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RMG An Open Source Electronic Structure Code for Multi-Petaflops Calculations EMIL BRIGGS, WENCHANG LU, MIROSLAV HODAK, JERZY BERNHOLC, North Carolina State Univ — RMG (Real-space Multigrid) is an open source, density functional theory code for quantum simulations of materials. It solves the Kohn-Sham equations on real-space grids, which allows for natural parallelization via domain decomposition. Either subspace or Davidson diagonalization, coupled with multigrid methods, are used to accelerate convergence. RMG is a cross platform open source package which has been used in the study of a wide range of systems, including semiconductors, biomolecules, and nanoscale electronic devices. It can optionally use GPU accelerators to improve performance on systems where they are available. The recently released versions (>2.0) support multiple GPU's per compute node, have improved performance and scalability, enhanced accuracy and support for additional hardware platforms. New versions of the code are regularly released at <http://www.rmgdft.org>. The releases include binaries for Linux, Windows and MacIntosh systems, automated builds for clusters using cmake, as well as versions adapted to the major supercomputing installations and platforms. Several recent, large-scale applications of RMG will be discussed.

Emil Briggs
North Carolina State Univ

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