R&D field: Nano science

Analysis of Electron States of Proteins in Solution with the 3D-RISM/FMO Method

- Program name: RISM/3D-RISM
- Developer
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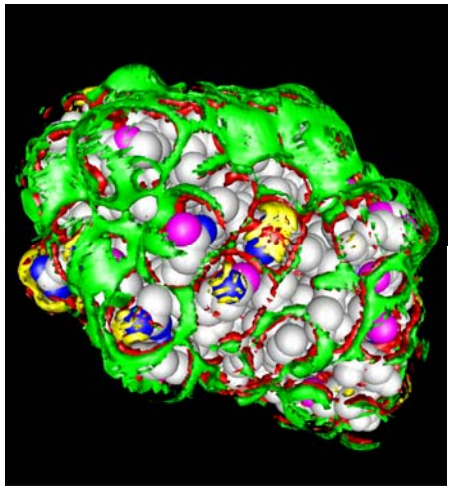
- Abstract
  - Estimation of electron states, solvation structure, and free energy of substances contained in enzyme reaction.
  - All-electron structure calculation of proteins in solution.
  - Coupled calculation of 3D-RISM (a statistical method for solution distribution) and FMO (a quantum chemistry method for large-scale molecules).
- Algorithm
  - FORTRAN77/90.
  - 3D-RISM: Parallelization of three-dimensional fast Fourier transformation.
  - FMO: Parallel calculation of each fragment decomposing protein into a few fragments of residues.
- Current computation size
  - 3D-RISM: Lattice points 512x512x512x2.
  - Protein size: 250 residues (3,000 atoms and 30,000 bases).
  - Memory 60 GB (one parameter set).
- Future computation size in 2010
  - 3D-RISM: Lattice points 1024x1024x1024x4.
  - Protein size: 1000 residues (10,000 atoms and 100,000 bases).
  - Memory 600 GB (one parameter set in an enzyme-reaction coordinate system).



Distribution of waters and ions around lysozyme

- Expected results
  - Ab-initio description of enzyme reactions with 3D-RISM/FMO.
  - Identification of effective reaction conditions and finding of new reaction paths.
  - Development of new enzymes having high reaction rate based on prediction of enzyme reaction on protein mutants.
- Reference
  - http://daisy.ims.ac.jp/indexj.html