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Linear-scaling density-functional theory with wavelets: challenges and opportunities for petascale and beyond LAURA RATCLIFF, Leadership Computing Facility, Argonne National Laboratory, LUIGI GENOVESE, STEPHAN MOHR, THIERRY DEUTSCH, CEA, INAC-SP2M, L Sim, Grenoble, France — Density-functional theory (DFT) has been used to study a wide range of materials in simulations with a moderate level of parallelism. A common approach divides the electronic orbitals between MPI tasks, however this limits the number of tasks that can be used for a given system. The most straightforward path to exploiting petascale machines is therefore to increase the size of the system being studied. However, standard implementations of DFT scale cubically with the number of atoms so that the time rapidly increases for large systems. Algorithms must therefore be designed with reduced scaling, such as the linear-scaling approach in BigDFT, which uses an adaptive localized basis set that is itself represented in an underlying wavelet basis set. It thus retains all the benefits of wavelets, such as systematic convergence, while also presenting some new advantages, e.g. the definition of a fragment approach. Nonetheless, as we move towards the exascale, there remain a number of challenges associated both with increasing parallelism and the treatment of large systems. We will outline the algorithms and parallelization used in BigDFT and present some recent results which have been facilitated by this approach, as well as discussing some of the future challenges.

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