# NSCI SI2-SSE: Multiscale Software for Quantum Simulations of Nanostructured Materials and Devices

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**Objectives:** (1) Open source, highly scalable software for supercomputers and clusters (2) More features implementations to serve the community

## Large-Scale Quantum Simulations of Materials and Devices

- "Real" materials structures are often complex and cannot be reduced to a few hundreds of atoms
  - Process simulation requires large systems
- Materials Genome – White House initiative to "deploy advanced materials twice as fast, at a fraction of the cost"
- National Strategic Computing Initiative (NSCI)
  - Pre-exascale, 150-300 pflops ~2018; Sustained exaflop ~2021
- National Quantum Initiative, signed Dec 21, 2018
  - Establishes a coordinated multiagency program to support research and training in quantum information science (QIS).
  - Involves NSF, DOE, NIST
  - Our RMG (real-space multigrid) code is capable of simulating quantum materials and devices at scale on the latest pre-exascale and exascale multi-core/multi-GPU supercomputers, e.g., the IBM-NVIDIA Summit.

## Real-space Multigrid (RMG) Code Development and Release

- Gamma and k-point calculations, spin polarization
- Runs on Linux/Unix, Windows and Mac
- Highly scalable to thousands of nodes and hundreds of thousands of CPU cores
- GPU accelerated: supports thousands of GPU-containing nodes with multiple GPU's per node
- Optional Openbabel support for importing atomic structures
- Supports both ultrasoft and norm-conserving pseudopotentials
- Wide choice of DFT functionals, including hybrid functionals, van der Waals via vdW-DF and spin-orbit coupling
- Accurate Hellman-Feynman forces, structure optimization and molecular dynamics
- Novel, electronic-structure-specific parallel diagonalizer
  - Partitioned Folded Spectrum Method (PFSM)
  - Up to 10x faster for repeated diagonalization

Website: www.rmgdft.org
Hosted on https://github.com/rmgdft

## Accuracy across the periodic table

**Reproducibility of DFT calculations for solids**
**(Lajaehgere et al, Science 2016)**
**40 DFT codes compared to highly converged all-electron Wien2k results**
**Δ [meV] = measure of difference in Equation of State results between two different codes**

**RMG vs Wien2K (all-electron code)**

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H 1.852 | | | | | | | | | | | | | | | | | He --- |
| Li --- | Be 0.831 | | | | | | | | | | | B --- | C 0.047 | N 4.558 | O --- | F --- | Ne --- |
| Na --- | Mg 0.492 | | | | | | | | | | | Al --- | Si 0.407 | P 0.502 | S --- | Cl 0.259 | Ar --- |
| K 0.010 | Ca 0.105 | Sc 0.260 | Ti 0.107 | V 0.582 | Cr 1.749 | Mn 2.146 | Fe 2.203 | Co 0.173 | Ni 0.378 | Cu 0.927 | Zn 0.031 | Ga 0.214 | Ge 0.577 | As 1.656 | Se 0.055 | Br 0.886 | Kr --- |
| Rb 0.111 | Sr 0.184 | Y 0.177 | Zr 0.081 | Nb 1.108 | Mo 1.025 | Tc 0.731 | Ru 1.417 | Rh 1.689 | Pd 1.638 | Ag 0.675 | Cd 0.818 | In 0.290 | Sn 0.417 | Sb --- | Te 0.406 | I 0.096 | Xe --- |
| Cs 0.031 | Ba 0.353 | Lu --- | Hf 1.408 | Ta 0.735 | W 0.489 | Re 0.618 | Os 1.439 | Ir 0.713 | Pt 0.905 | Au 1.559 | Hg 0.056 | Tl 0.037 | Pb 1.010 | Bi --- | Po --- | At --- | Rn --- |

**RMG vs QuantumEspresso (plane wave code)**

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H 0.075 | | | | | | | | | | | | | | | | | He --- |
| Li --- | Be 0.023 | | | | | | | | | | | B --- | C 0.202 | N 0.042 | O --- | F --- | Ne --- |
| Na --- | Mg 0.450 | | | | | | | | | | | Al --- | Si 0.066 | P 4.216 | S --- | Cl 0.243 | Ar --- |
| K 0.018 | Ca 0.082 | Sc 0.104 | Ti 0.039 | V 0.083 | Cr 1.644 | Mn 3.834 | Fe 1.898 | Co 0.073 | Ni 0.256 | Cu 0.130 | Zn 0.332 | Ga 0.120 | Ge 0.059 | As 0.041 | Se 0.017 | Br 0.119 | Kr --- |
| Rb 0.013 | Sr 0.169 | Y 0.119 | Zr 0.059 | Nb 0.054 | Mo 0.145 | Tc --- | Ru 0.117 | Rh 0.199 | Pd 0.438 | Ag 0.135 | Cd 0.084 | In 0.149 | Sn 0.035 | Sb --- | Te 0.047 | I 0.206 | Xe --- |
| Cs 0.066 | Ba 0.044 | Lu --- | Hf 0.058 | Ta 0.166 | W 0.023 | Re 0.137 | Os 0.129 | Ir 0.751 | Pt 1.321 | Au 0.071 | Hg 0.166 | Tl 0.056 | Pb 0.099 | Bi --- | Po --- | At --- | Rn --- |

## Code Restructuring for the Exascale Era

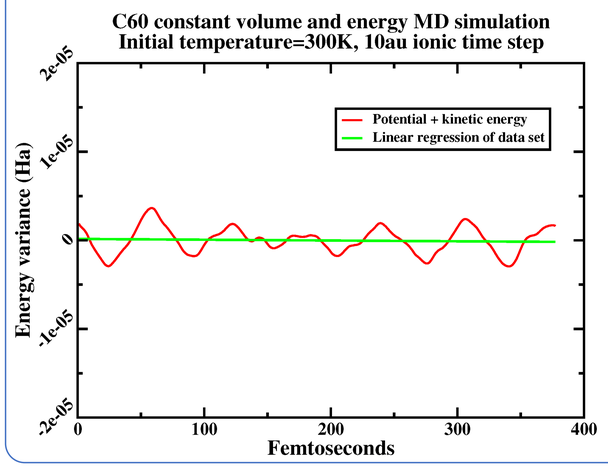
RMG code base was refactored and substantially rewritten in templated C++
- Significantly shorter, more transparent code
- Portable *cmake* build process for a variety of architectures
- Mixed parallel programming model: MPI, OpenMP and C++11 threads

Programming models CPU vs GPU
- CPU - high clock speed, smaller number of powerful execution units.
- Memory latency hidden by caches and out of order execution.
- Good single threaded performance.

GPU – lower clock speed, large number of weaker execution units.
Memory latency hidden by high thread counts.
Poor single-threaded performance.

Large fraction of RMG code base is well adapted for the GPU model
- Uses vendor libraries as much as possible
- NVIDIA specific optimizations
- Cuda-managed memory
- Small amounts of custom GPU code in critical sections
- GPU Direct support

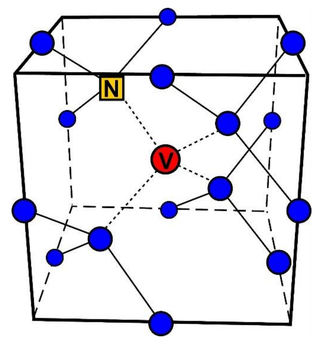
## *Ab Initio* Molecular Dynamics With RMG Energy Conservation




## RMG Performance Comparison

Prior generation machine Titan vs current Summit at ORNL

Test Case Nitrogen-vacancy center in diamond 4096 atom unit cell




Titan: 70 secs/scf step on 1728 nodes with GPUs.
Summit: 31 secs/scf step on 48 nodes with GPUs.
100 secs/scf step on 48 nodes CPU only.

RMG v3.0 is 13.5x faster per GPU and 81X faster per node on Summit. GPU version is 3.1x faster than CPU.

Speedup exceeded raw performance ratio!

**Summary: Quantum simulation software can be used to predict, evaluate and optimize new nano materials and nano devices. The open-source RMG code (www.rmgdft.org) performs at multipetaflops level and scales from desktops to exascale supercomputers. The developers are happy to help deploy RMG on users' systems and to collaborate on projects of mutual interest.**