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Ab initio electronic structure calculations of metals by the finite element method[1] JOHN E. PASK, PHILIP A. STERNE, University of California, Lawrence Livermore National Laboratory, USA — The finite-element (FE) method is a general approach for the solution of partial differential equations. Like the planewave (PW) method, the FE method is a systematically improvable expansion approach. Unlike the PW method, however, its basis functions are strictly local in real space, which allows for variable resolution in real space and facilitates massively parallel implementation. We discuss the application of the FE method to *ab initio* electronic-structure calculations of metals. In particular, we discuss the use of nonlocal pseudopotentials in crystalline calculations, the handling of long-range interactions in the construction of the Kohn-Sham effective potential and total energy, and the synthesis of the metallic charge density. We show that the total energy converges variationally and at the optimal theoretical rate consistent with the cubic completeness of the basis.

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