Comment on “Accurate and Scalable O(N) Algorithm for First-Principles Molecular-Dynamics Computations on Large Parallel Computers”

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While we acknowledge the progress made by Osei-Kuffuor and Fattebert in developing their O(N) algorithm[1], a number of the claims and statements made in the paper appear to us to be questionable, in particular that they have presented the first truly scalable O(N) molecular dynamics algorithm. The claims that we wish to discuss in detail are: controllable accuracy; non-global communications and scalability; the approach to inversion of the overlap matrix; and their results.

There are a number of O(N) codes already available which offer controllable accuracy in the basis set. The ONETEP code[2] uses periodic sinc or psinc functions[3], while the CONQUEST code[4, 5] uses b-spline functions[6] and the FEMTECK code[7] uses finite elements[8]. In all these codes, the accuracy is systematically controlled using a grid spacing which is directly equivalent to a plane-wave cutoff, and involves no approximation in the kinetic energy (whereas a finite difference approach approximates the kinetic energy[9]).

The principle of removing global communications to achieve scalability is well established (and papers on sparse matrix multiplication[10, 11] and sparse, parallel matrix multiplication in the FreeON[12, 13], ONETEP[14], CP2K[15] and CONQUEST codes[16] show that this is strongly developed in the O(N) community).

We disagree with the authors’ assertion that “the parallel implementation of [algorithms to invert the S matrix] generally require some global coupling”. There are a number of existing approaches to inverting the S matrix, including the orbital minimisation method (OMM)[17, 18] used by FEMTECK, the method used in OpenMX[19], and Hotelling’s or Schultz’s method (which will be scalable and O(N) with sparse matrix algebra), as well as the approximate inverse methods cited by the authors. We note that the approach that the authors suggest is essentially the same as used in 1994 by Stechel et al.[20].

Moreover, it is important to recall that one of the major efforts in the O(N) community in recent years has been to develop locally communicating, scalable codes. The CP2K code has recently demonstrated calculations on 1,000,000 atoms with density functional tight binding (DFTB) and 96,000 water molecules with DFT, scaling to 46656 cores[13]. The CONQUEST code has demonstrated scaling to over 2,000,000 atoms[21] on 4,096 processors, and recently scaled to 196,000 cores on the K computer[22] as shown in Fig. 1. In the data in Fig. 2 presented by Osei-Kuffuor and Fattebert, there seems to be a slow increase in wall clock time with system size on the IBM BGQ which indicates some residual problems with scalability in the implementation.

FIG. 1: Weak scaling for CONQUEST on the K computer, showing scaling to around 200,000 cores

The accurate, efficient calculation of molecular dynamics with O(N) complexity is a significant challenge, with problems including energy conservation and efficiency of re-use of electronic structure[23] and efficient load balancing. We note that, despite the title of the paper, the authors do not actually show any results from molecular dynamics, while these have been shown by others. Tsuchida demonstrated MD on 1,000 atoms of ethanol (though this used a direct inversion of S, which is not scalable)[24] while Cawkwell and Niklasson have shown

FIG. 2: Wall time (sec/MD step) versus number of atoms (log scale) for CONQUEST on the K computer for different atom counts
accurate, energy conserving O(N) MD (without testing scalability). We have demonstrated efficient relaxation of large nanostructures with systems of 26,000 atoms, recently extended to over 100,000 atoms, and have recently implemented efficient, energy conserving molecular dynamics in Conquest.

In all our comments we simply want to note that there have been other demonstrations of scalable, efficient linear scaling approaches to electronic structure calculations including ab initio molecular dynamics, which should have been referenced and acknowledged by the authors of the present paper.

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