R&D field: Life science

Ab initio Molecular Dynamics Calculation in Large-Scale Protein Systems

- Program name: ProteinDF
- Developer
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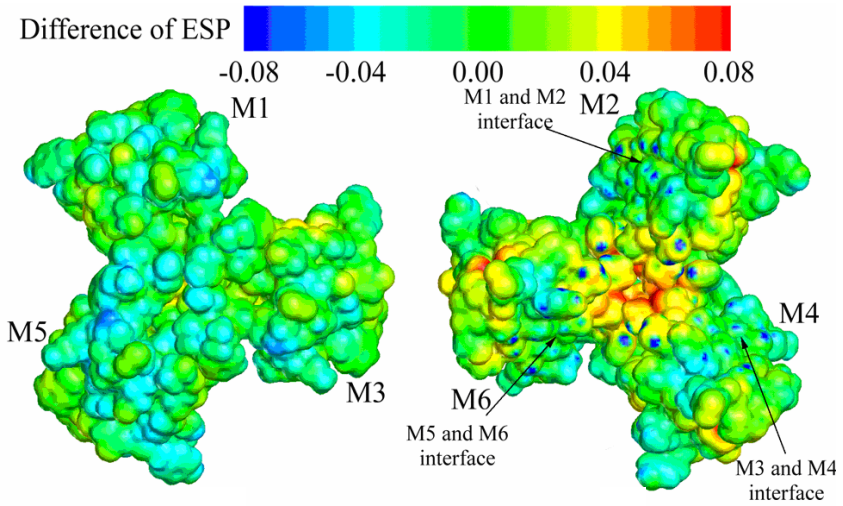
- Abstract
  - Precise and large-scale calculation of all-electron structure of complex proteins with canonical orbitals based on the density functional method.
  - Simulation of excited states, electron transition, and chemical reactions based on ab initio molecular dynamics calculation of excited states in addition to ground states.
- Algorithm
  - Ground states: canonical SCF calculation of molecular/XC integrals and matrix operations. The computation amount is proportional to the cube of the number of orbitals.
  - Excited states: The above plus the AO-direct algorithm. The computation amount is proportional to the fifth of the number of orbitals.
  - C++ and MPI (the existing library for matrix operations, atom decomposition for XC integrals, and the RT algorithm plus uniform decomposition with the shell-type classification for molecular integrals).
- Current computation size
  - 306 residues, 27,000 orbitals (ground states, the world's largest)
  - Sustained performance 300 GFlops (64 CPUs of Altix3700).
  - Memory 256 GB and disk 1 TB.
- Future computation size in 2010
  - Three times of the current computation size to deal with almost all proteins.
  - Analysis of dynamics of excited and ground states.
  - Memory 10 PB and disk 10 PB (excited states).



Difference with a classical result of electrostatic potential for the insulin hexamer

- Expected results
  - Improvement of quality and efficiency of drug development as well as increase of reliability of fundamental research of drug discovery.
  - Creation of next-generation R&D models for drug discovery.
  - Establishment of superiority to western countries over business-method and business-model patents.
  - Application of the method to catalysts, molecular device, and environmental substances.
- Reference
  - http://www.rss21.iis.u-tokyo.ac.jp/