

RMG version 2.2 electronic structure code

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RMG (Real-space MultiGrid) is an open source, DFT-based electronic structure code that discretizes the Kohn Sham equations on real-space grids. Either norm-conserving or ultrasoft pseudopotentials can be used to represent the atomic species. An extensive default set of pseudopotentials is provided with the download package. The Kohn-Sham equations are solved using *Multigrid* preconditioning techniques coupled with subspace diagonalization methods. RMG has been efficiently parallelized for a wide range of computer and cluster architectures. It runs well on systems ranging from standard workstations up to the largest supercomputers available today, where a peak performance in excess of 6.5 Pflops was demonstrated using an earlier version of the code. When present, GPU accelerators can be used to improve performance. Both Nvidia and Intel variants are supported. RMG has been selected to be a part of NSF's Sustained Petascale Performance Benchmarks, which are being used to help select NSF's future Leadership Class supercomputers. Version 2.2 of RMG is a maintenance release that includes bug fixes and performance improvements as well as refinements to existing functionality, such as better handling of spin polarized calculations, updated GPU accelerator support, convergence enhancements and reduced memory usage.

RMG is available for download at www.rmgdft.org. Documentation, wiki, user forums, installation and getting started support are also provided. In addition to the source code, binary packages are supplied for various common Linux distributions, Macs and Windows. For Cray systems, a portal for RMG has been established at <http://bluewaters.ncsa.illinois.edu/rmg>. Similar portals will be created for other major supercomputer sites and architectures.

An RMG hand-on tutorial will be presented at 6 pm on Monday. Free pizza will be provided, please email elbriggs@ncsu.edu, so that we order an appropriate amount.