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Superbox method for order-N electronic structure calculations for very large systems KALMAN VARGA, Physics Depertment, University of Tennessee, and Condensed Matter Science Division, Oak Ridge National Laboratory, S.T. PANTELIDES, Vanderbilt University and Condensed Matter Science Division, Oak Ridge National Laboratory — We have developed a superbox method for ab initio electronic structure calculations for very large systems. The method is applicable to density-fucntional or Hartree-Fock-based calculations. In this approach a molecule, a cluster, or a large supercell of a crystal is divided into a number of boxes. Self-consistent calculations are then carried out in parallel for each box, treating it either as a supercell or as a free unit. The wave function or the Green's function of the total system is then constructed by connecting the solutions obtained in the individual boxes by a rigorous and formally exact procedure that yields a self- consistent solution for the entire system. The method has been implemented by using the recently introduced Lagrange-function basis [1]. Examples will be presented using density functional theory to demonstrate the linear scaling of the approach with respect to the number of atoms in the system. [1] K. Varga, Z. Zhang, and S. T. Pantelides, Phys. Rev. Lett. 93, 176403 (2004).

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