# Parallel Adaptive Finite Element Algorithms for Electronic Structure Computing based on Density Functional Theory

**Lihua Shen**

## Abstract

This thesis proposes some parallel adaptive finite element algorithms for Kohn-Sham equation. First, for the finite element approximation of the linear Schroedinger equation, we discuss the convergence, postprocessing techniques, a posteriori error estimation, and adaptive algorithms. Then we design some parallel adaptive algorithms for both the linear Schroedinger equation and the Kohn-Sham equation. We give the theoretical analysis of our algorithms for the linear Schroedinger equation, whereas we prove the validity of the algorithm for the Kohn-Sham equation by numerical evidence. Indeed, it is the superiority of the mesh distribution of the adaptive method and the highly-efficient parallel property that would make our algorithms be potentially competitive in electronic structure computation.

**Keywords: electronic structure computation, Kohn-Sham equation, density functional theory, finite element method, adaptive method, parallel computation, a posteriori error estimation**