
Structure-Aware Calculation of Many-Electron Wave Function Overlaps on Multicore Processors

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We introduce a new algorithm that exploits the relationship between the determinants of a sequence of matrices that appear in the calculation of many-electron wave function overlaps, yielding a considerable reduction of the theoretical cost. The resulting enhanced algorithm is embarrassingly parallel and our comparison against the (embarrassingly parallel version of) the original algorithm, on a computer node with 40 physical cores, shows acceleration factors which are close to 9-10x for the largest problems, consistent with the theoretical difference.

Keywords: Wave functions, LU factorization, multicore processors.