OAK RIDGE National Laboratory

Advances in Theory for Nuclear Data Evaluations

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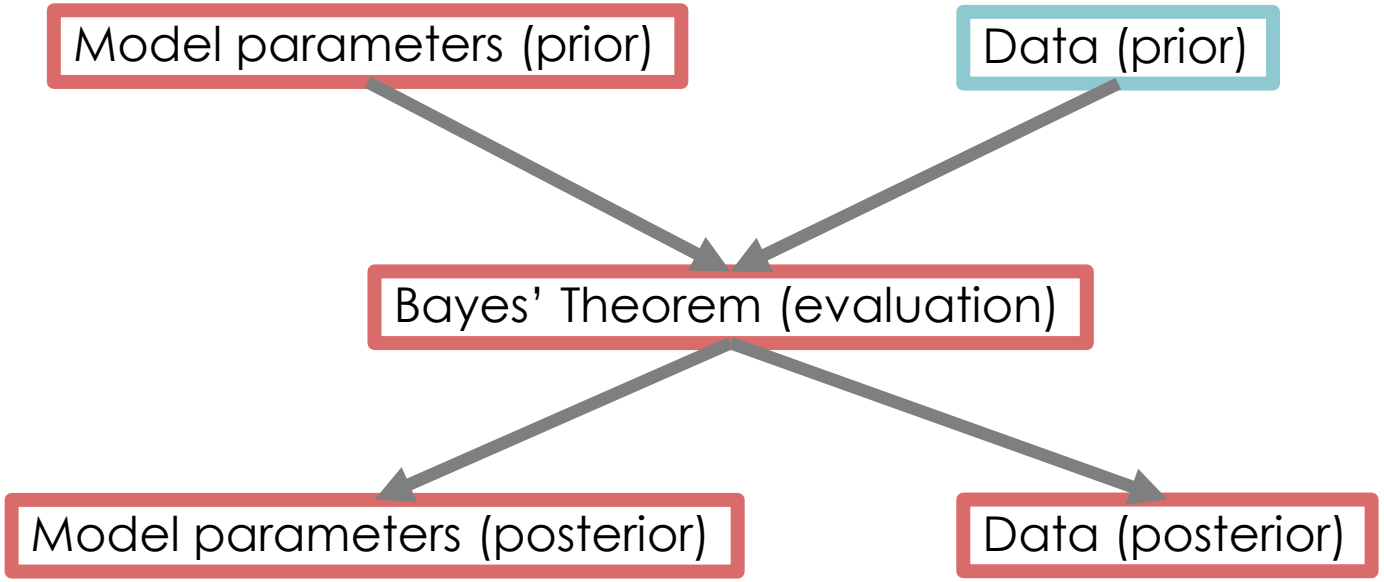
Introduction and Overview

- 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:

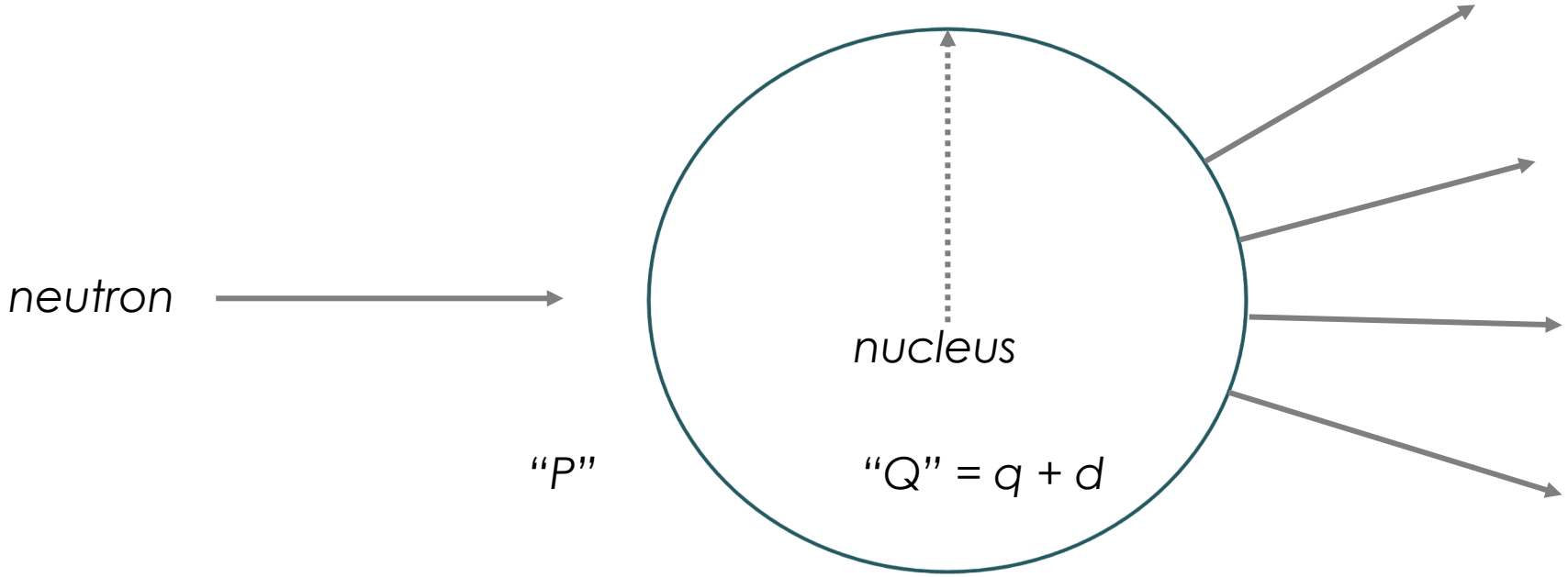
see Jesse Brown's talk on the Bayesian Monte Carlo evaluation of RRR

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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