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Ab initio methods for nuclear properties - a computational physics approach[1]

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A microscopic theory for the structure and reactions of light nuclei poses formidable challenges for high-performance computing. Several ab-initio methods have now emerged that provide nearly exact solutions for some nuclear properties. The ab-initio no-core full configuration (NCFC) approach is based on basis space expansion methods and uses Slater determinants of single-nucleon basis functions to express the nuclear wave function. In this approach, the quantum many-particle problem becomes a large sparse matrix eigenvalue problem. The eigenvalues of this matrix give us the binding energies, and the corresponding eigenvectors the nuclear wave functions. These wave functions can be employed to evaluate experimental quantities. In order to reach numerical convergence for fundamental problems of interest, the matrix dimension often exceeds 1 billion, and the number of nonzero matrix elements may saturate available storage on present-day leadership class facilities. I discuss different strategies for distributing and solving this large sparse matrix on current multicore computer architectures, including methods to deal with with memory bottleneck. Several of these strategies have been implemented in the code MFDn, which is a parallel fortran code for nuclear structure calculations. I will show scaling behavior and compare the performance of the pure MPI version with the hybrid MPI/OpenMP code on Cray XT4 and XT5 platforms. For large core counts (typically 5,000 and above), the hybrid version is more efficient than pure MPI. With this code, we have been able to predict properties of the unstable nucleus 14F, which have since been confirmed by experiments. I will also give an overview of other recent results for nuclei in the A = 6 to 16 range with 2- and 3-body interactions.

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