Introductory Remarks: Linear Scaling Methods

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PREFACE

Introductory Remarks: Linear Scaling Methods

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It has been just over twenty years since the publication of the seminal paper on molecular dynamics with *ab initio* methods by Car and Parrinello [1], and the contribution of density functional theory (DFT) and the related techniques to physics, chemistry, materials science, earth science and biochemistry has been huge. Nevertheless, significant improvements are still being made to the performance of these standard techniques; recent work suggests that speed improvements of one or even two orders of magnitude are possible [2]. One of the areas where major progress has long been expected is in $O(N)$, or linear scaling, DFT, in which the computer effort is proportional to the number of atoms. Linear scaling DFT methods have been in development for over ten years [3], but we are now in an exciting period where more and more research groups are working on these methods. Naturally there is a strong and continuing effort to improve the efficiency of the methods and to make them more robust. But there is also a growing ambition to apply them to challenging real-life problems.

This special issue contains papers submitted following the CECAM Workshop 'Linear-scaling *ab initio* calculations: applications and future directions', held in Lyon from 3–6 September 2007. A noteworthy feature of the workshop is that it included a significant number of presentations involving real applications of $O(N)$ methods, as well as work to extend $O(N)$ methods into areas of greater accuracy (correlated wavefunction methods, quantum Monte Carlo, TDDFT) and large scale computer architectures.

As well as explicitly linear scaling methods, the conference included presentations on techniques designed to accelerate and improve the efficiency of standard (that is non-linear-scaling) methods; this highlights the important question of crossover—that is, at what size of system does it become more efficient to use a linear-scaling method? As well as fundamental algorithmic questions, this brings up implementation questions relating to parallelization (particularly with multi-core processors starting to dominate the market) and inherent scaling and basis sets (in both normal and linear scaling codes). For now, the answer seems to lie between 100–1,000 atoms, though this depends on the type of simulation used among other factors.

Basis sets are still a problematic question in the area of electronic structure calculations. The linear scaling community has largely split into two camps: those using relatively small basis sets based on local atomic-like functions (where systematic convergence to the full basis set limit is hard to achieve); and those that use necessarily larger basis sets which allow convergence systematically and therefore are the localised equivalent of plane waves. Related to basis sets is the study of Wannier functions, on which some linear scaling methods are based and which give a good point of contact with traditional techniques; they are particularly interesting for modelling unoccupied states with linear scaling methods.

There are, of course, as many approaches to linear scaling solution for the density matrix as there are groups in the area, though there are various broad areas: McWeeny-based methods, fragment-based methods, recursion methods, and combinations of these. While many ideas have been in development for several years, there are still improvements emerging, as shown by the rich variety of the talks below.

Applications using $O(N)$ DFT methods are now starting to emerge, though they are still clearly not trivial. Once systems to be simulated cross the 10,000 atom barrier, only linear scaling methods can be applied, even with the most efficient standard techniques. One of the most challenging problems remaining, now that *ab initio* methods can be applied to large systems, is the long timescale problem.

Although much of the work presented was concerned with improving the performance of the codes, and applying them to scientifically important problems, there was another important theme: extending functionality. The search for greater accuracy has given an implementation of density functional designed to model van der Waals interactions accurately as well as local correlation, TDDFT and QMC and GW methods which, while not explicitly $O(N)$, take advantage of localisation.

All speakers at the workshop were invited to contribute to this issue, but not all were able to do this. Hence it is useful to give a complete list of the talks presented, with the names of the sessions; however, many talks fell within more than one area. This is an exciting time for linear scaling methods, which are already starting to contribute significantly to important scientific problems.

Applications to nanostructures and biomolecules

- A DFT study on the structural stability of Ge 3D nanostructures on Si(001) using `CONQUEST` *Tsuyoshi Miyazaki, D R Bowler, M J Gillan, T Otsuka and T Ohno*
- Large scale electronic structure calculation theory and several applications *Takeo Fujiwara and Takeo Hoshi*
- `ONETEP`: Linear-scaling DFT with plane waves *Chris-Kriton Skylaris, Peter D Haynes, Arash A Mostofi, Mike C Payne*
- Maximally-localised Wannier functions as building blocks for large-scale electronic structure calculations *Arash A Mostofi and Nicola Marzari*
- A linear scaling three dimensional fragment method for *ab initio* calculations *Lin-Wang Wang, Zhengji Zhao, Juan Meza*
- Peta-scalable reactive Molecular dynamics simulation of mechanochemical processes *Aiichiro Nakano, Rajiv K Kalia, Ken-ichi Nomura, Fuyuki Shimojo and Priya Vashishta*
- Recent developments and applications of the real-space multigrid (RMG) method *Jerzy Bernholc, M Hodak, W Lu, and F Ribeiro*

Energy minimisation functionals and algorithms

- `CONQUEST`: A linear scaling DFT Code *David R Bowler, Tsuyoshi Miyazaki, Antonio Torralba, Veronika Brazdova, Milica Todorovic, Takao Otsuka and Mike Gillan*
- Kernel optimisation and the physical significance of optimised local orbitals in the `ONETEP` code *Peter Haynes, Chris-Kriton Skylaris, Arash Mostofi and Mike Payne*

- A miscellaneous overview of SIESTA algorithms *Jose M Soler*
- Wavelets as a basis set for electronic structure calculations and electrostatic problems *Stefan Goedecker*
- Wavelets as a basis set for linear scaling electronic structure calculations *Mark Rayson*
- $O(N)$ Krylov subspace method for large-scale *ab initio* electronic structure calculations *Taisuke Ozaki*
- Linear scaling calculations with the divide-and-conquer approach and with non-orthogonal localized orbitals *Weitao Yang*
- Toward efficient wavefunction based linear scaling energy minimization *Valery Weber*
- Accurate $O(N)$ first-principles DFT calculations using finite differences and confined orbitals *Jean-Luc Fattebert*

Linear-scaling methods in dynamics simulations or beyond DFT and ground state properties

- An $O(N)$ time-domain algorithm for TDDFT *Guan Hua Chen*
- Local correlation theory and electronic delocalization *Joseph Subotnik*
- *Ab initio* molecular dynamics with linear scaling: foundations and applications *Eiji Tsuchida*
- Towards a linear scaling Car–Parrinello-like approach to Born–Oppenheimer molecular dynamics *Thomas Kühne, Michele Ceriotti, Matthias Krack and Michele Parrinello*
- Partial linear scaling for quantum Monte Carlo calculations on condensed matter *Mike Gillan*
- Exact embedding of local defects in crystals using maximally localized Wannier functions *Eric Cancès*
- Faster GW calculations in larger model structures using ultralocalized nonorthogonal Wannier functions *Paolo Umari*

Other approaches for linear-scaling, including methods for metals

- Partition-of-unity finite element method for large, accurate electronic-structure calculations of metals *John E Pask and Natarajan Sukumar*
- Semiclassical approach to density functional theory *Kieron Burke*
- *Ab initio* transport calculations in defected carbon nanotubes using $O(N)$ techniques *Blanca Biel, F J Garcia-Vidal, A Rubio and F Flores*
- Large-scale calculations with the tight-binding (screened) KKR method *Rudolf Zeller*

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References

[1] Car R and Parrinello M 1985 *Phys. Rev. Lett.* **55** 2471
[2] Kühne T D, Krack M, Mohamed F R and Parrinello M 2007 *Phys. Rev. Lett.* **98** 066401
[3] Goedecker S 1999 *Rev. Mod. Phys.* **71** 1085