

Sensitivity and Uncertainty Propagation Needs Beyond Criticality

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Monte Carlo Codes, XCP-3

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**Covariance/Sensitivity/Uncertainty/Validation
and Its Impact on Applications**



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Ideal Nuclear Data Pipeline

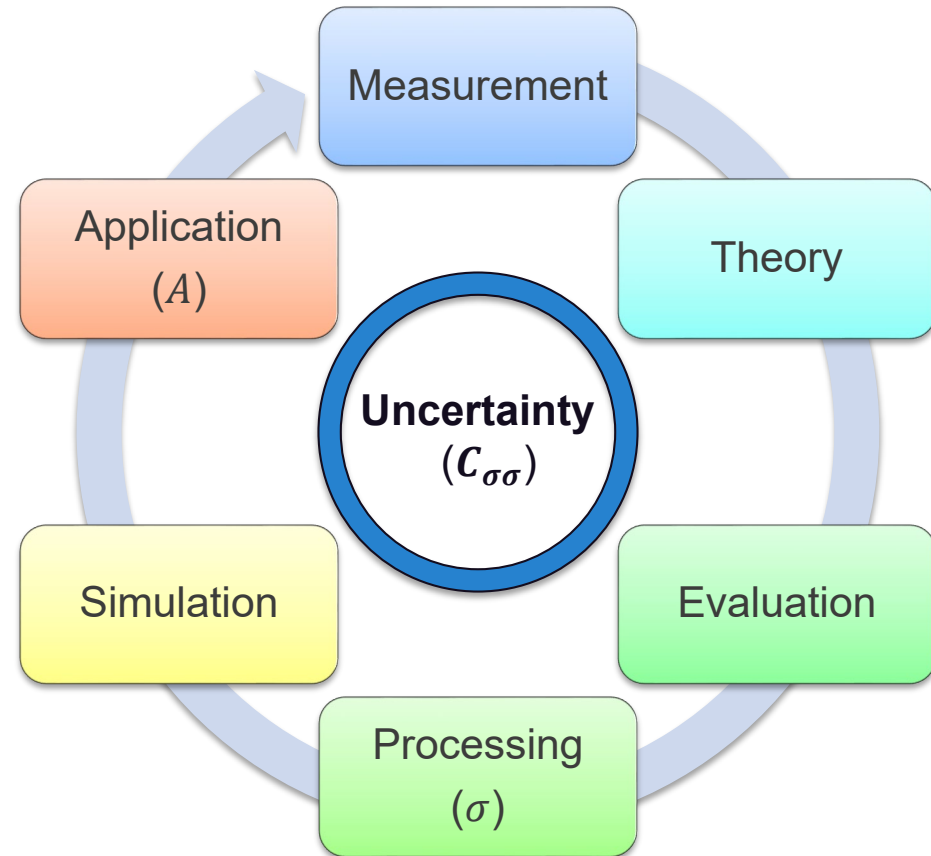
Sensitivity/perturbation methods provide efficient uncertainty propagation (UP) to applications and efficient feedback (FB) to the nuclear data evaluation community.

$$\text{UP: } \text{Var}(A) = S_{A,\sigma}^T \mathbf{C}_{\sigma\sigma} S_{A,\sigma}$$

$$\text{FB: } A, \sigma, \mathbf{C}_{\sigma\sigma} \xrightarrow{\text{GLLS}(S_{A,\sigma})} A', \sigma', \mathbf{C}'_{\sigma\sigma}$$

Many established methods to compute $S_{A,\sigma}$ for a variety of applications (some limitations).

Each piece of the ND pipeline needs sensitivity/perturbation capabilities.



Impact of new measurement campaign should be quantified *a priori*

Focus of Sensitivity/Perturbation Capabilities Has Been Somewhat Limited – Need More Diverse Applications

For both ND uncertainty propagation and feedback, in general:

- Most focus on neutron data (covariances $C_{\sigma\sigma}$), transport simulations (k-eigenvalue) and criticality applications (ICSBEP, reactors)

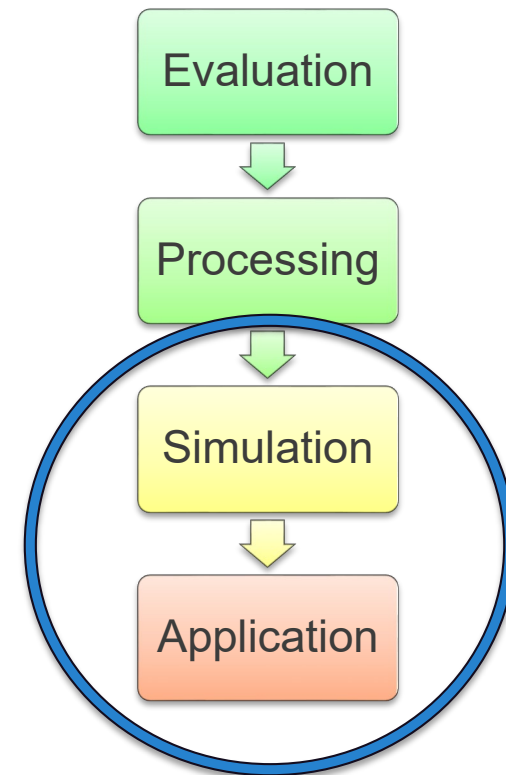
Many simulation codes (e.g. MCNP, SCALE, Serpent, OpenMC, etc.) can compute various sensitivities/perturbations to ND:

- Fixed-source, k-, and α -eigenvalue
- General responses: current, flux, dose, reaction rates
- Other responses
 - diffusion and void reactivity coefficients
 - effective prompt neutron lifetime and delayed neutron fraction

Applications beyond just transport

- Production-depletion
- Time-dependent accident/excursion
- Coupled particle physics
- Advanced detector physics

Higher-Order Sensitivity Methods Will Be Needed!



Focus of Sensitivity/Perturbation Capabilities Has Been Somewhat Limited – Need Developments in Processing

In general, a direct connection between the application and the evaluated ND for both uncertainty propagation and feedback is lacking

Sensitivity/perturbation methods applied to ND processing

– Improved connection between

- Evaluated ND (parameters), p
- Processed ND, σ

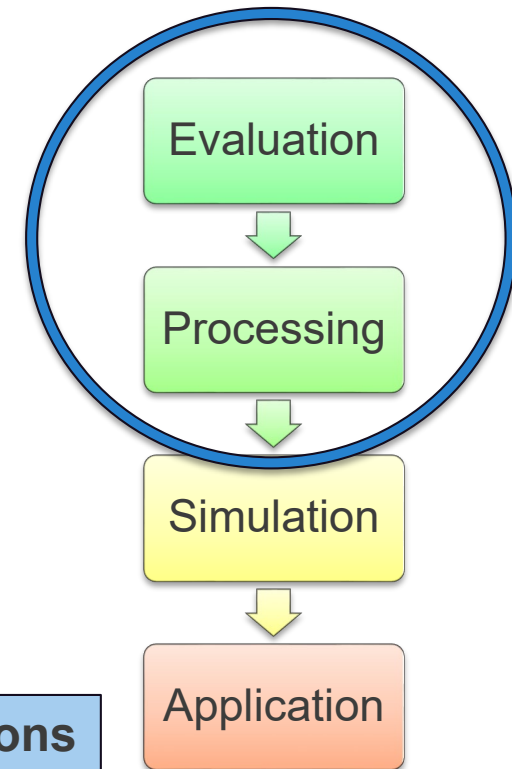
$$S_{A,p} \sim S_{A,\sigma} S_{\sigma,p}$$

– Applies to evaluated ND and covariances

Applications of sensitivity/perturbation processing

- Resonance parameters
- Thermal scattering
- Temperature (doppler broadening)
- Multigroup weighting function

Direct and Efficient UP from Evaluation to Applications
Direct and Efficient FB from Applications to Evaluation



Without Sensitivities, All Is Not Lost – Sampling-Based (Derivative-Free) Methods Are Good Too

Uncertainty Propagation, Evaluation → Application

- Monte Carlo methods
 - Brute force
 - MCMC
 - LHS
- Stochastic collocation methods
- Central differencing (sensitivities)

Feedback to ND, Application → Evaluation

- Monte Carlo methods
 - Total MC (TMC)
 - Unified MC (UMC)
 - TMC+UMC
- Derivative-free optimization
 - MADS, NOMAD
 - Genetic algorithms
 - Other ML/AI methods

Benefits

- **Creating replica data is generally straightforward**
- **Processing and simulation steps need no change**
- **Handles nonlinearities in complex applications**
- **When converged, provides accurate results**

Limitations

- **Non-physical replicas**
- **Can be orders of magnitude more computationally expensive (potentially intractable)**