

Abstract Submitted  
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***Ab initio* no core configuration interaction calculations in the natural orbital basis**<sup>1</sup> CHRYSOVALANTIS CONSTANTINOU, MARK A. CAPRIO, University of Notre Dame, JAMES P. VARY, PIETER MARIS, Iowa State University — The natural orbital basis has been successfully used in the past in atomic and molecular structure calculations. The natural orbitals used in those calculations are calculated by diagonalizing the electron one-body density matrix. Here we develop natural orbitals for nuclear no-core configuration interaction (NCCI) calculations. A NCCI calculation using an initial single particle basis, such as the harmonic oscillator basis, must first be performed in order to obtain a one-body density matrix. The eigenvectors of the one-body density matrix are the natural orbitals, and the corresponding eigenvalues are the occupations of these natural orbitals in the nuclear wave function. According to these occupancies, the most important natural orbitals, in the sense of the most occupied, can then be selected and used in a NCCI calculation. We discuss *ab initio* nuclear NCCI calculations for light nuclei and assess their ability to provide faster convergence.

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