Introduction

Our task: To provide internationally recommended and validated data for A+M+PMI/PSI processes relevant to fusion. Before recommendation comes evaluation. Evaluation has multiple facets: documentation, traceability, data integrity, domain of validity, quantification of uncertainty. Uncertainty assessment is well established for experimental data; needs work for theoretical data.

Challenge: Develop methods to estimate uncertainties of calculated data that do not require huge additional computational effort.

This presentation: One approach from the nuclear data community; Unified Monte Carlo.

Verification, Validation and UQ

Verification. The process of determining how accurately a computer program (“code”) correctly solves the equations of the mathematical model.

Validation. The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

Uncertainty quantification (UQ). The process of quantifying uncertainties associated with model calculations of true, physical QOIs, with the goals of accounting for all sources of uncertainty and quantifying the contributions of specific sources to the overall uncertainty.


Unified Monte Carlo Approach for Nuclear Data

Following R. Capote, presentation at IAEA, 2013-05-06

\[ p(\sigma) = C \times L(y_E, V_E | \sigma) \times p_0(\sigma | \sigma_C, V_C) \]

\[ p_0(\sigma | \sigma_C, V_C) \sim \exp\left\{ -\frac{1}{2} \left[ (\sigma - \sigma_C)^T \left( V_C^{-1} \right) (\sigma - \sigma_C) \right] \right\} \]

\[ L(y_E, V_E | \sigma) \sim \exp\left\{ -\frac{1}{2} \left[ (y - y_E)^T \left( V_E^{-1} \right) (y - y_E) \right] \right\} \]

• \( y_E, V_E \): measured quantities with \( n \) elements

• \( y_C, V_C \): calculated using nuclear models with \( m \) elements

Use Metropolis (Markov chain) sampling for \( \sigma \).

Unified Monte Carlo Approach for Nuclear Data

From D. Neudecker, S. Gundacker, H. Leeb et al., ND2010, Jeju Island, Korea; Via R. Capote, presentation at IAEA, 2013-05-06

Outline of UMC for Rovibrational Spectroscopy

Starting point: MULTIMODE code

Unified Monte Carlo Approach for Nuclear Data

Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

- If the authors claim high accuracy, or improvements on the accuracy of previous work.

- If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.

- If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

Rovibrational molecular spectrum is obtained from solution of the nuclear Schrödinger equation:

$$\frac{\hbar^2}{2M} \Delta \Psi + V \cdot \Psi = E \cdot \Psi$$

Here, $\Psi$ is the nuclear wavefunction (say for $N$ nuclei) and $V(x)$ is the solution of the electronic S.E. for nuclear configuration $x$ (Born-Oppenheimer approximation).

**Watson hamiltonian**: expansion in rotational states leaving $3N - 6$ independent nuclear coordinates.

Solution of nuclear S.E. (eigenvalue problem) provides spectrum and (dipole, etc.) matrix elements.

Sources of error and uncertainty

- Ab initio electronic structure calculations
- Fitted potential energy surface
- Solution of nuclear Schrödinger equation
- Validity of Born-Oppenheimer approximation

Approach via Unified Monte Carlo

- Treat the PES as the model prior
- MULTIMODE supplies the posterior
- Need some accurate lines to evaluate likelihood of the posterior

Prior:

Consider a linear model for ease of exposition. The coefficients $c_i$ are uncertain.

$$V(x) = \sum_i c_i f_i(x)$$

$c = c^{(0)} + \text{Gaussian}(0, M)$

(Dispersion matrix $M$ may be obtained along with least squares determination of $c^{(0)}$.)

If a nonlinear model is used, or a more complicated expression for the prior uncertainty, then one may need Metropolis sampling to obtain $c$. In practice the model for $V$ may have a few nonlinear and many linear parameters; then combine Metropolis and analytical.

Posterior:

For any coefficients $c$ sampled from the prior

- Set up and solve the nuclear Schrödinger equation [*];
- Evaluate rms deviation for selected known lines;
- Evaluate likelihood; accept or reject vector $c$.

Evaluate complete $\text{spec}(H)$ and relevant matrix elements and an estimated uncertainty from the (Metropolis) statistics.

[*] Maybe solve the S.E. only once, for a reference vector $c$, and then assume a linear response to changes in $c$.

For consideration: Could anything similar work for scattering data?

Thank you for your attention!