# Large-Scale Electronic Structure Calculations on the BlueGene/L Computer

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The scalability of Qbox, a parallel First-Principles Molecular Dynamics (FPMD) code, was recently demonstrated on 128k CPUs on the Lawrence Livermore National Laboratory BlueGene/L platform [1]. This experiment provided new insights into the performance bottlenecks that will likely be encountered on future petascale platforms. We present the strategy adopted in the design of Qbox, and discuss some of the performance bottlenecks that appear when using $O(10^5)$ processors.

Current trends in the architecture of new massively parallel computers emphasizes the need for new scalable algorithms for electronic structure calculations. The need to shift focus from floating point performance to data locality is well known in parallel application development, but becomes acute at the petascale.

We present a new algorithm for the calculation of compact representations of Kohn-Sham invariant subspaces. The method allows one to reduce the volume of the data used to describe a set of Kohn-Sham orbitals, with *a priori* control of the error caused by the reduction process. When applied to Kohn-Sham wavefunctions expanded on a plane-wave basis, this approach leads to a substantial reduction of the size of the datasets used to restart first-principles simulations, with controlled loss of accuracy. We also discuss a new scalable parallel implementation of a simultaneous diagonalization algorithm used in computations of Maximally Localized Wannier Functions (MLWFs) and Generalized Minimum Spread Wavefunctions (GMSWFs)[2].

[1] F. Gygi, E. W. Draeger, M. Schulz, B. R. de Supinski, F. Franchetti, S. Kral, J. Lorenz, C. Ueberhuber, J. A. Gunnels, J. C. Sexton, V. Austel, Large-Scale Electronic Structure Calculations of High-Z Metals on the BlueGene/L Platform", Proceedings of the 2006 ACM/IEEE Conference on Supercomputing, Tampa, FL, Nov. 2006.

[2] F. Gygi, J.-L. Fattebert and E. Schwegler, Comput. Phys. Comm. **155**, 1 (2003).