

# Parallelization of Triple and Quadruple Perturbation Corrections to Multireference CISD

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Triple and quadruple (TQ) perturbative corrections to multireference configuration interaction including single and double excitations calculation, the most time-consuming part of MRCISD(TQ) calculations, was parallelized using Message Passing Interface (MPI). The MRCISD(TQ) method is organized in the framework of macroconfigurations, which both allows the use of incomplete reference spaces and provides an efficient means of screening large number of noninteracting configuration state functions. A previously unexploited feature is its actual connection to MPI parallelization. The test calculations show that the parallel code can achieve close to linear speed-up when the number of configuration state functions in each macroconfiguration is small. The speed-up suffers when large numbers of configuration state functions exist in the macroconfigurations.