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Editorial: Uncertainty quantification in nuclear physics

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Editorial on the Research Topic
Uncertainty quantification in nuclear physics

Uncertainty quantification (UQ) has emerged as a crucial aspect of the interface between theory and experiment in nuclear physics. Over the past decade the field has undergone a transformative shift into the "precision era" due to advancements in *ab initio* many-body methods, computing power, sophisticated theoretical techniques, and the advent of a new generation of experiments.

With experimental procedures now capable of probing observables with greater precision, and in some cases even where data is lacking, the need for theoretical predictions with well-quantified error bars has become more pronounced. This requirement extends not only to ongoing experiments but also to future endeavors seeking accurate measurements of more exotic processes including precision tests of the Standard Model as well as Beyond the Standard Model searches.

The employment of Bayesian approaches, efficient emulators to overcome computational limitations, and machine learning methods has sparked a surge of interest in UQ, revolutionizing the field. These techniques have enabled researchers to assess uncertainties in different theoretical domains, ranging from lattice quantum chromodynamics to nuclear many-body forces to properties of atomic nuclei. Moreover, they have enabled quantitative insights into the role played by future astrophysics and gravitational observations for constraining the equation of state for neutron matter, the determination of nucleon resonances in experimental data, and the development of reliable nuclear-energy-density functionals for extrapolations into unexplored nuclear territories.

To consolidate the expertise and achievements in nuclear physics UQ, this Research Topic aimed to bring together leading contributors in the field. We have received an outstanding Research Topic that highlight recent accomplishments along this line of research and that provide insights into the methodologies being developed and employed.

The Research Topic features 15 articles. Several contributions focus on the uncertainty quantification in nuclear structure calculations. For instance, Alnamlah et al. discuss an effective field theory (EFT) for rotational bands in odd-mass nuclei and employ a Bayesian analysis to estimate uncertainties in rotational energy levels. They consider both experimental and EFT truncation uncertainties, utilizing Markov Chain Monte Carlo (MCMC) sampling to infer low-energy constants and the breakdown scale of the EFT. Becker et al. investigate alpha clustering and collective properties in nuclei using emulators within the *ab initio* symmetry-adapted no-core shell model framework. Their work highlights the importance of such emulators in quantifying uncertainties and improving the precision of nuclear structure calculations. They utilize the eigenvector continuation technique to study various nuclear properties in ^{6}Li and ^{12}C including excitation energies, point-proton root-mean-square radii, electric quadrupole moments, and transitions.

Furthermore, Maris et al. examine uncertainties in theoretical ground state energies of p-shell nuclei using interactions from chiral EFT. They investigate the dependence of these energies on the chiral order and analyze two- and three-body data for fitting, addressing uncertainties stemming from basis truncations, omitted induced many-body forces, and EFT truncation. Acharya et al. focus on quantifying theoretical uncertainties in *ab initio* calculations of electromagnetic observables in light and medium-mass nuclei. They discuss different sources of uncertainties including approximations introduced by few- and many-body solvers and the truncation of the chiral EFT expansion.

Regarding reactions in nuclei, some contributions are particularly noteworthy. Skibiński et al. investigate the nucleon-induced deuteron breakup reaction using the Faddeev approach at specific laboratory energies. They focus on quantifying theoretical uncertainties associated with the predicted cross-section, particularly in relation to the regulator cutoff parameter. Ceccarelli et al. concentrate on UQ for the muon capture reaction $\mu^- + d \rightarrow n + n + \nu_\mu$ in the doublet hyperfine state. They address four sources of theoretical uncertainty including model dependence, chiral-order convergence, uncertainty in the single-nucleon axial form factor, and numerical techniques used for solving the $A = 2$ systems.

Furthermore, Odell et al. focus on the estimation of uncertainties in resolved resonance cross section data in nuclear physics using the R-matrix framework. They introduce the Bayesian R-matrix Inference Code Kit (BRICK) by implementing a MCMC sampler, specifically the emcee algorithm, into the R-matrix code AZURE2. They apply Bayesian uncertainty estimation to simultaneously fit the ^{3}He(α, γ) ^{7}Be and ^{3}He(α, α)^{3}He reactions, aiming to gain insights into the fitting of capture and scattering data. The data from both reactions are relevant to constrain the values of the bound state α-particle asymptotic normalization coefficients in ^{7}Be. Baker et al. investigate the effective interaction between a nucleon and a nucleus based on optical potentials, with a UQ perspective. They extracted elastic scattering observables for ^{4}He, ^{12}C, and ^{16}O at projectile energies between 65 and 200 MeV. Lastly, Vassh et al. employ a MCMC procedure to predict ground state masses for nucleosynthesis calculations and investigate conditions capable of producing the observed solar r-process rare-earth abundance peak. They examine how mass predictions change when using a few different sets of r-process solar abundance residuals that have been reported in the literature, with focus on uncertainty propagation.

The Research Topic also includes a review article by Ekström et al. that provides a historical overview of the notion of *ab initio* in nuclear physics and discusses its current relationship with theoretical UQ.

Furthermore some of the article discuss various advancements in UQ methodology. One of the topics covered is the use of projection-based, reduced-order emulators as fast surrogate models for complex high-fidelity models. Drischler et al. present a pedagogical introduction to these emulators, which effectively approximate complex models and offer an efficient approach to calculations while addressing the challenges of UQ. Additionally, Rothkopf discusses state-of-the-art methods for extracting spectral functions using Bayesian inference, highlighting the importance of prior domain knowledge for regularization. The use of machine learning for spectral function reconstruction is also mentioned, noting its contribution to the Bayesian community's understanding of the topic.

Verriere et al. focus on the challenges in studying atomic nuclei and the potential of nuclear density functional theory to accurately describe their properties with uncertainties. They explore the application of machine learning and artificial intelligence techniques to enhance DFT calculations and accelerate the understanding of nuclear phenomena. In the paper by Giuliani et al., the authors showcase the application of a principled Bayesian statistical framework for UQ in nuclear physics. By employing the reduced-based emulator and calibrating the energy density functional, they provide accurate model calculations with estimated uncertainties, supporting the nuclear theory community in delivering reliable predictions in the face of increasing data availability.

Lastly, Jiang et al. address the usefulness of the sampling/importance resampling method in UQ for nuclear theory applications. By employing sampling/importance resampling to realistic scenarios, the authors demonstrate its effectiveness in inferring posterior distributions and estimating the predictive probability distribution of observables. Researchers in nuclear theory can benefit from employing this Bayesian sampling method to gain insights into uncertainties and make informed decisions based on the obtained posterior distributions.

In conclusion, this Research Topic presents a comprehensive collection of articles that contributes to the advancement of UQ in nuclear physics. The diverse range of topics and methodologies highlights the progress made in addressing uncertainties and provides a solid foundation for future developments in the field. We are grateful to all the scientists participating in this project and hope that the reader will enjoy this Research Topic.

Author contributions

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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