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A Large Scale Molecular Orbital Calculation Using Fragment Molecular Orbital Method - Method and Performance Evaluation -

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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 fragment molecular orbital method [1], 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 [2]. 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. Elapsed time of Hartree-Fock calculation of Lysozyme (129 amino-acid residues, 1961 atoms) with FMO/HF/STO-3G (6005 basis functions) is listed in Table 1. Performance of the method was improved by parallel processing.

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Table1 E-time (sec.) for FMO-MO calc. of Lysozyme ^{a, b}			
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		# of proc.	E-time
FMO calculation		544	549
Fock matrix generation		512	515
eigenvalue and eigenvector of Fock matrix	Cholesky decomposition + Householder + bisection ^b	1	370
	Sakurai-Sugiura method	1	610
		16	64

^a; CPU type is Opteron (model 246, 2.0GHz).
^b; Lapack & BLAS routines in ACML2.5.0 were used.

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

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