Distinguished Lecture of

Professor James P. Vary

Computational Nuclear Physics:
Key To Discovery Opportunities

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Distinguished Lecture:

Computational Nuclear Physics: Key to Discovery Opportunities

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Abstract

The vision of solving the nuclear many-body problem with fundamental interactions tied to QCD via Chiral Perturbation Theory appears to be gaining support. The goals are to preserve the predictive power of the underlying theory, to test fundamental symmetries with the nucleus as laboratory and to develop new understandings of the full range of complex nuclear phenomena. Advances in theoretical frameworks (renormalization and many-body methods) as well as in computational resources (new algorithms and leadership-class parallel computers) signal a new generation of theory and simulations that will yield profound insights into the origins of nuclear shell structure, collective phenomena and complex reaction dynamics. Fundamental discovery opportunities also exist in such areas as physics beyond the Standard Model of Elementary Particles, the transition between hadronic and quark-gluon dominated dynamics in nuclei and signals that characterize dark matter. I will review some recent achievements and present ambitious consensus plans along with their challenges for a coming decade of research that will build new links between theory, simulations and experiment.

Keywords: *Computational Physics, ab initio Nuclear Theory*

1 Introduction

Computational Physics has joined Theoretical and Experimental Physics to form a foundation that supports advances in Physics. According to the recent National Academy Report [1], "High Performance Computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes the third leg supporting the field of nuclear physics."

Many of the forefront questions that we address in nuclear physics require advances in theory as well as advances in both computational algorithms and hardware to address. Here are some of my personal favorites for these questions.

1. What controls nuclear saturation?
2. How do the nuclear shell and collective models emerge from the underlying theory?
3. What are the properties of nuclei with extreme neutron/proton ratios?
4. Can we predict useful cross sections that cannot be measured?

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http://www.ntse-2013.khb.ru/Proc/JPVary.pdf.

5. Can nuclei provide precision tests of the fundamental laws of nature?
6. Can we solve QCD to describe hadronic structures and interactions?

Before I delve into specific issues, let us address a general question: "What is Computational Physics?". I propose that Computational Physics is the field that takes a physics problem through the following stages leading to its solution.

1. Theoretical developments leading to the Problem Statement.
2. Computational hardware and resource assessments.
3. Algorithm developments and/or selections.
4. Software developments and/or selections including validation and verification.
5. Generation of results, analysis of the results and uncertainty quantification.
6. Conclusion with the problem's solution.

There are many prominent examples where computational nuclear physics has become a leading route to discovery. A few examples will suffice:

1. Core-collapse supernova simulation.
2. Hadronic structures and interactions from Lattice QCD.
3. Quark-gluon plasma simulations in Lattice QCD.
4. *Ab initio* nuclear structure and nuclear reactions.
5. Energy density functional simulation of neutron and proton drip lines.
6. Nuclear fission dynamics.

It may be useful to visualize the challenges we face from the long-term perspective of the overarching goal of nuclear physics which I posit as "If the Standard Model of Elementary Particles is correct, we should be able to accurately describe all nuclear processes." For our long-term goal, I propose that we aim to use all the fundamental interactions, including yet-to-be-discovered interactions, to construct a model for the evolution of the entire universe. In my view, the purpose of this international conference is to assess the current progress with theory and the associated supercomputer simulations that highlight our journey along this path.

Since my specific goal here is to address the question of the discovery potential using supercomputer simulations in nuclear theory, I will begin with my particular problem statement: solve the quantum many-body Hamiltonian with strong interactions. Here, I am including both the conventional non-relativistic nuclear many-body Hamiltonian formulation as well as the fully relativistic light-front Hamiltonian approach.

In order to provide one concrete set of examples, I show in Fig. 1 the projected goals of calculating the Nuclear Matrix Elements (NMEs) needed for interpreting experiments on neutrinoless double beta-decay. The goals are laid out along an axis of estimated computational resources needed to perform *ab initio* nuclear structure calculations that retain the predictive power of the underlying microscopic Hamiltonian. The need for reliable NMEs, free from phenomenology and associated uncertainties, to interpret the experimental data is well established [3].

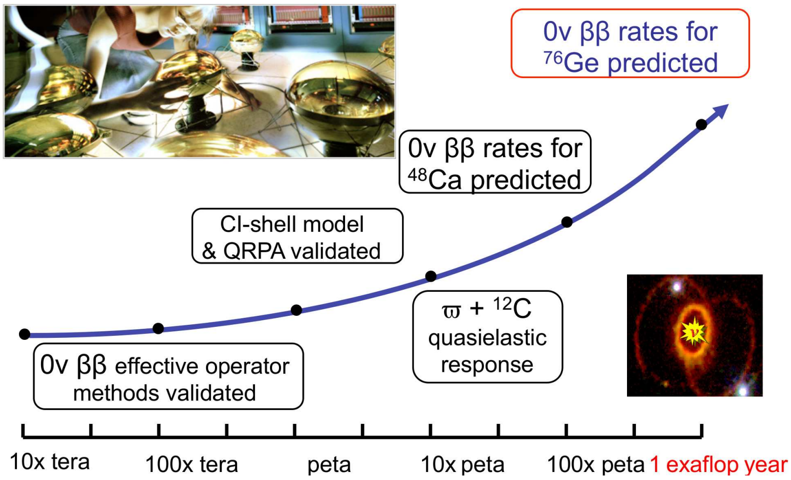

Figure 1: As more computational resources become available (horizontal axis in units of sustained flops × year) we anticipate the indicated research highlights will be achieved under the banner "Nuclei as neutrino physics laboratories" [2].

2 No Core Shell Model

The *ab initio* No Core Shell Model (NCSM) first appeared in Refs. [4,5] where realistic NN interactions, suitably renormalized to a finite Hamiltonian matrix in the harmonic oscillator (HO) basis, were employed to solve for the spectroscopy of ^{12}C in modest basis spaces that were nevertheless sufficient to demonstrate good convergence of the low-lying excitation spectra. Since that time, there has been rapid progress for increasing the basis space in order to address additional observables with increasing precision and to solve for the properties of a wide range of light nuclei. Recent progress has evolved along many semi-independent lines of research aimed at achieving improved accuracy and/or reducing the demands on computational resources.

Fig. 2 displays a snapshot of methods that have appeared that relate in some way

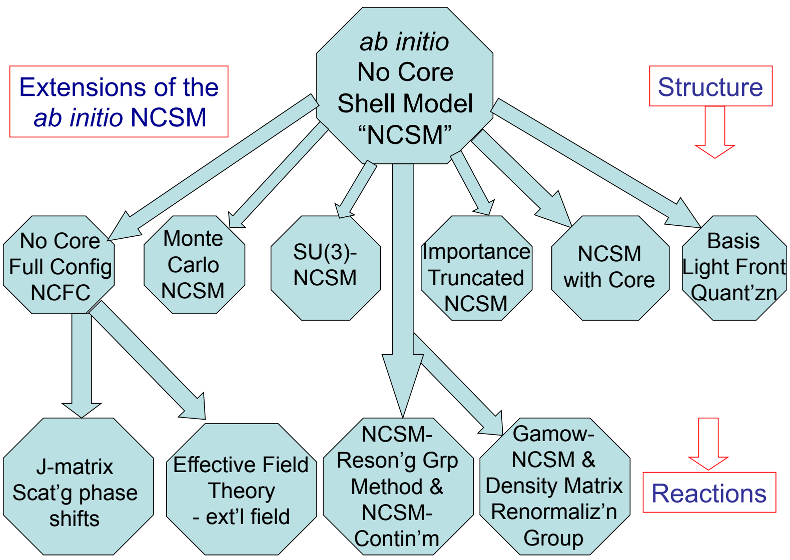

Figure 2: *Ab initio* No Core Shell Model with nuclear structure and nuclear reactions methods based on the NCSM [13]. See the text for additional details.

to the NCSM. At present, some address primarily nuclear structure applications while others address nuclear reactions. I will mention each with a short review.

Ref. [6] introduces the *ab initio* No Core Full Configuration (NCFC) method that adopts the given microscopic strong interaction suitable for an infinite basis space and performs a sequence of increasing finite basis space calculations. The NCFC then features an extrapolation to the infinite basis limit to arrive at the predicted spectra and observables. A significant success of this approach was the accurate prediction of the spectroscopy for the proton-unstable nucleus ^{14}F [7] which was later confirmed by an experiment at Texas A&M University [8]. For a recent review of applications to properties of p-shell see Ref. [9].

The Monte Carlo No Core Shell Model (MCSM) was recently introduced and benchmarked with the NCSM in Ref. [10]. The MCSM has advantageous scaling properties for solving heavier nuclei and is summarized by Abe at this conference [11]. To date, successful benchmark calculations have been performed for p-shell nuclei using the realistic NN interaction, JISP16 [12].

Light nuclei exhibit collective motion and this provides a challenge for the NCSM in a HO basis. This has motivated the development and application of the SU(3)-NCSM as summarized by Draayer [14] and by Dytrych [15] at this conference. In the SU(3)-NCSM one truncates the basis space by including only the leading irreducible representations of SU(3) that are motivated by the collective degrees of freedom dominating the low-lying eigenstates. This approach has led to successful *ab initio* descriptions of collective states in light nuclei with highly truncated basis spaces [16].

Roth and collaborators have introduced the Importance Truncated No Core Shell Model (IT-NCSM) in order to facilitate convergence by sampling larger basis spaces and retaining configurations making significant contributions to the low-lying eigenstates [17–19]. The prospects for this method are very strong and recent developments are presented by Roth at this meeting [20]

The drive to extend the *ab initio* NCSM to heavier nuclei has led to the development of a method that re-introduces the core in order to cut down on the basis space dimensions. Specifically, the *ab initio* Shell Model with a Core method [21, 22] carries out a second renormalization procedure to develop a valence-nucleon Hamiltonian suitable for solving nuclei beyond doubly-magic reference systems. The method is currently being developed for nuclei in the *sd*-shell [23].

Since these Hamiltonian many-body methods have shown great flexibility and applicability, it is natural to seek applications to subfields outside of nuclear structure and nuclear reactions. Not surprisingly, a parallel line of developments has emerged in Hamiltonian light-front field theory with a basis function approach. This has been termed Basis Light-Front Quantization (BLFQ) [24, 25] and several papers at this conference present results from this approach [26–28]. The central theme is that non-perturbative solutions of bound state and scattering problems are achievable in BLFQ and in a time-dependent BLFQ (tBLFQ) [29].

3 No Core Shell Model — applications to reactions

The *ab initio* theory of nuclear reactions has dramatically advanced in recent years based, in part, on the successes of the *ab initio* NCSM. Selected examples are listed on the bottom row of Fig. 2 showing their connections with related no-core structure methods. Space does not permit to review of additional *ab initio* reaction methods based on other *ab initio* structure methods such as the Green's Function Monte Carlo (GFMC) and Coupled Cluster (CC) methods.

The J-matrix inverse scattering approach has been introduced and employed with a HO basis representation to analyze scattering phase shifts and extract resonance energies and widths from experimental data. One of the main advantages of the J-matrix formalism is that it provides eigenstates directly related to the eigenstates of the NCSM in a given model space and with a given value of the oscillator spacing. In Ref. [30] we discussed the J-matrix inverse scattering technique, extended it for the case of charged colliding particles, and applied it to the analysis of $n-\alpha$ and to $p-\alpha$ scattering. We then compared the J-matrix eigenvalues extracted from experimental phase shifts with the NCSM calculations of ^{5}He and ^{5}Li based on the JISP16 NN interaction and found a remarkably good correlation between J-matrix eigenstates and the NCSM eigenvalues. We anticipate that with improved Hamiltonians that more accurately predict binding energies, the NCSM eigenstates will become predictive components of scattering phase shifts within the J-matrix formalism.

By employing the techniques of EFT and confining our scattering problem to an external HO potential, we may extract the elastic scattering phase shifts as demonstrated in Ref. [31]. An analytic expression that relates the eigenvalues of two interacting particles confined by a HO potential to the scattering phase shift at those energies, analogous to "Lüscher's method" [32,33] allows one to extract the phase shift in the limit that the oscillator length is large compared to the range of nuclear forces. The requirements for demonstrating high accuracy with the NN phase shift application [31] suggests more work is needed to reduce the computational requirements for this method.

Major efforts are underway to develop and apply a hybrid NCSM and Resonating Group Method (RGM) approach called NCSM/RGM [34–36]. The aim is to simultaneously describe both bound and scattering states in light nuclei by combining these two approaches. The goal is to eventually achieve *ab initio* descriptions of scattering and reactions of two light nuclei with three-body breakup channels included [37].

Another major set of efforts aims to develop and apply the Gamow Shell Model (GSM) [38, 39] where a discretized representation of continuum single-particle states are included with conventional bound single-particle states in the many-body basis. The first *ab initio* no core Gamow Shell Model (NCGSM) application has recently appeared [40] and shows great promise for producing *ab initio* descriptions of resonances in light nuclei.

The field of *ab initio* nuclear reaction theory is emerging as a vibrant area of activity with many new ideas showing great promise. For example, direct calculation of microscopic reaction amplitudes in an extended NCSM approach is under intensive investigation [37, 41, 42].

4 Selection of recent results

Since this conference features many excellent talks presenting results from the theoretical approaches that I outlined above as well as from additional *ab initio* approaches, I will select a few examples to illustrate some recent results that complement those discussed by others. The results that I select use realistic interactions from chiral EFT and from inverse scattering.

However, before diving into these results it is also worthwhile to survey the landscape of the research closely related to the *ab initio* approaches, their goals and the computational issues associated with them. This is best illustrated in Fig. 3 that overviews the current research activities in the SciDAC-NUCLEI project [43], a set of collaborations among nuclear theorists, computational scientists and applied mathematicians supported by DOE. Clearly, there is a broad scope of linked research efforts depicted and that scope requires a large set of collaborative enterprises to be successful.

In a recent effort, we examined the properties on $A = 7$ and 8 nuclei in the NCSM [44]. We compared results with chiral NN interaction only [45, 46] and those with chiral $NN+NNN$ interactions [47] (in the local form of Ref. [48]) using $N_{\max} = 8$

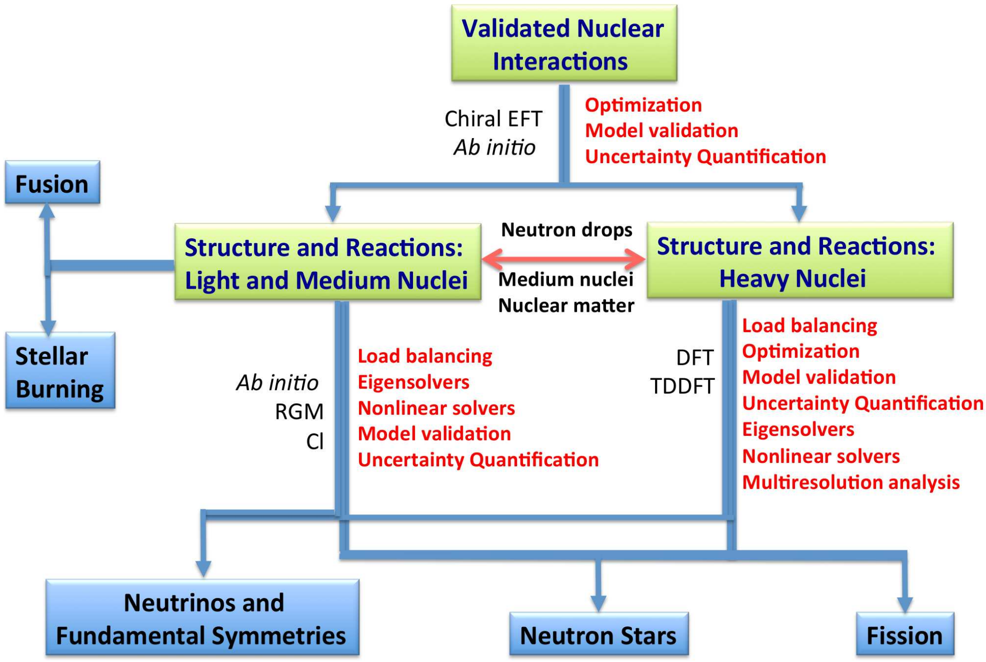

Figure 3: Overview of the workflow of the SciDAC-NUCLEI project [43]. The items in red identify computational and applied mathematics topics related to that particular branch of the workflow. Note that the links extend from fundamental interactions based on QCD at the top to large amplitude nuclear phenomena at the bottom and on the left.

basis spaces. Note that the chiral NN interaction is complete though N3LO while the chiral NNN interaction is complete through N2LO. These are the most advanced chiral interactions available at the present time.

We showed [44] that including the chiral EFT NNN interaction in the Hamiltonian improves overall agreement with experimental binding energies, excitation spectra, transitions and electromagnetic moments. We also predicted states that exhibit sensitivity to including the chiral EFT NNN interaction but are not yet known experimentally.

In order to soften the chiral interactions to render them suitable for the many-body basis spaces currently accessible, we adopted the Okubo–Lee–Suzuki (OLS) [49, 50] renormalization procedure. We review this and alternative renormalization procedures in detail in Ref. [13]. It is worth remarking that the OLS renormalization approach generates induced multi-nucleon interactions that are needed to preserve many-body unitarity. It is our practice to date to retain at most the induced NNN interactions along with the initial NNN interactions. That is, we ignore the induced $4N$ interactions as well as higher-body interactions. While all indirect signs (such as convergence trends) are encouraging, there is a definite need to further investigate this approximation in the future by retaining induced $4N$ interactions.

One should also note there are a number of additional freedoms in the OLS procedure [51, 52] as, indeed, there are in other renormalization procedures. First, there is the choice of the states from the full space calculations with non-vanishing components in the model space. This choice goes into the definition of the similarity transformation and is not unique. Second, there is the additional freedom of a unitary transformation of the resulting effective Hamiltonian within the model space [52]. Third, there is the freedom in the selection of an additional interaction to add and subtract at various stages of the solution of the decoupling equations. The second and third freedom are related. These freedoms remain as opportunities for future

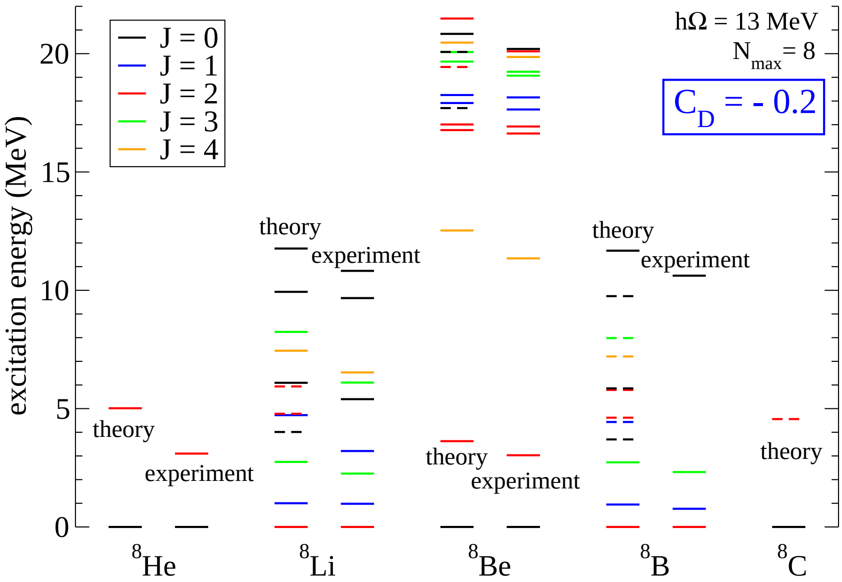

Figure 4: *Ab initio* No Core Shell Model results for $A = 8$ nuclei using chiral $NN + NNN$ interactions in an $N_{\max} = 8$ HO basis with HO energy $\hbar\Omega = 13$ MeV. The solid lines indicate states that are identified both in the theory and the experimental results. The dashed lines indicate additional states predicted by the theory. See the text and Ref. [44] for additional details.

investigations.

While the binding energies are generally close to agreement with experiment, it is easier to view the comparison between theoretical and experimental spectra by lining up the energies of the ground states and displaying just the excitation energies. Therefore, we show in Fig. 4 the excitation spectra of the $A = 8$ nuclei where we compare theory and experiment. For the chiral NNN interaction we adopt the low-energy constants (indicated by $c_D = -0.2$ on the figure) that are tuned to the binding energy and half-life of tritium [53]. The states predicted by the theory, for which there is no apparent experimental counterpart, appear as dashed lines in Fig. 4. Note that these states are in the continuum. We interpret the energies of these states as indications of the resonance widths but we are not able to predict the widths themselves at the present time. We expect that the predictions will be more accurate for the states with narrow widths. We plan to implement the continuum physics in the future and to predict the widths of states appearing above breakup threshold. Among the many options we are considering, several are well-represented here at this meeting [38–41, 54].

In another set of investigations, we have adopted the Similarity Renormalization Group (SRG) [55, 56] approach for decoupling the high momenta components of the inter-nucleon interactions from the low momenta components. As in the OLS renormalization approach mentioned above, this is intended to facilitate convergence of the *ab initio* many-body calculations at the “cost” of calculating induced multi-nucleon interactions and of requiring a corresponding treatment of other operators corresponding to observables that we intend to evaluate with the resulting *ab initio* wavefunctions. We have investigated the detailed predictions and the convergence properties of no-core full configuration calculations with SRG-evolved interactions in p-shell nuclei over a wide range of softening [57, 58]. The dependence on the degree of softening (the SRG resolution scale) allows us to assess convergence properties, to investigate extrapolation techniques, and to infer the role of neglected induced higher-body contributions.

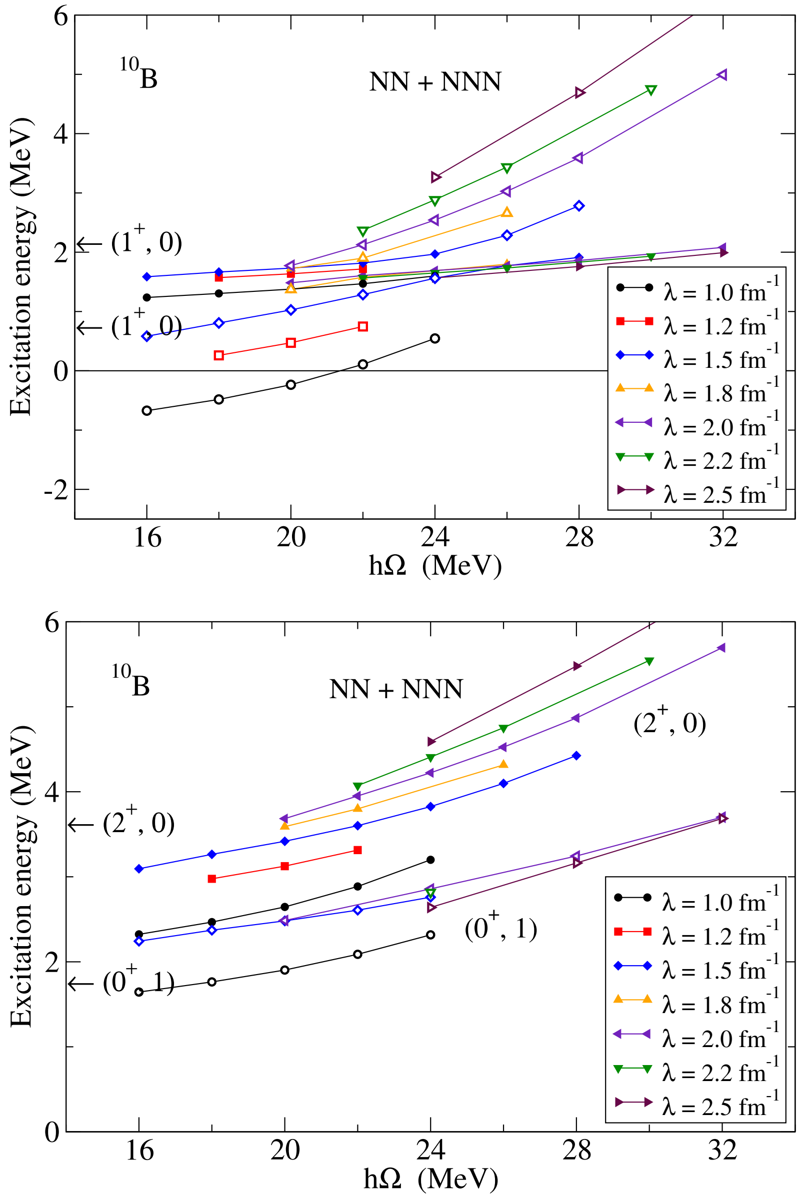

Figure 5: Lowest excited states of ^{10}B as a function of $\hbar\Omega$ for each SRG λ value at $N_{\max} = 8$. The small black arrows on the left shows the experimental values. Each color and shape of the symbol represents a value of λ as defined in the legend. Two excited states are shown in each panel, one with an open symbol and the other with a closed symbol. See Ref. [58] for additional details.

Here, we use the same chiral $NN + NNN$ interaction as in the applications to $A = 7$ and 8 nuclei discussed above using the OLS renormalization. In this case, we are using SRG with a range of evolution scales, λ from 2.5 fm^{-1} down to 1.0 fm^{-1}. This evolution scale dictates the approximate range of momentum transfer retained in the NN T-matrix while preserving the on-shell phase shifts. Generally speaking, we expect induced NNN interactions to increase as we decrease λ. Experience with these chiral $NN + NNN$ interactions indicates non-trivial induced NNN interaction contributions even with $\lambda = 2.5$ fm^{-1}.

Once we adopt the approximation to retain the induced NNN interactions but to neglect induced $4N$ interactions, it is natural to retain the "bare" chiral NNN interaction defined by the underlying chiral EFT. Figure 5 presents a sample of excited states in ^{10}B relative to the lowest calculated $(3^+, 0)$ state which is the experimental ground state. Note that the ground state spin for ^{10}B has become a highly-cited example of an observable that is sensitive to the inclusion of NNN interactions [59]. Realistic NN interactions, without NNN interactions, tend to predict a ground state spin of $(1^+, 0)$. We see in the upper panel of Fig. 5 that the correct ground state spin is obtained, within the results shown, for all but one value of the SRG λ scale parameter over the range of $\hbar\Omega$ depicted. The spread in the predictions as a function of λ and the dependence on $\hbar\Omega$ are indicators of the role of neglected induced $4N$ and/or higher-body interactions. Thus, with these $N_{\rm max} = 8$ results in the SRG treatment, it is not reliably established that the NNN interactions produce the correct ground state spin of ^{10}B. Clearly more work is needed to include the induced $4N$ interactions which we expect to produce stronger indication of the fully converged result.

Another feature evident in the upper panel of Fig. 5 is the difference in the trends of two states with the same spin and parity $(1^+, 0)$ in ^{10}B. One state appears to be better converged than the other — that is less reliant on induced 4-body interactions and/or basis space increases. This indicates that these two states have very different structure. A more detailed analysis is needed to disentangle those differences. For example, future work may reveal that the "spin content" of these two states, when decomposed into neutron and proton spin and orbital components as in Ref. [9] for other states in other systems, is distinctively different.

The lower panel of Fig. 5 displays the excitation energy of the $(0^+, 1)$ and $(2^+, 0)$ states compared with experiment. The former appears to be less sensitive to the SRG λ scale parameter, indicating less sensitivity to neglected induced $4N$ interactions. Both states reveal approximately the same dependence on the basis $\hbar\Omega$ indicating approximately the same level of convergence with increasing basis space cutoff $N_{\rm max}$.

The residual discrepancies between theory based on chiral EFT and experiment, as seen in the results presented here as well as many other results presented at this meeting, are indicators of shortcomings of the present chiral EFT interactions. At present, we use chiral NNN interactions only at N2LO while the NN interactions are at the level of N3LO, which was found important for an accurate description of the NN phase shift data. Thus, we will have consistency once we include the chiral NNN interaction itself at N3LO so that it is at the same order of chiral perturbation theory as the NN interaction. In this context, it is worth noting the large-scale international efforts that are underway to develop and apply these next-generation chiral EFT interactions [60]. Here again, a workflow diagram (see Fig. 6 is useful to illustrate the complexity and diversity of such a project. This workflow indicates the multifaceted challenges and the need for bringing the expertise of many groups into the project to achieve the project goals.

In closing this section with a sample of recent results that help indicate future directions, I will briefly discuss the challenges of clustering phenomena in light nuclei. These phenomena are a particular challenge to the *ab initio* NCSM since clustering implies intermediate range correlations which require large HO basis spaces for accurate descriptions [61,62]. For the Hoyle state, the $(0^+, 0)$ state at 7.66 MeV excitation energy in ^{12}C which is just above the threshold for breakup into three alpha particles, the predominant thinking is that it is dominated by a three-alpha cluster and is the leading resonance for ^{12}C production in astrophysical settings. Many cluster-based models provide successful descriptions of the Hoyle state with the three-alpha configuration. Currently, our hope for extending the *ab initio* NCSM within the HO basis to describe cluster states, like the Hoyle state, is to adopt the SA-NCSM or the MC-NCSM approach discussed above.

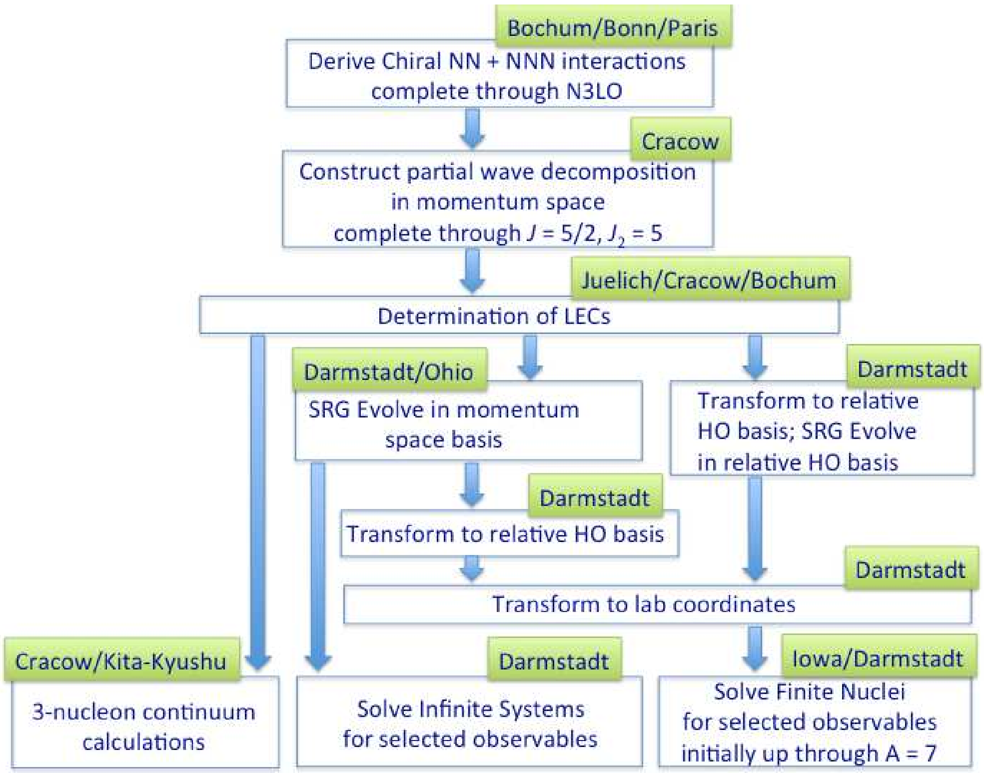

Figure 6: Workflow for the Low Energy Nuclear Physics International Collaboration (LENPIC) showing the development and implementation of the next-generation chiral EFT interactions complete and consistent through Next-to-Next-to-Next-to Leading Order (N3LO). See the text and Ref. [60] for additional details.

5 Reaching for the infinite basis limit

There has been intense recent activity addressing the convergence properties of *ab initio* no-core approaches [63–68]. Clearly, understanding the convergence properties will help us predict results with greater precision using the available computational resources and will help us quantify the uncertainties in these predictions.

While most of this research has focused on extrapolating the ground state energy obtained in a no-core approach within the HO basis to the infinite basis limit, there is also considerable progress in understanding the convergence properties of the root-mean-square (rms) radius. Electromagnetic matrix elements are of particular interest since they are challenging to describe in the HO basis as they are, typically, long-range operators that are sensitive to the asymptotic properties of the nuclear wavefunction. For this reason, the rms radius has served as the initial testing ground for the long-range electromagnetic operators.

For the ground state energy, a simple exponential in $N_{\rm max}$ at fixed $\hbar\Omega$ has proven to be a useful extrapolation tool [6, 58, 69]. Current thinking implies this is a useful phenomenological extrapolation tool for the ultraviolet (UV) properties but a different functional form, a simple exponential in $\sqrt{N_{\rm max}}$ is theoretically supported for the infrared (IR) properties [65]. The physical argument for the IR behavior of the wavefunction is appealing — we know from elementary quantum mechanics that the long-range tail of a single-particle wavefunction for a bound state in a finite potential well has an exponential form with a decay constant dictated by the binding energy. The step to the many-body problem involves examining the highest HO single-particle state in the basis and identifying the appropriate exponential tail for that state as it will dominate the longest range component of the many-body wavefunction. Following, the *ab initio* results through a sequence of many-body cutoffs (i. e. systematically raising the highest HO single-particle state in the basis) allows one to optimize the choice of the constants that go with this exponential in $\sqrt{N_{\max}}$

Let us examine the case of the ground state energy of ^{6}Li calculated in the *ab initio* NCSM with the bare JISP16 interaction [12] as a function of the many-body cutoff $N_{\max}$. This same case was examined in some detail in Refs. [6, 70] and a recent extrapolation has been presented in Ref. [9]. Each of these papers extends the preceding paper either with results calculated at higher $N_{\max}$ values to reduce the uncertainties or with improvements in the uncertainty estimation procedure. Each uses the simple exponential in $N_{\max}$ (i. e. phenomenological form alone) for the fit function. The results are consistent with each other — that is the fall within each others' uncertainty estimates: -31.45 ± 0.05 MeV in Ref. [6] with the maximum $N_{\max} = 14$; -31.49 ± 0.03 MeV in Ref. [70] with the maximum $N_{\max} = 16$; -31.49 ± 0.06 MeV in Ref. [9] with the maximum $N_{\max} = 16$. Note that the experimental ground state energy is -31.994 MeV so JISP16 is clearly underbinding this nucleus by about 0.5 MeV.

A new set of calculations is underway to extend the calculated results to $N_{\max} = 18$ and to further improve the extrapolation procedure by combining both a phenomenological function for the UV and the derived function for the IR. In addition to the ground state energy, extrapolations of the rms radii will be included. The aim is to further reduce the quantified uncertainties by relying on additional theoretical input.

Figure 7 provides an indicator of recent progress in the research on extrapolation methods. Here, I am following the line of developments introduced as "Extrapolation A" in Ref. [6]. In this approach, one identifies the minimum in the ground state energy as a function of $\hbar\Omega$ for each $N_{\max}$ beginning with $N_{\max} = 8$ where one works with increments of 2.5 MeV in $\hbar\Omega$. Then one uses the the 5 consecutive data sets spanning 10 MeV in $\hbar\Omega$ that begin with the $\hbar\Omega$ value below that minimum and extend

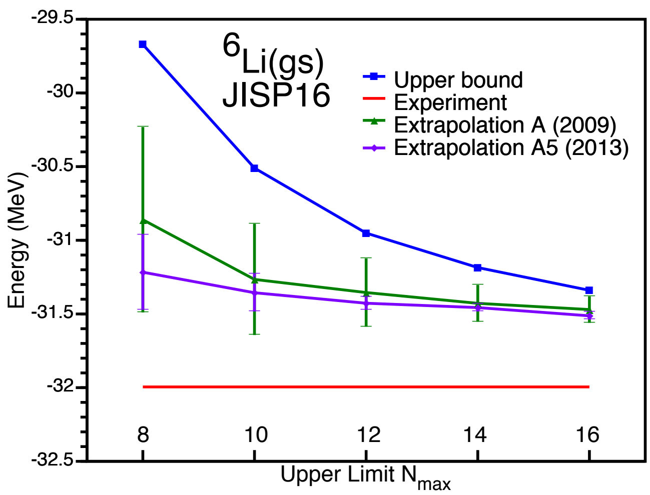

Figure 7: Extrapolations of the *ab initio* No Core Shell Model ground state energy for ^{6}Li using the JISP16 NN interaction [12] as a function of the upper limit on the $N_{\max}$ cutoff of the energies used in the extrapolation. "Extrapolation A (2009)" is the quantity E_∞ from Eq. (1) as reported in Ref. [6]. "Extrapolation A5 (2013)" employs an improved UV + IR functional form using 5 free parameters that is under development. For reference, the variational upper bound (minimum in the ground state energy as a function of $\hbar\Omega$) is shown for each $N_{\max}$ providing a sense of the magnitude of the extrapolation. The A5 extrapolation is -31.51 ± 0.03 MeV at $N_{\max} = 16$. See the text for additional details.

to larger values of $\hbar\Omega$. Results at the 3 increments in $N_{\max}$ below that upper limit in $N_{\max}$ are also included yielding a total of 20 calculated ground state energies (4 $N_{\max}$ values and 5 $\hbar\Omega$ values) for determining the 3 fit parameters of the function:

$$E(N_{\max}) = E_\infty + a\exp(-bN_{\max}). \tag{1}$$

For Extrapolation A, one then uses Eq. (1) to fit the 4 ground state energies at each of the 5 $\hbar\Omega$ values separately. This determines a spread of the values of E_∞ and half of that spread is defined as the uncertainty in the Extrapolation A result at that upper limit in $N_{\max}$. This procedure was tested extensively with JISP16 results for ground state energies of light nuclei and the evaluated uncertainties were found to be consistent with each other with increasing upper limit in $N_{\max}$ [6]. This is seen in Fig. 7 by the overlapping error bars of the Extrapolation A points.

Extrapolation A5 builds on the experience with Extrapolation A and includes an additional term to better simulate the IR behavior as motivated by the developments of Refs. [63, 65, 67]. That is, I adopt a 5 parameter function which, for sufficiently large $N_{\max}$ can be represented by:

$$E(N_{\max}) = E_\infty + a\exp(-bN_{\max}) + c\exp\Big(-b\sqrt{N_{\max}}\Big). \tag{2}$$

The detailed functional form of the IR term added in Eq. (2) $\Big[\exp\Big(-b\sqrt{N_{\max}}\Big)\Big]$ is more involved since it closely follows the forms advocated in Ref. [67]. However, the difference effects mainly the behavior at lower $N_{\max}$ and I use Eq. (2) to indicate the primary dependence at large $N_{\max}$.

Since two more parameters must now be determined, the procedure defined in Ref. [6] is further extended in several ways. First, I include 5 sets of $N_{\max}$ at each of 5 $\hbar\Omega$ values. The range of the $\hbar\Omega$ values is shifted upwards by +5 MeV compared to Extrapolation A as this was found to produce more reliable in tests with ground state energy results in ^{4}He. The need for 5 sets of $N_{\max}$ values is clear in order to adequately determine the spread in a manner analogous to the spread determination in Extrapolation A. The data point for Extrapolation A5 at the upper limit $N_{\max} = 8$ is a special case as I continue the practice of omitting the $N_{\max} = 0$ calculated ground state energies in the fits. For $N_{\max} = 8$, the total data set is then only 20 calculated points. The uncertainty assigned to the data point at the upper limit $N_{\max} = 8$ for Extrapolation A5 is simply taken to be twice the uncertainty calculated for the next higher data point in Fig. 7.

Note that Extrapolation A and Extrapolation A5 produce results that are consistent with each other — that is they fall within each others' uncertainties. However, both Extrapolation A and Extrapolation A5 produce a noticeable downward drift in the values of E_∞ with increasing upper limit in $N_{\max}$. This indicates the need for additional research to develop improved extrapolation forms and procedures.

6 Conclusion and Outlook

Computational physics and forefront simulations have developed rapidly to become one of the key areas of research in nuclear physics, approaching a par with experiment and theory. Many breakthroughs in our understanding of fundamental nuclear processes have emerged from recent advances and any listing would not do justice to the field. In fact, I have generated with the help of colleagues, a list of more than 90 Physical Review Letters to date that have focused on *ab initio* nuclear structure and nuclear reactions. Many of these are joint experiment and theory letters. Therefore, I will simply select examples that specifically focus on the developing bridge provided by chiral EFT between QCD and low-energy nuclear properties. Each of these achievements, indicated in the title, is the focus of a Physical Review Letter that appears below in a chronological sequence.

1. "The three nucleon and four nucleon systems from chiral effective field theory" [71].
2. "Structure of $A = 10{-}13$ nuclei with two plus three-nucleon interactions from chiral effective field theory" [59].
3. "*Ab Initio* many-body calculations of n-^{3}H, n-^{4}He, p-^{3,4}He, and n-^{10}Be scattering" [34].
4. "Medium-mass nuclei from chiral nucleon-nucleon interactions" [72].
5. "Evolution of nuclear many-body forces with the Similarity Renormalization Group" [73].
6. "Three-nucleon low-energy constants from the consistency of interactions and currents in Chiral Effective Field Theory" [53].
7. "Ground-state and single-particle energies of nuclei around ^{16}O, ^{40}Ca, and ^{56}Ni from realistic nucleon-nucleon forces" [74].
8. "Role of long-range correlations on the quenching of spectroscopic factors" [75].
9. "Lattice effective field theory calculations for $A = 3$, 4, 6, 12 nuclei" [76].
10. "*Ab initio* computation of the ^{17}F proton halo state and resonances in $A = 17$ nuclei" [77].
11. "Constraints on neutron star radii based on chiral effective field theory interactions" [78].
12. "Thermal neutron captures on d and ^{3}He" [79].
13. "*Ab initio* calculation of the Hoyle state" [80].
14. "Origin of the anomalous long lifetime of ^{14}C" [81].
15. "In-medium Similarity Renormalization Group for open-shell nuclei" [82].
16. "Quenching of spectroscopic factors for proton removal in oxygen isotopes" [83].
17. "Similarity-transformed chiral NN+3N Interactions for the *ab initio* description of ^{12}C and ^{16}O" [84].
18. "Measurements of the differential cross sections for the elastic n-^{3}H and n-^{2}H scattering at 14.1 MeV by using an inertial confinement fusion facility" [85].
19. "Chiral two-body currents in nuclei: Gamow–Teller transitions and neutrinoless double-beta decay" [86].
20. "*Ab initio* many-body calculations of the ^{3}H$(d,n)^4$He and ^{3}He$(d,p)^4$He fusion" [87].
21. "First direct mass measurement of the two-neutron halo nucleus ^{6}He and improved mass for the four-neutron halo ^{8}He" [88].
22. "Continuum effects and three-nucleon forces in neutron-rich oxygen isotopes" [89].
23. "Evolution of shell structure in neutron-rich calcium isotopes" [90].
24. "New precision mass measurements of neutron-rich calcium and potassium isotopes and three-nucleon forces" [91].
25. "Medium-mass nuclei with normal-ordered chiral $NN + 3N$ interactions" [92].

26. “Structure and rotations of the Hoyle state” [93].

27. “Three-body forces and proton-rich nuclei” [94].

28. “*Ab initio* description of the exotic unbound ^{7}He nucleus” [95].

29. “Neutron matter at next-to-next-to-next-to-leading order in chiral effective field theory” [96].

30. “Spectroscopy of ^{26}F to probe proton-neutron forces close to the drip line” [97].

31. “The isoscalar monopole resonance of the alpha particle: a prism to nuclear Hamiltonians” [98].

32. “Viability of carbon-based life as a function of the light quark mass” [99].

33. “An optimized chiral nucleon-nucleon interaction at next-to-next-to-leading order” [100].

34. “*Ab initio* calculations of even oxygen isotopes with chiral two- plus three-nucleon interactions” [101].

35. “Quantum Monte Carlo calculations with chiral effective field theory interactions” [102].

36. “Isotopic chains around oxygen from evolved chiral two- and three-nucleon interactions” [103].

37. “First principles description of the giant dipole resonance in ^{16}O” [104].

These are indicators of a broader set of recent achievements that portend the discovery opportunities in computational nuclear physics. Continued close collaboration among nuclear theorists, computational scientists and applied mathematicians will be essential to fully exploit the potential of the rapid growth in computational resources. These collaborations are critical to devising new algorithms and their efficient realizations in order to generate and capitalize upon the full discovery potential. Further close collaboration with experimentalists is needed to fully exploit the predictive power that is emerging along with the opening of new frontier experimental facilities in order to devise and plan critical tests of the theoretical foundations. Joint planning activities will be valuable to efficiently utilize personnel, computational resources and experimental facilities in order to maximize the discovery potential of the field.

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