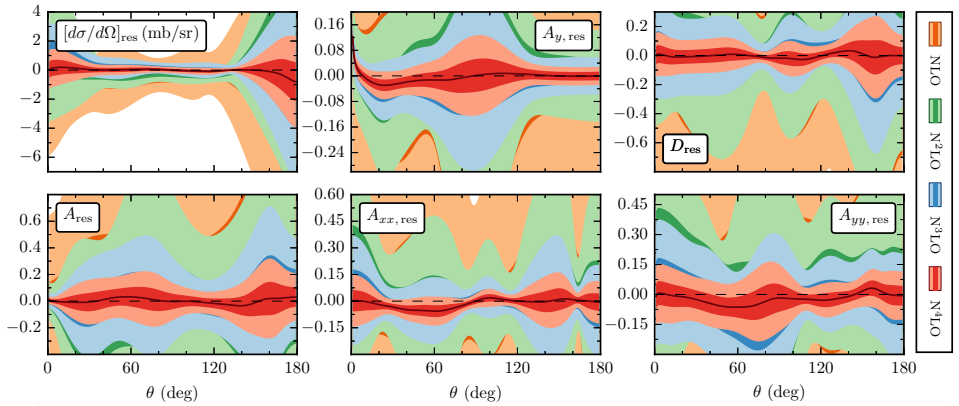
U.S. DEPARTMENT OF ENERGY | Office of Science

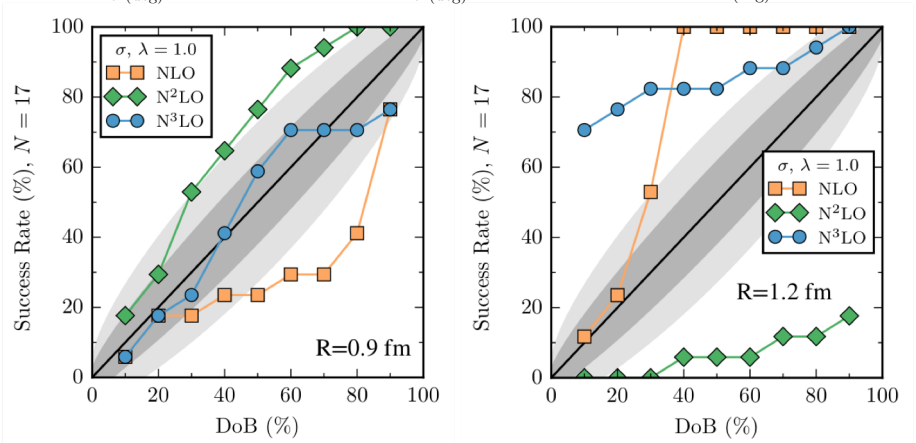
Theory errors for nuclear calculations using Bayesian statistics

NUCLEI Nuclear Computational Low-Energy Initiative

Objectives

- The precision calculations of nuclei enabled by NUCLEI advances in algorithms and HPC also need uncertainty quantification for the theory input.
- Develop and validate a statistical approach to theory truncation errors and develop diagnostics to identify deficiencies in effective field theory (EFT) models.





Impact

- Bayesian methods to account for truncated EFT expansions were developed and successfully tested for nucleon-nucleon (NN) observables.
- New model checking procedures provide diagnostics for EFTs and our statistical model.
- For the first time the breakdown scale of the EFT expansion has been estimated from the convergence pattern.
- The new methods will be applied to many-body calculations of nuclei and nuclear matter.

Accomplishments

- Publication: J. Melendez, S. Wesolowski, and R.J. Furnstahl, Phys. Rev. C 96, 024003 (2017).
- Highlighted as Editors' suggestion.
- Featured as March, 2018 picture on APS calendar.

Figures: The top figure shows that the order-by-order residual error from theoretical calculations of NN observables is correctly predicted by the Bayesian estimates. The lower figures show how model checking validates one EFT implementation (left) while revealing deficiencies in another (right).