Recent Developments in the Linear Scaling DFT Code CONQUEST: Constrained DFT, TDDFT, and Basis Sets

D. R. Bowler,[1,2,3] T. Miyazaki,[4] C. O'Rourke,[1,2,3] and M. Gillan[1,2,3]

[3] *London Centre for Nanotechnology, UCL, London WC1H 0AH, UK.*
[2] *Department of Physics & Astronomy, UCL, London WC1E 6BT, UK.*
[3] *Thomas Young Centre, UCL, London WC1E 6BT, UK.*
[4] *National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0047, Japan.*

Linear scaling or O(N) electronic structure codes have been under development for around fifteen years [1]. After an initial explosion of interest, the practical difficulties of implementation and efficiency have led to a slow down in development and applications. In this talk I will present details of recent developments in the massively parallel CONQUEST linear scaling DFT code, and make some comments on the linear scaling field in general.

The CONQUEST code [2] is one of the leading O(N) codes, and has demonstrated not only excellent scaling to over two million atoms and many thousands of cores [3] but also practical applications to nanostructures on semiconductor surfaces [4], and recently to biological systems. I will describe the details of the CONQUEST code, including recent developments in basis functions and parallelisation. I will also discuss recent improvements including constrained DFT [5], exact exchange and TDDFT, all of which have been implemented with linear scaling.

[1] D. R. Bowler and T. Miyazaki, Rep. Prog. Phys. **75**, 036503 (2012).

[2] D. R. Bowler, R. Choudhury, M. J. Gillan, and T. Miyazaki, phys. stat. sol. b **243**, 989 (2006).

[3] D. R. Bowler and T. Miyazaki, J. Phys.: Condens. Matter **22**, 074207 (2010).

[4] T. Miyazaki, D. R. Bowler, M. J. Gillan, and T. Ohno, J. Phys. Soc. Jpn. **77**, 123706 (2008).

[5] A. M. P. Sena, T. Miyazaki, and D. R. Bowler, J. Chem. Theory Comput. **7**, 884 (2011).

Contact: david.bowler@ucl.ac.uk