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Improving Performance of Basis-set-free Hartree-Fock Calculations Through Grid-based Massively Parallel Techniques

Friday, February 26, 2016 10:00 AM (15 minutes)

Multicenter numerical integration scheme for polyatomic molecules has been implemented as an initial step to develop a complete basis-set-free Hartree-Fock (HF) software. The validation of the integration scheme includes the integration of the total density and the calculation of Coulomb potentials for several diatomic molecules. A finite difference method is used to solve Poisson's equation for the Coulomb potential on numerical orbitals expanded on the interlocking multicenter quadrature grid. The implementation which rely on OpenMP and CUDA shows a speedup up to 30x.

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