Iowa State University – Final Report for SciDAC3/NUCLEI

The Iowa State University (ISU) contributions to the NUCLEI project are focused on developing, implementing and running an efficient and scalable configuration interaction code (Many-Fermion Dynamics – nuclear or MFDn) for leadership class supercomputers addressing forefront research problems in low-energy nuclear physics. We investigate nuclear structure and reactions with realistic nucleon-nucleon (NN) and three-nucleon (3N) interactions. We select a few highlights from our work that has produced a total of more than 82 refereed publications and more than 109 invited talks under SciDAC3/NUCLEI. Since our works are built upon previous successes, it is most useful to review the highlights of the most recent years of SciDAC3/NUCLEI.

(1) The SciDAC-NUCLEI team at ISU participates in the Low Energy Nuclear Physics International Collaboration (LENPIC, http://www.lenpic.org/) to develop and apply a new generation of chiral Effective Field Theory (EFT) nucleon-nucleon (NN) and three-nucleon (3N) interactions. We completed and published an initial investigation of the chiral EFT NN interaction through fifth order (N4LO). The ISU team solved for the properties of light nuclei up through A = 6 as a function of the retained chiral order and as a function of the local regulator. We performed analyses of ground state energies, excitation energies and selected electromagnetic observables. This LENPIC project includes solutions for scattering observables in 3-body systems to quantify the chiral and regulator uncertainties. All results point to consistent behavior of the chiral EFT interactions with increasing chiral order and to the need for chiral 3N interactions at the N2LO order and above. We also tested and applied the Similarity Renormalization Group approach to soften the NN interactions, generate induced NNN interactions and achieve converged results for bound state properties in these light nuclei. This first LENPIC project has been published (S. Binder, et al., LENPIC collaboration, Phys. Rev. C 93, 044002 (2016). A second LENPIC project, extending the results of the first paper to a wide range of nuclei and including many additional observables has been submitted to Physical Review C and is available online (S. Binder, et al., LENPIC collaboration, arXiv:1802.08584). A third paper is in preparation solving for properties of nuclei with LENPIC NN + 3N interactions consistent through N2LO.

(2) Ab initio calculations of nuclei face the challenge of simultaneously describing strong short-range internucleon correlations and the long-range properties of weakly-bound halo nucleons. Natural orbitals, which diagonalize the one-body density matrix, provide a basis which is better matched to the physical structure of the many-body wave function. Together with Mark Caprio and his student, Chrysovalantis Constantinou, at Notre Dame University, we demonstrated that the use of natural orbitals significantly improves convergence for ab initio no-core configuration interaction calculations of the neutron halo nucleus 6He, relative to a harmonic oscillator basis (Chrysovalantis Constantinou, Mark A. Caprio, James P. Vary and Pieter Maris, "Natural orbital description of the halo nucleus 6He," Nuclear Science and Techniques (NST) 28, 179 (2017) [arXiv:1605.04976].)

(3) In collaboration with the SciDAC SUPER Institute, the LBNL team continued its work on the optimization of sparse matrix-multiple vectors multiplication, which aimed at improving the performance of sparse block eigensolvers for MFDn. This has led to major improvements

in the last year and to a publication in 2018 of the major findings. (M. Shao, H.M. Aktulga, C. Yang, E.G. Ng, P. Maris and J.P. Vary, "Accelerating nuclear configuration interaction calculations through a preconditioned block iterative eigensolver," Computational Physics Communications 222, 1 (2018) [arXiv:1609.01689]). In particular, we demonstrated the benefit of using a preconditioned block iterative method to replace the Lanczos algorithm that has traditionally been used to perform this type of computation. The rapid convergence of the block iterative method is achieved by a proper choice of starting guesses of the eigenvectors and the construction of an effective preconditioner. These acceleration techniques take advantage of special structure of the nuclear configuration interaction problem which we discuss in detail. The use of a block method also allows us to improve the concurrency of the computation, and take advantage of the memory hierarchy of modern microprocessors to increase the arithmetic intensity of the computation relative to data movement. We also demonstrated that implementation details are critical to achieving high performance on massively parallel multi-core supercomputers, and we demonstrated that the new block iterative solver is two to three times faster than the Lanczos based algorithm for problems of moderate sizes on a Cray XC30 system.

(4) In collaboration Bruce Barrett, Andrey Shirokov and others we have developed and successfully applied an extension of the NCSM that restores the core in a theoretically controllable way and enables access to heavier nuclei in standard shell model (valence nucleon) calculations (E. Dikmen, A. F. Lisetskiy, B. R. Barrett, P. Maris, A. M. Shirokov and J. P. Vary, "Ab initio effective interactions for sd-shell valence nucleons," Phys. Rev. C 91, 064301 (2015); arXiv:1502.00700).

(5) The ISU and Old Dominion University (ODU) teams have developed an application which combines the code POUNDERs with MFDn to search for improved NN interactions through phase-shift-equivalent transformations. During year 4, we succeeded in applying this application to develop a new NN interaction, "Daejeon 16". We used phase-equivalent transformations to adjust off-shell properties of similarity renormalization group evolved chiral EFT NN interaction (Idaho N3LO) to describe binding energies and spectra of light nuclei without NNN forces. (A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris and J.P. Vary, "N3LO NN interaction adjusted to light nuclei in *ab exitu* approach," Phys. Letts. B 761, 87 (2016); arXiv: 1605.02819).

(6) We utilized various ab initio approaches to search for a low-lying resonance in the four-neutron (4n) system using the JISP16 realistic NN interaction. Our most accurate prediction was obtained using a J-matrix extension of the no-core shell model and suggests a 4n resonant state at an energy near E = 0.8 MeV with a width of approximately Γ = 1.4 MeV. (A.M. Shirokov, G. Papadimitriou, A.I. Mazur, I.A. Mazur, R. Roth and J.P. Vary, "Prediction for a four-neutron resonance," Phys. Rev. Letts. **117**, 182502 (2016); arXiv: 1607.05631).