

FMO calculations with ABINIT-MP on K-computer

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The K-computer, one of the fastest peta-scale supercomputers in the world, processes huge amounts of tasks at once with its massive parallelism and have started being utilized for drug discovery primarily based on the classical mechanical approaches.

On the other hand, fragment molecular orbital (FMO) method proposed by Kitaura *et al.* in 1999 has revealed the electronic properties of large biomolecular systems quantum-mechanically and has a great expectation for application to drug discovery. Especially, the four-body corrected FMO method (FMO4) [1], which is implemented to an FMO processing program, ABINIT-MP, enables us to divide a molecular system more finely with keeping good accuracy and analyze inter-fragment interactions with higher resolution favorable to the structure-based drug design (SBDD) [2]. While the number of tetrameric combinations of fragments needed for four-body correction voluminously increases as the whole system size, one can simultaneously complete all the tasks of processing the combinations in a moment by using the K-computer.

The Cholesky decomposition (CD) technique for two-electron repulsion integral approximation [3] is essential to accelerate the second-order Moeller-Plesset perturbation processes in FMO calculations by keeping the Cholesky basis on memory and executing the DGEMM operations. For saving memory and further acceleration, we introduce the CD approximation with one-center Cholesky basis (1C-CD) [4], which limits the atomic orbital pairs as the Cholesky basis to those on the same atoms. The computational times in Hartree-Fock processes are also reduced successfully by applying the 1C-CD approximation.

Details of our trials and applications with ABINIT-MP on the K-computer will be shown in the poster session.

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