Tutorial at ES2016 on open-source RMG version 2.0 electronic structure code

There will be an optional tutorial on the Real Space Multigrid (RMG) version 2.0 code at ES2016 on Monday evening, starting at about 5:45 pm. RMG is an open-source real-space DFT-based electronic structure code. Designed for scalability, it has been run successfully on systems with thousands of GPU nodes and hundreds of thousands of CPU cores, reaching multipetaflops performance. An extensive default set of pseudopotentials, both norm-conserving and ultrasoft, is built-in. RMG is highly portable and runs on Linux/UNIX, Windows and Mac OS X workstations and desktops, as well supercomputers. A future release will include non-equilibrium Green's function module for self-consistent calculations of ballistic transport.

Version 2.0 of RMG, which will be launched on the first day of ES2016 together with a hands-on tutorial, has a number of new features and enhancements. These include a new eigensolver for small to medium-size systems, additional density mixing algorithms, vdW-DF exchange-correlation functional, dramatically faster force calculation as well as other performance and memory usage optimizations. As the result, time to solution has been cut by a factor of 3 to 5.

RMG is available for download from https://sourceforge.net/projects/rmgdft. Documentation, wiki, user forums, installation and getting started support are also provided. In addition to the source code, binary packages are supplied for the common Linux distributions, Macs and Windows. For the 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.

The tutorial will consist of short presentations and a hands-on session. Attendees will be able to test RMG on their laptops and on remote GPU-enabled workstations, as well as receive installation help on their own systems.

Free pizza will be provided. Please let us know that you will be attending (email: elbriggs@ncsu.edu), so that we order an appropriate amount.

Thank you very much,
Jerry Bernholc, Emil Briggs, Wenchang Lu, Miro Hodak