RMG – Multi-Petasflops Open Source Materials Simulations Code
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RMG Open Source Code
Most of the code rewritten in templated C++, uses C++11 threads
CPU and GPU data transfers encapsulated for easier porting
Much reduced memory footprint
Part I: portable library of C++ routines for HPC including
GIAM decomposition across MPI nodes
Threading on a node
Porta interfacing (Multithreading and central operators)
Profile performance of pseudopotential impact
Resolves MultiGrid solver with support routines
Elaborates data types including fast, double, complex
Omkara build system, BSD-type license
Part II: full-code release (GPL license) including:
Real space electronic structure code
Multithread and non-blocking pseudopotential library
Portable library and DFT part released:
versions: 1.0 1/15, 1.1 6/15, 1.2 10/15
Quantum transport and linear-scaling parts planned for 2016

Performance improvements
Test case: 256 atom Cu cell, N=1664, 64 nodes of Cray XK7
LAPACK
Total time
Eigensolver time
Scalapack comparison:
Larger system: 4000 atom Al cell, N=212,512 nodes of Cray XK7
Total time
Eigensolver time
Scalapack comparison:

Quantum Transport Implementation and Applications
Multi-Terminal Ballistic Devices

Handling Systems with Thousands of Atoms

Nanoribbon Transistor Simulation
Best nanoribbon for transistor: mod(3,5) = 0 family of armchair nanoribbons

SI Nanowire p-n Junction
Nanoribbon: 18 atomic-layers wide
Bulk Graphene as source and drain
2 layers of BN as insulator
A few layers of Al as the gate
450 atoms in NEGF calculation

Si nanowire p-n junction
24 nm long and 3 nm diameter
more than 10,000 atoms in NEGF calculation
Forward bias:
Source-drain bias increases exponentially.
Backward bias:
nearly zero current