NTSE-2013 Summary Talk:

Conference Summary

Bruce R. Barrett

Department of Physics, PO Box 210081, University of Arizona, Tucson, AZ 85721-0081

Abstract

The conference summary observes how the presented talks reflect the diverse research interests of Professor James P. Vary and how, as a whole, they lead to the underlying goals of the International Conference on Nuclear Theory in the Supercomputing Era — 2013.

Keywords: *Conference summary; goals; high performance computing; light front quantization; ab initio nuclear theory*

1 Introduction

As the schedule for the International Conference on Nuclear Theory in the Supercomputing Era — 2013 (NTSE-2013) clearly shows, this was an exciting, diverse and highly informative conference, reflecting, appropriately, the research interests of Professor James P. Vary, the meeting honoree, on his 70th birthday. (See the conference schedule of presented talks, appearing earlier in these proceedings.) Looking back on the 50 talks presented over the last five days, I see the synthesis of the three major themes of this meeting, i. e., 1) High Performance Computing, 2) from Quantum Chromodynamics (QCD) to Nuclear Structure, and 3) *ab initio* Nuclear Structure and Reaction Theory, into one underlying goal, or *physics driver*, as James would say. I would state this goal as "the collaboration of computer scientists and nuclear physicists (both theorists and experimentalists) to determine the nucleon-nucleon (NN) and higher-nucleon interactions, based on QCD, and to use these interactions in microscopic calculations of nuclear properties for structure and reactions with predictive power and error quantification," i. e., we want a reliable, predictive theory of nuclei with proper error estimates.

One could say that James' research program is like a three-legged stool, in which all three legs are necessary in order to have a stable, final entity. I will consider these three legs in the order given in the previous paragraph, instead of the order of the talks, as given during the conference.

2 High performance computing: Large scale computational science in support of nuclear physics

Speakers: {Ng, Çatalyürek, Fann, Nam, Sosonkina, Yang}

Performing calculations at the forefront of computing technology has always been a priority for James Vary, so it is no surprise that he quickly adapted to the new

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

paradigm that physical scientists will need to collaborate with computer scientists, if the former want to take full advantage of the new developments in computer hardware and software.

Exascale computing is coming, roughly between 2016 and 2020. When it does arrive, it will produce a time of disruptive change. Although it will be difficult and challenging, it will also be a *perfect storm* of opportunities for new investigations. As the speakers in this section made clear, collaborations between nuclear theorists and computer scientists will be crucial in the exascale era. Or as one slide in the keynote talk by Esmond Ng indicted — in the form of a demonstrator with a sign reading "Collaborate or Die!".

Even though there is much to do to get ready for the exascale era, we should remember that high performance computers, such as Titan, currently exist, as well as Graphics Processing Units (GPUs). These tools should be used now for training and preparation for the exascale era.

3 From Quantum Chromodynamics to nuclear structure

The scales of nuclear physics go from the quark and gluon degrees of freedom to those of the nucleons, the interactions among the nucleons and nuclear structure. One of the principal goals of nuclear physics is to unite the physics of quarks and gluons, i. e., Quantum Chromodynamics in the form of the QCD Lagrangian, with nuclear structure, i. e., the physics of nucleons and mesons in nuclei. Two approaches to achieving this goal were discussed during NTSE-2013: 1) Lattice Gauge Theory (or Lattice QCD) and 2) Light Front QCD.

3.1 Lattice QCD

Speakers: {Savage, Qiu}

In recent years, significant progress and advances have been made in Lattice QCD. As the keynote talk by Martin Savage made clear, everything that is required to do calculations at the physical quark masses now exists. What is required are *more* resources in order to perform these calculations. Doing this will allow Lattice QCD, combined with chiral Effective Field Theory and nuclear many-body techniques, to provide first principles, predictive capabilities for nuclear physics with quantifiable uncertainties. Consequently, the main, outstanding problem for nuclear physicists is to determine how to optimally match the results of Lattice QCD calculations, namely, well-calculated energy eigenvalues, to the nuclear many-body machinery. This is a current, major problem of interest in nuclear physics and rapid progress is being made in attacking it.

3.2 Light front QCD

Speakers: {Brodsky, Chakrabarti, Honkanen, Karmanov, D. S. Kulshreshtha, U. Kulshreshtha, Li, Vary, Wiecki, Zhao}

The second approach, Light Front QCD, is the method being investigated by James Vary and his collaborators. The keynote talk on this topic by Stanley Brodsky emphasized the fact that AdS + Light Front Holography yields an analytic first approximation to QCD, which is as simple as Schrödinger theory in atomic physics. This talk was then followed by a number of presentations by Iowa State University physicists and other collaborators on numerous applications of this Basic Light Front Quantization.

4 *Ab initio* nuclear structure and reaction theory

I will divide this section into three major parts: 1) the efforts to determine the fundamental interactions among the nucleons, 2) many-body nuclear-structure theory and experiment, and 3) nuclear-reaction theory and experiment: scattering, reactions, loosely bound/unbound nuclei.

4.1 NN, NNN, and higher-N interactions

Speakers: {Machleidt, Epelbaum, Polyzou, Sauer}

The keynote talk by Ruprecht Machleidt gave a comprehensive overview of the origin and properties of strong inter-nucleon interactions, both historically and theoretically. One of the facts, which was clearly brought forward at this conference, is that the field of nuclear physics is still waiting for QCD based strong interactions, i. e., based on lattice QCD and/or Light Front QCD. Until then, one will need to use the best-fit NN and NNN interactions to the scattering data. Fortunately, the new POUNDerS (Practical Optimization Using No Derivatives) routine is now providing truly high quality fits to the experimental data.

Talks at this meeting also pointed out that NN and NNN interactions derived from Effective Field Theory and Chiral Perturbation Theory (CPT) still have some unresolved problems, which need to be addressed. In this regard, the important role of NNN interactions in understanding nuclear structure microscopically has become apparent. Consequently, CPT NN interactions need consistent NNN interactions at the same order, e. g., next-to-next-to-next-lowest order (N3LO). There is also the problem of whether or not to include deltas into the CPT expansion.

4.2 Many-body nuclear-structure theory and experiment

Speakers: {Hagen, Draayer, Abe, Bogner, Caprio, Carlson, Coon, Dean, Dytrych, Furnstahl, Ginocchio, Hjorth-Jensen, Kim, Maris, Miller, Otsuka, Pieper, Papenbrock, Roth, Rotureau, Schwenk, Sosonkina, Tuchin, Vary, Weidenmüller, Wiringa}

As pointed out in the keynote presentation by Gaute Hagen, many excellent *ab initio* nuclear many-body approaches now exist, such as, Quantum Monte Carlo, Lattice EFT, NCSM (both Effective Interaction and Configuration Interaction), Monte Carlo NCSM, NCSM with the Continuum (NCSMC), NCSM with a Core, NC-Gamow-SM (NCGSM), Coupled Cluster method (CCM), In-Medium Similarity Renormalization Group (SRG), Self-Consistent Green's Functions, Effective Interaction Hyperspherical Harmonics method, etc. All these methods compete with each other and at the same time complement each other. As such, it is definitely time to start new benchmark calculations among these different approaches, such as between the In-Medium SRG and the NCSM with a Core and among the NCSMC, the NCGSM and the CCM with the Berggren basis.

The important role of symmetry in understanding nuclear structure and the strong interaction was emphasized in the keynote talk by Jerry Draayer. Nuclear shell models and nuclear collective models were shown to be complementary methods. This led to the application of symmetry approaches to the NCSM, in what is known as the Symmetry Adapted NCSM (SA-NCSM), which builds on the exact and approximate symmetries of nuclei.

These improved many-body techniques along with the latest high-performance computers have made much more accurate calculations possible. These results coupled with theory-guided extrapolation methods have made possible theoretical predictions with quantified error estimates. Consequently, it is now possible to perform calculations to guide future experiments and to make meaningful predictions in *terra incognita*.

As mentioned earlier, collaborations between nuclear theorists and computer scientists play a crucial role in these calculations and have proven to be most beneficial. Indeed, supercomputing has become an essential part of nuclear theory.

4.3 Nuclear-reaction theory and experiment: Scattering, reactions, loosely bound/unbound nuclei

Speakers: {Navrátil, Hill, Leidemann, Polyzou, Rotureau, Shirokov}

The keynote address by Petr Navrátil presented an overview of some of the numerous *ab initio* approaches that now exist for studying nuclear reactions, such as the NCSM + Resonating Group Method (NCSM/RGM), the NCSMC, the QMC/GFMC, the CCM with Berggren basis, the Fermionic Molecular Dynamics (FMD) approach, etc., while other talks discussed approaches, such as the Lorentz Integral Transform + Effective Interaction Hyperspherical Harmonics (LIT/EIHH) method, the LIT/NCSM, the Gamow Shell + NCSM (NCGSM), etc. Significant progress has been made with the NCSM/RGM and NCSMC approaches, which can now include NNN forces and can handle three-body clusters. The LIT approach has the advantage of having a controlled resolution, and it can also be used for *ab initio* calculations far into the continuum. The NCGSM and the CCM methods have demonstrated the usefulness of the Berggren basis for including the continuum into nuclear structure and reaction calculations.

5 Summary of recent advances

I list below a few of the numerous recent advances in *ab initio* microscopic nuclear structure and reaction theory. Although it is an impressive list, it is far from being a complete list.

1. Petascale computers and GPUs
2. Increasing collaborations among nuclear theorists and computers scientists
3. First basis Light Front Quantization applications
4. Lattice QCD calculations with physical masses
5. Best fit (POUNDerS) NN interactions
6. Many excellent *ab initio* many-body methods
7. In-Medium SRG approach and results
8. UV and IR limits and extrapolations of results
9. NCSM/RGM and NCSMC with three-body clusters
10. New *ab initio* methods for nuclear-reaction theory

6 Some remaining challenges

As in Section 5, I will simply list a few of the remaining challenges that are faced in *ab initio* nuclear structure and reaction theory. As before, this is only a partial list of such challenges.

1. Making the transition to exascale computers, GPUs, etc.
2. Finding the resources for Lattice QCD calculations with the physical pion mass
3. Determining how to link Lattice QCD and LFQCD with the nuclear many-body machinery
4. Obtaining consistent NN and NNN interactions for all current potential approaches (AV18, EFT/CPT interactions, etc.)
5. Extending successful *ab initio* approaches for $0p$-shell nuclei to heavier mass nuclei
6. Developing error quantification for theoretical results
7. Establishing new collaborations, especially with computer scientists
8. And most important of all, recruiting more young physicists into nuclear-physics research

7 Conclusions

The talks at this conference, along with the honoring of James Vary on his 70th birthday, have reminded me of the closing statement by my *Thesis Grandfather*, Victor F. Weisskopf, i. e., the thesis advisor of my thesis advisor, in his summary talk for the International Conference on Nuclear Structure, held in Kingston, Canada, August 29 to September 3, 1960.

"But don't let yourself be talked into believing that the nucleus is not interesting. It is so small and it has so few parts and still it shows a tremendous variety of phenomena. Its investigation requires the whole arsenal of presently available experimental techniques and its understanding makes use of almost all branches of theoretical physics. What a marvelous invention! It is worth devoting a lifetime to it." [1].

James Vary has, indeed, devoted his professional life to this challenging system. We all wish him many more years of excellent health and excitement, as he continues this task. Happy 70th birthday, James!

References

[1] V. F. Weisskopf, in *Proc. Int. Conf. Nuclear Structure, Kingston, Canada, August 29 — September 3, 1960*, edited by D. A. Bromley and E. W. Vogt. University of Toronto Press, Toronto, 1960, p. 905.