

# *ab initio* Electronic Structure Calculations on the BG/L Supercomputer

C. Bekas A. Curioni W. Andreoni  
IBM Research Division, Zurich Research Laboratory  
Säumerstrasse 4, CH-8803, Rüschlikon, Switzerland

June 13, 2006

Electronic structure calculations, in the framework of Density Functional Theory (DFT) [2, 4], have proven remarkably accurate in providing a wealth of information concerning several important physical properties of complex materials. However, DFT calculations are extremely demanding and have stretched our computational capabilities to their very limits. Therefore, advances in better simulation techniques and algorithms as well as advanced supercomputer architectures receive much of attention in this very active field of research.

The advent of the BG/L supercomputer has triggered a lot of excitement in the electronic structure calculation community, mainly caused by the prospect of highly increased scalability as compared to rival supercomputer architectures. Here we report our progress in scaling the CPV code [1, 5], which is part of the **quantum Espresso** package<sup>1</sup>, on the recently installed BG/L supercomputer at EPFL, Lausanne, Switzerland<sup>2</sup>.

The core problem in **ab initio** DFT calculations is the solution of the time independent Schrödinger equation

$$H_\rho \Psi_\rho = E \Psi_\rho, \quad (1)$$

where  $\rho$  is the charge density of the electrons distribution,  $H_\rho$  is the Hamiltonian operator,  $\Psi_\rho$  are the wavefunctions and  $E$  is the energy of the system. Observe that this is a nonlinear eigenvalue problem, since the Hamiltonian and the wavefunctions depend upon each other through the charge density  $\rho$ . The last decades have seen many methods that attempt to efficiently solve equation (1). All of them utilize some sort of iteration which aims to improve some initially selected wavefunctions so that at the end of the iteration the approximate energy  $E$  is as small as possible, or in other words the solution of equation (1) is self-consistent. The computational complexity of practical algorithms for this problem stems mainly from two factors:

---

<sup>1</sup><http://www.quantum-espresso.org/>

<sup>2</sup><http://bgl.epfl.ch>

**Discretization** The Hamiltonian operator and thus the wavefunctions have to be discretized in some suitably selected basis. This typically results in a very large discretized Hamiltonian (in the order of millions of degrees of freedom). Consequently, the eigensolvers for dense matrices, such as the ones in LAPACK, cannot be applied in this case. Thus, one has to utilize instead iterative techniques that only use the application of the discretized Hamiltonian operator on a likewise discretized function (i.e. vector). In plane wave implementations, such as the present case, this results in a sequence of inverse and forward 3D FFT transforms, the efficient implementation of which is crucial for overall performance. The CPV code uses a plane-wave basis to discretize the Schrödinger equation and thus relies on heavy use of 3D Fast Fourier transforms. We have investigated the efficient parallelization of 3D FFTs. In particular, we have adopted a scheme based on a task group parallelization strategy that concurrently performs several parallel 3D FFTs, one per each group of processors. Similar to the approach in [3] for the CPMD code<sup>3</sup>, we exploit opportunities for hierarchical parallelism in CPV.

**Orthogonality** The wavefunctions  $\Psi_\rho$  are orthogonal among each other. Thus, the approximate discretized wavefunctions must likewise form an orthogonal basis. This has the consequence that all iterative methods that target to solve the nonlinear eigenproblem (1) have to maintain a set of mutually orthogonal approximate wavefunctions at each iteration. Maintaining orthogonality will of course come at a cost, which scales as the cube of the total number of valence electrons in the system. BG/L nodes are equipped with two dual core PowerPC 440 processors at 700 MHz. Each processor can perform in parallel 4 fused multiply-add operations at each cycle, thus yielding a peak performance of 2.8 Gflops (5.6 Gflops per node). We have exploited on chip parallelization in order to compute the orthogonality constraints achieving close to optimal per node performance.

## References

- [1] R. Car and M. Parrinello. Unified approach for molecular dynamics and density-functional theory. *Phys. Rev. Lett.*, 55(22):2471–2474, 1985.
- [2] P. Hohenberg and W. Kohn. Inhomogeneous electron gas. *Phys. Rev.*, 136(3B):B864–B871, 1965.
- [3] J. Hutter and A. Curioni. Car-parinello molecular dynamics on massively parallel computers. *Chem. Phys. Chem.*, 6:1788–1793, 2005.
- [4] W. Kohn and L. J. Sham. Self-consistent equations including exchange and correlation effects. *Phys. Rev.*, 140(4A):A1133–A1138, 1965.
- [5] K. Laasonen, A. Pasquarello, R. Car, C. Lee, and D. Vanderbilt. Car-parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. *Phys. Rev. B*, 47(16):10142–10153, 1993.

---

<sup>3</sup><http://www.cpmid.org>