COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **4**, No. 5, pp. 1086-1105

Commun. Comput. Phys.
November 2008

Parallel Mesh Refinement of Higher Order Finite Elements for Electronic Structure Calculations†

Dier Zhang[1,*], Aihui Zhou[2] and Xin-Gao Gong[1]

[1] *Department of Physics, Fudan University, Shanghai 200433, China.*
[2] *LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China.*

Received 29 February 2008; Accepted (in revised version) 29 May 2008

Available online 16 July 2008

Abstract. The finite element method is a promising method for electronic structure calculations. In this paper, a new parallel mesh refinement method for electronic structure calculations is presented. Some properties of the method are investigated to make it more efficient and more convenient for implementation. Several practical issues such as distributed memory parallel computation, less tetrahedra prototypes, and the assignment of the mesh elements carried out independently in each sub-domain will be discussed. The numerical experiments on the periodic system, cluster and nano-tube are presented to demonstrate the effectiveness of the proposed method.

AMS subject classifications: 81Q05, 65L50

Key words: Tetrahedral mesh, adaptive mesh refinement, parallel algorithms, electronic structure calculations.

1 Introduction

The finite-element (FE) method has attracted much attention for electronic structure calculations. Using the compactly supported piecewise polynomials functions, the method allows for variable resolution in real space and produces well structured sparse matrices. Therefore it is very suitable for parallel implementation. On the other hand, the FE method has been so far limited by the huge number of basis functions, which uses much more degrees of freedoms than the traditional plane wave (PW) method [1] based on the Fourier basis. However, the significant strength of the finite element method lies in its

†Dedicated to Professor Xiantu He on the occasion of his 70th birthday.
*Corresponding author. *Email addresses:* dearzhang@fudan.edu.cn (D. Zhang), azhou@lsec.cc.ac.cn (A. Zhou), xggong@fudan.edu.cn (X.-G. Gong)

ability to place adaptive/local refinements in regions where the desired functions vary rapidly while treating the other zones with a coarser description [2–9].

In early works, White *et al.* [10] found that with uniform meshes as many as 10^5 basis functions per atom were required to achieve sufficient accuracy. To decrease the number of basis functions Tsuchida and Tsukada [2] had applied nonuniform hexahedron meshes on H_2 molecules. Beck [5, 11] studied the multigrid method based on such nonuniform hexahedron meshes. In these applications the grid can be made to vary logarithmically near the nuclei, but the smoothness of the wave function is not guaranteed for the non-conforming mesh. Afterward, Tsuchida and Tsukada [3, 4] proposed another approach with the adaptive curvilinear coordinates (ACC's), which was recently applied for the calculations of *ab initio* molecular dynamics. All the above adaptive coordinates are based on hexahedron meshes. In [12], we proposed an adaptive refinement method to generate conforming tetrahedra mesh. This method can create a very flexible mesh which could be locally refined in any interested regions. Moreover, the mesh conforming can be preserved during the refinements. With a posteriori error estimation of the eigenvalue problem [13], the refinement is carried out, automatically paying special attention to the spatial regions where the computed functions vary rapidly, especially near the nuclei. For this implementation the particular technique adopted for mesh refinement is very important. In order to perform large scale electronic structure calculations, we present a parallel algorithm for the adaptive construction of tetrahedral meshes in the finite element computations, which is technically assigned for the physics problem.

The serial refinement algorithms of simplicial meshes have been examined by many authors. However few works concerning parallel mesh refinements have been reported. Jones and Plassmann [14] proposed a parallel algorithm for adaptive local refinement of two-dimensional triangular meshes. Castaños and Savage [15] described the parallel algorithm for local adaptive refinement of tetrahedral meshes used in the PARED package. Zhang [16] proposed another parallel algorithm using the newest vertex approach.

For efficient electronic structure calculations, we will introduce a new direct parallel algorithm for the adaptive refinements. In our method the assignment of the FE nodes is applicable for interpolation during the calculations. Our parallel algorithm follows the simplicial bisection algorithm based on newest vertex approach. This approach was first developed by Bäsch [17] for the local tetrahedral mesh refinement. Later on, Maubach [18] and Horst [19] generalized the method to the case of arbitrary number of dimensions. Kossaczky [20], Liu and Joe [21], and Arnold *et al.* [22] also studied local refinement by bisection with different interpretations. The basic step in the refinement is tetrahedral bisection, as shown in Fig. 1. We adopt the notation and algorithm of the bisection refinement introduced in [22]. In this algorithm, with the data structure named *marked tetrahedron* the tetrahedra are classified into 5 types and the selection of refinement edge depends only on the type and the ordering of vertices for the tetrahedra. The parallelization of the refinement algorithm is based on a natural idea, i.e., to exchange the hanging vertices and edges on the interface of each sub-mesh, as used in the literatures [14–16].