Efficient *ab-initio* MD with a linear-scaling DFT technique

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First-principles simulations have been a practical tool and applied to a broad swath of materials to investigate their structures and physical properties with density functional theory (DFT). Their computational cost, however, increases rapidly with the third power of the number of atoms so the conventional DFT methods usually face a difficulty in calculating large systems. We have been developing a linear-scaling DFT code CONQUEST\textsuperscript{[1]}, which only raises the CPU cost linearly, thus it is capable of studying massive systems that $O(N^3)$ methods have not ever touched.

Here we shall present our studies on $O(N)$ *ab-initio* molecular dynamics (MD). It has recently become feasible to carry out efficient and stable Born-Oppenheimer dynamics with CONQUEST. It utilises the density matrix and imposes a spatial cutoff on it to achieve $O(N)$. Though this may cause a change in the number of neighbour atoms during a simulation, we have succeeded in running accurate and stable MD. We have overcome an intrinsic problem of energy drift by introducing additional electronic degrees of freedom to the Born-Oppenheimer Lagrangian\textsuperscript{[2]} and direct use of the optimised density matrices at the previous step to the present SCF calculation has resulted in a remarkably high efficiency. It will be shown that how computationally efficient it is now via a comparison with the calculated results by initialising density matrices at every step. Furthermore, we shall report the energy dependence on calculation conditions, such as SCF tolerance and cutoff values imposed on density matrices, and discuss the calculation stability in both micro canonical and canonical ensembles.

\textsuperscript{[2]} Anders. M. N. Niklasson, PRL 100, 123004 (2008)