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Ab initio calculations of ^{12}C and neutron drops[1]

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Ab initio calculations of nuclei, which treat a nucleus as a system of A nucleons interacting by realistic two- and three-nucleon forces, have made tremendous progress in the last 15 years. This is a result of better Hamiltonians, rapidly increasing computer power, and new or improved many-body methods. Three methods are principally being used: Green's function Monte Carlo (GFMC), no-core shell model, and coupled cluster. In the limit of large computer resources, all three methods produce exact eigenvalues of a given nuclear Hamiltonian. With DOE SciDAC and INCITE support, all three methods are using the largest computers available today. Under the UNEDF SciDAC grant, the Argonne GFMC program was modified to efficiently use more than 2000 processors. E. Lusk (Argonne), R.M. Butler (Middle Tennessee State U.) and I have developed an Asynchronous Dynamic Load-Balancing (ADLB) library. In addition all the cores in a node are used via OpenMP as one ADLB/MPI client. In this way we obtain very good scalability up to 30,000 processors on Argonne's IBM Blue Gene/P. Two systems of particular interest that require this computer power are ^{12}C and neutron drops. V.R. Pandharipande (UIUC, deceased), J. Carlson (LANL), R.B. Wiringa (Argonne), and I have developed new trial wave functions that explicitly contain the three-alpha particle structure of ^{12}C. These are being used with the Argonne V18 and Illinois-7 potentials which reproduce the energies of 51 states in $3 \leq A \leq 12$ nuclei with an rms error of 600 keV. Neutron drops are collections of neutrons confined in an artificial external well and interacting with realistic NN and NNN potentials. Their properties can be used as "experimental data" for developing energy-density functionals.

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