ONETEP: Linear Scaling DFT with Plane-Waves – Methods and Applications –

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We present ONETEP[1] (Order-N Electronic Total Energy Package), a density functional method, based on plane-waves, whose computational cost scales only linearly with the number of atoms.

Although at first sight the extended nature of plane-waves makes them appear unsuitable for representing the localised orbitals used in linear scaling methods – which is why localised basis sets such as Gaussians, numerical atomic orbitals, spherical waves and B-splines have been used commonly instead – we have developed a linear scaling method based on plane-waves which overcomes this difficulty and which can achieve the same accuracy and convergence rate as traditional plane-wave calculations[2].

We describe the main features of our method which result in its success, and present recent developments and results for realistic applications.

[1] Introducing ONETEP: Linear-scaling density functional simulations on parallel computers, *J. Chem. Phys.* **122**, 084119 (2005).

[2] Preconditioned iterative minimization for linear-scaling electronic structure calculations, *J. Chem. Phys.* **119**, 8842 (2003).