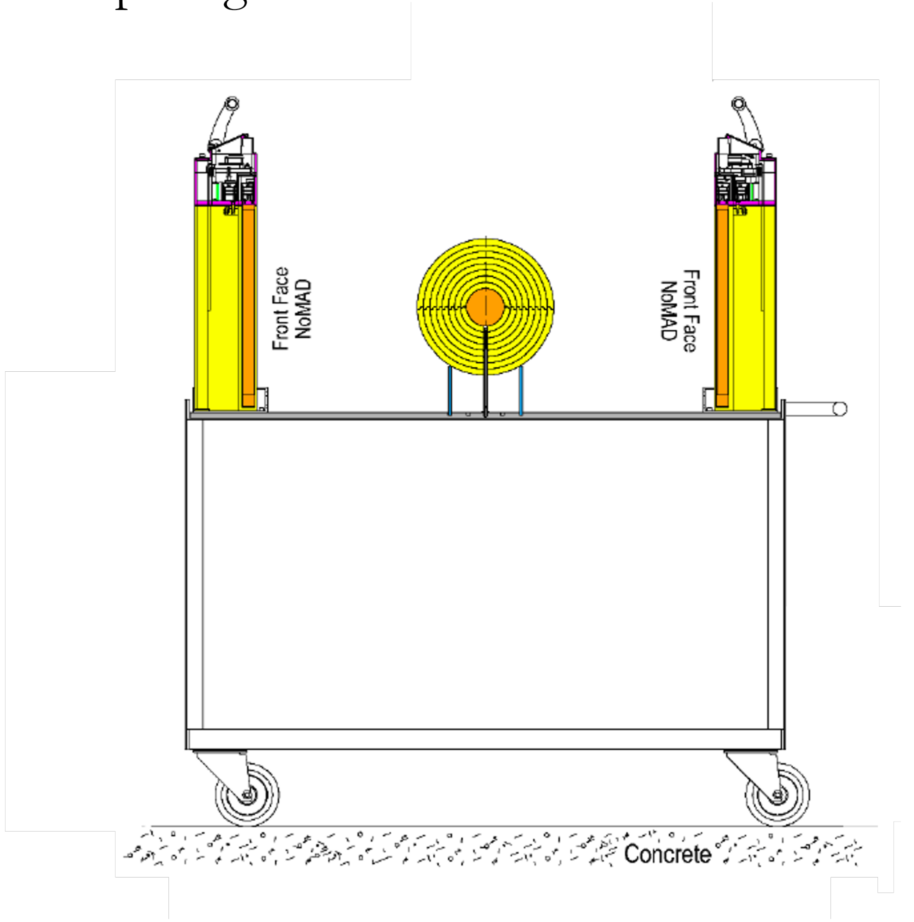
March 22nd, 2022

Jawad R. Moussa, Anil K. Prinja

Department of Nuclear Engineering
University of New Mexico

Introduction and Motivation

- Neutron multiplicity distributions are unique identifiers of SNM but computing these distributions can be expensive
- Low order statistical information is generally easier to obtain but has limited content
- Developed accurate and inexpensive methods for reconstructing multiplicity distributions from low order statistical information
    - orthogonal polynomial representation
    - maximum information entropy
- Reconstruction methods are agnostic to source of low-order information: point-kinetic, deterministic transport, Monte Carlo computation, or experiment
- Demonstrate with MCNP simulation of LANL SCRaP benchmark experiment



Modeling Approaches

- Hierarchy of modeling and simulation approaches provides comprehensive predictive capability and complements experimental measurements

Monte Carlo (ex. MCNP)
- Slow; Statistics
- General Geometry
- Continuous Energy
- Full Physics

Deterministic (ex. PARTISN)
- Faster
- Multi-group Data
- Space, Angle, Energy Discretization
- Limited Geometry

Point Kinetic Models
- Fastest
- Parameters Systematically Computed from MC and Deterministic Codes
- Geometry Sacrificed

Reconstructing the Count PDF

$\boldsymbol{P_n(D|s)}$ **:** The probability that n counts are registered in $D\colon \{t_{min}, t_{max}\}$ given that a spontaneous fission source is turned on at an earlier time s

- Factorial Moments: $M_k(D|s) = \overline{n(n-1)\ldots(n-k+1)}$

$$M_1(D|s) = \sum_{n=0}^{\infty} nP_n(D|s) = \overline{n}(D|s) \qquad (mean)$$

$$M_2(D|s) = \sum_{n=0}^{\infty} n(n-1)P_n(D|s) = \overline{n^2} - \overline{n} \qquad (gives\ variance)$$

- Two approaches were used to reconstruct the neutron count distribution for a fixed time gate
  - Maximum Entropy Method
  - Orthogonal Polynomial Method

Maximum Entropy Method

- Reconstructing probability distribution by maximizing the information (Shannon) entropy

$$Entropy: \quad S[P_n] = -\sum_{n=0}^{\infty} P_n \, lnP_n$$

- Neutron count pdf is approximated by maximizing the entropy subject to constraints
  - The first K exact normalized central moments
  - The first $n^{\star}$ exact discrete counts

$$\boldsymbol{\widetilde{P}_n(D|s) = \begin{cases} P_n; & 0 \leq n \leq n^{\star} \\ exp\left(-1 + \sum_{k=1}^{K} -\lambda_k \left(\frac{n}{\bar{n}} - 1\right)^k\right); & n > n^{\star} \end{cases}}$$

Orthogonal Polynomial Expansion

- Gamma distribution approximates neutron number distribution well with knowledge of just the mean and variance:

$$P^{(G)}(n;D|s) = \left[\frac{\eta}{\bar{n}}\right]^{\eta} \frac{n^{\eta-1}}{\Gamma(\eta)} \exp\left(-\frac{n\eta}{\bar{n}}\right); \qquad \eta = \frac{\bar{n}^2}{\sigma^2}$$

- Accuracy can be improved by preserving higher order moments through a truncated expansion in generalized Laguerre polynomials $L_r^k(x)$

$$\boxed{\boldsymbol{\tilde{P}_n(D|s) = P^{(G)}(n;D|s)\left\{1 + \sum_{k=3}^{K} a_k L_k^{\eta-1}\left(\frac{\eta n}{\bar{n}}\right)\right\}}}$$

- The expansion coefficients a_k are obtained by enforcing preservation of the true moments up to order K

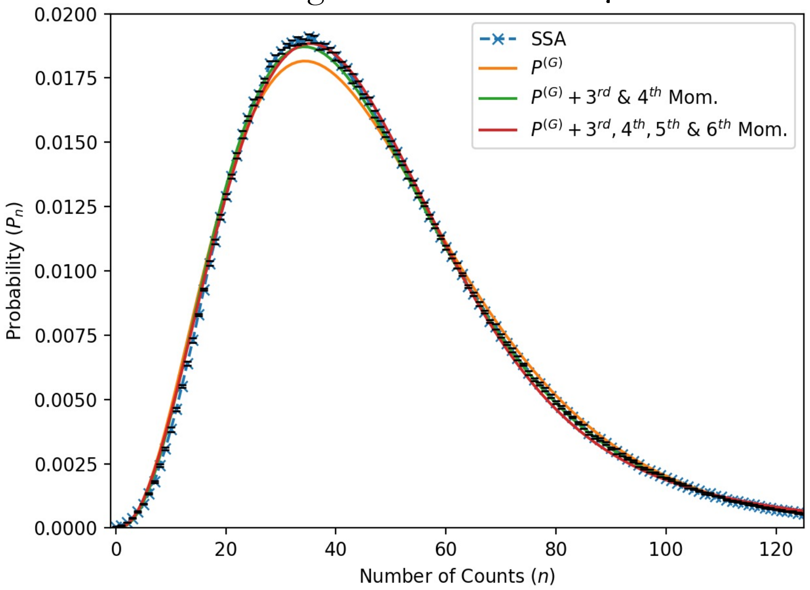
Point Kinetic Model Results

- Backward Master equation formulation yields explicit equations for count probabilities and factorial moments*

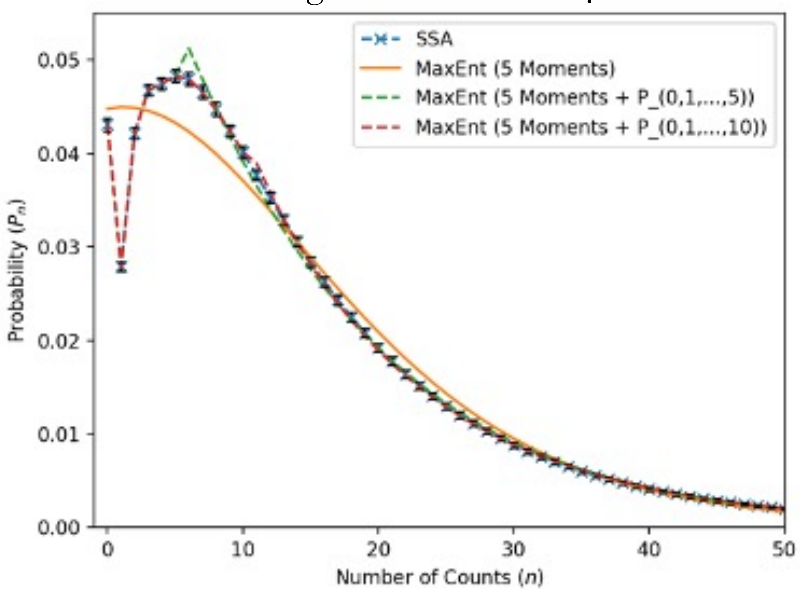
- Results are shown for an *80 wt%* ^{239}Pu *20 wt%* ^{240}Pu sample and are benchmarked against a Stochastic Simulation Algorithm (SSA)

- Point kinetic data was obtained from standard adjoint weighted 1D spherical geometry transport calculations

2680g – Time Gate = 19 μs



2680g – Time Gate = 6 μs



* Journal paper submitted to NIMA

Error Metrics

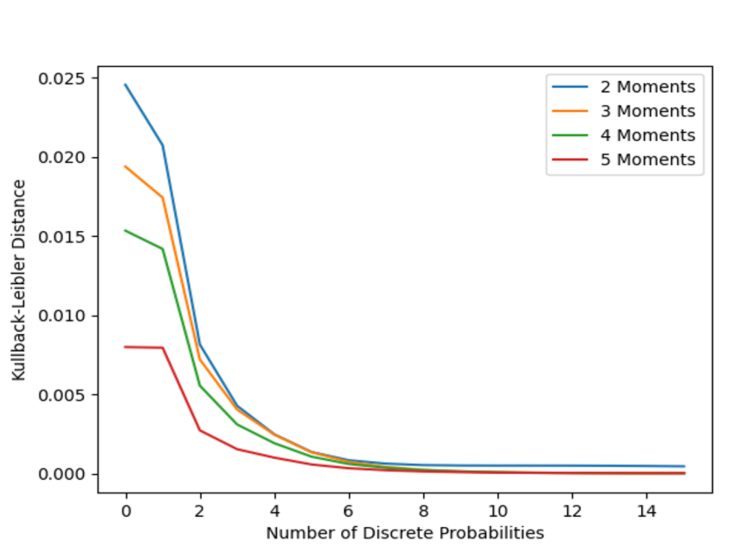
- Difference measures between two probability distributions are provided by:

  - The KL divergence (relative entropy)

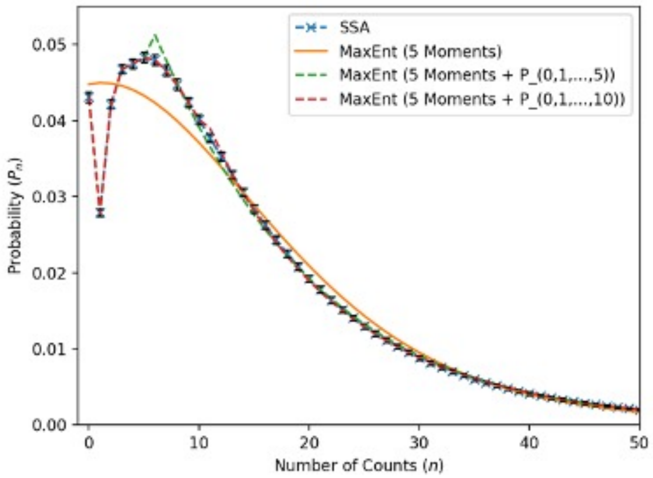
$$D_{KL}(P\,||\,Q) = \sum_{n=0}^{\infty} P_n \ln\left(\frac{P_n}{Q_n}\right)$$

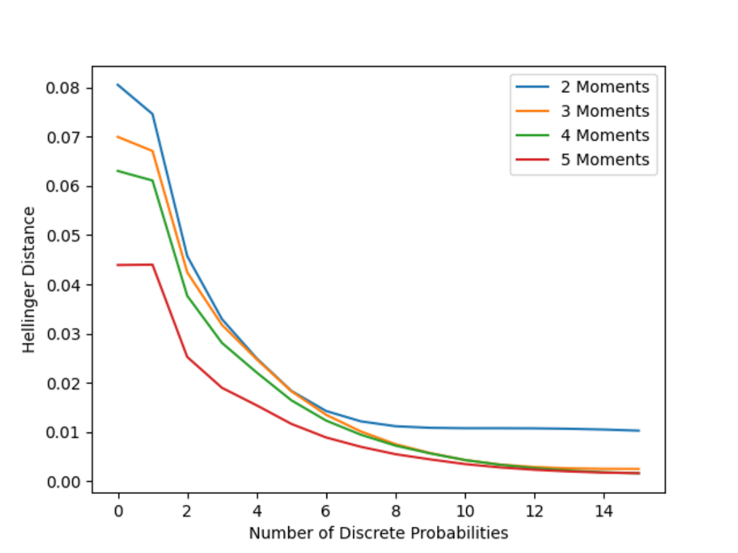
  - The Hellinger Distance

$$H(P\,||\,Q) = \sqrt{\frac{1}{2}\sum_{n=0}^{\infty}\left(\sqrt{P_n} - \sqrt{Q_n}\right)^2}$$



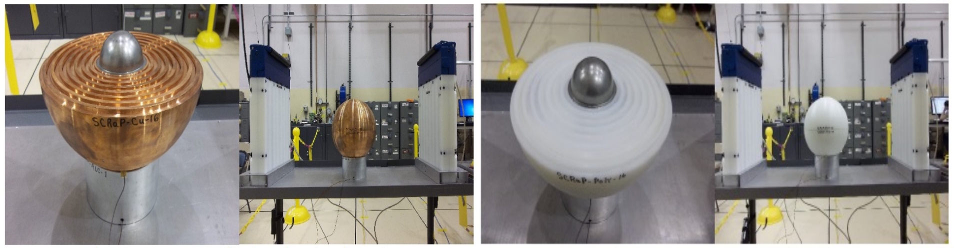
2680g – Time Gate = 6 μs

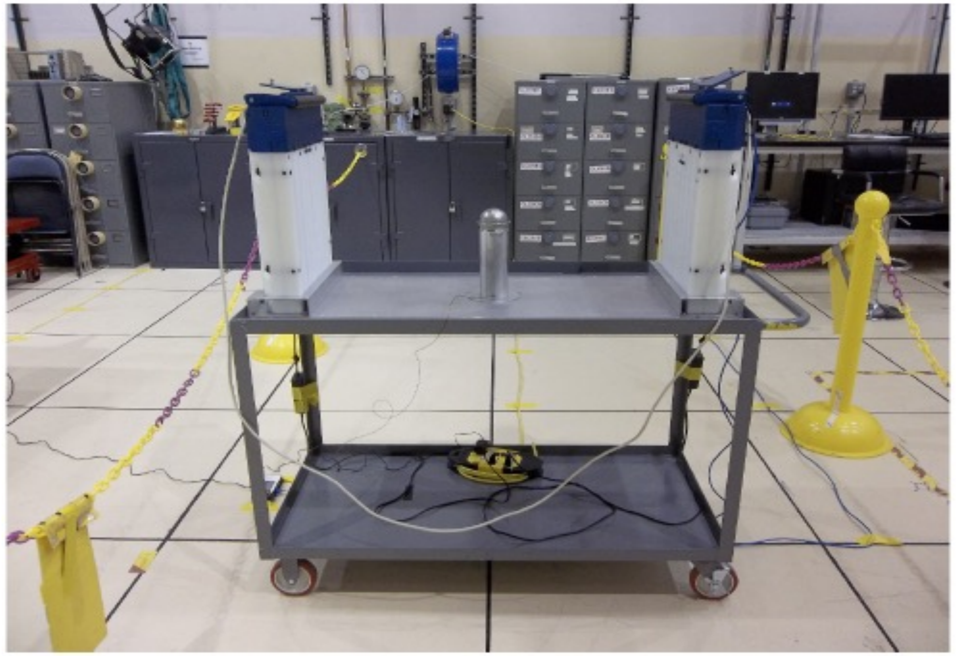




SCRaP Benchmark Experiment

- Three configurations simulated in MCNP to produce list mode data
  - bare metal sphere,
  - metal sphere reflected by a 4-inch Polyethylene layer; and
  - metal sphere reflected by a 4-inch Copper layer.
- Post processing makes it possible to analyze MCNP data as experimental data
  - MCNP output → LMX file
- Gate-dependent multiplicity moments and count probabilities extracted from Feynman histograms (*unnormalized* time-gated multiplicity distributions)
- Multiplicity distributions reconstructed and compared against distributions from Feynman histograms

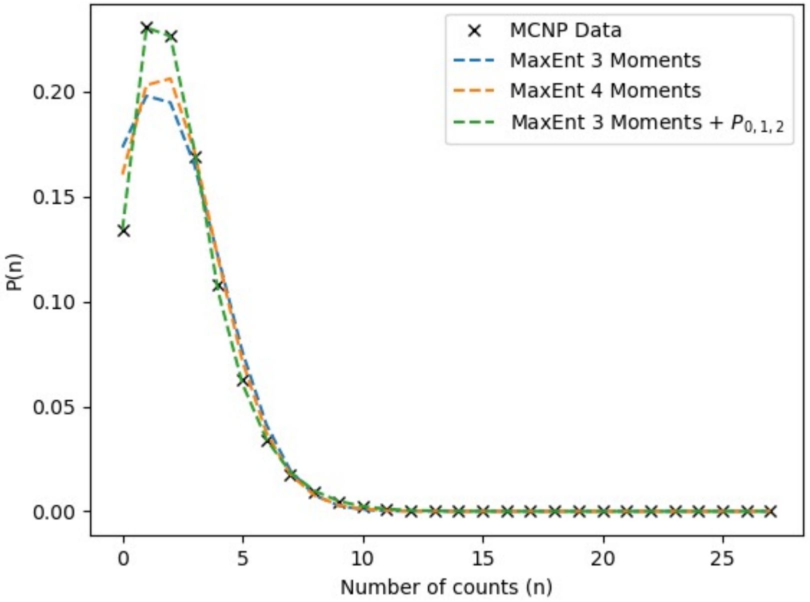




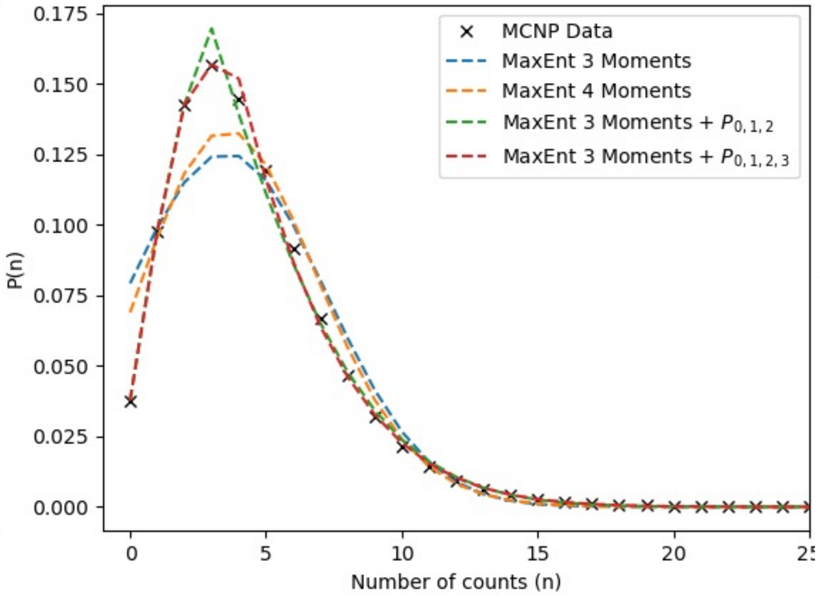
Maximum Entropy Reconstruction

128μs

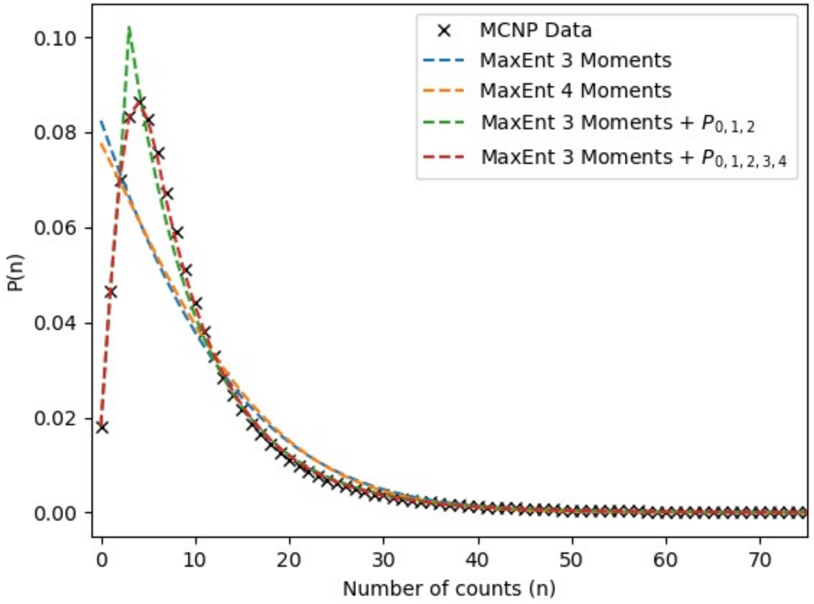
Bare Pu



4in Poly



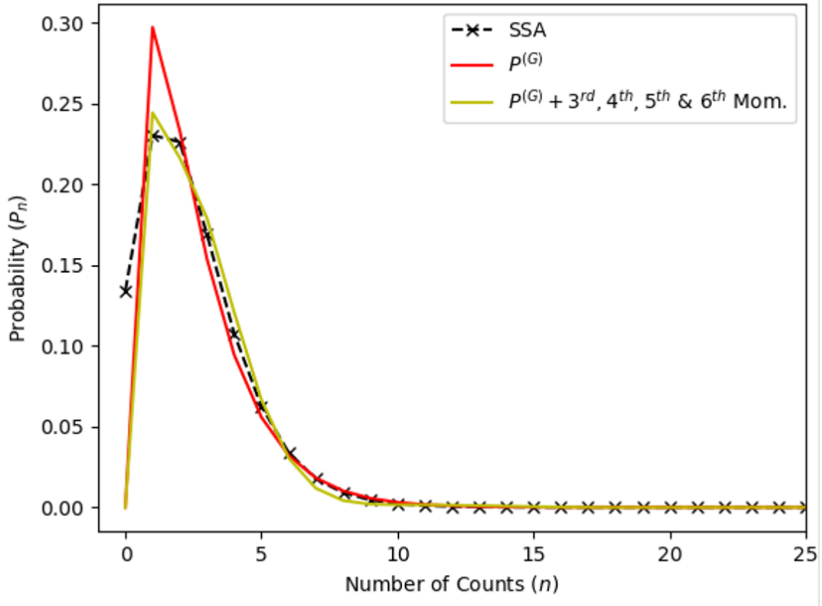
4in Cu



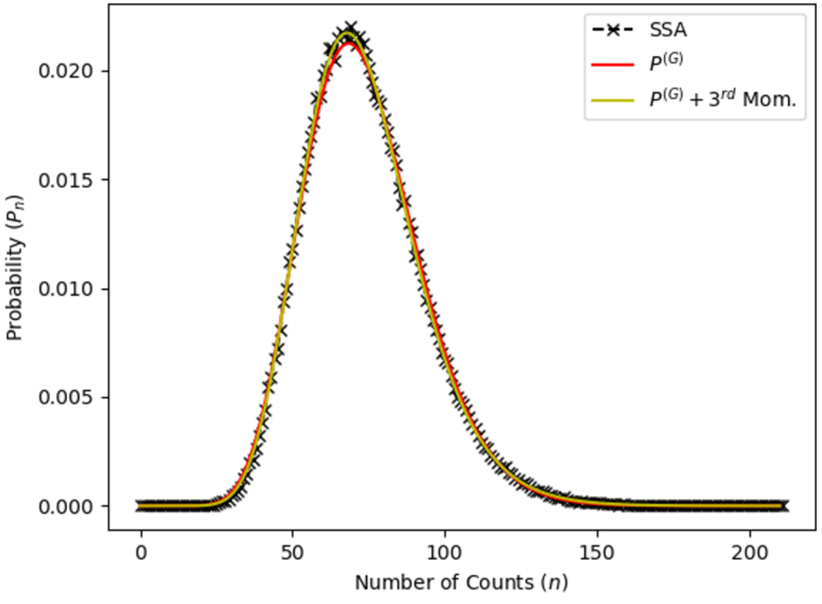
Jmoussa@unm.edu

Orthogonal Polynomial Reconstruction

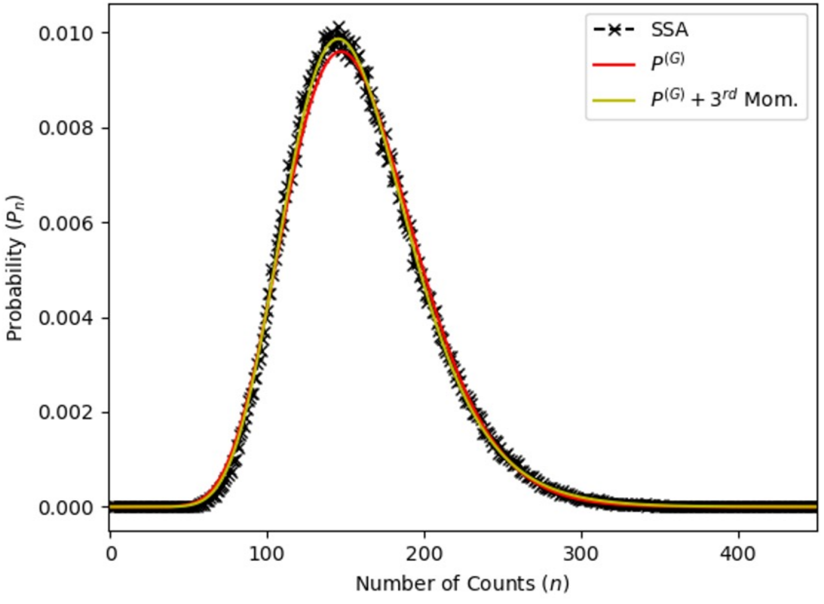
Bare Pu (128 μs)



4in Poly (2048μs)



4in Cu (2048μs)



Conclusions & Future Work

- Multiplicity distributions can be, accurately and efficiently, reconstructed from low-order factorial moments and low-order count probabilities
- Demonstrated that reconstruction methods can work with higher fidelity simulation models
- Monte Carlo calculations are computationally expensive and require extensive postprocessing
- Working with LANL (CCS-2) to add multiplicity distribution capability in deterministic transport code PARTISN
  - Moments and probabilities of neutron counts in external detectors
- Compare Monte Carlo vs. Deterministic vs. Point Model

Jmoussa@unm.edu

Acknowledgements

The Consortium for Monitoring, Technology, and Verification would like to thank the NNSA and DOE for the continued support of these research activities.

This work was funded by the Consortium for Monitoring, Technology, and Verification under Department of Energy National Nuclear Security Administration award number DE-NA0003920