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Introducing ONETEP: Linear-Scaling Density Functional Theory with Plane Waves

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In order to apply first principles quantum mechanical calculations to systems containing thousands of atoms we need linear-scaling techniques. In achieving this goal we must not lose the accuracy, efficiency and flexibility provided by conventional total energy schemes. Plane waves are a popular choice of basis set for many such schemes because their implementation is straightforward and the completeness of the basis set can be controlled systematically with a single parameter. However, the resulting calculations require a computational effort which scales as the cube of the number of atoms in the system, and as a result current simulations are limited to hundreds of atoms.

In this talk I will present ONETEP (Order-N Electronic Total Energy Package), a parallel implementation of our linear-scaling reformulation [1] of the plane wave pseudopotential approach. The linear-scaling is achieved by exploiting the real space localisation of the electronic system that is inherent in non-metallic materials. I will describe the theoretical developments that allow us to optimise with linear cost the strictly localised quantities expressed in terms of a delocalised plane-wave basis. These same localised quantities also lead us to a physical way of dividing the computational effort among many processors to allow calculations to be performed efficiently on parallel machines. It will be shown that the localisation is achieved in a controlled and mathematically consistent manner so that ONETEP provides the same accuracy as conventional cubic-scaling plane-wave approaches, and offers fast and stable convergence. The particular features of our method which result in its success will be highlighted and preliminary results for realistic biological and condensed matter applications will be presented.

[1] C.-K. Skylaris, A. A. Mostofi, P. D. Haynes, O. Diéguez and M. C. Payne, *Phys. Rev. B*, **66**, 035119 (2002).