Research interests and directions

Accurate solutions to the quantum many-body problem represent one of the great intellectual challenges of our day and pervade the sciences from materials and chemistry to nuclei. In nuclear physics, the recent world-wide push to investigate nuclei farther from the valley of beta-stability has already given us a taste of the discovery potential that lies ahead. With the advent of the Rare Isotope Accelerator (RIA) we are entering into a fascinating era of research and new discoveries. The unstable nuclei that are currently being produced at various facilities, and will be copiously produced at RIA, bring significant opportunities to nuclear theory. Our challenges are to develop methods and techniques that will extend to these systems, to make reliable predictions and guide experimental efforts, and to investigate the underlying nuclear effective forces that are employed in many-body theory. We also have the exciting challenge to understand nuclear processes and properties that enter into astrophysics (such as masses and lifetimes of r-process nuclei, or electron capture on nuclei present in core collapse). Clearly, we are entering a time of increasing collaboration and cooperation among various nuclear theory efforts in the U.S. and abroad in order to meet the challenges ahead.

The Nuclear Physics Theory Program at ORNL strives to meet the challenges that RIA will present through development and implementation of: coupled-cluster theory for nuclei; basis-optimization techniques (such as DMRG and factorization) for the shell model; Monte Carlo algorithms for the shell model; continuum shell-model approaches; and energy-density functionals for use in Hartree-Fock-Bogoluibov (HFB) calculations and extensions. In addition to these major thrusts, members of the Nuclear Theory Group also work in such diverse areas as quantum chaos, random Hamiltonians, Bose Einstein condensates, and quantum dots. In each case, the unifying theme involves the quantum many-body problem.

Our research efforts require significant computational capability. For example, the computation of the ground state energy of ^{16}O in seven oscillator shells using the coupled cluster theory in singles and doubles (CCSD) requires 0.5 Tflop-hours for convergence; ^{40}Ca in the same model space requires roughly 3 Tflop-hours for convergence. Computing a nuclear mass table for 3000 nuclei using deformed-oscillator HFB techniques requires 1 Tflop-hour. We are fortunate to have available resources to carry out such calculations both locally at the Center for Computational Sciences at ORNL and at NERSC. Investigations of open-shell neutron-rich nuclei and the inclusion of three-body interactions into our coupled-cluster methods, and the generation of the next generation of energy density functionals, including time-odd components, will significantly increase our computational needs in the coming 2-3 years.