THE DEVELOPMENT OF CODES FOR THE CALCULATION OF CI DENSITY MATRICES - PART I

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In this presentation the development of two codes whose purpose is the evaluation of reduced density matrices are described.
The first code, pciden, is a parallel implementation of the program ciden. The latter program was developed to calculate the 1- and 2- particle density matrices resulting from a multireference configuration interaction (MRCI) calculation, the most computationally expensive step in the calculation of MRCI energy gradients as it is implemented in the COLUMBUS suite of programs of which ciden is a part. Before the ciden code could be parallelized a large number of modifications were necessary mainly for the purpose of load balancing. Even before attempting to parallelize the ciden code these modifications have allowed it to be applied to a wider range of problems than was previously possible. The parallelization itself follows the same general philosophy to that which was used in the development of the pciudg program and is still in progress.
The purpose of the second code, density, is to calculate the 1-particle density matrix from a spin-orbit configuration interaction (SOCI) calculation. This density matrix can be used in the same manner as standard 1-particle density matrices with the added feature that the effects of spin-orbit coupling can be determined. The density matrix calculated by the density program has been used in a few of the more common applications of a 1-particle density matrix.

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