Tutorial on RMG -- a DFT/hybrid-DFT electronic structure code

RMG as an open-source code that discretizes the DFT equations on real-space grids distributed over the nodes of a massively parallel system via domain decomposition. Multigrid techniques dramatically accelerate convergence while only requiring nearest-neighbor communications, while a novel adaptive discretization of the kinetic energy operator leads to the same average accuracy as plane-wave codes on the Delta test (71 elements, https://doi.org/10.48550/arXiv.2303.01937). RMG uses all CPU cores and GPUs in each node, and scales from desktops and clusters to exascale supercomputers, including Frontier, Summit, and Perlmutter.

Current capabilities include gamma and k-point calculations for all crystal lattice types, accurate forces for structure optimization and molecular dynamics, spin-orbit coupling, and a novel parallel diagonalizer suitable for very large systems. An extensive default set of pseudopotentials is built-in. A wide range of DFT functionals can be used, including hybrids, DFT+U, and van der Waals. An interface to quantum Monte Carlo code QMCPACK has been developed, and semi-local pseudopotentials are also supported for QMCPACK input.

The tutorial will consist of a short review of RMG capabilities with recent examples and a hands-on session featuring an easy-to-use web-based RMG input generator and RMG output analyzer.

RMG is currently distributed via github.com/rmgdft. It was downloaded over 4,000 times.