Office of Science, U.S. Department of Energy
Office of Nuclear Physics
Nuclear Theory Division

BUILDING A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL (UNEDF)

SciDAC-2 Project
Project Period: 1 Dec 2006 – 30 Jun 2012

Final Report

On behalf of UNEDF prepared by the UNEDF Council

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I. INTRODUCTION

An understanding of the properties of atomic nuclei is crucial for a complete nuclear theory, for element formation, for properties of stars, and for present and future energy and defense applications. During the period of Dec. 1 2006 – Jun. 30, 2012, the UNEDF collaboration carried out a comprehensive study of all nuclei, based on the most accurate knowledge of the strong nuclear interaction, the most reliable theoretical approaches, the most advanced algorithms, and extensive computational resources, with a view towards scaling to the petaflop platforms and beyond. Until recently such an undertaking was hard to imagine, and even at the present time such an ambitious endeavor would be far beyond what a single researcher or a traditional research group could carry out.

The long-term vision initiated with UNEDF is to arrive at a comprehensive, quantitative, and unified description of nuclei and their reactions, grounded in the fundamental interactions between the constituent nucleons. We seek to replace current phenomenological models of nuclear structure and reactions with a well-founded microscopic theory that delivers maximum predictive power with well-quantified uncertainties. Specifically, the mission of this project has been three-fold:

- First, to find an optimal energy density functional (EDF) using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.
- Second, to apply the EDF theory and its extensions to validate the functional using all the available relevant nuclear structure and reaction data.
- Third, to apply the validated theory to properties of interest that cannot be measured, in particular the properties needed for reaction theory.

The main physics areas of UNEDF, defined at the beginning of the project, were:

- Ab initio structure
- Ab initio functionals
- DFT applications
- DFT extensions
- Reactions

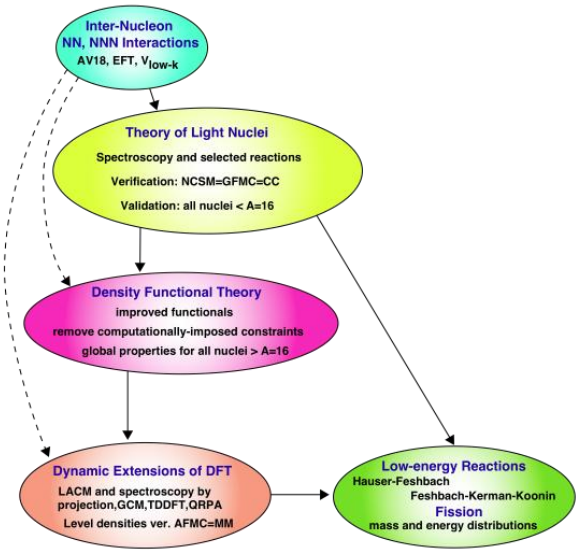

Figure 1: UNEDF in 2007.

Figure 1 shows the UNEDF strategy diagram during Year-1 of the project. The main efforts are indicated but very few connections existed at that time. However, as UNEDF matured, it was gratifying to see increased coherence within the effort. Indeed, the project has created and facilitated an increasing interplay among the major sections where none existed previously. Each of the main physics areas now includes on-going collaborations that cross over into other sectors. These interconnections, which will be detailed in this report, are highlighted in the summary diagram of the UNEDF strategy shown in Figure 2. In addition to physics links, numerous

computer science/applied mathematics (CS/AM) interconnections were established within UNEDF as tools developed in one area of UNEDF were used in other parts of the program. Some of the unique computational/mathematical tools developed under UNEDF, motivated by nuclear needs, are likely to be used in other areas of science.

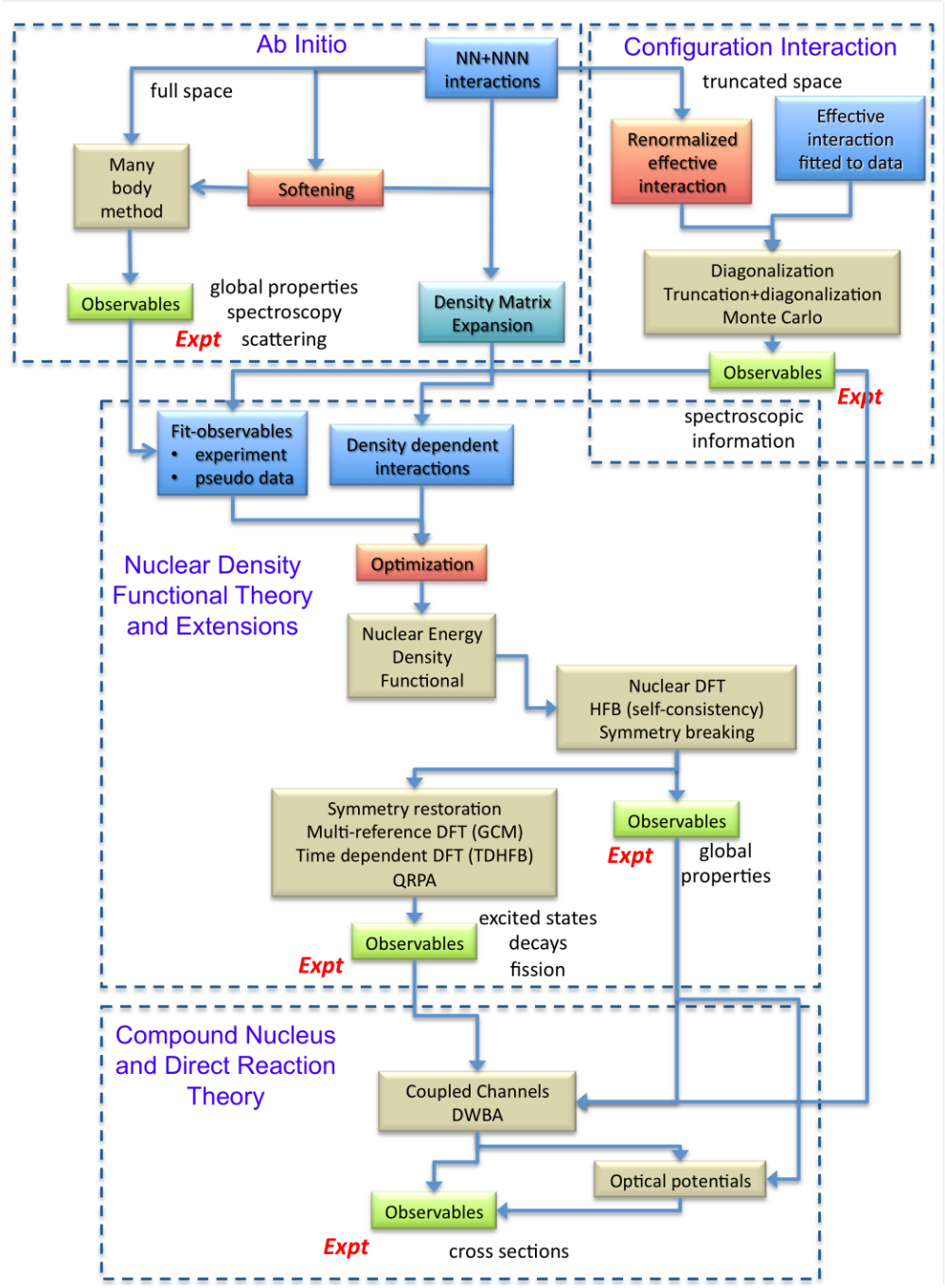

Figure 2: UNEDF strategy diagram in 2012. Active connections between various research areas are marked by arrows. Many of these connections were nonexistent at the project inception.

The UNEDF SciDAC project has developed several key computational codes and algorithms for reaching the goal of solving the nuclear quantum many-body problem throughout the chart of nuclei. Without such developments, scientific progress would not be possible. Specific examples include the development of the Asynchronous Dynamic Load Balancing Library that enable Greens Function Monte Carlo calculations to scale to the full BG/P platform at ANL and investigate the Hoyle state in ^{12}C that is crucial for understanding $^{12}C(\alpha,\gamma)^{16}O$ reaction; improvements in Krylov methods and load balancing on the Jaguar at ORNL, BG/P, Thunder and Atlas (LLNL), and Franklin (NERSC) that accelerate converged ground-state and excited-state computations of light nuclei using the No Core Shell Model (NCSM) approaches, enabling computations of ^{14}C beta decay; load-balancing efforts that enable the angular momentum coupled-cluster with triples corrections and the three-body force to eventually calculate neutron-rich ^{78}Ni on Jaguar and Kraken at ORNL; developments of multi-wavelet basis states for nuclear DFT that enable maximally converged calculations of nuclear properties across the nuclear chart including properties of very weakly bound nuclei; determination of the best energy density functional using model-based optimization algorithms with efficient implementation for parallel runs across Jaguar, Kraken, and Franklin.

Access to leadership-class computing resources and large compute time allocations has been critical for the scientific investigations of UNEDF members. Through the competitive INCITE program, many UNEDF members have been awarded large allocations at the Oak Ridge Leadership Computing Facility (OLCF) and the Argonne Leadership Computing Facility (ALCF). The INCITE resources, particularly those at OLCCF, have increased rapidly. In 2012, our nuclear theory INCITE was sixth largest out of 60 awards for 2012. A summary of INCITE allocations and utilization for UNEDF collaborators over the course of the project is given in Figure 3.

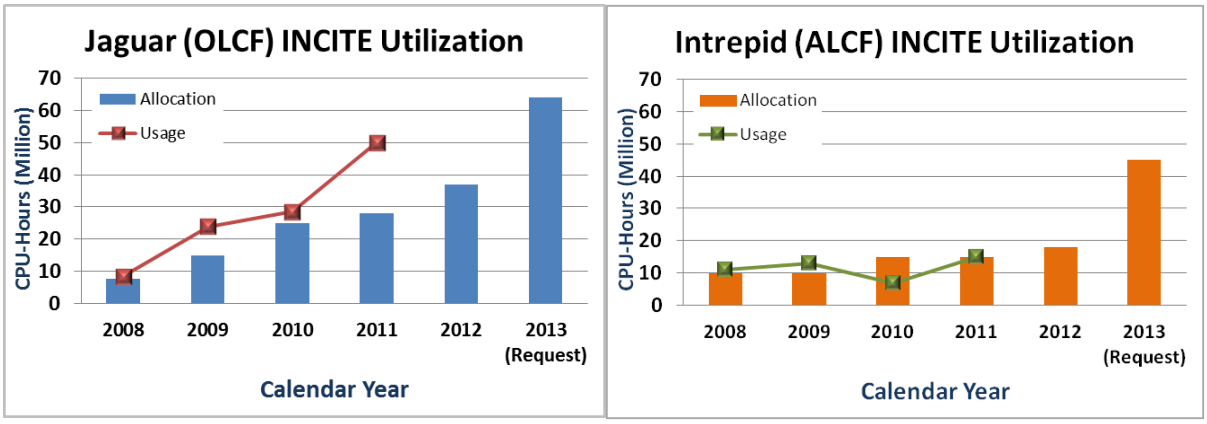

Figure 3: INCITE allocation and utilization of the Jaguar supercomputer at the OLCF (left) and of the Intrepid supercomputer at the ALCF (right).

At the intersection of the ab-initio techniques and the DFT techniques are comparisons of observables among the various approaches, particularly through constraints on the density. Such calculations have not been performed before and require significant computational capability and an increasing sophistication of data manipulation. Research on the nuclear problem would be incomplete without a serious effort to understand the nuclear interactions involved and their connection to DFT; therefore the UNEDF project also included elements that required less computational capability, but which are integral to the project, such as the development of nuclear

forces using renormalization group approaches. Research on nuclear reaction properties requires the use and development of algorithms for the largest computers and more conventional computing that still requires algorithmic breakthroughs.

Another new aspect to the low-energy theory effort driven by SciDAC is the greatly enhanced degree of quality control. 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 crosschecking of different theoretical methods and codes (e.g., GFMC vs. AFDMC vs. NCFC), the use of multiple DFT solvers with benchmarking, and the confrontation of ab initio functionals with ab initio structure using the same Hamiltonian. A new way to estimate theory error bars was to use multiple Hamiltonians with different cutoffs and then analyze the cutoff dependence of calculated observables. The UNEDF assessment component has required the development and application of statistical tools to deliver uncertainty quantification and error analysis for theoretical studies as well as to assess the significance of new experimental data. For example, quantifying the sensitivity of optimized functionals to particular data is now possible. Such technologies were virtually unknown in the low-energy nuclear theory community until UNEDF, but are essential as new theories and computational tools are applied to entirely new nuclear systems and to conditions that are not accessible to experiment. UNEDF also made strides in the preservation, enhancement, and dissemination of computational infrastructure for the community. A prime example is the Leadership Class Configuration Interaction (LCCI) framework (described below), which provides a user-friendly environment for researchers to download and run state-of-the-art CI codes and to archive results from large-scale production runs.

The SciDAC program fosters transformative science and this goal has been fulfilled by the new capabilities stemming from UNEDF. The scientific highlights of UNEDF are summarized in Sec. II. But the outcomes reach beyond the many particular compelling calculations for nuclear structure and reactions. UNEDF has changed for the better the way that low-energy nuclear theory is carried out, analogous to the shift in experimental programs, moving from many small groups working independently to large-scale collaborative efforts. The successes of the SciDAC UNEDF project were built upon certain best practices, some implemented originally and some learned by experience, in organizing and implementing the scientific effort. These are summarized in Sec.III. This is followed by a comprehensive list of junior members of UNEDF (students and postdocs) in Sec.IV, prizes and awards (Sec. V), and cumulative lists of deliverables (publication, codes and databases, and presentations) in Sec. VI. Section VII contains a budget summary table. The UNEDF charter is included in Sec. VIII. Finally, Sec. IX reviews annual accomplishments in the major areas of UNEDF during Year-5. For a high-level description of UNDEF, see Nuclear Physics News, DOE Office of Science "Science Highlights Series", and SciDAC Review.

II. HIGHLIGHTS OF UNEDF DELIVERABLES

The main deliverables of UNEDF are publications, reports, conference presentations, and computer codes, as well as trained young scientists. The project has been very productive, with over 250 publications (see Figure 4 for the yearly rates), including 50 *Physical Review Letters*, a *Science* article in 2011, and a *Nature* article in 2012. Cumulative lists of publications, talks, and codes are given in Sec. VI of this report.

A number of important milestones have been met by UNEDF during 2007-2012. Below, we list examples of achievements. The detailed descriptions of those from Years 1-4 are given in the corresponding Annual Reports. The recent highlights are discussed in some detail in Sec. IX of this document.

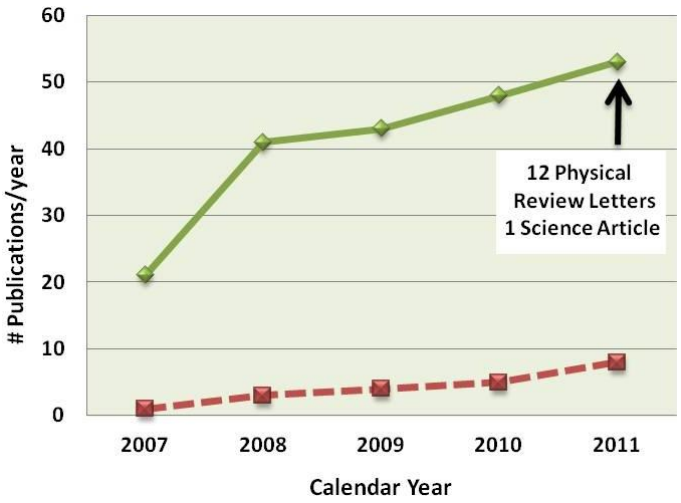

Figure 4: Publications produced yearly through the UNEDF collaborations. The solid line shows all publications and the dashed-line shows papers jointly authored by physicists and mathematicians or computer scientists.

DISCOVERIES ENABLED THROUGH PHYSICS-CS/AM COLLABORATIONS IN UNEDF

Year-5

- Much improved GFMC calculations of the 0^+ (Hoyle) excited state of ^{12}C and development work on BG/Q to dramatically improve performance.
- A weak scaling study (in which the work done is increased in proportion to the number of nodes used), based on our ^{12}C calculation, of the GFMC+ADLB code gave perfect scaling from 512 to 16,384 nodes on Argonne's IBM Blue Gene/P. At 32,768 nodes (131,072 cores) the time increased by only 8%.
- Demonstrated critical role of three-nucleon forces in producing the anomalously long but useful lifetime of ^{14}C. Collaboration between multiple UNEDF institutions produced this high-profile paper based on more than 30 million cpu hours of leadership class computing on Jaguar at ORNL. See New Scientist, ScienceDaily.
- Achieved the milestone of a final overall factor of 4 improvement in the leadership class code MFDn running ^{13}C with three-nucleon forces through a series of collaborative developments among UNEDF physicists, computer scientists and applied mathematicians. These developments culminated in Year-5 but spanned the entire UNEDF 5 year program.

- Developed energy density functional UNEDF1 that simultaneously reproduces ab-initio calculations of inhomogeneous neutron matter, and significantly advance our abilities to reproduce fission barriers and fission half-lives. See Stockpile Stewardship Quarterly and ANL PR.
- We used DFT with six nuclear energy density functionals and ORNL's Jaguar supercomputer to map the nuclear landscape. By using several models, we were able for the first time to quantify uncertainties of predicted drip lines. Model extrapolations turned out to be unexpectedly consistent between the current effective interactions, leading the team to estimate that the number of bound nuclei with Z between 2 and 120 is 6,900±500. See Nature NewsBlog, LiveScience, ScienceDaily, UTK PR.
- Introduced a comprehensive theoretical framework for the fermionic superfluid dynamics, grounded on a local extension of the time-dependent density functional theory. With this approach, we described the generation and the real-time evolution and interaction of quantized vortices. See PhysicsToday, ScienceDaily, PNL PR.
- A new official release of the HFODD DFT solver was published in Computer Physics Communications in 2012.
- The benchmarking of MADNESS on realistic self-consistent HFB problems for cold fermions and nuclei has been accomplished. We solved the HFB equations of the SLDA and ASLDA density functionals for cold Fermions, testing against the HFB-AX code that uses B-spline techniques.
- The systematic study of quadrupole vibrations in heavy nuclei with the deformed Skyrme-QRPA was completed, examining the performance of the QRPA framework itself and of individual Skyrme functionals.
- A fully symmetry unrestricted superfluid Time-Dependent DFT was used to calculate properties of the isovector giant dipole resonances of the deformed open-shell heavy nuclei. This is the first calculation of the linear response of open-shell triaxial systems.
- Using an ab initio approach based on Quantum Monte Carlo, we showed that the pseudogap phase sets in ultracold Fermi gases close to the unitary limit.
- We demonstrated that in the collision of two superfluid fermionic atomic clouds, of a total of approximately 750 fermions, one observes the formation of quantum shock waves as discontinuities in the number density and collective flow velocity.

Year-4

- A weak scaling study (in which the work done is increased in proportion to the number of nodes used), based on our ^{12}C calculation, of the GFMC+ADLB code gave perfect scaling from 512 to 16,384 nodes on Argonne's IBM Blue Gene/P. At 32,768 nodes (131,072 cores) the time increased by only 8%. See SciDAC Review.
- Development of the Leadership Class Configuration Interaction (LCCI) project and establishment of the LCCI database with current release versions of key codes, scripts

and test cases. Development and implementation of a Database Management System for storing and accessing meta-data on large CI production runs under the LCCI project.

- Development of a coupled total angular momentum (J) version of MFDn running on parallel processors with continuing efforts to improve load-balancing and scalability.
- Completed and published ab initio predictions for the highly-unstable proton rich nucleus ^{14}F for which experimental results are expected in the near future. See INCITE in Review, Science NewsLine.
- Completed an extensive set of calculations of the anomalously long half-life of ^{14}C using NN + NNN interactions with some runs carried out on more than 200,000 cores on Jaguar.
- Energies and one-body densities of superfluid neutron drops in external potentials have been calculated with GFMC (up to 16 neutrons) and AFDMC (up to 54 neutrons), leading to crucial constraints for energy density functionals developed by UNEDF.
- We developed the derivative-free optimization algorithm POUNDERS that yields substantial computational savings over alternative optimization methods. By adding the capability to restrict the search space to finite ranges for some of the parameters of the energy density functional (EDF), we obtained excellent fits to diverse data on 72 nuclei. See DEIXIS.
- For sensitivity analysis of optimized EDFs, we established a covariance technique for determining the correlations, standard errors, and sensitivity to perturbations of the data. These calculations are highly scalable and we have computed correlations using 5616 cores at NERSC, in the same wall-time as a single nucleus simulation.
- Using the UNEDF Experimental Database and the optimized solver HFBTHO, the Skyrme functional was optimized using the POUNDERS algorithm. The resulting parameterization UNEDF0 yields good agreement with a number of nuclear ground-state properties. See DEIXIS.
- The recently developed HFB-MADNESS solver has been applied to cold Fermions and tested against the HFB-AX code based on B-splines. This benchmark demonstrated the first practical application of MADNESS for 3D Fermi systems with broken time-reversal symmetry and pairing regularization (using zero-boundary conditions). The code has been scaled up to 4000 processors, with several improvements on performance compared to last year.
- We have developed a highly parallelized ASLDA DFT solver, which performs efficiently the diagonalization of the full 3D HFB matrix in parallel. The existing code can currently handle nuclear cubic volumes up to ~50^3 fm^3, with no self-consistent symmetries imposed.
- The time-dependent DFT software has been completed and successfully tested at scale on Jaguar to describe vortex formation and dynamics of unitary Fermi gas systems. The software has been used for production simulations on over 97% of the entire machine.

The code has achieved checkpointing~ 10TB of time-dependent simulation data at over 10GBps rates.

- A proton-neutron algorithm for the MPI JMoments code was designed and implemented, which improved its scalability to tens of thousands of cores, and increased its overall performance by a factor of more than 10,000. This development opens the possibility of calculating accurate shell model nuclear level densities and reaction rates for a large class of nuclei.

Year-3

- By applying a new approach to dynamic load balancing (ALDB) necessary for large scale computing, we calculated the ^{12}C ground state with the most realistic two- and three-nucleon interactions. The ground-state energy is within 1 MeV of the experimental results, and the calculated proton radius and densities are in excellent agreement with experiment.
- A weak-scaling test of ALDB for neutron drops reached 90% efficiency on 16K cores and 80% efficiency on 32K cores on Intrepid at Argonne (IBM BG/P). In these calculations, a thousand cores of the 32K available are used as servers. This is a dramatic improvement over last year, when efficiency peaked at 80% at around 900 cores.
- For the Many-Fermion Dynamics code, the total time has been reduced by approximately a factor of 3 from April 2007 to January 2009 through improvements in data structures and algorithms. Nearly ideal strong scaling has been achieved up to 7626 cores. The first successful ^{14}C and ^{14}N calculations with chiral NN + NNN interactions in Nmax =8 basis spaces have been performed on 110K and 143K cores, respectively.
- Calculations of neutron drops in external wells have been completed from 8 to 40 neutrons using MFDn, GFMC, and AFDMC methods. Excellent agreement has been achieved for the smaller systems (up to N=12) even for quite different NN interactions, confirming the fact that the three-nucleon interactions have little impact for the systems considered.
- The prototype 3D symmetry-free nuclear DFT solver HFB-MADNESS, based on advanced mathematical techniques such as low separation rank approximations and multiresolution analysis, has been demonstrated on the Cray XT-5 supercomputers, Jaguar at ORNL and Franklin at NERSC. High performance and scalability on computers with large number of cores and nodes have been demonstrated.
- Performance optimization of HFB codes enabled large-scale mass table calculations on 9,060 processors for over 840,000 configurations in 9,000 nuclei in a 14-hour run.
- We developed a new optimization algorithm, MFQNLS, and created a prototype code for obtaining the complete set of pairwise correlations between EDF parameters. Using Skyrme-DFT codes, we conducted 5 CPU-years worth of calculations to estimate 10

EDF parameters when simultaneously fitting experimental binding energies, rms radii, and pairing gaps for 72 deformed and spherical nuclei.

- Using the TD-SLDA framework, we have established that a unitary Fermi gas has a surprisingly rich spectrum of large amplitude modes of the pairing field. We showed that Higgs mode of the pairing field is strongly coupled to density oscillations in the case of strong pairing.

Year-2

- By applying a new approach to dynamic load balancing necessary for large scale computing, we achieved speedup efficiency of 83% in Quantum Monte Carlo calculations on over 16,000 processors for neutron droplets with N=14.
- Using the configuration interaction approach, we computed the ten lowest states in ^{14}F at 2 billion dimension on 30,628 processor cores by quadrupling MFD's speed.
- Performance optimization of HFB codes enabled large-scale mass table calculations on 4,000 processors for over 800,000 configurations in 9,000 nuclei in a day and the first multi-dimensional DFT symmetry-unrestricted calculations of multi-dimensional fission pathways.
- We developed a unique computational infrastructure for large-scale DFT calculations, including the most accurate, general-purpose 3D symmetry-free nuclear DFT solver for petascale computers. This solver is based on advanced mathematical techniques such as low separation rank approximations and multiresolution analysis.
- We applied the Broyden's iterative method to solve equations with limited memory and guaranteed convergence in various problems arising from nuclear structure calculations. The number of unknown variables reached ~3,000,000 in DFT and ~108 in Coupled Cluster applications

Year-1

- We benchmarked various *ab initio* methods (GFMC, NCSM, CC) on a common set of nuclei and NN interactions. For A=6, NCSM and GFMC gave binding energies very closed to each other (29.0-29.4 MeV). The CC method was tested against others for the first time with excellent results for ^{4}He in the CCSD(T) approximation.
- There has been much progress calculating the energy of the trapped gas, most recently for small numbers of particles. Within GFMC, we studied EOS and pairing gap of the unitary gas.
- We continued developing the tools of DFT and its extensions. An important computational question was the choice of basis to represent the orbitals of DFT. We assessed the relative merits of three choices: harmonic oscillator basis, 3D mesh basis, and wavelet basis.

- We initiated mass table calculations for odd-A nuclei using the HFODD HFB solver that does the full HFB treatment of the pairing and releases commonly used approximations for the fields including invariance on time reversal and axial symmetry.
- We carried out the survey are the first 2^+ excited states of even-even nuclei using QRPA and GCM

OTHER UNEDF HIGHLIGHTS

Year-5

- QMC calculations of a very large number of asymptotic normalizations and magnetic moments completed, excellent agreement with experiment.
- Coupled-Cluster calculations of the binding of neutron-rich Ca isotopes including better coupling to the continuum and effective three-nucleon interactions provide an excellent description of the approach to the neutron drip line. See UTK PR.
- NCSM/RGM calculations of several low-energy reactions in A=4,5,8 including initial studies with three nucleon interaction. See Physics.aps.org Synopsis
- Joint CI/QMC calculations of neutron drops in many external wells for several different interactions, extracted shell closures, spin-orbit splitting, and pairing signals.
- Calculations of neutron matter Equation of State used to compare to astrophysical observations; excellent agreement with mass/radius relationship
- Calculations of effective range coefficient in cold atoms allows for more exact comparison of cold atoms and neutron matter over a wider density range
- Completed first successful comparison between ab initio no core full configuration and density matrix expansion calculations of neutron drops in external potentials. Developed, implemented, and published the Coulomb-Sturmian basis for ab initio no core full configuration (NCFC) calculations and demonstrated improved convergence of long-range observables.
- Completed extensive investigation of the Lithium isotopes and published tables showing favorable comparisons with experiment where available and published 23 separate predictions for future experiments.
- Completed and published development and testing of ab initio no-core Monte Carlo Shell Model (MCSM) and benchmarked results with full configuration interaction (FCI) and with no-core full configuration (NCFC) results.
- Achieved up to a factor of two speedup of MFDn's Lanczos iterations in large scale applications by designing and implementing a new topology for core assignments.
- Completed and submitted for publication extensive investigation of the infra-red and ultra-violet properties of the no-core shell model (NCSM) calculations in a harmonic

oscillator basis. Identified key parameters and universal features for efficient and accurate extrapolations of eigenvalues to the infinite matrix limit.

- SRG NNN potentials consistently softened in an oscillator basis were applied in the p-shell through ^{12}C with initial chiral EFT potentials, with successful convergence but showing hints that four-body interactions may be important in heavier nuclei. To address this issue and to extend applications to infinite matter, the first momentum-space SRG evolution of NNN potentials was achieved.
- Local projections of soft non-local NN potentials were demonstrated, making future quantum Monte Carlo applications feasible.
- The framework for evolving consistent operators for use with SRG wave functions was further developed with successful tests of long-distance operators (e.g., the radius) in A=3 and A=4 nuclei.
- The in-medium SRG (IMSRG) was extended to open-shell systems and used to generate semi-microscopic shell model Hamiltonians, which outperformed those derived from many-body perturbation theory.
- Density matrix expansion calculations of neutron drops in external potentials were extended to larger systems with successful comparisons to ab initio auxiliary field Monte Carlo and coupled cluster calculations.
- Within HFB, we studied the structure of the unbound quasiparticle spectrum of weakly bound nuclei within several methods that do not rely on imposing scattering or outgoing boundary conditions. Various approximations were implemented and examined to estimate resonance widths.
- We studied the bulk deformation properties of the Skyrme nuclear energy density functionals. Following simple arguments based on the leptodermous expansion and liquid drop model, we applied the nuclear density functional theory to assess the role of the surface symmetry energy in nuclei. We concluded that its proper determination is crucial for the stability of deformed phases of the neutron- rich matter and description of fission rates for r-process nucleosynthesis
- A charge-changing version of the deformed-Skyrme-QRPA code was constructed, which is being also used for beta and double-beta decays.
- A new algorithm hass been implemented that calculates the 2nd moments of the Hamiltonian. These widths can be further used to calculate nuclear level densities free of center-of-mass contribution. The new algorithm was integrated in the JMoments code and was validated for several sd-shell nuclei, either by comparing with exact shell model results or with experimental data. Using this algorithm, shell model nuclear level densities for unnatural parity states of sd-shell nuclei have been calculated.

Year-4

- Completed first successful comparison between ab initio no core full configuration and density matrix expansion calculations of neutron drops in external potentials.
- Introduced and successfully tested new ab-initio scattering method for nuclear systems in a harmonic trap enabling bound state scattering solutions to produce scattering phase shifts.
- Coupled-cluster theory was used to calculate the proton halo state and resonances in A=17 nuclei using the Gamow basis and to calculate spectroscopic factors. See ScienceDaily.
- Softened SRG NNN potentials were extended to a Slater-determinant basis with the first applications to p-shell nuclei. Procedures for consistently evolved SRG operators were developed with factorization demonstrated. In-medium SRG diagonalization of closed-shell nuclei such as ^{40}Ca comparable to CCSD(T).
- We developed a portable Fortran 90 module implementing the DME of chiral effective interactions in DFT solvers. The module has been tested against analytical formulas in Mathematica.
- First implementation of orbital-based DFT for nuclei with successful comparisons to Hartree-Fock and beyond.
- The first hybrid EDF with long-range chiral EFT contributions combined with a short-range Skyrme-like parametrization was successfully demonstrated, with good agreement with ab initio results for test interactions in neutron drops.
- By applying naïve dimensional analysis based on chiral effective theory, a large sample of Skyrme parametrizations was examined for naturalness. The best current functionals are consistent with naturalness and a momentum scale of ~700 MeV/c.
- The coordinate-space code HFB-AX has been used to study the competition between normal superfluidity and Larkin-Ovchinnikov (LO) phases of polarized Fermi gases at unitarity in extremely elongated traps. We find families of LO type of solutions with prominent transversal oscillation of the pairing potential. Those states coexist with a superfluid state having a smooth pairing potential.
- Scattering ab initio calculations were performed for n-^{8}He, n-^{9}Li using the resonating group method with similarity-renormalization-group interactions.
- We calculated reaction cross sections for nucleons on a range of nuclei A=40-144 by coupled-channel calculations, and were able to reproduce ~100% of that observed, by including couplings to correlated QRPA states as well as one-nucleon transfer channels.
- We developed a procedure to compute non-local optical potentials for use in general reaction models of nucleons on heavy nuclei.
- Coupled channels sets up to 20,000 partial-wave channels solved for nucleon-nucleus scattering.

Year-3

- Completed first successful comparison between ab initio no core full configuration and density matrix expansion calculations of neutron drops in external potentials.
- A solution to the center-of-mass problem in the coupled-cluster method has been found.
- By implementing a Λ-CCSD(T) Coupled Cluster scheme, we obtained converged results for ^{40}Ca with the bare N^{3}LO chiral interaction.
- We carried out a full three-dimensional evolution of SRG NNN potentials. Studies of the triton and the alpha particle verify that evolving the full Hamiltonian leaves energies unchanged (at the 40 keV level in ^{4}He) and establishes that an initial hierarchy of many-body forces (as from chiral EFT) is maintained in the evolution.
- The scalar-isoscalar part of an ab initio EDF, based on the density matrix expansion and adapted to use a chiral EFT interaction softened using RG methods by generalizing to momentum space and NNN interactions, was completed. A new phase space averaging approach has been implemented that has led to reduction of relative errors in integrated quantities by a factor of ~ 5-10 across many different isotope chains.
- We derived the most general long-range DME-based EDF from chiral EFT through N^{2}LO. The evolution to low momentum does not change the long-range (pion) NN and NNN contributions to the EDF, which is therefore universal.
- We carried out a number of large-scale surveys based on DFT, including (i) odd-even nuclear binding energy staggering using several treatments of the pairing interaction, (ii) one-quasiparticle states in odd-*A* nuclei; and (iii) low-excitation energy spectra of even-even nuclei.
- Using the axial coordinate-space parallel solver HFB-AX, we investigated the isentropic fission barriers in the heaviest and superheavy nuclei. For nuclei produced in "cold fusion" reactions, we predicted a more rapid decrease of fission barriers with excitation energy as compared to the nuclei synthesized in "hot fusion" experiments.
- We have constructed an accurate EDF for the asymmetric unitary gas and presented strong theoretical evidence that a new phase of matter, the Larkin-Ovchinnikov pairing phase, is favored over the homogeneous superfluid and normal phases in three-dimensional unitary Fermi systems.
- The serial version of the Moments CI code was parallelized using MPI and a load-balancing algorithm. The domain decomposition was done along the collection of many-body configurations built on spherical single particle orbits. The new code was benchmarked on Franklin at NERSC, and it showed very good strong scaling up to 256 cores for the case of ^{56}Fe, which has only 475 configurations.
- Scattering ab initio calculations were performed for *n*-^{4}He, *p*-^{4}He, *n*-^{7}Li, *p*-^{12}C, and *n*-^{16}O using the resonating group method with similarity-renormalization-group interactions.

- We performed coupled-channel calculations for the reactions n, p + ^{90}Zr and ^{208}Pb by including couplings to uncorrelated particle-hole states and to correlated RPA states.

Year-2

- Using Quantum Monte Carlo and Superfluid Local Density Approximation, we calculated the Equation-of-State pairing gap of dilute neutron matter.
- By implementing a CCSD J-coupled Coupled Cluster scheme, we obtained converged results for medium-mass nuclei ^{40,48}Ca and ^{48}Ni with the bare N3LO chiral interaction.
- Fits of the N2LO NNN parameters have been obtained for the first time for $V_{low\text{-}k}$ and SRG NN interactions that start from chiral EFT potentials, with realistic calculations of nuclear matter. The first density matrix expansion functionals with NN and NNN interactions have been constructed.
- Ab initio reactions are a new UNEDF activity. Scattering ab initio calculations were performed for n-^{3}H, n-^{4}He, p-^{3,4}He, and n-^{16}O using the resonating group method with similarity-renormalization-group interactions.
- The moments approach based on the configuration interaction method was successfully adapted to calculate nuclear level densities.

Year-1

- Within SRG method, we studied nuclear matter using a well-regulated realistic NN interaction. By adding a perturbative NNN interaction we achieved saturation properties.
- We have constructed an LDA energy functional for the unitary gas and compared with GFMC calculations.
- We studied inelastic scattering of protons on ^{90}Zr at 40 MeV incident energy using RPA transition densities.
- The semidirect mechanism for capture of energetic neutrons was calculated using DFT input with satisfactory results.

IMPACTS BEYOND NUCLEAR PHYSICS

The UNEDF project had a significant impact beyond nuclear physics. One example is the applications of nuclear physics to neutron stars as discussed below. Another important example is the application of methods developed during UNEDF to cold atoms. Cold atoms are very similar to neutron matter at very low density because the binary interaction can be tuned to produce a zero-energy bound state; this system is called the 'unitary Fermi gas'. Many experiments and calculations have been performed in this limit.

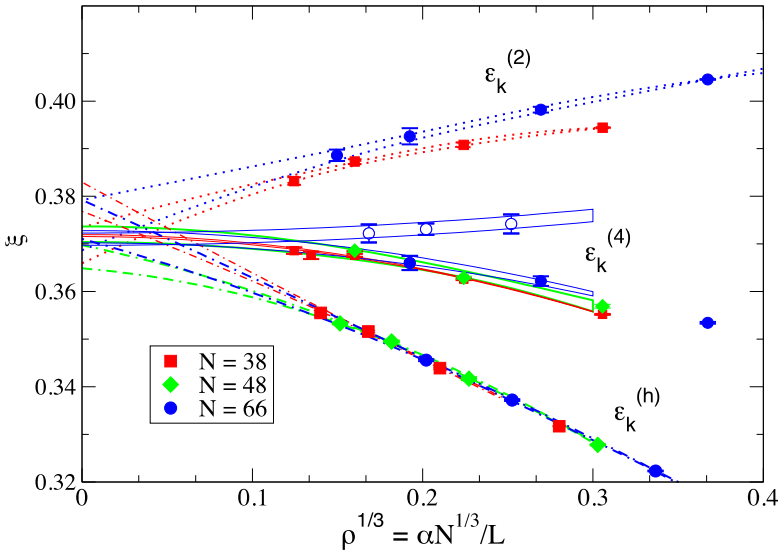

Figure 5: Equation of state of the unitary Fermi gas.

The UNEDF collaboration have performed the most accurate calculations of several universal parameters describing the unitary Fermi Gas, including the equation of state ("Bertsch parameter"), the contact, and the superfluid pairing gap at T=0. Figure 5 shows new lattice calculations of the Bertsch parameter. The different curves represent different interactions with the same continuum limit. The extrapolated value agrees well with recent MIT experiments.

The slope is a new universal parameter associated with the effective range of the interaction. We have also examined quantities at finite temperature, including the superfluid-to-normal phase transition and its associated critical temperature, and the pseudo-gap phase above the critical temperature where pairing still exists but the system is no longer superfluid.

The close coupling between ab-initio and density functional theories in UNEDF also made it possible to connect these ab-initio calculations to density functionals designed for cold atoms, in

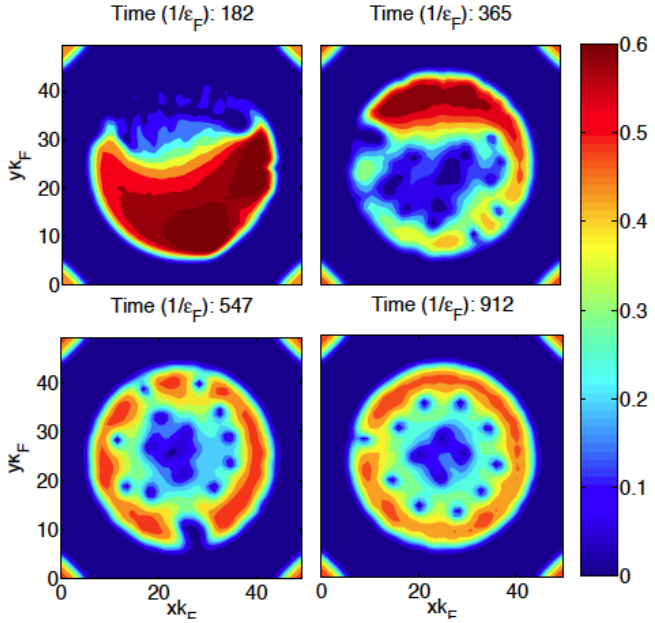

Figure 6: Vortex dynamics in the unitary Fermi gas.

particular the ASLDA theory. This superfluid local density approximation is particularly accurate for cold atoms; it has been used to study vortex dynamics in cold atom systems. For the first time one could recreate the real-time creation of vortices and their evolution into lattice structures (see Figure 6).

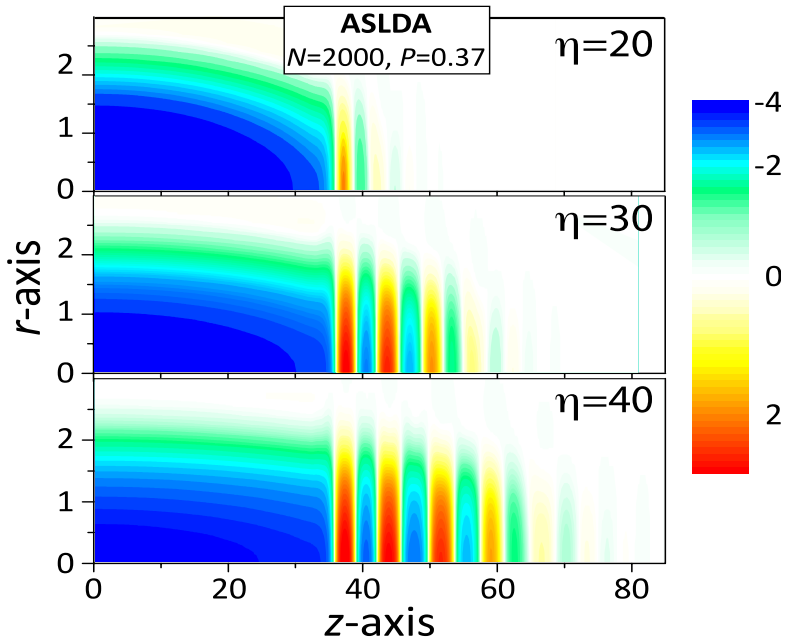

Figure 7: Inhomogeneous superfluid phases in cold atom systems.

We also studied exotic superfluid phases in UNEDF (see Figure 7). These inhomogeneous superfluid phases have been postulated to exist in cold atomic gases and in QCD at high chemical potential and low temperature. Density functional theory allowed us to cover the large ratio of scales between the interparticle distance and the scale of pairing oscillations.

The UNEDF project, focused on advancing the capabilities of nuclear physics simulations and the tight coupling between ab-initio and density functional theory, as well as the tight coupling between applied mathematicians and computer scientists with nuclear theorists, enabled us to make rapid progress on this important area with clear overlap with nuclear physics.

III. BEST PRACTICES AND LESSONS LEARNED

UNEDF was a successful SciDAC project. These successes were built upon certain best practices, some implemented originally and some learned by experience, in organizing and implementing the scientific effort.

CLOSE ALIGNMENT OF PHYSICS WITH CS/AM

To foster the close alignment of the necessary **applied mathematics and computer science research** with the necessary **physics research**, multiple direct partnerships were formed consisting of computer scientists and applied mathematicians linked with specific physicists. In each partnership, mathematicians/computer scientists collaborated with physicists to remove barriers to progress on the computational/algorithmic physics side. All of these interactions have success stories, from greatly improved load balancing on leadership class, to dramatically improved algorithms for optimization of functionals and for finding eigenvalues/eigenfunctions of extremely large matrices, to new DFT solver technologies, and more. There have been over 20 joint publications and most of the scientific highlights of UNEDF were directly enabled by one of these partnerships.

MANAGEMENT

To oversee the project, a representative council of senior scientists and a charter were established. The UNEDF charter, which established the functions, organizational structure, and responsibilities within the UNEDF project, is given below in Sec. VIII. Council consisted of the Director and co-Directors (Bertsch in Year-1; Lusk and Nazarewicz in Years 2-5), and additional members drawn from the Collaboration (Carlson, Furnstahl, Horoi, Ng, Thompson, Vary; and Bulgac and Dean in Year-1). The UNEDF Council met regularly (typically once per month) through conference calls and also during annual collaboration meetings. The main role of these conferences was to discuss the progress, assess the goals, and, when needed, redirect the collaboration's effort through periodic assessments. The UNEDF Council coordinated the expansion of the partnership activity within the existing set of participants. The integration of various shell-model activities under UNEDF into the "Leadership-Class Configuration Interaction" (LCCI) research area in Year-3 was such a development. Progress in the LCCI effort in Year-5 is described in a separate section below.

The UNEDF Council also served as a facilitator of new research directions by receiving proposals for new partnerships consisting of new researchers, either physicists or mathematicians and computer scientists, which could advance the overall goals of the project. If it considered these worthy, such proposals were conveyed to the relevant program offices for their review and possible addition to the SciDAC program under the UNEDF umbrella. The addition in Year-3 of the Lattice QCD LLNL effort by Tom Luu, which bridges lattice results and inter-nucleon potentials, was an example of such an extension.

UNEDF WEBSITE: COMMUNICATION AND INTEGRATION TOOL

The collaboration's website (unedf.org) has been an important communication tool for UNEDF and an outreach window into UNEDF science. Improvements and enhancements to the website were implemented throughout the project to increase the visibility of SciDAC, to emphasize the relevance of UNEDF research, and to reach a wide audience including the general public. The website is divided into public and user sections, with the user pages accessible to all collaboration members through a common username and password. (Stronger security than this has not been necessary.) Screenshots of the homepage are shown in Figure 8 and Figure 9. Clickable brief highlights are available at the top (Figure 8) with news items and announcements below (Figure 9).

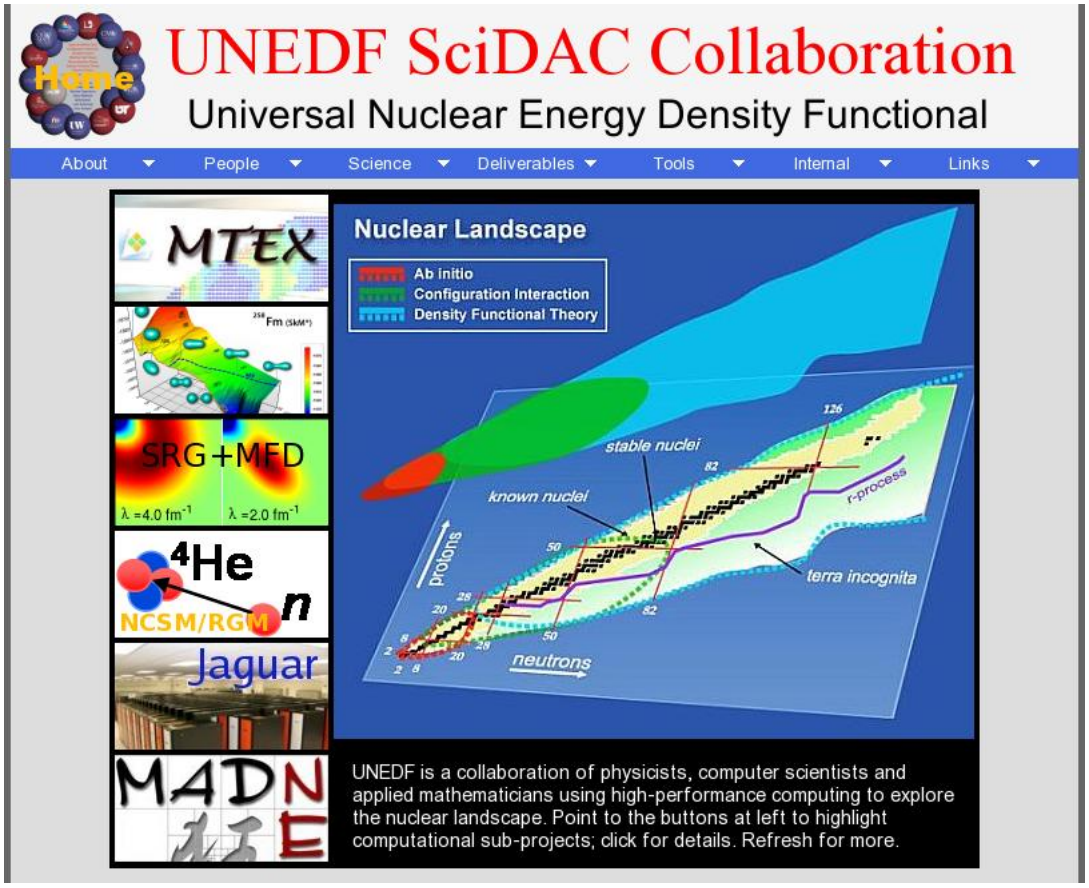

Figure 8: UNEDF website unedf.org home page, featuring clickable highlights of the project. Navigation is via the dropdown menus across the top.

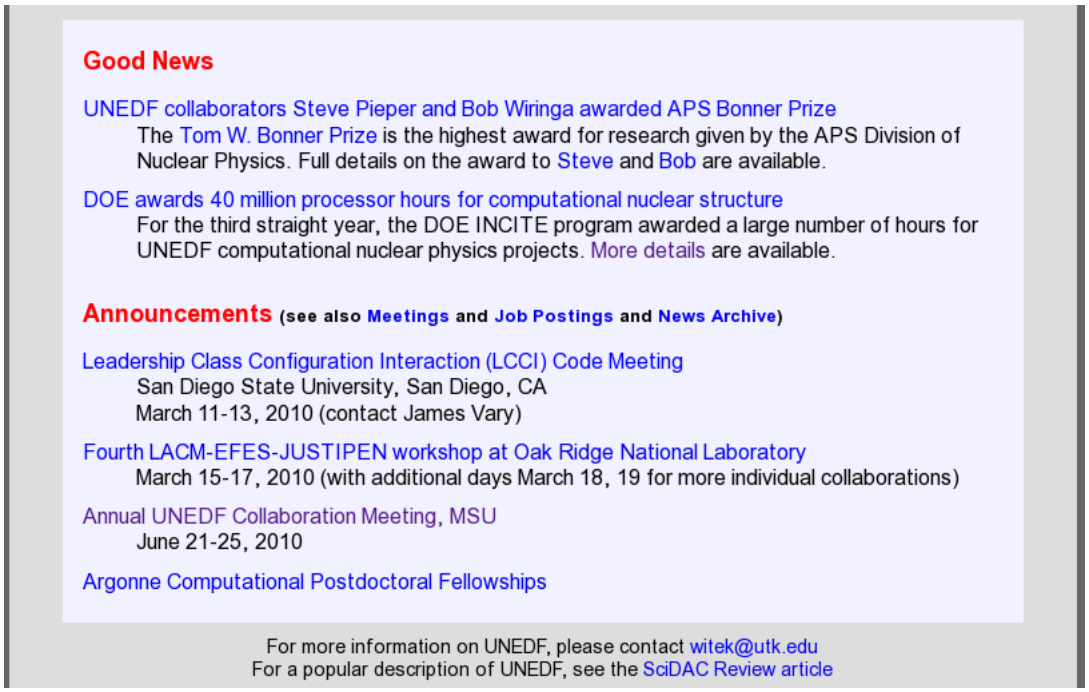

Figure 9: Additional content on unedf.org home page. "Good News" gives brief summaries and links to recent accomplishments or recognitions in the project. "Announcements" link to upcoming meetings or opportunities.

Navigation of the website is through dropdown menus that are part of the header common to every page. An example of a menu is shown in Figure 10. Here we summarize the content under each menu heading.

- About — A brief overview of the UNEDF project and a strategy diagram, as well as links to overviews of the science and the organization of the project (research areas, the UNEDF Council, the UNEDF Charter, annual meetings).
- People — Participating institutions and investigators as well as foreign collaborators (including a worldwide map with their distribution), members of the UNEDF Council, job opportunities.
- Science — Descriptions of the physics, applied mathematics, and computer science aspects of the UNEDF project, overview articles, and highlights. The highlights are one-page slides, in some cases with supplementary notes, which describe in pictures and broadly accessible language one notable result from the UNEDF project. The target audiences include the DOE offices, fellow scientists, congressional staff, and the general public.
- Deliverables — Continually updated lists of publications (organized by year and title), presentations (chronologically), computer codes, and one-page highlights.
- Tools — Links to the UNEDF SVN repository, public codes, databases of relevant nuclear properties (e.g., masses and fission barriers), Mass Explorer, and various other tools.
- Internal — Collaboration-only (password protected user pages) material, including minutes of Council meetings, proceedings from UNEDF Annual

Meetings, internal projects and white papers, and information for the DOE offices.

- Links — General related links and outreach.

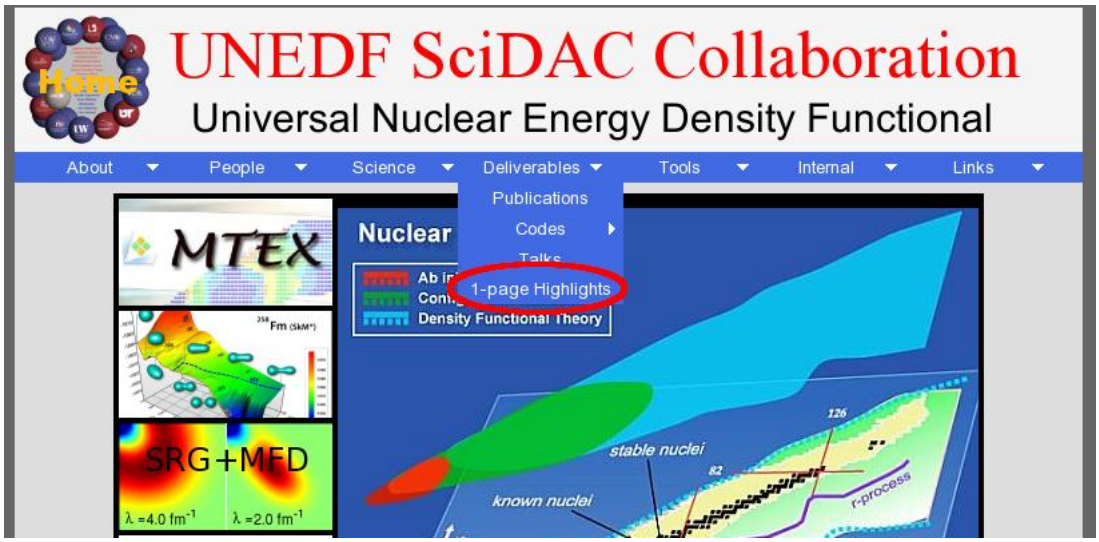

Figure 10: Deliverables menu, featuring the link to one-page highlights.

The unedf.org website was easy to maintain and update (basically by one person; Furnstahl) because of the technical design. The important aspects are described here.

- The website is hosted at Ohio State University on an Apache server running Linux, with daily backups. The computer is a dedicated machine for serving OSU Physics Department web pages. The server hardware is maintained by the OSU computer staff.
- The pages are written in PHP for both static and dynamic content. For a uniform appearance and easy, consistent updates, a common header and footer file is input to every page. This includes the UNEDF banner at the top (which is an image map with links) and the drop-down menus.
- The drop-down navigation menus are implemented as CSS, which is more robust than javascript. The content is simple to change by editing a single text file.
- Access to the internal user pages is restricted using .htaccess files with a common username and password for all collaboration members. Indexing of content by external search engines is restricted by a robots.txt file.
- Static content is modified by directly editing the corresponding php pages (rather than using a webpage building software).
- Details of deliverables (publications, talks) and the collaboration (investigators, institutions, and foreign collaborators) are stored in a MySQL database, which is accessed by PHP pages. Changes to the database are made through forms-based administration web pages, which are accessed via a separate username and password.

COLLABORATION MEETINGS

The annual meetings were crucial for the effort's integration. The main objectives were to: (i) assess progress towards next year and final deliverables; (ii) decide the next steps of specific research plans to be undertaken; (iii) create opportunities for new collaborations; (iv) broaden the scientific horizons and increase coherence of the effort; (v) provide a global view through guest presentations; (vi) solicit information from collaboration members on how to improve practices; and (vii) provide opportunities to interact with funding agencies and FRIB management. Five annual meetings were held:

- August 13-16, 2007, Pack Forest, WA; 47 participants incl. 8 guests
- June 23-26, 2008, Pack Forest, WA; 50 participants incl. 6 guests
- June 22-25, 2009, Pack Forest, WA; 66 participants incl. 8 guests
- June 21-25, 2010, MSU campus, MI; 58 participants incl. 10 guests
- June 20-24, 2011, MSU campus, MI; 56 participants incl. 12 guests

All meetings were supported by UNEDF internal funds; the Year-5 meeting received a contribution from FRIB/NSCL. An important role of the last meeting was to prepare the collaboration for the anticipated SciDAC-3 solicitation.

UNEDF members attending the APS/DNP annual meetings organized satellite meetings to discuss progress and exchange information on UNEDF contributions. In addition, there were many other meetings between subsets of UNEDF. For instance, the Leadership Class Configuration Interaction (LCCI) group met regularly to discuss recent progress and the integration of the LCCI codes. Besides the special gatherings at the UNEDF annual meetings, the LCCI group (ca. 15 members) met separately 3 times: SDSU, March 11-13, 2009; SDSU, March 11-13, 2010; and LBNL March 17-19, 2011.

KEEPING SPONSORS INFORMED

To increase the awareness of funding agencies of our progress and research goals, visits of the UNEDF Council to DOE (e.g., in October 2010) and interactions with DOE leadership at APS/DNP meetings were important and valuable. These meetings provided focused opportunities to discuss our transformational science targeting extreme-scale computing. In particular, the Council presented the collaboration's computational and scientific accomplishments during past years, discussed milestones for the next year, and presented the long-term strategy.

MENTORING AND TRAINING

One of the most important deliverables from the UNEDF project has been the training of young scientists. Annually the project provided support to 30 young researchers (11 students and 19 postdocs), who are among the best in low-energy nuclear theory. Below in Section IV we list all of the young scientists (students and postdocs) who have participated in the research, which reveals many success stories. The UNEDF experience has been a springboard for advancement, as UNEDF postdocs have obtained permanent positions at U.S. universities (S. Bogner, J. Drut, P. Maris), at National Laboratories (S. Gandolfi, E. Jurgenson, L. Platter, S. Quaglioni, I. Stetcu, N. Schunck, S. Wild), and at foreign institutions worldwide (A. Gezerlis, J. Pei, J. Terasaki).

Here we quote one of those success stories, Dr. Nicolas Schunck, who discusses how aspects of the UNEDF project were beneficial. On careers:

> *"Clearly, there were new postdocs positions opened almost every year, so it was great. But what was really useful was the 5 year duration of the project: it meant that postdocs could be given extra time to find a job if needed. I spent 3 and half years at ORNL/UTK, others moved from one institution to another while remaining funded under UNEDF and continuing their work. In such a difficult economic environment, this job security, or job continuity, was very valuable. I believe it is one of the factors why so many young scientists were hired at universities/labs."*

On science:

> *"UNEDF annual meetings were truly fantastic opportunities for postdocs. Because UNEDF is a transversal project (from nucleon forces to ab initio/shell model to DFT to reactions), our meetings were like a giant crash course on nuclear theory and HPC methods, both taken really in their broadest sense, and given by the most experts in the field. In fact, if I had a student funded from a different source, I would try to send him/her to these meetings anyway, they are so much more useful than any workshop or conference. In fact, I don't think there is any equivalent to these meetings. On a personal level, that's where I started to get really interested in nuclear physics and HPC."*

The UNEDF project has also been a springboard for new training options in nuclear theory and computational sciences. The TALENT initiative (Training in Advanced Low Energy Nuclear Theory), which took form at a UNEDF collaboration meeting and subsequent discussions between UNEDF members and European collaborators, will provide 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 intensive 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 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 the 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 multithreading in numerical computing, lattice simulations, advanced parallelization for multicore and GPU processing for linear systems and eigenvalue calculations, and challenges and approaches for heterogeneous HPC. Several additional TALENT courses are planned for 2013. Other training opportunities that UNEDF members took advantage of include

workshops such as the 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.

INTERNATIONAL IMPACT

The UNEDF collaboration, through its scope, size, and structure is unique worldwide in the field of low-energy nuclear theory. UNEDF has collaborated closely with a number of foreign efforts and individual scientists sharing similar fundamental science goals. Such collaborations include joint software development and benchmarking. Representatives of Foreign Collaborating Projects regularly attended the UNEDF annual meeting. The UNEDF activities have had positive (leveraging) effects on our foreign partners. Examples include the joint UNEDF-JUSTIPEN and UNEDF-FIDIPRO efforts and a new initiative involving low-energy nuclear theory in France, FUSTIPEN. The worldwide impact of the UNEDF is clearly seen at international meetings and workshops, such as the 2010 INPC meeting in Vancouver, where our highlights were quoted in several plenary talks (including a keynote talk by Peter Brown-Munzinger from Darmstadt).

IV. JUNIOR SCIENTISTS in UNEDF

Support and successful careers for junior scientists have been an important goal of our 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. Below we list the junior scientists in UNEDF, and indicate their present positions (if known). It is critical to maintain this stream of young people, and to provide a balance across types and fields of positions.

STUDENTS

- Eric Anderson, OSU (PhD 2012, Postdoc at UNC)
- Noah Birge, UTK (undergrad)
- Juan Burgos-Vasquez, MSU
- Justin Cantley, CMU (PhD student at U. Florida)
- Chase Cockrell, ISU (PhD 2012, Postdoc at Univ. Chicago in Biophysics)
- Biruk Gebremariam, MSU (industry at SAS from 6/2010)
- Alex Gezerlis, UI/Urbana/LANL (PhD 2009, Postdoc at INT, TU Darmstadt)
- Eric Jurgenson, OSU (PhD 2009, Postdoc then staff at LLNL)
- Jagjeet Kaur, CMU (PhD student at WMU)
- Nikhil Laghave, Ames Lab
- Yuan Lung (Alan) Luo, UW
- Jordan McDonnell, UTK, NNSA SSGF fellow (PhD 2012, Postdoc at LLNL)
- Alina Negoita, ISU (PhD 2010, Computer Science PhD candidate at ISU)
- Nicola Nikolov, UTK, supported by NNSA SSAA (PhD 2011, Postdoc at LSU)
- Erik Olsen, UTK, supported by NNSA SSAA
- Alex Perhac, UTK (undergrad)
- Mike Scott, MSU (PhD student at MSU)
- Avinash Srinivasa, Ames Lab
- Joshua Staker, SDSU
- Karthik Ushkhala, TAMU-C
- Kyle Wendt, OSU, supported by DOE graduate fellowship
- Sukjin Yoon, UW (Postdoc Asia-Pacific Center for Theoretical Physics, Pohang)

POST-DOCTORAL ASSOCIATES

- Hasan Metin Aktulga, LBNL
- Simone Baroni, UW (Postdoc at ULB, Brussels)
- Scott Bogner, OSU (Faculty at MSU)
- Ivan Brida, ANL (on leave from LANL postdoc)
- Christopher Calderon, LBNL (Staff, Numerica)

- Joaquin Drut, OSU, LANL Fellow (Faculty at UNC)
- Jochen Erler, UTK/ORNL (German Cancer Research Center since 2012)
- Stefano Gandolfi, LANL (Staff at LANL)
- Zaochun Gao, CMU (China Inst. of Atomic Energy)
- Alex Gezerlis, INT (now at TU Darmstadt, next year faculty at Guelph)
- Kai Hebeler, OSU
- Heiko Hergert, MSU (Postdoc at OSU)
- Jason Holt, UTK/ORNL (Postdoc at TUD Darmstadt)
- Eric Jurgenson, LLNL (Staff at LLNL)
- Markus Kortelainen, UTK/ORNL (Research Prof. at U. Jyväskylä)
- Plamen Krastev, SDSU/LLNL (Computational scientist Harvard)
- Thomas Lesinski, UT/ORNL (Postdoc at Warsaw U.)
- Pieter Maris, ISU (Research Assoc. Prof. of Physics, ISU since 2011)
- Eric McDonald, MSU (software engineer at MSU)
- Sergej Moroz, UW
- Mika Mustonen, UNC and CMU (Postdoc UNC)
- Gustavo Nobre, LLNL (Postdoc at BNL, NNDC)
- Junchen Pei, UTK/ORNL (Professor at Peking U.)
- Lucas Platter, OSU (Staff at ANL)
- Nicolas Schunck, UTK/ORNL (Staff at LLNL)
- Roman Senkov, MSU (Fixed-term faculty CMU)
- Ionel Stetcu, UW (Staff at LANL)
- Jun Terasaki, UNC (Assoc. Prof. at Tsukuba U.)
- Stefan Wild, ANL (Staff at ANL)
- Gabriel Wlazłowski, UW/Warsaw University

V. PRIZES and AWARDS

UNEDF scientists have won significant awards during the past several years. Notable accomplishments include:

- Joaquin Drut (OSU), who was awarded the Hermann Kümmel Early Achievement Award in Many-Body Physics in 2009.
- Steve Pieper and Robert Wiringa (ANL), who received the Tom W. Bonner Prize in Nuclear Physics in 2010 *"For development of quantitative, ab initio calculations of the properties of nuclei from A=6 to A=12, including deep physical insight into the nature of nuclear forces and the application of state-of-the-art computational physics."*
- Sofia Quaglioni (LLNL), who received a prestigious DOE Early Career award in 2011.
- Witold Nazarewicz (UTK/ORNL), who received the Tom W. Bonner Prize in Nuclear Physics in 2012 *"For his foundational work in developing and applying nuclear Density Functional Theory, motivating experiments and interpreting their results, and implementing a comprehensive theoretical framework for the physics of exotic nuclei."*
- 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.

VI. DELIVERABLES

PUBLICATIONS (ALL YEARS)

Joint publications between physicists and applied mathematicians or computer scientists are highlighted in red.

1. *A High-Performance Algorithm to Calculate Spin- and Parity-Dependent Nuclear Level Densities*, R. Senkov and M. Horoi, Phys. Rev. C 82, 024304 (2010) [arXiv:1004.5027].
2. *A High-Performance Fortran code to Calculate Spin- and Parity-Dependent Nuclear Level Densities*, R. Senkov, M. Horoi, and V. Zelevinsky, Comp. Phys. Comm. (2012) in press [arXiv:1206.4583].
3. *A Unitary Fermi Supersolid: The Larkin-Ovchinnikov Phase*, A. Bulgac and M.M. Forbes, Phys. Rev. Lett. 101, 215301 (2008) [arXiv:0804:3364].
4. *Ab initio approach to effective single-particle energies in doubly closed shell nuclei*, T. Duguet and G. Hagen, Phys. Rev. C 85, 034330 (2012) [arXiv:1110.2468].
5. *Ab initio computation of circular quantum dots*, M. Pedersen Lohne, G. Hagen, M. Hjorth-Jensen, S. Kvaal, and F. Pederiva, Phys. Rev. B 84, 115302 (2011) [arXiv:1009.4833].
6. *Ab initio computation of the ^{17}F proton-halo state and resonances in A = 17 nuclei*, G. Hagen, T. Papenbrock, and M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010) [arXiv:1003.1995].
7. *Ab initio coupled-cluster approach to nuclear structure with modern nucleon-nucleon interactions*, G. Hagen, T. Papenbrock, D. J. Dean, and M. Hjorth-Jensen, Phys. Rev. C 82, 034330 (2010).
8. *Ab initio many-body calculation of the $^{7}Be(p,\gamma)^{8}B$ radiative capture*, P. Navratil, R. Roth and S. Quaglioni, Phys. Lett. B 704, 379 (2011).
9. *Ab Initio Many-Body Calculations of n-H-3, n-He-4, p-He-3,4, and n-Be-10 Scattering*, S. Quaglioni and P. Navratil, Phys. Rev. Lett. 101, 092501 (2008) [arXiv:0804.1560].
10. *Ab initio many-body calculations of nucleon-nucleus scattering*, S. Quaglioni, P. Navratil, Phys. Rev. C 79, 044606 (2009).
11. *Ab Initio Many-Body Calculations of the 3H(d,n)4He and 3He(d,p)4He Fusion Reactions*, P. Navratil and S. Quaglioni, Phys. Rev. Lett. 108, 042503 (2012) [arXiv:1110.0460].
12. *Ab initio no-core full configuration calculations of light nuclei*, P. Maris, J.P. Vary and A.M. Shirokov, Phys. Rev. C 79, 014308 (2009) [arXiv:0808.3420].
13. *Ab initio no-core shell model and microscopic reactions: Recent achievements*, S. Quaglioni and P. Navratil, Few-Body Syst. 44, 337 (2008) [arXiv:0712.0855].
14. *Ab initio nuclear structure simulations: the speculative ^{14}F nucleus*, P. Maris, A.M. Shirokov, and J.P. Vary, Phys. Rev. C 81, 021301 (2010) [arXiv:0911.2281].
15. *Ab initio nuclear structure: The Large sparse matrix eigenvalue problem*, J.P. Vary, P. Maris, E. Ng, C. Yang, and M. Sosonkina, J. Phys. Conf. Ser. 180, 012083 (2009) [arXiv:0907.0209].
16. *Ab initio nuclear theory – progress and prospects from quarks to the cosmos*, J.P. Vary, Acta Physica Polonica B 42, 397 (2011).
17. *Ab initio shell model with a core*, A.F. Lisetskiy, B.R. Barrett, M.K.G. Kruse, P. Navratil, I. Stetcu, J. P. Vary, Phys. Rev. C 78, 044302 (2008) [arXiv:0808.2187].

18. *Ab initio study of Ca-40 with an importance truncated no-core shell model*, R. Roth and P. Navratil, Phys. Rev. Lett. 99, 092501 (2007).
19. *Ab-initio computation of neutron-rich oxygen isotopes*, G. Hagen, T. Papenbrock, D.J. Dean, M. Hjorth-Jensen, and B. Velamur Asokan, Phys. Rev. C 80, 021306 (2009) [arXiv:0907.4167].
20. *Accelerating Configuration Interaction Calculations for Nuclear Structure*, P. Sternberg, E.G. Ng, C. Yang, P. Maris, J.P. Vary, M. Sosonkina and H.V. Le, Proceedings of the 2008 ACM/IEEE Conference on Supercomputing (Austin, Texas, November 15 - 21, 2008), (2008).
21. *Accuracy of BCS-based approximations for pairing in small Fermi systems*, N. Sandulescu and G.F. Bertsch, Phys. Rev. C 78, 064318 (2008).
22. *Advancing Nuclear Physics Through TOPS Solvers and Tools*, E. Ng, J. Sarich, S.M. Wild, T. Munson, H. Aktulga, C. Yang, P. Maris, J.P. Vary, M. Kortelainen, W. Nazarewicz, T. Papenbrock, N. Schunck, M.V. Stoitsov, and M.G. Bertolli, Proceedings of the 2011 SciDAC Conference, Denver, CO, (2011).
23. *An effective field theory approach to two trapped particles*, I. Stetcu, J. Rotureau, B.R. Barrett, and U. van Kolck, Ann. Phys. 325, 1644 (2010) [arXiv:1001.5071].
24. *An improved density matrix expansion for spin-unsaturated nuclei*, B. Gebremariam, T. Duguet and S.K. Bogner, Phys. Rev. C 82, 014305 (2010) [arXiv:0910.4979].
25. *An Out-of-core Eigensolver on SSD-equipped Clusters*, E. Saule, H. M. Aktulga, Z. Zhou, C. Yang, E. G. Ng, P. Maris, J. P. Vary and U. Catalyurek, 2012 International Conference on Parallel Processing (ICPP) Workshops, Fifth International Workshop on Parallel Programming Models and Systems Software for High-End Computing (P2S2), (2012).
26. *An Update of B(E2) Evaluation for 0_1^+ --> 2_1^+ Transitions in Even-Even Nuclei near N~Z~28*, B. Pritychenko, J. Choquette, M. Horoi, B. Karamy, B. Singh, At. Data. Nucl. Data. Tab. 92, 798 (2012) [arXiv:1102.3365].
27. *Angular momentum projected configuration interaction with realistic Hamiltonians*, Z.-C. Gao and M. Horoi, Phys. Rev. C 79, 014311 (2009).
28. *Are low-energy nuclear observables sensitive to high-energy phase shifts?*, S.K. Bogner, R.J. Furnstahl, R.J. Perry, and A. Schwenk, Phys. Lett. B 649, 488 (2007).
29. *Augmented Lagrangian Method for Constrained Nuclear Density Functional Theory*, A. Staszczak, M.Stoitsov, A. Baran, and W. Nazarewicz, Eur. Phys. J. A 46, 85 (2010) [arXiv:1006.4137].
30. *Auxiliary Field quantum Monte Carlo for Strongly Paired Fermions*, J. Carlson, Stefano Gandolfi, Kevin E. Schmidt, and Shiwei Zhang, Phys. Rev. A 84, 061602 (2011) [arXiv:1107.5848].
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SOFTWARE DEVELOPMENT AND DATABASES

ADLB (Asynchronous Dynamic Load Balancing) is an MPI-based library that implements a simple master/slave programming model in a scalable way. It has been used this year to scale GFMC (Green's Function Monte Carlo) to 132,000 cores on Argonne's BG/P, enabling accurate calculations for ^{12}C. In Year-4 we have begun to explore a new implementation of ADLB based on MPI's passive-target one-sided operations in order to reduce the memory required for ADLB.

ASLDA developments. ASLDA is a coordinate representation DFT solver in a DVR basis, developed by Magierski. During Year-2, the code has been extended to allow for an additional spin-orbit potential, the pairing potential has been implemented; various tests concerning the accuracy of the code have been performed; the nonlinear couplings in the set of differential equations have been introduced by making the equations dependent on nuclear densities. Finally, Broyden's method has been implemented.

BIGSTICK developments. BIGSTICK is a general-purpose configuration-interaction shell model code, developed primarily by Ormand and Johnson, using on-the-fly algorithms, which require less memory. During year 4 the SDSU/LLNL group analyzed the performance and significantly reorganized the code. The two-body setup is ten times faster and the Hamiltonian application for Lanczos is at least twice as fast. In the past year, SDSU/LLNL group succeeded the parallelization the code using MPI, and the matvec operation for two-body interactions scales well up to 10,000 cores. The current computational barrier is reorthogonalization; collaboration with applied mathematicians, notably Yang and Ng of Lawrence Berkeley have started, and established specific plans for further improvement.

CIDM. Ab-initio CI Data Management tool for accessing the results of calculations along with the the information to reproduce them. The tool is being developed by the Ames Lab and ISU teams. Its design includes (a) interface with nuclear physics ab-initio code output; (b) database manager and server targeting large amounts of data; (c) web-based graphical user interface to enter queries and retrieve results. The three components make CIDM a key player in the LCCI project as an interface among its software packages. During Year-4, the component (a) has been implemented for the MFDn code, and a complete prototype of CIDM, available from http://nuclear.physics.iastate.edu/info/, has been tested with MFDn to record production runs.

Experimental Database to optimize EDF. The database of essential experimental data to be used to fine-tune the EDF has been organized by Schunck: http://orph02.phy.ornl.gov/workshops/lacm08/UNEDF/database.html. It contains data explanation and a set of Fortran subroutines that read the data in the proper format.

ev8_odd. This code is an DFT solver that can treat odd-A nuclei in the blocked BCS approximation. The code (Bertsch, Bertulani) is based on the published ev8 code, written by an Orsay/Saclay/Brussels group. The orbital representation is a 3D grid in an octant of real space, permitting axial and triaxial deformations.

FAM Developments: We have developed a Fortran 90 module for HFBTHO for the finite amplitude method (FAM) QRPA. At the present, FAM module can calculate electric monopole transition strengths in axially deformed nuclei. In the future, we plan to expand the module to

handle higher multipole modes and also transition modes with non-zero values of *K*. Another future development is to parallelize the FAM module for large-scale calculation across the whole nuclear landscape. This work is currently ongoing. We also plan to further expand FAM module to handle beta decays.

FRESCO developments. FRESCO is a general-purpose coupled-channels solver developed by Thompson, and UNEDF work with Summers has produced a MPI version of this for the LLNL computers. In Year-4, MPI sub-parallelization of inner loops and linear algebra has been implemented, allowing larger coupled-channels sets than with OPENMP coding.

GFMC developments. The Argonne Green's Function Monte Carlo program does ab initio nuclear calculations by propagating a starting variational trial wave function in imaginary time to find an exact eigenfunction. It can be used up to ^{12}C using realistic two- and three-nucleon potentials. Under this SciDAC, the ADLB library is being developed and used to enable GFMC to efficiently use the full power of leadership class computers.

HFBRAD Developments. HFBRAD is mostly used as a test DFT solver, or for large-scale pre-optimizations. In the latest version, the energy functional and the associated Kohn-Sham potentials are defined in a separate, portable, Fortran 90 module (Kortelainen, Stoitsov). Another recent development is the inclusion of external fields, which has been used in calculations of neutron droplets and will also be utilized in the future neutron droplet studies.

HFB-AX developments. HFB-AX is a 2D DFT solver, based on B-splines, that preserves axial symmetry and space inversion developed by Pei. The ASLDA has been implemented to treat polarized Fermi systems in extremely elongated traps. The hybrid parallel programming (MPI+OpenMP) has been implemented to treat large box sizes for weakly bound heavy nuclei based on multi-core architectures. The continuum contributions to nucleonic densities have been successfully estimated using the Thomas-Fermi approximation.

HFBTHO Developments. A new version of the code has been submitted to Computer Physics Communications under a joint publication between ORNL, UTK, ANL and LLNL involving both physicists and computer scientists. The new version includes advanced multi-threading support, which reduces the cost of one HFB calculation by a factor 6 on 8 threads.

HFODD Developments. A new official release of the HFODD DFT solver, version 2.49t, was published in Computer Physics Communications in 2012. This is the first natively parallel version of the code. It is based on a hybrid MPI/OpenMP programming model and supports 3 different layers of parallelism. This architecture is implemented using MPI communicators and groups. Multi-threading provides a factor 2-3 acceleration.

JIVE. Two-step code developed by Thompson to calculate non-local optical potentials from couplings to doorway states calculated in QRPA models. Extended to include non-local couplings to transfer channels.

JMOMENTS developments. JMOMENTS is a general-purpose code developed by Horoi et al. that calculates the angular momentum (J) projected 1st and 2nd configuration moment of a two-body nuclear Hamiltonian. The moments are further used to accurately calculate nuclear level

densities. The code was parallelized using MPI and a simple, but very efficient load-balancing algorithm. The domain decomposition was done along the collection of many-body configurations on the spherical single particle orbits. With Senkov, a new proton-neutron formalism was implemented, which makes the code significantly more scalable. The new code was benchmarked on Franklin at NERSC and it shows very good strong scaling up to 4,096 cores for the case of ^{26}Si. The present study indicates that the new algorithm could scale to tens and hundreds of thousands of cores, but good effective interactions for larger model spaces are necessary. In year 5 a new version of the code was developed that calculates the moments of the nuclear Hamiltonian in restricted many-body subspaces, such as $N\hbar\omega$ configuration, which can be used to remove the center-of-mass spurious states from the nuclear level density.

LCCI database includes key codes of SciDAC/UNEDF being developed into a leadership-class configuration interaction (LCCI) code suite. The database includes introductory material, README files, scripts and test runs as well as current release versions of the codes. For example, the LCCI database includes current versions of BIGSTICK, MFDn, NuShellX, and TRDENS. The database resides at NERSC in the directory /project/projectdirs/unedf/lcci and is described in a section of this report. Additional materials, including the white paper that guides the development of the LCCI database, are found on the UNEDF web page.

Low-momentum interactions. A code to generate the latest $V_{low\text{-}k}$ and SRG NN interactions has been developed at OSU and made available to the UNEDF collaboration.

MADNESS-DFT is a scalable fully parallel, symmetry free, and adaptive multiwavelet-based 3-D HFB solver employing the Multiresolution ADaptive Numerical Environment for Scientific Simulation (MADNESS) computational framework. In Year-4, the benchmarking of MADNESS on realistic self-consistent HFB problems has been accomplished by Fann, Pei, Harrison (ORNL/UTK), and others. We solved the HFB equations of the SLDA and ASLDA density functionals for cold Fermions, testing against HFB-AX. Skyrme functionals have also been implemented, and are being tested. The ASLDA-MADNESS has been scaled up to 4,000 processors, with several improvements on performance compared to last year. We are also developing an interface to ScaLAPACK so that we can solve large systems with 20,000 more eigenstates and better scaling performance.

MassTableExplorer. Stoitsov developed a Java-based visualization tool "Mass Table Explorer" which facilitates the processing of huge datasets produced in these large-scale mass table calculations. The tool is also available for download through the website massexplorer.org. New features include an online converter to natural units where one can browse and convert the Skyrme forces to check whether they are natural.

MFDn is a general purpose configuration interaction code developed initially by Vary and improved significantly during Years 1-4 in a multi-faceted collaboration between ISU and CS/AM groups at LBNL and Ames Lab. It is highly scalable and portable, running on laptops to leadership class machines. It is optimized for storing the full Hamiltonian, enabling convergence of a large set of eigenstates, and has options for compute-on-the-fly and external field capabilities. Extensive improvements are underway to continue improving its speed and expanding its capabilities. MFDn has become a significant component of the LCCI project during Year-4 and is available to

SciDAC/UNEDF researchers via the unedf project space at NERSC, including scripts and test cases.

NuShellX. This is a CI code written by Rae in 2007-2008. It starts with a NuShell calculation for protons and neutrons separately, then uses angular momentum coupling to construct the angular momentum coupled basis for protons and neutrons that has a fixed total *J* value. The proton-neutron interaction is transformed into the particle-hole form. The calculation of the Hamiltonian matrix elements can be calculated "on-the-fly" eliminating the need for storage of the large matrix. Eigenvalues and eigenvectors are obtained with the thick-restart Lanczos method. OpenMP is used to efficiently distribute the calculation over many cores (up to 64 have been tested). NuShellX@MSU (Brown) provides a user-friendly wrapper for Oxbash style input and output. Matrix elements for one and two nucleon transfer, one-body transitions densities and Hamiltonian overlaps provide a complete set of observables. In year 4 parts of the code were rewritten with the goal of maximizing the efficiency for many cores. In the summer of 2009 Alexander Litsetsky converted the OpenMP loops to MPI. Eric McDonald, who started to work on the project half-time, made the modifications required to work with the PGI compiler. This has made the code more portable, and opened a path to experiment with GPU acceleration via CUDA. Alex Brown worked on the wrapper code, which will be integrated with LCCI codes.

PCI developments. PCI is a Projected Configuration Interaction code that uses a deformed single particle basis with axial symmetry developed by Gao and Horoi. The code was developed during Years-1 and 2 of UNEDF. The performance of the code was significantly improved by implementing a new Lanczos algorithm for real symmetric generalized eigenvalue problems, and by increasing the efficiency of that part of the code that calculates the projected matrix elements of the Hamiltonian and norm. A new algorithm for an improved basis selection and treatment of parity in mixed-shells model spaces was recently integrated.

POUNDERS (Practical Optimization Using No Derivatives, for Squares) is a method developed by Argonne mathematicians for solving nonlinear least squares problems when derivatives are unavailable. POUNDERS was the first model-based, derivative-free method implemented in the open-source Toolkit for Advanced Optimization (TAO). TAO is designed to solve large-scale optimization problems on high-performance, distributed architectures. TAO solvers have been used to solve computational science problems in a wide variety of areas; details can be found in the impact section at www.mcs.anl.gov/tao. The incorporation of POUNDERS in TAO allows UNEDF collaborators throughout the world access to an implementation of POUNDERS that is flexible and portable, able to run on anything from laptops to leadership class computing facilities.

Python Data Analysis Tool. To process the massive amount of data generated by HFBTHO and HFODD, data analysis software has been developed by McDonnell using the Python scripting language. The program has a simple GUI interface that allows the user to extract and plot all relevant data, in particular the one-quasiparticle states in odd-A nuclei. A porting of this interface is under progress.

QRPAdef developments: QRPAdef calculates excited-state energies and transition strengths in axially symmetric nuclei with arbitray Skyrme-like energy-density functionals. The code constructs and diagonalizes the usual A and B QRPA matrices in a deformed two-quasiparticle basis. The matrices are large and constructing them in many nuclei requires petascale resources. In

year 4 QRPAdef was tuned for a better scaling, and it was shows good strong scaling up to 10,000 cores.

QRPAsph solves the spherically coupled QRPA equations. In Year-4 the Livermore reactions group used this fully parallelized the code to calculate microscopic nucleon-nucleus optical potentials.

REDSTICK developments. REDSTICK is a general-purpose configuration-interaction shell model code, developed primarily by Ormand and Johnson, using on-the-fly algorithms which require less memory. During Year-3 we have analyzed the performance and significantly reorganized the code. The two-body setup is ten times faster and the Hamiltonian application for Lanczos is at least twice as fast. We are in the process of parallelized the improved algorithm, done by P. G. Krastev, a postdoc supported by UNEDF.

TDSLDA – 3D time-dependent DFT solver. This is the first parallel code developed within UNEDF from scratch for the leadership class computers. The size of the basis set it can handle is already 2-3 orders of magnitude larger than any other nuclear calculations ever or currently performed. This is essentially the first ever implementation of the so-called TDHFB problem in 3D without any symmetry restrictions. It was demonstrated that it was already achieved an extremely efficient implementation of this complex mathematical problem on JaguarPf using so far up to 217,800 PEs, which represent 97% of the entire machine. The suites of SLDA/TDSLDA codes has been chosen as one of the four applications used in the FY2010 DOE/ASCR Joule metric on computational effectiveness and has been awarded so far approximately 45M CPU hours.

TPFOLD. This code reads QRPA transition densities and folds them with a selection of nucleon-nucleon interaction to obtain the corresponding transition potential, of the form to be used by the code FRESCO.

TRCCF. This code, developed primarily by Nobre and Thompson, calculates RPA transition densities and transition potentials for transitions from the ground state to excited states and also between excited states, by folding these calculated densities with a nucleon-nucleon interaction. The transition potentials can be directly used by the code FRESCO. Transition densities and potentials for 1-particle—1-hole states without RPA correlation may also be calculated.

TRDENS. An MPI fortran 90 code for calculations of one- and two-body transition densities from ab initio no-core shell model wave functions obtained by various shell model codes. These densities are input for the ab initio NCSM/RGM reactions calculations. A new more efficient algorithm based on hashing search implemented. Runs on LLNL's LC machines Hera, Zeus and Atlas. Tested using up 1024 processors. In Year-2, capability to calculate three-body densities that serve as an input into the RGM integration kernel calculations for the deuteron-triton and deuteron-alpha scattering was implemented. In Year-3, we implemented a distribution of two-body density structure over groups of processors. This made it possible to calculate densities in significantly larger model spaces and also for more excited states. In collaboration with C. Johnson, we developed an interface between the CI code BIGSTICK and the TRDENS. In Year-4, in collaboration with P. Maris, we developed interface between the CI code MFDn and the TRDENS. The TRDENS code now works with wave functions obtained from the CI codes NCSD, Antoine, BIGSTICK, MFDn and the Darmstadt IT-NCSM code.

PRESENTATIONS (ALL YEARS)

1. *Ab-initio no-core shell model – an overview*, J.P. Vary, Argonne National Laboratory, January 18, 2007.
2. *GFMC Calculations of Nuclei*, S.C. Pieper, Chicago Town Meeting presentation, Chicago, IL, January 20, 2007.
3. *Atomic nuclei and mesoscopic science: Challenges to an ab initio approach*, D.J. Dean, presented at the "Femtoscience: from nuclei to nuclear medicine" symposium of the AAAS Annual Meeting, San Francisco, CA, February 15-19, 2007.
4. *Spin Polarized Cold Fermi Atoms*, J. Carlson, Workshop on the Intersections of Cold Atom and RHIC Physics, Trento, Italy, March 2007.
5. *Multiresolution Analysis for Solving Electronic Structure*, G. Fann, R. Harrison, G. Beylk, et al., Joint JUSTIPEN-LACM Workshop, Oak Ridge, TN, March 5-8, 2007.
6. *Ab-initio Calculations of Light Nuclei*, S.C. Pieper, Texas A&M Colloquium, College Station, TX, March 6, 2007.
7. *Long-range phenomena in the No-Core Shell Model*, J.P. Vary, Workshop on Three-Nucleon Interactions from Few- to Many-Body Systems, TRIUMF, Vancouver, Canada, March 12-16, 2007.
8. *Applications of chiral NN and 3N interactions to p-shell nuclei*, P. Navratil, Workshop on Three-Nucleon Interactions from Few- to Many-Body Systems, TRIUMF, Vancouver, Canada, March 12-16, 2007.
9. *Coupled-cluster theory with three-body forces*, T. Papenbrock, TRIUMF workshop on Three-Nucleon Forces, Vancouver, BC, March 12-16, 2007.
10. *Light Nuclei and 3N reactions*, R.B. Wiringa, Workshop on Three-Nucleon Interactions from Few- to Many-Body Systems, TRIUMF, Vancouver, Canada, March 12-16, 2007.
11. *Local density functional theory for superfluid fermionic systems:the unitary gas*, A. Bulgac, Seminar, Physics, UW, Seattle, WA, April 5, 2007.
12. *Large-scale calculations of nuclear-structure data for simulation databases*, P. Möller, R. Bengtsson, K.-L. Kratz, and H. Sagawa, Invited Talk, Proc. International Conference on Nuclear Data and Technology, Nice, France, April 22-27, 2007.
13. *Density Functional Theory in Nuclear Binding and Structure*, G.F. Bertsch, Colloquium, Argonne National Laboratory, May 2007.
14. *GFMC Then and Now in Nuclear Physics*, J. Carlson, Workshop on the 40th anniversary of GFMC, New York, NY, May, 2007.
15. *Improving the self-consistent calculations of Fermion systems*, A. Bulgac and M.M. Forbes, UNEDF seminar, May 7, 2007.
16. *Local density functional theory for superfluid fermionic systems:the unitary gas*, A. Bulgac, Workshop, Many-Body Correlations in Nuclear and other Mesoscopic Systems, NIPNE, Bucharest, May 14, 2007.
17. *The nuclear many-body problem: Challenges of, and vision for an an initio approach: coupled cluster theory*, D.J. Dean, Workshop on Open Quantum Many-Body Systems, ECT*, Trento, Italy, May 14-18, 2007.
18. *Why strongly interacting fermion gases are inetresting to a many-body theorist?*, A. Bulgac, Bothe colloquium, MPI Heidelberg, May 16, 2007.
19. *Ab-initio and ab-exitu no-core shell model*, J.P. Vary, Changing Facets of Nuclear Structure, Vico Equesne, Italy, May 20-24, 2007.

20. *Nuclear structure calculations for fission cross sections*, H. Olofsson and P. Möller, T-16 Nuclear Data Discussion, May 21, 2007.
21. *Large-Scale calculations of nuclear-structure data for simulation databases*, P. Möller, Invited Talk, First CARINA-JINA Collaboration Meeting on "Nuclear Physics Data Compilation for Nucleosynthesis Modeling," Trento, Italy, May 29-June 1, 2007.
22. *Building a Universal Nuclear Energy Density Functional*, G.F. Bertsch, Invited Talk, SciDAC conference, June 2007.
23. *Pairing Gaps in Low Density Neutron Matter and in Cold Atoms*, J. Carlson, INT Program 07-2a: The Neutron Star Crust and Surface, Institute for Nuclear Theory, University of Washington, Seattle WA, June, 2007.
24. *Progress and Challenges in the Theory of Nuclei*, D.J. Dean, International Nuclear Physics Conference, Tokyo, Japan, June 3-8, 2007.
25. *Taming the Savage Dineutron and the Miller's Correlation Tail*, R.B. Wiringa, INT-07-01: Fundamental Neutron Physics Seminar, Institute for Nuclear Theory, University of Washington, Seattle, WA, June 7, 2007.
26. *Long-Range Planning for Physics and Nuclear Astrophysics*, D.J. Dean, Jefferson Laboratory Users Group Meeting, Newport News, VA, June 18-20, 2007.
27. *Local density functional theory for superfluid fermionic systems:the unitary gas*, A. Bulgac, Seminar, Trimestre Quantum Gases, Institute Henri Poincare, Paris, June 21, 2007.
28. *Optimization in SciDAC Applications*, J. Moré, Scientific Discovery through Advanced Computing Conference, June 24-28, 2007.
29. *Spectroscopy of light nuclei with realistic NN interaction JISP*, A.I. Mazur, A. M. Shirokov, J. P. Vary, T. A. Weber, LVII International Conference on Nuclear Physics NUCLEUS-2007, Voronezh, Russia, June 25-29, 2007.
30. *Induced p--wave superfluidity in asymmetric Fermi gases*, A. Bulgac, Conference on "Recent Progress in the Study of Quantum Gases: theory and experiment," Paris, June 27, 2007.
31. *Large-scale calculations of nuclear-structure data for simulation databases*, P. Möller, R. Bengtsson, K.-L. Kratz, and H. Sagawa, LLNL, June 28, 2007.
32. *Present status of the no-core shell model*, P. Navratil, Workshop on Advanced Many-Body Methods for Nuclear Structure, EFT*, Trento, Italy, July 2-6, 2007.
33. *Large-scale calculations of nuclear-structure data for simulation databases*, P. Möller, Invited Talk, INT Program 07-2a: Workshop on the Neutron Star Crust and Surface: Observations and Models, Institute for Nuclear Theory, University of Washington, Seattle, WA, July 3, 2007.
34. *Dependence of Nuclear Binding on Hadronic Mass Variation*, R.B. Wiringa, Argonne National Laboratory, Argonne, IL, July 10, 2007.
35. *Local density functional theory for superfluid fermionic systems:the unitary gas*, A. Bulgac, Seminar, Institute de Physique Nucleaire, Orsay, France, July 11, 2007.
36. *Progress and challenges in the theory of nuclei*, D.J. Dean, Gordon Research Conference, Salva Regina University, Newport, RI, July 15-20, 2007.
37. *Developing New Many-Body Approaches for No-Core Shell Model Calculations*, B.R. Barrett, A.F. Lisetskiy, P. Navratil, I. Stetcu and J.P. Vary, International Conference on Recent Progress in Many-body Theories 14 (RPMBT14), Barcelona, Spain, July 16-20, 2007.

38. *Coupled-cluster approach to an ab initio description of nuclei*, D.J. Dean, G. Hagen, M. Hjorth-Jensen, and T. Papenbrock, International Conference on Recent Progress in Many-Body Theories, Barcelona, Spain, July 16-20, 2007.
39. *Ab Initio No-Core Shell Model Calculations for Light Nuclei*, P. Navratil, International School of Physics "Enrico Fermi," Varenna, Italy, July 17-27, 2007.
40. *Quantum Monte Carlo Calculations of Light Nuclei*, S.C. Pieper, Two Varenna summer school lectures, Varenna, Italy, July 17-20, 2007.
41. *Dependence of Nuclear Binding on Hadronic Mass Variation*, R.B. Wiringa, Los Alamos National Laboratory, Los Alamos, NM, August 1, 2007.
42. *Local Density Functional Theory for Superfluid Fermionic Systems: The Unitary FermiGas*, A. Bulgac, First Annual UNEDF general meeting, Pack Forest, WA, August 12-17, 2007.
43. *Optical potentials from CC Calculations*, G. Arbanas, UNEDF Annual Meeting, Pack Forest, WA, August 13-16, 2007.
44. *Benchmarks with HFODD and EV8_ODD*, C. Bertulani, UNEDF Annual Meeting, Pack Forest, WA, August 13-16, 2007.
45. *Equation of State and Pairing Gaps in Low-Density Neutron Matter and Cold Atoms*, J. Carlson, UNEDF Annual Meeting, Pack Forest, WA, August 13-16, 2007.
46. *Nuclear Masses*, P. Möller, UNEDF Annual Meeting, Pack Forest, WA, August 13-16, 2007.
47. *Density Functional Theory: Summary and goals for year 2*, W. Nazarewicz, UNEDF Annual Meeting, Pack Forest, WA, August 13-16, 2007.
48. *QMC Results for the Benchmark NN Potentials*, S.C. Pieper, UNEDF Annual Meeting, Pack Forest, WA, August 13-16, 2007.
49. *Realistic NN and NNN interactions and the nuclear single-particle basis*, J.P. Vary, Carpathian Summer School of Physics 2007, Sinaia, Romania, "Advances in Nuclear and Particle Astrophysics", August 30, 2007.
50. *Effective interactions and operators – recent progress in the ab-initio no-core shell model*, J.P. Vary, Carpathian Summer School of Physics 2007, Sinaia, Romania, "Advances in Nuclear and Particle Astrophysics", August 31, 2007.
51. *Light nuclei from chiral EFT interactions*, P. Navratil, 20th European Conference on Few-Body Problems in Physics (EFB20), Pisa, Italy, September 2007.
52. *Light nuclei from chiral EFT interactions*, P. Navratil, 19th Indian-Summer School on Few-Body Techniques and Effective Field Theories, Rez/Prague, Czech Republic, September 2007.
53. *Ab-initio no-core shell model*, J.P. Vary, XXX Meeting of the Brazilian Physical Society, Águas de Lindóia, Brazil, September 4, 2007.
54. *Local density functional theory for superfluid fermionic systems:the unitary gas*, A. Bulgac, Argonne National Labooratory, Argonne, IL, September, 5, 2007.
55. *Equation of State and Pairing Gaps in Low-Density Neutron Matter and Cold Atoms*, J. Carlson, MSU Workshop on Mesoscopic Physics, October, 2007.
56. *Coupled-cluster theory for medium-mass nuclei*, T. Papenbrock, INT program ``Nuclear Many-body Approaches for the 21st Century", Seattle, WA, October 2007.
57. *Extracting the continuum limit of the no-core shell model*, J.P. Vary, Mid-West Theory Get-Together, Argonne National Laboratory, Oct 5-6, 2007.
58. *Progress and challenges in the theory of nuclei*, D.J. Dean, eRIBS07 International Workshop, Newport News, VA, October 10, 2007.

59. *GFMC Calculations of Isospin-Mixing in ^{8}Be*, R.B. Wiringa, 2007 Meeting of the Division of Nuclear Physics, American Physical Society, Newport News, VA, October 11-13, 2007.
60. *Kawai-Kerman-McVoy Statistical Theory of Nuclear Reactions*, G. Arbanas, CNR-2007, Fish Camp, CA, October 22-26, 2007.
61. *Local density functional theory for superfluid fermionic systems:the unitary gas*, A. Bulgac, First FIDIPRO-JSPS workshop on energy density functionals in nuclei, Keuruu, Finland, October 25-27, 2007.
62. *Nuclear DFT: questions and challenges*, W. Nazarewicz, First FIDIPRO-JSPS Workshop on Energy Density Functionals in Nuclei, Keurusselka, Finland, October 25-27, 2007.
63. *Ab Initio No Core Shell Model (NCSM) and the route to constraints on the Nuclear Energy Density Functional*, J.P. Vary, First FIDIPRO-JSPS Workshop On Energy Density Functionals In Nuclei, Jyväskylä, Finland, October 25-27, 2007.
64. *Nucleon (and Δ) Momentum Distributions in Nuclei*, R.B. Wiringa, SRC 2007 Workshop on Short-Range Structure of Nuclei at 12 GeV, Jefferson Laboratory, Newport News, VA, October 26, 2007.
65. *The Illinois Extension to the Fujita-Miyazawa Three Nucleon Force*, S.C. Pieper, International Symposium on New Facet of Three Nucleon Force - 50 Years of Fujita-Miyazawa Three Nucleon Force, Tokyo, Japan, October 29, 2007.
66. *Large Scale Computing for Nuclear Structure*, P. Maris, nuclear physics seminar at Kent State University, Kent, OH, Nov. 2007.
67. *Statistical properties of Kawai-Kerman-McVoy T-matrix*, G. Arbanas, Compound Nuclear Reactions and Related Topics Conference, November 2007.
68. *Understanding nuclei: progress and challenges*, D.J. Dean, Compound Nuclear Reactions and Related Topics Conference, November 2007.
69. *No-core shell model with JISP16 NN interaction: spectroscopy of light nuclei and neutron-nucleus sca*, A.M. Shirokov, INT Program 07-3: Nuclear Many-Body Approaches for the 21st Century, Institute for Nuclear Theory, University of Washington, Seattle, WA, November 2, 2007.
70. *Ab Initio solutions of the properties of light nuclei*, J.P. Vary, University of Iowa Colloquium, Iowa City, Iowa, November 5, 2007.
71. *Benchmark calculations of nuclear mass tables*, C. Bertulani, INT Program 07-3: Nuclear Many-Body Approaches for the 21st Century, Institute for Nuclear Theory, University of Washington, Seattle, WA, November 7, 2007.
72. *Nuclear Forces and the Destiny of the Universe*, R.B. Wiringa, Physics Colloquium, University of Iowa, Iowa City, IA, November 12, 2007.
73. *Light nuclei from chiral EFT interactions*, P. Navratil, INT Program 07-3, Nuclear Many-body Approaches for the 21st Century, Institute for Nuclear Theory, University of Washington, Seattle, WA, November 13, 2007.
74. *Hamiltonian Light-Front QCD*, J.P. Vary, XIX Reunião de Trabalho sobre INterações HAdrônicas, CBPF, Rio de Janeiro, Brazil, November 19-20, 2007.
75. *Advances in microscopic nuclear theory using ab initio methods*, J.P. Vary, ITA - Instituto Tecnológico de Aeronáutica, Sao Paulo, Brazil, November 21, 2007.
76. *Ab initio solutions of the properties of light nuclei*, J.P. Vary, Instituto de ísica Teórica, Sao Paulo, Brazil, November 23, 2007.
77. *Convergence of full configuration calculations for N3LO NN interactions*, P. Maris, Workshop on Hamiltonians for ab-initio nuclear physics, Oak Ridge, TN, Dec. 2007.

78. *Nuclear Structure '07: Exciting, Broad, Relevant*, W. Nazarewicz, JUSTIPEN, RIKEN, Wako, Japan, December 2007.
79. *New Global Calculations of Nuclear Masses and Fission Barriers for Astrophysical Applications*, P. Möller, OMEGO7, Hokkaido University, Sapporo, Japan, December 4-7, 2007.
80. *Full Configuration Interaction (CI) approach - convergence*, J.P. Vary, Workshop on Hamiltonians for ab-initio nuclear physics, ORNL, Tennessee, December 6, 2007.
81. *Unified calculations of nuclear-structure properties: Ground-state masses and deformations, fission*, P. Möller, RIKEN, Wako, Japan, December 17, 2007.
82. *Density Functional Theory in Nuclear Physics*, G.F. Bertsch, Colloquium, Rutgers University, January, 2008.
83. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, Physics Colloquium, University of Tennessee, Knoxville, TN, January, 2008.
84. *The UNEDF Project*, R.J. Furnstahl, TRIUMF nuclear theory seminar, Vancouver, BC, March 2008.
85. *Recent Advances in ab initio calculations in nuclear structure*, P. Maris, Modern Aspects in Nuclear Structure and Reactions, Hirschegg, Austria, Jan. 2008.
86. *Coupled-cluster Theory for Medium Mass Nuclei*, T. Papenbrock, Hirschegg 2008, International Workshop XXXVI on Gross Properties of Nuclei and Nuclear Excitations, January 13-19, 2008.
87. *Complementary aspects of EDF and CI methods*, B.A. Brown, Hirshegg 2008, Modern Aspects of Nuclear Structure and Reactions, Jan. 13-19, 2008.
88. *Strategies for Extracting Optimal Effective Hamiltonians for CI and Skyrme EDF Applications*, B.A. Brown, DFT-UNEDF Workshop on the Determination of the Nuclear Energy Functional: Optimization, Strategy, Essential Experimental Data and Chi-Squared Metrics, Oak Ridge National Laboratory, Oak Ridge, TN, January 22, 2008.
89. *Parameter Estimation in Nuclear Fission*, J. Moré, DFT-UNEDF Workshop on the Determination of the Nuclear Energy Functional: Optimization Strategy, Essential Experimental Data and Chi-Squared Metrics, Oak Ridge National Laboratory, Oak Ridge, TN, January 22, 2008.
90. *Ab-initio calculations with an external field - initial results*, J.P. Vary, UNEDF-DFT Workshop, Oak Ridge National Laboratory, January 22, 2008.
91. *Coupled-cluster Theory for Light Nuclei*, G. Hagen, 2nd Annual LACM-EFES-JUSTIPEN Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, January 23-25, 2008.
92. *A Short Guide to Optimization Technology on High-Performance Architectures*, J. Moré, JUSTIPEN Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, Jan. 23-25, 2008.
93. *Spectroscopy of Odd-Mass Nuclei in Energy Density Functional Theory – Impact of Terascale Computing*, N. Schunck, JUSTIPEN Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, Jan. 23-25, 2008.
94. *Full Configuration Interaction studies of light nuclei - opportunities and challenges*, J.P. Vary, JUSTIPEN Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, Jan. 23-25, 2008.
95. *Benchmark calculations of nuclear mass tables*, C. Bertulani, DFT-UNEDF Workshop, The 2nd Joint LACM-EFES-JUSTIPEN Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, January 25, 2008.
96. *Microscopic Description of Spontaneous Fission*, W. Nazarewicz, SSAA Seminar, NNSA, Washington, DC, January 29, 2008.

97. *Progresses and challenges in nuclear theory*, D.J. Dean, Colloquium at Vanderbilt University, Nashville, TN, January 31, 2008.
98. *QMC vs. Experiment*, R.B. Wiringa, Physics Division Seminar, Argonne National Laboratory, Argonne, IL, February 18, 2008.
99. *Progresses and challenges in nuclear theory*, D.J. Dean, Colloquium at Argonne National Laboratory, Argonne, IL, February 20, 2008.
100. *High Performance Nuclear Structure Computation*, P. Sternberg, SIAM Parallel Processing Conference, March, 2008.
101. *Solving 3-D and 6-D Schrödinger's Equations Using Multiresolution Adaptive Pseudo-spectral Methods on Leadership Class Computers*, G. Fann, SIAM Conference on Parallel Processing for Scientific Computing, Atlanta, GA, March 12-14, 2008.
102. *Dependence of Nuclear Binding on Hadronic Mass Variation*, R.B. Wiringa, Theoretical Physics Seminar, Jefferson Laboratory, Newport News, VA, March 17, 2008.
103. *UNEDF: building a microscopic nuclear energy density functional*, W. Nazarewicz, Warsaw University, Warsaw, Poland, March 19, 2008.
104. *Ab initio calculations of light nuclei with JISP16 NN interaction*, A.M. Shirokov, Cyclotron Institute, Texax A&M University, College Station, TX, March 20, 2008.
105. *Full configuration calculations of light nuclei*, P. Maris, APS spring meeting, St.Louis, MO, April 2008.
106. *Computing Atomic Nuclei*, W. Nazarewicz, IOP Annual Nuclear Physics Group Conference, Liverpool, UK, April 1, 2008.
107. *Quantum Monte Carlo Calculations of Light Nuclei*, R.B. Wiringa, Theoretical Physics Seminar, Brookhaven National Laboratory, Upton, NY, April 4, 2008.
108. *Derivative-Free Optimization Solvers: A Shootout*, J. Moré, Tenth Copper Mountain Conference on Iterative Methods, Copper Mountain, Colorado, April 11-17, 2008.
109. *Ab initio no-core shell model with continuum*, P. Navratil, APS Meeting, Saint Louis, MO, April 11-15, 2008.
110. *Odd-Even Mass Nuclei in Energy Density Functional Theory; Steps Towards a Universal Energy Density Functional*, N. Schunck, APS Meeting, Saint Louis, MO, April 11-15, 2008.
111. *Beyond the shell model: computing nuclei with coupled cluster theory*, D.J. Dean, Invited Talk, APS Meeting, Saint Louis, MO, April 11-15, 2008.
112. *Odd-Even Mass Nuclei in Energy Density Functional Theory – Steps Towards a Universal Energy Den*, N. Schunck, APS Meeting, Saint Louis, MO, April 11-15, 2008.
113. *Science of rare isotopes: connecting nuclei with the universe*, W. Nazarewicz, Plenary Talk, APS Meeting, Saint Louis, MO, April 12, 2008.
114. *UNEDF Panel Review: Introduction*, G.F. Bertsch, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
115. *UNEDF SCIDAC ab-initio progress*, J. Carlson, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
116. *Microscopic Input to Energy Functionals*, R.J. Furnstahl, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
117. *Using the Functionals: Towards Spectroscopic-Quality NEDF (DFT Applications)*, W. Nazarewicz, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
118. *DFT Extensions for Dynamics, Excited States*, M. Horoi, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.

119. *Reaction Theory in UNEDF Optical Potentials from DFT Models*, I. Thompson, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
120. *Computer Science in UNEDF*, R. Lusk, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
121. *The Asynchronous Dynamic Load-Balancing Library*, R. Lusk, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
122. *Ab-initio Calculations of Microscopic Structure of Nuclei*, J.P. Vary, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
123. *Computational Infrastructure for Nuclear Energy Density Functional Theory*, J. Moré, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
124. *Computer Science Research and Software Development: Superfluid Local Density Approximation; Coupled Cluster*, K. Roche, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
125. *International Impact*, W. Nazarewicz, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
126. *Future Computing Needs for Reactions*, I. Thompson, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
127. *UNEDF Panel Review: Answers to Homework Questions*, UNEDF Collaboration, UNEDF Panel Review, Rockville, MD, April 17-18, 2008.
128. *High-Performance Nuclear Structure Calculations*, E. Ng, The 9th International Workshop on State-of-the-Art in Scientific and Parallel Computing, Trondheim, Norway, May, 2008.
129. *Effective Field Theory and Density Functional Theory*, R.J. Furnstahl, Conference on "From quarks to the nuclear many-body problem", Oslo, Norway, May 21-24, 2008.
130. *Large-scale shell model calculations and coupled cluster calculations*, M. Horoi, invited talk at the international Conference “From Quarks to the Nuclear Many-Body Problem”, Oslo University, May 21-24, 2008.
131. *Ab initio studies of light nuclei with Green's function Monte Carlo*, S.C. Pieper, Conference on "From Quarks to the Nuclear Many-Body Problem" University of Oslo, Norway, May 21-24, 2008.
132. *Towards incorporating nuclear pairing on an ab initio basis into the nuclear EDF*, A. Bulgac, Mass Olympics, ECT*, Trento, Italy, May 26-30, 2008.
133. *Angular Momentum Projected Configuration Interaction of Different Shapes*, Z. Gao and M. Horoi, Nuclear Structure 2008, East Lansing, MI, June 3-6, 2008.
134. *Application of the Shell-Model Code NushellX to the Structure of 56Ni in the full pf shell and a Truncation within a Diagonlized Proton-Neutron Basis*, M. Horoi, B.A. Brown and W. Rae, Nuclear Structure 2008, East Lansing, MI, June 3-6, 2008.
135. *ENST Lecture series on the Quasiparticle Random Phase Approximation*, J. Engel, CEA/SPhN, June 18-20, 2008.
136. *Static and TD (A)SLDA for cold atoms and nuclei*, A. Bulgac, The second annual UNEDF meeting, Pack Forest, WA, June 23-26, 2008.
137. *Nuclear Forces and Spectra (and Scattering)*, R.B. Wiringa, Elba X Workshop on Electron-Nucleus Scattering EIPC, Marciana Marina, Elba, Italy, June 23-27 2008.
138. *Comparison of Nuclear Configuration Interaction Calculations and Coupled Cluster Calculations*, M. Horoi, invited talk at the International Symposium on "50 Years of Coupled Cluster Theory", INT Seattle, WA, June 30 - July 2.

139. *Ab initio density functional theory for nuclei*, R.J. Furnstahl, workshop on "Ab-Initio Nuclear Structure - Where do we stand?", Bad Honnef, Germany, July, 2008.
140. *No-core Full Configuration basis results for nuclei and neutron droplets in external fields*, P. Maris, JUSTIPEN--EFES--Hokudai--UNEDF workshop, Onuma-koen, Hokkaido, Japan, July 2008.
141. *Ab Initio Many-Body Calculations of Nucleon Nucleus Scattering*, P. Navratil, 410. WE-Heraeus Workshop Ab-Initio Nuclear Structure - Where do we stand??, BadHonnef, Germany, July, 2008.
142. *Coupled-cluster theory for medium-mass nuclei*, T. Papenbrock, INT Program ``Atomic, Chemical, and Nuclear Developments in Coupled Cluster Methods", Seattle, WA, July 2008.
143. *Coupled-cluster theory for medium-mass nuclei*, T. Papenbrock, Heraeus workshop "Ab-initio nuclear structure - Where do we stand?", Bad Honnef, Germany, July 2008.
144. *Accurate description of the spin- and parity-dependent nuclear level*, M. Horoi, invited talk at the International Workshop on Statistical Nuclear Physics and its Applications in Astrophysics and Technology, Ohio University, Athens OH, July 8-11, 2008.
145. *The Incredible Many Facets of the Unitary Fermi Gas*, A. Bulgac, Extreme QCD 2008, Raleigh, NC, July 21-23, 2008.
146. *New Approaches to Configuration Interaction*, M. Horoi, Hokudai-TORIJIN-JUSTIPEN-EFES workshop & JUSTIPEN-EFES-Hokudai-UNEDF meeting, Hokkaido, Japan, July 21-25, 2008.
147. *Accurate Nuclear Level Densities for Nuclear Reactions*, M. Horoi, Hokudai-TORIJIN-JUSTIPEN-EFES workshop & JUSTIPEN-EFES-Hokudai-UNEDF meeting, Hokkaido, Japan, July 21-25, 2008.
148. *Parity Dependent Shell Model Level Densities for Nuclear Astrophysics*, M. Scott and M. Horoi, International Symposium on Nuclear Astrophysics ”Nuclei in the Cosmos - IX”, Mackinac Island, July 25 - August 1, 2008.
149. *Neutron radii of atomic nuclei and the neutron matter EOS*, B.A. Brown, Lead Radius Experiment (PREX) Workshop and Neutron Rich Matter in the Heavens and on Earth, Thomas Jefferson National Accelerator Facility, August 17-19, 2008.
150. *Theory of neutron-rich nuclei and nuclear radii*, W. Nazarewicz, Lead Radius Experiment (PREX) Workshop and Neutron Rich Matter in the Heavens and on Earth, Jefferson Lab, Newport News, VA, Aug. 17-19, 2008.
151. *UNEDF Project: Towards a Universal Nuclear Energy Density Functional*, P. Magierski, 25th International Physics Congress (Turkish Physical Society), Bodrum, Turkey, August 25-29, 2008.
152. *Computing atomic nuclei*, W. Nazarewicz, Zakopane Conference on Nuclear Physics, Zakopane, Poland, Sep. 1-4, 2008.
153. *The Incredible Many Facets of the Unitary Fermi Gas*, A. Bulgac, Seminar, Cyclotron Lab, Texas A&M, September 2, 2008.
154. *A unitary quantum supersolid*, A. Bulgac, Seminar, Department of Physics, Texas A&M, September 2, 2008.
155. *Nuclear Coupled-Cluster approach*, G. Hagen, The Fifth International Conference on Exotic Nuclei and Atomic Masses ENAM'2008, Ryn, Poland, Sep. 7-15, 2008.
156. *Summary Talk*, W. Nazarewicz, The Fifth International Conference on Exotic Nuclei and Atomic Masses ENAM'2008, Ryn, Poland, Sep. 7-15, 2008.

157. *Derivative-free solvers for simulation-based optimization problems*, J. Moré, Societa' Italiana di Matematica Applicata e Industriale, SIMAI, Roma, Italy, September 16, 2008.
158. *Computing atomic nuclei*, W. Nazarewicz, Colloquium, University of Jyvaskyla, Jyvaskyla, Finland, October 2008.
159. *Light nuclei without a core*, P. Maris, Fall Meeting of the Division of Nuclear Physics of the APS, Oakland, CA, Oct. 2008.
160. *Thermodynamics Properties and Phase Transitions in Dilute Fermion Matter*, A. Bulgac, DNP Meeting, Oakland, CA, October 23-26, 2008.
161. *UNEDF Project: Towards a Universal Nuclear Energy Density Functional*, P. Magierski, Warsaw University of Technology, Warsaw, Poland, October 28, 2008.
162. *Ab initio calculations of light nuclei*, P. Maris, seminar at the KVI, Groningen, the Netherlands, Nov. 2008.
163. *Science of rare isotopes: connecting nuclei with the universe*, W. Nazarewicz, Rutgers Physics Colloquium, Rutgers University, NJ, Nov. 2008.
164. *Accelerating Configuration Interaction Calculations for Nuclear Structure*, C. Yang, Supercomputing Conference, Austin, TX, November, 2008.
165. *Systematics of the First 2+ Excitation in Spherical Nuclei with Skyrme-QRPA*, J. Terasaki, 5th ANL/MSU/JINA/INT FRIB Workshop on Bulk Nuclear Properties, Michigan State University, November 19-22, 2008.
166. *Recent Developments in Nuclear Quantum Monte Carlo*, R.B. Wiringa, 5th ANL/MSU/JINA/INT FRIB Workshop Michigan State University, East Lansing, MI, November 19-22, 2008.
167. *Nuclear structure input for nuclear reactions*, M. Horoi, International Conference on Interfacing Structure and Reactions at the Center of the Atom, Queenstown, New Zealand, December 1-5, 2008.
168. *Ab initio calculations for light nuclei and neutron droplets*, P. Maris, seminar at Michican State University, East Lansing, MI, Jan. 2009.
169. *No-Core Shell-Model and No-Core Full Configuration calculations in nuclear physics*, P. Maris, Extreme Scale Computing Workshop - nuclear physics, Washington D.C., Jan. 2009.
170. *Ab Initio Approaches to Nuclear Reactions*, P. Navratil, Forefront Questions in NuclearScience and the Role of High Performance Computing, Washington, DC, January, 2009.
171. *The Incredible Many Facets of the Unitary Fermi Gas*, A. Bulgac, Physics of Quantum Electronics, Snowbird, Utah, January 4-8, 2009.
172. *Today's atomic nucleus - bridge from quarks to the cosmos*, J.P. Vary, University of Delhi colloquium, Delhi, India, January 9, 2009.
173. *Some arguments for the need of exascale computing for nuclear structure and reactions and for a comprehensive many-body approach to fermionic superfluid phenomena in general*, A. Bulgac, Forefront Questions in Nuclear Science and the Role of High Perfomance Computing, Washington, DC, January 26-28, 2009.
174. *Ab initio Nuclear Structure and Reactions - New Science through Extreme Scale Computing*, J.P. Vary, DOE Workshop on Forefront Questions in Nuclear Science and the Role of High Performance Computing, Gaithersburg, MD, January 26-28, 2009.
175. *The Optimized Effective Potential*, J. Drut, Oak Ridge National Laboratory, Knoxville, TN, February, 2009.

176. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, Nuclear Seminar, Ohio Univ., Athens, OH, February, 2009.
177. *Ab Initio Many-Body Calculations of Nucleon Scattering on Light Nuclei*, P. Navratil, 2009 Mardi Gras Nuclear Physics Workshop, Baton Rouge, LA, February, 2009.
178. *Ab initio no core approach to the properties of light nuclei*, J.P. Vary, Mardi Gras Nuclear Physics Workshop, Baton Rouge, LA, Feb. 18-20, 2009.
179. *Coupled-cluster theory for nuclei*, G. Hagen, 3rd LACM-EFES-JUSTIPEN Workshop, JIHIR, Oak Ridge, February 23-25, 2009.
180. *Non-empirical pairing energy functional*, T. Lesinski, 3rd LACM-EFES-JUSTIPEN Workshop, JIHIR, Oak Ridge, .
181. *Pairing of a trapped unitary Fermi gas*, J. Pei, 3rd LACM-EFES-JUSTIPEN Workshop, JIHIR, Oak Ridge, February 23-25, 2009.
182. *Getting nuclear DFT ready for the exascale age*, N. Schunck, 3rd LACM-EFES-JUSTIPEN Workshop, JIHIR, Oak Ridge, February 23-25, 2009.
183. *Recent developments in the large-scale DFT calculations for odd-even mass differences*, M.V. Stoitsov, 3rd LACM-EFES-JUSTIPEN Workshop, JIHIR, Oak Ridge, February 23-25, 2009.
184. *Recent ab initio NCSM and NCFC results*, J.P. Vary, LACM-EFES-JUSTIPEN Workshop, Oak Ridge National Lab, Feb. 23-25, 2009.
185. *Recent developments in parameter estimation for complex simulations*, J. Moré, The 3rd LACM-EFES-JUSTIPEN Workshop, Oak Ridge, TN., February 24, 2009.
186. *Skyrme functional fitting at 13% of the computational expense*, S. Wild, The 3rd LACM-EFES-JUSTIPEN Workshop, Oak Ridge, TN., February 25, 2009.
187. *Density Functional Theory (DFT) for Nuclei -- What About EFT?*, R.J. Furnstahl, INT Program on Effective Field Theory and the Many-Body Problem, Seattle, WA, March, 2009.
188. *Distributed matrix storage algorithms and MFD*, P. Maris, Leadership Class CI codes workshop, San Diego, CA, March 2009.
189. *TRDENS Density Matrix Code and Importance Sampling*, P. Navratil, Workshop on Leadership Class Configuration Interaction Code, San Diego, CA, March, 2009.
190. *Model-Based Optimization Algorithms for Expensive Simulation-Driven Problems*, S. Wild, Iowa State University Nuclear Physics Seminar, Ames, IA, March 5, 2009.
191. *The Many Facets of the Nuclear CI*, M. Horoi, invited talk at the UNEDF workshop on Leadership Class CI Codes, San Diego State University, March 11-14, 2009.
192. *Computing the nucleus of the atom from first principles*, J.P. Vary, Colloquium at the Computational Science Research Center, San Diego State University, San Diego, CA, March 13, 2009.
193. *Similarity Renormalization Group and Evolution of Many-Body Forces*, E.D. Jurgenson, INT Program on Effective Field Theory and the Many-Body Problem, Seattle, WA, March 31, 2009.
194. *Ab-initio calculations in nuclear physics*, P. Maris, NCCS Users Meeting, Oak Ridge, TN, April 2009.
195. *From EFT Interactions to a Unified Ab Initio Description of Light Nuclei*, P. Navratil, INT Program on Effective Field Theory and the Many-body Problem, Seattle, WA, April, 2009.
196. *The static and dynamic extension of DFT to superfluid fermionic systems: SLDA, ASLDA and TDSLDA*, A. Bulgac, Effective Field Theories and the Many-Body problem, INT program, Seattle, April 2nd, 2009.

197. *Non-empirical pairing energy functional*, T. Lesinski, INT Program on Effective Field Theory and the Many-Body Problem, Seattle, WA, April 10, 2009.
198. *Toward Microscopically Enriched and Constrained EDF*, B. Gebremariam, INT Program on Effective Field Theory and the Many-Body Problem, Seattle, WA, April 16, 2009.
199. *Time-Dependent Superfluid Local Density Approximation: A Status Report on the Full 3D Implementation and Applications*, I. Stetcu, Arctic FIDIPRO-EFES Workshop, Saariselkä, Finland, April 20-24, 2009.
200. *Fission Barriers of Compound Heavy Nuclei; Pairing Reentrance Phenomenon in Heated Rotating Nuclei*, W. Nazarewicz, GANIL, Caen, France, May 2009.
201. *Tentative solution of the center of mass problem*, T. Papenbrock, INT Program on Effective Field Theory and the Many-Body Problem, Seattle, WA , May 2009.
202. *Nuclear Quantum Monte Carlo*, R.B. Wiringa, INT Program on Effective Field Theory and the Many-Body Problem University of Washington, Seattle, WA, May 6, 2009.
203. *Ab initio no core nuclear structure: progress and plans*, J.P. Vary, Seminar, Institute for Nuclear Theory, University of Washington, Seattle, WA, May 11, 2009.
204. *Unexpected aspects of large amplitude nuclear collective motion*, A. Bulgac, FISSION 2009, Chateau de Cadarache, Saint-Paul-lez-Durance, France, May 13-16, 2009.
205. *Coupled-cluster theory for nuclei*, G. Hagen, CEA Workshop on Many-Body open quantum systems, Saclay, May 18-20, 2009.
206. *Symmetry-Conserving Spherical Gogny HFB Calculations in a Woods-Saxon Basis*, N. Schunck, Importance of continuum coupling for nuclei close to the drip-lines, CEA Workshop on Many-Body open quantum systems, Saclay, May 18-20, 2009.
207. *Benefits of Parallel I/O in Ab Initio Nuclear Physics Calculations*, N. Laghave, M. Sosonkina, P. Maris and J.P. Vary, International Conference on Computational Science (ICCS) 2009, Baton Rouge, LA, May 25-27, 2009.
208. *Ab Initio Many-Body Calculations of Nucleon Scattering on Light Nuclei*, P. Navratil, RNB8, Grand Rapids, MI, May 25-26, 2009.
209. *Exact Pairing in a Deformed Hartree-Fock Basis*, R. Senkov, B. A. Brown, V. Zelevinsky, G. Bertsch and Y.L. Luo, 2009 APS April Meeting, Denver, CO, May 25, 2009.
210. *Coupled-cluster theory for medium-mass nuclei*, T. Papenbrock, 8th International Conference on Radioactive Ion Beams (RNB-8), Grand Rapids, MI, May 26-30, 2009.
211. *Ab initio no core calculations of light nuclei*, J. Vary, CIPANP, May 25-30, 2009.
212. *Similarity renormalization group and low-momentum interactions for nuclei*, S.K. Bogner, CIPANP 2009, May 25-30, 2009.
213. *Ab Initio Reactions of Nucleons on Light Nuclei*, P. Navratil, UNEDF SCIDAC meeting, Pack Forest, WA, June, 2009.
214. *Ab Initio Many-Body Calculations of Light Ion Reactions*, P. Navratil, TRIUMF, Vancouver, Canada, June, 2009.
215. *Ab initio nuclear structure - the large sparse matrix eigenvalue problem*, J.P. Vary, SciDAC 2009, San Diego, CA, June 15-18, 2009.
216. *Simulation-based Nonlinear Least Squares Fitting*, S. Wild, SIAM Conference on Math. & Computational Issues in the Geosciences, Leipzig, Germany, June 15, 2009.
217. *Computing Atomic Nuclei*, W. Nazarewicz, National Nuclear Physics Summer School, June 28-July 10, 2009.
218. *Solving ab-initio nuclear structure problems with configuration interaction methods*, P. Maris, Invited talk in session on Extreme Scale Computing in Large-scale Scientific

Applications at the 2009 SIAM (Society for Industrial and Applied Mathematics) annual meeting, Denver, CO, July 6 - 10, 2009.

219. *Nuclear Structure Theory 2009: Progress Report and Challenges*, W. Nazarewicz, SUPA Lecture; University of the West of Scotland, Paisley, July 15, 2009.
220. *Discussion and concluding remarks*, W. Nazarewicz, Workshop on Structure and astrophysics from nuclear reactions with exotic nuclei, University of the West of Scotland, Paisley, July 15, 2009.
221. *The Unitary Fermi Gas: so simple yet so complex!*, A. Bulgac, Colloquium, CNLS, Los Alamos National Lab, July 20, 2009.
222. *Some Open Problems in Nuclear Large Amplitude Collective Motion (including fission)*, A. Bulgac, Seminar T2, Los Alamos National Lab, July 21, 2009.
223. *The Unitary Fermi Gas: so simple yet so complex!*, A. Bulgac, The XXVII International Symposium on Lattice Field Theory, Beijing, China, July 25-31, 2009.
224. *The properties of the unitary Fermi gas at finite temperatures - Quantum Monte Carlo approach*, P. Magierski, INT Program: From Femtoscience to Nanoscience: Nuclei, Quantum Dots and Nanostructures Seattle, USA, July 20- August 28, 2009.
225. *Multi-resolution computing platform of nuclear energy density functional*, J. Pei, CScADS 2009 Workshop, CA, Aug.3, 2009.
226. *Estimating Computational Noise in Simulation-Based Optimization Problems*, J. Moré, Linear and Numerical Linear Algebra Theory, Methods, and Applications, Northern Illinois University, August 12, 2009.
227. *Recent progress in ab initio Hamiltonian approaches to nuclear structure and light front field theory*, J.P. Vary, Technische Universitaet Darmstadt, Darmstadt, Germany, August 13, 2009.
228. *Computing Atomic Nuclei: Status and Challenges*, W. Nazarewicz, Lecture at the Department of Technical Physics, School of Physics, Peking University, Aug. 14, 2009.
229. *Frontiers of nuclear physics*, W. Nazarewicz, The 10th International Conference on Nucleus-Nucleus collisions, Beijing, China, Aug. 16-21, 2009.
230. *Fission barriers of compound superheavy nuclei*, J. Pei, The 10th International Conference on Nucleus-Nucleus collisions, Beijing, China, Aug. 16-21, 2009.
231. *Realistic NN and NNN interactions and the nuclear single-particle basis*, J.P. Vary, Lecture 1, International Summer School on Subatomic Physics, Beijing, China, August 23-27, 2009.
232. *ab initio No Core Nuclear Structure: Progress and Plans*, J.P. Vary, Lecture 2, International Summer School on Subatomic Physics, Beijing, China, August 23-27, 2009.
233. *Derivative-Free Optimization Methods for Simulation-Based Optimization Problems*, J. Moré, 20th International Symposium on Mathematica Programming, Chicago, IL, August 25, 2009.
234. *Variable Numbers of Interpolation Points in Model-based Algorithms*, S. Wild, 20th International Symposium on Mathematical Programming, Chicago, IL, August 25, 2009.
235. *Estimating Computational Noise in Simulation-Based Optimization Problems*, J. Moré, Tercer Congreso Latinoamericano de Matem\'aticos, Santiago, Chile, September 1, 2009.
236. *Designer nuclei: Connecting the femto-world with the Universe*, W. Nazarewicz, Physics Colloquium, University of Delaware, Newark, DE, Sep. 2009.
237. *Effective Field Theory and the no-core shell model*, I. Stetcu, plenary talk at the 9th International IUPAP Conference on Few-Body Problems in Physics, University of Bonn, Germany, August-September 2009.

238. *Turning Weeks Into Days: Parameter Estimation For Expensive Nuclear Energy Density Functionals*, S. Wild, ANLPS, Argonne, IL, September 10, 2009.
239. *Large Amplitude Superfluid Dynamics of a Unitary Fermi Gas*, A. Bulgac, Finite-Temperature Non-Equilibrium Superfluid Systems, Durham, September 14-17, 2009.
240. *Relativistic three-body bound state calculations in Bethe-Salpeter and lightfront formalism*, P. Maris, ECT* Workshop on Relativistic Description of Two- and Three-Body Systems in Nuclear Physics, Trento, Italy, Oct. 2009.
241. *Microscopic description of nuclear fission*, W. Nazarewicz, Meeting on Scientific Grand Challenges in National Security: The Role of Computing at the Extreme Scale, Washington D.C., October, 2009.
242. *Some Open Problems in Nuclear Large Amplitude Collective Motion*, A Bulgac, Scientific Grand Challenges in National Security: the Role of Computing at the Extreme Scale, Gaithersburg, MD, October 6-8, 2009.
243. *Inelastic and Transfer Couplings in Nucleon Induced Reactions*, G.P.A. Nobre, DNP 2009 Meeting in Waikoloa, Hawaii, October 14, 2009.
244. *Estimating Computational Noise in Numerical Simulations*, S. Wild, Lehigh University Department of Industrial and Systems Engineering Seminar, Lehigh, PA, October 16, 2009.
245. *Spin- and Parity-Dependent Nuclear Level Densities for rp-Process Nuclei*, M. Horoi, invited talk at the National Superconducting National Lab, MSU, October 22, 2009.
246. *Ab Initio Nuclear Structure Calculations of C, N, and other light nuclei*, P. Maris, invited talk in the ORNL booth at SuperComputing 2009, Portland, OR, November, 2009.
247. *Designer Nuclei-And How to Use Them*, W. Nazarewicz, University of Tennessee Science Forum, Knoxville, TN, November, 2009.
248. *The Unitary Fermi Gas: so simple yet so complex!*, A. Bulgac, Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, November 16, 2009.
249. *Extended Energy Density Functionals*, M. Kortelainen, MSU/NSCL Nuclear Physics Seminar, Michigan State University, Dec. 1, 2009.
250. *Extended Energy Density Functionals*, M. Kortelainen, Justipen-EFES Workshop, Riken, Japan, Dec. 7, 2009.
251. *Microscopic Description of the Fission Process*, W. Nazarewicz, 2010 SSAA Symposium, Washington, DC, Jan. 2010.
252. *Five Lectures on Nuclear Structure Theory*, B.A. Brown, School on Topics in Nuclear Many-Body Theory, from Lattice QCD to Nuclei, Gala, Norway, January 4-9 2010.
253. *Ab initio Hamiltonian approach to nuclear physics and to light-front field theory*, J.P. Vary, High Energy Physics in the LHC Era HEP-2010, Valparaiso, Chil, January 4-8, 2010.
254. *Density Functional Theory for Atomic Nuclei*, R.J. Furnstahl, Physics Colloquium, Argonne National Lab, Jan. 22, 2010.
255. *Computational Noise in Simulation-Based Optimization Problems*, J. Moré, International Conference on Analysis and Applications, Sultan Qaboos University, Muscat, Oman, January 24, 2010.
256. *Ab Initio No Core Full Configuration approach: recent results*, P. Maris, EFES-Iowa mini-workshop on nuclear structure, Ames, IA, February, 2010.
257. *Ab initio nuclear structure calculations with configuration interaction methods*, P. Maris, seminar, Iowa State University, Ames, IA, Feb. 2010.
258. *Fission Barriers of Compound Superheavy Nuclei*, W. Nazarewicz, invited talk at the APS April Meeting 2010, Washington, DC, February, 2010.

259. *Universal interactions in atomic and low-energy few-nucleon systems*, I. Stetcu, invited talk at the April Meeting of APS, Washington DC, February 2010.
260. *Shell Model Analysis of the Double Beta Decay Half-Life*, M. Horoi, EFES-NSCL workshop on "Perspectives on the modern shell model and related experimental topics", NSCL/MSU, February 4-6, 2010.
261. *Improving convergence of ab initio no core nuclear structure methods*, G. Negoita, Nuclear Physics seminar at University of Arizona, Tucson, Arizona, February 10, 2010.
262. *Improving convergence of ab initio no core nuclear structure methods*, G. Negoita, EFES-Iowa mini symposium on the ab initio Monte Carlo Shell Model, Feb. 26-27, 2010.
263. *No core shell model – recent progress and future prospects*, J.P. Vary, EFES-Iowa mini symposium on the ab initio Monte Carlo Shell Model, Feb. 26-27, 2010.
264. *Scalability and performance of MFDn -- recent and future developments*, P. Maris, Second Leadership Class CI Codes workshop, San Diego, CA, March 2010.
265. *Computing Atomic Nuclei on the Cray XT5*, H.A. Nam, Proc. 51st Cray User Group Conference 2009 (www.cug.org), March, 2010.
266. *MFDn – future prospects as an LCCI code*, J.P. Vary, LCCI development workshop, San Diego State University, San Diego, CA, March 11-13, 2010.
267. *Progress and problems with projected basis CI*, M. Horoi, Leadership Class CI codes workshop, San Diego State University, March 12, 2010.
268. *What do we know about the unitary Fermi gas?*, A. Bulgac, Invited talk - APS March Meeting, Portland, OR, March 15-19, 2010.
269. *Natural Units in the Nuclear Energy Density Functional Theory*, M. Kortelainen, 4th LACM-EFES-Justipen Workshop, ORNL, Mar. 15, 2010.
270. *Instabilities in the Nuclear Energy Density Functional Theory*, T. Lesinski, 4th LACM-EFES-Justipen Workshop, ORNL, Mar. 15, 2010.
271. *Augmented Lagrangian Method for Precise Constrained Density Functional Theory Calculations*, M. Stoitsov, 4th LACM-EFES-Justipen Workshop, ORNL, Mar. 15, 2010.
272. *Skyrme QRPA calculation of deformed nuclei*, J. Terasaki, 4th LACM-EFES-JUSTIPEN workshop, ORNL, March 15-17, 2010.
273. *Frontiers in Nuclear Physics*, W. Nazarewicz, KTH Stockholm, Colloquium, March 19, 2010.
274. *Frontiers in nuclear structure theory from a FAIR perspective*, W. Nazarewicz, Nordic Winter Meeting on PHYSICS @ FAIR, Björkliden, Sweden, March 22-26, 2010.
275. *Non-empirical energy density functionals for nuclei*, S. Bogner, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.
276. *Some Open Problems in Nuclear Large Amplitude Collective Motion (including fission)*, A. Bulgac, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.
277. *Neutron Matter from Low to High Densities*, J. Carlson, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.
278. *Energy Density Functionals for Nuclei*, R.J. Furnstahl, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23 - 26, 2010.
279. *Novel High Performance Computational Aspects of the Shell Model Approach for Medium Nuclei*, M. Horoi, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.
280. *How shall we program very large machines?*, R. Lusk, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.

281. *Ab initio no core full configuration approach to the structure of light nuclei*, P. Maris, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23 - 26, 2010.
282. *Ab initio many-body calculations of light-ion reactions*, P. Navratil, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.
283. *Ab-initio coupled cluster computations of nuclei*, T. Papenbrock, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.
284. *Ab initio no core shell model - status and prospects*, J. Vary, Computational Forefront in Nuclear Theory: Preparing for FRIB, Argonne National Laboratory, March 23-26, 2010.
285. *Novel High Performance Computational Aspects of the Shell Model Approach for Medium Nuclei*, M. Horoi, 6th ANL/MSU/JINA/INT FRIB Theory Workshop, ANL, March 25, 2010.
286. *Building bridges from quarks to the cosmos*, J.P. Vary, Colloquium at the University of Missouri, Rolla, MO, April 15, 2010.
287. *Frontiers in Nuclear Physics*, W. Nazarewicz, Physics Colloquium, Texas A&M University, Commerce, TX, May, 2010.
288. *Computing Atomic Nuclei*, W. Nazarewicz, Physics Colloquium, Ohio State University, May, 2010.
289. *Ab initio theory - Building bridges from quarks to the cosmos*, J.P. Vary, Theory Group Seminar, Saha Institute of Nuclear Physics, Calcutta, India, May 3, 2010.
290. *Computational Noise in Complex Simulations: Theory and Impact*, J. Moré, 2010 DOE Applied Mathematics Program Meeting, Berkeley, CA, May 4, 2010.
291. *Model-Based Derivative-Free Optimization Using Existing Expensive Evaluations*, S. Wild, 2010 DOE Applied Mathematics Program Meeting, Berkeley, CA, May 4, 2010.
292. *Shell Model Predictions of Double Beta Decay Half-Lifes*, M. Horoi, invited talk at RCNP, University of Osaka, May 12, 2010.
293. *Improving convergence of ab initio no core nuclear structure methods*, G. Negoita, Nuclear Physics seminar at Washington University, St. Louis, MO, May 14, 2010.
294. *Novel Computational Aspects of the Shell Model Nuclear Level Densities and Reaction Rates*, M. Horoi, invited talk at RIKEN, Saitama, Japan, May 20, 2010.
295. *New Approaches for Shell Model Level Densities and Reaction Rates*, M. Horoi, invited talk at University of Tokyo, May 20, 2010.
296. *Renormalized Interactions with EDF Single-Particle Basis States and NuShellX@MSU*, B.A. Brown, 10th International Spring Seminar on Nuclear Physics, New Quests in Nuclear Structure, Vietri Sul Mare, Italy, May 21-25, 2010.
297. *Pairing in low density fermion systems: Open problems, Next Frontier - Time-dependent probes*, A. Bulgac, Superfluidity in nuclear-matter, finite nuclei and ultra cold fermion gases, CEA-Saclay, FRANCE, May 31-June 4, 2010.
298. *Pairing in cold atoms from Monte Carlo calculations; finite temperature aspects*, P. Magierski, Workshop: Superfluidity in nuclear matter, finite nuclei and ultra-cold fermion gases, Saclay, France, May 31- June 4, 2010.
299. *Scaling of ab-initio nuclear physics calculations on multicore computer architectures*, P. Maris, ICCS2010, Amsterdam, the Netherlands, June 2010.
300. *Pairing in nuclear systems; observables, phenomenology and microscopic calculations*, W. Nazarewicz, Workshop on Superfluidity in nuclear matter, finite nuclei and ultra-cold fermion gases, Espace de Structure Nucléaire Théorique at Saclay, May-June, 2010.

301. *New developments of realistic J-matrix inverse scattering NN interaction and ab initio description of light nuclei*, A.M. Shirokov, NPAE-2010, Kiev, Ukraine, June 2010.
302. *Pairing from Effective Field Theory and Density Functional Theory*, R.J. Furnstahl, workshop on "Superfluidity in nuclear matter, finite nuclei and ultra-cold fermion gases", CEA Saclay, June 2, 2010.
303. *Ab initio light-front field theory based on the no core shell model*, J.P. Vary, LC2010, Valencia, Spain, June 13-19, 2010.
304. *Coupled Channels: From Nuclear Structure to Reaction Observables*, G.P.A. Nobre, LLNL Post-doc Seminar Series, June 15, 2010.
305. *Renormalized Interactions for CI constrained by EDF methods and NuShellX@MSU*, B.A. Brown, Carpathian Summer School of Physics 2010, Exotic Nuclei and Nuclear/Particle Astrophysics (III), From Nuclei to Stars, Sinaia, Romania, June 20 – July 3, 2010.
306. *Nuclear Shell Model Analyses and Predictions of Double Beta Decay Observables*, M. Horoi, the Carpathian Summer School of Physics 2010, Exotic Nuclei and Nuclear/Particle Astrophysics (III), From Nuclei to Stars, Sinaia, Romania, June 20 – July 3, 2010.
307. *Model independent computation of atomic nuclei: status and perspectives*, T. Papenbrock, "The INT at 20 years: The Future of Nuclear Physics and its Intersections," Seattle, WA, July 1-2, 2010.
308. *Static Properties and Dynamics of Strongly Interacting Many Fermion Systems*, A. Bulgac, Summer School on Nuclear Collective Dynamics V, F.Gursey Institute for Theoretical Physics, Istambul Turkey, July 4-10, 2010.
309. *Three-Nucleon Forces for Neutron-Rich, Medium-Mass Nuclei*, J. Holt, International Nuclear Physics Conference Vancouver, BC, Canada, July 4, 2010.
310. *Large-Scale Computations of Nuclear Dynamics*, J.P. Carlson, SCIDAC 2010, July 12-16, 2010.
311. *Generation and dynamics of vortices in superfluid Fermi gases*, A. Bulgac, Quantum solids, liquids, and gases, Stockholm, Sweden, July 19 - August 27, 2010.
312. *The Role of Shell Model Nuclear Level Densities for Nuclear Astrophysics*, M. Horoi, 11th International Symposium on Nuclei in Cosmos, Heidelberg, Germany, July 19-23, 2010.
313. *Three-Nucleon Forces for Medium Mass Nuclei Towards the Driplines*, J. Holt, Pan-American Advanced Studies Institute on Rare Isotopes, Joao Pessoa, Brazil, August 1, 2010.
314. *Ab initio nuclear theory - requirements and science goals for sustained petascale simulations*, J.P. Vary, SciApps - 10 Challenges and Opportunities for Scientific Applications: learning to sustain the Petaflop with eyes on the Exaflop horizon, Oak Ridge National Laboratory, August 6, 2010.
315. *Optimization Without Derivatives for Expensive Simulation-Based Problems*, S. Wild, ICIS Workshop on Optimization in Energy Systems, Snowbird, UT, August 6, 2010.
316. *Coupled-cluster approach to medium-mass and neutron-rich nuclei*, G. Hagen, Nuclear Structure 2010 (NS2010), Clark-Kerr Campus, U. C. Berkeley, CA, August 8-13, 2010.
317. *TAO Tutorial*, J. Sarich, Eleventh Workshop on the DOE ACTS Collection, Lawrence Berkeley National Laboratory, Berkeley, CA, August 18, 2010.
318. *Computing atomic nuclei*, W. Nazarewicz, NUCL Symposium: Radiochemistry at the Facility for Rare Isotope Beams (FRIB), Fall 2010 ACS National Meeting, Boston, MA, Aug. 22, 2010.

319. *Coupled-cluster approach to medium-mass and neutron-rich nuclei*, G. Hagen, Frontiers In NUclear STructure, Astrophysics and Reactions (FINUSTAR 3), Rhodes, Greece, August 23-27, 2010.
320. *Ab initio nuclear theory – progress and prospects*, J.P. Vary, Plenary talk, Zakopane Conference on Nuclear Physics, Extremes of the Nuclear Landscape, Zakopane, Poland, August 30 – September 4, 201.
321. *No-Core Full Configuration Nuclear Structure Calculations*, P. Maris, Mid--West Nuclear Theory get-together, Argonne, IL, September, 2010.
322. *Nuclear structure and dynamics in a time-dependent SLDA framework*, I. Stetcu, seminars at MSU, Warsaw Inst. Tech., NIPNE-HH Bucharest, Sept.-Nov. 2010.
323. *Ab initio theory - Building bridges from quarks to the cosmos*, J.P. Vary, GANIL, Caen, France, September 6, 2010.
324. *Least Squares Parameter Fitting Without Derivatives*, S. Wild, 2nd International Conference on Engineering Optimization, Lisbon, Portugal, September 7, 2010.
325. *Surprising features of ultra cold atomic gases at BCS-BEC crossover,* P. Magierski, 27th International Physics Congress (Turkish Physical Society), Istanbul, Turkey, 14-17 September 2010.
326. *Spontaneously broken symmetries in nuclear systems -are there any?*, P. Magierski, 17th Nuclear Physics Workshop, Kazimierz, Poland, 22-26 September 2010.
327. *Pairing properties, pseudogap phase and dynamics of vortices in a unitary Fermi gas*, P. Magierski, Workshop: Ultracold Quantum Gases beyond Equilibrium, International Institute of Physics, Natal, Brasil, Sept. 27 -Oct. 1, 2010.
328. *Operator Evolution for Light Nuclei with the Similarity Renormalization Group*, R.J. Furnstahl, ECT* workshop on The Limits of Existence of Light Nuclei, October, 2010.
329. *Add, multiply, divide, and conquer*, C.W. Johnson, UCSD Quantum Chemistry Seminar, October, 2010.
330. *Nuclear Structure Calculations with JISP16 for light nuclei*, P. Maris, seminar at the Universtiy of Iowa, Iowa City, IA, October, 2010.
331. *The road from trapped cold atoms to nuclear physics*, I. Stetcu, ECT* workshop on "The limits of existence of light nuclei," Trento, Italy, Oct. 2010.
332. *Probing the driplines with ab-initio Coupled-Cluster theory,* G. Hagen, ECT* Workshop on Limits of existence of Light nuclei, ECT*, Trento, Italy, October 25, 2010.
333. *Three-Nucleon Forces and the Evolution of Nuclear Structure Towards the Driplines*, J. Holt, ECT* Workshop: "The Limits of Existence of Light Nuclei", Trento, Italy, October 27, 2010.
334. *Structure Theory for the Facility of Rare Isotope Beams,* M. Horoi, invited talk at the Annual Meeting of Division of Nuclear Physics of the American Physical Society, Santa Fe, New Mexico, November 4, 2010.
335. *Estimating Derivatives of Computationally Noisy Functions*, S. Wild, INFORMS Annual Meeting, Austin, TX, November 7, 2010.
336. *Superfluidity of Imbalanced Fermi Gas*, J.C. Pei, UTK nuclear physics seminar, UTK, November 8, 2010.
337. *Configuration Interactions Constrained by Energy-Density Functionals*, B.A. Brown, University of Aizu- JUSTIPEN - EFES Symposium on Cutting-Edge Physics of Unstable Nuclei, University of Aizu, Aizuwakamatsu, Fukushima, Japan, November 10-13, 2010.

338. *Natural units and neutron droplets as constraints in the EDF optimization*, M. Kortelainen, Aizu-JUSTIPEN-EFES Symposium on "Cutting-Edge Physics of Unstable Nuclei", University of Aizu (Aizu-Wakamatsu, Japan), November 10-13, 2010.
339. *Information content of a new observable*, W. Nazarewicz, Aizu-JUSTIPEN-EFES Symposium on "Cutting-Edge Physics of Unstable Nuclei", University of Aizu (Aizu-Wakamatsu, Japan), November 10-13, 2010.
340. *Microscopically Based Nuclear Energy Density Functionals Using The Density Matrix Expansion*, M. Stoitsov, Aizu-JUSTIPEN-EFES Symposium on "Cutting-Edge Physics of Unstable Nuclei", University of Aizu (Aizu-Wakamatsu, Japan), November 10-13, 2010.
341. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, EMMI workshop on Strongly Coupled Systems, GSI, Darmstadt, Germany, Nov. 15-17, 2010.
342. *Computing exotic nuclei*, W. Nazarewicz, International Symposium on "New Faces of Atomic Nuclei", Okinawa Institute of Science and Technology (OIST), Okinawa, Japan, November 15-17, 2010.
343. *Ab initio nuclear structure calculations*, T. Papenbrock, EMMI workshop "Strongly coupled systems," GSI, Darmstadt, Germany, November 15-17, 2010.
344. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, Bonn University Physics Colloquium, Nov. 18, 2010.
345. *Proton-neutron pairing correlations in nuclei: a shell model perspective*, M. Horoi, invited talk at the International Workshop Probing Proton-Neutron Pair Correlations held at Nishina Center, RIKEN Wako-shi campus, Japan, November 19-20, 2010.
346. *Ab initio theory - Building bridges from quarks to the cosmos*, J.P. Vary, Theory Seminar, Indian Institute of Technology (IIT) -Mumbai, India, Nov. 19, 2010.
347. *Introduction to ab initio theory of nuclei - I and II*, J.P. Vary, Workshop preceding conference on NN Interaction and the Nuclear Many-Body Problem, Mumbai, India, Nov. 22-26, 2010.
348. *Ab initio nuclear theory -- recent progress and future prospects*, J.P. Vary, NN Interaction and the Nuclear Many-Body Problem, Tata Institute of Fundamental Research, Mumbai, India, Nov. 22-26, 2010.
349. *Computational Nuclear Structure and Reactions - Progress and Opportunities on Leadership Class Computers from a US Perspective*, J.P. Vary, International Symposium "From Quarks to Supernovae", Izu-Atagawa, Japan, Nov. 28-30, 2010.
350. *Three-Nucleon Forces and the Evolution of Nuclear Structure in Exotic Nuclei*, J. Holt, Nuclear Theory / EMMI Seminar; Technical University Darmstadt, Darmstadt, Germany, November 29, 2010.
351. *Frontiers in nuclear structure theory*, T. Papenbrock, Physics Colloquium, Technische Universität Darmstadt, Darmstadt, Germany, December 3, 2010.
352. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, JLab Theory Seminar, Dec. 6, 2010.
353. *Ab initio calculations of radiative capture*, P. Navratil, CAWONAPS 2010, TRIUMF, December 9-10, 2010.
354. *Computing exotic nuclei*, W. Nazarewicz, Colloquium, Saha Institute of Nuclear Physics, Kolkata, India, Dec. 9, 2010.
355. *Information content of a new observable*, W. Nazarewicz, Invited Seminar, GANIL, Caen, France, Dec. 17, 2010.
356. *Generation and dynamics of vortices in a superfluid unitary Fermi gas*, A. Bulgac, Frontiers of condensed matter physics, Stockholm, Sweden, January 3-8, 2011.

357. *The nuclear many-body problem*, G. Hagen, five lectures at the Second Uio-MSU-ORNL-UT School on Topics in Nuclear Physics: Many-Body Theory, Connections to Experiment and Nuclear Astrophysics, MSU, January 3-7, 2011.
358. *Ab initio theory of light-ion reactions*, P. Navratil, XXXIV Symposium on Nuclear Physics, Cocoyoc, January 3-7, 2011.
359. *Static and Time-Dependent Density Functional Theory with Applications to Nuclear and Cold Atom Physics*, A. Bulgac, 14th Taiwan Nuclear Physics School, Taiwan, January 17-22, 2011.
360. *Science Overview - Needs for Large Collaborations in Nuclear Theory*, W. Nazarewicz, FUSTIPEN Inauguration Meeting, GANIL, Caen, France, Jan. 18, 2011.
361. *Similarity Renormalization Group Techniques for the Nuclear Many-Body Problem*, H. Hergert, TRIUMF, Vancouver, Canada, January 20, 2011.
362. *Nuclear Structure Theory Relevant to the Facility for Rare Isotope Beams*, M. Horoi, colloquium at Western Michigan University, Kalamazoo, MI, January 24, 2011.
363. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, Ohio State University Physics colloqium, Feb. 1, 2011.
364. *Large sparse matrix techniques in ab initio approaches to nuclear structure*, P. Maris, 2nd EFES-Iowa mini-workshop on nuclear structure, Ames, IA, February, 2011.
365. *Solving Large-scale Eigenvalue Problems in Nuclear Structure Calculation*, C. Yang, Linear Algebra Seminar, UC Berkeley, Feb, 2011.
366. *Exploring Neutron-Rich Exotic Nuclei with Three-Nucleon Forces*, J. Holt, Nuclear Physics Seminar Instituto de Fisica Teorica Universidad Autonoma de Madrid, Madrid, Spain, February 2, 2011.
367. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, workshop on Perspectives of the Ab Initio No-Core Shell Model, TRIUMF, Feb. 10-12, 2011.
368. *Factorization algorithms in large scale shell model calculations*, C.W. Johnson, workshop on Perspectives of the Ab Initio No-Core Shell Model, TRIUMF, Feb. 10-12, 2011.
369. *No-core full configuration calculations for neutrons in a H.O. trap*, P. Maris, workshop on Perspectives of the Ab Initio No-Core Shell Model, TRIUMF, Feb. 10-12, 2011.
370. *NCSM for trapped few-body systems*, I. Stetcu, workshop on Perspectives of the Ab Initio No-Core Shell Model, TRIUMF, Feb. 10-12, 2011.
371. *Origin of the anomalous long lifetime of 14C*, J.P. Vary, workshop on Perspectives of the Ab Initio No-Core Shell Model, TRIUMF, Feb. 10-12, 2011.
372. *Ab Initio Theory of Light-Ion Reactions*, P. Navratil, The 48th Winter Nuclear and Particle Physics Conference, Banff, Alberta, February 18-20, 2011.
373. *Reaction theory for neutron-deficient nuclei*, C. Bertulani, EURISOL topical meeting, Valencia, Spain, February 22, 2011.
374. *Similarity Renormalization Group Techniques for the Nuclear Many-Body Problem*, H. Hergert, Ohio State University, Columbus, OH, February 22, 2011.
375. *What keeps the 14C clock ticking for 5730 years?*, J.P. Vary, EFES-Iowa workshop on the ab initio Monte Carlo Shell Model, Ames, Iowa, February 23, 2011.
376. *Toward model-independent nuclear structure computations*, T. Papenbrock, Physics seminar, Universität Frankfurt, Frankfurt, Germany, February 24, 2011.
377. *Renormalization Group in Nuclear Physics*, R.J. Furnstahl, lectures at the Schladming Winter School, Schladming, Austria, March, 2011.
378. *Chiral three-nucleon forces in nucleonic matter*, K. Hebeler, ECT* workshop on Effective theories and the nuclear many-body program, Trento, Italy, March, 2011.

379. *New Frontiers in Nuclear Physics*, K. Hebeler, invited seminar at TU Darmstadt, March, 2011.
380. *Harmonic EFT, the beginning: from nuclei to trapped atoms*, I. Stetcu, ECT* workshop on Effective theories and the nuclear many-body problem, Trento, Italy, March, 2011.
381. *Cold atomic gases and effective interactions*, C.W. Johnson, Benchmarking the many-body problem, Institute for Nuclear Theory/University of Washington, March, 2011.
382. *Large Sparse Matrix Problems in Ab-initio Nuclear Physics*, P. Maris, invited talk at SIAM/CSE11, Reno, NV, March 2011.
383. *Update on MFDn*, P. Maris, third Leadership Class CI codes workshop, Berkeley, CA, March 2011.
384. *Harmonic EFT, the beginning: from nuclei to trapped atoms*, I. Stetcu, ECT* workshop on "Effective theories and the nuclear many-body problem," Trento, Italy, March 2011.
385. *Model-independent approaches to nuclear structure*, T. Papenbrock, Annual NuSTAR meeting, GSI, Darmstadt, Germany, March 2-4, 2011.
386. *Applied Optimization Without Derivatives*, S. Wild, SIAM Conference on Computational Science & Engineering, Reno, NV, March 3, 2011.
387. *Nuclear physics in the cosmos*, C. Bertulani, Department of Physics, University of Texas at Arlington, March 4, 2011.
388. *Towards ab initio structure and reactions in neutron rich nuclei with coupled-cluster theory*, G. Hagen, ECT workshop on Effective theories and the nuclear many-body problem, ECT, Trento, Italy, March 7-11, 2011.
389. *Three-Body Forces and Shell Structure in Exotic Nuclei*, J. Holt, ECT* Workshop: "Effective Theories and The Nuclear Many-Body Problem", Trento, Italy, March 7, 2011.
390. *Effective Forces Responsible for Enhanced Proton-Neutron Correlations in N ~= Z Nuclei*, M. Horoi, ECT* workshop on Effective Theories and the Nuclear Many-Body Problem, Trento, Italy, March 7-11, 2011.
391. *Exploration of Fission in Superheavy Elements Using the Skyrme-Hartree-Fock Model*, J. Erler, The fifth LACM-EFES-JUSTIPEN Workshop, March 15-17, 2011.
392. *Test of Skyrme Energy Functionals with QRPA in Low-Lying States of Rare-Earth Nuclei*, J. Terasaki, 5th LACM EFES JUSTIPEN Workshop, Oak Ridge, TN, March 15, 2011.
393. *Origin of the anomalous lifetime of 14C*, J.P. Vary, Fifth LACM-EFES-JUSTIPEN Workshop, Oak Ridge, Tennessee, March 15-17, 2011.
394. *The Hunt for Missing Derivatives: Reward Offered!*, S. Wild, 5th LACM-EFES-JUSTIPEN Workshop, Oak Ridge, TN, March 16, 2011.
395. *Three-Nucleon Forces and the Evolution of Nuclear Structure in Exotic Nuclei*, J. Holt, The Fifth LACM-EFES-JUSTIPEN Workshop Oak Ridge, TN, March 17, 2011.
396. *Updates on Nushellx*, M. Horoi, LCCI collaboration meeting, BLNL, March 17-19, 2011.
397. *Quasiparticle continuum and resonances in HFB theory*, J.C. Pei, 5th LACM-EFS-JUSTIPEN Workshop, Oak Ridge, March 17, 2011.
398. *Overview of the Leadership Class Configuration Interaction (LCCI) code development project*, J.P. Vary, 2011 LCCI meeting, Lawrence Berkeley National Laboratory, Berkeley, CA, March 17-19, 2011.
399. *Information content of a new observable*, W. Nazarewicz, Colloquium, LBNL, Nuclear Science Division, March 23, 2011.
400. *Ab initio methods for nuclear properties - a computational physics approach*, P. Maris, invited talk, joint DCOMP-DNP session at APS spring meeting, Anaheim, CA, April 2011.

401. *Frontiers of nuclear physics*, W. Nazarewicz, IOP Nuclear and Particle Physics Divisional Conference, University of Glasgow, Glasgow, UK, April 4-7, 2011.
402. *Spectroscopic information form reactions with unstable nuclei*, C. Bertulani, International Conference on "Nuclear Physics in Astrophysics V", Eilat, Israel, April 5, 2011.
403. *Adventures in Load-Balancing at Large Scale: Successes, Fizzles, and Next Steps*, E. Lusk, Invited talk at 9th Annual Workshop on Charm++ and its Applications. University of Illinois, Champagne, IL, April 19, 2011.
404. *Chiral Three-Nucleon Forces: From Neutron Matter to Neutron Stars*, K. Hebeler, NT program on ``Fermions from Cold Atoms to Neutron Stars: Benchmarking the Many-Body Problem," Seattle, May, 2011.
405. *Nuclear dynamics in real time*, I. Stetcu, the International Workshop on Nuclear Physics, Stellen¬bosch, South Africa, May, 2011.
406. *Nuclear dynamics in real time*, I. Stetcu, invited talk at the International Workshop on Nuclear Physics, Stellenbosch, South Africa, May 2011.
407. *Model-independent nuclear structure computations*, T. Papenbrock, HISKP Colloquium, Universität Bonn, Bonn, Germany, May 12, 2011.
408. *Coordinate-space HFB description of superfluid Fermi systems*, J.C. Pei, INT-11-1 program "Fermions from Cold Atoms to Neutron Stars", INT Seattle, May 12, 2011.
409. *Towards ab initio structure and reactions in neutron rich nuclei with coupled-cluster theory*, G. Hagen, invited seminar talk at CEA, CEA, Saclay, France, May 13, 2011.
410. *Pseudogap from Path Integral Monte Carlo (PIMC) on the lattice*, P. Magierski, INT Symposium: Fermions from Cold Atoms to Neutron Stars: Benchmarking the Many-Body Problem, Seattle, USA, May 14-20, 2011.
411. *Thermodynamics and Pairing Properties of a Unitary Fermi Gas*, P. Magierski, INT Symposium: Fermions from Cold Atoms to Neutron Stars: Benchmarking the Many-Body Problem, Seattle, USA, May 14-20, 2011.
412. *Real Time Dynamics of the Unitary Fermi Gas*, A. Bulgac, INT Ultra-Cold Atoms Symposium, May, 16-20, 2011.
413. *Introduction to Nuclear Structure Theory*, W. Nazarewicz, International Workshop on Nuclear Physics, Stellenbosch Institute for Advanced Study, Stellenbosch, South Africa, May 16-27, 2011.
414. *Coupled-channels Neutron Reactions on Nuclei*, I.J. Thompson, University of Surrey, UK, May 17, 2011.
415. *Bench¬marking the Many-body Problem: Precision bounds on the Equation of State*, M.M. Forbes, INT Program 11-1: Fermions from Cold Atoms to Neu¬tron Stars: Benchmarking the Many-Body Problem, Seattle, May 18, 2011.
416. *Optimization With Some Derivatives*, S. Wild, SIAM Conference on Optimization, Darmstadt, Germany, May 18, 2011.
417. *Hamiltonian Light Front Field Theory: Recent Progress and Tantalizing Prospects*, J.P. Vary, Invited talk at the Light Cone 2011 Meeting, Dallas, TX, May 23-27, 2011.
418. *Towards a unified description of nuclear structure and reactions with coupled-cluster theory*, G. Hagen, FUSTIPEN Topical Meeting "Structure and reactions at the drip lines", GANIL, Caen, France, May 24-25, 2011.
419. *Large-scale calculations of nuclear excited states using density functional method*, J. Terasaki, Computational Science Colloquium, Center for Computational Science, University of Tsukuba, Japan, May 24, 2011.

420. *Chiral Three-Nucleon Forces: From Neutron Matter to Neutron Stars*, K. Hebeler, International Workshop ``Microphysics in Computational Relativistic Astrophysics," Waterloo, Canada, June, 2011.
421. *Ab initio calculations of weakly bound nuclei*, G. Hagen, The first International Conference on Advances in Radioactive Isotope Science (ARIS - 2011), Leuven, Belgium, June 1, 2011.
422. *No Core CI Calculations for light nuclear systems*, P. Maris, INT program on Extreme Computing and its Implications for the Nuclear Physics/Applied Mathematics/Computer Science Interface, Seattle, WA, June 2011.
423. *Computational Issues in ab initio Nuclear Structure*, P. Maris, INT Exascale workshop, Seattle, WA, June 2011.
424. *Solving Large-scale Eigenvalue Problems in Nuclear Structure Calculations*, C. Yang, invited talk at the INT workshop on Extreme Computing and its Implications for the Nuclear Physics/Applied Mathematics/Computer Science Interface, June, 2011.
425. *Nuclear Configuration Interaction Calculation using ARPACK*, C. Yang, Invited talk at the Workshop in honor Danny Sorensen's 65th birthday, Reno, NV, June, 2011.
426. *Charge-Changing Processes and Nuclear Response*, J. Engel, collaboration meeting of the DOE topical center on hot-and-dense matter, June 3, 2011.
427. *Recent progress and new challenges in ab initio nuclear structure and nuclear reactions*, J.P. Vary, Invited talk at the Institute of Nuclear Theory Program on Extreme Computing and its Applications, Seattle, WA, June 6, 2011.
428. *Toward model-independent nuclear structure computations*, T. Papenbrock, ECT* workshop on "Nuclear many-body open quantum systems," Trento, Italy, June 7, 2011.
429. *Nuclear physics in the cosmos*, C. Bertulani, Meeting of the Brazilian Physical Society, Iguassu Falls, Brazil, June 9, 2011.
430. *Challenges for a reliable shell-model description of the neutrinoless double beta decay matrix elements*, M. Horoi, MEDEX'11 Workshop, Prague, June 13-16, 2011.
431. *Nuclear structure at the neutron drip-line*, G. Hagen, Gordon Research Conferences, Intersections Between Structure and Reactions: Pushing the Frontiers of Nuclear Science, Colby-Sawyer College, New London, CT, June 14, 2011.
432. *Renormalization group methods in nuclear few- and many-body problems*, S. Bogner, National Nuclear Physics Summer School 2011, Chapel Hill, NC, June 27-29, 2011.
433. *Real-Time Dynamics of Fermionic Superfluid Systems: from Deterministic Petascale to Stochastic Exascale Simulations*, A. Bulgac, INT Workshop on the Nuclear Physics-Applied Math-Computer Science Interface, June 27 -July 1, 2011.
434. *Ab initio calculations of light-ion reactions: Application to 7Be(p,γ)8B capture*, P. Navratil, IKP, TU Darmstadt, June 29, 2011.
435. *Tests of Skyrme energy density functionals in low-energy vibrational states of rare-earth nuclei using QRPA*, J. Terasaki, RUBF ULIC and CNS Symposium on Frontier of gamma-ray spectroscopy, RIKEN, Wako, Japan, June 30 - July 2, 2011.
436. *New Frontiers in Nuclear Physics*, K. Hebeler, colloquium at the University of Guelph, July, 2011.
437. *Large-scale Parallel Null Space Calculation for Nuclear Configuration Interaction*, H.M. Aktulga, 2011 High Performance Computing and Simulation Conference (HPCS 2011), Istanbul, Turkey, July, 2011.

438. *UNEDF: Building Nuclei from the ground up*, W. Nazarewicz, INT 11-2a program "Extreme Computing and its Implications for Nuclear Physics/Applied Mathematics/Computer Science Interface", INT Seattle, July 7, 2011.
439. *Physics with Rare Isotope beams, an overview*, W. Nazarewicz, Tenth Exotic Beam Summer School - EBSS2011, NSCL/MSU, July 25-30, 2011.
440. *Making Sense of Structure/Reaction `Non-observables*, R.J. Furnstahl, 2011 INT/FRIB workshop, INT, Seattle, August, 2011.
441. *Status of Nuclear Theory*, R.J. Furnstahl, Superusers Workshop, Michigan State University, August, 2011.
442. *Chiral three-body forces and neutron-rich matter*, K. Hebeler, INT program ``Astrophysical Transients: Multi-messenger Probes of Nuclear Physics," Seattle, August, 2011.
443. *New Applications of Renormalization Group Methods in Nuclear Physics*, K. Hebeler, International workshop ``Renormalization Group Approach from Ultra-Cold Atoms to the Hot QGP," Kyoto, Japan, August, 2011.
444. *On Reducing I/O Overheads in Large-Scale Invariant Subspace Projections*, H.M. Aktulga, 2011 High Performance Scientific Software Workshop (HPSS 2011), Bordeaux, France, August, 2011.
445. *How robust is big bang nucleosynthesis?*, C. Bertulani, Laboratori Nationali del Sud, Catania, Italy, August 2, 2011.
446. *Ab initio reaction theory for light nuclei*, P. Navratil, 7th ANL/INT/JINA/MSU annual FRIB workshop; INT Program INT-11-2d: Interfaces between structure and reactions for rare sotopes and nuclear astrophysics, Seattle, August 8, 2011.
447. *Reactions at Intermediate Energies*, C. Bertulani, 7th ANL/INT/JINA/MSU Annual FRIB Workshop, INT, University of Washington, Seattle, August 17, 2011.
448. *Theoretical nuclear physics*, W. Nazarewicz, Four lectures at the16th UK Nuclear Physics Postgraduate Summer School, St Andrews, Scotland, UK, Sep. 3-6, 2011.
449. *Real-Time Dynamics of Superfluid Unitary Fermi Gases*, A. Bulgac, Finite-temperature Non-Equilibrium Superfluid Systems, Heidelberg, Germany, September 18-21, 2011.
450. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, Physics Colloquium, Indiana University, October, 2011.
451. *New Applications of Renormalization Group Methods in Nuclear Physics*, K. Hebeler, invited talk at the 2011 Fall Meeting, APS Division of Nuclear Physics, East Lansing, MI, October, 2011.
452. *Ab initio calculations of light-ion reactions*, P. Navratil, Frontier Issues in Physics of Exotic Nuclei (YKIS2011), Kyoto, Oct. 11, 2011.
453. *Challenges in Computational Nuclear Structure*, W. Nazarewicz, Frontier Issues in Physics of Exotic Nuclei (YKIS2011), Yukawa Institute for Theoretical Physics, Kyoto, Japan, October 14, 2011.
454. *Opening the Blackbox in Simulation-based Optimization*, S. Wild, University of Colorado-Denver, Operations Research Seminar, Denver, CO., October 25, 2011.
455. *Direct reactions with rare isotopes*, C. Bertulani, YIPQS Long-term workshop, Dynamics and Correlations in Exotic Nuclei (DCEN2011), Yukawa Institute for Theoretical Physics, Kyoto, Japan, October 28, 2011.
456. *From nucleons to nuclei to fusion reactions*, S. Quaglioni, Conference on Computational Physics 2011, Gatlinburg, Tennessee, Oct. 31 – Nov. 3, 2011.

457. *Ab Initio Nuclear Structure Calculations of Light Nuclei*, P. Maris, Conference on Computational Physics 2011, Gatlinburg, Tennessee, Oct. 31 – Nov. 3, 2011.
458. *Computational nuclear structure in the eve of exascale*, W. Nazarewicz, Physics Seminar, Physics Division, Brookhaven National Laboratory, Nov. 22, 2011.
459. *Towards an implementation of a real-time path-integral for interacting fermions*, A. Bulgac, Workshop The Stochastic Schroedinger Equation in Selected Physics Problems, CEA/SPhN, Gif-sur-Yvette, France, December, 6-7, 2011.
460. *Teoria struktury jadra atomowego w przededniu ery eksaflopow (in Polish)*, W. Nazarewicz, IX Sympozjum Instytutu Fizyki Teoretycznej, IFT, Warsaw University, Dec. 9, 2011.
461. *Effective theory for deformed nuclei*, T. Papenbrock, XXXV Symposium on Nuclear Physics, Cocoyoc, Mexico, January 3-6, 2012.
462. *Time-dependent density functional theory approach to (induced) nuclear fission and its extension*, A. Bulgac, FUSTIPEN workshop on nuclear fission, GANIL, Caen, France, January 4-6, 2012.
463. *Microscopic description of fission process within the Nuclear Density Functional Theory*, W. Nazarewicz, Topical Meeting on Theory of Nuclear Fission, GANIL, Caen, France, January 4-6, 2012.
464. *In-medium Similarity Renormalization Group for Nuclei*, S. Bogner, Facets of Strong-Interaction Physics: International Workshop on Gross Properties of Nuclei and Nuclear Excitations, Hirschegg, Austria, January 15-21, 2012.
465. *Towards model independent description of nuclei with coupled-cluster theory*, G. Hagen, Physics Colloquium Ohio University, Athens, January 17, 2012.
466. *Similarity Renormalization Group and All That*, S. Bogner, Third UiO-MSU-ORNL-UT School on Topics in Nuclear Physics: The computational quantum many-body problem, Oak Ridge, TN, January 23-27, 2012.
467. *Atomic Nuclei at Low Resolution*, R.J. Furnstahl, Physics Colloquium, Virginia Tech University, February, 2012.
468. *Making Sense of Scale- and Scheme-Dependent Observables in Low-Energy Nuclear Physics*, R.J. Furnstahl, NSCL Seminar, Michigan State University, February, 2012.
469. *Towards model independent description of nuclei with coupled-cluster theory*, G. Hagen, Physics Colloquium University of Maryland, College Park, February 8, 2012.
470. *Realistic NN and NNN Interactions and their range of validity*, J.P. Vary, Lecture at the DST-SERC School on "Modern Trends in Nuclear Structure and Dynamics" at the Indian Institute of Technology-Roorkee, India, February 13, 2012.
471. *IR/UV Regulators and Renormalization Methods*, J.P. Vary, Lecture at the DST-SERC School on "Modern Trends in Nuclear Structure and Dynamics" at the Indian Institute of Technology-Roorkee, India, February 14, 2012.
472. *Ab initio Configuration Interaction calculations for Nuclear Structure*, P. Maris, SIAM conference on Parallel Processing for Scientific Computing, Savannah, Georgia, February 15-17, 2012.
473. *Extreme Single-Particle Model*, J.P. Vary, Lecture at the DST-SERC School on "Modern Trends in Nuclear Structure and Dynamics" at the Indian Institute of Technology-Roorkee, India, February 15, 2012.
474. *Leadership class computing & techniques for large sparse matrix diagonlization*, J.P. Vary, Lecture at the DST-SERC School on "Modern Trends in Nuclear Structure and Dynamics" at the Indian Institute of Technology-Roorkee, India, February 16, 2012.

475. *Recent results in light nuclei with ab initio no core methods*, J.P. Vary, Lecture at the DST-SERC School on "Modern Trends in Nuclear Structure and Dynamics" at the Indian Institute of Technology-Roorkee, India, February 17, 2012.
476. *Towards nuclear reactions with coupled-cluster theory*, G. Hagen, Nuclear Physics Seminar University of Tennessee, February 20, 2012.
477. *Microscopic Description of Fission Process*, W. Nazarewicz, 2012 SSAA Symposium, Washington DC, Feb. 22-23, 2012.
478. *Towards nuclear reactions with coupled-cluster theory*, G. Hagen, Perspectives of the Ab Initio No-Core Shell Model, TRIUMF, Vancouver, BC, Canada, February 23-25, 2012.
479. *Large-scale ab initio CI calculations for light nuclei*, P. Maris, Workshop on Perspectives on the Ab Initio No-Core Shell Model, TRIUMF, Vancouver, BC, Canada, February 23-25, 2012.
480. *Role of the particle continuum and of three-nucleon forces in oxygen isotopes*, T. Papenbrock, Progress in Ab-Initio Techniques in Nuclear Physics, TRIUMF, Vancouver, February 23-25 2012.
481. *Convergence properties of no-core nuclear calculations*, J.P. Vary, Workshop on Perspectives on the Ab Initio No-Core Shell Model, TRIUMF, Vancouver, BC, Canada, February 23-25, 2012.
482. *Recent developments of the NCSM/RGM approach to nuclear reactions*, P. Navratil, Workshop on Perspectives on the /Ab Initio/ No-Core Shell Model, TRIUMF, Vancouver, BC, February 24, 2012.
483. *The onset of the pseudogap regime and shear viscosity from ab initio calculations in ultra cold Fermi gases*, A. Bulgac, APS March meeting, Boston, MA, Feb. 27-Mar. 2, 2012.
484. *Opening the Blackbox in Simulation-based Optimization*, S. M. Wild, Department of Applied Mathematics and Statistics Colloquium, University of California-Santa Cruz, Santa Cruz, CA, February 27, 2012.
485. *Solving Large-scale Eigenvalue problems in Nuclear Structure Calculations*, H.M. Aktulga, 12th Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, March, 2012.
486. *Simulating the Atomic Nucleus*, J.P. Vary, Joint Mathematics and Physics Colloquium, Florida International University, Miami, FL, March 2, 2012.
487. *Nuclear Quantum Monte Carlo*, S. Pieper, WE-Heraeus Seminar. Nuclear Ground-State Properties of the Lightest Nuclei ," Physikzentrum Bad Honnef, Germany, March 20, 2012.
488. *Ab initio calculations of light-ion reactions*, P. Navratil, DREB 2012, March 26, 2012.
489. *The limits of the nuclear landscape*, W. Nazarewicz, APS April Meeting 2012, Atlanta, GA, March 31-April 3, 2012.
490. *Sparse Linear Algebra on an SSD-equipped Testbed*, H.M. Aktulga, CRD All-Hands Meeting, LBNL, April, 2012.
491. *Information content of a nuclear observable and systematic and statistical errors of nuclear DFT*, W. Nazarewicz, Inter-collaboration meeting, CEA Saclay, France, April 10-11, 2012.
492. *Understanding Nuclei from First Principles*, P. Navratil, Department of Physics, Simon Fraser University, April 13, 2012.
493. *Nuclear Physics -- Bridging from Quarks to the Cosmos*, J.P. Vary, Department of Physics, Colloquium, Brookhaven National Laboratory, Upton, LI, NY, April 17, 2012.
494. *The limits of the nuclear landscape*, W. Nazarewicz, Physics Colloquium, University of Massachusetts, Amherst, April 18, 2012.

495. *Toward a model-independent approach to nuclear structure*, T. Papenbrock, Theory Seminar, National Superconducting Cyclotron Laboratory at Michigan State University, April 24, 2012.
496. *Towards nuclear reactions with coupled-cluster theory*, G. Hagen, The Extreme Matter Physics of Nuclei: From Universal Properties to Neutron-Rich Extremes, EMMI, GSI, Darmstadt, Germany, April 26, 2012.
497. *Science of rare isotopes: connecting nuclei with the universe*, W. Nazarewicz, Physics Colloquium, Ohio University, Athens, OH, April 27, 2012.
498. *Neutron-rich isotopes of oxygen and calcium*, T. Papenbrock, The Extreme Matter Physics of Nuclei: From Universal Properties to Neutron-Rich Extremes, Darmstadt, Germany, April 30-May 4 2012.
499. *Ab initio nuclear structure and reactions - perspectives and challenges*, J.P. Vary, Theory of Nuclear Physics Related to the RI Facilities Workshop, Institute of Basic Sciences, Daejeon, Korea, May 11-12, 2012.
500. *Theory, a Summary*, W. Nazarewicz, FUSHE 2012 – ENSAR-ECOS Workshop on FUture SuperHeavy Element Strategy, Erbismühle – Weilrod, Germany, May 13-16, 2012.
501. *Information content of a new observable and systematic and statistical errors of nuclear DFT*, W. Nazarewicz, physics seminar, Technische Universität Darmstadt, Germany, May 18, 2012.
502. *Theoretical Nuclear Structure (4 lectures)*, T. Papenbrock, Nuclear Structure Week, TU Darmstadt, Germany, May 21-24, 2012.
503. *Ab initio calculations of light-ion fusion reactions*, S. Quaglioni, JLab Theory Seminar, May 21, 2012.
504. *From QCD to ab initio nuclear structure with point nucleons and back again*, J.P. Vary, Thomas Jefferson Laboratory, May 25, 2012.
505. *Towards nuclear reactions with coupled-cluster theory*, G. Hagen, The 11'th International Conference on Nucleon-Nucleus Collisions, San Antonio TX, May 27-June 1, 2012.
506. *Finite-Size Instabilities in Odd-Mass Nuclei*, N. Schunck, Linear Response Theory: from infinite nuclear matter to finite nuclei, Espace de Structure Nucleaire Theorique, Saclay, May 30, 2012.
507. *Understanding Nuclei from First Principles*, P. Navratil, Eleventh Conference on the Intersections of Particle and Nuclear Physics CIPANP 2012, St. Petersburg, FL, June 2, 2012.
508. *Real-time vortex generation and dynamics in a time-dependent density functional theory approach*, A. Bulgac, CompStar2012 -the physics and astrophysics of compact stars, Tahiti, June 4-8, 2012.
509. *Towards nuclear reactions with coupled-cluster theory*, G. Hagen, Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics , New Orleans, Louisiana, June 4-7, 2012.
510. *Large-scale ab initio CI calculations for light nuclei*, P. Maris, Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics , New Orleans, Louisiana, June 4-7, 2012.
511. *A practical guide to accelerating nuclear structure calculations*, H. Nam, Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics , New Orleans, Louisiana, June 4-7, 2012.

512. *Nuclear structure approaches for the 21st century*, W. Nazarewicz, Conference on Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics, New Orleans, Louisiana, June 4-7, 2012.
513. *Toward model-independent nuclear structure computations*, T. Papenbrock, Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics , New Orleans, Louisiana, June 4-7, 2012.
514. *Nuclear Quantum Monte Carlo*, S. Pieper, Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics , New Orleans, Louisiana, June 4-7, 2012.
515. *Nuclear structure and dynamics in a unified approach*, I. Stetcu, Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics , New Orleans, Louisiana, June 4-7, 2012.
516. *Ab initio no-core solutions for nuclear structure - perspectives and challenges*, J.P. Vary, Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics , New Orleans, Louisiana, June 4-7, 2012.
517. *Atomic Nuclei: Many-Body Open Quantum Systems*, W. Nazarewicz, Nobel Symposium NS 152 - Physics with Radioactive Beams, Gothenburg, Sweden, June 10-15, 2012.
518. *Ab initio calculations of light-ion reactions*, P. Navratil, 13th INTERNATIONAL CONFERENCE ON NUCLEAR REACTION MECHANISMS, Varenna, Italy, June 11-15, 2012.
519. *From QCD to ab initio nuclear structure with point nucleons and back again*, J.P. Vary, Institute for Nuclear Physics, Moscow State University, June 15, 2012.
520. *Ab initio nuclear structure - recent developments*, J.P. Vary, Nuclear Theory in the Supercomputing Era Conference, Pacific National University (PNU) in Khabarovsk, Russia, June 18 - 22, 2012.
521. *New perspectives on the atomic nucleus*, J.P. Vary, Public Lecture at Pacific National University, Khabarovsk, Russia, June 19, 2012.
522. *Low-Energy Multipole Strength and Fundamental Physics*, J. Engel, invited talk at ECT* workshop on "The Nuclear Dipole Polarizability and its Impact on Nuclear Structure and Astrophysics", June 21, 2012.
523. *The Double Beta Decay: Theoretical Challenges*, M. Horoi, International Summer School of Physics", Sinaia, Romania, June 24 – July 7, 2012.
524. *Ab initio calculations of light-ion reactions*, P. Navratil, Workshop on "Electron-Nucleus Scattering XII", Elba, Italy, June 25-29, 2012.

1. VII. UNEDF BUDGET YEARS 1-5 SUMMARY TABLE

The UNEDF budget for Years 1-5 is shown below, together with the list of participating institutions and PIs. Other senior investigators were: Wiringa, Sarich, and Wild (ANL); Kawano and Möller (LANL), Hagen (ORNL); Escher, Quaglioni, Schunck, and Thompson (LLNL); Bogner (MSU); Papenbrock and Stoitsov (UTK); and Bertsch (UW).

UNEDF Budget

Institution-PI	Year-1	Year-2	Year-3	Year-4	Year-5
Argonne NL Pieper	133	133	133	133	133
Los Alamos NL Carlson	232	239	239	239	239
Livermore NL Ormand	420	440	440	440	440
Oak Ridge NL Arbanas	31	62	62	62	62
Subtotal NL	**816**	**874**	**874**	**874**	**874**
Central Mich. U Horoi	83	49	90	90	90
Iowa State U Vary	136	136	136	136	136
Michigan State Brown	99	74	100	130	130
Ohio State U Furnstahl	86	100	100	88	100
San Diego SU Johnson	43	34	55	55	55
TAMU-C Bertulani	0	46.75	48	48	48
U North Carolina Engel	83	63	83	83	83
U Tennessee Nazarewicz	295	248	259	260	260
U Washington Bulgac	359	375.25	255	236	224
Subtotal UNI	**1184**	**1126**	**1126**	**1126**	**1126**
Subtotal (physics)	**2000**	**2000**	**2000**	**2000**	**2000**
Argonne NL Lusk	325	325	325	325	325
Ames NL Sosonkina	100	100	100	100	100
Berkeley NL Ng	175	175	175	175	175
Oak Ridge NL Fann	400	400	400	200	200
Pacific Northwest NL Roche				200	200
Subtotal CS/AM	**1000**	**1000**	**1000**	**1000**	**1000**

VIII. UNEDF CHARTER

During Year-2 of UNEDF, a number of organizational changes took place. A charter was developed and adopted, and the UNEDF Council was expanded to include physicists and computer scientists/applied mathematicians so as to effectively represent the multiple sub-projects and institutional stakeholders.

The charter below was accepted on August 14, 2008, by a ratification vote of the UNEDF voting members.

1. **Purpose of the Charter**
   This Charter establishes the functions, organizational structure, and responsibilities within the UNEDF Project.

2. **Project Director**
   The Director is appointed by the Agencies and has the overall responsibility for the UNEDF project. He/she is the primary point of contact with the Agencies.

3. **Co-Directors**
   The Co-Directors are nominated by the Project Director and approved by the Agencies. Their principal responsibility is to assist the Project Director with project management.

4. **UNEDF Council**
   The Council consists of the Director and co-Directors and additional members drawn from the Collaboration. The additional members are nominated by the Director and co-Directors and approved by the voting members (see **5.**) of the Collaboration. The Council represents different subfields and institutions of UNEDF science. The Council oversees project integration and coordination among the subfields. It coordinates the project timetables and deliverables. It also makes recommendations to DOE regarding the scientific direction of the project and its budget.

5. **Voting Members**
   The UNDEF collaboration members who are Principal Investigators (PIs), co-PIs, or senior investigators are voting members.

6. **Procedures**
   a. The Council will conduct its business in a democratic manner with one vote per Council member.
   b. Vacancies on the Council must be replaced immediately.
   c. The Council shall meet monthly by conference calls, or more often as needed. The conference calls are organized by the Project Director. The agenda for each conference call will be posted on UNEDF.org at least 3 business days prior to the call to enable consultations between voting members and Council members as needed. Minutes of the Council meetings are to be posted on UNEDF.org. Draft minutes are to be placed on UNEDF.org within one week following the conference call. Final minutes are posted within one day of the vote to accept the minutes at the following conference call.

d. To make the progress transparent and to integrate science across tasks, reports on the progress in UNEDF subfields, presented at the Council meetings, are to be posted on UNEDF.org.
e. A voting member may propose agenda items for Council meetings by contacting any Council member.
f. Any voting member may attend a Council meeting at the invitation of a Council member.
g. Certain Council meetings may be declared "open" for any voting member to attend without specific invitation. These will be indicated when the agenda is posted on the web site.

7. NERSC Computational Resources

To help assure adequate computing resources, a NERSC coordinator will be appointed by the Director. The task is to obtain allocations from NERSC, maintain a NERSC repository, and distribute allotments as needed for UNEDF computation.

8. Website

The collaboration website, UNEDF.org, shall serve as a communication tool and as an outreach window into the UNEDF science. It is supervised by a member of UNEDF appointed by the Council and maintained by a communication coordinator.

9. Annual Meeting

The UNEDF collaboration meeting is to be held annually. It is organized by the UNEDF Director and co-Directors or designated collaboration members. The reports presented during the meeting summarize scientific progress of the Project and serve as a basic input to the Continuation Annual Report.

10. **Foreign Collaborators**

UNEDF collaborates closely with a number of foreign efforts and individual scientists sharing similar scientific goals. Such collaborations include joint software developments and benchmarking. Representatives of Foreign Collaborating Projects are invited to attend the UNEDF annual meeting. The license status of joint software developments is subject to **12b**.

11. Continuation Annual Report

The Continuation Annual Report is put together by the Project Director and co-Directors. It contains i) scientific progress, ii) new work plans, and iii) proposed budgets for the following year.

12. Deliverables

The main deliverables of UNEDF are publications, reports, conference presentations, and computer codes.

a. Publications and Talks: All deliverables should contain the acknowledgement to the appropriate DOE Grant number(s).
b. Computer codes: The final versions of computer codes (i.e. meeting all benchmarks required) developed under UNEDF are to be released as open source software, using

one of the standard open source licenses (GNU, BSD-like, etc.) to ensure that the community as a whole benefits from the software developed under UNEDF funding. Releases are expected to contain documentation, installation instructions for each platform on which the code runs, and input and output files for test cases.

13. Amendments

a. Amendments to this charter must originate from the UNEDF Council or from a group of five voting members sending statements of support to the Council.
b. Amendments to the charter may be adopted by a vote of voting members (plurality required) or unanimous vote of the Council. If the amendment passes by Council vote, a group of ten at-large voting members may request a vote by the entire Collaboration and the amendment in question is suspended until the vote can be held. Upon notification of the passage of the amendment, all voting members will have two weeks to request the vote.

14. Ratification

This Charter shall be accepted as a document providing guidance and rules of operation for the UNEDF Collaboration following a ratification vote in which 2/3 voting members favor adoption of the charter. The UNEDF Council shall administer the ratification vote.

IX. YEAR-5 REPORT

The UNEDF project completed with another successful year. As documented in this report, a number of crucial milestones were reached and important scientific deliverables produced. There was also other excellent news. The DOE INCITE program once again awarded a large number of hours for UNEDF computational nuclear physics projects. The UNEDF project was featured in numerous articles (referenced on unedf.org) including Nuclear Physics News, NNSA highlights, ScienceNewsline, MSNBC.com, Live Science, Supercomputing Online, New Scientist, PhysOrg.com, and highlight articles at Oak Ridge National Lab, Argonne National Lab, and the DOE Office of Science.

AB-INITIO STRUCTURE AND REACTIONS

The primary goal of the ab-initio UNEDF effort is to constrain the nuclear density functional by performing microscopic calculations based on realistic interactions. Ab-initio theory for nuclear interactions and structure can be used to connect directly from high-momentum scales of QCD and high-momentum scale interactions to the lower momentum scales where the nuclear energy density functional operates. Nuclei can be studied in external potentials and periodic boundary conditions to connect to lattice QCD and to extract information on the three-nucleon force. Ab-initio calculations provide direct guidance to density functionals through the introduction of external fields. Medium-mass nuclei, more directly applicable to density-functional techniques, are particularly valuable in this regard. These methods can also probe the density functionals at the extreme isospin limit by studying pure neutron systems in external fields. Finally, ab-initio calculations are critical in their own right to understand processes in light nuclear systems, particularly light-ion scattering and reactions. Figure 11 shows where ab-initio structure calculations fit into the overall UNEDF strategy.

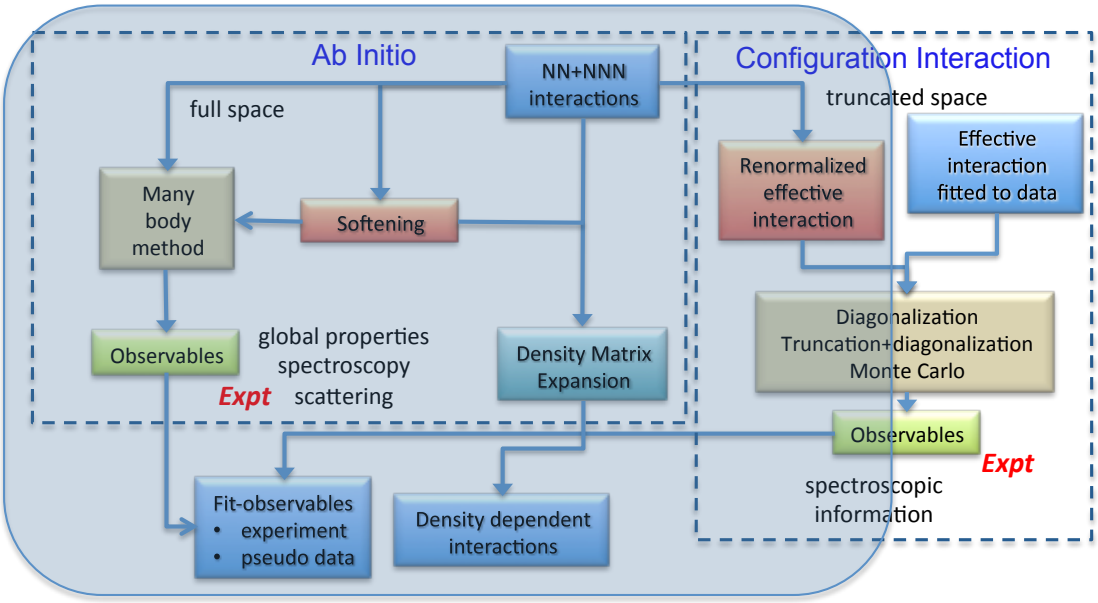

Figure 11: Ab-initio Structure in the UNEDF strategy diagram.

Ab-Initio Calculations of Light Nuclei

The UNEDF project has made important progress in the ab-initio calculation of light nuclei and their reactions. Quantum Monte Carlo, Configuration Interaction and Coupled Cluster methods start with microscopic two- and three-nucleon interactions and obtain physical quantities including spectra, transition rates and cross sections. The close coupling of computer scientists, applied mathematicians and physicists have been extremely valuable in this regard.

At the start of the UNEDF project, ab-initio calculations with realistic interactions had provided an excellent description of the spectra of the lightest nuclei, up to A=10. Over the course of the project, we have demonstrated that these same interactions, combined with consistent one- and two-nucleon current operators, can describe a much richer set of observables, including magnetic moments, form factors, asymptotic normalizations, and decay rates.

Calculations of many important observables in light nuclei have continued during the UNEDF project. New methods have been developed to calculate quantities that depend upon the long-distance behavior of the state. Calculations in ab initio no-core configuration interaction (NCCI) approaches, such as the no-core shell model (NCSM) or no-core full configuration (NCFC) methods, have conventionally been carried out using the harmonic-oscillator many-body basis. However, the rapid falloff (Gaussian asymptotics) of the oscillator functions at large radius makes them poorly suited for the description of the asymptotic properties of the nuclear wave function. During the past year, we have established the foundations for carrying out NCCI calculations with an alternative many-body basis built from Coulomb-Sturmian functions, and have presented results for ^{6}Li.

No-core configuration interaction calculations have also been performed for the Lithium isotopes with A=6,7,8. Calculations of observables including radii, moments, transition probabilities, and magnetic moments have been obtained and compared to experiment. In addition, benchmark calculations of 7 light nuclei using a variety of methods have been performed using the JISP16 nucleon-nucleon interaction.

Our previous work with the no core full configuration (NCFC) method indicates a simple exponential extrapolation of the ground state energies was adequate for that particular observable but a more extensive investigation is needed to isolate the convergence rates of operators sensitive to long range physics. Working in collaboration with Sid Coon and Bira van Kolck (University of Arizona) we are carrying out an investigation of the infrared (IR) and ultraviolet (UV) behavior of a set of observables in the *ab initio* NCFC approach. The first paper on this work has been accepted for publication by Physical Review C.

In order to obtain quantitative predictions for some electro-weak observables, in particular magnetic moments, two-nucleon currents must be included. Many of these had been qualitatively understood in terms of the simple shell model previously, but in specific cases (e.g., ^{9}Li) experiment and theory did not agree. In Figure 12, the magnetic moments including one- and two-nucleon currents are compared with experiment. The experimental results are in black, the single-nucleon currents alone in blue, and the complete calculation in red. The Quantum Monte Carlo calculations, combined with the realistic two-nucleon current operators, quantitatively reproduce the magnetic moments of all these nuclei. In some cases, including ^{9}Be, the two-nucleon currents are particularly important. The ratios of calculated to experimental magnetic moments are shown at right.

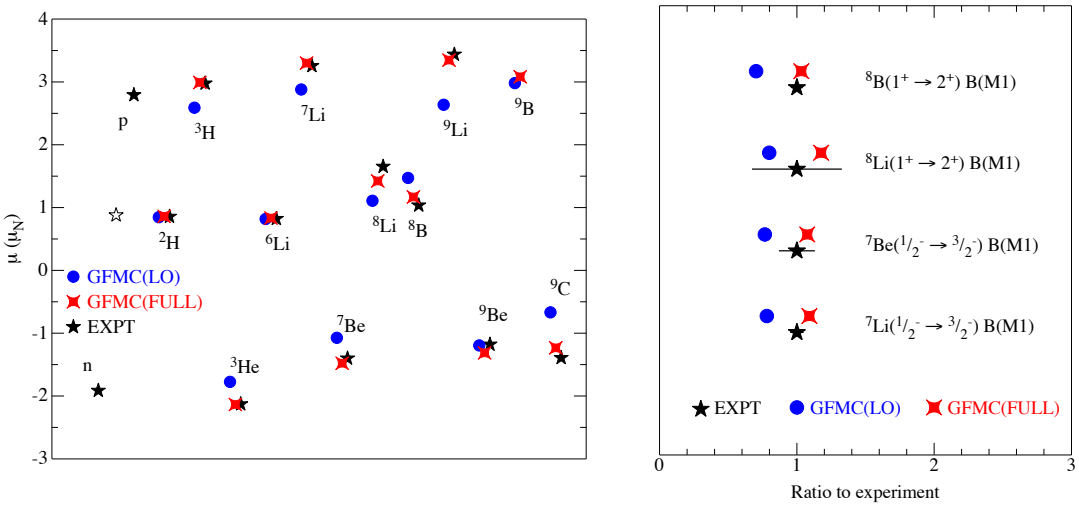

Figure 12: Calculated versus experimental magnetic moments of light nuclei

An important theme developed during the UNEDF project is the increasing attention paid to three-nucleon interactions. These are critically important to obtain the spectra of light nuclei. They are also critical for understanding the weak decays of ^{14}C, an important highlight of the UNEDF project. As shown below, three-nucleon interactions also play a critical role in understanding the binding of neutron-rich nuclei and the neutron star matter.

The decay of ^{14}C to ^{14}N is the basis of carbon dating, as the lifetime of ^{14}C is abnormally large. No-core shell model calculations of the structure of these A=14 nuclei demonstrate that the three-nucleon interaction is critical to obtaining this long lifetime. The decay matrix element as a function of the number of included shells is shown in Figure 13. With two-nucleon forces alone, the matrix element is large and the decay would occur quite rapidly. The three-nucleon interaction induces large cancellations with the p-shell between different contributions to the beta decay, reducing the matrix element by an order of magnitude.

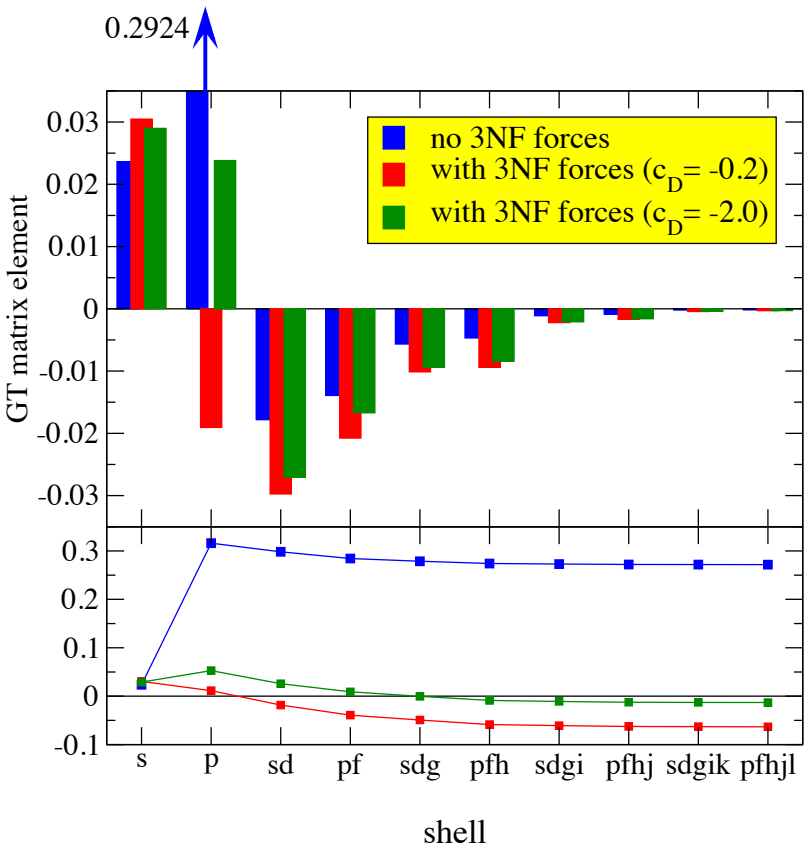

Figure 13: Contributions (top) and cumulative sum (bottom) to the matrix element describing ^{14}C beta decay

During the past year new methods have also been developed to calculate the asymptotic normalizations of light nuclei. These overlaps describe the amplitude of a nucleus being pulled apart into two clusters with specific quantum numbers, and are extremely relevant to studies of low-energy reactions. These asymptotic normalizations are well-defined observables that can be directly compared with experiment. Results for a large number of asymptotic normalizations are presented in Figure 14, scaled to the experimentally observed values.

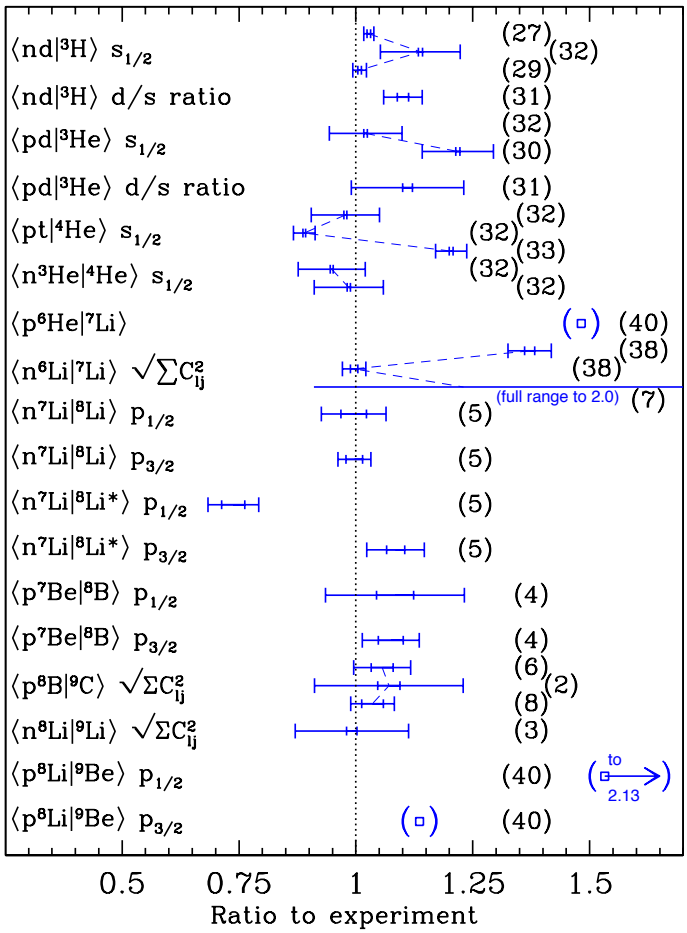

Figure 14: Ratio of calculated to experimental asymptotic normalizations in light nuclei

Some of the most difficult calculations of light nuclei attempted during the UNEDF project were to understand the ground-state and low-lying 0^+ excitation ('Hoyle state') of ^{12}C. The Hoyle state is very close to the threshold of breaking up ^{12}C into three alpha particles, making its description in standard mean-field or shell model approaches quite difficult. Quantum Monte Carlo methods are quite flexible in describing the clustering of light nuclei, having been previously been used to explore the structure of ^{8}Be, which is near the threshold of breakup into two alpha particles.

In order to perform these calculations, a new software library was developed that could deal with a very large number of loosely coupled processes. These types of problems are ubiquitous in large-scale computing, and Green's function Monte Carlo provides a very valuable test bed. This algorithm has a very large number of branching random walks; the walks are independent but the branching requires an efficient load-balancing mechanism particularly for the largest calculations like ^{12}C.

The Asynchronous Dynamic Load Balancing Library (ADLB) was created to address these kinds of problems. Figure 15 shows the scaling progress achieved with ADLB on GFMC codes over the course of the UNEDF project. This progress was a direct result of close coupling between computer scientists and physicists working together on ADLB and GFMC. In some cases attempts at new architectures for ADLB did not succeed, but recently excellent progress has been achieved

on the new BG/Q machine at ANL. Not all scaling results can be shown yet, but in Figure 16 we show scaling of the Open-MP part of the code on a node of BG/Q. Very good scaling is apparent up to 70 threads.

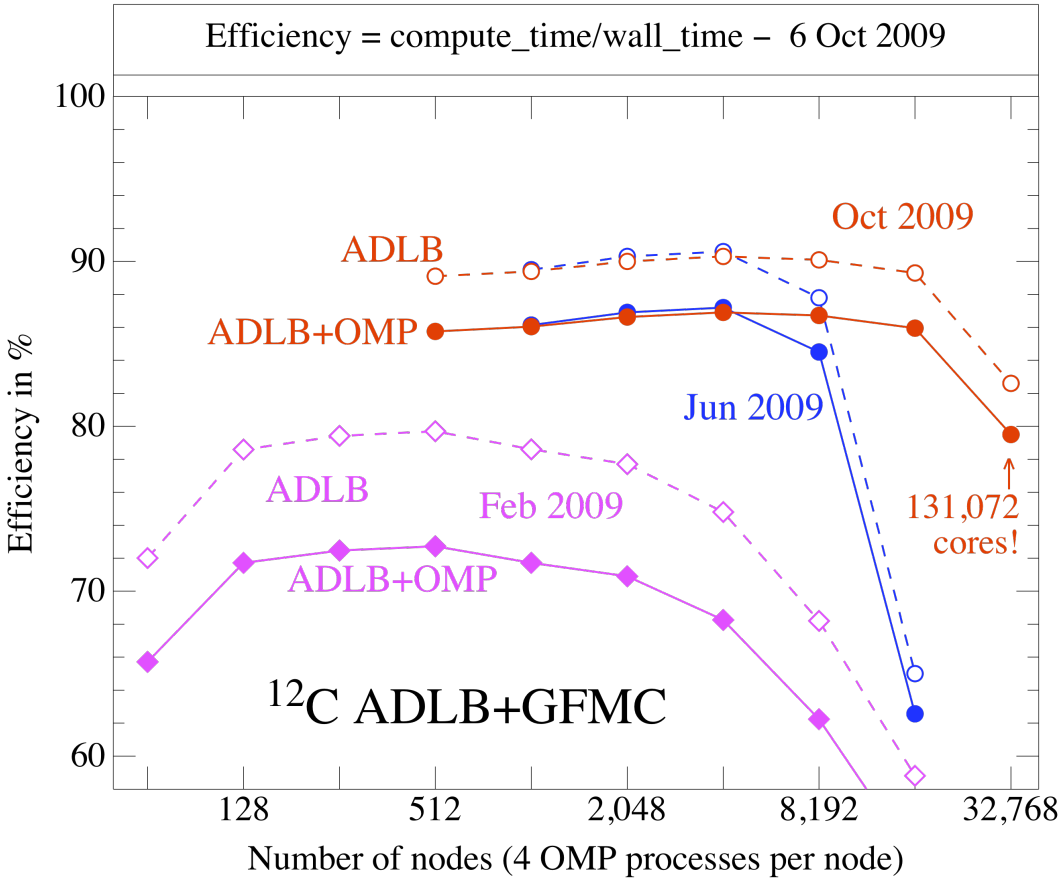

Figure 15: Scaling of GFMC and ADLB on Blue Gene P during UNEDF

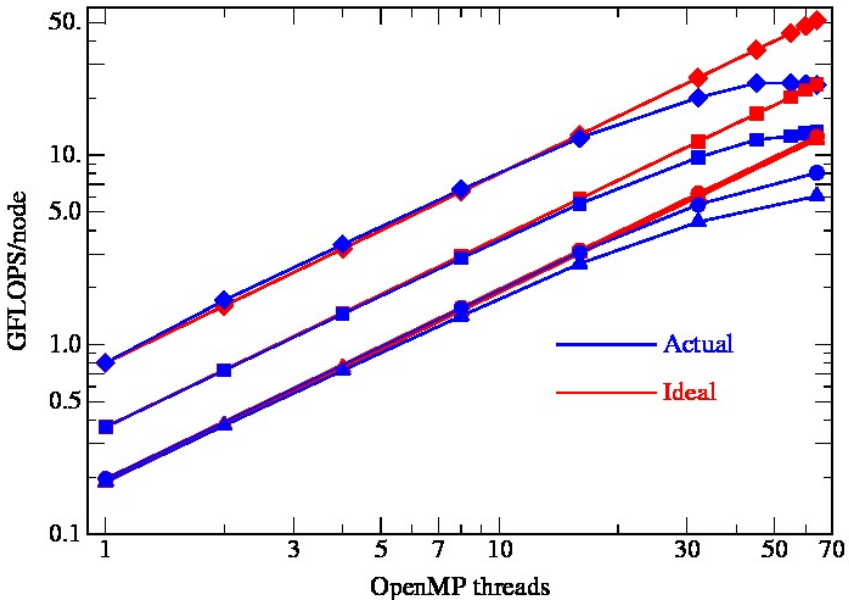

Figure 16: Scaling on one node of Blue Gene Q

The ground-state calculations have been completed and they describe both the energy and the observed ground-state charge density of ^{12}C. In order to obtain this agreement, it is necessary to incorporate both the traditional shell model picture of light nuclei and specific three-alpha components into the initial trial function. We find that the same Hamiltonian that predicts the spectra and other observables described above also correctly predicts the charge density of the ground state. Figure 17 compares the extracted point proton density (solid line) with the QMC calculations.

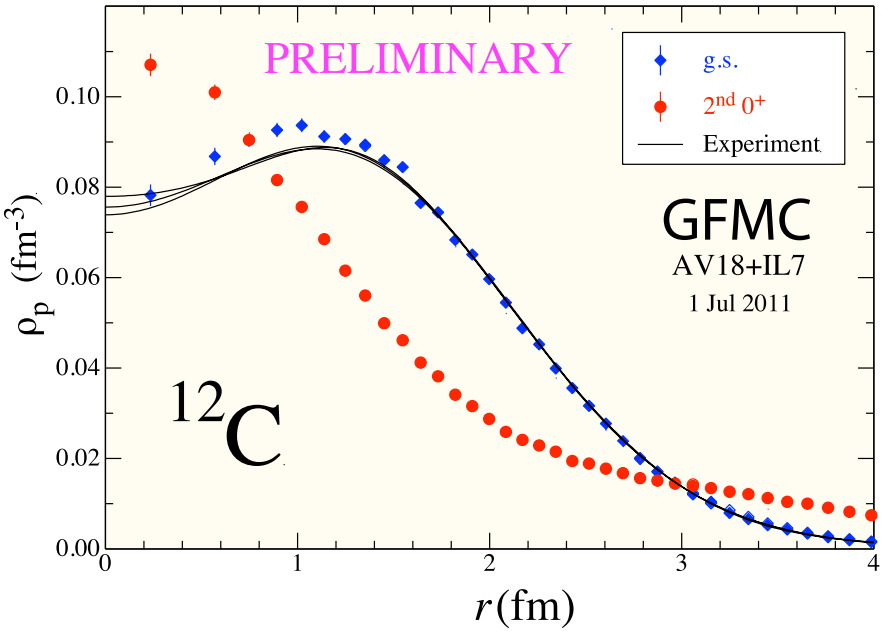

Figure 17: Proton density of the ground state and Hoyle state of ^{12}C

The Hoyle state is more difficult to treat because of its very extended nature. In these calculations the Hoyle state has a peak in the point proton density at the origin, in contrast to the small dip in the ground state. These differences, along with the measured transition form factors, provide further clues to the structure of the Hoyle state.

We have performed several calculations of both the ground and excited states using different initial trial states. If the calculations are converged the energy and other observables should be nearly independent of this trial state. The convergence of the energy with imaginary time is shown in Figure 18. Both the Hoyle and the ground state are fairly independent of the choice of initial state, and the QMC results describe the very low energy of the excited state.

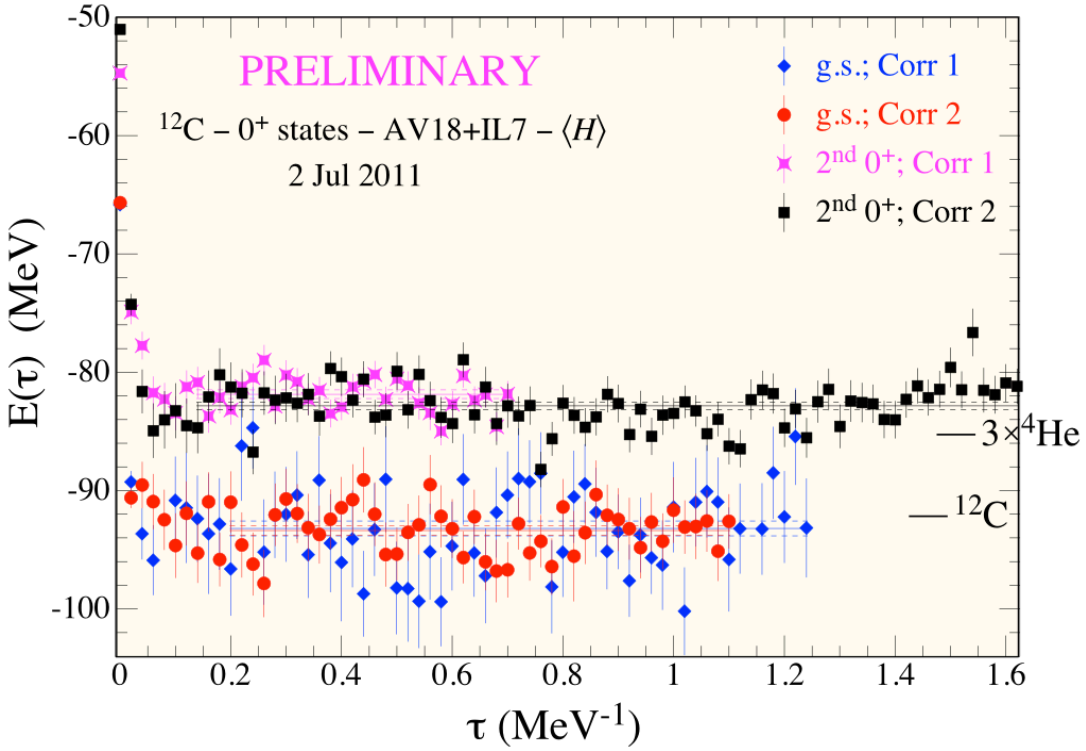

Figure 18: Convergence of GFMC calculations of the ground state (lower curves) and the excited 0+ state (upper curves) for different initial states.

The ground- and excited-states of ^{12}C have also been studied in a lattice Quantum Monte Carlo approach. They also found a low-lying 0+ (Hoyle) state, and a low-lying 2+ excited state as well. The approaches are complementary, as the lattice calculations use an alternative nuclear interaction. The present calculations use a large lattice spacing of ~ 2 fm and propagate for 0.1 MeV^{-1}, yielding somewhat larger uncertainties in energy, radii and form factors. They have demonstrated that they can describe the entire low-lying structure of ^{12}C with these low-momentum chiral interactions.

Reactions in light nuclei

Some of the most important advances in the UNEDF project have come in the studies of reactions in light nuclei. Previously studies of nuclear reactions in the lightest nuclei have mostly been

undertaken in simple models not directly connected to the ab-initio calculations of nuclear structure and decays described above. During the UNEDF project, R-matrix methods have been coupled to CI calculations to describe reactions in a host of light nuclei. The direct connection to ab-initio calculations with realistic interactions give these methods much more predictive power than with R-matrix or other simple models alone.

Low-energy reactions in light nuclei are important in several contexts, including astrophysics such as big-bang nucleosynthesis and stellar neutrinos. They are also critical in nuclear applications relevant to NNSA and the National Ignition Facility (NIF). In Figure 19 we show experiments, evaluations, and calculations of n-^{3}H scattering at 14 MeV. The experimental results have significant scatter. The RGM/NCSM calculations removed a great deal of uncertainty in this reaction, enabling a better understanding of NIF diagnostics.

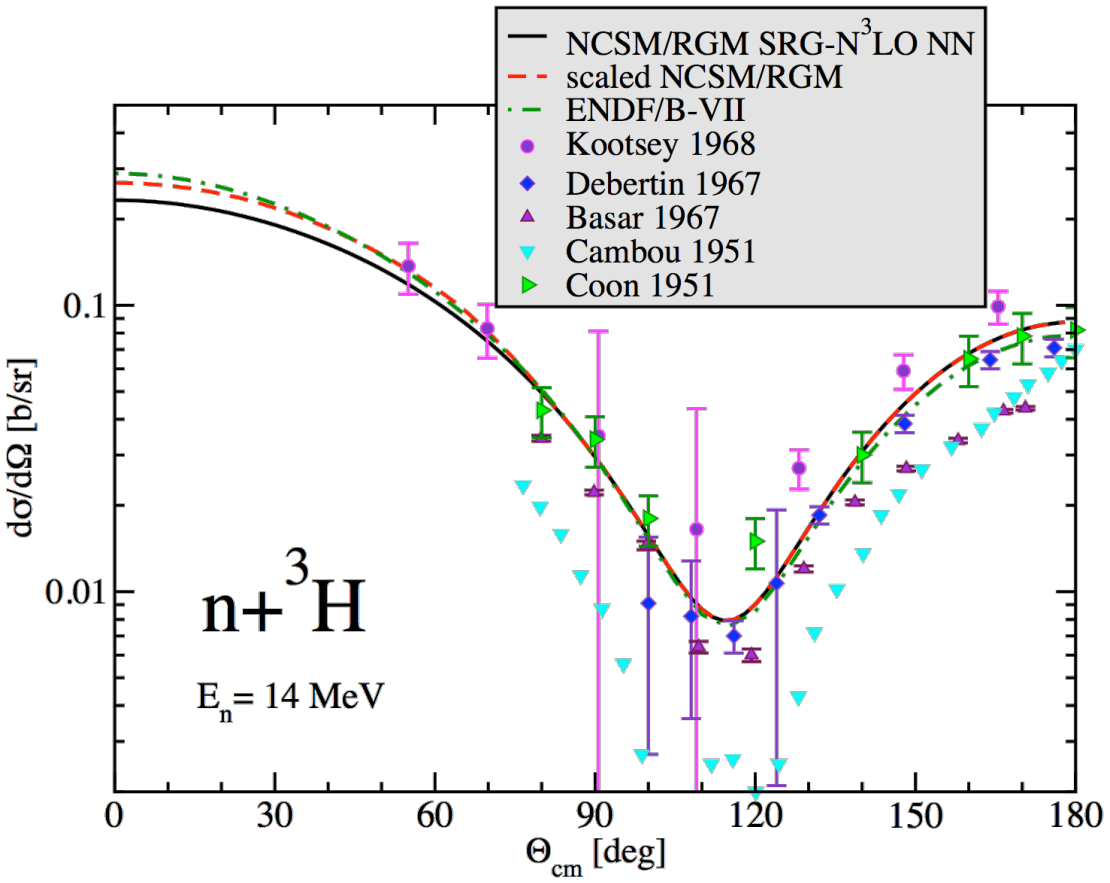

Figure 19: Differential cross section for n+3H, experiments (points), data libraries (green dot-dash line) and theory (back and red dashed curves).

The RGM/NCSM approach has been used to study a variety of important reactions, including inelastic reactions like d+^{3}He -> p + ^{4}He. The astrophysical S-factor, a coulomb-corrected representation of the cross-section is shown in Figure 20 for a variety of experiments. The different curves represent calculations with an increasing number of channels. The calculations with a large number of channels do a very good job of describing the data in the resonance region around 200 keV. Even more advanced calculations including three-nucleon interactions, and three-cluster breakup, are underway.

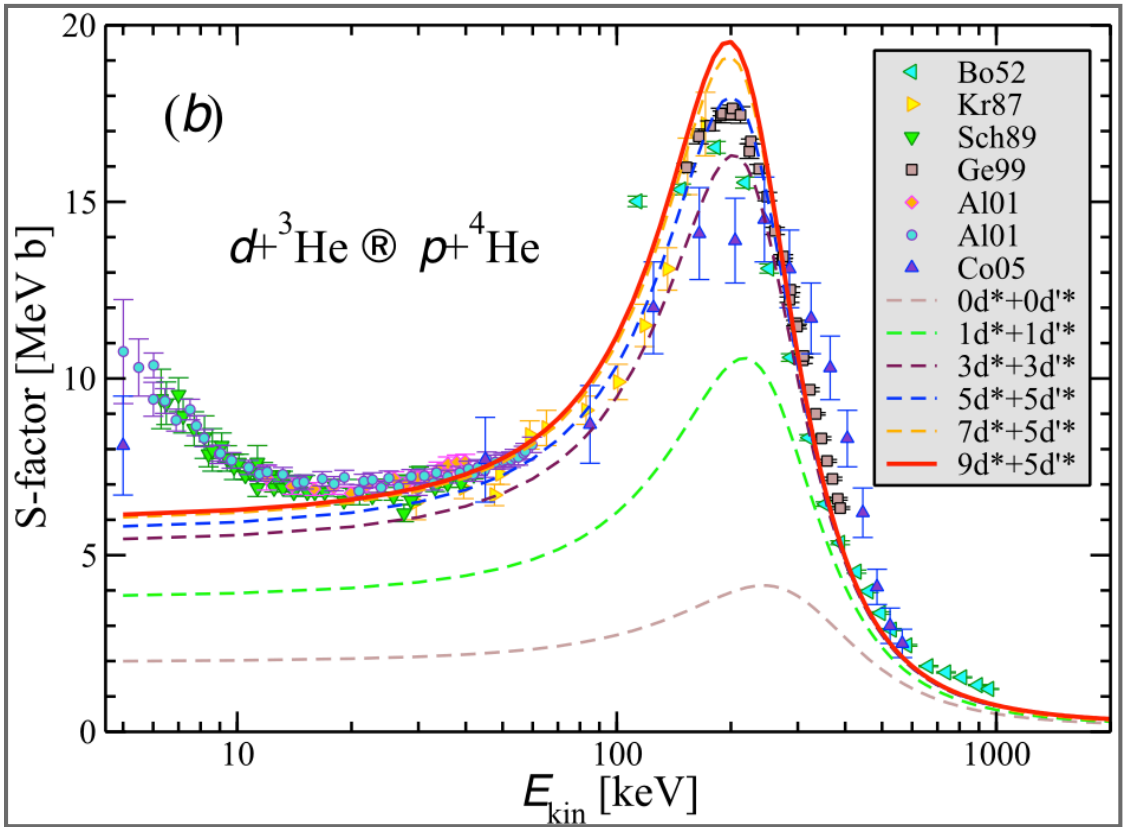

Figure 20: S-factor for the d+^{3}He -> p + ^{4}He reaction versus energy. Experimental data are points with error bars, lines indicate calculations with increasing numbers of channels.

Ab-Initio approaches to medium-mass nuclei

At the start of the UNEDF project, ab-initio calculations were mostly limited to mass A~10. During the course of this project, though, additional methods advanced rapidly to enable us to study medium mass nuclei directly using realistic interactions. The coupled cluster approach, originally developed in nuclear physics, now commonly employed in atomic and molecular systems, has taken a firm foothold in nuclear physics again.

One very important issue in nuclear physics is the structure and decays of very neutron-rich nuclei. Neutron-rich nuclei are critical to r-process nucleosynthesis thought to take place in core-collapse supernovae or neutron star mergers, and are a main point of emphasis for the new Facility for Rare Isotope Beams (FRIB) under construction at Michigan State University.

Using two-nucleon interactions alone, the line of stability describing the boundary between bound and unbound nuclei can be wildly inaccurate. In addition, the ability to couple to the continuum is very critical to the properties of neutron-rich nuclei. During the past year, Coupled-Cluster methods have incorporated both a better treatment of the continuum and an effective three-nucleon interaction to do a much better job of describing the binding of the neutron-rich isotopes of Calcium (see Figure 21).

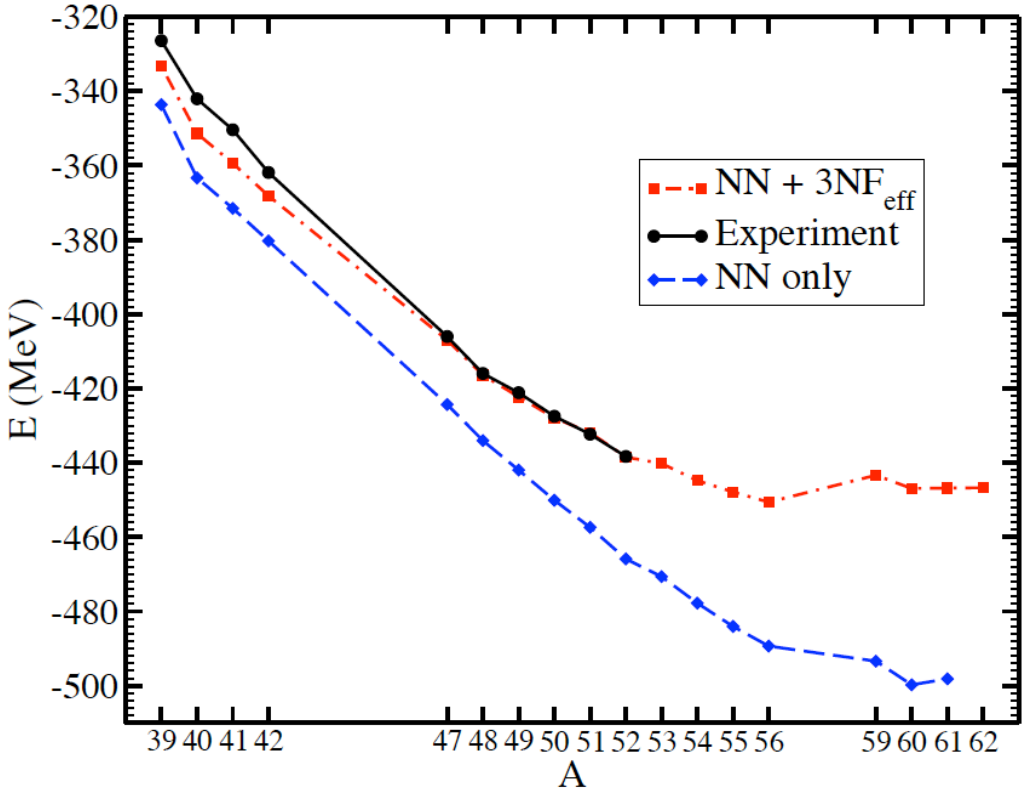

Figure 21: Energies of Calcium isotopes from coupled cluster calculations with NN interactions alone (blue) and with NNN interactions (red) compared to experiment (black)

The same three-nucleon interaction is critical in light nuclei, as describe above, and in neutron matter important for neutron stars. The UNEDF project has made significant progress in forming a more coherent picture of nucleonic matter across the entire nuclear chart.

Neutron matter EOS and inhomogeneous neutron matter

The UNEDF project made a concerted effort to tie ab-initio microscopic many-body theory to nuclear density functional theory used to calculate the properties of large neutron-rich nuclei. A major avenue for this connection is homogeneous and inhomogeneous neutron matter. During the course of the UNEDF project, we have refined the calculations of neutron matter at low- and moderate-densities, putting significant constraints on the equation of state (EOS) of neutron matter in the regime where the three-neutron interactions are modest. We have also calculated the $^1S_0$ pairing gap in neutron matter, and compared both the EOS and pairing gap to cold atoms where definitive experiments are available on these strongly-paired superfluids.

During the UNEDF project, we have performed the most accurate calculations of several of the universal parameters in cold atoms, including the Bertsch parameter and the contact describing the equation of state, as well as the pairing gap. During the past year, we have further developed the connection between cold atoms and neutron matter by including the effective range corrections in the calculations of dilute fermions. These terms can also be tested in cold atom experiments.

Figure 22 compares the equation of state for neutron matter and cold atoms, where the solid blue curve is a fit to the cold atom equation of state for zero effective range, and the dashed curve includes the gradient correction.

At higher densities, the equation of state becomes relevant for neutron stars, including the crust and at higher densities, the mass/radius relationship. The equation of state is also connected, through the symmetry energy and its derivative, to experimental observables including the dipole polarizability of lead and the neutron skin measured in the PREX experiment at Jefferson Lab. We have calculated the equation of state of neutron matter for a variety of three-nucleon interactions, in each case the parameters of the three-neutron interaction have been adjusted to produce a specific symmetry energy, or equivalently the energy of neutron matter at nuclear saturation density (see Figure 23). The shaded areas represent the error associated with uncertainties in the three-neutron interaction for specific values of the symmetry energy.

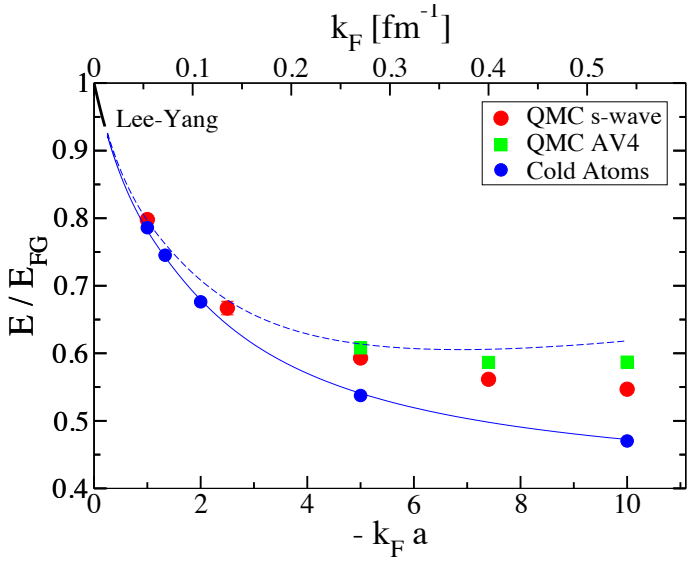

Figure 22: Equation of state for cold atoms and neutron matter at low density

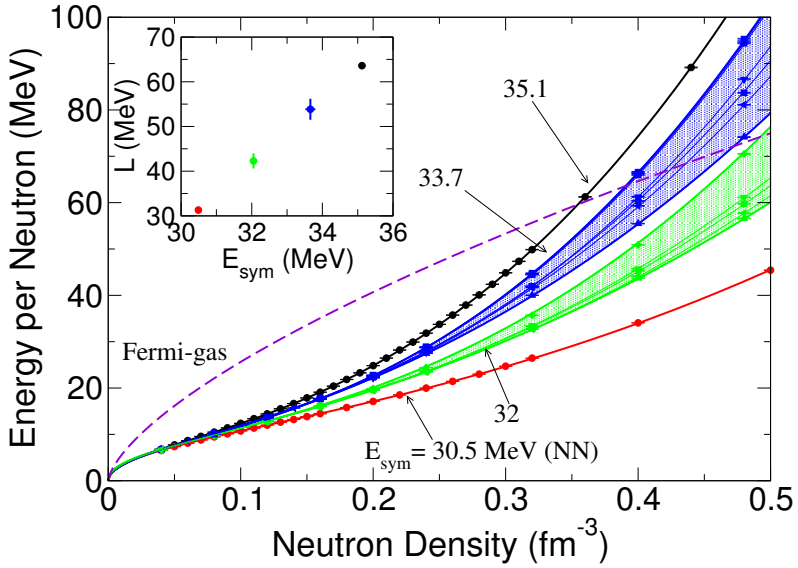

Figure 23: Equations of state for various models of nucleon-nucleon plus three-nucleon interactions with a given symmetry energy. The inset shows the implied relation between the symmetry energy at saturation density and its derivative.

The mass-radius relations obtained from these equations of state are shown in Figure 24. The two-neutron interaction alone does not allow for a two solar mass neutron star, as has been recently observed. The three-neutron interaction is required to give sufficient pressure to support a two solar mass neutron star. The blue and green bands below, with moderate values of the three-neutron repulsion, are consistent with both the two solar mass neutron star and constraints obtained through astrophysical observations.

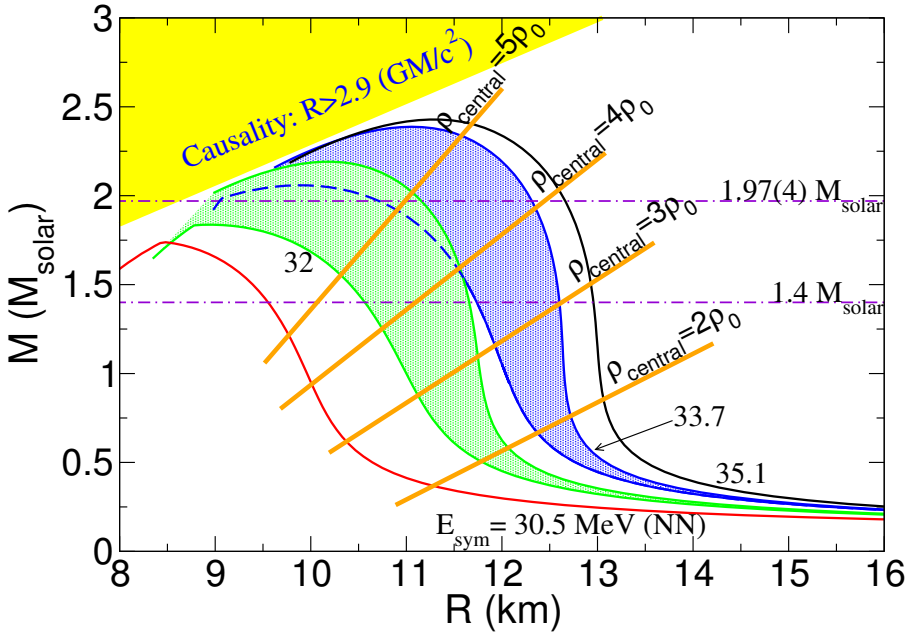

Figure 24: Mass/radius relations for the same equations of state. Orange bands indicate approximate values of the central density for a neutron star with a given mass.

The properties of inhomogeneous neutron matter are also critical to understand the properties of neutron-rich nuclei. In the UNEDF project we have spent significant effort studying systems of neutrons confined in various external fields. In order for neutron drops to provide a useful benchmark, we have to understand the uncertainties in the interactions and the uncertainties in the many-body methods employed. We have recently compared neutron drops confined in harmonic wells using a variety of interactions and many-body techniques. The results are summarized in Figure 25. The (compressed) vertical scale shows the energy scaled by the harmonic oscillator frequency and the number of particles to the 4/3rd power. The Thomas-Fermi (local density) approximation for such a system with an equation of state scaling like the density to the 2/3 would be a horizontal line. The NN and NNN interactions span a wide range, and include both repulsive (UIX) and attractive (IL7) three-neutron interactions. The microscopic results all lie within approximately 10% for up to approximately 30 particles, meaning that the uncertainties in methods and interactions are fairly modest. We have also completed calculations comparing shell closures, pairing, spin-orbit splitting, and radii for systems up to 40 neutrons.

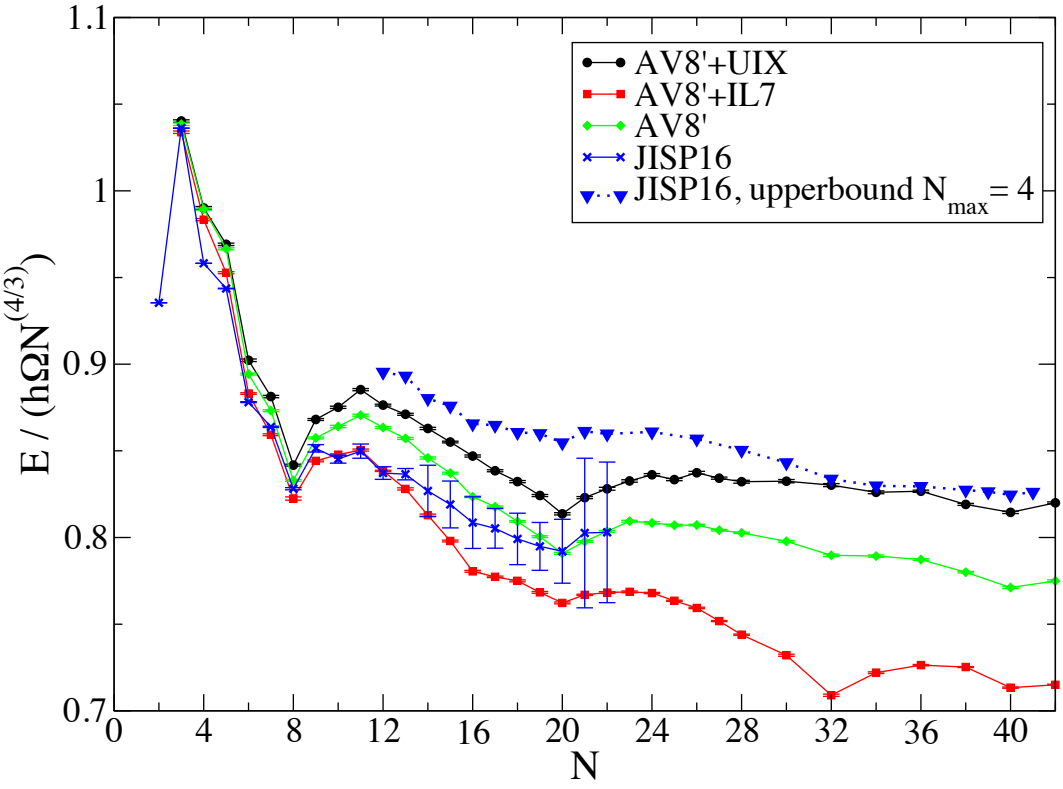

Figure 25: Scaled Energy for neutrons confined in a 10 MeV harmonic well

LEADERSHIP CLASS CONFIGURATION INTERACTION CODES

LCCI Project Overview

The project to develop a single environment for leadership class configuration interaction (LCCI) calculations emerged from a broad range of UNEDF planning activities conducted after UNEDF became operational. Through a sequence of several meetings during years 2 and 3 of UNEDF, we developed a white paper that outlined many of the key elements that were incorporated into the project. The white paper has been posted on the UNEDF website.

The LCCI project was officially launched as the sixth major component of UNEDF at the annual meeting in June 2009 and appears in our 2009 CPR with goals set for Year-4. After Year-4, additional goals were set for Year-5. The LCCI participants met two times per year during Years 3–5 of UNEDF, in addition to the UNEDF annual meeting, and summaries of these meetings are also available through the UNEDF website.

The overarching goals of the project were, broadly speaking:

1. To develop a leadership class configuration interaction code(s) leading to the capability of performing the configuration interaction (CI) calculations outlined in the DOE white paper: http://extremecomputing.labworks.org/nuclearphysics/report.stm;
2. To make these resources available to the broader community;
3. To develop a prototype database management system (DBMS) for large-scale production runs that documents the runs and their results for further use following original publication.

These LCCI goals have been achieved during Years 3-5, though much work remains to achieve all the aims of the original UNEDF white paper. It is noteworthy that the LCCI project, by virtue of maintaining forefront codes in operational condition for current research projects, enabled many of the physics accomplishments reported in other sections of the CPRs and this closeout report.

In order to put the LCCI project in context, we highlight in Figure 26 the areas of the UNEDF workflow where the LCCI project supports the main goals. Note that there are additional major codes of this domain outside the scope of LCCI – such as the GFMC and CC codes summarized elsewhere in this report.

The progress within the LCCI project has been accomplished through close collaborations between many physics, computer science and applied math groups within UNEDF. Participants at the working meetings included representatives of the groups at Ames Lab, ISU, LLNL, LBNL, MSU/WMU, and SDSU.

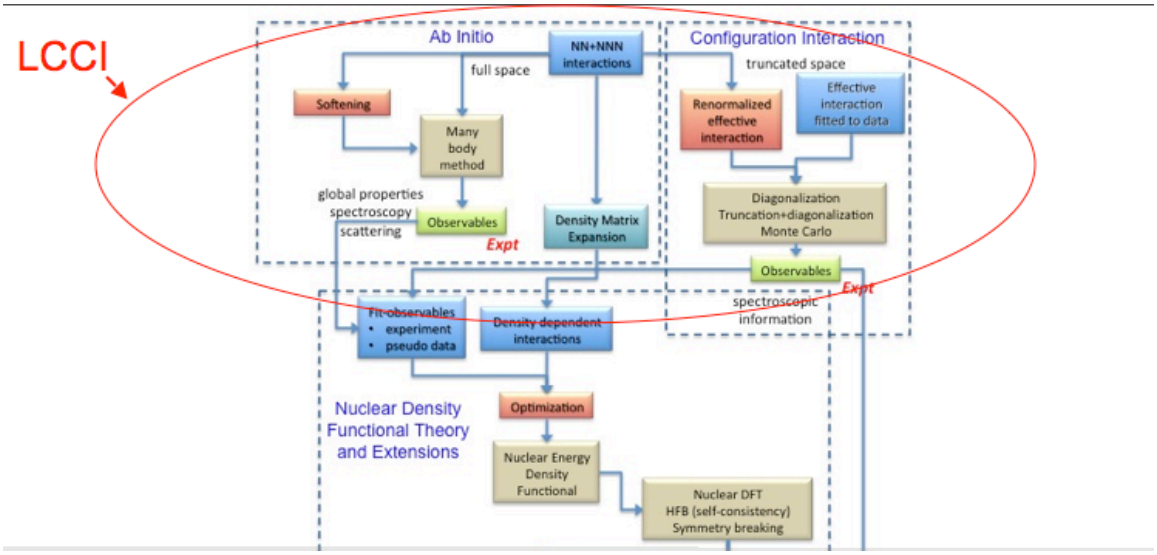

Figure 26: The UNEDF areas where the LCCI project shares the goals (region within the oval). The developed CI codes are made available to other researchers through the LCCI project along with sample scripts and test cases.

LCCI Code and Script Development

All LCCI codes, scripts and test cases have been deposited and updated on the UNEDF shared project space at NERSC. Table 1 provides a listing of the codes and the primary contact for additional information. Introductory materials are available in the main directory (/project/projectdirs/unedf/lcci). Source codes, sample scripts, a README file, and test outputs are available in subdirectories for each code.

Table 1: List of source codes deposited in LCCI directory at NERSC with scripts and test outputs. The primary contact and the most recent updates are indicated. Typically, updates under UNEDF occurred on 6-month cycles. Previous versions are retained for archival reference.

Code	Contact	Last Update
BIGSTICK	Calvin Johnson	June 2011
MFDn	Pieter Maris	September 2012
NuShellX	Mihai Horoi	March 2011
trdens	Petr Navratil	April 2010
Ncsmv2eff	Petr Navratil	July 2011
LCCI-wrapper	Pieter Maris/Calvin Johnson	July 2011

The smooth interconnectivity of these codes was still under development at the completion of UNEDF. The achieved workflows between codes are indicated in Figure 27 and Figure 28. Figure 27 shows workflows for runs using MFDn or BIGSTICK that may include three-nucleon interactions. Figure 28 shows workflow for runs that are valence model space runs using NuShellX.

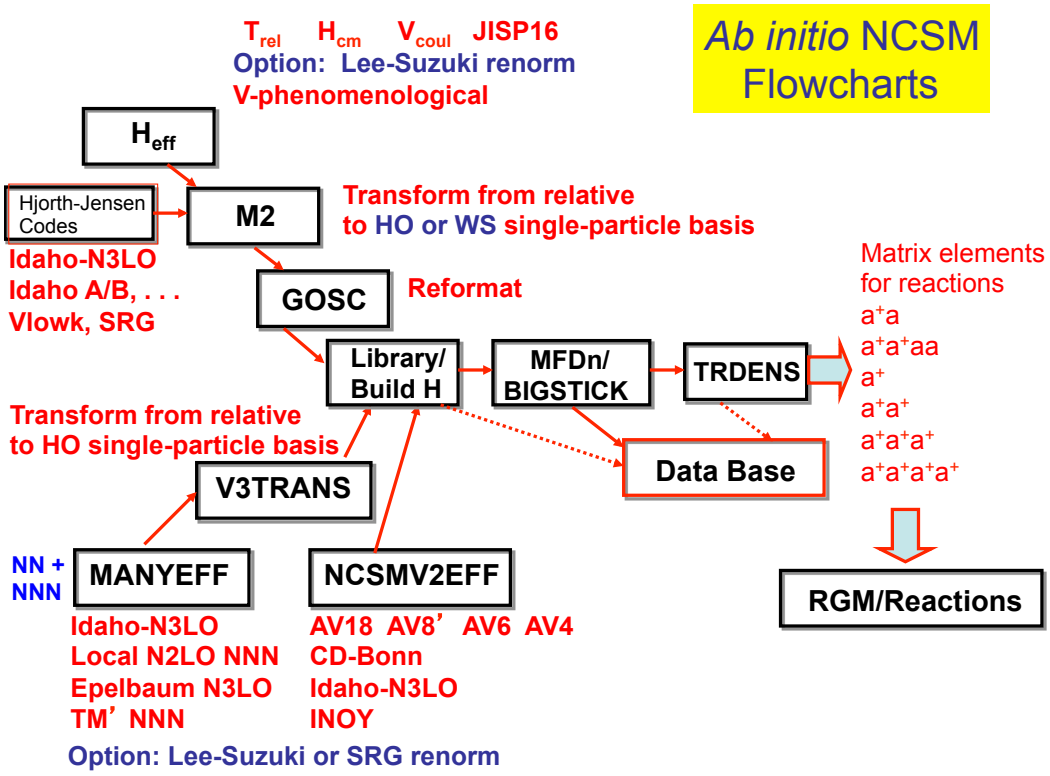

Figure 27: Workflow for CI calculations of LCCI project. NN, NNN and NN+NNN interaction files are generated by sets of codes to the left of center. Either MFDn or BIGSTICK performs the many-body calculation producing wave function files and initial suites of observables. TRDENS reads wave function files and computes additional observables and matrix elements for reactions. The details of calculations may be documented in the prototype Database Management System (DBMS, labeled as "Data Base" above) by depositing an info file (produced by the LCCI script) into the DBMS.

In an ab initio no-core shell model (NCSM) calculation, one begins by evaluating two-body and/or three-body interaction matrix element files for input to the many-body calculation that is performed by either MFDn or BIGSTICK. One may also select from libraries of previously evaluated interaction files.

Figure 27 shows how the six main codes used for these "upstream" efforts generate interaction files for the MFDn/BIGSTICK calculations in M-scheme, the most resource-intensive stage of the calculation.

The workflow diagram for NuShellX is shown in Figure 28. Here, one either selects from a library of existing interaction files or generates new interaction files that are used by NuShellX in the many-body calculation, which is also the most resource-intensive stage of the calculation. NuShellX performs the many-body calculations in a coupled-J basis.

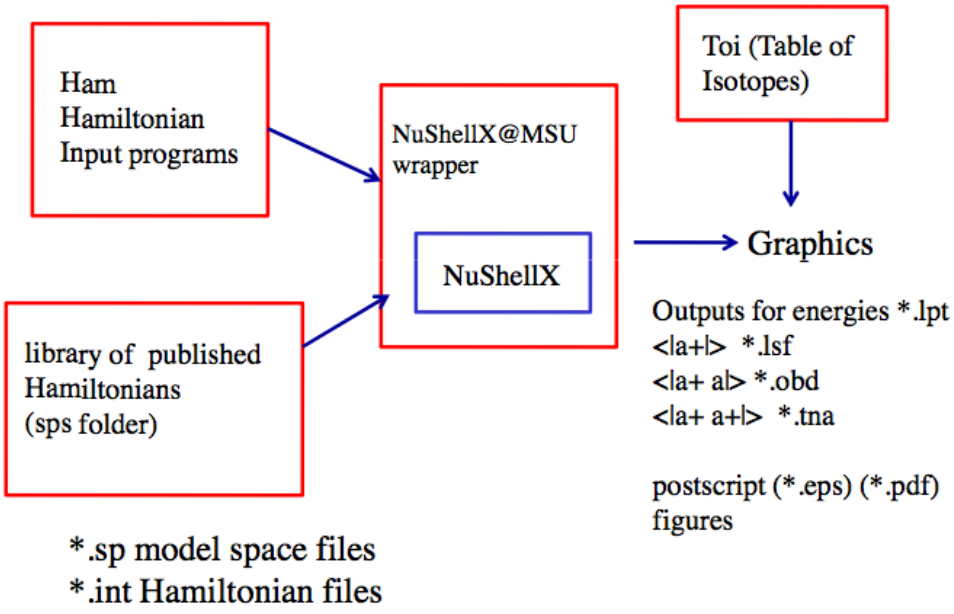

Figure 28: Workflow for CI calculations using NuShellX. Interactions are evaluated or taken from a library as indicated to the left of center and are fed into NuShellX. Output files include a suite of observables and matrix elements for reaction applications. There are options to produce figures for comparisons between theory and experiment using the Table of Isotopes.

The three resource-intensive components (BIGSTICK, MFDn, NuShellX) represent three different algorithm designs. The differences include in-memory storage of matrix elements versus on-the-fly recalculation, uncoupled M-scheme versus coupled J-scheme bases, and two-body interactions only versus three-body interaction capabilities. The codes therefore have different strengths and weaknesses, potentially different target applications, and potentially different approaches to architecture exploitation. Close cooperation under LCCI is leading to cross-fertilization of ideas key to developing optimal strategies for next-generation architectures. Each algorithm is capable of solving problems with or without a core.

A prototype LCCI python script was developed (ISU/SDSU) to provide flexibility for the user to select the algorithm most appropriate to his/her application and available architecture. The user launches the python script interactively and responds to a series of prompts for information that defines the calculation and produces a script for submission to the batch queue. The initial prototype was designed for running with interaction files from libraries and the MFDn/BIGSTICK codes as indicated in Figure 27. A future effort will be needed to include the NuShellX workflow of Figure 28.

During the 2010 SciDAC/UNEDF annual meeting, LCCI team members provided tutorials on the use of these codes. During 2011, LCCI team members have worked to streamline the scripts to

increase their ease of use with enhanced tables listing options during the interactive session that builds the run script.

In accordance with our planned milestone for Year-5, we delivered final UNEDF versions of LCCI codes, scripts, and test cases to UNEDF. We also completed the prototype python script that facilitate running these codes.

Prototype Database Management System (DBMS)

During Year-4 and Year-5, a collaboration between the ISU and Ames Laboratory groups designed, developed, tested, and implemented a prototype Database Management System, which is available for access at http://nuclear.physics.iastate.edu/info/. The DBMS aims to address problems encountered when multiple researchers are using large codes to make production runs with major investments of personnel and computational resources. Currently, CI codes run on different platforms, and results are often stored under different usernames and directories making it difficult to locate and retrieve information that has been calculated and stored. In addition, records on what went into a given production run are often incomplete or inadequate.

The long-term goals of the DBMS are: (i) to provide an efficient tool for retrieving output from previous CI calculations. The aim is to develop a single digital index to record key information on CI production runs; (ii) to provide an initial step towards replicable research. The ultimate aim is to record not only results, but also how those results are obtained so they may be fully replicated by independent researchers, referred to as “provenance”.

When discussing the DBMS, we distinguish between “data” and “meta-data”. The data are results from LCCI codes, typically stored on platforms where the runs are performed (physical observables, wave functions, one-body density matrices, etc.). The meta-data contain key information about each run (neutron number, proton number, interactions, basis space, platform, directories for results, user who performed the run, date of the run, etc.).

In the DBMS prototype developed and deployed under UNEDF, records of the meta-data of every run in the database are consolidated and formatted into a single file and a searchable master index. Anyone can access this database over the web and find out whether the runs of his/her interest have been performed. If the answer is yes, the DBMS provides information on where the results are located. Figure 29 provides an overview of the DBMS prototype at the Nuclear Physics Server at Iowa State University.

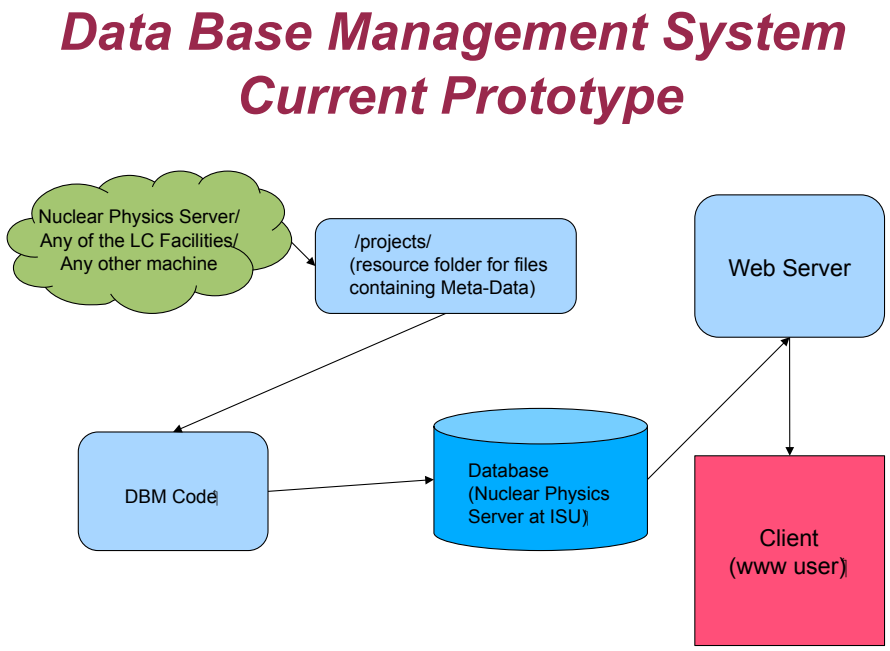

Figure 29: Overview of the prototype Database Management System currently at the Nuclear Physics Server at Iowa State University http://nuclear.physics.iastate.edu/info/.

Figure 30 presents the workflows of the prototype DBMS. Users make deposits of info files into a "drop-box" on the server. Note that a user running the LCCI script accessing MFDn will automatically generate this info file tailored to the syntax of the DBMS. Once the user is satisfied that the run is successful, the user then deposits this auto-generated info file into the DBMS dropbox. The DBMS periodically sweeps for newly deposited meta-data files and updates the database according to the workflow of the left panel of Figure 30. Database queries are processed through an online search form according to the workflow of the right panel of Figure 30. All runs logged into the database that satisfy the search criteria are presented in table form to the user's www client. Clicking on an entry in that table displays the info file with all the recorded meta-data – typically 1-2 pages of information about the run. As an alternative, the user may select a listing of all runs logged into the database. A table of all the runs is then presented to the user who can then click on any single entry and inspect the details of that run. Various pull-down menus allow the user to generate a list of a defined subset of all runs in the data base such as all runs with a particular interaction or by a specific user, etc.

The specific example in the left panel of Figure 30 illustrates the case for a run of MFDn in the prototype DBMS. A future redesign of the MFDn.info formats and new designs for the BIGSTICK.info and NuShellX.info formats are feasible.

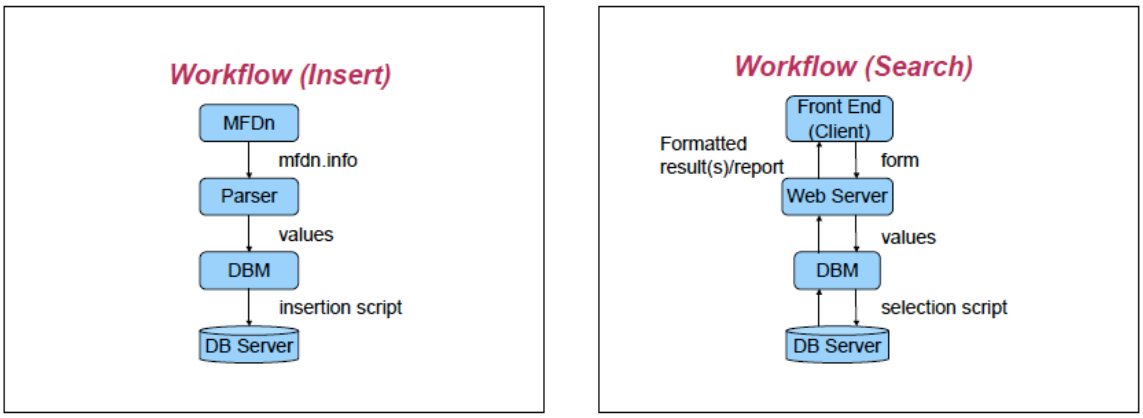

Figure 30: Workflow for insert mode (left panel) for the specific example of an MFDn run that produces the file mfdn.info with the meta-data for that run, and workflow for the user-initiated search (right panel) that queries the database of all recorded runs.

During Year-4 and Year-5 we designed and implemented revisions that accommodate data in a relational database to improve organization and flexibility in the database. We achieved the Year-5 milestone of a developed and deployed prototype DBMS. The DBMS software is released and available upon request.

LCCI (MFDn) collaborations between ISU, Ames Lab, LBNL and ANL

MFDn – major code developments

We have developed and implemented a python script for interactive setup of production runs on various platforms including automatic generation of scripts for post-processing of results and generation of log-file (the "mfdn.info" file) for the Data Base Management System (see below). This script facilitates the training of new users of the production code MFDn-Version 13, and we have initiated several new collaborative research projects.

We have developed an initial version of a stand-alone code (BuildH) to pre-process the input Hamiltonian components (results of "upstream codes") into a single file for input to MFDn in order to facilitate calculations using a more general single-particle basis than the H.O. basis, see Phys. Rev. C 86, 034312 (2012). In addition, the format of the output of BuildH reduces the memory for the input to MFDn, and saves on both memory and processing time in the setup phase of MFDn.

Major code improvements to MFDn have been developed, implemented and tested in collaboration with the LBNL group (Ng, Yang, Aktulga). In year-4 and the beginning of year-5, we have made significant improvements in the efficiency of constructing a basis of good total angular momentum for MFDn (rather than an M-scheme basis) by using different algorithms depending on the size of the invariant subspaces. We also improved the load-balancing and scalability, and as a result we now have MFDn-Total-J, a version of MFDn using a basis of good total J.

The extremely large size of the Hamiltonian matrices involved in ab initio no-core calculations may hinder the scalability of the Lanczos-based eigensolver in MFDn. In a recent investigation,

we quantitatively show that topology-aware mapping of computational tasks to physical processors significantly reduces the communication overheads in the eigensolve phase. For typical large-scale eigenvalue calculations in MFDn, we obtain up to a factor of 2.5 improvements in overall performance by using a topology-aware mapping.

The many-body Hamiltonian in MFDn is a highly unstructured sparse matrix. This requires broadcasting/reducing the entire Lanczos vector over large processor groups. Therefore the overall communication overheads in large-scale MFDn runs can be very high, even with the topology-aware mapping techniques mentioned above. In a follow-up investigation, we have developed a novel strategy to overlap the expensive communication operations with sparse matrix-vector multiply (SpMV) computations on multicore platforms. In addition, using a 1D hierarchical decomposition approach, we have reduced the communication overheads during basis orthogonalization significantly compared to an earlier version of MFDn. These improvements lead to over 80% computational efficiency in large-scale runs.

To gain an impression of our accomplishments over the entire 5-year period of the SciDAC/UNEDF award, we display in Figure 31 the cumulative time for a total production run of MFDn that includes pre-processing (setting up basis space, evaluating/storing many-body Hamiltonian), diagonalization via the Lanczos algorithm and post-processing (transforming eigenfunctions to original basis representation, evaluation of a suite of observables, generating output files). The improved strong scaling (i.e. the same problem solved on different numbers of cores) is observed through the improved flattening of the curve and its overall decrease with newer versions. Significant gains have been achieved by switching over to the recently implemented hybrid MPI/OMP mode, and, most recently, by employing a topology-aware mapping of the processors. This latest version of MFDn-Version 13 scales to more than 200,000 cores on Jaguar (see Figure 32) and has been uploaded to NERSC under UNEDF with script and test cases as part of Leadership Class Configuration Interaction (LCCI) code project.

The emergence of clusters equipped with non-volatile NAND-flash memory based solid state drives (SSD) presents unique opportunities. In recent investigations, we have developed an out-of-core eigensolver for MFDn using a novel distributed out-of-core linear algebra framework, called DOoC+LAF. The framework provides an easy-to-use high-level application interface for linear algebra operations while providing efficient execution by orchestrating pipelined execution of computation, communication and I/O. We have shown that our out-of-core eigensolver running on an SSD-equipped cluster can achieve computational efficiencies comparable to those of the in-core implementation running on modern supercomputers for actual MFDn computations.

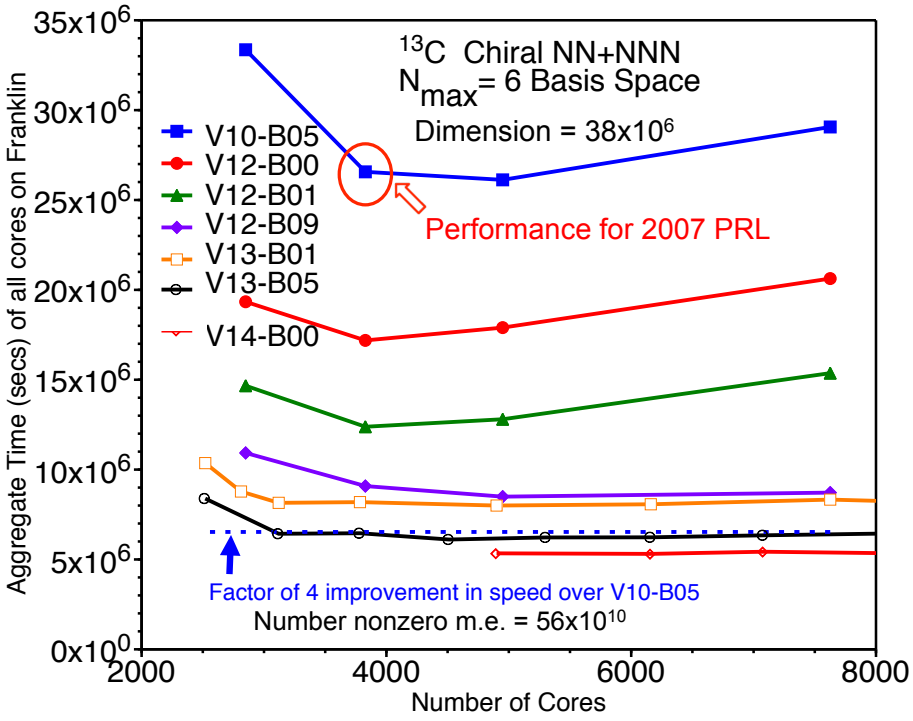

Figure 31: Total CPU time on Cray XT4 for test case marking the improved performance of MFDn on Franklin (NERSC) over the 5-year period of this SciDAC/UNEDF grant. Successive stages of code development are indicated in the legend by increasing "version" numbers and "beta" edition numbers. The test case uses chiral NN + NNN interactions, a matrix dimension of 3.8×10^7 and 5.6×10^{11} nonzero many-body matrix elements that are computed and stored.

Finally, we have started the development of a new version, MFDn-Version 14, which is based on a different 2-dimensional distribution of the basis (and hence of the matrix) over the processors than MFDn-Version 13 and before. The key difference is that in Version 14 we group states together in order to retain some of the natural structure of the sparse matrix. This leads to significant speedups during the construction of the matrix, as well as a moderate improvement during the Lanczos iterations (most likely due to a better cache performance).

Iowa State-Ames collaboration continued to develop, test, and implement the prototype Data Base Management System (DBMS). It is available at http://nuclear.physics.iastate.edu/info/. The goal of the DBMS project is to record all production runs of ab initio no-core calculations under the LCCI component of SciDAC/UNDEF and to make available the outputs of those runs (spectra, observables, wavefunctions, one-body transition densities, etc.) to other researchers. This system has logged 1038 production runs on 68 distinct nuclei with a total of 7405 separate calculations as of the time of writing this report. While the logs of runs are publicly available, detailed results (e.g. calculated observables) are available only to SciDAC/UNEDF researchers at the present time. Over time, and with additional support in the future we plan to increase the functionality of the DBMS and the access by other researchers.

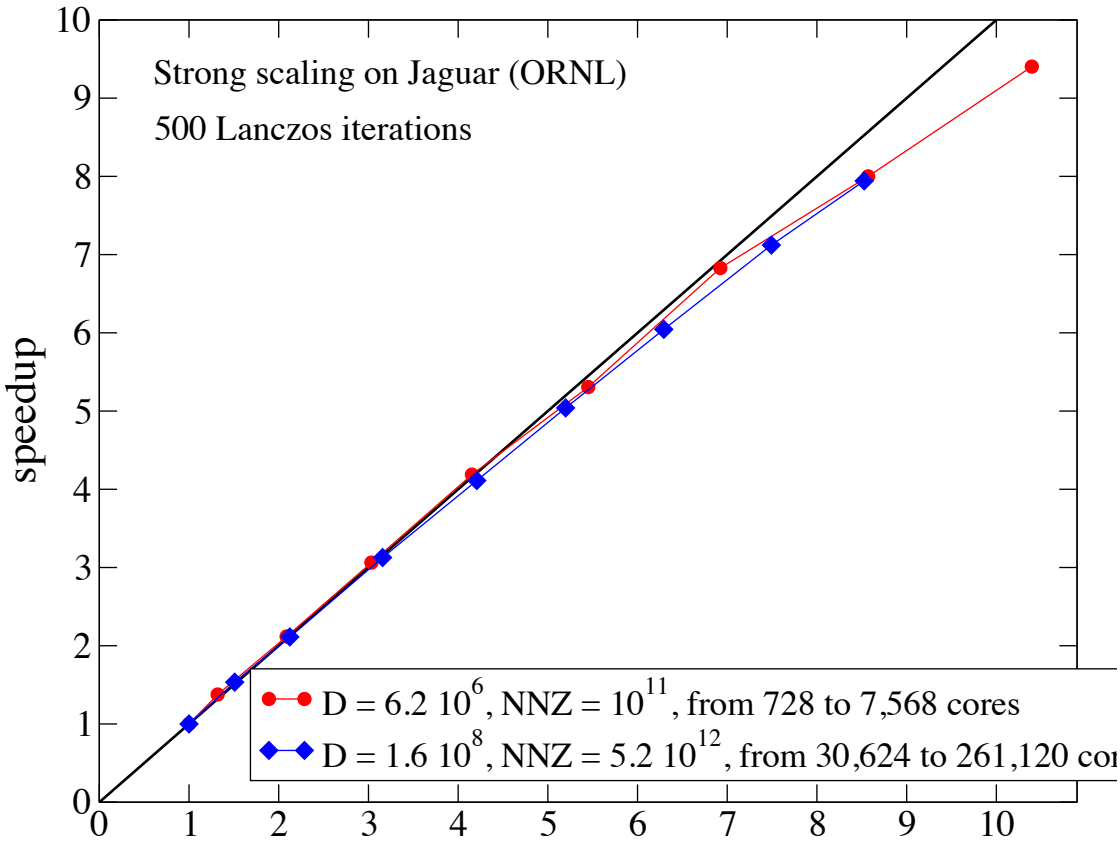

Figure 32: Strong scaling for MFDn: speedup for 500 Lanczos iterations (the most time-consuming phase of the code). Shown are two problem sizes: ^{7}Li with a dimension of 6.2 million and 118 billion nonzero matrix elements; and ^{10}B with a dimension of 160 million and 5.2 trillion nonzero matrix elements. The runs where performed with 2 MPI processors per node, and 8 threads per MPI processor. The smaller problem needs at least 1 TB in order to store all nonzero matrix elements in core, and needs therefore at least 91 MPI processors (728 cores) to fit the problem in core. The larger problem needs at least 42 TB, and we used 3828 MPI processors or more for that problem.

Jointly with the University of Indiana a prototype of web services and scientific workflow was developed to address the needs of the LCCI project. The proposed abstractions and interfaces will enable rapid involvement of new collaborators and graduate students in productive research. The workflow infrastructure democratizes the access to the nuclear physics simulations executing on remote supercomputing resources since the infrastructure was built on open-community workflow systems that were enhanced with advanced features to facilitate parametric sweeps and provenance collection for nuclear physics applications. Additionally, dynamic workflow reconfiguration was implemented.

Memory-pinning strategies have been investigated for nonuniform memory access (NUMA) architectures. Since the access time to the shared data structures may be detrimental to the scalability, it is imperative to carefully map large shared arrays to specific memory banks based on the nature of the computation and the multithreaded parallelism characteristics. In particular, we have proposed strategies pertinent to sparse matrix-vector multiplication and vector

orthogonalization phases from the MFDn package. Several nuclei and nuclear interactions were considered in the large-scale test cases. Performance gains of up to 25% were observed with the proposed strategies as compared to the default memory placement policy when static threading was used in the Lanczos algorithm.

In the March 2011 meeting of LCCI teams at LBNL, we decided to approach the National Nuclear Data Center to investigate a possible partnership for long-term sustainability of the LCCI codes and DBMS. This goal was reaffirmed in the meeting in the Fall of 2011. For this purpose, Vary presented the LCCI project to the National Nuclear Data Meeting at MSU following the DNP meeting in October 2011. Based on the favorable responses and expressions of interest, Vary visited NNDC in April of 2012 and met with the leadership of NNDC and its key staff members. These discussions revealed potential additional avenues to jointly pursue, leading to a white paper and to a joint proposal to DOE. Aspects of "Big Data" surfaced in discussions of the possible interest in storing large scale ab initio wave functions for access by broader research communities. Further discussions and meetings are planned.

AB INITIO DFT

The main goals of this part of UNEDF are to: (i) Develop low-momentum NN and NNN interactions and operators as input to ab initio wave function methods and nuclear matter; (ii) Develop nuclear matter calculations with controlled theoretical errors as input to microscopic functionals; (iii) Construct ab initio functionals in the form of a generalized Skyrme interaction, with theoretical error bars, and understand conceptual issues; (iv) Validate the functionals against ab initio wave function methods; and (v) Provide guidance to DFT Applications on novel density dependencies for EDF's based on microscopic input. Milestones in Year-5 addressing these goals are described below. The multiple interconnections of Ab Initio DFT with other UNEDF efforts span the region shown in Figure 33 (e.g., "Softening", "Density Matrix Expansion").

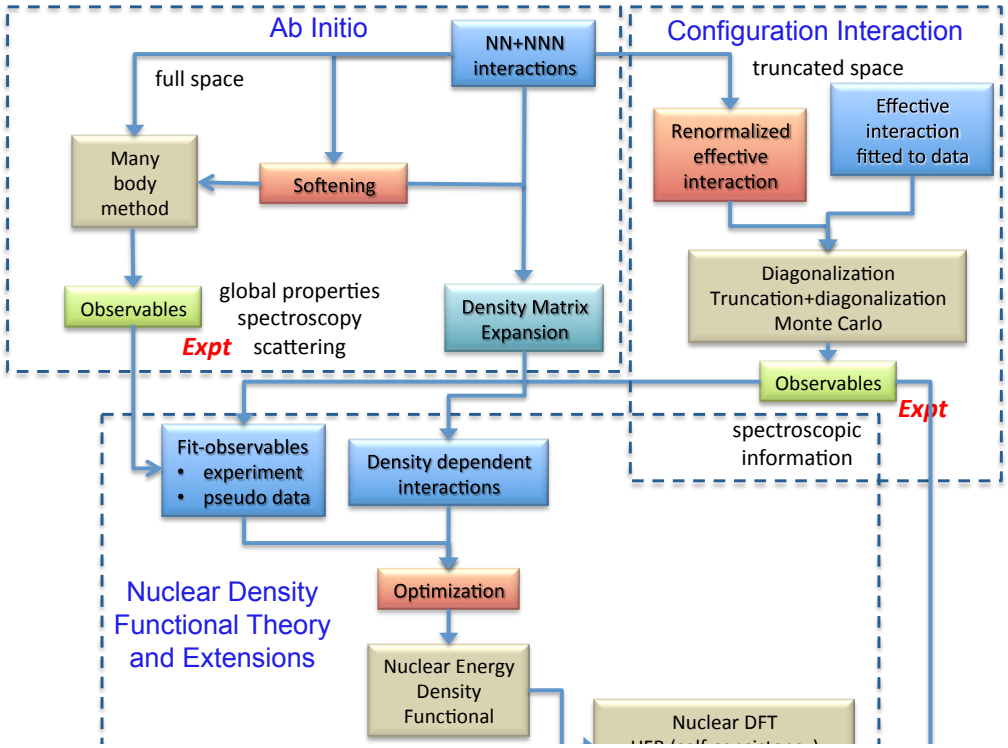

Figure 33: UNEDF's Ab Initio DFT Effort on the UNEDF strategy diagram

The main groups in Year 5 were at Ohio State (Anderson, Furnstahl, Hebeler, Hergert [starting at OSU in 9/2011], and Wendt) and Michigan State (Bogner, Burgos-Vasquez, Hergert) with significant collaboration with international groups at Saclay (Duguet) and Darmstadt (Roth, Schwenk), and with former UNEDF collaborators (Drut, Lesinski, Platter). Much of the Ab Initio DFT effort was in close collaboration with the Ab Initio Wave Function and DFT Applications groups. The computational needs for developing the interactions and the functionals have grown through the course of the project but have not required leadership class resources. However, the validation and optimization of the functionals relies critically on the large-scale computing capabilities in the other groups (e.g., coupled cluster and configuration interaction calculations

with NNN forces and fast DFT solvers) and collaboration with CS/AM scientists (e.g., for efficient optimization).

Low-Momentum Interactions And Operators

The low-momentum $V_{low\text{-}k}$ and Similarity Renormalization Group (SRG) interactions based on initial chiral effective field theory (EFT) potentials are used for rapid convergence of coupled cluster and NCSM calculations as well as for the microscopic construction of the energy functional. The ability to vary cutoffs provides a diagnostic tool and error estimates for the many-body approximations. Furnstahl gave a series of four lectures on "The Renormalization Group in Nuclear Physics" at the 2011 Schladming Winter School, which were published in Nuclear Physics B proceedings.

Evolution and Application of NNN

In Year 5, work continued on development of the SRG flow equation method, which evolves internucleon interactions and operators toward softer forms. The SRG evolution of NNN interactions was first achieved in a harmonic oscillator basis by Jurgenson, Navratil, and Furnstahl, while Jurgenson was a graduate student at Ohio State. The SRG evolution for A=2 and 3 is carried out in a Jacobi harmonic oscillator basis, using the recursive anti-symmetrization formalism developed by Navratil and NCSM collaborators. As a postdoc at LLNL, Jurgenson, together with Navratil and Furnstahl, applied the potentials to p-shell nuclei, with the first paper published in Year 5. Another paper with Year 5 results, which now includes Maris and Vary as collaborators, is being finalized. This includes results for nuclei through ^{12}C.

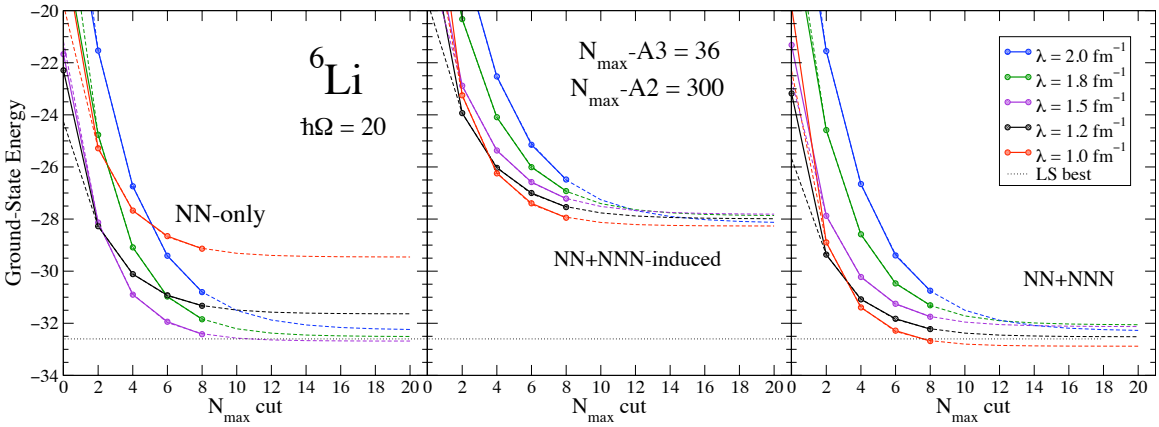

Figure 34: SRG evolution in ^{6}Li including NNN.

The application to p-shell nuclei such as ^{6}Li (see Figure 34, dotted lines show simple extrapolation to large N_{max}) tracks the growth of induced many-body forces at larger A. The NN-only ^{6}Li results (left panel) show a large spread, demonstrating the same scale dependence as observed in previous momentum-representation-evolved calculations. The spread decreases significantly when induced NNN matrix elements are included (center panel) and initial NNN interactions bring the extrapolated results close to experiment (right panel). In Figure 35, the calculated ground-state energy for ^{10}B is shown as a function of the SRG flow parameter. When initial three-body forces are included (NN+NNN), the energies are remarkably constant over the range shown. However,

for larger nuclei there are indications that four-body (NNNN) interactions may be growing significant. This has led to an investigation of alternative SRG generators and to the development of technology to evolve NNN interactions in a momentum basis. The importance of using a consistent generator in the presence of deep bound states was demonstrated (Wendt, Furnstahl, Perry) and novel generators that greatly improved the speed of the evolution were identified and tested (Li, Anderson, Furnstahl).

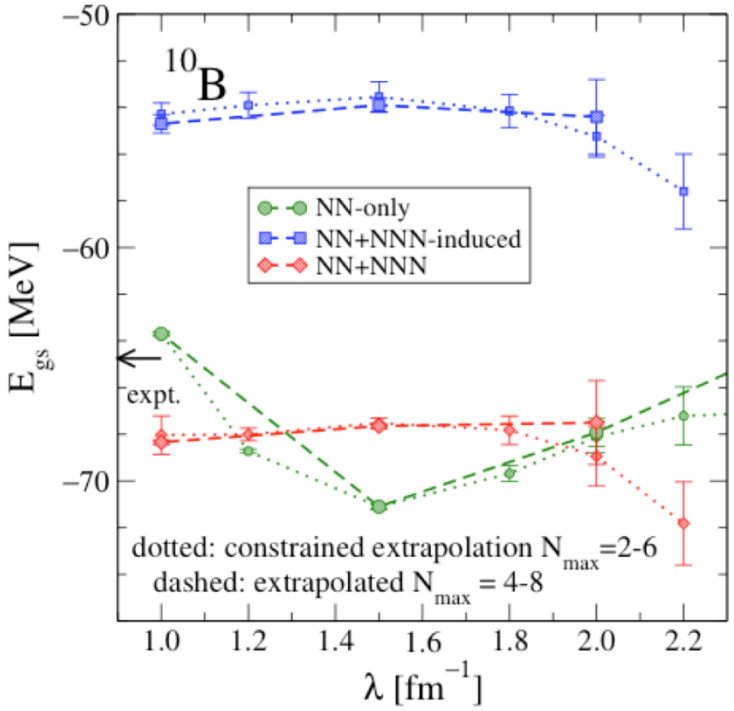

Figure 35: (Preliminary) Ground-state energy in ^{10}B as a function of the SRG flow parameter for just two-body interactions (NN-only), including the induced 3NF (NN+NNN-induced), and with an initial 3NF (NN+NNN).

The first evolution in a partial-wave momentum basis was achieved by Hebeler in Year-5. This opens the door to important tests of the evolution in the harmonic-oscillator basis, allows SRG generators not previously possible, and enables calculations of neutron matter with 3NF, which will be used to constrain functionals. Among the interesting physics results are a first-time demonstration of (partial) universality in the NNN interaction, as illustrated in Figure 36. Another development by Wendt and Furnstahl was of local projections of non-local low-momentum potentials. This provides the first clear visualization of the "melting" of the repulsive core in traditional NN potentials (see Figure 37) but may also lead to the use of soft potentials with Green's function and auxiliary field Monte Carlo methods.

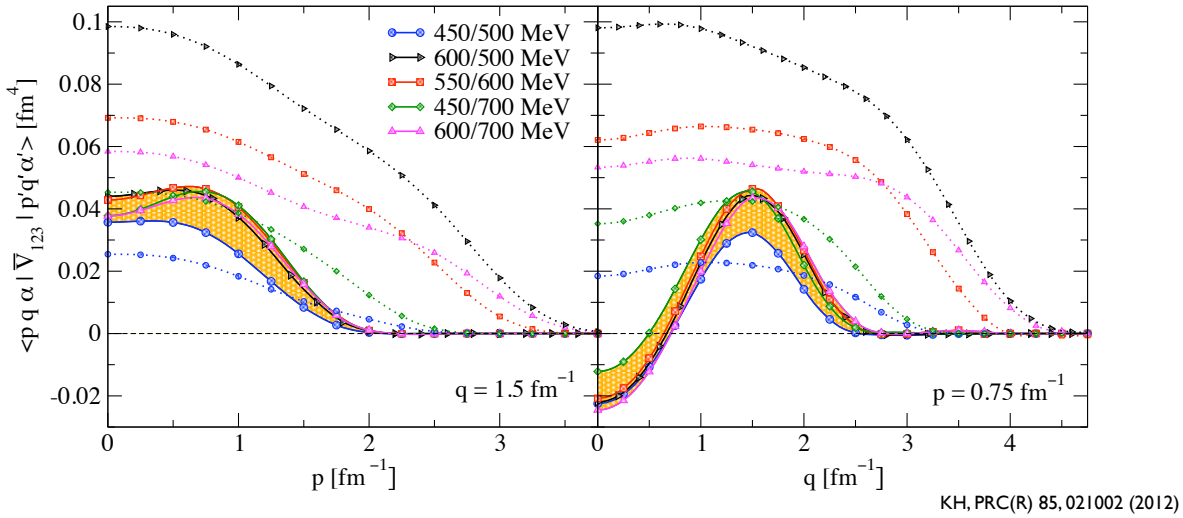

Figure 36: (Partial) collapse of representative three-body matrix elements evolved from five different initial NN and NNN interactions. The widely spread initial values fall, after evolution, into relatively narrow bands with non-trivial shapes.

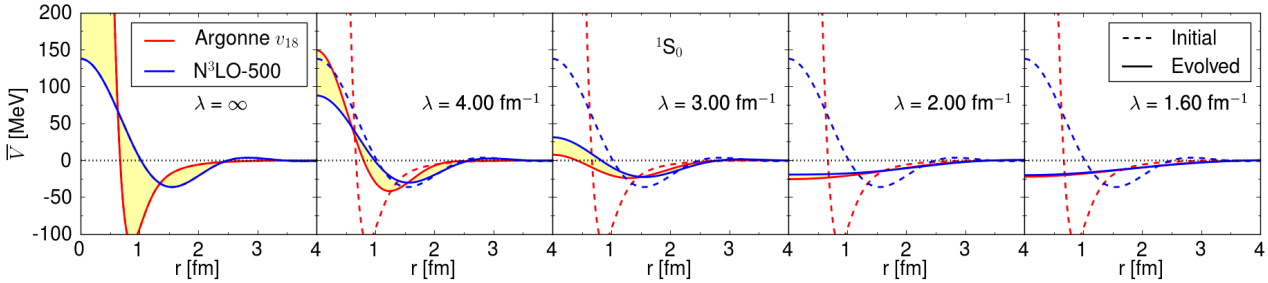

Figure 37: SRG evolution of the local projection of the Argonne V18 and chiral EFT (N3LO-500 MeV) NN potentials.

Operator Evolution via the SRG

The consistent evolution of SRG operators in few-body was demonstrated for the first time in model systems in Year 4 by Anderson, Bogner, Furnstahl, and Perry, with a paper published in Year 5. To use the wave functions produced by the SRG-evolved interactions to calculate other matrix elements of interest, we must account for the associated change in operators. These operators evolve according to the same equation as the Hamiltonian, and can thus be efficiently computed. The evolution of few-body interactions is critically important for the SRG Hamiltonian (as shown in Year-3) and the same is true of other operators. In Year-4, a computational framework was developed at OSU for evolving generic few-body operators and extracting their few-body components for use in existing solvers of few- and many-particle systems (see Figure 38 for a schematic diagram of this process). This framework is based on the unitary transformation constructed from the evolution of the Hamiltonian in successively larger few-particle bases and accounts for boost corrections necessary to embed some operators in a larger basis.

It was also demonstrated that decoupling of high- and low-momentum basis states, which leads to the improved convergence of binding energies, is maintained in the calculation of operator expectation values. Nevertheless, the calculation of long-range operators in a harmonic oscillator

model space presents additional challenges. Computational simplifications have been identified through factorization of the SRG-evolved operators, which occurs when there is a scale separation between the initial operator and the wave function momentum scales. This factorization leads to a universal function of the operator expectation value at high momentum, as well as an alternative interpretation to the role of short-range correlations.

A computational framework was developed for evolving generic few-body operators and extracting their few-body components for use in existing solver of few- and many-particle systems with the first applications to 3D calculations in a harmonic oscillator basis in Year 5 with planned explorations of alternative SRG generators and factorization of electroweak and other operators.

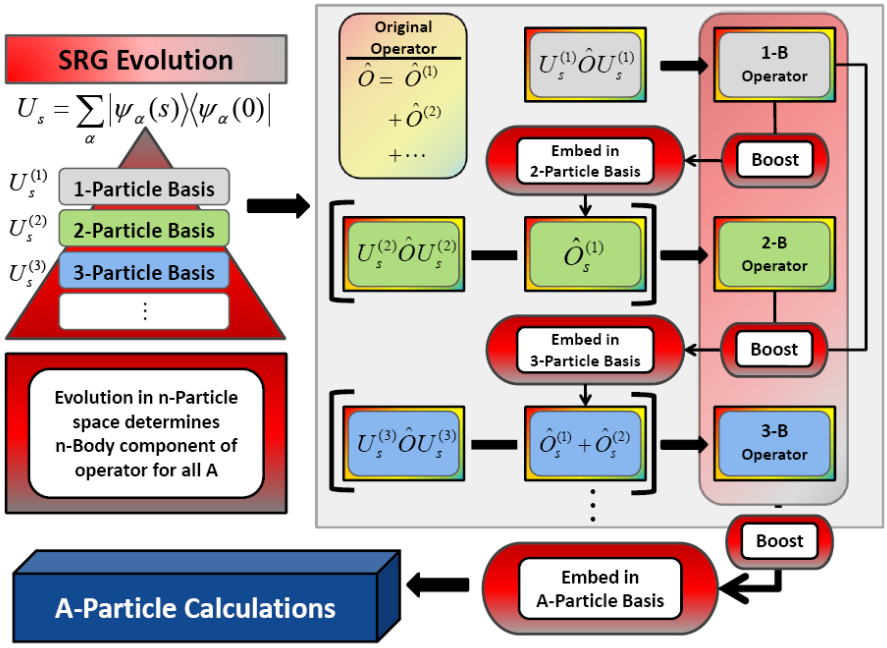

Figure 38: Operator Evolution, extraction, and embedding process for A-body calculations

In-Medium SRG

Continuing work that was initiated in Year 4, Bogner and external collaborators Tsukiyama and Schwenk completed proof-of-principle calculations where the in-medium SRG (IMSRG) was adapted to construct effective Hamiltonians for shell model applications. Initial calculations for ^{6}Li (see Figure 39) demonstrated that the IMSRG gives consistently better agreement with the exact spectra (obtained by large-scale NCSM diagonalization) compared to shell model Hamiltonians derived from many-body perturbation theory. In conjunction with the ^{6}Li calculations, which were fully microscopic and parameter-free, the IMSRG was also used to generate semi-microscopic shell model hamiltonians for ^{18}O in which empirical single-particle energies were used in place of the microscopically generated values. Once again, the IMSRG shell model Hamiltonians outperformed those derived from MBPT, indicating the importance of the higher-order contributions that are implicitly summed in the IMSRG approach.

In addition to the development of IMSRG shell model Hamiltonians for open-shell systems, Bogner and collaborators implemented a modified truncation scheme for closed-shell IMSRG calculations so that "hard" or "bare" input interactions can be used. The original formulation, for which the bulk of the years 3 and 4 calculations were carried out with, was limited to soft NN interactions. The modified truncation scheme gives good agreement between IMSRG and CCSD calculations of ^{4}He, ^{16}O and ^{40}Ca using the bare N^{3}LO(500) NN potential of Machleidt, and it does not alter the excellent agreement that was found in the original IMSRG truncation for soft NN potentials in Year 4 (see Figure 40).

Together with the coupled-cluster theory group at ORNL/UTK (Papenbrock and Hagen), the CI group at ISU (Vary and Maris) and external collaborator Carlo Barbieri (Self-consistent Green's Function Method), benchmark calculations were performed for the ground states of ^{8}He, ^{12}C, ^{16}O, ^{18}O and ^{40}Ca using several input NN interactions. For the lighter nuclei, the IMSRG, CC, and SCGF methods all gave reasonably good agreement with the exact CI results. For the heavier nuclei beyond the reach of exact CI, the IMSRG, CC, and SCGF also gave rather similar results. While the quantification of uncertainties due to the truncation errors of the different methods and basis extrapolations are still open questions, the qualitative agreement amongst the different many-body methods is, to the best of our knowledge, the first benchmark of its kind for medium-mass nuclei.

Finally, in Year 5 substantial computational improvements in the IMSRG codes were made by UNEDF researcher Heiko Hergert (Ohio State University). With these advances, calculations can now be performed in up to 15 major harmonic oscillator shells. Previous calculations in years 3 and 4 were limited to 10 major shells.

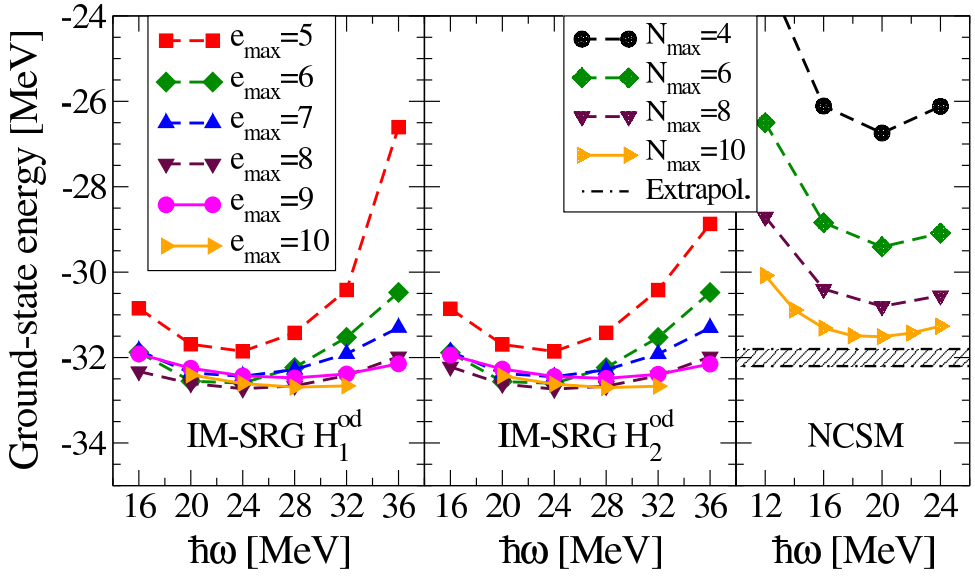

Figure 39: Ground-state energy of ^{6}Li versus harmonic-oscillator parameter from a diagonalization of the IM-SRG Hamiltonian in the p-shell (left and center), compared to the convergence of the no-core shell model (NCSM) with N_{max} (extrapolation is the band).

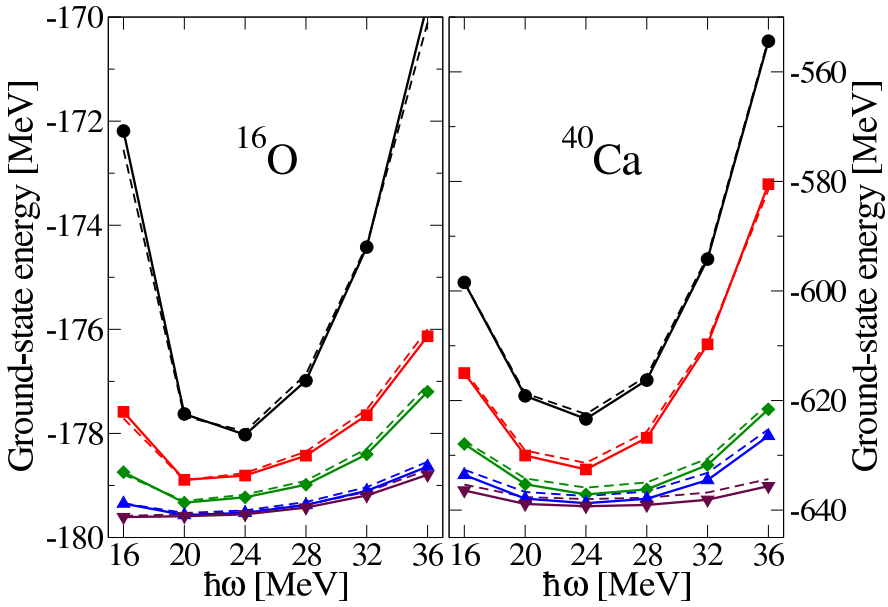

Figure 40: Convergence of the IM-SRG energy in ^{16}O and ^{40}Ca for in-medium SRG (solid) and CCSD (dashed) for emax from 4 to 8 (black to violet).

Nuclear Matter

A derivation of a density-dependent approximation for NNN has been completed and incorporated in many-body calculations of neutron and nuclear matter calculations based on $V_{low\text{-}k}$ and SRG NN interactions. These calculations, led by Hebeler extend previous work by Bogner, Furnstahl, Nogga (Jülich) and Schwenk by a full treatment of all exchange terms, the study of error bands due to uncertainties in many-body forces and the inclusion of 3rd order contributions, indicating the convergence of the many-body expansion scheme. This parameter-free calculation gives an encouraging description of nuclear matter saturation (see Figure 41). Hebeler continued applications to neutron matter (and neutron stars) in Year 5 and he also published work on the impact of chiral three-nucleon forces on pairing in nuclei.

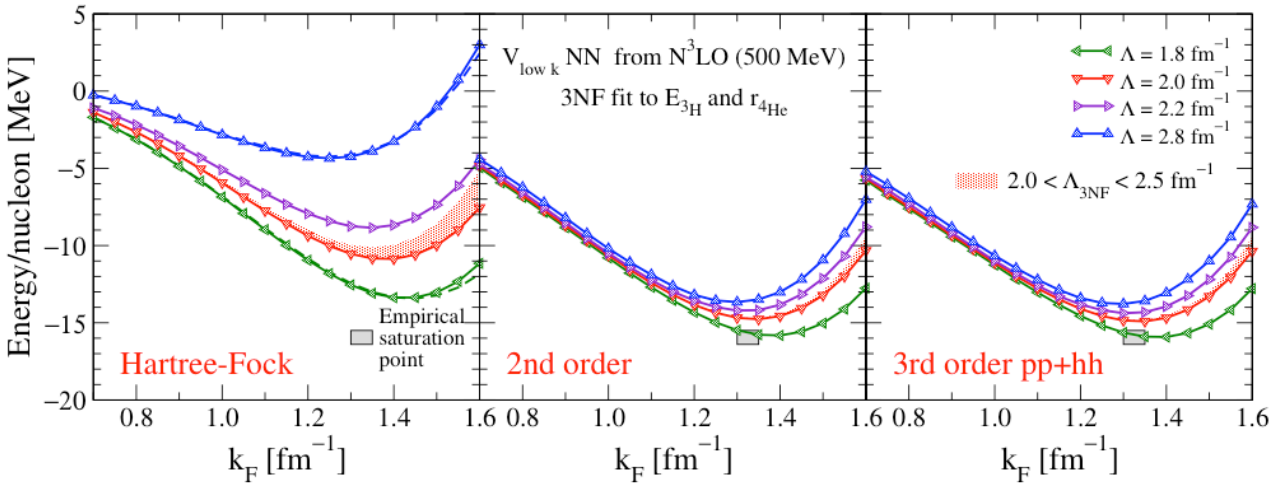

Figure 41: Nuclear matter in three approximations showing cutoff dependence.

Development of DFT Functionals

Beyond NV-DME (Π-DME) and Comparisons to Ab Initio Calculations

The scalar-isoscalar part of an ab initio EDF, based on the Negele-Vautherin density matrix expansion (NV DME) and adapted to use a chiral EFT interaction softened using RG methods by generalizing to momentum space and NNN interactions, was developed by Bogner, Furnstahl, and Platter in Years 2 and 3. Comparisons were made with ab initio coupled cluster and NCSM wave function (wf) calculations using the same Hamiltonian and varying parameters and an external potential. These comparisons showed some clear deficiencies in the DME implementation. The standard NV-DME suffers from several problems, the most severe being an extremely poor description of the vector part of the density matrix. Gebremariam, Bogner, and Duguet traced the problems to an inadequate phase space averaging (PSA) used in previous DME approaches. Their new parameter-free PSA was tested and documented in several papers published in Years 3 and 4. The improvements are substantial, typically reducing relative errors in integrated quantities by a factor of ~ 5-10 across many different isotope chains. The improvement is especially striking for the vector density matrices, where the original NV DME can give relative errors in excess of 40%.

Starting in Year-4 and continuing through Year-5 (and on-going), the improved PSA DME of Gebremariam, Bogner, and Duguet was used to benchmark ab-initio DFT calculations against ab-initio wave-function calculations of neutron drops in external fields. Studies of closed-shell droplets (N=8 and N=20) using the semi-realistic Minnesota NN potential found that the DME functional (derived at the HF level) reproduces radii at the 1-3% level and energies at the 3-5%, while the DME functional at the BHF level gives a substantial improvement, reproducing radii at the .5-2% level and energies at the .5-1% level. A paper describing the implementation and pre-optimization of DME-based energy density functionals was published with the UT/ORNL, and MSU groups (and T. Duguet from Saclay, an international UNEDF collaborator). New comparisons of DME calculations with auxiliary field Monte Carlo and coupled cluster calculations were initiated in Year 5, with a first publication in preparation.

Orbital-Based DFT for Nuclei

Because the fully DME-based DFT may simply be inadequate compared to ab initio calculations, a sub-project to develop an orbital-based DFT was started in Years 2-3 and is on-going. Drut and Platter (also a former UNEDF postdoc) have been the main developers, and published in Year 5 (based partly on work Drut did while still at OSU) the first paper on exact exchange for nuclear DFT using a model interaction in neutron drops. Comparison tests are being made of the DME, the Optimized Effective Potential framework developed by quantum chemists to overcome deficiencies of DFT functionals based on gradient expansions, which are the analog of the DME functionals, and approximations to the OEP (such as KLI), starting with neutron drops in external fields, where ab initio results are available. In Year 5 the issues of symmetry breaking self-interaction were addressed in this formalism by Drut and Furnstahl with an extension to pairing and more realistic microscopic interactions. This work is on-going.

Before leaving OSU for LANL, Drut started a new line of research to explore how to apply Hybrid Monte Carlo (HMC) to the non-relativistic many-body problem. This approach, which is used in state-of-the-art Lattice QCD codes, offers improved scaling compared to Determinantal Monte Carlo (DMC). Benchmarking tests were made in related problems such as the unitary Fermi gas (UFG) and graphene. A paper surveying preconditioning strategies, which are key to the successful adaptation of HMC, was published during Year 5. Work on using graphical processor units (GPU) for HMC calculations continued through Year 5 with OSU student Kyle Wendt, with one paper published and another paper in preparation.

Generalized Skyrme Functional with Universal Long-Range DME

Gebremariam, Bogner, and Duguet derived a non-empirical nuclear energy density functional by applying the Density Matrix Expansion (DME) to the Hartree-Fock energy obtained from chiral effective field theory (EFT) two-and three-nucleon interactions. Due to the structure of the chiral interactions, each coupling in the DME functional is given as the sum of a coupling constant arising from zero-range contact interactions and a coupling function of the density arising from the finite-range pion exchanges. All expressions for the couplings are analytic (even the complicated NNN part), which was carried out using fully automated symbolic tools (Mathematica) that have been published. Since the contact contributions are very similar to the structure of empirical Skyrme functionals, a microscopically-guided Skyrme phenomenology follows from releasing the contact terms in the DME functional for optimization to finite-density observables to capture short-range correlation energy contributions from beyond Hartree-Fock. The optimization, testing, and benchmarking of this new, next-generation hybrid functional is being carried out as a collaboration between the DFT team at UT/ORNL, the team developing an ab initio DFT (MSU/OSU/Saclay) and computer scientists at ANL. The roadmap for this on-going sub-project is shown in Figure 42.

The DME-based functional has been implemented in the DFT solvers HFBRAD (by Kortelainen) and HFBTHO (by Stoitsov) in leading order (LO), next-to-leading order (NLO), and next-to-next-leading order (N2LO) approximations. HFBRAD is a very fast solver (CPU seconds per nucleus) for spherical nuclei and density-dependent local density approximations, while HFBTHO needs about 10-15 CPU minutes per nucleus but calculates spherical and axially deformed nuclei, and can handle additional gradient corrections to the local density approximation.

Kortelainen and Stoitsov developed a new Fortran module for the density-dependent parts of the EDF from the DME applied to chiral effective potentials but which can also handle other functionals. This module allows details of the EDF and the HFB solver to be separated with the same module used for different HFB solvers. It has been implemented and tested so far for HFBRAD and HFBTHO and a paper on the module will be published in Computer Physics Communications. A regression algorithm has been applied as a pre-optimization procedure based on nuclear masses and the HFBRAD solver. The optimization parameters entering the volume of the functional are expressed in terms of infinite nuclear matter saturation properties. In progress is work towards a more advanced pre-optimization procedure based on a genetic algorithm for spherical nuclei (Lesinski, Schunck), which can include a larger variety of nuclear characteristics.

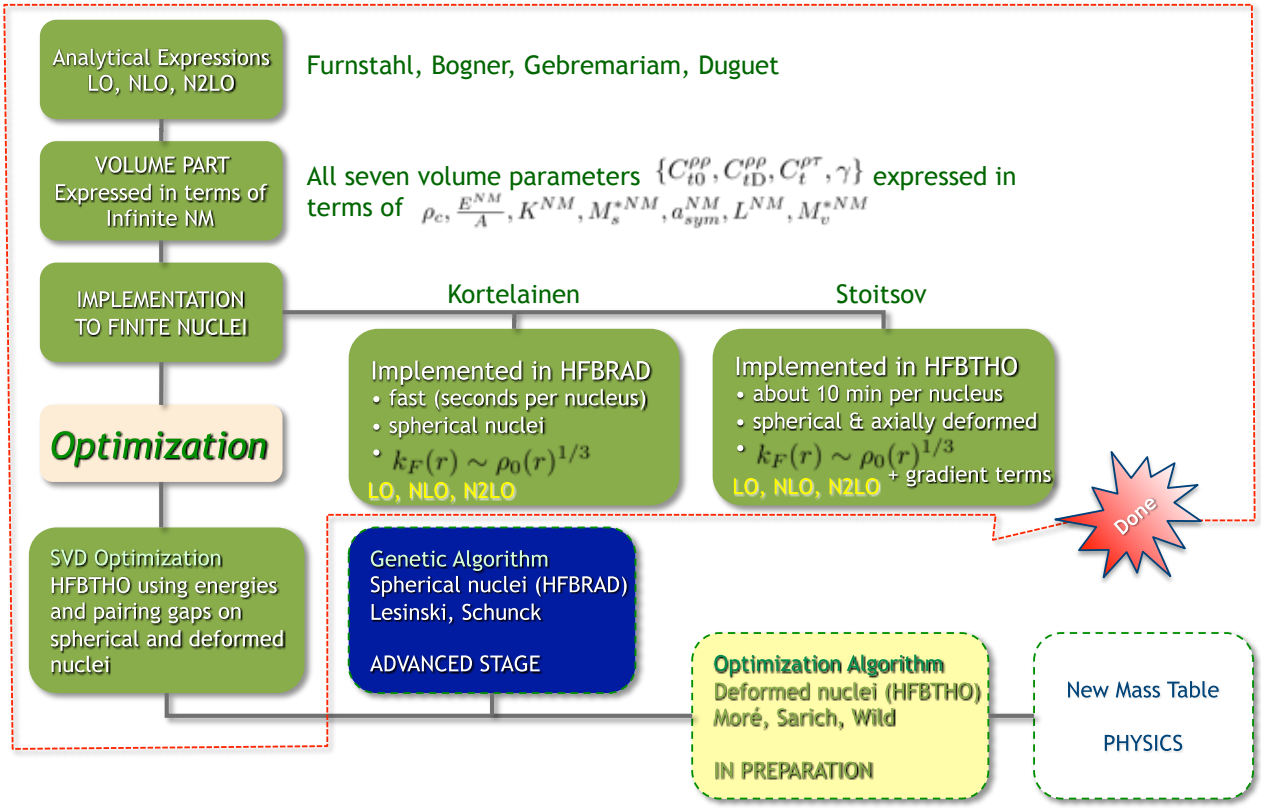

Figure 42: Roadmap for DME functional implementation and optimization.

The first steps have been taken to test the ability of the new hybrid DME functional, which has a much richer set of density dependencies than traditional Skyrme functionals, to generate sensible and stable results for nuclear applications. The results of the first proof-of-principle calculations are encouraging and numerous practical issues related to the implementation of the new functional in existing Skyrme codes have been worked out. Using a restricted singular value decomposition (SVD) optimization procedure, it was found that the new DME functional gives numerically stable results, and exhibits a small but systematic reduction in chi-squared compared to standard Skyrme functionals, thus validating its suitability for future global optimizations and large-scale calculations. It is already apparent that the new density dependences will lead to modification of observables compared to standard Skyrme functionals, such as in the deformability of nuclei (see Figure 43). A paper on these results has been published.

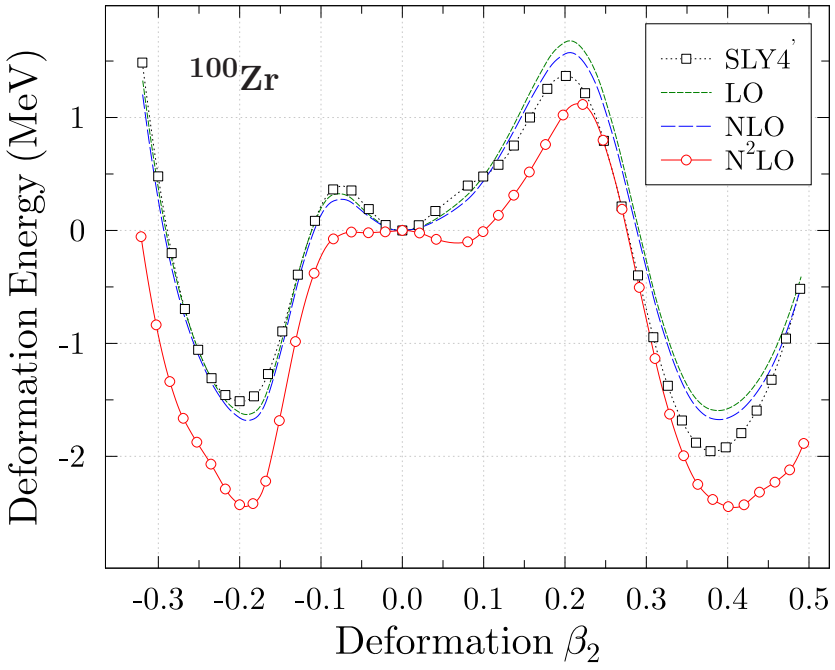

Figure 43: Deformability of ^{100}Zr for SLy4 Skyrme EDF and the hybrid DME functional at LO, NLO, and N2LO.

DFT APPLICATIONS

The main goals of this part of UNEDF are: (i) Develop modern computational infrastructure for nuclear DFT to calculate observables (global properties and spectroscopy); (ii) Define the form of EDF; (iii) Optimize the EDF to theoretical and experimental data; (iv) Develop technology to estimate theoretical uncertainties, in particular when extrapolating to unknown regions; and (v) Through large-scale nuclear DFT calculations guide experimental efforts. The general organization of DFT-Applications and the underlying computational strategy are shown in Figure 44.

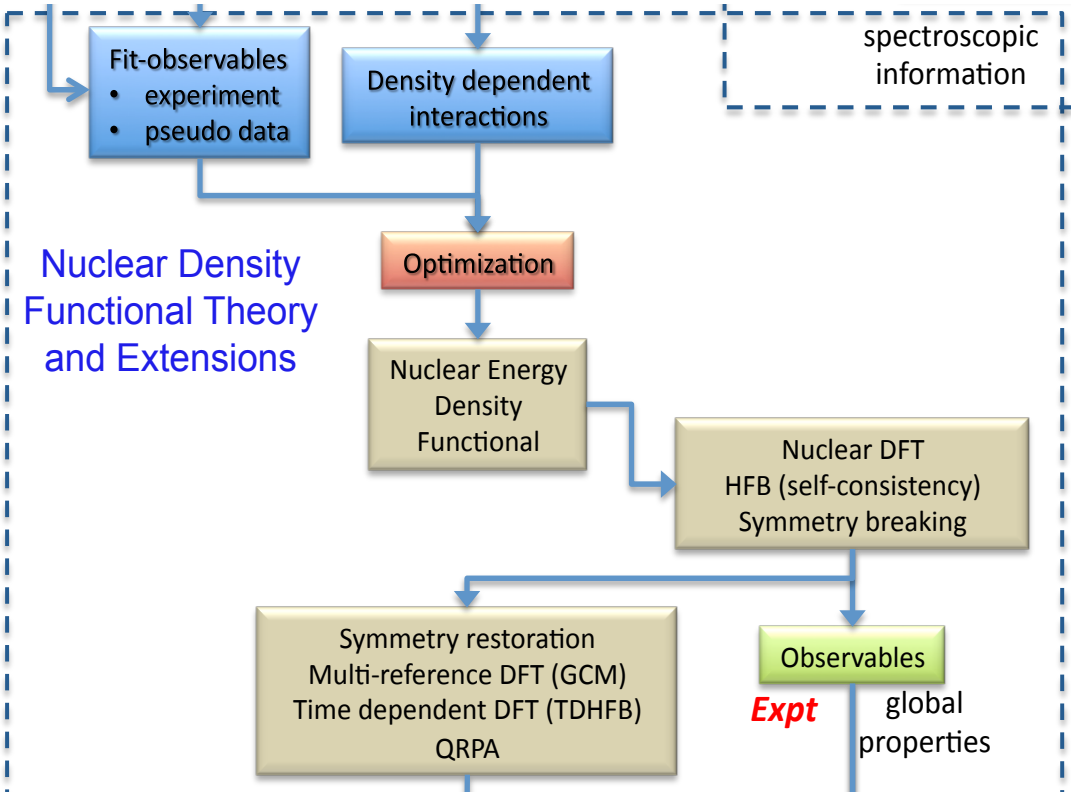

Figure 44: UNEDF's DFT Applications Computational Strategy on the UNEDF strategy diagram

This work was carried out by UTK/ORNL (Erler, Kortelainen, McDonnell, Nazarewicz, Nikolov, Olsen, Pei, Stoitsov), Schunck (LLNL), ANL CS/AM (Sarich, Wild), Bertulani (TAMU-C), with significant collaboration with international groups at Warsaw/Jyvaskyla (Dobaczewski, Satula), Lublin (Baran, Staszczak, Warda), and Reinhard (Erlangen).

During Year-5, several milestones have been accomplished in all areas of DFT-Applications activity. The numerical and computational achievements are discussed first. This is followed by an overview of benchmarking work and large-scale surveys.

Numerical and Computational Developments

HFODD solver development

A new official release of the HFODD DFT solver was published in Computer Physics Communications in 2012. Among many new features, version 2.49t of HFODD contains: a method to compute efficiently multi-dimensional potential energy surfaces using the readjustment of constraints based on the RPA matrix, the finite-temperature formalism, the shell correction, and isospin mixing and projection of the Hartree-Fock states. This is the first natively parallel version of the code. It is based on a hybrid MPI/OpenMP programming model and supports 3 different layers of parallelism: (i) the outer-most layer handles the various nuclear configurations (nuclei, deformations, etc.); (ii) the middle layer spreads the diagonalization of the HFB matrix across several cores using the ScaLAPACK library; (iii) the inner-most layer adds multi-threading capabilities via OpenMP instructions. This architecture is implemented using MPI communicators and groups. Multi-threading offers a factor 2-3 acceleration. Current work involves the development of the proton-neutron mixing HFB formalism, the acceleration of routines dealing with finite-range effective forces, the development of a natively parallel I/O layer based on the ADIOS library, the implementation of an interface to GPU architectures, and the development of a general toolkit for large-scale fission calculations. The code is the official DFT solver for the "Computational Nuclear Structure and Reactions" Incite award.

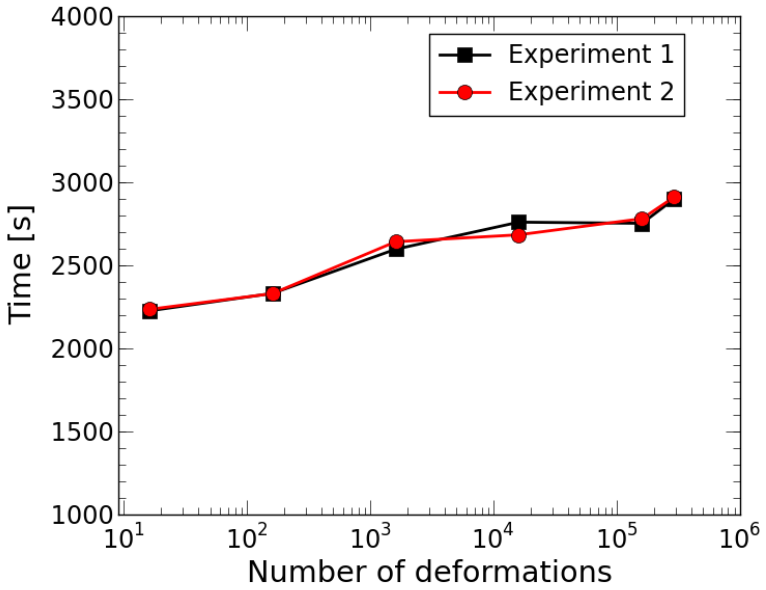

Figure 45: Scaling of HFODD on Titan (early access). Using large-scale parallelism enables to compute much larger potential energy surfaces at a near-constant computational cost. In these experiments, the code ran at the full scale of the ORNL Titan leadership class computer.

HFBTHO solver development

A new version of the code has been submitted to Computer Physics Communications under a joint publication between ORNL, UTK, ANL and LLNL involving both physicists and computer scientists. The new version includes advanced multi-threading support, which reduces the cost of one HFB calculation by a factor 6 on 8 threads. It is much more deeply integrated with our main

DFT solvers HFODD and contains a number of important new features such as the treatment of odd-mass nuclei, the finite-temperature HFB formalism, generalized Skyrme functionals and a method to compute multi-dimensional potential energy surfaces based on the readjustment of the constraints using the cranking approximation of the RPA matrix. HFBTHO is used primarily for large-scale optimization analyzes of Skyrme functionals, mass table computations, and as a pre-conditioner for potential energy surfaces in fission calculations.

Multi-resolution 3D HFB approach and its applications to superfluid Fermi systems

The goal of MADNESS-HFB project is to develop a high-precision, parallel, portable, symmetry-unrestricted 3D code based on multiresolution wavelet technology for determining nuclear structures and reactions in complex geometry and topologies. In Year-5, the benchmarking of MADNESS on realistic self-consistent HFB problems for cold fermions and nuclei has been accomplished by Fann, Pei, and others. We solved the HFB equations of the SLDA and ASLDA density functionals for cold Fermions, testing against the HFB-AX code that uses B-spline techniques. This benchmark demonstrated the first practical application of MADNESS for 3D Fermi systems with broken time-reversal symmetry, spin polarization, and pairing regularization (using zero-boundary conditions). Skyrme functionals for nuclei have also been implemented. We carried out the first implementation of an adaptive parallel pseudo-spectral method for 3D complex quasi-paricle wave functions; the nonlinear Hartree-Fock-Bogoliubov equations are solved, accurately and self-consistently, using integral scattering operators and adaptive approximations of nonlinear partial differential equations.

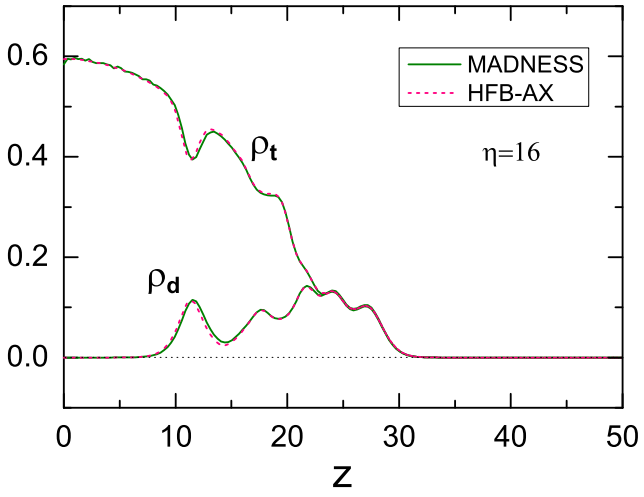

Figure 46: Benchmark of MADNESS with HFB-AX. Calculated total densities and polarized densities of 100 particles in an elongated trap with the aspect ratio η=16, assuming polarization P=0.2.

The constrained 3D Skyrme-HFB- MADNESS theory will be implemented and used for fission calculations.

Quasiparticle continuum and resonances in the Hartree-Fock-Bogoliubov theory

The quasiparticle energy spectrum of the HFB equations contains discrete bound states, resonances, and nonresonant continuum states. We studied the structure of the unbound

quasiparticle spectrum of weakly bound nuclei within several methods that do not rely on imposing scattering or outgoing boundary conditions. Various approximations were examined to estimate resonance widths. It was shown that the stabilization method works well for all HFB resonances except for very narrow ones. The Thomas-Fermi approximation to the nonresonant continuum has been shown to be very effective, especially for coordinate-space HFB calculations in large boxes that involve huge amounts of discretized quasiparticle continuum states.

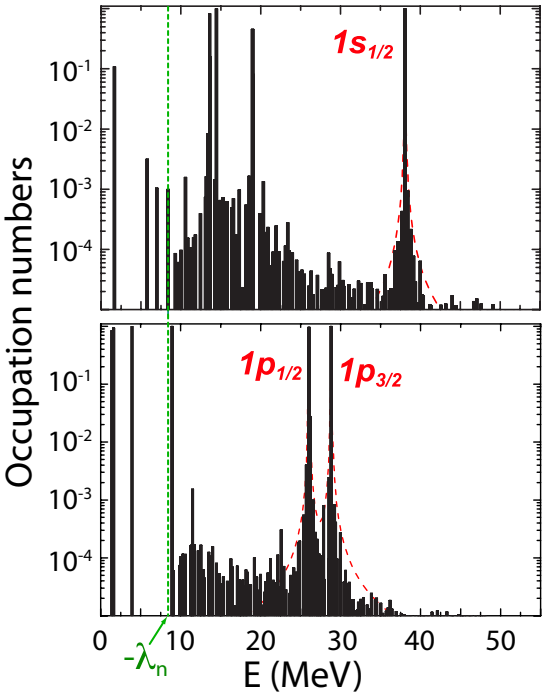

Figure 47: Occupation numbers of the discretized neutron quasiparticle continuum states in ^{70}Zn. The corresponding Breit-Wigner envelopes are indicated by dashed lines. The $-\lambda_n$ threshold is marked by a dotted line.

Benchmarking and Large-Scale Surveys

The Limits of the Nuclear Landscape

A team from UTK and ORNL used DFT with six nuclear energy density functionals and ORNL's Jaguar supercomputer to map the nuclear landscape. Earlier estimates of the nuclear landscape varied from as few as 5,000 to as many as 12,000 possible nuclei. Because most of these nuclei are beyond our experimental reach, models must conform to known nuclei in a way that allows researchers to extrapolate results for exotic nuclei. Insights on the nature of most exotic nuclei must be, in turn, extrapolated from those well-calibrated models.

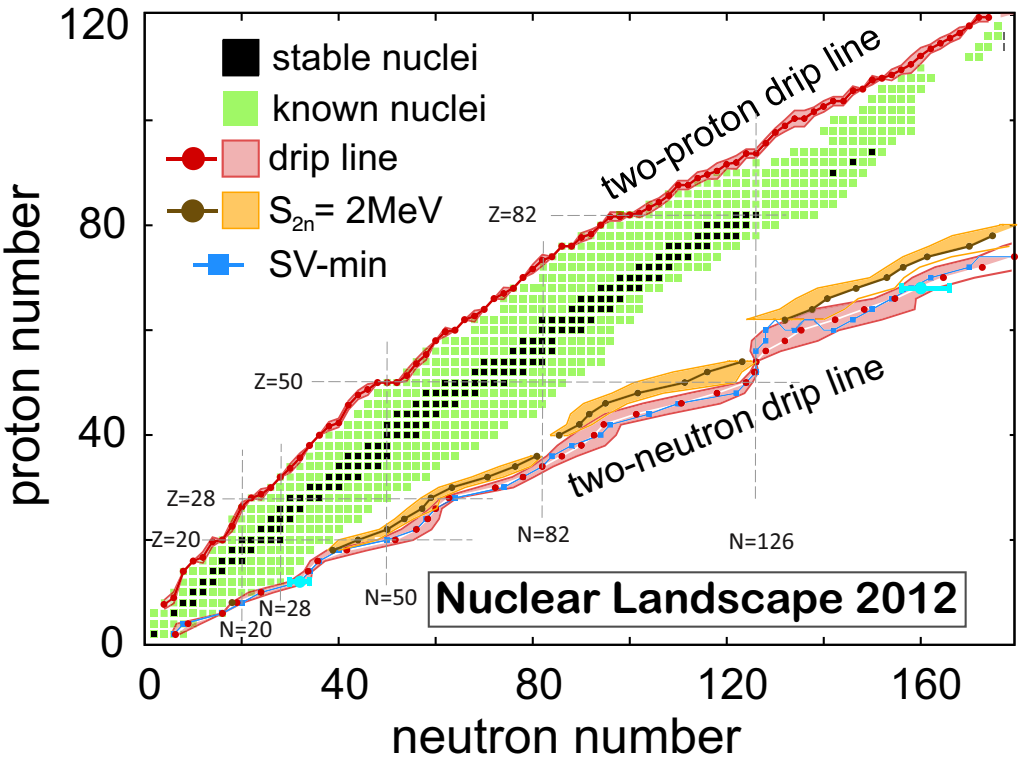

Figure 48: Map of bound even-even nuclei as a function of the proton number Z and the neutron number N. There are 767 even-even isotopes known experimentally: both stable (black squares) and radioactive (green squares). Mean drip lines and their uncertainties (red) were obtained by averaging the results of different models. The two-neutron drip line of SV-min (blue) is shown together with the statistical uncertainties at Z=12 and 68 (blue error bars). The S_{2n}=2 MeV line is also shown (brown) together with its systematic uncertainty (orange).

The calculations themselves were massive, with each set of nuclei taking about two hours to calculate on the 244,256-processor Jaguar system. Each of these runs needed to include about 250,000 possible nuclear configurations. By using several models, we were able for the first time to quantify uncertainties of predicted drip lines. The error on the position of the neutron drip line was shown to grow steadily with distance from the valley of stability. Model extrapolations turned out to be unexpectedly consistent between the current effective interactions, leading the team to estimate that the number of bound nuclei with Z between 2 and 120 is 6,900±500.

Global investigation of odd-even mass differences and radii with isospin-dependent pairing interactions

Neutron and proton odd-even mass differences are systematically studied with HF+BCS calculations with Skyrme interactions and an isospin-dependent contact pairing interaction. The strength of pairing interactions is determined to reproduce empirical odd-even mass differences in a wide region of the mass table. The importance of the isospin dependence of the pairing interaction is singled out for odd-even mass differences in medium and heavy isotopes. Proton and neutron radii are studied systematically using the same model.

Surface Symmetry Energy of Nuclear Energy Density Functionals

We studied the bulk deformation properties of the Skyrme nuclear energy density functionals. Following simple arguments based on the leptodermous expansion and liquid drop model, we applied the nuclear density functional theory to assess the role of the surface symmetry energy in nuclei. To this end, we validated the commonly used functional parametrizations against the data on excitation energies of superdeformed band-heads in Hg and Pb isotopes, and fission isomers in actinide nuclei. After subtracting shell effects, the results of our self-consistent calculations are consistent with macroscopic arguments and indicate that experimental data on strongly deformed configurations in neutron-rich nuclei are essential for optimizing future nuclear energy density functionals. The resulting survey provides a useful

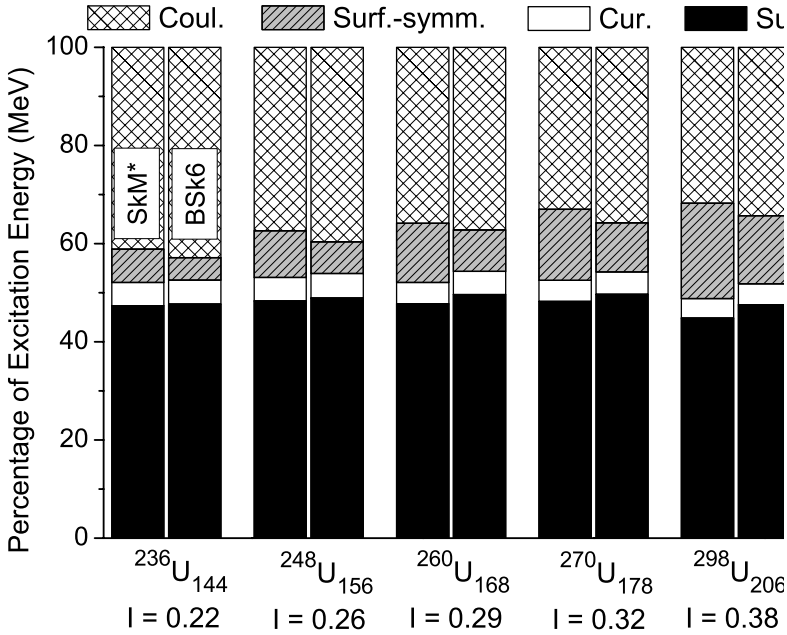

Figure 49: Relative contributions of the Coulomb, surface symmetry, curvature, and surface terms to the equivalent LDM excitation energy of fission isomers for the selected U isotopes. Calculations are based on SkM* and BSk6 EDFs.

benchmark for further theoretical improvements. Unlike in nuclei close to the stability valley, whose macroscopic deformability hangs on the balance of surface and Coulomb terms, the deformability of neutron-rich nuclei strongly depends on the surface-symmetry energy; hence, its proper determination is crucial for the stability of deformed phases of the neutron- rich matter and description of fission rates for r-process nucleosynthesis.

Optimization of Skyrme functionals for Nuclear Fission

We completed the optimization of generalized Skyrme functionals, and set up the infrastructure for optimizing more complicated functionals rooted in the Density Matrix Expansion (DME) of Chiral interactions.

During Year-5, using the UNEDF Experimental Database and the fast DFT solver HFBTHO, a new Skyrme-like energy density suitable for studies of strongly elongated nuclei was determined in the framework of the Hartree-Fock-Bogoliubov theory using the recently developed model-based, derivative-free optimization algorithm POUNDerS. A sensitivity analysis at the optimal solution has revealed the importance of states at large deformations in driving the parameterization of the functional. The good agreement with experimental data on masses and separation energies, achieved with the previous parameterization UNEDF0, is largely preserved. In addition, the new energy density UNEDF1 gives a much-improved description of the fission barriers in ^{240}Pu and neighboring nuclei. Furthermore, UNEDF1's new status as the input of choice when it comes to the microscopic study of the nuclear fission process sacrifices little. Indeed, UNEDF1 provides a

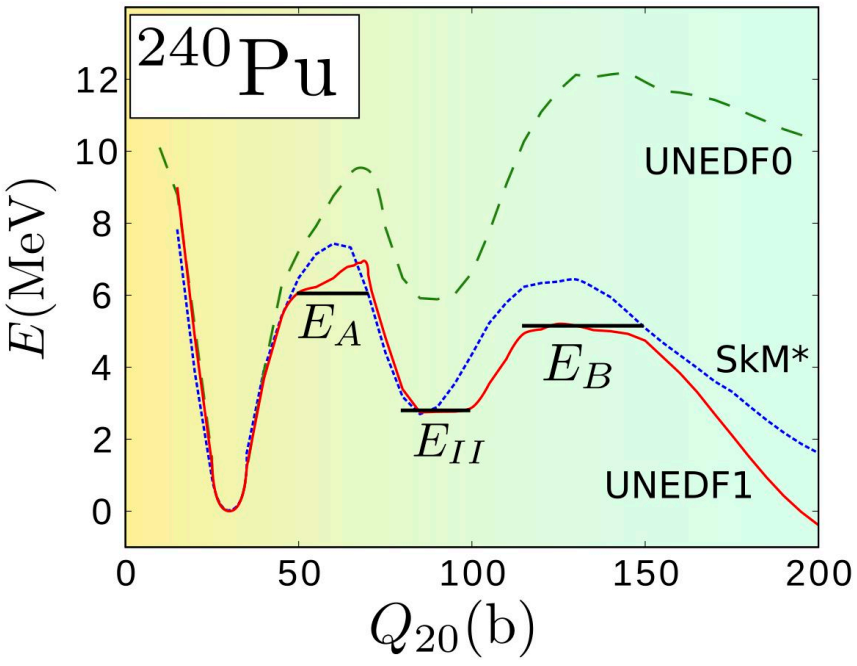

Figure 50: Fission pathway for ^{240}Pu along the mass quadrupole moment calculated with the SkM*, UNEDF0, and UNEDF1 energy density functionals. EII, EA, and EB denote the experimental energy of the fission isomer and the inner and outer barrier heights, respectively.

description of global nuclear properties that is almost as good as that of UNEDF0. Researchers are encouraged by the finding that deformation properties of the functional can be well-constrained by including only a handful of data relevant to fission. Although the quest for the microscopic fission theory is far from over, a crucial milestone towards this lofty goal has been reached.

Recently, the experimental dataset has been enhanced by adding data related to shell structure (spin-orbit splitting in closed shell nuclei), giant resonances, and neutron droplets pseudo-data from ab-initio calculations. generalized Skyrme functionals and DME functionals will be optimized on this new set. The new UNEDF functional will be used in large-scale surveys, spectroscopy, and description of fission.

Fission modes of mercury isotopes

Recent experiments on β-delayed fission in the mercury-lead region and the discovery of asymmetric fission in ^{180}Hg have stimulated theoretical interest in the mechanism of fission in heavy nuclei. We applied nuclear DFT employing Skyrme and Gogny energy density functionals to study fission modes and fusion valleys in ^{180}Hg and ^{198}Hg to reveal the role of shell effects in the prescission region and explain the experimentally observed fragment mass asymmetry and its variation with mass. The potential energy surfaces in multidimensional space of collective coordinates, including elongation, triaxiality, reflection-asymmetry, and necking, were calculated;

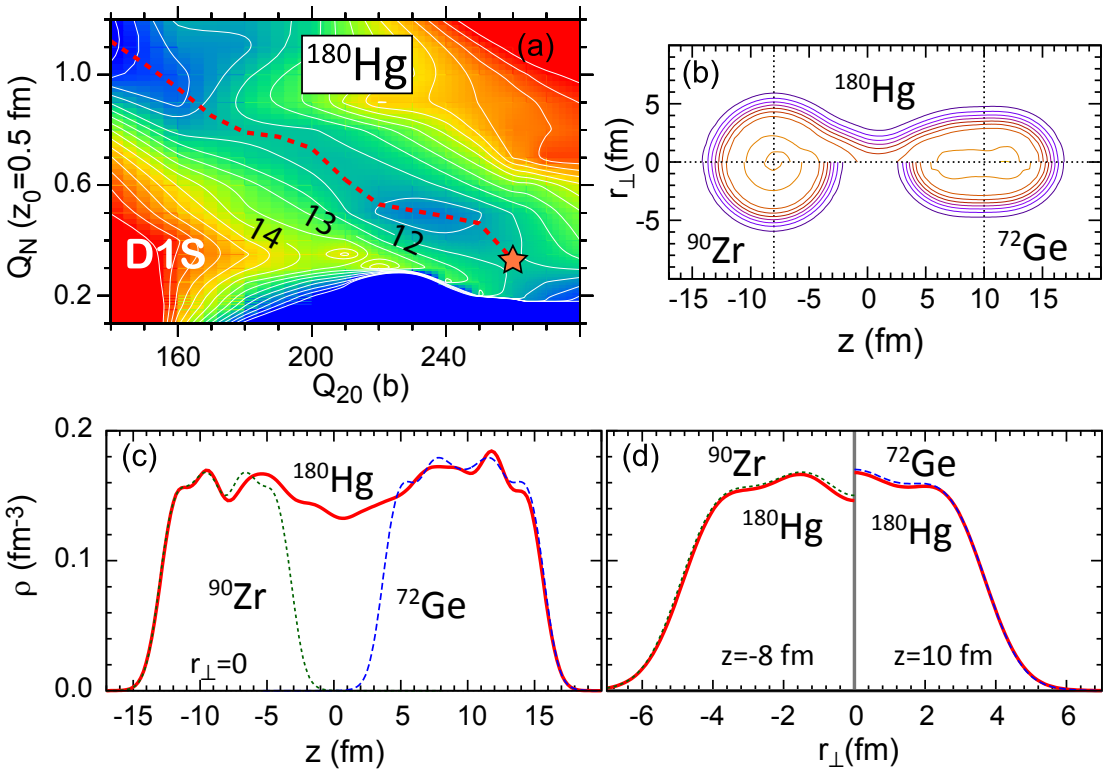

Figure 51: (a) PES of ^{180}Hg in the (Q_{20},Q_N) plane computed in HFB-D1S in the scission region. (b) Density distribution in ^{180}Hg close to scission [marked by a star in panel (a)] compared to density distributions of ^{90}Zr (in its spherical ground state) and ^{72}Ge (in the excited deformed configuration). The density profiles for $r\perp = 0$ (c), and for $z = -8$ fm and $z = 10$ fm (d) along the cuts marked by dotted lines in panel (b).

the asymmetric fission valleys — well separated from fusion valleys associated with nearly spherical fragments — were found in both cases. The density distributions at scission configurations were studied and related to the experimentally observed mass splits. The EDFs SkM* and D1S give a very consistent description of the fission process. We predict a transition from asymmetric fission in ^{180}Hg toward a more symmetric distribution of fission fragments in ^{198}Hg. For ^{180}Hg, both models yield ^{100}Ru/^{80}Kr as the most probable split.

Quadrupole collective inertia in nuclear fission: Cranking approximation

A collective mass tensor derived from the cranking approximation to the adiabatic time-dependent Hartree- Fock-Bogoliubov (ATDHFB) approach is compared with that obtained in the Gaussian overlap approximation (GOA) to the generator coordinate method. Illustrative calculations are carried out for one-dimensional quadrupole fission pathways in ^{256}Fm. It was shown that the collective mass exhibits strong variations with the quadrupole collective coordinate. These variations are related to the changes in the intrinsic shell structure. The differences between collective inertia obtained in cranking and perturbative cranking approximations to ATDHFB, and within GOA, were discussed.

Monopole strength function of deformed superfluid nuclei

We have proposed an efficient method for calculating strength functions using the finite amplitude method (FAM) for deformed superfluid heavy nuclei within the framework of the nuclear density functional theory. We demonstrated that FAM reproduces strength functions obtained with the

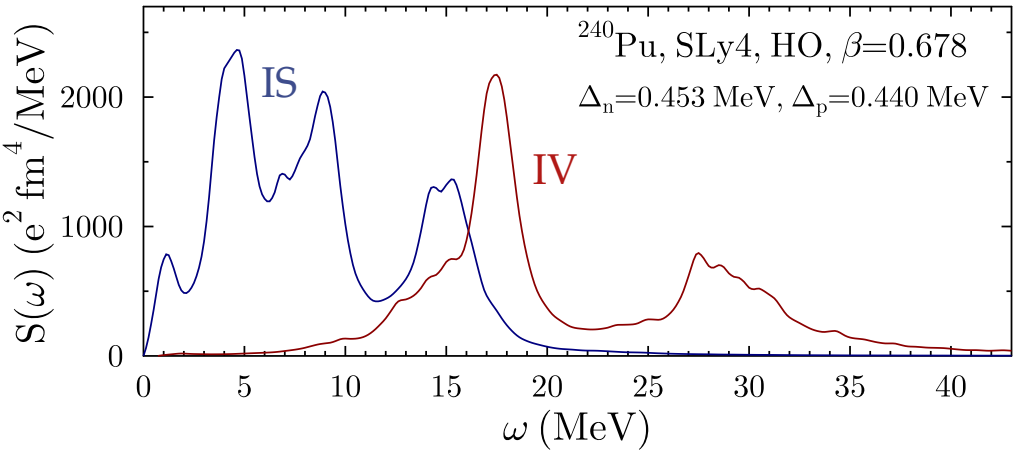

Figure 52: Isoscalar (IS) and isovector (IV) monopole strength in the superdeformed fission isomer of ^{240}Pu obtained in FAM-QRPA.

fully self-consistent quasi-particle random-phase approximation (QRPA) at a fraction of computational cost. As a demonstration, we computed the isoscalar and isovector monopole strength for strongly deformed configurations in ^{240}Pu by considering huge quasi-particle QRPA spaces. Our approach to FAM, based on Broyden's iterative procedure, opens the possibility for large-scale calculations of strength distributions in well-bound and weakly bound nuclei across the nuclear landscape

The extension of FAM to higher-multipolarity modes and to beta decay strength is in progress.

Other DFT Applications

Microscopic Calculations of Isospin-Breaking Corrections to Superallowed Beta Decay

The superallowed β-decay rates that provide stringent constraints on physics beyond the standard model of particle physics are affected by nuclear structure effects through isospin-breaking corrections. The self-consistent isospin- and angular-momentum-projected nuclear DFT, with no adjustable parameters, was used for the first time to compute those corrections for a number of Fermi transitions in nuclei from A=10 to A=74. The resulting leading element of the Cabibbo-Kobayashi-Maskawa matrix, $|V_{ud}|$=0.974 47(23), agrees well with the earlier benchmarks and implies that unitarity of the CKM matrix is satisfied with precision of 0.1%.

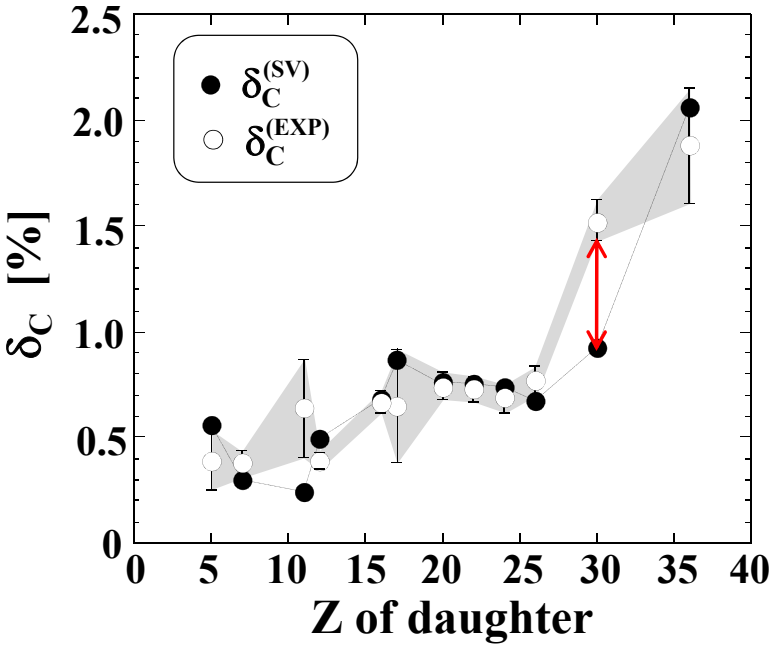

Figure 53: Calculated (black dots) and empirical (white dots, with error bars) values of isospin-breaking corrections as function of proton number in the daughter nuclei.

Occupation-number-based energy functional for nuclear masses

We developed an energy functional with shell-model occupations as the relevant degrees of freedom and compute nuclear masses across the nuclear chart. The functional is based on Hohenberg-Kohn theory with phenomenologically motivated terms. A global fit of the 17-parameter functional to 2049 nuclear masses yields a root-mean-square deviation of χ=1.31 MeV. Nuclear radii are computed within a model that employs the resulting occupation numbers.

DFT EXTENSIONS

The main goals of the DFTE research area of UNEDF are: (i) Develop modern computational infrastructure for extending the nuclear DFT to calculate excited states and their associated observables (transition probabilities, level densities, etc); (ii) Investigate the connection between EDFs and the CI effective Hamiltonians; (iii) Optimize the extensions of EDFs to theoretical and experimental data; (iv) Develop the technology to estimate theoretical uncertainties, especially when extrapolating to unknown regions; and (v) Through large-scale calculations guide experimental efforts, and provide input to the UNEDF nuclear reaction group. The areas covered by DFT-Extensions activity can be identified in the general UNEDF diagram and are shown in Figure 54.

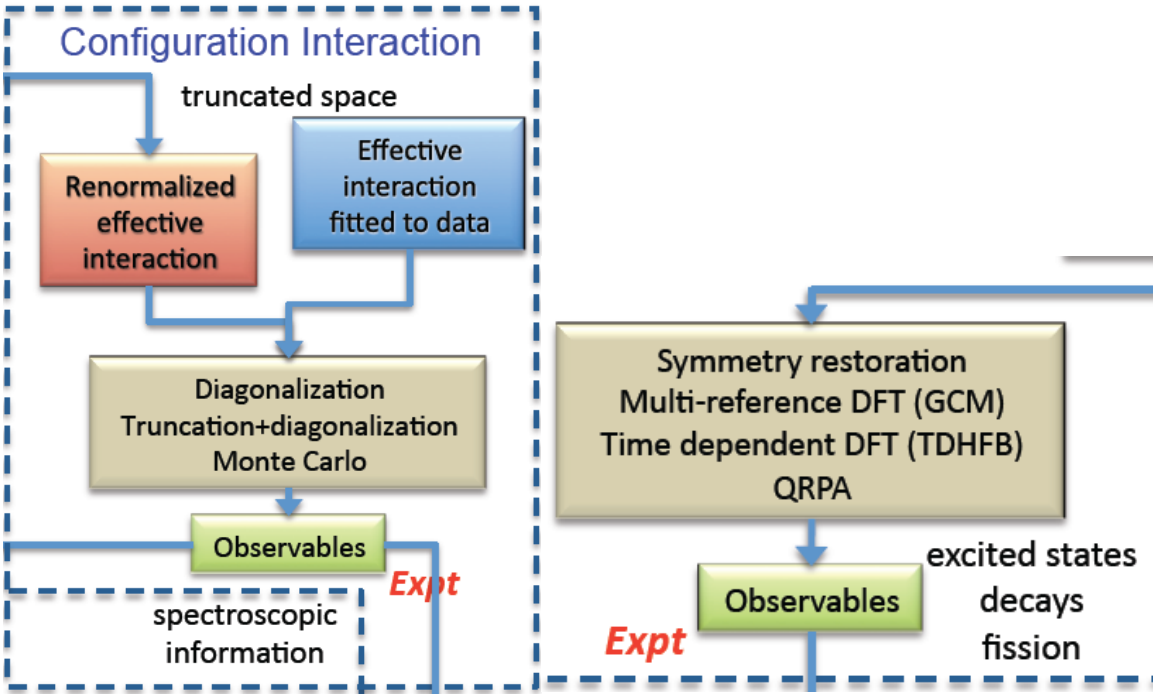

Figure 54: UNEDF's DFT EXTENSIONS Effort

During year 5 of the UNEDF project, several milestones have been accomplished in all areas of the DFT-Extensions activity. They are discussed below. The numerical and computational achievements are discussed first, followed by an overview of benchmarking work and large-scale surveys.

Numerical and Computational Developments

QRPA Calculations of Excited States in Deformed Nuclei

The UNC group experienced significant turnover in Year 5, as Terasaki left his postdoc position at the beginning of April 2011 for a position in Tsukuba, Japan. In July 2011,

Mustonen came from Finland to UNC as a postdoc. The interruption slowed progress toward Year-5 milestones, but nevertheless there were significant accomplishments in Year 5. In the spring of 2011, the first-ever systematic study in heavy nuclei with the deformed Skyrme-QRPA was completed, examining the performance of the QRPA framework itself and of individual Skyrme functionals in quadrupole vibrations across the rare-earth region of the isotopic chart. Later, a charge-changing version of the deformed-Skyrme-QRPA code was constructed, which is being also used for beta and double-beta decays. Figure 55 shows some of the results of the systematic vibration study. The functional SkM* turns out to reproduce the data well — better than the functional SLy4 — but not as well as a calculation that treats the vibrations as large amplitude motion in collective variables. (The QRPA is a small-amplitude approximation.) These results indicate that low-lying quadrupole states do indeed have a large-amplitude (multi-particle-multi-hole) component.

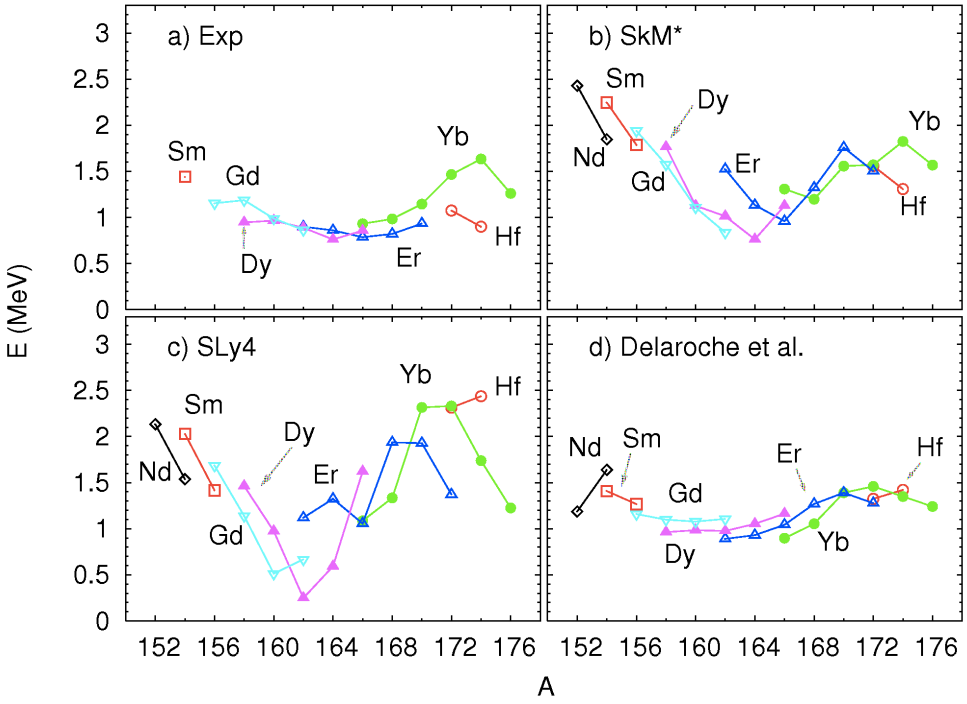

Figure 55: Energies of the lowest 2+ states in a wide-range of rare-earth nuclei. Panel a) shows the experimental results, panel b) the predictions of the QRPA with SKM*, panel c) the predictions with SLy4, and panel d) the results of a Gogny-based collective-model calculation that allowed large-amplitude motion.

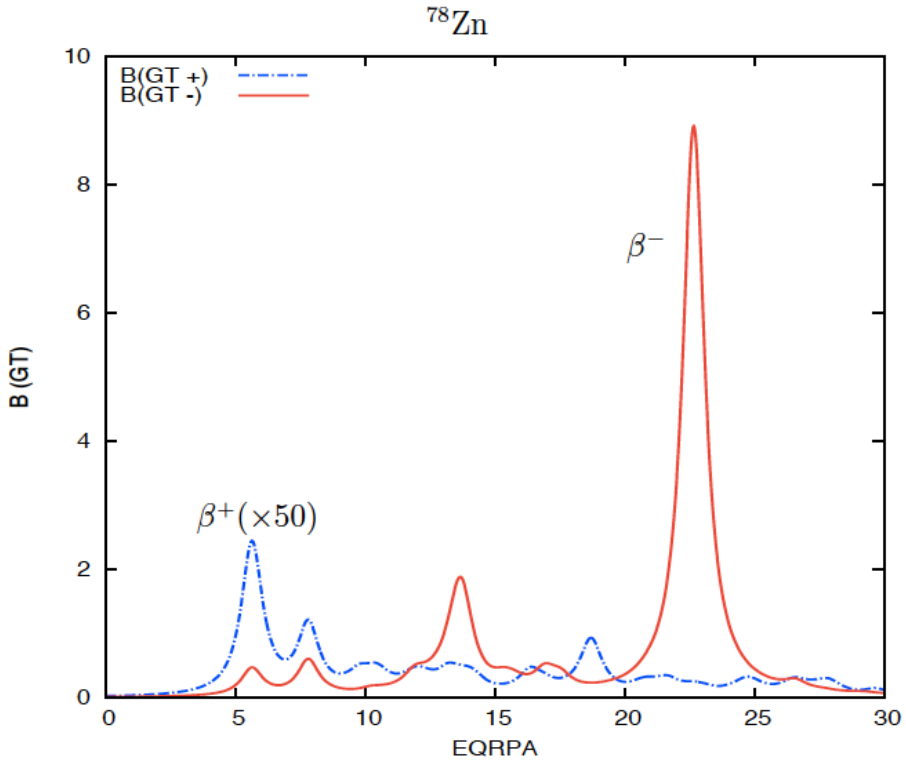

Figure 56: β^- and β^+ strength distributions in ^{78}Zn, calculated with a modified version of the Skyrme functional SkM* in our new charge-changing deformed-Skyrme QRPA.

The UNC group is leveraging 10M hours of Kraken time to apply the charge-changing code, which is now producing β-and ββ-decay rates for publication. Figure 56 shows an example: the β^- and β^+ strength distributions in the nucleus ^{78}Zn. Nuclei in this region are playing a large role in the synthesis of r-process elements in the first abundance peak. The calculations of ββ decay in ^{76}Ge, ^{130}Te, ^{136}Xe, and ^{150}Nd, the first with modern energy-density functionals, are nearly complete as well. The deformed QRPA code, QRPAdef, was under development by the UNC group (Engel and Terasaki).

TD SLDA Developments

The effort during Year 5 was directed in achieving the full implementation of the nuclear TDSLDA with all terms of the forces needed to perform realistic calculations. The University of Washington (UW) group, represented by Bulgac and Stetcu with the CS expertise of Roche (now at PNNL), has further optimized and improved the SLDA and TDSLDA codes and most of them have been re-written in C. During the last two years the UW group used more than 75M CPU hours on JaguarPF at NCCS and more than 8M CPU hours on Hopper at NERSC. The use of the computer cluster Hyak at UW, funded by an NSF MRI grant and UW, a cluster with 1120 PEs (140 nodes with double quad PEs), played a crucial role in their work. They performed a wide range of calculations of dilute Fermi gases and nuclei.

New collaborations with Bertulani (TAMU-C), J.E. Drut (UNC), Yu (Wuhan), Wlazlowski (Warsaw, who joined the NT group as a postdoc at the beginning and after that as UW visiting assistant professor), Moroz (who joined the UW NT group September 16th, 2011 as a postdoc), Nakatsukasa (RIKEN), and Reddy (INT) were initiated.

Some highlights of this effort:

- In Phys. Rev. C 84, 051309(R) (2011) a fully symmetry unrestricted Time-Dependent Density Functional Theory extended to include pairing correlations was used to calculate properties of the isovector giant dipole resonances of the deformed open-shell nuclei 172Yb, 188Os, and 238U, and to demonstrate good agreement with experimental data on nuclear photo-absorption cross-sections for two different Skyrme force parameterizations of the energy density functional: SkP and SLy4. This is the first calculation of the linear response of an open-shell triaxial nucleus. In particular, TDSLDA is a theoretical framework unique in theoretical physics. The numerical implementation is also unique and exceeds by a factor of 1000-2000 any TDHF codes. The code solves approximately 500,000 time- dependent 3D nonlinear coupled PDEs, a mathematical problem of unique complexity, apparently unparalleled in the literature.
- In Phys. Rev. Lett. 108, 150401 (2012) it was shown that in the collision of two superfluid fermionic atomic clouds, with a total of approximately 750 fermions, one observes the formation of quantum shock waves as discontinuities in the number density and collective flow velocity. Domain walls, which are topological excitations of the superfluid order parameter, are also generated and exhibit abrupt phase changes by π and slower motion than the shock waves. The domain walls are distinct from the gray soliton train or number density ripples formed in the wake of the shock waves and observed in the collisions of superfluid bosonic atomic clouds. Domain walls with opposite phase jumps collide elastically.
- In Phys. Rev. Lett. 107, 145304 (2011) it was shown, using an ab initio approach based on Quantum Monte Carlo techniques, that the pseudogap phase sets in for ultracold Fermi gases close to the unitary point. The onset of this phase at a value of the interaction strength corresponding to $(k_F a)^{-1} \approx -0.05$ (where "a" is the scattering length) was located. The evolution of the gap as a function of temperature and interaction strength in the Fermi gas around the unitary limit was determined and it was shown that the results exhibit a remarkable agreement with the recent wave-vector-resolved radio frequency spectroscopy data. The results indicate that the finite temperature structure of the Fermi gas around unitarity is more complicated and involves the presence of the phase with preformed Cooper pairs, which however do not contribute to the long-range order. This is the first ab initio calculation of a realistic strongly interacting Fermion system that demonstrates pairing correlations similar to those observed in high-temperature superconductors.

Benchmarking and Large-Scale Surveys

Nuclear Level Densities: Moments Code

Senkov and Horoi implemented a new algorithm that calculates the 2nd moments of the Hamiltonian, i.e. the widths, for pure $N\hbar\omega$ configurations. These widths can be further used to calculate nuclear level densities free of center-of-mass spurious contribution via an algorithm developed by Horoi and Zelevinsky. The new algorithm was integrated into the JMoments code and was validated for several sd-shell nuclei, either by comparing with exact shell model results or with experimental data. Using this algorithm, spurious-free shell model nuclear level densities for un-natural parity states of nuclei in the middle of the sd-shell were calculated for the first time. An example for the 1^- states in ^{26}Al is presented in Figure 58. The JMoments code was parallelized using MPI and a simple, but efficient, load-balancing algorithm. The domain decomposition was performed along the collection of many-body configurations built on spherical single-particle orbits. The new code was benchmarked on Franklin at NERSC and it showed good strong scaling up to 4,096 cores for the case of ^{26}Si (see Figure 57). The results were published in Physics Letters B. A report describing the algorithm and the usage of the code was submitted to Computer Physics Communication.

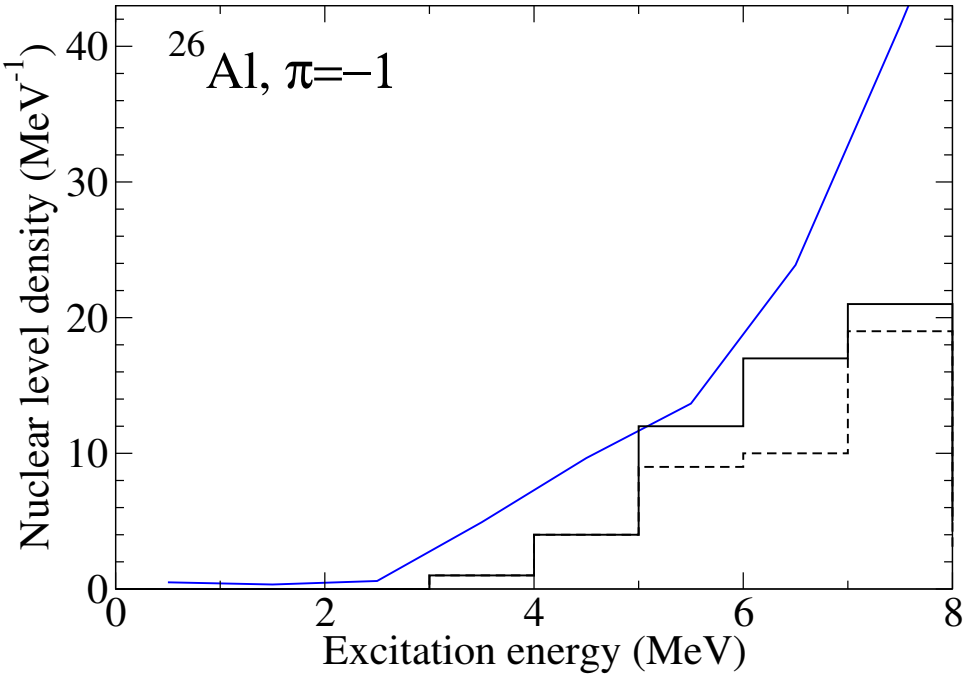

Figure 58: **Calculated level density of the 1^- states in ^{26}Al (blue line), compared with the available experimental data (staircases). Dashed staircases set the experimental lower limit.**

The benchmark indicates that the almost-perfect scaling could be extended to tens (and possibly hundreds) of thousands of cores. Tests with many cores would require reliable

effective interactions in larger valence spaces, which would span more than one major shell. Horoi also collaborated with Brown and McDonald to validate, port, and benchmark the new CI code NuShellX to MPI. NuShellX was used by Senkov to calculate exact CI level densities, to validate the results of the moments method.

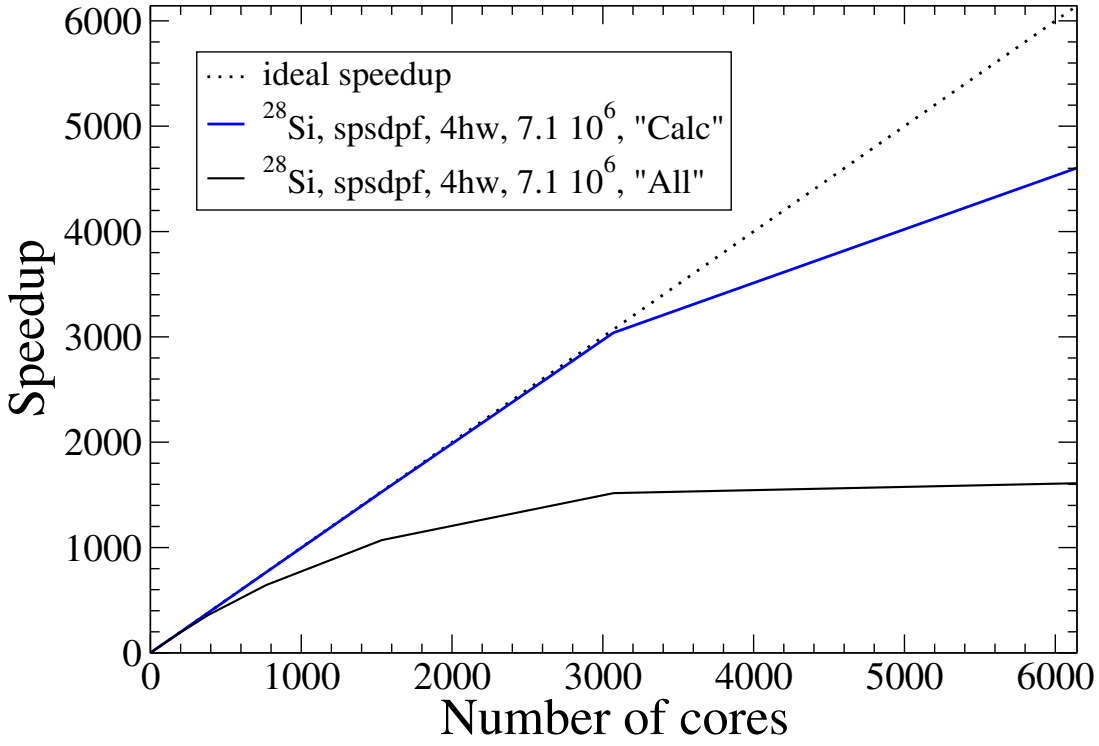

Figure 59: Hard scaling of the MPI version of the JMoments code used to calculate spin- and parity-projected nuclear level densities. "All" designate the total time needed to complete the calculation, while "Calc" excludes the time needed for some preparations that does not yet scale efficiently.

Investigation of performance of the J-scheme CI code NuShellX

UNEDF supported the computational development of the LCCI code NuShellX. This code works in a basis with protons of angular momentum J_p and neutrons with angular momentum J_n coupled to a total angular momentum J. The Hamiltonian matrix is calculated "on-the-fly." The original code written by Bill Rae uses OpenMP and was written for the Intel compiler, ifort. The developmental work on NuShellX was primarily carried out by the MSU group, and is one of the main computational tools used for the development of CI methods and for the collaborations with the experimental groups. In February of 2010 McDonald started to work on the project half-time with the other half supported as a consultant at the Institute for Cyber Enabled Research at MSU. The first task was to make the modifications required to work with the PGI compiler. This has made the code more portable.

Brown has worked on the wrapper code. This now includes integration with a database for the table of isotopes with automated graphics for comparison between theory and experiment. Also, a new Hamiltonian code was started that generates starting interactions for new model spaces based on both microscopic nucleon-nucleon interactions and DFT results.

During Year 5, Bill Rae produced a new OpenMP version of NuShellX. This version was organized to be more portable to MPI. Eric McDonald successfully performed the port from the reorganized OpenMP-only code to a MPI/OpenMP hybrid code. The Year 5 goals of analyzing the scalability constraints of the code, evaluating options for reaching the petascale level, and producing a working MPI/OpenMP hybrid version were met. The hybrid version has been shown to scale to a much larger number of cores that the original OpneMP-only code.

Benchmarking and Extending the Capabilities of the BIGSTICK CI code

SDSU's primary role in UNEDF, in collaboration with Erich Ormand of Lawrence Livermore National Lab, was developing BIGSTICK (successor to REDSTICK), a configuration-interaction shell-model (CI-SM) code, for *ab initio* calculations of energies and densities of light nuclei to be used to constrain and validate the EDF. The UNEDF grant to SDSU supported half of Krastev's salary, with the remainder coming from LLNL. The Office of Science grant supports travel for both the PI and for Krastev, as the UNEDF grant does not cover travel. However, Krastev left in summer 2011 for a permanent staff position in scientific computing support at Harvard. We received permission to rebudget the remaining amount to buying out the PI's teaching time to finish the project. This was supplemented by a buyout from Livermore.

We have made significant progress in the new code, with three-body forces implemented in a scalar version. While the mat-vec multiple operation is well-parallelized, our orthogonalization is still a drag on the code. Investigation shows this is largely due to I/O. (Unfortunately part of the investigation was done by computer scientists at Oak Ridge in late 2010, but the report got lost in e-mail and we only received it in June 2011.) Comparison with the MFD code suggests storage of the Lanczos vectors is the best route to avoid I/O. The parallel distribution of the mat-vec operations have been rewritten with additional instrumentation of the timing. With a modest (500k hours) Director's Discretion grant on Jaguar at ORNL, the code's scalability has been investigated. The efficiency of the matvec operation is above 70-80% up to 16000 cores.

REACTIONS

The main goal of this part of UNEDF has been to develop modern reaction theory based on microscopic nuclear structure input. For light nuclei, *ab initio* scattering (described in part above in the Ab-Initio Structure and Reactions section) calculations are now possible that can guide developments in medium-mass and heavy nuclei. The coupling between structure and reactions is accomplished by (i) using structural Hamiltonian matrix elements directly in microscopic calculations for scattering; (ii) using QRPA occupation amplitudes for ground and excited states to calculate matrix elements for neutron excitation; (iii) adapting the density functional itself to give effective interactions between continuum states; (iv) using QRPA amplitudes to give the transition potentials for a full coupled-channels (CCh) calculation of scattering; (v) to extract the optical potential, and also to (vi) to examine the statistical methods needed to average over compound-nucleus resonances for the optical potentials. We alternatively used a two-step model to simplify steps (iv-v). The general organization of parts (ii-vi) is shown in Figure 60. Our reaction work required large-scale parallel computing, in particular in the final year.

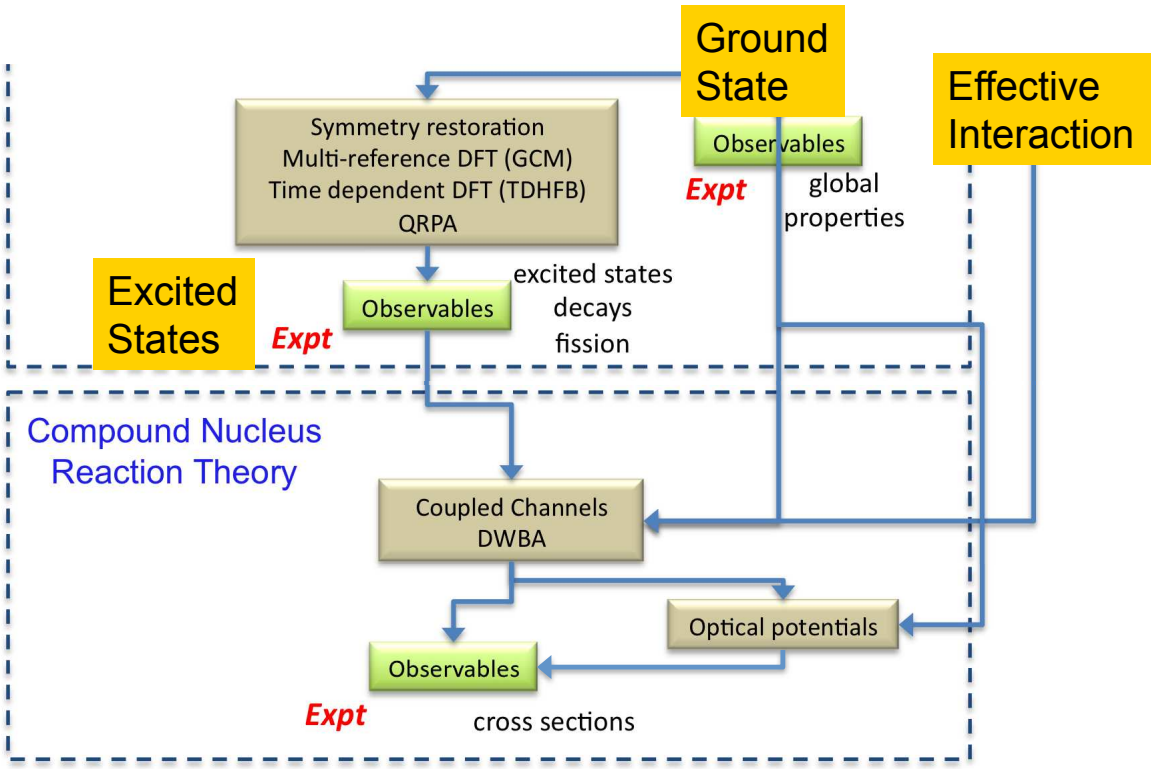

Figure 60: Workflow for reaction theory using the structure results of the gold-colored boxes.

Ab Initio Reactions

We continued the development and application of *ab initio* many-body reaction theory through the merging of the NCSM and the RGM. Navratil and Quaglioni were principally involved in this work and collaborated with Roth (Darmstadt) and Kruse (University of Arizona, now LLNL) by using the importance truncation method to improve the nuclear structure calculations. Based on our previous study of p+^{7}Be scattering, performed under UNEDF, we applied the NCSM/RGM approach to the astrophysically important reaction ^{7}Be(p,γ)^{8}B and obtained the first *ab initio* many-body calculation of this cross section starting from a Similarity Renormalization Group (SRG) evolved chiral nucleon-nucleon interaction (with Λ=1.86 fm^{-1}) that describes accurately two-nucleon data. Our calculations predict simultaneously both the normalization and the shape of the S-factor that, at zero energy, assumes the value $S_{17}(0)$ = 19.4(7) eV b, on the lower side of, but consistent with, the latest evaluation of 20.8 ± 0.7 (expt.) ± 1.4 (Theory). These results were obtained with the largest realistic model space currently achievable, including the five lowest eigenstates of ^{7}Be in an harmonic oscillator basis size N_{max}= 10. The influence of higher ^{7}Be excited states and/or of larger harmonic oscillator excitations was explored and used to estimate our uncertainty in the obtained value of $S_{17}(0)$. This work has been published. Continuing on our past UNEDF efforts to arrive at a far more unified description of both bound and scattering states, we have completed nucleon-^{8}He calculations to study the impact of continuum states on the low-lying structure of ^{9}He. Our n+^{8}He results indicate that the ground state of ^{9}He is a positive-parity ½+ state (*S*-wave scattering length of -12.59 fm, most likely due to the softness of the potential adopted – SRG evolved chiral nucleon-nucleon interaction with Λ=2.0 fm^{-1}). The *P*-wave resonance, found at about 1.7 MeV, is in a good agreement with experiment and is quite stable with respect to the number of ^{8}He excited states included in the calculation. Experimentally, the parity of the ground-state is still under debate. A paper on this subject is in preparation. Other applications of NCSM/RGM to reactions in light nuclei are described in the Ab-Initio Structure and Reactions section.

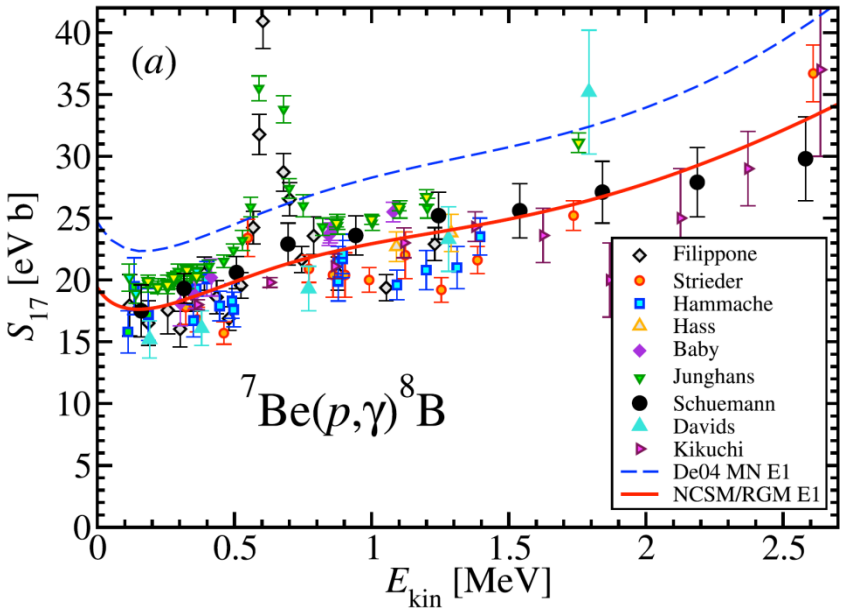

Figure 61 Calculated S-factor for the ^{7}Be(p,γ)^{8}B radiative capture obtained with an SRG evolved interaction from chiral EFT N^{3}LO interaction with Λ=1.86 fm^{-1}. *Ab initio* theory predict simultaneously both normalization and shape of S_{17}.

Coupled-Channels Calculations

Effective interactions for coupled-channels scattering

Nobre (LLNL) and Thompson (LLNL) performed large-scale coupled-channels calculations for the determination of cross sections or the extraction of optical-model potentials, which required (diagonal and off-diagonal) coupling potentials as input, and in turn contained information on the structure of the target nucleus and on the effective NN interaction between the projectile (nucleon) and target nucleons. While the former could be obtained from QRPA nuclear-structure calculations based on DFT results, the latter were not determined in a straightforward manner. One of the UNEDF goals was to determine effective interactions appropriate for large-scale reaction calculations and to incorporate these into the reaction codes. In Year-4, the folding formalism and codes were extended by Escher (LLNL) to handle several forms of density-dependent interactions, and local approximations for the treatment of the exchange terms has been investigated. We found that the density dependence is particularly important even to set the depth of the diagonal monopole folded potentials. We also implemented coupled-channels scattering methods using the radius-dependent effective masses inspired by Skyrme density functionals, and found that the renormalization of the coupling lead to a reduction in the effective couplings strengths.

Coupled-channels excitations

The methods of Nobre (LLNL) and Thompson (LLNL) for the microscopic calculation of the optical potentials for neutron-nucleus scattering by explicitly calculating the couplings between the elastic channel and all the channels reached by moving one particle either within the target, or (in a transfer reaction) to the projectile. With recent computational developments with Summers (LLNL), we performed very large coupled-channel calculations for neutron and proton reactions on the range of nuclear masses A=40, 48, 58, 90 and 144. Couplings were calculated to correlated QRPA states, for target excitations up to limits in the range of 10–60 MeV for projectile energies from 5 to 60 MeV (lab). We found that the couplings *between* RPA excited states were not significant at energies above 10 MeV, so focused on large coupled-channels calculations with couplings from and back to the elastic channel. Large-scale computing was necessary to include all the RPA channels as well as the non-local transfer couplings to the deuteron channels, with up to 20000 partial waves in a coupled-channels set.

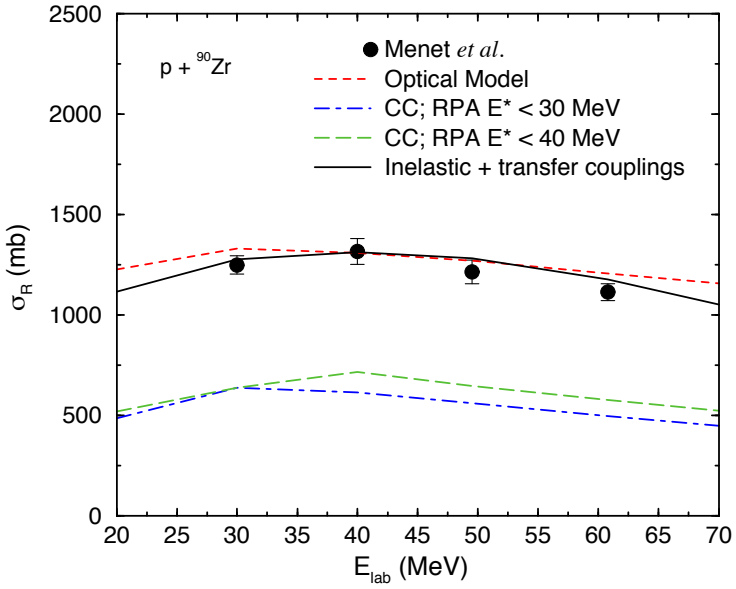

Figure 62 Total reaction cross-section as a function of the incident energy for the reaction p + 90Zr using the Gogny D1S force. The results are shown for couplings to the inelastic RPA states lying below 30 (dash-dotted line) and 40 MeV (dashed line), and to the inelastic and transfer channels with non-orthogonality corrections (solid line). The Koning-Delaroche optical model calculations are shown as short-dashed lines.

Our calculations showed that reaction cross sections calculated in this approach compared well to predictions of a fitted optical potential and to experimental data. For the first time observed reaction cross-sections are completely accounted for by explicit channel coupling, for incident energies between 20 and 70 MeV, as shown in Figure 62. The resulting work has been published in Physical Review Letters and a longer paper in Physical Review C. The most recent work has been to fit local optical potentials to reproduce the cross sections of the coupled-channels calculations, and to use these local

potentials consistently in the deuteron channel by means of the Johnson-Soper approximation.

Nonlocal Optical Potentials

The success of the above reproduction of reaction cross sections without the couplings between the RPA states supported a 'doorway approximation' that models the elastic optical potential in terms of its first-order couplings only. In the doorway approximation the further decay of the RPA doorway states, whether to nucleon escape or to compound-nucleus production, does not affect the flux that they take from the elastic channel. Thompson (LLNL) therefore developed, alongside the coupled channels methods, a two-step model to calculate optical potentials directly in terms of the QRPA couplings and occupied mean-field states. This model enabled the ready production of non-local optical potentials from the mean-field structure models being produced by the UNEDF collaboration. In Year 4, he also developed new systematic methods for *using* the non-local optical potentials within FRESCO, his standard scattering code. This enables the new non-local potentials to be used as entrance optical potentials in wide range of elastic, inelastic, transfer and breakup calculations. We find surprising large L-dependence in these potentials, even though the range of non-locality is not more than 2 or 3 fm. This work has now been taken over as the PhD project of Luke Titus at Michigan State University, in order to systematically examine the role of optical-potential L-dependences & non-localities in direct reaction calculations, in particular (N,γ) capture reactions which are sensitive to the scattering wave functions in the low partial waves. Results will be compared with the use of local equivalent potentials without L-dependence.

Statistical Theories of Nuclear Reactions and Hauser-Feshbach

Arbanas (ORNL), Bertulani (Tamu-Commerce), Roche (PNL), Kerman (MIT) and Ushkhala (Tamu-Commerce) extended and applied the KKM (Kawai, Kerman and McVoy) model to doorway states. They prototyped doorway states on 1 CPU. Energy dependence was introduced into KKM expressions for more accurate energy averaging, and was implemented in a parallel code that relies on an eigensolver for "ensemble" of complex symmetric matrices developed by K. Roche. This led to a potentially useful computational tool for other parts of the UNEDF effort: a parallel eigensolver for large sets of complex symmetric matrices. A new paper also examines the effect of energy-dependence of eigensolutions in the expansion for the KKM theory. The KKM theory was formally extended to intermediate structure via doorway states; this result provides a formal justification for using intermediate structure (doorway) optical potentials.