Linear-scaling Density-functional Theory with Plane Waves

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Plane-waves are a popular choice of basis set for simulations based on density-functional theory because the implementation is straightforward and the completeness can be controlled systematically with a single parameter. The resulting simulations require a computational effort which scales as the cube of the system-size, which makes the cost of large-scale calculations prohibitive. Extended basis functions would appear to be an inappropriate choice for expanding the localised orbitals of linear-scaling methods or for embedding the calculation within a larger model, and so localised basis sets such as Gaussians or atomic orbitals have been used instead.

In spite of this, we present a linear-scaling method based on plane-waves\textsuperscript{1,2} which can achieve the same accuracy and convergence rate as traditional plane-wave calculations, and which overcomes the apparent difficulties mentioned above. The particular features of our method which result in its success will be highlighted, and preliminary results for realistic biological and condensed matter applications from the ONETEP parallel code will be presented.
