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Calculations for millions of atoms with density functional theory: linear scaling shows its potential

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Abstract
An overview of the CONQUEST linear scaling density functional theory (DFT) code is given, focusing particularly on the scaling behaviour on modern high-performance computing platforms. We demonstrate that essentially perfect linear scaling and weak parallel scaling (with fixed number of atoms per processor core) can be achieved, and that DFT calculations on millions of atoms are now possible.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Linear scaling approaches to atomistic calculations have their origin in molecular dynamics codes with force fields: the idea that, by calculating interactions for each atom only within a local part of space, computational effort scales with a local volume leads to efficient increases in system size; this also leads to natural parallelization schemes. It is well known that, for systems with a gap or metals at finite temperature, electronic structure is local, and falls off exponentially with distance—summed up in Kohn's 'nearsightedness' principle [1]. This realization led to linear scaling tight binding methods in the 1980s. Methods for $O(N)$ or linear scaling DFT calculations [2] were first proposed over 15 years ago [3–9], but it is only in the last five years that practical calculations using these methods have begun to appear. The developments which have enabled these calculations will be surveyed in detail in section 2. In brief, the algorithms used to find the ground state have converged on a few main methods, while there has been more work on the local orbitals used to represent the density matrix. Local basis sets, and their efficient implementation and minimization, are key to performance in linear scaling codes.

Part of the reason for the slow development of practical codes is that parallelization is extremely important. If calculations on tens of thousands or hundreds of thousands of atoms are to be performed, this will require hundreds or thousands of processors (or cores in the case of multi-core processors, as is becoming almost universal). The efficient implementation of linear scaling codes on parallel machines has received attention before [10–14]; in this paper, we will explore how far scaling can be extended efficiently. We find that there is every reason to believe that linear scaling DFT will make extremely good use of the hundreds of thousands of cores which are becoming available with petascale computers[5]. In this paper, we will consider the performance of our linear scaling DFT code CONQUEST [9, 10, 15–20], but there are other linear scaling DFT codes under development, for instance Siesta [21], OpenMX [22] and ONETEP [23]. As will be described in section 2, most linear scaling methods work by using a reformulation of DFT in terms of the density matrix, and apply localization constraints to achieve good scaling with system size.

In section 2, we give an overview of the CONQUEST methodology, covering the fundamental theory as well as

[5] The Jaguar Cray machine installed at Oak Ridge National Laboratory in America is the first petaflop machine, and has 150 000 cores, while the next-generation supercomputer in Japan, which is scheduled for completion in 2011, will have a peak performance of over 10 petaflops and will require several hundred thousand cores.

details of the implementation. Section 3 forms the central part of the paper, presenting scaling data both with respect to number of cores and numbers of atoms. We conclude with a brief look forward.

2. Methodology

The ideas underlying CONQUEST have been presented before [9, 10, 15–20], but we will give an overview here for convenience and to help explain the implementation details given below; the interested reader is referred to previous publications for full details. As is common with many linear scaling codes, CONQUEST works directly with the density matrix rather than wavefunctions, and writes it in a separable form:

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{i\alpha, j\beta} \phi_{i\alpha}(\mathbf{r}) K_{i\alpha j\beta} \phi_{j\beta}(\mathbf{r}'), \tag{1}$$

where $\phi_{i\alpha}(\mathbf{r})$ is a strictly local function centred on atom i called a *support function*; multiple support functions on the same atom are notated with α. The support functions are not orthogonal, and there is an associated overlap matrix:

$$S_{i\alpha j\beta} = \int \mathrm{d}\mathbf{r}\, \phi_{i\alpha}(\mathbf{r}) \phi_{j\beta}(\mathbf{r}). \tag{2}$$

The density matrix in the basis of support functions is written $K_{i\alpha j\beta}$. Locality is imposed in CONQUEST via a spherical cutoff on the support functions R_{cut} and a distance-based criterion on the elements of an auxiliary density matrix from which K is derived.

For a given set of support functions, the ground state is found by varying the elements of K to minimize the energy subject to various conditions:

(i) Self-consistency between the charge density and potential.
(ii) Correct electron number, $N_{\mathrm{e}} = 2\mathrm{Tr}[KS]$.
(iii) Idempotency of the density matrix.

The first of these conditions is a standard problem within electronic structure, and while not trivial, has been widely explored in other contexts [20, 24, 25]. The second is relatively easy to impose, and can be incorporated within the minimization [10, 15]. The final condition is extremely hard to impose, and we instead use the ideas of McWeeny [26] to impose weak idempotency. By writing K in terms of an auxiliary density matrix (ADM), L, we ensure that its eigenvalues lie between 0 and 1 and converge towards these extrema as the minimization proceeds [5, 8, 16, 26]:

$$K = 3LSL - 2LSLSL. \tag{3}$$

This method for achieving idempotency is sometimes known as the ADM or LNV method.

Practically, the localization on the density matrix is imposed on L, so that $L_{ij} = 0, |\mathbf{R}_i - \mathbf{R}_j| > R_L$. By using sparse matrices, and carefully constructed sparse matrix methods [12], the computational time and memory required for minimization of energy with respect to the elements of K (and ultimately L) scale linearly with the number of atoms in the system.

This is one area where CONQUEST differs from other linear scaling DFT codes (though it is not the only linear scaling DFT code to use the ADM method: the ONETEP code [23], for instance, also uses it). The orbital minimization method (OMM) [7, 6, 27] is another variational approach, though it is not commonly used (it is implemented in the SIESTA code [28] and used by Tsuchida [29]). Non-variational methods commonly used include the divide-and-conquer [3] (D&C) method and the trace-correcting family of methods [30]. These are the main methods used for the density matrix search.

The representation of the support functions or local orbitals is an important problem within linear scaling electronic structure techniques, and is another area where CONQUEST differs from other codes. The codes now available [18, 22, 23, 28] are of two types: those that use basis sets akin to plane waves (including blips or B-splines [31], finite element approaches [32–34], periodic sinc functions [35] and wavelets [36]), which allow systematic basis-set convergence; and those that use pseudo-atomic orbitals (PAOs) as basis sets [22, 28, 37–40], for which systematic convergence is usually significantly harder, but which have smaller basis sizes. An important feature of our own CONQUEST code [18–20] is that both types of basis are implemented, and this means that rapid, though semi-quantitative calculations can be performed for exploratory purposes, but precise calculations are also possible. The support functions are written:

$$\phi_{i\alpha}(\mathbf{r}) = \sum_s b_{i\alpha s} \chi_s(\mathbf{r}) \tag{4}$$

where $\chi_s(\mathbf{r})$ is a basis function centred on atom i.

The quantitative basis set uses blip functions, specifically b-splines, on a cubic regular grid defined within the support region for each atoms [31], which can be related to a plane-wave energy cutoff; it is, however, perfectly possible to use different spacings for different atoms. By increasing the support region radius and the L matrix cutoff systematically, it is possible to achieve plane-wave accuracy linear scaling calculations [10, 31, 41].

The different computational operations in CONQUEST can be summarized as:

(i) Matrix multiplication (e.g. $K_{ij} = L_{ik} S_{kl} L_{lj}$).
(ii) Integration on a grid (which is regular, and defined along the simulation cell lattice vectors).
(iii) Basis function operations: analytic integrals or basis-to-grid transformations.
(iv) Fast Fourier transforms (performed on the same grid as integration).
(v) Communication of information between cores.

The parallelization strategy in CONQUEST [10, 12, 17] relies on the division of the computational cell into small groups of atoms (partitions) and integration grid points (blocks); typically a partition will contain ∼5–20 atoms, and a block will have size of $3\times3\times3$–$8\times8\times8$ grid points. These are assembled into groups (bundles of partitions and domains of blocks) which should be both localized and overlapping for good

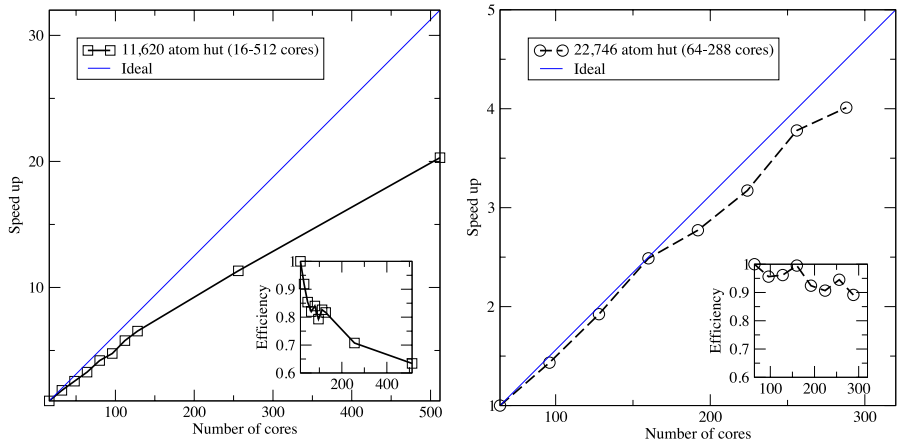

Figure 1. Scaling using automated Hilbert partitioning for two different hut clusters. (a) Hut cluster with 11 620 atoms on 16–512 cores (increasing by 32 times); (b) hut cluster with 22 746 atoms on 64–288 cores (increasing by 4.5 times).

performance, and assigned to cores (for multi-core CPUs). The assembly of domains and bundles, and the assignment of these groups to cores can strongly affect the efficiency of the code. We have implemented a default partitioning scheme based on Hilbert curves [13] which allows calculations without detailed optimization of load balancing; examples of the efficiency of parallel scaling with this scheme are given below in section 3. Details of partitioning can be optimized externally to CONQUEST, and this allows different approaches to be taken. There are some computational cells where the assignment of domains and bundles to cores is obvious (for instance the cubic cells used for scaling tests up to millions of atoms), and a simple script will allow the optimal distribution to be created. We also have an optimizing code which uses simulated annealing to load-balance the system.

CONQUEST can operate at different levels of accuracy, depending on the basis set chosen, and other factors. If PAOs are used, with only a minimal basis set and no self-consistency, then we have non-self-consistent *ab initio* tight binding (NSC-AITB). If self-consistency is introduced and the basis set expanded somewhat then the code runs at the level of self-consistent AITB. For full PAO basis sets and blip functions with full basis optimization we achieve full DFT accuracy, and when cutoffs are taken to convergence we can recover plane-wave accuracy. CONQUEST has the PBE GGA functional implemented as well as LDA, at all levels [42]. Forces are calculated exactly as derivatives of the energy [19, 42] and are implemented at all levels of accuracy, both for LDA and GGA [42].

Many of the calculations in this paper operate at the NSC-AITB level, as this uses the full functionality of the code and permits good scaling tests. This does not mean, however, that this is how we anticipate using the code; indeed, we have performed self-consistent calculations on cells up to 262 144 atoms (described below) with no decrease in the scaling. Optimization of support functions scales in a similar manner.

3. Results

The results in this section are intended to demonstrate the scaling performance of the CONQUEST code. We have recently used the code for a series of calculations on the Ge(105) surface [43] and on the energetics of self-assembly of Ge hut clusters on Si(001) [44], and we draw many example systems from these studies. Details of the systems are given in the papers already published. Linear scaling methods are also ideal for application to ionic materials (which often have large band gaps) and we have successfully performed exploratory self-consistent calculations on MgO surfaces with defects. We are also using CONQUEST to perform calculations on other systems, such as biomolecules, and we are actively pursuing this area [42, 45, 46].

We start by considering the strong scaling performance on the current UK HPC facility HECToR (a Cray XT4): that is increasing the number of cores used in a calculation while keeping the system size fixed. For these tests, we have used two of the Ge hut cluster systems, containing 11 620 and 22 746 atoms respectively. The unit cells are far from cubic, which presents a non-ideal situation for the default partitioner which uses a 3D Hilbert curve and performs best for cells close to cubic[6]. The smaller system allows somewhat better assignment of atoms to cores, and we have tested the parallel scaling more extensively on this system.

Results are shown in figure 1. In figure 1(a) we show the speed-up of the code for the smaller hut cluster, as we increase the number of cores by a factor of up to 32. For an increase of a factor of up to 8, the scaling is excellent with an efficiency (defined as speed-up measured divided by increase in number of cores) of about 80%. For further increases in numbers of cores we see smaller efficiencies, but the efficiency is still over 60%. In figure 1(b) we show the scaling for the larger hut cluster, as the number of cores is increased by a factor of up to 4.5. This scaling is excellent, and remains at over 90%.

We can understand the strong scaling behaviour from the parallelization strategy. The main computational load in CONQUEST is the sparse matrix multiplication, which we have optimized extensively [12]. The time required for multiplies scales with the number of neighbours of each atom as well as the number of atoms per core; in the hut cluster system

[6] We are developing improvements to the partitioner to allow us to move away from this restriction, but these are still at a preliminary stage.

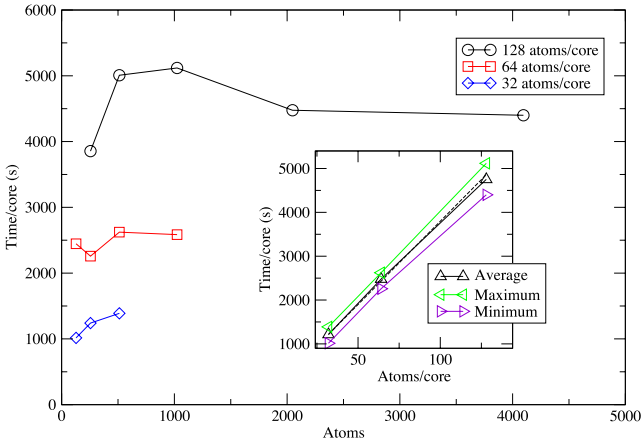

Figure 2. Scaling on LCN cluster (dual-core Opteron, Myrinet interconnect). Main graph shows time per core for different atoms per core (reaching 4096 atoms on 32 cores); inset shows the change of time/core with increasing numbers of atoms/core, with a linear increase for the average shown with a dashed line.

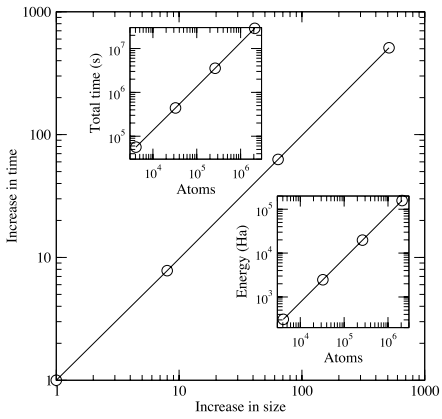

Figure 3. Linear and parallel scaling for bulk silicon on 512–4096 cores. The insets show total time and total energy (made positive to enable log plot) while main graph shows increase in time with system size. Exact data values are given in table 1.

shown above, some atoms are near the surface of the system with fewer neighbours, while others are in the bulk with more neighbours. With less than 20 atoms per core, it is rather hard to achieve good load balancing. Good load balancing also requires that the bundles of atoms assigned to cores are compact, and this is difficult to achieve with small numbers of atoms per core. Also, as the number of atoms per core decreases, communications overhead will start to dominate. This behaviour is clearly seen in figure 1, where there are only ∼20 atoms/core at the largest number of cores. The most efficient results are seen for 40 or more atoms per core.

In practical calculations, we usually increase the number of cores proportionately with the number of atoms in the system. Therefore, more realistic tests of the scaling are to fix the number of atoms per core, and increase the number of cores at the same time as increasing the number of atoms; this is known as weak scaling. Results for this mode of operation on a local HPC cluster (based on dual processor, dual-core Sun servers with Myrinet interconnects) are shown in figure 2. The system being tested is bulk silicon, which while not scientifically interesting, is simple to prepare and contains all the essential physics we wish to test. The main graph shows the time per core plotted against number of atoms in the system for different numbers of atoms per core: 32 atoms/core, 64 atoms/core and 128 atoms/core. A number of important points come out of this plot: first, the time per core is effectively constant for the systems considered; second, communication becomes unimportant for 64 atoms/core or more (as seen in figure 1 as well); third, as shown in the inset, the linear scaling performance of the code is excellent, lying on the ideal linear curve.

Finally, we are concerned to show that this good scaling behaviour persists to extremely large systems, so we have taken a system which can be easily partitioned and scaled and scaled to over 4000 cores and over 2000 000 atoms. We show increase in total time (i.e. time/core summed over cores) versus increase in system size, as well as total time and total energy plotted against number of atoms in figure 3. These were run on HECToR, using between 8 and 4096 cores with 512 atoms/core, giving 2097 152 atoms as the largest cell considered. Details of times, energies and numbers of cores are given in table 1.[7]

Table 1. Times and energies for CONQUEST runs with 512 atoms/core. The energy per atom takes a constant value of 0.075 261 Ha.

Atoms	Time/core (s)	Total energy (Ha)	Cores
4 096	7068.878	−308.268 785	8
32 768	6893.759	−2 466.150 282	64
262 144	6931.418	−19 729.202 254	512
2097 152	7032.496	−157 833.618 033	4096

The most important result from this calculation is that DFT calculations on millions of atoms are now possible. We see that the time per core does not increase with system size, and that the energy per atom is constant. There are parts of the CONQUEST code which are not strictly linear scaling: we use an Ewald sum for electrostatic interactions (which can be easily replaced with a scheme such as the neutral atom potential [28, 37]) which scales as $\mathcal{O}(N^{3/2})$ and fast Fourier transforms which scale as $N \log(N)$, but even for the 2097 152 atom unit cell these are negligible (approximately 3 s for all FFT-related work and 50 s for Ewald sum). We note that orbital-free DFT calculations have recently been performed on a supercell of 1012 500 atoms of bulk Al [47].

We have also performed self-consistent $O(N)$ calculations on this system (actually for the first three cells), and find that they require four to five times as long, with our current implementation (in this case, the variational nature of the minimization means that, as self-consistency is approached, less time is spent finding the density matrix); the scaling of the code when performing self-consistent calculations, is identical to non-self-consistent calculations. The main challenge now is

[7] The grid spacing used was a little coarser than we would normally choose, to reduce memory requirements; however, we note that this will not affect the convergence or scaling, and have tested the smaller systems with finer grids to ensure that there is no effect from this.

to improve the efficiency of the code, and reduce the number of atoms per core which can be run without communications becoming a heavy burden. We will focus on three main areas: first, efficient re-use of variational data such as the L matrix to reduce the time to the ground state; second, robustness and stability of the calculations; and finally, more efficient automatic partitioning [13]. This will allow us to consider real scientific problems which require tens or hundreds of thousands of atoms, and to perform molecular dynamics simulations using petascale computer platforms.

4. Conclusions

Linear scaling approaches to DFT have been under development for about fifteen years, and are now starting to show their promise in real calculations, and in their applicability to petascale computers. This special issue of Journal of Physics: Condensed Matter is in honour of Professor Mike Gillan's 65th birthday, and it is appropriate to celebrate the considerable contribution which he has made to the development of linear scaling DFT, both through the theory and implementation [9, 10, 12, 15–20, 31, 39, 43–45, 48, 49]. The results in this paper show that linear scaling DFT is realizing its potential, and that Mike Gillan's contributions have underpinned all that has gone on in the field.

It has been noted [50] that applications of linear scaling methods to real problems are starting to emerge; the challenge now is to make linear scaling methods sufficiently robust and efficient that they can be used as routinely as standard DFT methods, and to find applications which demonstrate their power. Examples of applications of these methods include work on DNA with Siesta [51] and CONQUEST [45], biomolecules with ONETEP [52] and CONQUEST [42, 46] and our work on Ge on Si(001) with CONQUEST, extending to over 20 000 atoms [43, 44]. Among other applications, we intend to extend the Ge work to the transition from hut clusters to domes, as well as applying CONQUEST to biomolecules [46]. The code will also be released under a GPL licence in the near future.

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