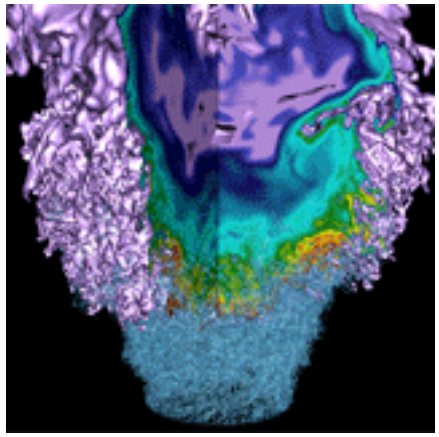
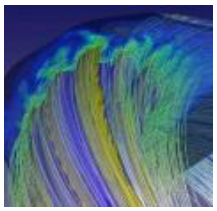
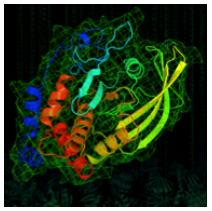
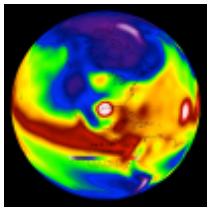
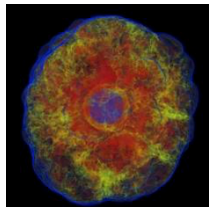
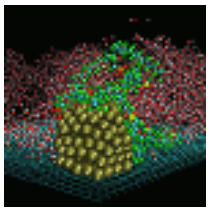
Improved Implementation of Exact Exchange in Quantum Espresso



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January 9, 2017

U.S. DEPARTMENT OF ENERGY | Office of Science

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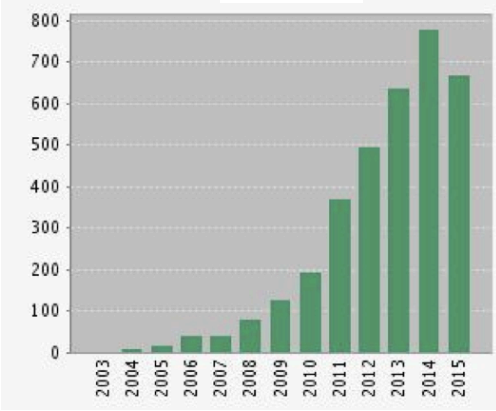
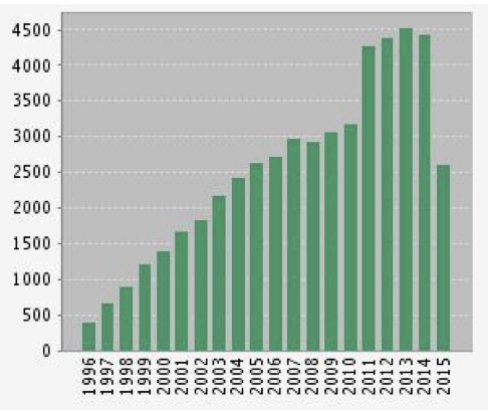
Introduction

Exact Exchange Citations

HSE



B3LYP



Goals

Prepare QE for large-scale execution on the KNL architecture, with a particular focus on improving the implementation of hybrid exchange

Local DFT:

Approximate exchange functional

$$\mathrm{K}\ \psi_i(x_1) = v_{\mathrm{xe}}[\rho(x_1)]\,\psi_i(x_1)$$

Hybrid DFT:

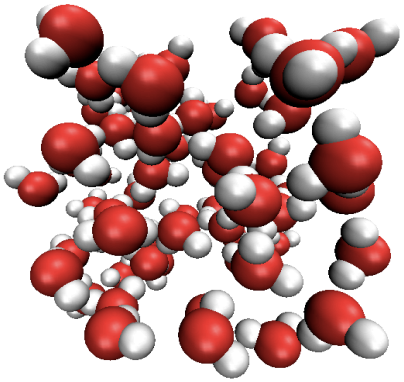
Exact exchange operator

$$\mathrm{K}_j\,\psi_i(x_1) = \left[\int \frac{\psi_i(x_2)\,\psi_j(x_2)}{|x_2 - x_1|}\,dx_1\right]\psi_j(x_1)$$

Importance of Band Groups

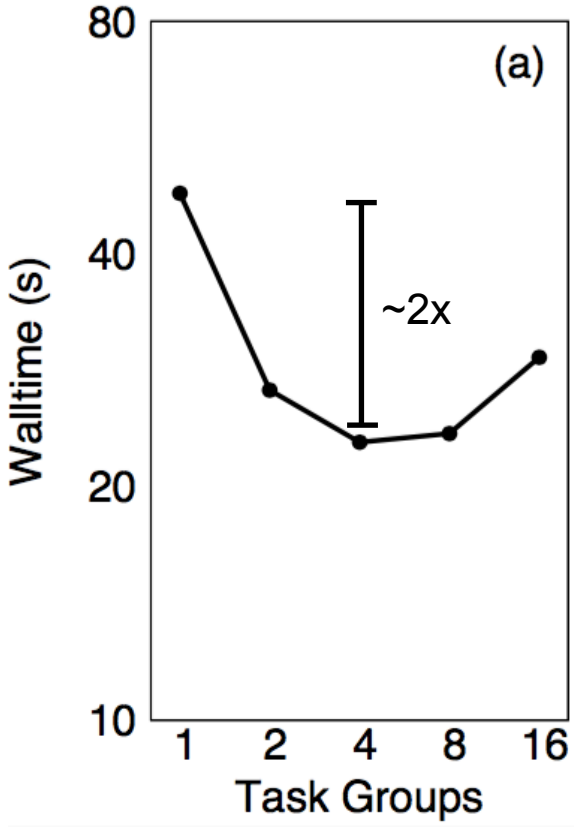
Total walltime for local and hybrid DFT calculations running on 64 Haswell nodes, for different levels of band parallelization.

System

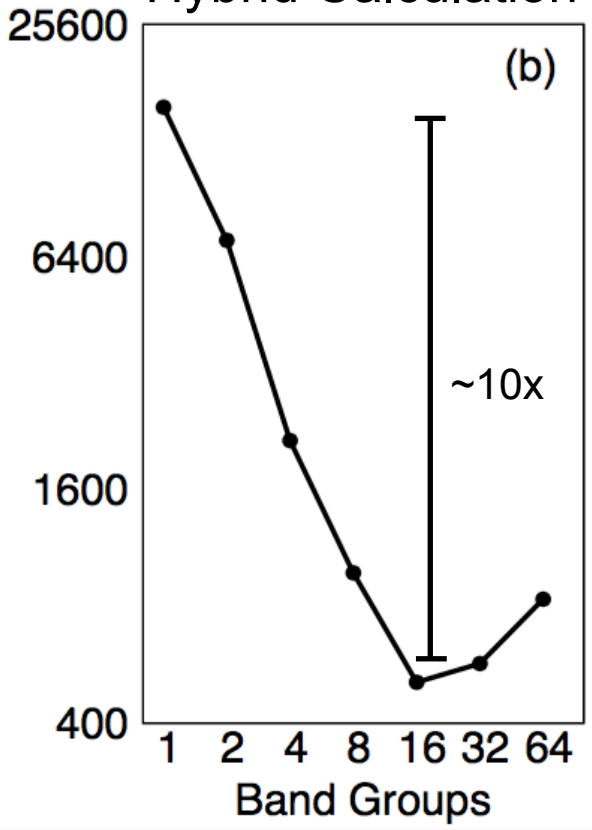


64 water molecules
256 electrons
ecutwfc=80.0 Ry
ecutfock=90.0 Ry
Norm-Conserving PP

Local Calculation

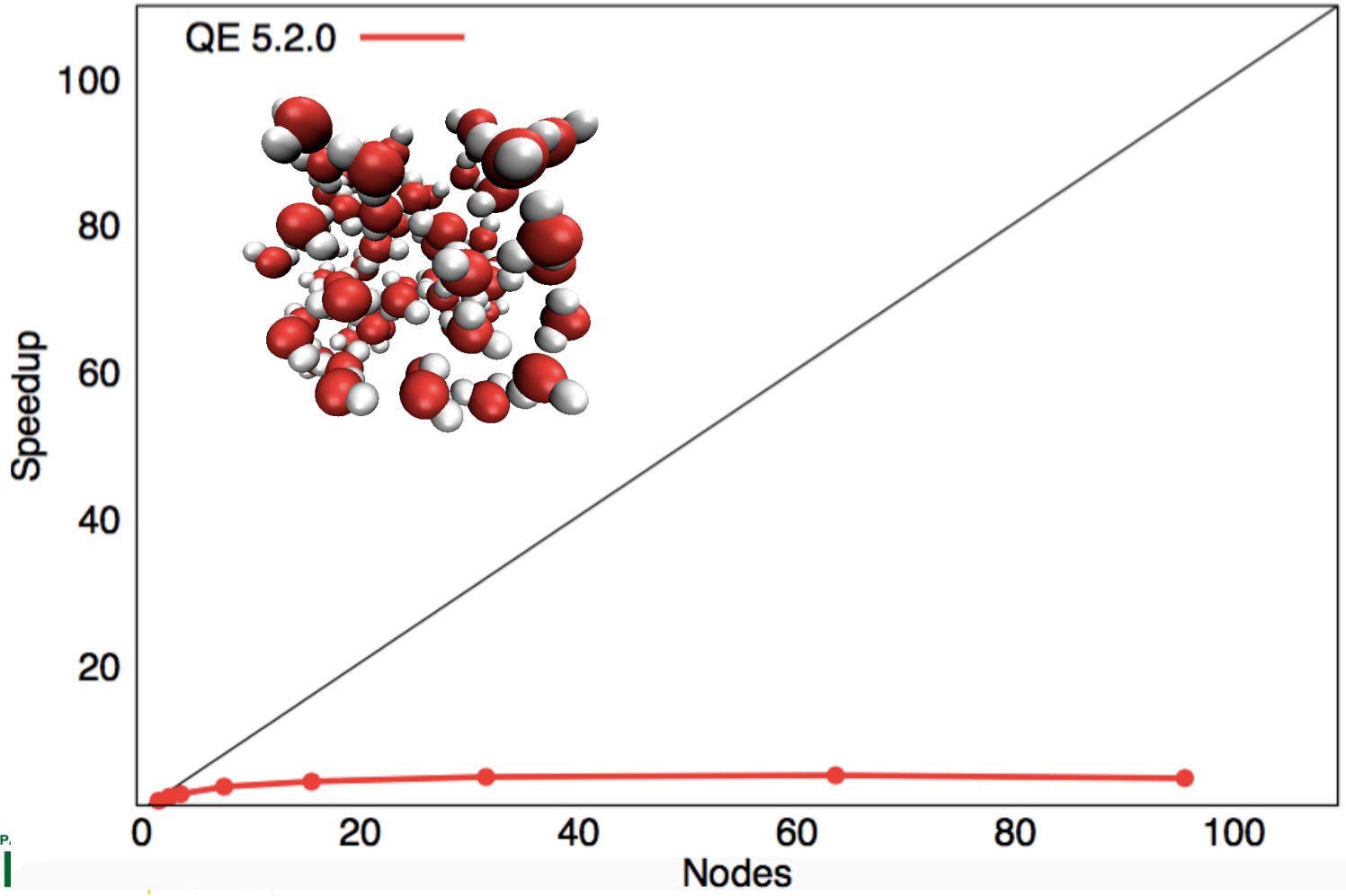


Hybrid Calculation

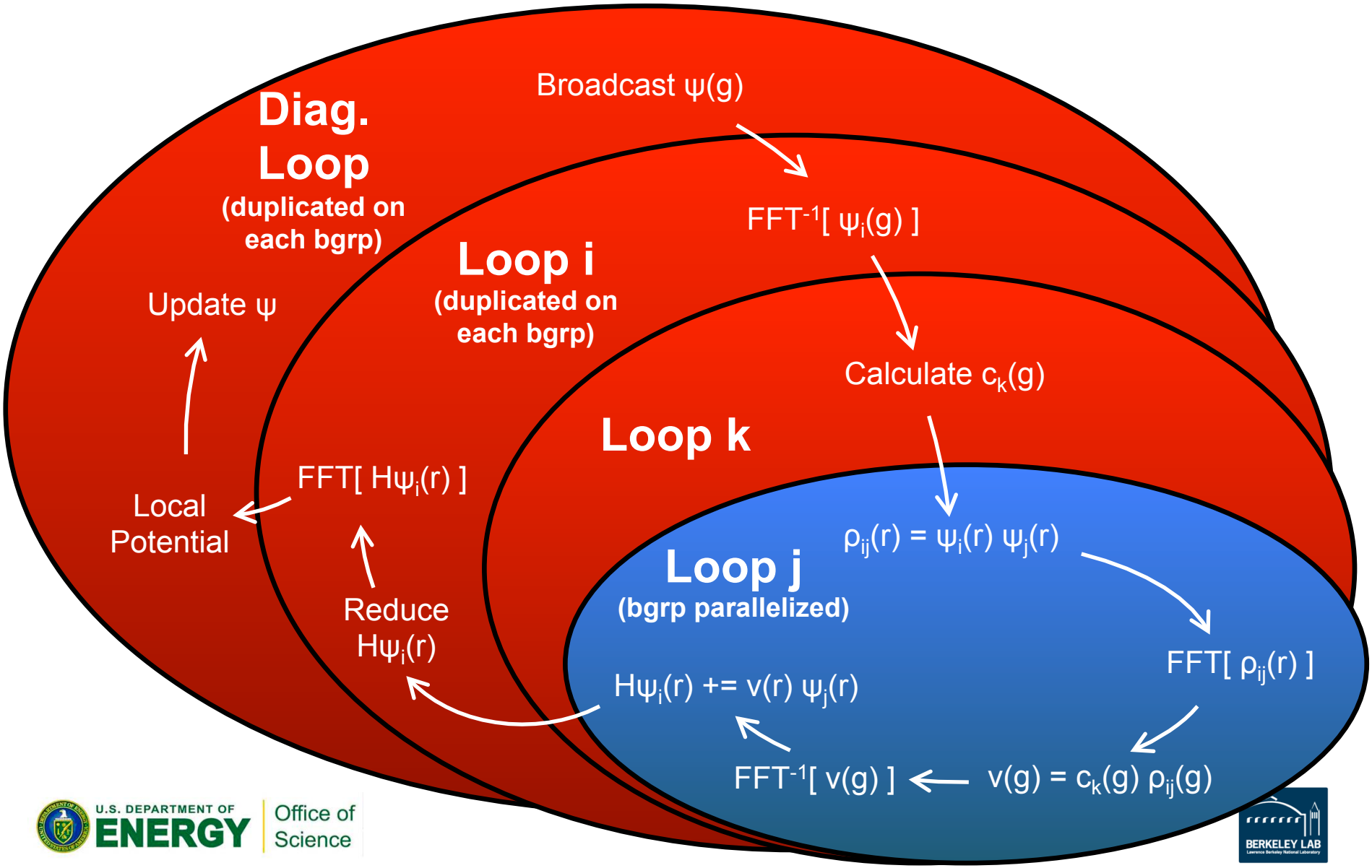


Strong Scaling of QE

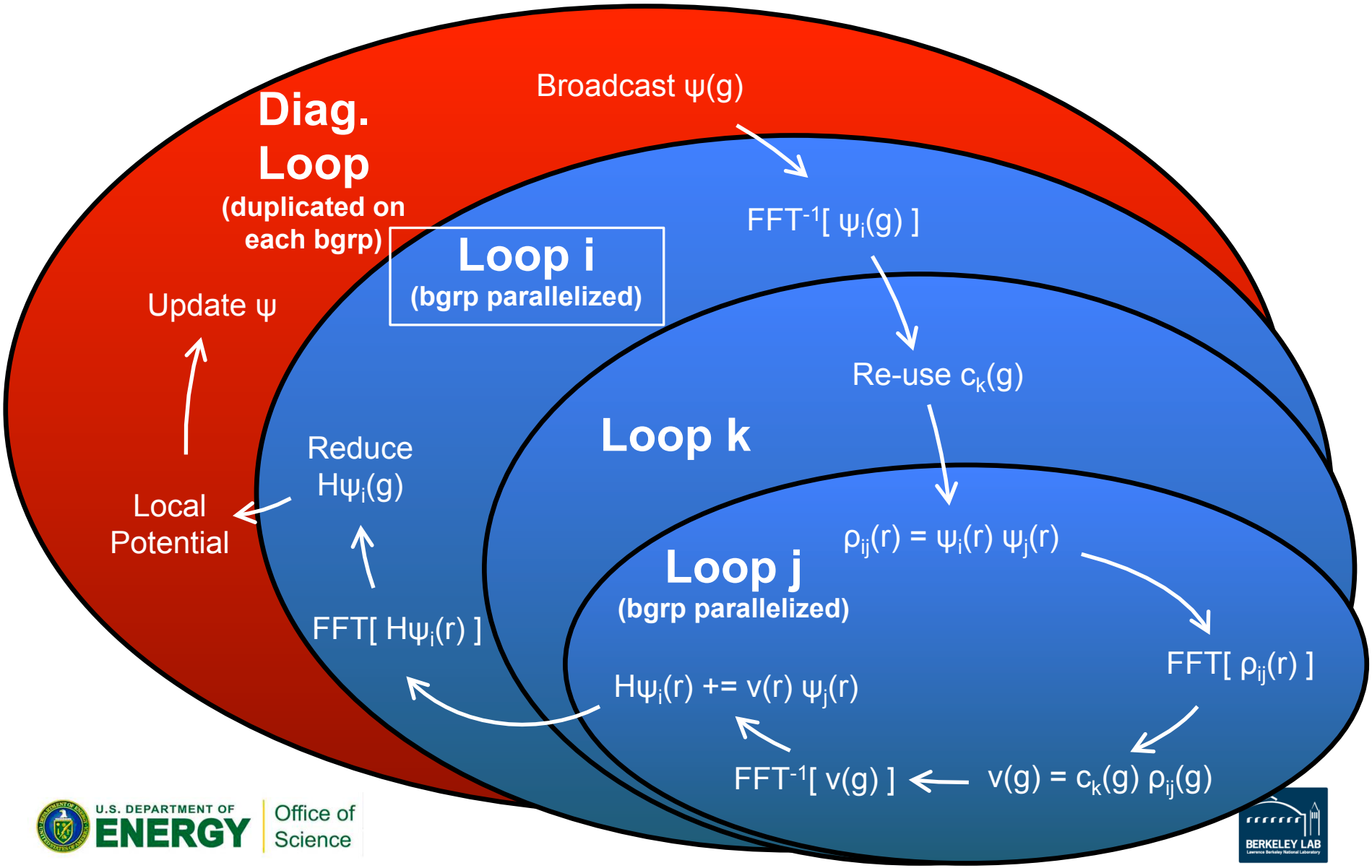
Strong scaling of QE on Ivy Bridge, using pure MPI mode and 1 band group per node:



Overview of Existing Code



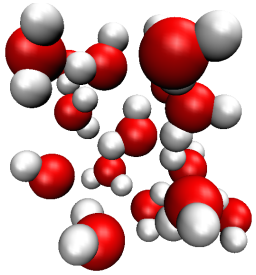
Pair Parallelization



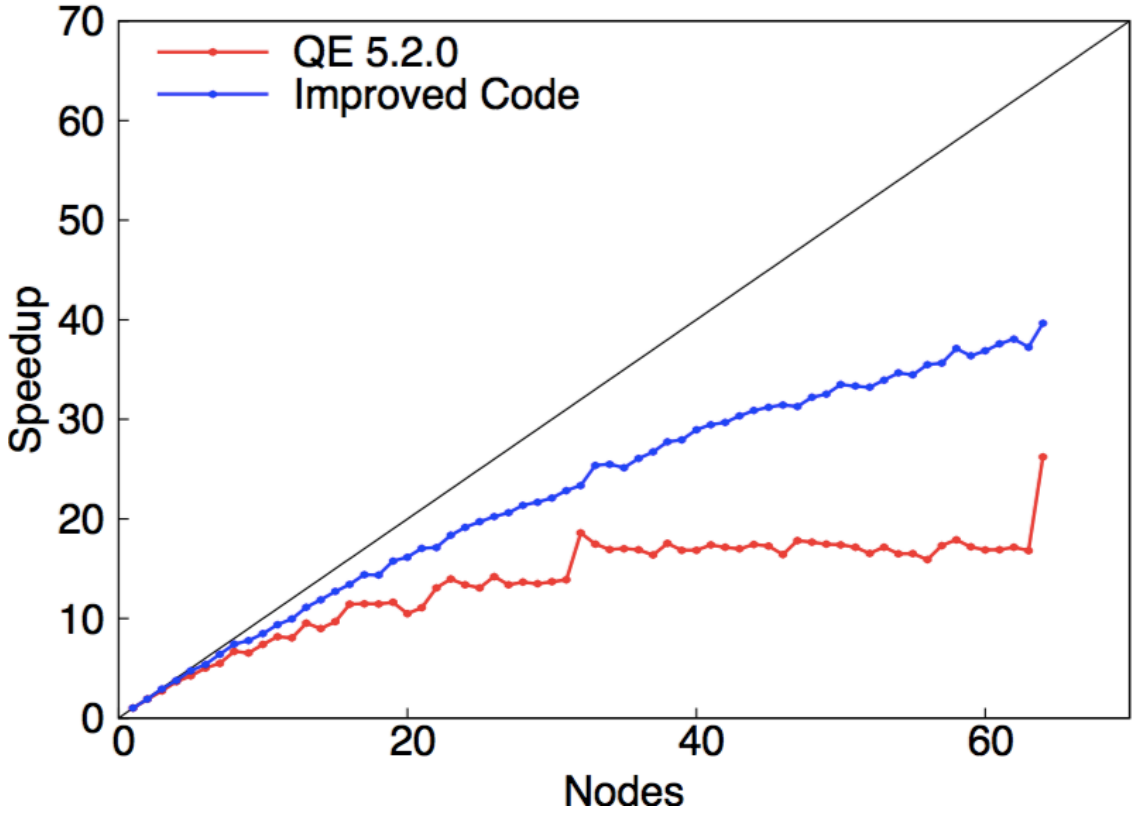
Pair Parallelization Performance

Strong scaling of the exact exchange part of the code on Ivy Bridge, with 1 band group per node:

System

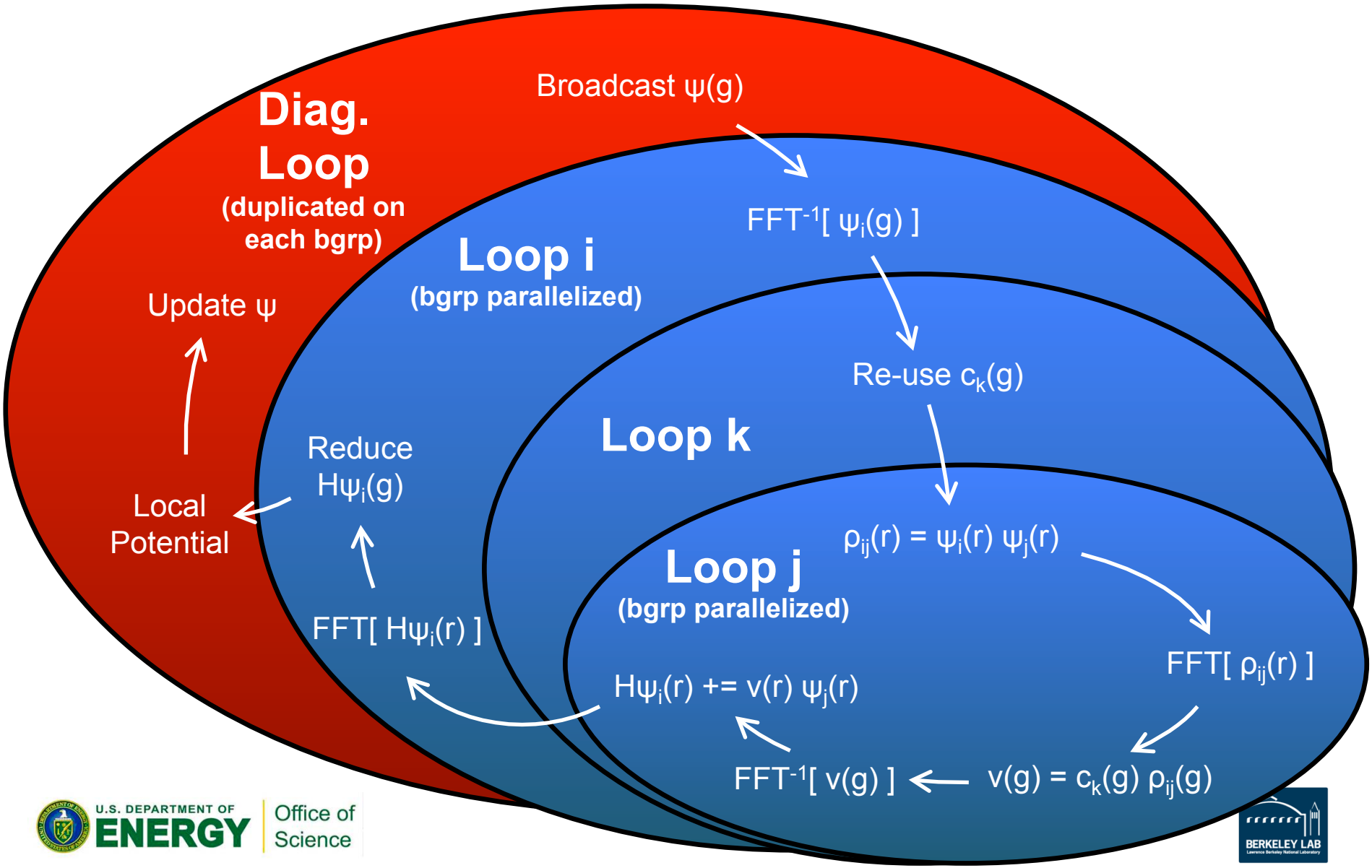


16 water molecules
64 electrons
ecutwfc=80.0 Ry
ecutfock=90.0 Ry
Norm-Conserving PP



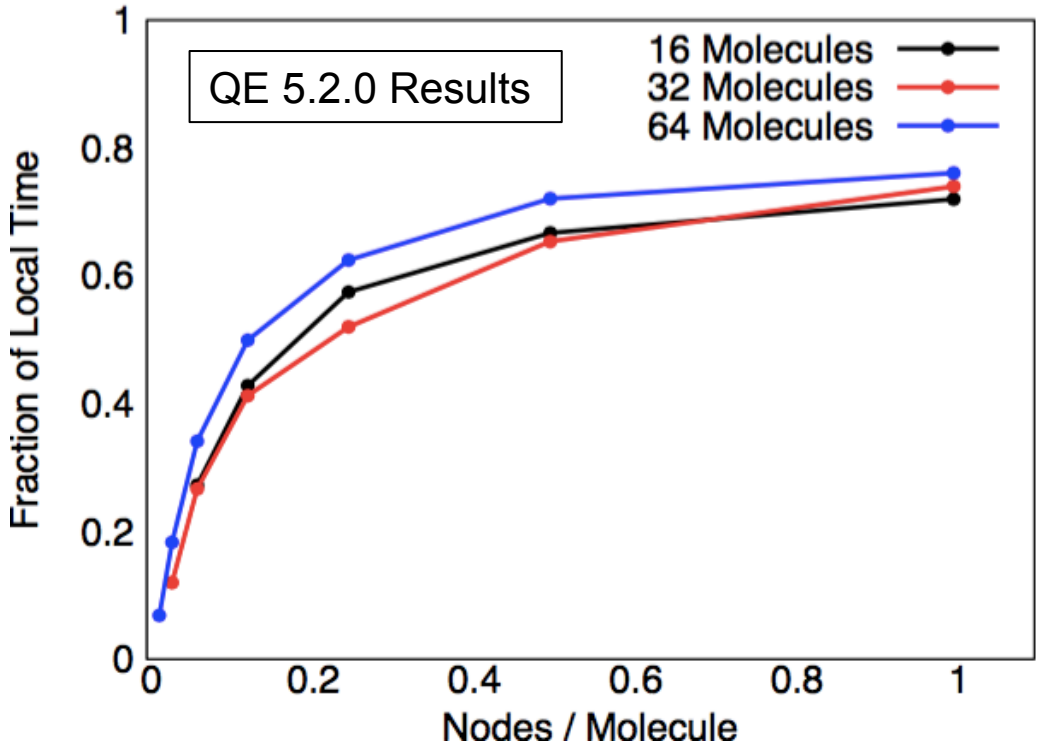
Parallelization over band pairs both improves the strong scaling of the code and also improves the load balancing.

Code Overview



Cost of the Local Calculation

Fraction of total walltime spent in local regions of the code, using 1 band group per node on Haswell:

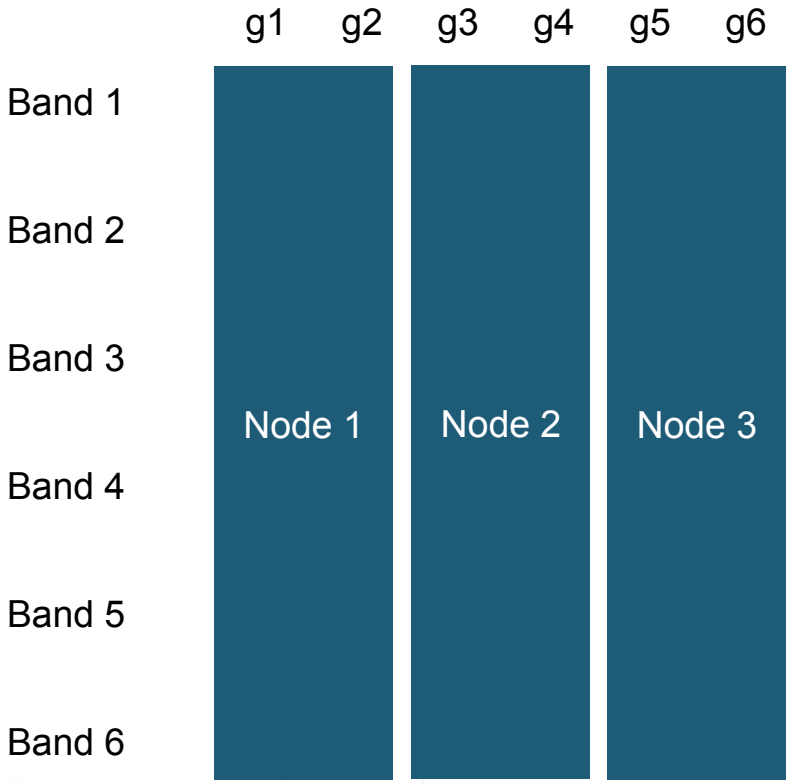


Unintuitively, local regions of the code dominate the cost of the calculation when using large numbers of nodes. This is because the local regions of the code a run in serial with respect to band groups.

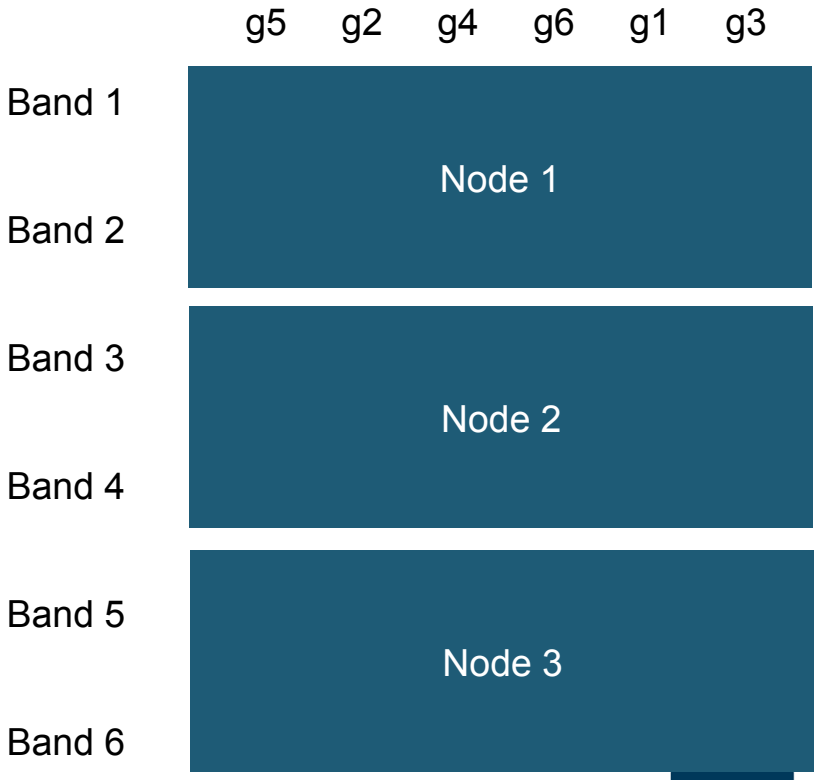
Independent Parallelization of the Local Code

Enabling parallelization of the local regions of the code across band groups requires on-the-fly transformation of the data structures between local and exact exchange regions of the code.

Data structure of Ψ(g), in local code:

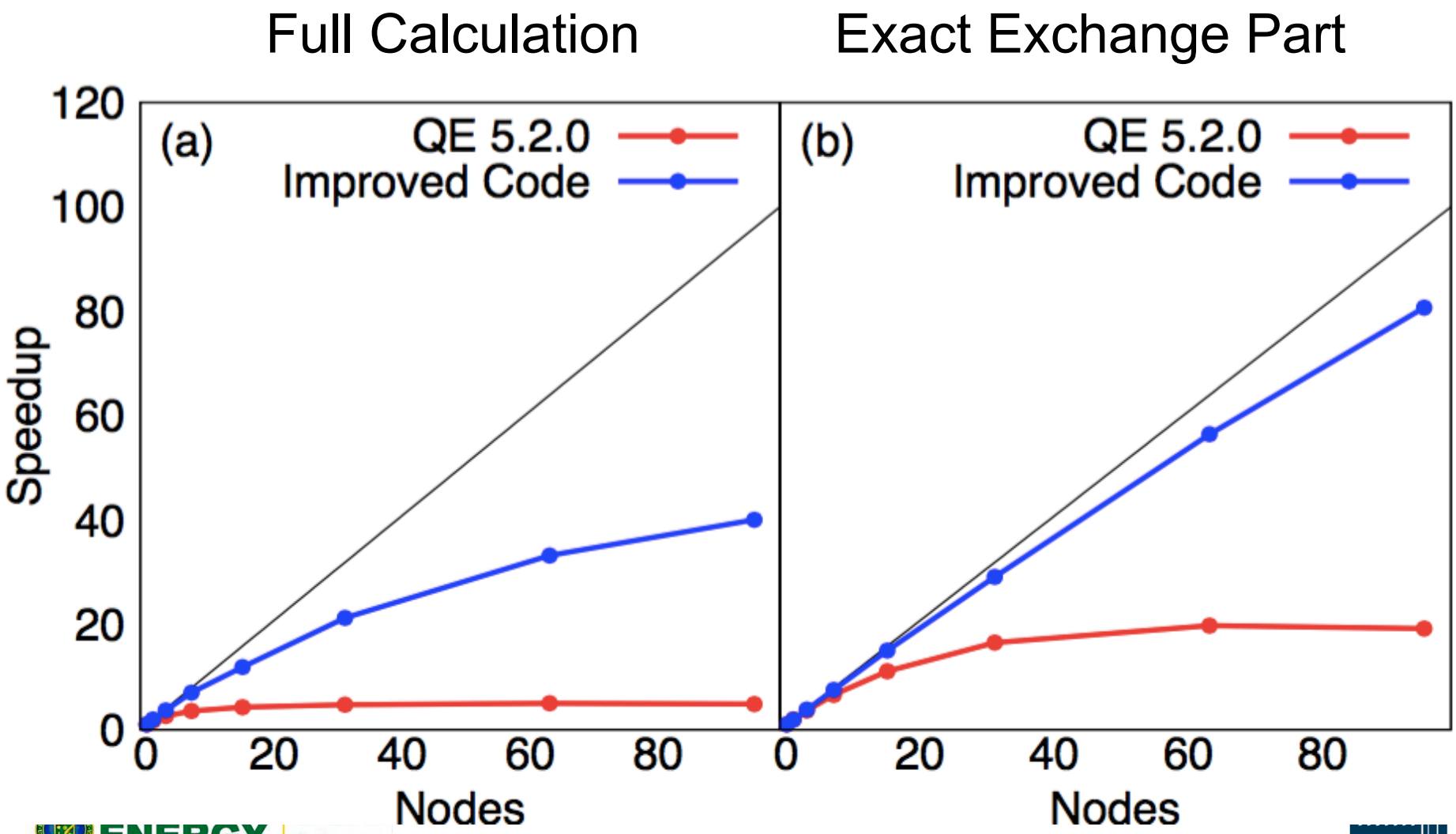


Data structure of Ψ(g), in exact exchange code:

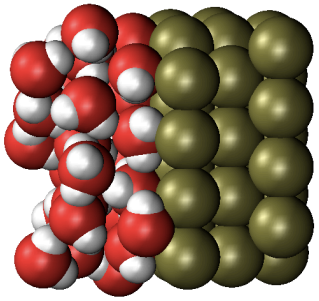


Improved Strong Scaling

Strong scaling on Ivy Bridge, with 1 band group per node:



Real-World Applications



QE 5.2.0:

Walltime: 37 hours

CPU Hours: 110,000 hours

Improved Code:

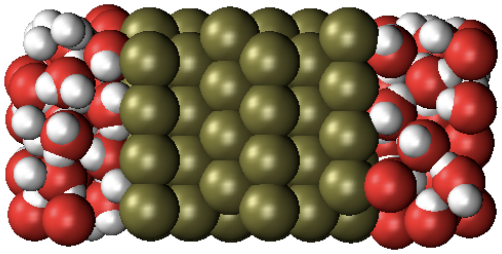
Walltime: 3 hours

CPU Hours: 10,000 hours

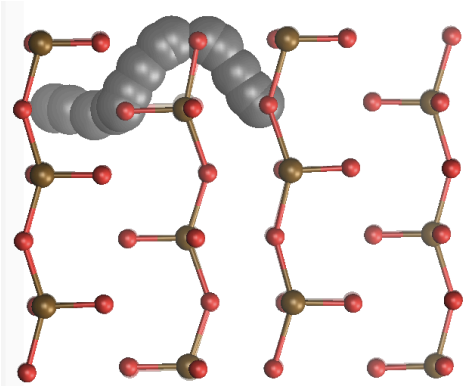
Improved Code, with ACE:

Walltime: 0.3 hours

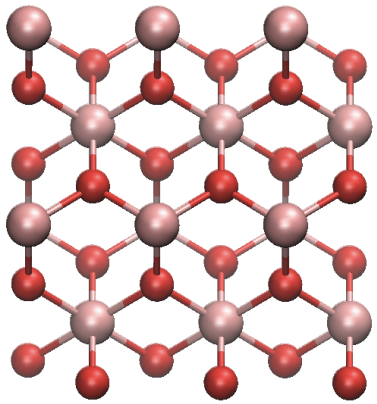
CPU Hours: 1,000 hours



MD Simulation of Water on a Pt Surface



NEB Analysis of Mg Diffusion in MoO_3



XAS Simulation of MnO_2

Summary

- We have improved the scaling of the exact exchange code by improving the parallelization and data layouts.
- Order-of-magnitude improvements are achieved for some systems.
- These changes have been contributed in a patch for inclusion in the development branch.
- Suggestions for improvements are welcome.

Papers:

Barnes, T., et al. Evaluating and optimizing the NERSC workload on Knights Landing. *SC Conference, 7th International Workshop on Performance Modeling, Benchmarking and Simulation of HPC Systems,* (2016) pp. 43-53.

Barnes, T., et al. Improved Treatment of Exact Exchange in Quantum ESPRESSO. *Comp. Phys. Comm.,* accepted.

Inter-Band Group Communication

Source of communication costs:

QE 5.2.0 – Broadcast ψ and reduce Hψ

Improved Code – Transform data structure of ψ and Hψ