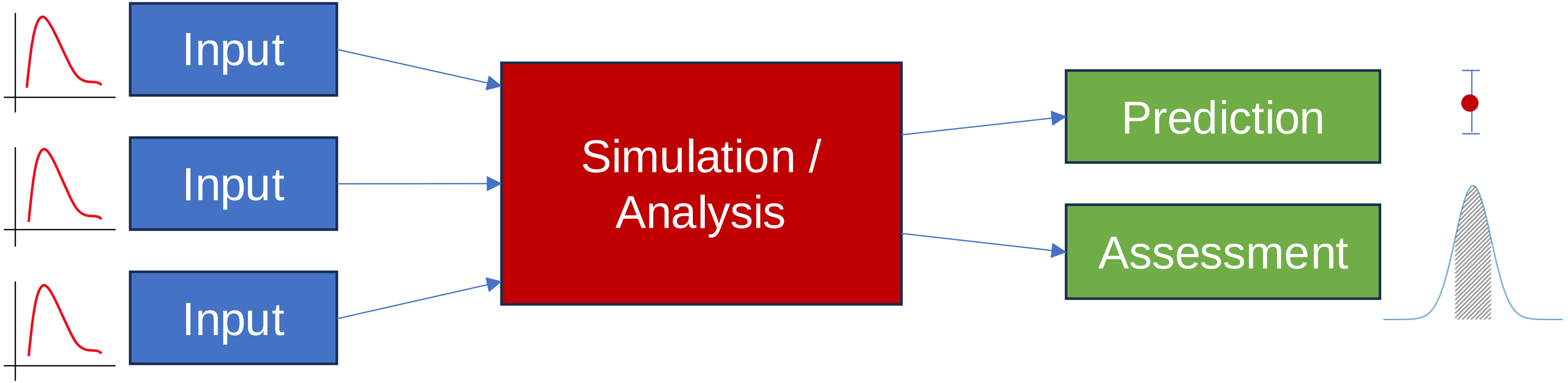
Los Alamos NATIONAL LABORATORY

Propagation of Uncertainties from Nuclear Data

Nathan A. Gibson, XCP-5

Tuesday, December 17, 2024

Uncertainties in Applications



Nuclear Data Applications

Energy
Reactor design
Reactor operation
Reactor safety

Materials Handling
Criticality safety
Waste storage

National Security
Stockpile stewardship
Safeguards
Nuclear forensics

Types of Uncertainty Quantification

Forward propagation

- Estimating uncertainty on a predicted output
- Requires knowledge of all sources of uncertainties
- Used for design and certification

Scenario:
Can we demonstrate the safety of introducing a new material into a plutonium manufacturing process? What controls need to be put in place?

Sensitivity Analysis

- Estimating impact of particular input uncertainty on an output
- Only requires individual source of uncertainty
- Used to motivate improvements in data or modeling

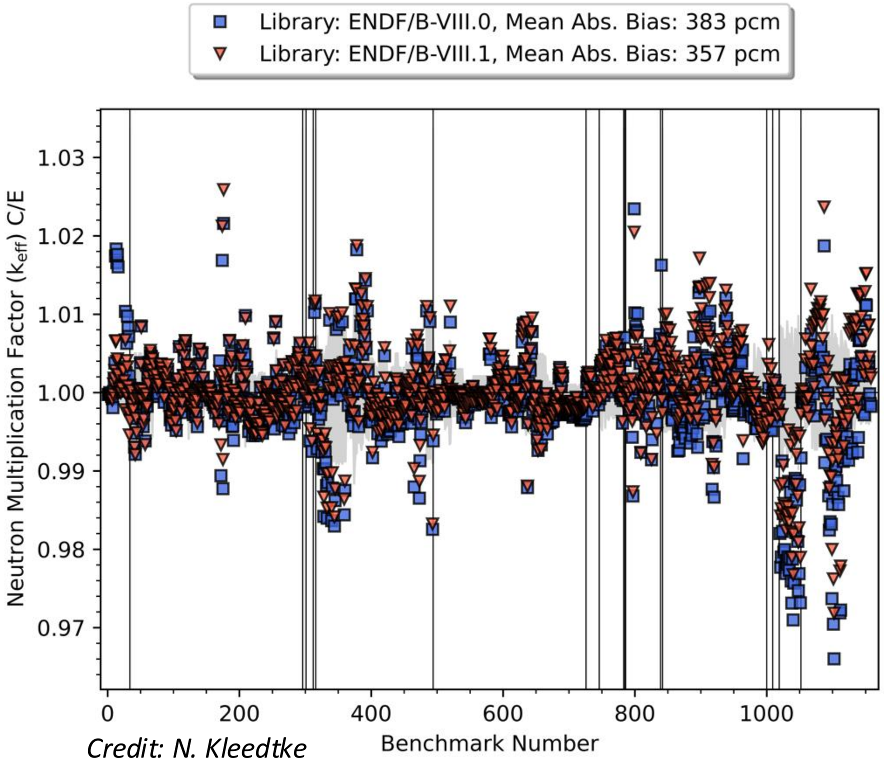
Scenario:
Does the expected uncertainty reduction from a new cross section measurement justify its cost to a programmatic sponsor?

Nuclear Data Evaluation

Typical workflow (especially for LANL fast region work)

- Prior taken from theory models
- Differential experimental database curated
- Kalman filter used to update parameters based on differential data observations
- Model stiffness may require cross section updates
- Resulting uncertainties may need to be scaled if unrealistic
- Validation performed by calculations of critical assemblies

Validation or Adjustment?



Credit: N. Kleedtke

Observations

1. ENDF library performs very well on integral benchmarks, much better than reported uncertainties would suggest
2. Evaluators openly adjust nu-bar to match Jezebel and Godiva
3. Evaluators generally aware of decisions that improve or hurt integral performance

Corollaries

1. ENDF includes information from integral data without formal adjustment procedure
2. Uncertainty information reported does not represent our complete knowledge

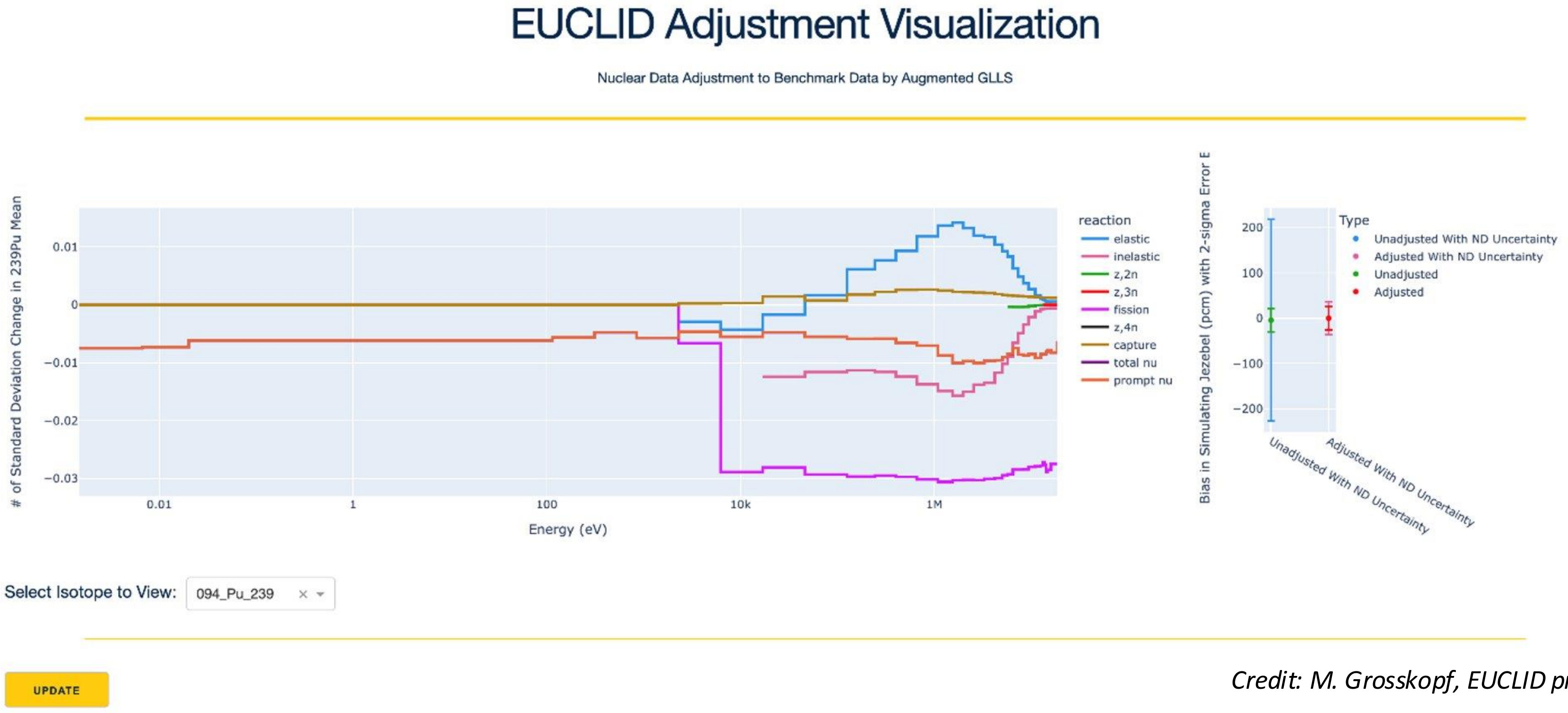
Los Alamos NATIONAL LABORATORY

Nuclear Data Adjustment

For real-world UQ needs, ENDF covariance data not including all our knowledge is a problem. Fixing this is an open area of research.

- Methods like Generalized Least Squares are most common
- Sampling-based approaches also used
- Ignore fact that integral data may have influenced mean values previously, rely on covariances not previously including integral data
- Evaluator (adjustor?) needs to make similar decisions as with differential data
  - How to handle discrepant datasets?
  - Which datasets are most relevant? Most trusted?
  - Do adjustments make sense?
- Still a controversial topic in the nuclear data community

Adjustment Example



Credit: M. Grosskopf, EUCLID project

Sensitivity-Based Methods

Calculating Sensitivities

$$S_{R;\alpha_i} = \frac{\partial R}{\partial \alpha_i}$$

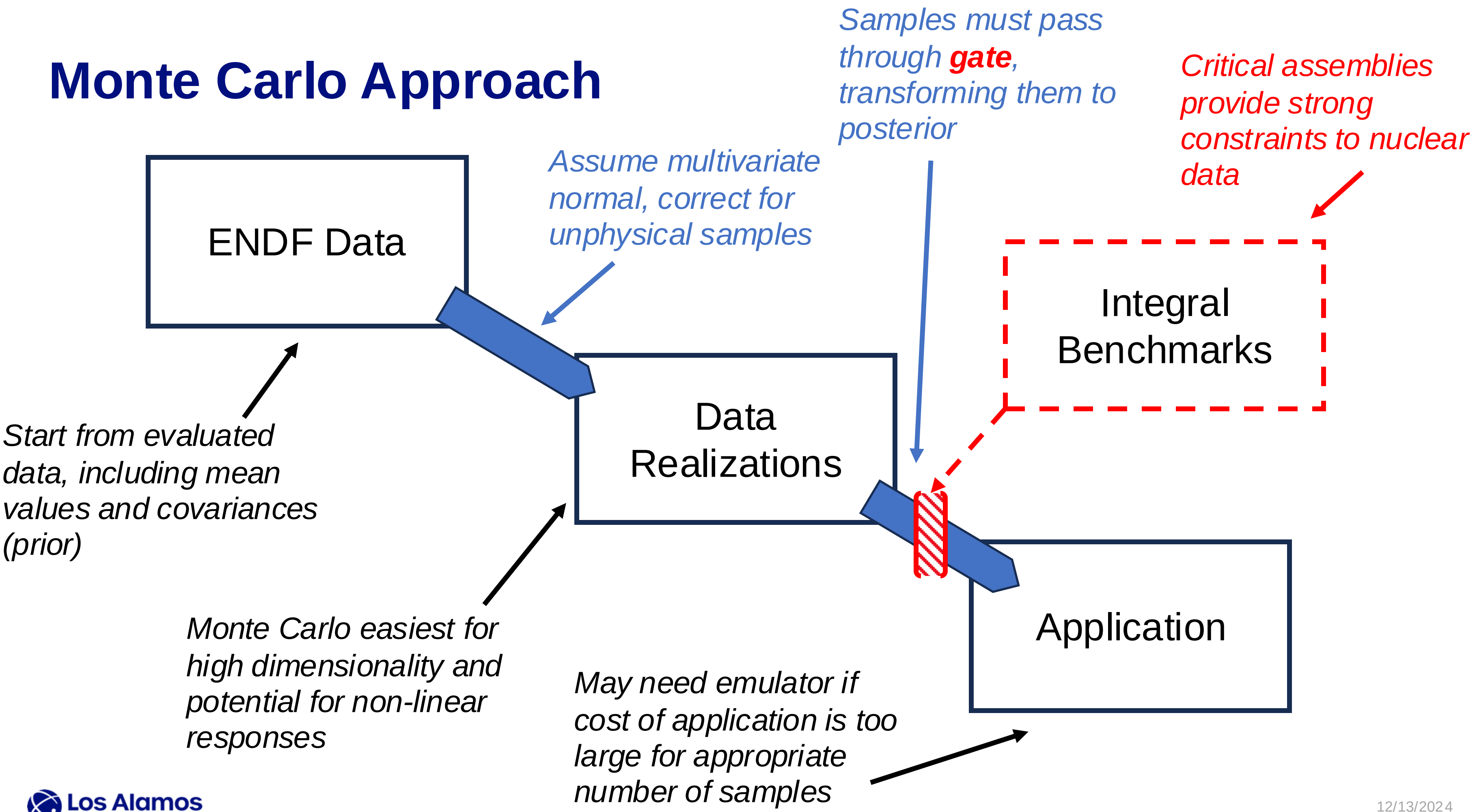
- Finite differences
  - Lots of simulation runs
- Adjoint-based methods
  - e.g. KSEN in MCNP

Sandwich Rule

$$\Delta R = S_{R;\alpha} C_{\alpha\alpha} S_{R;\alpha}^T$$

- If sensitivities are available, very simple
- Assumes linear responses
- Requires any adjustments to be reflected in covariance matrix

Monte Carlo Approach



Los Alamos NATIONAL LABORATORY

Practical Considerations

In no particular order…

- Computing sensitivities for large numbers of problems (e.g., ICSBEP benchmark suite) is very difficult, requires storage and re-use
- Sensitivities are a function of the mean values used
- Adjusted data contains correlations across channels and isotopes that is difficult to represent in ENDF and make usable
- Much of UQ is still exploratory and customers haven’t fully embraced it
- Changing the way an established field operates requires careful planning, communication, and patience

Conclusions

- Propagating a given uncertainty to an application is typically interesting to the data owner
- Solving real-world UQ problems requires more wholistic understanding of uncertainties
- Theory, differential data, and integral data all provide contributions to uncertainties and can’t be ignored
- Focused research needed to tie all the pieces together