EX01

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

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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. In our method, the entire Fock matrix is generated by the technique based on the FMO method [1]. To solve the large scale generalized eigenproblem, we use the Sakurai-Sugiura method [2]. Because this method solves several number of liner equation which has a large granularity and master-worker type of execution, the method is efficient for parallel processing on the distributed memory parallel computer. 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. Elapsed time of Hartree-Fock calculation of Lysozyme (129 amino-acid residues and solvent molecules, total 8258 atoms) with FMO/HF/STO-3G (20758 basis functions) is listed in Table 1. Molecular structure of Lysozyme is depicted with HOMO (Lower left) and LUMO (Center) in Figure 1. Performance of the method was improved drastically by parallel processing.

Table1 E-time for FMO-MO calc. of Lysozyme

		CPU type	#proc.	E-time
FMO calculation		Opteron[a]	128	6.3 hour
Fock matrix generation		Opteron[a]	64	42.3 hour
Eigenvalue and eigenvector of Fock matrix	Cholesky decomposition + Householder + bisection.	Opteron[a]	1	4.1 hour
	Sakurai-Sugiura method	Xeon[b]	1	44.5 min
		Xeon[b]	128	1.9 min

[a]Opteron :model 246, 2.0GHz, [b] 2.0GHz Xeon: 3.06GHz

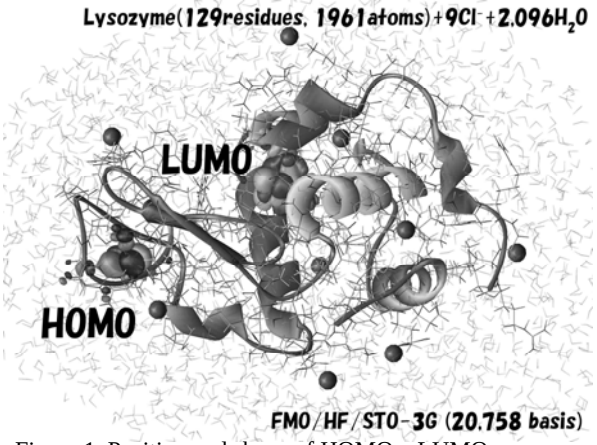

Figure 1. Position and shape of HOMO　LUMO of Lyzozyme

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