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Deterministic alternatives to the full configuration interaction quantum Monte Carlo method for strongly correlated systems[1] NORM TUBMAN, BIRGITTA WHALEY, University of California, Berkeley — The development of exponential scaling methods has seen great progress in tackling larger systems than previously thought possible. One such technique, full configuration interaction quantum Monte Carlo, allows exact diagonalization through stochastically sampling of determinants. The method derives its utility from the information in the matrix elements of the Hamiltonian, together with a stochastic projected wave function, which are used to explore the important parts of Hilbert space. However, a stochastic representation of the wave function is not required to search Hilbert space efficiently and new deterministic approaches have recently been shown to efficiently find the important parts of determinant space. We shall discuss the technique of Adaptive Sampling Configuration Interaction (ASCI) and the related heat-bath Configuration Interaction approach for ground state and excited state simulations. We will present several applications for strongly correlated Hamiltonians.

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