**Massively Parallel and GPU-accelerated Implementation of the Cluster Perturbation Method for Excitation Energies**

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**Abstract**

The coupled cluster singles and doubles (CCSD) method has been shown to be a reliable means of calculating molecular energies and properties, including excitation energies. However, the calculation of excitation energies requires solving the CCSD response eigenvalue equation via an iterative method which scales as N6, often making these calculations prohibitively expensive for larger molecular systems. Cluster perturbation (CP) theory[1] seeks to overcome this scaling by avoiding explicitly solving the doubles eigenvalue problems required to obtain the full spectrum of excitation energies. Instead, excitation energies from coupled cluster singles (CCS) calculations are perturbatively corrected one at a time in orders of the fluctuation potential to achieve CCSD quality. This series of corrections has been termed the CPS(D) series and has been applied out to the 6th order correction. Calculations have shown that the third-order correction, CPS(D-3) results in energies of CCSD quality in a fraction of the computational time.[2] Here we present a massively parallel implementation of the CPS(D-3) method within the LS-Dalton program.[3] We find good agreement with previously reported small molecule benchmark studies of CCSD excitation energies. Additionally, we report excitation energies for various configurations of retinal calculated with a triple-Î¶ basis as well as efforts to implement efficient GPU-acceleration of expensive tensor contractions within the CPS(D-3) calculation.