Computational Nuclear Physics Town Meeting

SURA Headquarters, Washington DC, July 23-24, 2012

REPORT

Prepared by the Computational Nuclear Physics Town Meeting Organizing Committee

A. Burrows, J. Carlson, R. Edwards, W. Nazarewicz, P. Petreczky, D. Richards, M. J. Savage

1 Preamble

Large scale numerical calculations in theoretical nuclear physics play an increasingly prominent role in our understanding of the physics of strongly interacting systems from hadrons and nuclei to hot and dense matter. These calculations not only impact our theoretical understanding but often also guide present and future experimental programs. The importance of computational approach in nuclear physics was recognized in the 2007 Long Range plan. It is further reinforced in the vision presented in the recent National Academy of Sciences (NAS) report "Exploring the Heart of Matter":

> *High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes a third leg supporting the field of nuclear physics.*

and its consequent recommendation:

> *A plan should be developed within the theoretical community and enabled by the appropriate sponsors that permits forefront computing resources to be exploited by nuclear science researchers, and establishes the infrastructure and collaborations needed to take advantage of exascale capabilities as they become available.*

An article in HPCwire on *Meet the Exascale Apps* identifies potential application areas for exa-scale development. It notes the emergence of nuclear physics as a driver that was not evident in the 1990s (Fig. 2 therein).

2 Computational Nuclear Physics Town Meeting

In light of the integral role of computational nuclear physics across the nuclear physics program, and of the establishment of a NSAC subcommittee charged with providing advice on implementing the priorities and recommendations of the 2007 NSAC Long Range Plan, a Computational Nuclear Physics Meeting was held at the headquarters of the Southeastern Universities Research Association, Washington DC on July 23-24, 2012. The objectives of the meeting were to highlight the accomplishments of the community, to identify outstanding opportunities for computational physics, to advance our understanding of nuclear physics, and to identify the resources needed to achieve these advances.

The meeting attracted $\sim$50 attendees encompassing domain scientists representing the major thrusts of computational nuclear physics, members of the applied mathematics and computational science communities that are key to our work, and representatives of the DOE and NSF, and of the national leadership-class computing facilities. The first day comprised four review talks describing the main computational areas: hadron structure, spectroscopy and interactions through lattice QCD ("Cold QCD"), the phase structure of QCD at finite temperature and density ("Hot QCD"), nuclear structure and reactions, and nuclear astrophysics. This was followed by contributed talks that presented new and emerging opportunities for computational nuclear physics. The session concluded with a general discussion aimed at distilling the important issues raised throughout the day.

The second day comprised two working sessions, the first devoted to the identifying the computational and manpower requirements of our field, and the second devoted to identifying the expected evolution of the field and of its impact on nuclear physics, on other areas of physics, and on computational science more generally. The meeting concluded with the unanimous adoption of two resolutions and three recommendations:

- **Resolution 1:** The opportunities for nuclear physics provided by high performance computing and partnerships with computer science and applied mathematics are unprecedented. The Town Meeting strongly endorses the vision stated in the NAS report: *"High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes a third leg supporting the field of nuclear physics."*

- **Resolution 2:** The Town Meeting strongly supports the recommendation of the NAS report: *"Recommendation: A plan should be developed within the theoretical community and enabled by the appropriate sponsors that permits forefront computing resources to be exploited by nuclear science researchers, and establishes the infrastructure and collaborations needed to take advantage of exascale capabilities as they become available."*

- **Recommendation 1:** The nuclear physics community should work with DOE and NSF to increase funding for the Nuclear Physics (NP) SciDAC programs and other cyber-related initiatives, and to foster partnerships with ASCR, NNSA, OCI, and other agencies to strengthen the impact of these programs. In addition to enabling new physics, these partnerships also open new avenues in the areas of computer science and applied mathematics.

- **Recommendation 2:** Collaboration amongst the fields of computational nuclear physics, experimental nuclear physics and analytic theory is critical. In particular, new experimental initiatives should be integrated with large-scale theoretical computations to maximize the combined science output.

- **Recommendation 3:** Concrete steps should be taken to educate and train the next generation of computational nuclear physicists, and to increase the cross-fertilization between the various efforts, exploiting synergies in physics, computer science and applied mathematics. The options include, but are not limited to: computational nuclear physics meetings, workshops, and schools; enhanced connections between SciDAC projects; and student exchanges

A recurrent element in discussions during the Town Meeting was the importance of the trained workforce and computational infrastructure. It was emphasized that the FY13 budget is insufficient to maintain viable programs across several areas of computational nuclear physics; the Town Meeting has urged funding agencies *to restore support for computational nuclear physics to a level at least commensurate with the historical level of support that has created such a world-class computational nuclear physics program.*

2.1 Science

Below we describe some of the activities that contribute to the vision for the field presented at the meeting, and the computational requisites to satisfy it. The details pertaining to the major computational efforts are contained in Appendices A-C.

2.1.1 Hadrons, Nuclei and Nuclear Matter from First Principles

Quantum Chromodynamics (QCD) is the underlying theory of the strong interactions that, together with the electroweak force, describes the structure of nuclei, the nature of their constituent hadrons, and the phases of strongly interacting matter. The powerful numerical technique of lattice gauge calculations enables key properties of the world around us to be computed from first principles. Thus lattice QCD calculations can compute the bound states of the theory, and describe how the fundamental quarks and gluons of QCD give rise to the observed protons, neutrons, pions, and the other hadrons. They can determine how charge, current, and matter are distributed within a hadron, and contribute to the building of a three-dimensional picture of the proton. The emergence of the nuclear force from QCD can be resolved, and first-principle calculations can be made for very light nuclei. The phase structure of strongly interacting matter can be investigated, describing how the relevant degrees of freedom of QCD change under conditions of high temperature and/or high density, and the role these phases play in the cosmos can be elucidated.

Lattice calculations have a key role both in predicting the outcomes of future experiments, and in fully capitalizing on the current and future DOE experimental nuclear physics programs. Lattice QCD calculations will predict the spectrum and properties of so-called exotic mesons, in which the gluonic degrees of freedom are manifestly exposed, that are the target of the GlueX experiment at the 12 GeV upgrade of Jefferson Laboratory. Calculations of nucleon form factors, generalized parton distributions, and transverse-momentum-dependent distributions will provide a more complete three-dimensional tomography of the nucleon than can the experimental programs at JLab and at RHIC-spin provide alone. Calculations of the cross-over temperature at small baryon densities and of fluctuations of conserved charges will enable the exploration of freeze-out conditions at RHIC. Finally, lattice studies of the interactions between hadrons will provide a first-principles QCD underpinning to studies of nuclear structure and reactions and to nuclear astrophysics, and provide data for key interactions, such as those of hypernuclei, for which there is a glaring paucity of empirical data.

2.1.2 Nuclear Structure and Reactions

Large-scale nuclear physics computations are dramatically increasing our understanding of nuclear structure and reactions, and of the properties of nuclear matter. In light nuclei, *ab initio* calculations of reactions, including those for fission and electroweak processes, are being used to systematically reduce uncertainties and to predict experimentally inaccessible data and processes. *Ab initio* approaches are being extended to reactions on medium-mass nuclei. Density Functional Theory and its extensions are being applied to medium-mass and heavy nuclei, including neutron-rich systems, nuclear matter, and the structure of neutron star crust. The suite of computational methods, including Quantum Monte Carlo, Configuration Interaction, Coupled Cluster, and Density Functional Theory, now scale efficiently to the largest computers.

These studies will have a direct impact on the experimental nuclear physics program. Computational studies of the strongly correlated matter found in nuclei and neutron stars impact the current experimental programs at NSCL and ATLAS, and guide the future program at FRIB. Computations of the neutron distribution in nuclei and of electroweak process are key to the interpretation of results at JLab, and of light-ion thermonuclear reactions to the program at NIF. Precise calculations of nuclear matrix elements provide crucial input for the interpretation of fundamental interaction experiments. Finally, accurate solutions of the strongly interacting quantum many-body systems will yield new insights and the ability to calculate phenomena, processes, and states of matter that are difficult or impossible to measure experimentally, such as the crust of a neutron star or the core of a fission reactor.

2.1.3 Nuclear Astrophysics

A central goal of nuclear physics is the explanation in detail of the origin of the elements and of their isotopes. Overwhelmingly, these elements are produced in stars, either during quiescent thermonuclear burning stages, or explosively, as in core-collapse and thermonuclear supernovae. Most of the elements up to the iron peak are ejected in supernova explosions, and an understanding of stellar explosions and stellar evolution is central to an understanding of the abundance pattern of the nuclei around us. Stellar evolution calculations involve both nuclear ratio rates generated either theoretically or through experiment, and three-dimensional turbulence and magnetic interactions. Stellar explosions are always multi-dimensional requiring state-of-the-art radiation/hydrodynamical simulations. As a consequence, addressing this key nuclear physics goal of the origin of the elements entails the sophisticated numerical simulations employing the latest computational tools and the exploiting the most powerful supercomputers.

Computational nuclear physics is essential to capitalize on the DOE Office of Nuclear Physics experimental programs. The astrophysics of neutron-rich nuclei is one of four scientific pillars of FRIB. Comparisons of supernova calculations with flagship experimental observations at the Intensity Frontier of the DOE High Energy Physics (HEP) program could reveal new physics beyond the Standard Model. Finally, investigations of the nuclear equation of state can be compared with experiments such as those at JLab aimed at measuring the weak charge radius of lead and calcium.

2.2 Computational Resources

This ambitious program in computational nuclear physics requires substantial computational resources. Advanced calculations that can resolve the key issues of nuclear physics require leadership computing at the largest scales (capability computing), medium scales (capacity computing), and a software infrastructure to effectively exploit that computing. The nuclear physics community has aggressively pursued these resources and thereby received substantial allocations on leadership-class facilities such as those under DOE's INCITE program, and programs within the NSF and NNSA. It is through the generous access to such large scale computational resources, and the recognition of the need for a range of computational capabilities to exploit them, such as the dedicated facilities of USQCD, that such impressive progress has been made. However, as outlined in the 2009 Nuclear Physics Exascale Report substantially more computational resources will be needed to capitalize on the scientific potential made possible by computational nuclear physics.

Over the last year, on the order of 1 Billion CPU-hours have been made available to all of theoretical computational nuclear physics within the U.S., including QCD, nuclear structure, and nuclear astrophysics. This corresponds to about 0.1 Petaflop-years which places this field at the earliest part of the time-line described in the 2009 Nuclear Physics Exascale Report. New generations of calculations will require substantially more computing time as the fidelity of the simulations improves. As discussed below, major investments in computer science and applied mathematics manpower are needed to maintain this momentum. These investments will be crucial in transitions to new computational architectures and programming models beyond the petascale.

2.3 Personnel, Funding, Leveraging

Computational nuclear physics bridges many areas of science, and as such, the expertise of a broad range of individuals including physicists, computer scientists, applied mathematicians, as well as students, is vital to the success of the program. As computational environments become more diverse, it is crucial that the work force include those individuals with skills sufficient to master these challenges. This work force will follow the emerging trends in these architectures and will develop the algorithms and software infrastructure to enable their exploitation and advance the overall program. Interdisciplinary programs such as SciDAC will become even more crucial in the future to help foster such collaborations.

The U.S. DOE SciDAC program has enabled significant advances in computational nuclear physics within the U.S. in the past few years, precisely because it has brought together leading domain specialists and computational scientists to focus on algorithmic improvement as well as improving domain codes for NP. These SciDAC funded positions are cost effective and highly leveraged; namely, many domain scientists are supported out of some base funding. The SciDAC programs thus enable the support of a very special class of collaborators - ones not typically covered under base funding. Notably, the algorithmic advances and highly optimized codes that SciDAC has facilitated, have been key to the leveraging of substantial leadership-class computational resources.

In FY13, the historical level of NP funding for SciDAC has been reduced by a factor of nearly three; *key areas of computational nuclear physics now lack support for the development of the computational infrastructure, with the potential loss of leadership not only in the computational domain, but also in the* *corresponding experimental and theoretical domains.*

The education of future computational scientists is also of major importance in the field as these junior staff will be the future leaders. As such, we strongly support new programs such as the TALENT initiative, and also SciDAC SCADS summer workshops on Petascale Architectures. In addition, the support of university based HPC infrastructure, such as courses and computational hardware, help to train the future generations of researchers.

A Hadrons, Nuclei and Nuclear Matter from First Principles

Numerical calculations in discretized versions of Quantum Chromodynamics, called lattice QCD, allow to study the properties and interactions of strongly interacting matter from first principles, along with quantification of the uncertainties. Lattice QCD allows for the calculations of the hadronic spectrum, nucleon properties and few nucleon interactions, as well as structure of some light nuclei. These calculations, referred to as "Cold QCD", are relevant for the experimental programs at existing and future facilities such as JLab, FAIR, J-PARC and FRIB. Lattice QCD can also predict the properties of strongly interacting matter at high temperatures and densities such as the transition temperature and equation of state (EoS). Such calculations are relevant for the relativistic heavy ion experiments at RHIC and LHC, and will be discussed in the subsection entitled "Hot QCD". While cold and hot lattice QCD calculations address somewhat different physics objectives, they are technically similar. Furthermore, the synergy between the above lattice QCD calculations relevant for the US NP Program and the lattice calculations relevant for HEP program is also fully explored. In 1999 the USQCD consortium was created for this purpose. The development of the software and operation of the dedicated hardware, as well as allocation of the external resources, proceeds through the USQCD consortium. In the past, the software development for lattice QCD was funded through joint HEP-NP SciDAC-2 project. Now the software development of nuclear physics lattice QCD is funded by the SciDAC-3 grant "Computing properties of hadrons, nuclei and nuclear matter from QCD", though some of the software development activities are coordinated through USQCD between HEP and NP.

A.1 Cold QCD

The main focus of the cold lattice QCD is the calculations of the bound state spectrum of QCD, study of the internal structure of the nucleon, and study of interactions between nucleons, including two and higher body interactions. The calculations of the QCD spectrum will be relevant to the interpretation of the experimental results from the GlueX as well as for the search of so-called missing resonances at CLAS experiments. Lattice calculations of the nucleon structure are closely related to the experimental efforts in the RHIC spin physics program, measurements of Generalized Parton Distribution functions in JLab and measurements of single spin asymmetries in COMPAS and HERMES experiments. A better understanding of interactions between nucleons is important for ab-initio nuclear structure calculations and experiments in J-PARC and FAIR facilities. Lattice QCD is a way to, not only understand, but to rigorously refine the interactions between nucleons from first principles. The major accomplishments of cold lattice QCD calculations since 2007 include (at unphysical light-quark masses, in the absence of electromagnetism and without isospin breaking):

- The isovector meson spectrum, hinting towards existence of hybrid mesons
- The low lying nucleon and Δ spectrum that show consistency with quark model predictions
- Moment of the generalized parton distributions in the nucleon, and determination of the proton spin composition
- Exploratory studies of transverse momentum-dependent distributions of the nucleon
- Studies of the nucleon-nucleon and hyperon-nucleon interactions
- Determinations of the pion-pion scattering length and phase-shifts
- Studies of finite-density Bose condensed multi-meson systems
- The spectrum of the lightest nuclei and hypernuclei

A.2 Hot QCD

A central goal of contemporary research in Nuclear Physics is to understand properties of nuclear matter at densities several times that inside a nucleus and at temperatures more than a million times that of the sun. In the US, a large experimental program at the Relativistic Heavy Ion Collider has been in place for the last 12 years. Complementary programs have started in Europe (LHC, Switzerland), and future programs are planned in Germany (FAIR) and Russia (NICA).

Large scale numerical calculations on leadership-class computers, as well as compute clusters with specialized, graphic card (GPU) enhanced compute nodes are needed to perform theoretical studies that relate to this experimental program and address the fundamental questions raised in the 2007 Nuclear Science Long Range Plan:

1. *What are the phases of strongly interacting matter, and what role do they play in the cosmos ?*

2. *What does QCD predict for the properties of strongly interacting matter ?*

Numerical lattice QCD calculations are essential in answering these questions and in providing guidance to the experimental heavy ion program. In particular, the beam energy scan program at RHIC, to a large extent, was motivated by lattice QCD calculations which provided first hints for the possible existence of a critical point at non-vanishing net baryon density, where the smooth cross-over observed at vanishing baryon density turns into a first order phase transition. Establishing the existence of this point is crucial for our understanding of the QCD phase diagram and is one of the main goals of the RHIC beam-energy scan program. Lattice QCD results will be essential for the interpretation of the experimental results on fluctuations of conserved charges measured in the RHIC beam energy scan, which provide a direct probe of the temperature and baryon density of the created system.

Calculations of real time quantities, such as transport coefficients and in-medium hadron spectral functions, are also important to the heavy ion program. Lattice calculations of these quantities are particularly challenging since the extraction of spectral functions from the imaginary time correlation functions, that are presently accessible in numerical calculations, requires significant "data sets" and extremely fine discretization grids.

Major accomplishments of lattice QCD calculations at non-zero temperature and density since the 2007 Long Range Plan include:

- the detailed understanding of the chiral and deconfinement aspects of the crossover in QCD and determination of the chiral crossover temperature, $T_c = 154(9)$MeV.

- the calculations of the equation of state at several lattice spacings, which soon will allow to provide reliable equation of state in the continuum limit.

- a study of fluctuations of conserved charges on course lattices and determination of the crossover temperature at small baryon density, that allows to explore freeze-out conditions in RHIC

- Exploratory calculations of the hadronic spectral functions and determination of some transport coefficients neglecting the effect of dynamical quarks.

Clearly many of the above calculations need to be refined (reducing their associated uncertainties) with the increasing computational resources in the US. As emphasized in the 2012 NAS report "Exploring the heart of matter" quantitatively reliable calculations on the QCD phase diagram, at non-zero net baryon density, hadronic spectral functions and transport coefficients will be essential for theoretical interpretation of present and future experimental results.

Table 1: Recent hires in lattice QCD

Person	Institution
Andrei Alexandru	George Washington University
Christopher Aubin	Fordham University
Silas Beane	University of New Hampshire
Saumen Datta	Tata Institute
Will Detmold	College of William and Mary, JLab (recently hired by MIT)
Jozef Dudek	Old Dominion University
Shinji Ejiri	Niigata University
Bálint Joó	JLab
Jimmy Juge	University of the Pacific
Nilmani Mathur	Tata Institute
Harvey Meyer	University of Mainz
Swagato Mukherjee	BNL
Kostas Orginos	College of William and Mary, JLab
James Osborn	ANL
Péter Petreczky	BNL, former RIKEN-BNL Fellow
Claudio Picca	University of Southern Denmark
Enno Scholz	University of Regensburg
Brian Tiburzi	City College New York, RIKEN-BNL Fellow
Takashi Umeda	Hiroshima University

A.3 Career Paths

In the past decade, many young researchers working within USQCD have obtained tenured/tenure track positions at universities and laboratories. The Jlab bridge and joint positions, and the RIKEN-BNL bridge positions, played an important role in facilitating these hires. Recent hires in lattice QCD are listed below in Table 1

A.4 Computational Resources and Personnel

A significant fraction of the computational resources for lattice QCD come from the dedicated capacity hardware operated by USQCD and funded jointly by NP and HEP. The total USQCD resources amount to 300M CPU core hours and 4.7M GPU hours. For typical lattice QCD applications the amount of the GPU time corresponds to about 140M CPU core hours. Roughly half of the total USQCD resources are available for nuclear physics. Therefore 220M core hours is available for nuclear physics calculations from USQCD hardware. Cold and Hot lattice QCD researchers also receive considerable resources from INCITE, NERSC, NSF, as well as institutional computational centers. The total computer time from these resources amounts to about 200M core hours. Thus, the total amount of computer time available for cold and hot lattice QCD in 2012 is approximately 420M core hours. If the computational resources available to this component of nuclear physics research increase no faster than Moore's law, the community will likely be unable to synchronously address the questions relevant to the experimental programs. It will require further significant algorithmic improvements to reach this goal. At the same time, optimizing codes for the new hardware architectures will be increasingly difficult. Investment in the personnel responsible for software development will be critical to ensure a viable lattice QCD program, and re-assure leadership-class facilities that computational resources provided to the community will be optimally exploited (thereby leading to at least Moore's Law growth in resources). This will require at least the same level of support that was provided to SciDAC-2, and hence a significant increase in the level of support currently being provided to SciDAC-3.

A.5 Education and Training

There are summer schools focused on lattice QCD which help train the next generation of researchers in the field, e.g.

- INT Summer School on Lattice QCD for Nuclear Physics, August 6 - 24, 2012, INT, Seattle.
- Lattice QCD, Hadron Structure and Hadronic Matter, Dubna International Advanced School of Theoretical Physics-Helmholtz International School, September 5 - 17, 2011, Dubna, Russia
- Summer School on Lattice QCD and its Applications, August 8 - 28, 2007, INT Seattle

Lattice QCD researchers from the US were actively involved as organizers and/or lecturers in these schools.

A.6 Prizes and Awards

This area of nuclear physics has received significant recognition for its research accomplishments: Silas Beane was awarded a NSF Career Award, Will Detmold and Kostas Orginos were awarded DOE OJI's, Jozef Dudek was awarded a DOE Early Career Award, Péter Petreczky was awarded the Zimanyi Medal, Robert Edwards became a Fellow of the APS, and Martin Savage was awarded a Humboldt Fellowship and an IBM Faculty Award. Further, numerous local awards have been made to researchers in this area. The NSF has supported MRI's for computational hardware for this research area: one at the College of William and Mary (Orginos), and one at the University of Washington (Kaplan, Bulgac, Reschke and Savage).

B Nuclear Structure and Reactions

Large-scale nuclear physics computations dramatically increase our understanding of nuclear structure and reactions and the properties of nucleonic matter. The physics research ranges from studies of the nuclear interaction to critical processes in light and heavy nuclei and nuclear astrophysics. In light nuclei, the focus is on *ab initio* calculations of reactions, including fusion and electroweak processes. *Ab initio* techniques are used to systematically reduce uncertainties and make predictions for experimentally inaccessible data and processes, including reactions on unstable nuclei. Computational approaches are being expanded to reactions on medium-mass nuclei. In heavy nuclei, the focus is on structure and reactions using density functional theory and its extensions. The density functional work is closely tied to *ab initio* studies of experimentally inaccessible systems such as neutron drops to enhance the predictive capabilities. Important areas of research are the structure and decays of very neutron-rich nuclei, the dynamics of the fission process in heavy nuclei, and the structure of neutron star crust. In the area of fundamental physics, the focus is on double-beta decay, hadronic weak interaction studies, and neutrino scattering from nuclei.

The current Quantum Monte Carlo, Configuration Interaction, Coupled Cluster, and Density Functional codes – used in advanced nuclear structure computations – now scale efficiently to the largest computers available. Computational studies of the strongly correlated matter found in nuclei and neutron stars impact experimental programs throughout the U.S., including FRIB (the structure of heavy neutron-rich nuclei and related astrophysical environments), ATLAS and other low-energy nuclear physics facilities (structure and reactions of nuclei and nuclear astrophysics), TJNAF (the neutron distribution in nuclei, few body systems, and electroweak processes), NIF (light-ion thermonuclear reactions in a terrestrially controlled plasma environment), MAJORANA and FNPB (neutrinoless double-beta decay and physics beyond the Standard Model), LANSCE (studies on the properties of fission), and other nuclear physics and astrophysics facilities. Accurate solutions of the strongly interacting quantum many-body systems will yield new insights and the ability to calculate phenomena, processes, and states of matter that are difficult or impossible to measure experimentally, such as the crust of a neutron star or the core of a fission reactor.

Computational nuclear structure and reactions in the U.S. has advanced significantly through the UNEDF SciDAC-2 project, which joined forces of nuclear theorists, computer scientists and applied mathematicians. Integral to the UNEDF project was the verification of methods and codes, the estimation of uncertainties, and assessment. Methods to verify and validate included the cross checking of different theoretical methods and codes, the use of multiple DFT solvers with benchmarking, and the confrontation of *ab initio* functionals with *ab initio* structure using the same Hamiltonian. The UNEDF project helped form a coherent nuclear theory community, opened up new capabilities, fostered transformative science resulting in high-visibility publications, and advanced the careers of many junior scientists. The UNEDF experience has been a springboard for advancement, as UNEDF postdocs have obtained permanent positions at universities and national labs. Another new aspect to the low-energy theory effort driven by SciDAC is the greatly enhanced degree of quality control. The successor of UNEDF, the NUCLEI SciDAC-3 project, will bridge the scales from hadronic interactions to the structure and dynamics of heavy nuclei to neutron stars within a coherent framework. NUCLEI is strongly coupled to all of the SciDAC Institutes; aided by these connections, the collaboration will develop novel computational tools that are specifically needed to accomplish the physics goals.

B.1 Accomplishments

Major scientific achievements since 2007 include:

- Dramatic advances in *ab initio* studies of fusion reactions, combining the no-core shell model and resonating group techniques.

- The first *ab initio* calculations of important and unique light nuclear states and transitions, including the Hoyle state of ^{12}C and the life-time of ^{14}C.

- Critical accomplishments in *ab initio* calculations of medium-mass neutron-rich nuclei emphasizing the importance of three-nucleon interactions and particle continuum.

- Improved density functionals (UNEDF0 and UNEDF1) that simultaneously reproduce *ab initio* calculations of inhomogeneous neutron matter, and significantly advance our abilities to reproduce fission barriers and half-lifes.

- Calculations, including error estimates, of the full range of atomic nuclei, based upon these improved density functionals.

- Important impacts on other fields, particularly cold atom physics, in both *ab initio* and density functional calculations.

B.2 Computational Resources

These advances were made possible by a rapid increase in our ability to use the largest-scale computational resources, and in available computational resources. Large-scale usage in nuclear structure and reactions rose from 80M core-hr/year in 2009 to a requested 320M core-hr/year in 2013. INCITE resources, particularly those at OLCCF, have increased rapidly. In 2012, our nuclear theory INCITE was sixth largest out of 60 awards for 2012.

In addition there is a tremendous need for additional computational resources, as indicated by the expected 2013 requests. In the future our ability to use the largest-scale computers will require additional investments in manpower, particularly as we transition to new architectures.

B.3 Personnel, Funding, Leveraging

The issue of personnel in computational nuclear structure and reactions is critical. UNEDF brought together a big fraction of the nuclear theory community, and represented a significant increase in support for junior scientists. This was possible only through a tremendous leveraging of the base programs in Nuclear Physics and ASCR, and strong support from NNSA. The UNEDF SciDAC-2 project typically involved approximately 50 scientists in physics, computer, and applied mathematics, including full support for 11 students and 19 postdocs per year. Senior scientists were typically supported only a modest amount or not at all, depending upon particular laboratory and university situations. The full budget for UNEDF was $3 M per year, with NP, ASCR, and NNSA contributing $ 1 M each.

Due to the limited resources involved, the NUCLEI proposal was scaled back to $ 2.7 M per year. Final funding is $ 2.4 M per year (NNSA contribution is $ 0.5 M). This reduction, combined with inflation, will reduce our ability to support the next generation, endangering the program in future years. We estimate we will be able to initially support approximately 10 students and 12 postdocs per year; some will certainly be supported at a partial level. In addition, another scientifically strong SCIDAC-3 proposal in nuclear structure and reactions was not funded. Present funding is clearly insufficient to ensure a strong future for the field, support from other sources, including NP and ASCR base funding, and NNSA, will have to provide the rest.

We estimate a need for an additional 10 positions over 5 years in nuclear structure /reactions and associated computer science and applied math. Approximately 1/2 of these positions would be nuclear physicists and 1/2 computer science and applied math scientists. These new positions are critical to enable the effort to scale to the largest-scale machines heading toward exa-scale, and to support the FRIB and related experimental program in a timely manner. Given sufficient support, we can fundamentally change the future of the field, as demonstrated by the recent history outlined below.

B.4 Career Paths

Support and successful careers for junior scientists have been an important goal of the computational nuclear physics program. Junior scientists involved in UNEDF have been successful in obtaining positions at universities, in Office of Science and NNSA laboratory positions, and academic institutions and laboratories worldwide. Table 2 lists some of the junior scientists in UNEDF in 2010 and their career paths. It is critical to maintain this stream of young people, and to provide a balance across types and fields of positions.

B.5 Education: options for training and in computational sciences

The new TALENT initiative (Training in Advanced Low Energy Nuclear Theory;) aims at providing an advanced and comprehensive training to graduate students and young researchers in low-energy nuclear theory. The network aims at developing a broad curriculum that will provide the platform for a cutting-edge theory for understanding nuclei and nuclear reactions. These objectives will be met by offering series of lectures, commissioned from experienced teachers in nuclear theory, computer science, and applied mathematics. The educational material generated under this program will be collected in the form of WEB-based courses, textbooks, and a variety of modern educational resources. The characteristic feature of this initiative is training in multi-scale nuclear physics. This knowledge is crucial not only for a basic understanding

Table 2: Career paths of some junior researchers in UNEDF in 2010

Postdoc	previous location(s)	present position
Joaquin Drut	UW, OSU, LANL	Prof., UNC Chapel-Hill
Stefano Gandolfi	LANL	Staff, LANL
Alexandros Gezerlis	LANL, UW	Prof., U. Guelph
Eric Jurgenson	LLNL	Staff, LLNL
Markus Kortelainen	UTK	Research Prof., U. Jyväskylä
Plamen Krastev	ISU	Reseacher, Harvard
Pieter Maris	ISU	Research Prof. ISU
Eric McDonald	MSU	Research Prof. MSU
Gustavo Nobre	LLNL	Staff, BNL (NNDC)
Junchen Pei	UTK	Prof., Pekin U.
Nicolas Schunck	UTK	Staff, LLNL
Ionel Stetcu	UW	Staff, LANL
Jun Terasaki	UNC	Staff, U. Tsukuba
Stefan Wild	ANL	Staff, ANL

of atomic nuclei, but also for further development of knowledge-oriented industry; from nanotechnology and material science to biological sciences, to high performance computing. The first TALENT Course on Computational Many-body Methods for Nuclear Physics was held at ECT* in the period June 25 to July 13, 2012.

Another TALENT activity was the recent UiO-MSU-ORNL-UT School on the computational quantum many-body problem. The topics included: computational quantum chemistry, dynamic multi-threading in numerical computing, lattice simulations, advanced parallelization for multi-core and GPU processing for linear systems and eigenvalue calculations, and challenges and approaches for heterogeneous HPC.

Other training opportunities – that computational low-energy nuclear community took advantage of – include workshops, such as SciDAC Center for Scalable Application Development Software summer workshops on Petascale Architectures and Performance Strategies, summer training courses on high-performance computing fundamentals offered by the Oak Ridge Leadership Computing Facility and National Institute for Computational Sciences, and the Virtual School of Computational Science and Engineering.

Finally, nuclear theory students take advantage of university courses on high performance computing offered at several universities, including FSU, LSU, OSU, and UTK.

B.6 Prizes

Computational nuclear physicists have won significant awards during the past several years. Notable accomplishments include Sofia Quaglioni (LLNL), who received a prestigious DOE Early Career award in 2011; Steve Pieper and Robert Wiringa (ANL) who received the Tom W. Bonner Prize in Nuclear Physics in 2010; Witold Nazarewicz (UTK), who received the Tom W. Bonner Prize in Nuclear Physics in 2012; and Joaquin Drut who was awarded the Hermann Kümmel Early Achievement Award in Many-Body Physics in 2009. George Fann, a UNEDF member, is a co-leader of the MADNESS software development team that received a R&D 100 Award in 2011 presented by R&D Magazine. In addition, there were numerous local prizes awarded to UNEDF scientists at universities and national labs.

C Nuclear Astrophysics

A primary goal of nuclear astrophysics, and of Nuclear Physics at the DOE, is the explanation in detail of the origin of the elements and their isotopes. Overwhelmingly, the elements of Nature are produced in stars, either during quiescent thermonuclear burning stages or explosively, as in core-collapse and thermonuclear supernovae, gamma-ray bursts, X-ray bursts, and novae. Most of the elements up to the iron peak are ejected in supernova explosions. The r-process is thought to occur in core-collapse supernovae, but may be ejected when neutron stars in binaries merge or in gamma-ray bursts. The proton-rich nuclei of the rp-process seem to be produced in X-ray bursts. Therefore, whatever their origin and history, an understanding of stellar explosions and stellar evolution is central to an understanding of the abundance pattern of nuclei around us. Stellar evolution calculations for the entire range of stellar masses involve nuclear reaction rates generated theoretically or by nuclear experiment and the complexity of three-dimensional turbulence and magnetic interactions. Stellar explosions are always multi-dimensional, requiring state-of-the-art radiation/hydrodynamical simulations with significant nuclear physics input. As a consequence, much of nuclear astrophysics entails sophisticated numerical simulations employing the latest computational tools and the most powerful supercomputers of the DOE complex to address key goals of the Office of Nuclear Physics.

Computational nuclear astrophysics also supports important components of the DOE Office of Nuclear Physics experimental program. The astrophysics of neutron-rich nuclei is one of four scientific “legs” of the Facility for Rare Isotope Beams. FRIB experiments will determine the masses and beta-decay rates along much of the r-process path. However these data lose value if uncertainties in the r-process environment exceed those of the nuclear data. Since core-collapse supernovae (CCSN) and merging neutron stars are leading candidate sites for the r-process, the increased fidelity of CCSN and merging neutron-star simulations can be viewed as an important complement to FRIB efforts to better define the nuclear physics of the r-process.

The flagship experimental program in DOE’s Intensity Frontier program includes a megadetector that will allow experimentalists to follow the neutrino light curve from the next galactic supernova. There are novel neutrino flavor phenomena associated with supernovae – collective flavor oscillations sensitive to the neutrino hierarchy and a second MSW crossing associated with the mixing angle θ_{13} – that could emerge as new physics from detailed comparisons of supernova theory with observation.

The nuclear equation of state is a third intersection with the DOE experimental program. A JLab program to constrain the nuclear symmetry energy, and, thus, the EoS for neutron-rich matter, by measuring the weak charge radius of Pb has yielded first results. While the JLab experiment tests the symmetry energy at about half nuclear density, this data point still provides an important experimental test of the nuclear theory used in modeling the high-density supernova core and neutron stars.

To accomplish the computational astrophysics goals and projects articulated in the 2007 DOE Long-Range Plan for Nuclear Physics, the tight collaboration of computer scientists, applied mathematicians, and nuclear physicists to create efficient, highly-scalable, parallel simulation capabilities is required. Furthermore, access to resources on the petascale (in the near term), then exa-scale (on the decadel horizon), will be necessary to fully realize the stated astrophysical science goals of the Office of Nuclear Physics.

C.1 Accomplishments

Major scientific milestones since 2007 include:

- The development of 3D codes for the study of core-collapse supernovae, superseding the previous 2D capability
- The emergence of realistic whole-star 3D models for thermonuclear supernova explosions (Type Ias) with the deflagration to detonation transition

- The publication of the first detailed 2D and 3D stellar evolution calculations, going beyond the traditional 1D models with ad hoc mixing-length convection theory
- The first neutron-star/neutron-star merger simulations in full general relativity with magnetic fields.

C.2 Computational Resources

Many of these advances were made possible by generous access to the largest-scale computational resources available in the unclassified DOE complex. These include in 2012 $\sim$150 MCPU-hours of INCITE time and $\sim$35 MCPU-hours at NERSC. Adding in the $\sim$25 MCPU-hours of NSF Teragrid time, the total for nuclear astrophysics amounted to $\sim$200 MCPU-hours in 2012.

However, there is a growing demand for additional computational resources as three-dimensional radiation-hydrodynamic and massive nuclear network simulations for a variety of key nuclear astrophysics problems become conceivable and feasible. The major investments needed to maintain this momentum are in scientific and applied-mathematics manpower. These investments will be all the more crucial as we transition to new computational architectures and programming models beyond the petascale.

C.3 Personnel, Funding, Leveraging

As stated above, it is critical that the personnel issues needed to realize the potential of this next generation of nuclear astrophysics capabilities be addressed. In this regard, it is disappointing that no astrophysics proposals were funded during this last (2013) SciDAC round. This has left numerous groups scrambling to find alternate funding for their junior team members and to maintain their scientific viability. Currently, it is estimated that there are $\sim$50 mid-level researchers in the various previous SciDAC teams who are affected (directly or indirectly). While most of them will find (or have found) alternate employment and leveraging by alternate sources was indeed necessary in the past, the effect of this progressive defunding by the DOE over the last years has severely compromised the United States' ability to realize the progress envisioned in the context of previous DOE investments. We estimate that, factoring in University, NSF, and National Laboratory leveraging, nuclear astrophysics will now need additional support for $\sim 10-20$ junior nuclear astrophysicists and computational scientists to reestablish the momentum previously enabled by past DOE support. These new positions are crucial as we head toward the exa-scale, and to support the nuclear astrophysics component of the Office of Nuclear Physics experimental program. Failure to address this critical need will, over time, cede leadership in computational nuclear astrophysics to Japan and Germany, both of which are ramping up investment to establish both 1) the critical masses in manpower and 2) the access to the heaviest iron needed to realize the transformative potential exa-scale presents.

C.4 Prizes

Computational astrophysicists have garnered numerous awards and honors while funded under recent DOE awards, including membership in the U.S. National Academy of Sciences, the Bruno Rossi Prize, and numerous Gordon Bell Prizes and Early Career awards.