Finite Element Method in First-Principle Calculations

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The finite-element method (FEM), in which the wave functions are directly evaluated by strictly local piecewise-polynomial basis on real-space grid points, allows for variable resolution in real space; produces sparse,structured matrices; improved the accuracy with irregular mesh grids; and well suited for parallel implementation. We are developing a FEM package for solving Kohn-Sham equation, which applied self-adaptive mesh grid based on posteriori error estimation and highly-efficient parallel algorithm on mesh distribution. After solving some technical problems, as real-space pseudopotential etc , we proved the validity and exacti-tude of the algorithm by numerical evidence.

Kohn-Sham Equation

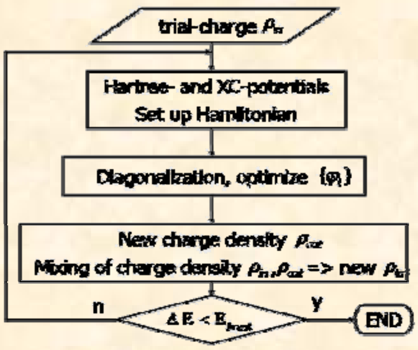
$$\left[-\frac{\nabla^2}{2}+V_{ionic}+V_{Hartree}(\rho)+V_{xc}(\rho)\right]\varphi_i=\varepsilon_i\varphi_i$$

$$\rho(r)=\sum_i n_i\left|\varphi_i(r)\right|^2$$

$$V_{Hartree}=\int\frac{\rho(r)}{|r-r'|}dr' \quad \text{or} \quad \nabla^2 V_{Hartree}=-4\pi\rho$$

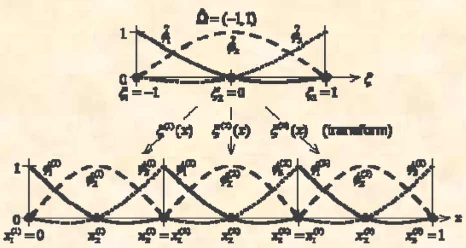
$$V_{xc}=V_x+V_c=\alpha\rho^{2/3}+\cdots$$

SCF calculation

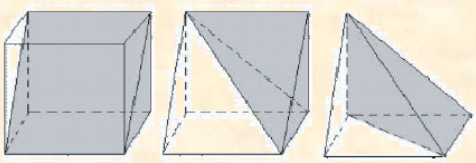


Finite Element Method

The FE method is a variational expansion approach, in which solutions are represented as a linear ombination of basis functions. It employs a basis of strictly local piecewise polynomials, each overlapping only its immediate neighbours.



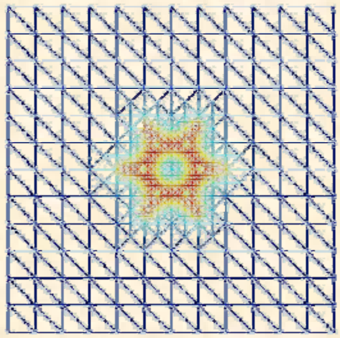
1-D Basis Functions



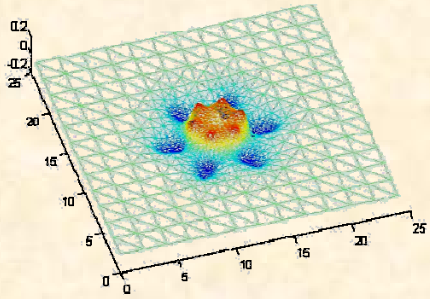
3-D space elements

Self-adaptive grid refinements

By refining the mesh according to the a posteriori error estimation, we can achieve an accurate approximation without too much cost.

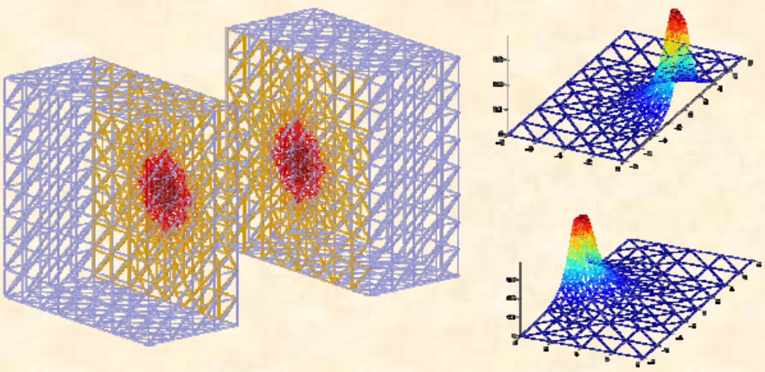


The mesh of a cut face on x-y plane



One of the wave functions

Parallel Calculations



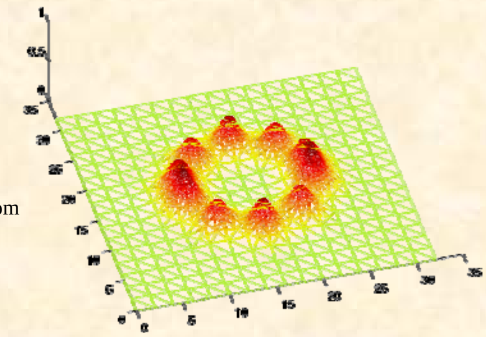
With dividing the solving region into several sub-domains we generate the mesh grids and the matrices on each ones. They are coupled on the boundary.

Numerical experiments

C60

free Energy=9.685 eV/atom

VASP result is 9.737 eV/atom



Density function on x-y plane