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Linear-Scaling Density Functional Theory Simulations of Nanomaterials with the ONETEP code: vdW-DF and PAW methodology and OpenMP/MPI hybrid parallelism NICHOLAS HINE, GABRIEL CONSTANTINESCU, MIKE PAYNE, University of Cambridge, U.K., LAMPROS ANDRINOPOULOS, ARASH MOSTOFI, PETER HAYNES, Imperial College London, U.K., KARL WILKINSON, JACEK DZIEDZIC, CHRIS-KRITON SKYLARIS, University of Southampton, U.K. — Methods based on traditional density functional theory (DFT) seek eigenstates of the Kohn-Sham Hamiltonian, and thus inevitably hit a scaling wall as system size increases, due to cubic scaling of the computational effort. However, useful contact with experiment in the study of nanomaterials (eg nanocrystals, interfaces, proteins, disordered molecular crystals) requires accurate calculations on systems comprising many thousands of atoms, beyond this scaling wall. Approaches based on the density matrix can exploit real-space localisation to achieve linear-scaling with system size and make such calculations feasible and highly parallel. The ONETEP Linear-Scaling DFT code [1] combines the benefits of linear-scaling, efficient parallelisation, and variational convergence akin to plane-wave approaches, with a wide-ranging set of features. I will present an overview of the code and recent developments: hybrid parallelism based on OpenMP and MPI, enabling scaling to tens of thousands of cores; Projector Augmented Wave methods, enabling study of transition metals; and van der Waals DF methods. These have combined to enable studies of C_{60} molecular crystals and Transition Metal Dichalcogenide interfaces eg $MoS_2/MoSe_2$. [1] C. Skylaris et al, JCP 122, 084119 (2005).

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