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Information and Statistics in Nuclear Experiment and Theory (ISNET)

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Introduction

As with all empirical sciences, nuclear physics operates in the virtuous cycle of the scientific method: observations inspire theoretical models; models lead to new predictions; predictions are tested in experiments; experiments lead to new observations; and so on. Evaluating what we are inferring, and how certain we are of it, is key to this process.

These requirements, and a general interest in applying novel statistical, mathematical, and computational techniques, led to the formation of a dedicated research community entitled "Information and Statistics in Nuclear Experiment and Theory (ISNET)" (https://isnet-series.github.io/), which now includes more than 300 members. While the community's interests lean toward nuclear theory, the unifying theme for this group is the inference of knowledge from data.

Input from beyond nuclear research has been critical to the success of the ISNET workshops. The most important contributions have come from statisticians and applied mathematicians, many of whom hail from the uncertainty quantification (UQ) community.

History

The series of ISNET meetings can be traced to a small workshop held at the Institute of Nuclear Physics in Krakow in 2012 to review the quantification of uncertainties in theoretical predictions; a response to an editorial in *Phys. Rev.* A [1] that highlighted "…the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities…"

This was followed by an extension to incorporate UQ in phenomenology and inference from experimental results, with a small workshop in Glasgow in 2013. The ISNET workshop series developed thereafter, including meetings at the European Centre for Theoretical Studies in Nuclear Physics and Related Areas in Trento, Italy; the Institute for Nuclear Theory (INT) in Seattle, USA; and Gothenburg, Sweden (see Figure 1). We are now approaching the 10th edition of ISNET at the Jiangwan Campus of Fudan University in Shanghai, China (https://napp.fudan.edu.cn/event/757/), in November 2024.

The first task was to learn how to speak each other's languages. For example, what statisticians call simulations, physicists call models, and whereas θ will trigger a statistician to think about a parameter, physicists imagine an angle. For Bayesians, probability represents uncertainty, and in the context of UQ, Bayesian credibility intervals should encompass all of our ignorance. This enables not just UQ for model parameters and predictions, but also probabilistic assessment of models themselves. Nuclear physicists were more used to frequentist confidence intervals. Despite these challenges, it was concluded that the different communities could benefit each other. A result of this was the compilation of ISNET-themed articles in two *Journal of Physics* G Focus issues [2, 3].

Figure 1. *Workshop participants, ISNET-7 in Gothenburg, Sweden.*

Culture Eats Strategy for Breakfast

From the outset, there has been an atmosphere of “there are no stupid questions,” and (we hope) this has led to a culture where the contributions from colleagues at all stages of their careers are welcome. We believe that the ISNET community is nonhierarchical, welcoming, and inclusive. It was thus a straightforward step to establishing a Code of Conduct that requires participants of meetings to adhere to respectful and inclusive standards of behavior. This requirement was introduced following the establishment of an ISNET "board" (chair 2022–2024 Daniel Phillips, chair 2024–2026 Andreas Ekström), which now oversees the decisions on meeting locations, provision of information, and training materials.

Developing a Toolbox

Many statistical methods used in nuclear physics are well known from undergraduate programs, but it is important to assess how additional techniques can be deployed. For example, parameter estimation and model calibration tasks are often performed by minimization of a sum of squared residuals (χ^2). But, if it is suspected that the data have correlated or non-Gaussian errors or if there is any multimodality and so on, new approaches are required. A Bayesian approach requires that we both examine the structure of the entire likelihood function and combine it with *a priori* information.

Bayesian inference was a key driver for the ISNET community, following on the heels of its successful deployment in fields such as astrophysics and cosmology. A Bayesian posterior can rarely be computed analytically, but it can be sampled using *Markov Chain Monte Carlo (MCMC)* methods (see, e.g., Ref. [4]). One of the first take-home messages from ISNET workshops was that these methods, developed by physicists in the 1950s, are now computationally straightforward and ubiquitous in statistics.

MCMC sampling of the posterior can be computationally expensive, and so the UQ community has for some time been using *emulators* extensively in inference problems. An emulator is a surrogate function that mimics the full calculation (“the simulator”) with minimal cost and quantified accuracy; that is, returns a value that is equal to that from the simulator, with an error that can then be accounted for in the uncertainty quantification of the overall inference.

Gaussian process (GP) [5] emulators were discussed extensively in early ISNET workshops. GPs are now regarded as a component of the machine-learning (ML) suite and are one of the key nonparametric approaches to interpolation and extrapolation. Recently, eigenvector continuation, a model-driven *reduced-basis method* [6], emerged in the nuclear theory community as a very useful technique for devising fast and accurate emulators.

History matching [7] is an iterative strategy that uses the power of emulators to shed light on computationally expensive simulations that depend on inputs living in high-dimensional parameter spaces. It does this by ruling out regions of parameter space that do not give acceptable matches between the emulator output and observed (i.e., historical), data. It thus identifies a “non-implausible region” of parameter space. History matching is one example of several so-called likelihood-free methods that were introduced to nuclear physicists by statisticians at ISNET meetings and have since been successfully imported into nuclear physics research.

Bayesian model averaging (BMA) [8] is sometimes suggested as the best way to formulate an assessment of model uncertainty. However, statisticians at ISNET meetings pointed out the limitations of BMA, and encouraged more general approaches, such as *stacking* [9], or *local Bayesian model mixing.* These strategies generalize the BMA approach in ways that locally leverage the strengths of different models.

Bayesian experimental design (BED) [10] explores a utility function that encodes the goal of an experimental campaign (e.g., to pin down certain parameters or refine a prediction). BED differs from *optimal experimental design* approaches in that it recognizes that there may be multiple maxima in the utility function, and that it can guide the sequential design of multiple, successive, experiments.

Projects Generated

Beyond Best-Fit Values for Mass-Model Parameters

Density functional theory (DFT) requires sophisticated optimization methods to be applied to χ^2-functions involving heterogeneous nuclear data if optimal DFT parameters are to be identified. GP emulators were leveraged, together with Bayesian inference and marginalization, to quantify and propagate parametric uncertainties in DFT predictions of nuclear masses, the two-neutron drip-line, and fission barriers; see Figure 2 [11]. The ability of Bayesian methods to combine information from multiple models has been used in DFT to provide a posterior probability for each nucleus to be stable against neutron emission, enabling probabilistic statements regarding the location of the neutron drip-line [12]. Future mass measurements that will yield the maximum reduction in uncertainty as to where the drip-line is have been identified [13].

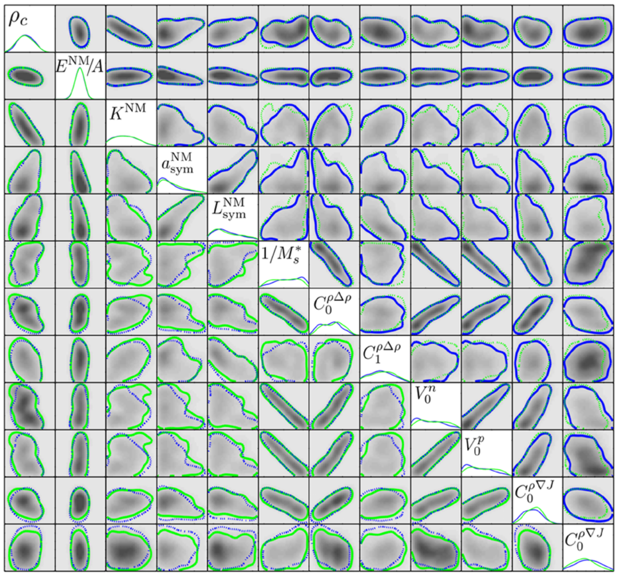

Figure 2. *Univariate and bivariate marginal posterior distribution for the 12-dimensional DFT parameter vector of the UNEDF1 parametrization. Figure from Ref. [11]; reprinted with permission, American Physical Society.*

History Matching and a Predictive Theory of Nuclear Structure

History matching has come to play a central role in the UQ of *ab initio* predictions of strongly interacting matter. Advances in quantum many-body methods and emulator technology based on eigenvector continuation [6] have enabled extensive exploration of different values for the low-energy constants entering effective field theory descriptions of the nuclear force. Coupled with history matching, this has enabled the formulation of likelihood-weighted ensembles of low-energy constants. This was recently used to quantify the uncertainty in the *ab initio* prediction of the neutron-skin thickness of ^{208}Pb, which provides a measure of the symmetry energy of nuclear matter at saturation density. The resulting posterior predictive distribution of the skin thickness is in mild tension with a recent parity-violating electron scattering measurement, but consistent with other experimental probes [14]; see Figure 3.

This exemplifies how to link microscopic nuclear forces to important properties of complex nuclei. History matching was also used to quantify a bivariate posterior predictive distribution for the ^{28}O to ^{24}O and ^{27}O to ^{28}O energy differences, requiring fine-tuning of nuclear forces to reproduce the experimental data [15]. ISNET workshops were instrumental in forming the collaboration with statistician Ian Vernon (Durham, UK) that developed these studies.

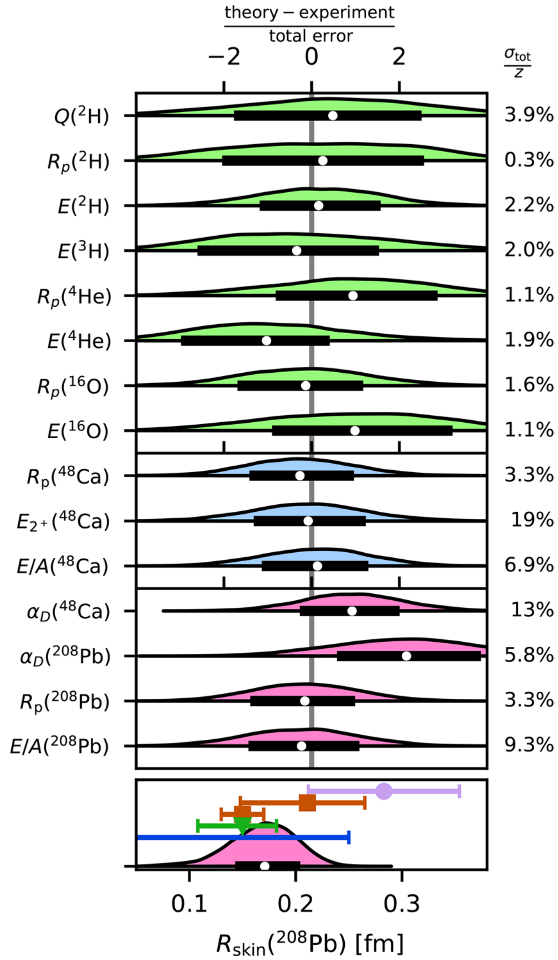

Figure 3. *Ab initio posterior predictive distributions for several observables in light- to heavy-mass nuclei. The neutron-skin thickness (R_{skin}) in ^{208}Pb in the bottom panel is on an absolute scale and compared to experimental results using electroweak (purple), hadronic (red), electromagnetic, and gravitational wave (blue) probes. Figure from Ref. [14].*

Complex Models Refine Inference of Fission Conditions

The average number of prompt (fast) neutrons, $\underline{\nu}$, emitted from fission has important correlations with the initial conditions of fission fragments, which cannot be measured directly. To first order, $\underline{\nu}$ is highly anticorrelated with the average total kinetic energy, $\underline{TKE}$, of the fission fragments. As $\underline{\nu}$ can be measured much more precisely than $\underline{TKE}$, it has been proposed that these anticorrelations be used to constrain $\underline{TKE}$ [16]. However, fission models such as *CGMF* [17] and *BeoH* [18] show that additional parameters can have a secondary impact on $\underline{\nu}$ that can loosen this constraint.

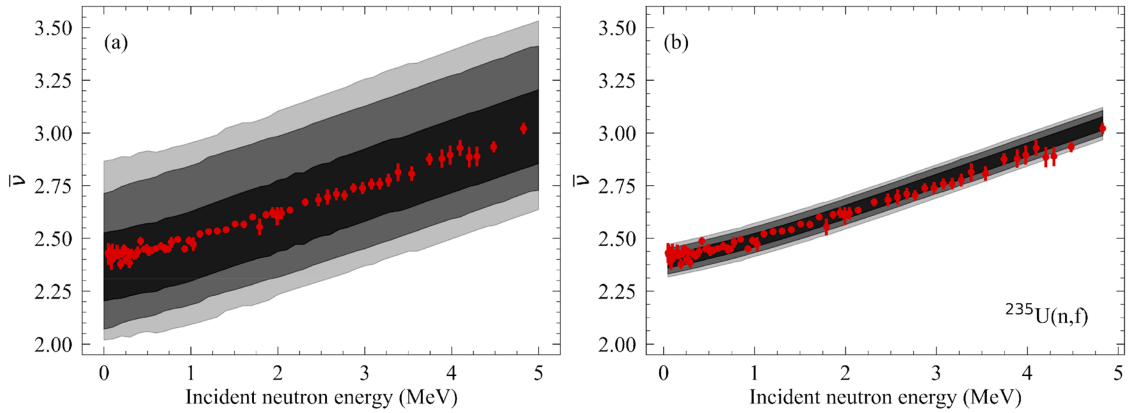

Figure 4. *The average number of emitted neutrons, $\underline{\nu}$, plus uncertainties without (a) and with (b) additional constraints imposed when using a GP emulator.*

Recent work [19], spurred by interactions at an ISNET meeting, constructed a GP emulator of the sophisticated fission fragment decay code *BeoH*. This emulator encoded the complex relationship between $\underline{TKE}$, $\underline{\nu}$, the fission fragment spin distribution, and the average number of emitted γ rays, $\underline{N}_\gamma$. Panel (a) of Figure 4 shows that optimising a parameterization that only depends on $\underline{TKE}$ to $\underline{\nu}$ reproduces the experimental data within wide error bars, because these data include dependencies on quantities other than $\underline{TKE}$. However, when both $\underline{\nu}$ and $\underline{N}_\gamma$ are included in the optimization, $\underline{\nu}$ is much better constrained, as shown in panel (b).

Quantitative and Rigorous Inference in Heavy Ion Physics

Since the turn of the century, the Relativistic Heavy Ion Collider (RHIC) has produced data of unprecedented quality and precision by colliding particles from protons and deuterons to gold and uranium. In response to this, the sophistication and accuracy of modeling took an enormous leap. Roughly 15 years ago, the accuracy of the theoretical models was sufficient to make qualitative statements that a novel form of matter, a strongly interacting quark–gluon plasma, had been created in RHIC's collisions. However, one could not infer properties such as the speed of sound or the viscosity of this new form of matter with meaningful uncertainties.

Because each observable was known to depend on multiple model inputs, and because each model input affected multiple observables, the data needed to be analyzed more globally. Emulators replaced expensive simulators, enabling the exploration of high-dimensional model-parameter spaces, and showing that much of the data could be understood in terms of a few principal components, thereby performing a data reduction on the vast RHIC data set.

ISNET meetings helped refine the emulator-based analysis by the Models and Data Analysis Initiative (MADAI) Collaboration to demonstrate rigorous constraints on the equation of state and the viscosity [20], as illustrated in Figure 5. The modeling of these collisions has now entered a precision era, with the Jet Energy-loss Tomography with a Statistically and Computationally Advanced Program Envelope (JETSCAPE) Collaboration producing the constraints on the bulk and shear viscosity of the quark–gluon fluid shown in Figure 6 [21].

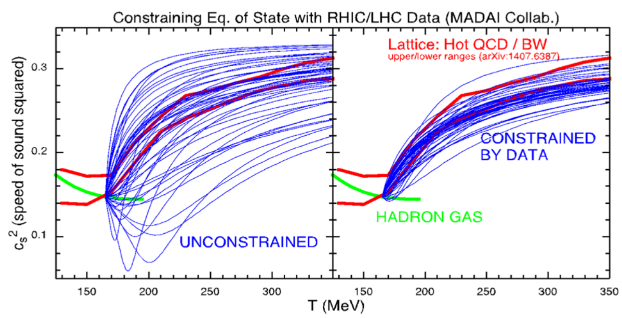

Figure 5. *Sample equations of state from the Bayesian posterior compared to those of the prior from Ref. 20.*

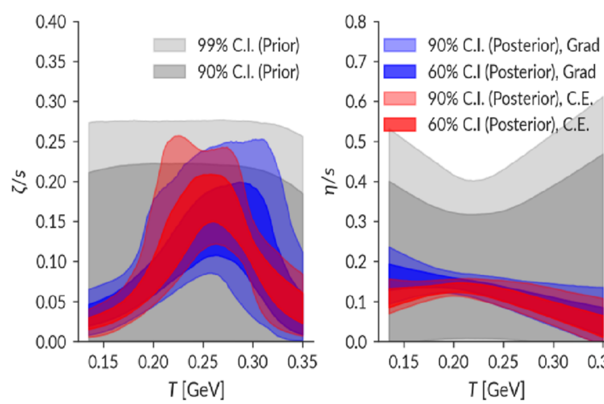

Figure 6. *Bulk and shear viscosities as constrained by JETSCAPE.*

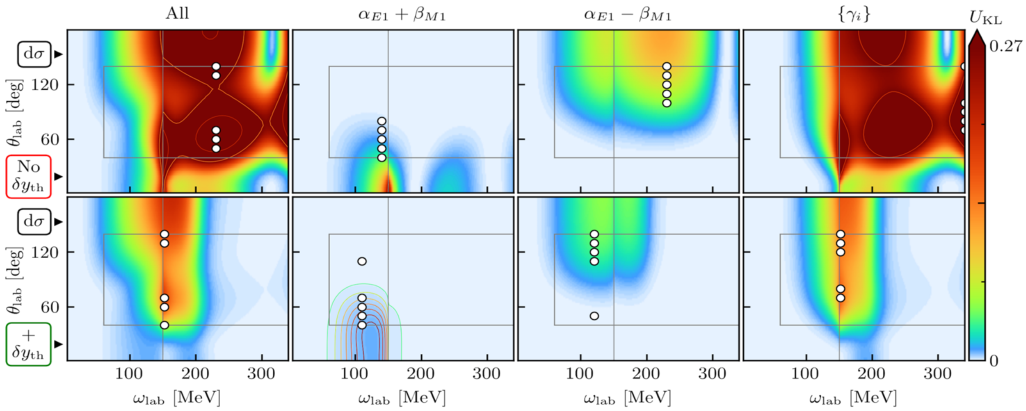

Figure 7. *The expected utility U_{KL} of proton Compton scattering differential cross-section measurements conducted at a particular kinematic point. The four panels in the top row do not account for effective field theory (EFT) truncation errors when assessing the information extracted, whereas the bottom row does include the EFT uncertainty in the computation of U_{KL}. For full details, see Ref. [22].*

Figure 8. *A BAND camp was held in conjunction with ISNET-9 at Washington University in St. Louis.*

Bayesian Experimental Design

Proton polarizabilities are fundamental parameters of quantum chromodynamics that measure the ability of electric and magnetic fields to induce different multipole moments. They can be extracted from Compton scattering data. The principles of BED were implemented in an assessment of the best kinematics for the extraction of proton polarizabilities from data in Ref. [22], where a utility function was defined that equated to the log of the reduction in the hypervolume in polarizability-space. Crucially, the assessment employed a discrepancy model, developed by the Bayesian Uncertainty Quantification: Errors in Your EFT (BUQEYE) Collaboration [23], that used GPs to account for the error induced when effective field theory computations are truncated at a particular order. Without this theoretical error included in the BED calculation, larger energies are preferred, but the interpretation of the data is subject to larger model errors there. The results of this study are summarized in Figure 7. They suggest it is best to focus on proton Compton scattering experiments at, or just below, the pion threshold.

Strike up the BAND

The Bayesian Analysis of Nuclear Dynamics (BAND) Collaboration was funded in 2020 by the National Science Foundation's Office of Advanced Cyberinfrastructure to create and curate software tools that make ISNET-initiated insights like the ones described in this article available to the larger nuclear physics community. BAND includes nuclear physicists, applied mathematicians, and statisticians, many of whom are veterans of the ISNET series. Its overall mission is discussed in Ref. [24]. The collaboration is building a set of software tools that enable emulation, including GP emulation, Bayesian model mixing, and BED. BAND conducts regular "BAND camps" during which attendees—who are mainly, but not exclusively, graduate students and postdocs—go through various examples of applications and learn how to use the software tools (Figure 8). The tools, examples, and BAND camp materials can be found at http://bandframework.github.io.

Future

ISNET began 12 years ago. Since then, UQ has gone from fringe to mainstream in nuclear theory, Bayesian methods find increasing application in both experiment and theory, and ML has become part of the nuclear physics toolkit. There are now multiple meetings every year that seek to leverage these methods to make progress on particular nuclear physics problems. In this landscape, ISNET continues to play a key role by providing an arena for statisticians and physicists to meet and have transdisciplinary conversation regarding better ways to make efficient and reliable use of the information content of nuclear physicists' very expensive experiments and huge computations. Please get in touch: you can sign up to join the ISNET community at the website https://isnet-series.github.io.

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Disclosure statement

No potential conflict of interest was reported by the author(s).

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