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Acceleration of screened-exchange density-functional calculations with approximate differential overlap[1] JONATHAN MOUSSA, PETER SCHULTZ, Sandia National Laboratories — We implement the Heyd-Scuseria-Ernzerhof (HSE) screened-exchange density functional in the SeqQuest electronic structure code. HSE calculations are accelerated by approximating differential overlap in the Fock exchange based on an atomic-orbital partitioning scheme. All one-center and two-center exchange integrals are calculated. A subset of three-center exchange integrals are calculated for one-center Fock exchange matrix elements and for exchange mediated by one-center density matrix elements. Four-center exchange integrals are not calculated. We test the validity of this approximation by examining the number and magnitude of these different classes of exchange integrals. Basis set and pseudopotential errors in HSE calculations are benchmarked on atoms. Differential overlap approximation errors are benchmarked on small molecules.

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