Uncertainty Quantification in Reaction Theory

A.E. Lovell, Los Alamos National Laboratory

August 9, 2022, LECM

LA-UR-22-28156
Reaction theory is crucial for interpreting experimental data

$^{12}\text{C}(n,n)^{12}\text{C}$ and $^{12}\text{C}(n,n^\ast)^{12}\text{C}(2^+_1)$ @ 28 MeV

$^{58}\text{Ni}(d,p)^{59}\text{Ni}$

Isotope Science Facility, white paper (2007)
To cover the full range of the nuclear chart, we are mostly limited to few-body approximations.

Model simplification and the phenomenological interactions that are used in these theories introduce uncertainties that should be rigorously quantified.
Elastic scattering and transfer reactions can use the same interactions

Optical Model Potentials (local, energy dependent)

\[ U(r) = V(r) + iW(r) + (V_{so}(r) + iW_{so}(r))(1 \cdot s) + V_C(r) \]

**Volume Term**

\[ V(r) = f(r; V_o, R_o, a_o) \]

**Surface and Spin-Orbit Terms**

\[ V(r) = \frac{d}{dr} f(r; V_o, R_o, a_o) \]

\[ f(r; V_o, R_o, a_o) = -\frac{V_o}{1 + e^{(r-R_o)/a_o}} \]

There is a non-linear relationship between the potential parameters and the observables (e.g. cross sections)
Comparing various potentials gives an incomplete picture of the full model uncertainty

\[ ^{132}\text{Sn}(d,d)^{132}\text{Sn} @ 9.46 \text{ MeV} \]

\[ ^{132}\text{Sn}(d,p)^{133}\text{Sn}(\text{g.s.}) @ 9.46 \text{ MeV} \]

χ² minimization and covariance propagation are widely used to construct uncertainties

12C(d,d) @ 11.8 MeV

...but this method relies on assumptions about the response of the model to the parameters and uncertainties can be underestimated.

Bayes’ Theorem can take into account the exact distributions

\[
P(H|D) = \frac{P(D|H)P(H)}{P(D)}
\]

\(48\text{Ca}(n,n)\) @ 12.0 MeV

\(48\text{Ca}(d,p)49\text{Ca}(\text{g.s.})\) @ 24 MeV

Interesting differences are seen between $\chi^2$ minimization and Bayesian optimization.

$^{48}\text{Ca}(n,n)$
@ 12 MeV

QUILTR: Quantified Uncertainties in Low-energy Theory for Reactions

Bayesian Markov Chain Monte Carlo wrapper around fresco (I. Thompson) but is being expanded

Completed studies:
• Elastic differential cross sections
• Transfer cross sections
• Reaction cross sections
• Polarization observables
• Principle Component Analysis
• Sensitivity analyses
• Bayesian evidence

Studies are still being extended:
• Asymptotic Normalization Coefficients (M. Catacora-Rios)
• Knockout reactions (C. Hebborn)
• Charge-exchange reactions (T. Whitehead)
• And more planned
Emulators are needed to perform robust UQ for computationally demanding models

Eigenvector Continuation for optical model

Classifier to determine neutron multiplicity from fission fragment initial conditions

Short fission time scales lead to necessary theory initial conditions being extracted from experimental data.

These uncertainties should be quantified and propagated through the models.

Fragment de-excitation models require information about the compound nucleus before fission and initial conditions of the fission fragments.

Prompt and delayed neutrons and \( \gamma \) rays can be measured, along with fission fragments after particle emission.

CGMF, P. Talou, et al., *CPC* 269, 108087 (2021)
Conclusions and future work

• Theory requires robust uncertainty quantification to make reliable predictions and perform reliable analysis.

• Over the last several years, UQ for optical potentials in direct reaction theory has been significantly upgraded, from comparing models, to $\chi^2$ minimization and covariance propagation, to Bayesian optimization.

• Differences between $\chi^2$ and Bayesian optimizations can be significant and should be investigated in other areas.

• Robust UQ of fission observables is the focus of a funded LANL LDRD Early Career Research project (5/2022-5/2024).
Acknowledgements

• Filomena Nunes, Garrett King, Manuel Catacora-Rios, Christian Drischler, Pablo Giuliani, Michael Quinonez (MSU/former MSU)

• Patrick Talou, Ionel Stetcu, Toshihiko Kawano, Mike Rising, Patrick Jaffke, Arvind Mohan, Denise Neudecker, Matthew Mumpower, Mike Grosskopf (LANL/former LANL)

This work was performed under the auspice of the U.S. Department of Energy by Los Alamos National Laboratory under Contract 89233218CNA000001 and was supported by the Laboratory Directed Research and Development program of Los Alamos National Laboratory, the Office of Defense Nuclear Nonproliferation Research and Development (DNN R&D), National Nuclear Security Administration, U.S. Department of Energy, and the DOE NNSA Stewardship Science Graduate Fellowship.