Large Scale DFT with PAW in Real-Space

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We present a new DFT tool developed in Julich and Osaka[1] that combines equidistant real-space grids and the Projector Augmented Wave (PAW) method[2]. The real-space treatment of wave functions, densities and potentials enables a simple and efficient parallelization with respect to communication and load balancing. It is especially well suited for massively parallel supercomputers that support nearest-neighbor communication on the hardware level (as e.g. the IBM BlueGene). The choice of boundary conditions in real-space is very flexible, i.e. we can handle isolated clusters, wire structures, surfaces and bulk on the same footing, which makes it a very universal tool for electronic structure calculations. We employ iterative diagonalization algorithms making use of the sparse and implicit representation of the Kohn-Sham Hamiltonian. By combining the PAW method, the frozen core approximation and the time-saving double-grid method[3], we can model the interactions close to the atom core properly and achieve all-electron accuracy at the costs of pseudopotential calculations. Aiming for systems consisting of several thousands of atoms, we have to parallelize over bands on top of the k-point parallelization and the real-space domain decomposition.

[1] K. Hirose, T. Ono, Y. Fujimoto, S. Tsukamoto, *First-Principles Calculations in Real-Space Formalism*, Imperial College Press, London (2005)

[2] P. E. Blochl, PRB **50**, 17953 (1994) [3]

[3] T. Ono, K. Hirose, PRL **82**, 5016 (1999) and PRB **72**, 085115 (2005)