NUCLEI

Nuclear Computational Low-Energy Initiative

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The NUCLEI (NUclear Computational Low-Energy Initiative) project will build upon recent successes in large-scale computations of atomic nuclei to provide results critical to nuclear science and nuclear astrophysics, and to nuclear applications in energy and national security. The large-scale computations we envision will transform the fields of low-energy nuclear physics and astrophysics. Physics topics to be addressed include nuclear interactions and their uncertainties, ab-initio studies of light nuclei and their reactions and of nucleonic matter and its astrophysical properties. We will also fundamentally advance the studies of neutron-rich nuclei and the fission of heavy nuclei, and the key nuclear physics issues in neutron stars and tests of fundamental symmetries.

All these efforts are closely coupled to research in mathematics and computer science, and to the large-scale simulations needed to accomplish our goals. We specifically focus on areas where large-scale simulations can have a critical impact on the experimental nuclear science program, nuclear applications, and the wider physics and computer science / applied mathematics communities.

Key computational codes include ab-initio and density-functional theories:

- Quantum Monte Carlo (GFMC and AFDMC)
- Configuration Interaction
- Configuration Interaction/Resonating Group approaches to scattering
- Coupled Cluster
- Density Functional Theory
- Time-Dependent Density Functional Theory

Key computer science and applied math questions to be addressed include:

- Load Balancing on the largest available machines
- Numerical and Performance Optimization
- Eigensolvers and Non-linear Solvers
- Model Validation
- Uncertainty Quantification
- Multiresolution Analysis

Ab-initio codes like GFMC, AFDMC, and CI scale well beyond 100K cores, and will allow us to study key physics issues including fusion reactions of astrophysical and applied physics interest, tests of fundamental symmetries, neutrino-nucleus scattering for astrophysics and for terrestrial experiments.

Density functional codes also scale to the largest machines available, and will allow us to study large neutron-rich nuclei including those relevant for r-process nucleosynthesis and including those to be produced at the Facility for Rare-Isotope Beams (FRIB). The ability to study dynamic processes including fission and heavy-ion fusion is critically important. Both the DFT work and the ab-initio work in light nuclei will require CS/AM support in load-balancing, numerical and performance optimization, uncertainty quantification, model validation, eigensolvers and nonlinear solvers, and multiresolution analysis. The project also requires a close coordination between ab-initio and DFT codes, including uncertainty quantification and numerical optimization. Only through a comprehensive SciDAC project such as NUCLEI can one take maximum advantage of advances in different areas of low-energy nuclear theory and significantly impact the experimental program at facilities and major experimets including FRIB, ATLAS, FNPB, MAJORANA, NIF, and TJNAF.