Ab Initio No-Core Shell Model with Leadership Class Supercomputers

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Nuclear structure and reaction theory is undergoing a major renaissance with the advent of high performance computing, advanced many-body methods and strong interactions with greatly improved links to Quantum Chromodynamics (QCD). Predictive power, with well-quantified uncertainty, is emerging from non-perturbative approaches along with the potential for new discoveries such as predicting nuclear phenomena before they are measured. I will present an overview of some the recent developments and discuss some of the challenges that lie ahead. Among my selection of topics, I will discuss: (1) strong interactions derived from chiral effective field theory; (2) large sparse matrix eigenvalue problem; (3) emergence of collective nuclear motion; (4) quantifying uncertainties; (5) coupling to continuum states; and (6) high-performance computer resource needs/utilization – especially leadership-class supercomputers. Recent reviews and research papers provide valuable background material [1-10]. This work was supported in part by the US Department of Energy [DESC0005248, DE-FC02-09ER41582 (Sci-DAC/UNEDF), DE-FG02-87ER40371], the National Energy Research Scientific Computing Center. This work was also supported by supercomputing resources under a DOE INCITE award for use of Mira at Argonne National Lab and Titan at Oak Ridge National Lab.

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