Advances in Theory for Nuclear Data Evaluations

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Introduction and Overview

• Theory of evaluations covers models/data/evaluations, UQ
  – Connects several NCSP Tasks presented at this TPR.

• Advances in R-matrix formalism (“model”):
  – Direct reactions
  – Doorway states

• Advances in evaluations (mean values and uncertainties)
  – Generalization of Bayes’ theorem with applications to
    • Differential cross section data
    • Integral benchmarks
Interplay of modeling, measured data, evaluations:

- Advances were made by generalizing
  1. Models: R-matrix formalism to include *direct* and *doorway* reactions
  2. Evaluation: Bayes’ theorem to account for *imperfect* data
    - New: The posterior model and data no longer forced to be equal
Benefits of the generalized form of the Bayes’ Theorem:

• Improves evaluation of any data:
  – differential cross sections (SAMMY) or integral benchmark data (TSURFER)

• Enables Bayesian Monte Carlo evaluation for large data sets
  – Presently not possible numerically due to large chi^2 values in EXP[-chi^2]
  – Useful for UQ of TSL evaluations: see Chris Chapmans talk on TSL

• Enables evaluators to incorporate expert judgment by defining:
  – Posterior expectation values of deviations between the model and data,
    and the covariance of deviations, to yield reasonable evaluated uncertainties that no longer need to be manually adjusted (increased).

• Enables sequential evaluations consistent with Bayes’ Theorem

Vital for accurate uncertainty quantification:

see Jesse Brown’s talk on the Bayesian Monte Carlo evaluation of RRR
Direct reactions in R-matrix formalism

- Conventional R-matrix accounts for resonant reactions only
- Parameterization of direct reactions in R-matrix was inspired by a 1967 paper Eugene Wigner, and was found to be analogous to a Feshbach’s parameterization of direct reactions in T-matrix
- Finally, a Reich-Moore approximation is extended to eliminate direct and resonant capture, simultaneously
- SAMMY adds direct capture to the resonant cross section, thus neglecting any interference between them
  - Direct reactions and capture to be implemented post-modernization
Doorway states in R-matrix formalism

• Generalized R-matrix formalism to parameterize doorway states:
  – Comparison of formal expressions for doorway state K-matrix (derived by Feshbach’s projection operator formalism) to the Brune’s alternative R-matrix has helped identify doorway state parameters in R-matrix:
    • Their widths and the strengths of their coupling to compound nuclear resonances

\[ P + Q = P + (q + d) = 1 \]
Summary and Conclusions:

- Several NCSP projects benefit from the presented advances:
  - Generalized form of the Bayes’ Theorem improves UQ for NCSP:
    - of differential and/or integral data evaluations, and of applications
      - See the presentation by Hany Abdel-Khalik on Safety Margins
      - is being implemented in an API for use by SCALE, SAMMY, etc.
        - See the presentations by Jesse Brown on Bayesian MC, and by C. Chapman on TSL.
  - Extended R-matrix formalism improves evaluations of RRR
    - Direct reactions, including direct capture, and the Reich-Moore approx.
    - Doorway state reactions with applications to RPI data on lead isotopes
    - To be implemented into SAMMY post modernization
      - See the presentation by D. Wiarda, A. Holcomb on SAMMY modernization

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