

Tutorial at ES2015 on open-source RMG code for electronic structure calculations

There will be an optional tutorial on the Real Space Multigrid (RMG) code at ES2015 on Monday evening, starting at about 5:40 pm. RMG is a newly released 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. RMG is highly portable and runs on Linux/UNIX, Windows and Mac OS X workstations and desktops. In addition to the usual features found in electronic structure codes, it provides an interface to BerkeleyGW and has a couple of graphical user interfaces for generation of input files and analyzing outputs.

RMG is currently installed on NSF Blue Waters as a community code and will soon be available at other centers as well. RMG can be found at <http://sourceforge.net/projects/rmgdft/> including source files, binaries, and documentation. A future release will include non-equilibrium Green's function module for self-consistent calculations of ballistic transport.

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,

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