Transactions of the Materials Research Society of Japan 24 [2] 209-212 (1999)

Efficient Parallelization of Tight Binding Methods

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We describe the design and implementation of parallel code of tight binding recursion methods, which show perfect locality. This improvement accelerates the time-consuming routine of local charge neutrality, which is crucial for simulating the lattice defects. We adopted the library 'pvm' developed at Oak Ridge National Laboratory, because it can be installed by the user and supports the heterogeneous configurations of cluster machines. The calculating times show almost the ideal inverse dependency on the number of proccessors.

1. INTRODUCTION

In materials science, the demands on understanding the mechanisms from the atomistic levels have been boosting the improvement of the atomic potentials, together with the knowledge of the first principles electronic structure calculations. For the realistic simulations on the phase transformations or the relaxations of atoms around the lattice defects, we need speedy atomic potentials which are expected to reflect the changes in the electronic structure. Thus the tight binding approximations have recently attracted the attentions of researchers[1].

We have been developing the program code ‘anbop' for static relaxations around the lattice defects. For energy calculations, this code uses the tight binding recursion method[2], which is very fast compared with the conventional *k*-space tight binding calculations. It still, however, takes much longer time than the empirical atomic potentials.

In this paper, we will report the efficiency of our parallel code for investigating realistic, and therefore huge systems. First we will explain tight binding formalism briefly, then the concept of the local charge neutrality (LCN), which is crucial for simulating the lattice defects. The results of the test model of Si 216 atoms show the expected inverse relations between CPU times and CPU numbers.

2. TIGHT BINDING MODEL AND LOCAL CHARGE NEUTRALITY

The two-center, orthogonal tight binding model expresses the total energy as follows[3]:

$$E_{\text{atom}} = E_{\text{repulsive}} + E_{\text{bond}} + E_{\text{promotion}} \ . \quad (1)$$

The first term is the simple pairwise interaction. The second term is bonding contributions of the electrons, and can be given by

$$E_{\text{bond}} = \sum_{\alpha} \int_{-\infty}^{E_F} \left(E - E_{\alpha}\right) n_{\alpha}\left(E\right) dE \quad (2)$$

where $n_{\alpha}(E)$ and E_{α} are the density of states and the self energy of the orbital α respectively, and E_F is the Fermi energy. The third term of eq. (1) is the promotion energy,

$$E_{\text{promotion}} = \sum_{\alpha} \left(N_{\alpha} - N_{\alpha}^{\text{atom}}\right) E_{\alpha} \quad (3)$$

which is associated with the change of occupancy of the atomic orbitals on forming the solid (N_{α}) from free isolated atoms (N_{α}^{atom}).

The density of states, $n_{\alpha}(E)$, in eq. (2) is the most time consuming to calculate. The conventional *k*-space tight binding performs it by diagonalizing the *k*-space Hamiltonian

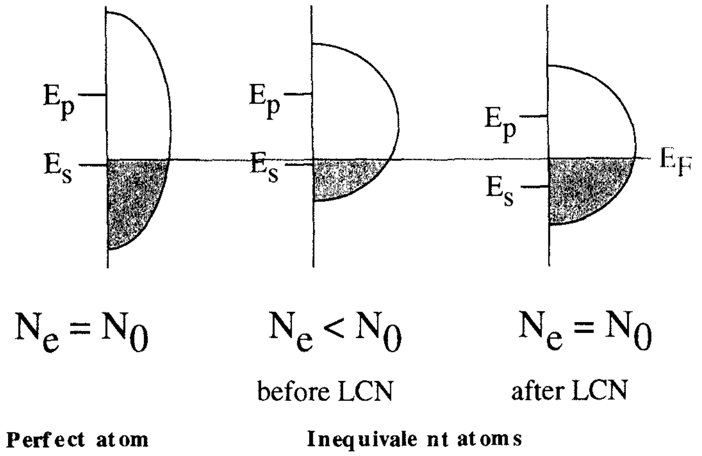

Fig. 1 Schematic drawings of the density of states of perfect atom(left), and atoms around the lattice defects before local charge neutrality(LCN) (middle), and after LCN(right). N_e represents the number of electrons on the site, and N_0 represents that of the isolated atom.

and integrating with the complicated tetrahedron method. Thus it shows $O(N^3)$ relations between independent atoms and calculating time. Recursion method, which uses Lanczos algorithm, shows excellent $O(N)$ dependency on the inequivalent atom[4]. Furthermore the locality of its Hamiltonian is perfect. When we parallelize the calculating code of recursion method, thus, the overhead of the data transfer is conceptually none.

For the realistic simulation, however, there have to achieve local charge neutrality for the metallic or covalent bonded systems[5]. We will see it in the model case of lattice defects. The band for the perfect lattice is shown in left hand panel of Fig. 1 and contains the same number of electron in an isolated atom. When the atom locates next to the defect site, the shape of the band modified by the different configurations alters the charge at this site. One way of local charge neutrality is achieved by shifting the self energy levels while keeping the energy difference constant until the total electron number is equal to the isolated atoms. This procedure needs self consistent calculations, because the shifting of the self energies at one site affects the surrounding sites. For the fast calculations, we parallelized this routine.

3. ALGORITHM OF ANBOP AND ITS EFFICIENCY

Many parallel libraries on the diagonalization of the matrixes have been developed, which are used in various programs. The usage of the parallelized routines does not make the calculation times reduced inversely on the CPU numbers. Because the localities of general matrixes are not perfect, the data transfers between the divided matrixes are necessary. As mentioned before, the tight binding recursion method shows perfect locality, thus it is not necessary to transfer data during the calculations of Hamiltonian. The transferring data is only about the values for achieving local charge neutrality .

For handling the data transfer and the configurations of parallel cluster machines, we use PVM (parallel virtual machine) library developed at Oak Ridge National Laboratory[6]. This library can be run on the heterogeneous machines and installed by the users not by the administrators. Fig. 2 shows the algorithm of parallelized local charge neutrality routine. The left hand side shows the common data, and the right hand side the paralleled routines. We employed the 'master-slave' configuration. The 'master' distributes atoms on each 'slave'. Each 'slave' machine gets the initial data at first, and

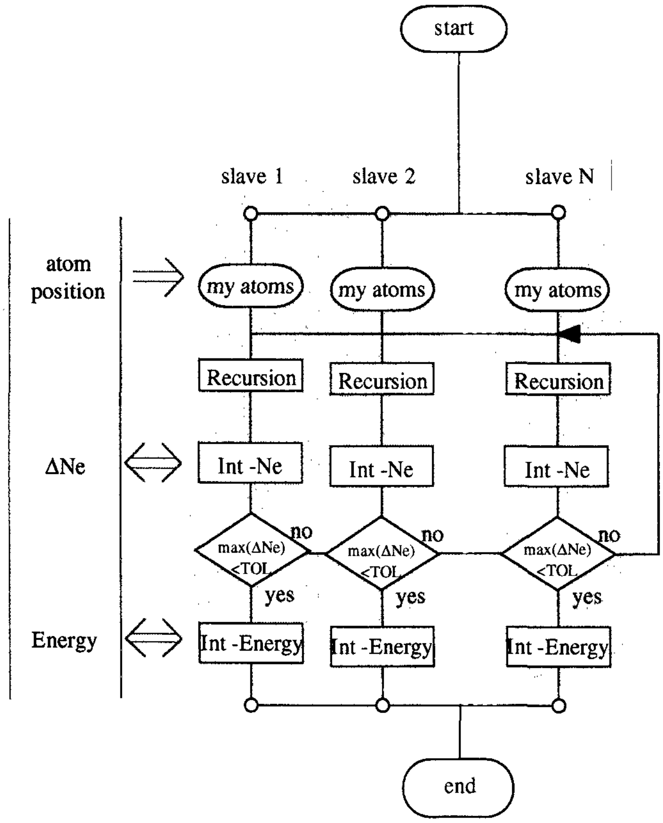

Fig.2 Algorithm and common data in the parallelized local charge neutrality routine of 'anbop'.

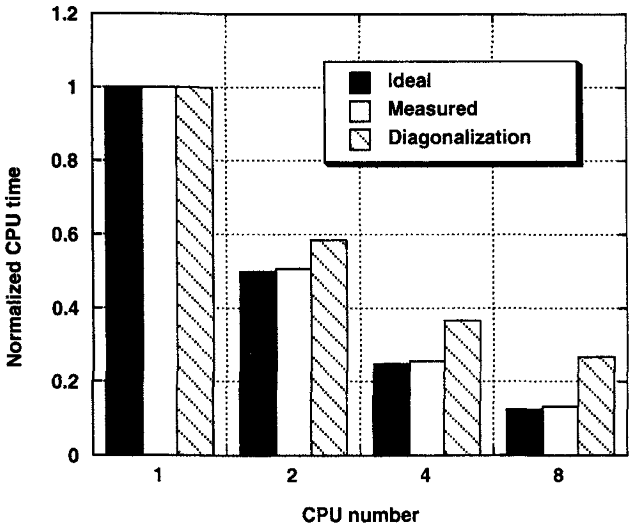

Fig.3 Dependence of the calculating time on CPU numbers. The values are normalized at those of one CPU. Ideal shows the calculated value from that of one CPU. The model calculations were performed on Si 216 atoms for achieving LCN once. The machine is SGI PowerChallenge 10000XL (CPU/clock:R10000/190MHz x 8, Cache:32KB/1024KB, Memory:2048MB, OS:IRIX6.2) of Kyoto University Data Processing Center. 'Diagonalization' shows the measured CPU times for getting eigen values with non-orthogonal bases of 100 Ag atoms by IBM SP2 using ScaLAPACK library[7].

perform the recursion algorithm (`Recursion`). Then they integrate DOS for getting the number of electrons (`Int-Ne`). The routine compares the difference between the number of electrons on each site and that of an isolated atom and adjusts the self energies, to achieve local charge neutrality self-consistently. After achieving the local charge neutrality on the whole system, they calculate the total energies of individual atoms (`Int-Energy`).

Figure 3 shows the measured CPU times on the realistic model of 216 Si atoms. The values are very close to those estimated from the one CPU time. Thus we can see the ideal job distribution is achieved. For the comparison, measuring times of *k*-space tight binding program are also shown in Fig. 3. This program uses a general library for parallel machines. For eight CPU, it takes almost double of the ideal time. Note that this program use the non-orthogonal bases, which means the locality of the matrixes are much worse than those with the orthogonal bases.

For the case of the cluster with cheap PCs, the communication among the machines takes more time. Even in the case, the amount of transferred data is designed as small as possible, the efficiency of parallelization is not so reduced.

5. CONCLUSION

The core routine of 'anbop' was ideally designed for parallelization and showed the almost perfect inverse relations between CPU times and CPU numbers. If we can obtain the tight binding parameters of the orthogonal bases describing the electronic structures of the system appropriately, we can simulate the reliable defect structures efficiently. Using higher recursion levels, the precision of the values obtained by the recursion method can approach to those obtained by the *k*-space calculations. When we use the truly empirical pair potentials, we can not escape from the ambiguity on the limit of the models. Using tight binding recursion method, however, we can judge it from the clear view points of physics. For ionic solids, the constraint of local charge neutrality will need to be relaxed for future research. For metalic solids, however, this program code is fast enough to treat huge systems for simulating realistic defect behavior and a convenient tool on the practical researches.

ACKNOWLEDGMENTS

The developing of 'anbop' is partially supported by the Grant-in-Aids for Scientific Research on Priority Areas, the Minister of Educations, Science, Sports and Culture, Japan, on "The Elucidation of Microscopic Mechanisms of Phase Transformations for the Microstructure Control of Materials". SRN appreciates the usage of computer facility of Kyoto University Data Processing Center.

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(Received December 11, 1998; accepted February 28, 1999)