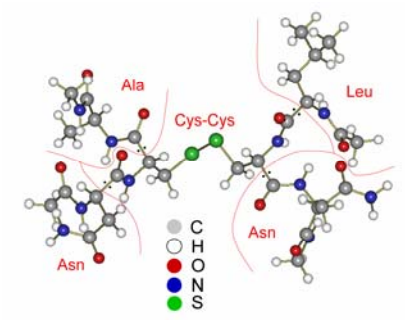
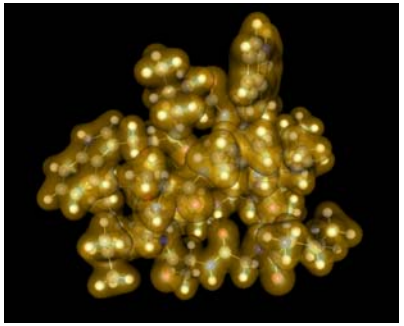
R&D field: Nano science

FMO Molecular Orbital Calculation

- Program name: GAMESS/FMO
- Developer
  - Kazuo Kitaura, D. G. Fedorov, and others, Scientists of Advanced Industrial Science and Technology (AIST)
- Abstract
  - Electron state calculation of large molecules such as protein.
  - Total energy calculation based on division of the target molecule into small fragments and on molecular orbital calculation of each fragment and fragment pair.
- Algorithm
  - Quantum chemistry calculation with the Hartree-Fock and other methods.
  - FORTRAN77 (partially C).
  - Parallelization with MPI.
- Current computation size
  - Each fragment is represented with 300 basis functions on the average.
  - The number of fragments is about 500.
  - It takes five or six days with 48 nodes of PC（Xeon 3GHz dual）.
  - Memory 500 MB (each process) and disk 300MB (each node).
- Future computation size in 2010
  - The number of fragments should be increased to around 20,000.
  - Estimated execution time is 60 hours with 10000 nodes of 100 CPUs.
  - Memory 6 GB (each process) and disk 15 GB (each node).



FMO method



Electron state of a protein

- Expected results
  - It will be possible to estimate electron states of protein with 0.6-0.8 million atoms and 20,000 fragments if each fragment is composed of 30-40 atoms on the average.
  - Screening for drug design will be performed with high accuracy based on results of detailed electron-state calculation for in-vivo molecules because realistic numbers of water molecules can be introduced to a protein model in water solution.
- Reference
  - http://www.msg.ameslab.gov/GAMESS/GAMESS.html