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Object-oriented Development of an All-electron Gaussian Basis DFT Code for Periodic Systems JOHN ALFORD, SAMUEL TRICKEY, Quantum Theory Project, Dept. of Physics, University of Florida — We report on the construction of an all-electron Gaussian-basis DFT code for systems periodic in one, two, and three dimensions. This is in part a reimplementation of algorithms in the serial code, GTOFF, which has been successfully applied to the study of crystalline solids, surfaces, and ultra-thin films. The current development is being carried out in an object-oriented parallel framework using C++ and MPI. Some rather special aspects of this code are the use of density fitting methodologies and the implementation of a generalized Ewald technique to do lattice summations of Coulomb integrals, which is typically more accurate than multipole methods. Important modules that have already been created will be described, for example, a flexible input parser and storage class that can parse and store generically tagged data (e.g. XML), an easy to use processor communication mechanism, and the integrals package. Though C++ is generally inferior to F77 in terms of optimization, we show that careful redesigning has allowed us to make up the run-time performance difference in the new code. Timing comparisons and scalability features will be presented. The purpose of this reconstruction is to facilitate the inclusion of new physics. Our goal is to study orbital currents using modified gaussian bases and external magnetic field effects in the weak and ultra-strong ($\sim 10^5$ T) field regimes. This work is supported by NSF-ITR DMR-0218957.

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