3D01　グリッド技術を用いた大規模分子シミュレーションプログラムの開発

Development of a Large Scale Molecular Simulation Program

for A Large Scale Molecular Orbital Calculation

using Fragment Molecular Orbital Method and Grid Computation Technique

Umpei Nagashima[a], Yuichi Inadomi[a], Hiroaki Umeda[a], Toshio Watanabe[a], Takayoshi Ishimoto[a], Tetsuya Sakurai[a,b] , Tsuneo Hirano[a], Mutsumi Tomonari[a,c]

[a] *Grid Technology Research Center, National Institute of Advanced Industrial Science and Technolog,, and Core Research for Evolutional Science and Technology (CREST), Japan Science and Technology Agency (JST)*

[b] *Department of Computer Science, Tsukuba University.*

[c] *Fundamental and Environmental Res. Labs., NEC Corporation.*

1. Introduction

We have been developing the computational tool to obtain the molecular orbitals for large molecules such as proteins and molecular clusters without excessive calculation costs. The most time consuming step of Hartree-Fock calculation is the molecular integral evaluation and Fock matrix gereration ($O(n^4)$). The actual cost of these steps has been reduced to $O(n^{2\sim3})$ by the fragment molecular orbital method [1] and parallel processing technique. The cost became the same or less for Fock matrix diagonalization ($O(n^3)$).

We have proposed FMO-MO method to obtain important MOs of large molecules cost-effectively [2]. In our method, the entire Fock matrix is generated by the technique based on the fragment molecular orbital method, which is applicable to large systems and suitable for the parallel processing. To solve the large scale generalized eigenproblem, we use the Sakurai-Sugiura method [3]. Because this method solves several number of liner equation which has a large granularity and master-worker type of execution, the method is sufficient for parallel processing on the computers of the distributed memory parallel architecture. And the method is favorable to calculate only a small number of eigenvalues and corresponding eigenvectors of the large scale matrix. Our method has high parallelization efficiency and the communication cost is negligible to the total calculation costs. Thus, this is one of the right applications for using the Grid technology.

2. Results

Elapsed time of FMO/HF/STO-3G of Lyzozyme (129 amino-acid residues, 1961 atoms, 6005 basis functions) and DNA model system (40 base pairs, 2636 atoms and 10108 basis functions) are shown in Table 1 where all calculation were executed on a PC cluster, AIST super-cluster system P32 consists of Opteron model 246, 2GHz x 1024 CPUs.

Total elapsed time for FMO-MO calculation of Lyzozyme is only about 17min. Since the elapsed time of the conventional method by GAMESS is almost 1 week (7 days = ~170 hours) on a PC cluster (Itanium II 3.06GHz x 64 CPUs), improvement of performance is more than 600 times..

Total elapsed time of DNA model is only about 56 min (~1 hour). Though the number of basis set of DNA is about twice of Lyzozyme, ratio of elapsed time is 3.3 times. It is suggested that the computational cost of FMO is proportional to square of the number of basis functions or less. Note that the computational cost of Fock matrix diagonalization of DNA model is the same as the Lyzozyme.

Table 1 E-time (sec.) for FMO-MO calc. of Lysozyme and DNA model system on a PC cluster consists of Opteron model 246, 2GHz x 1024 CPUs.

	Lyzozyme		DNA model system	
	No. of processor	E-time sec.	No. of processor	E-time sec.
FMO calculation	544	454	640	1182
Fock matrix gen.	512	515	256	1839
Fock matrix diag.	16	64	16	64
Total E-time		1033		3085

HOMO and LUMO of Lyzozyme are depicted in Figure 1. Reaction centers of Lyzozyme are clearly shown in the figure 1.

HOMO and LUMO of DNA model system are depicted in Figure 2. Because the molecular symmetry was slightly deformed, the LUMO is localized at the left hand side whereas the HOMO is at the center. The LUMO+1 is located at the right hand side though LUMO+1 is not shown in the figure 2.

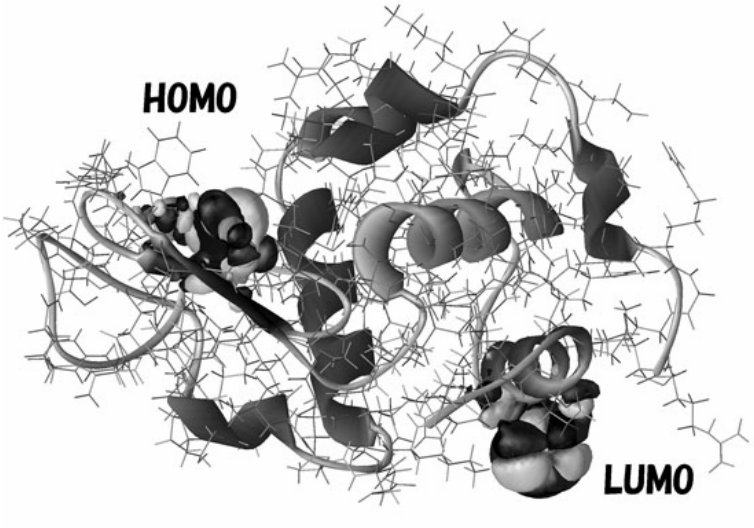

Figure 1. HOMO and LUMO of Lyzozyme

This work is supported by the research project, “Development of MO calculation system for large molecule on Grid”, CREST, JST. All numerical calculations were performed on the AIST super cluster.

[1] [T. Nakano, T. Kaminuma, T. Sato, K. Fukuzawa, Y. Akiyama, M. Uebayasi, and K. Kitaura, Chem. Phys. Lett., 2002, **351** , 475.

[2] Y. inadomi, T. Nakano, K. Kitaura and U. Nagashima, Chem. Phys. Lett., 2002, **364** 139-.

[3] T. Sakurai and H. Sugiura, J. Comput. Appl. Math., 2003, **159** 119-.

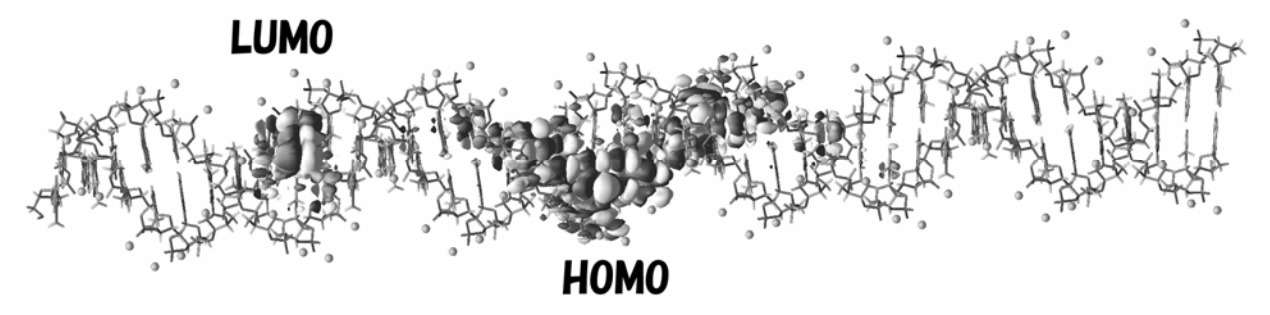

Figure 2. HOMO and LUMO of a model of DNA model consist of 40 base pairs