

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Real Space Multigrid (RMG) Open Source Software Suite for Multi-Petaflops Electronic Structure Calculations EMIL BRIGGS, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, YAN LI, North Carolina State University — RMG is a cross platform open source package for ab initio electronic structure calculations that uses real-space grids, multigrid preconditioning, and subspace diagonalization to solve the Kohn-Sham equations. The code has been successfully used for a wide range of problems ranging from complex bulk materials to multifunctional electronic devices and biological systems. RMG makes efficient use of GPU accelerators, if present, but does not require them. Recent work has extended GPU support to systems with multiple GPU's per computational node, as well as optimized both CPU and GPU memory usage to enable large problem sizes, which are no longer limited by the memory of the GPU board. Additional enhancements include increased portability, scalability and performance. New versions of the code are regularly released at sourceforge.net/projects/rmgdft/. 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.

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Date submitted: 06 Nov 2015

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