R&D field: Nanoscience

Massively-parallel multipurpose software for molecular dynamics calculation

- Program name: Modylas
- Developer
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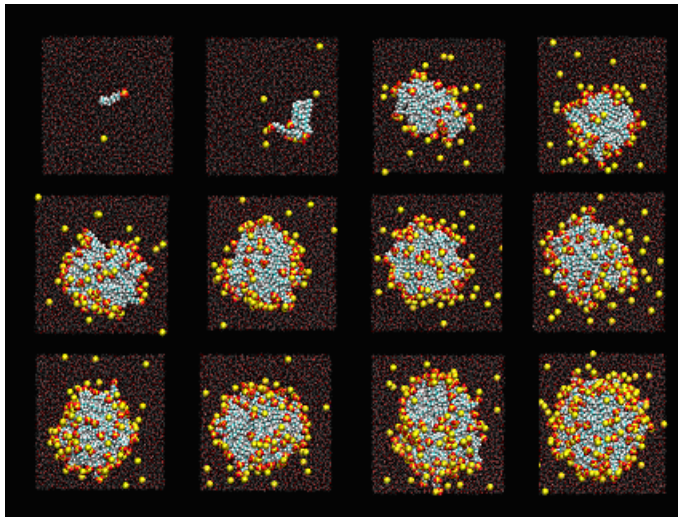
- Abstract
  - Multipurpose program of large-scale molecular-dynamics calculation for any molecular system.
  - Adopted various calculations necessary for nanoscience such as free-energy estimation.
- Algorithm
  - Long-range interaction : Particle mesh Ewald, Ewald, and tree method
  - Parallelization: domain decomposition and particle decomposition
  - Ensemble: NVE, NVT, and NPT (including rhombic cell)
  - Constraint: SHAKE, RATTLE, ROLL method
  - Time evolution: RESPA method
- Current computation size
  - PME: 2 sec/step with one million atoms (3 TFlops, 512 CPUs).
  - Tree: 20 sec/step with 10 million atoms (5 TFlops, 800 CPUs).
- Future computation size in 2010
  - Realization of long dynamics in each method from several hundred to thousand times based on massive parallelization.
  - Memory same as the current size.



Molecular dynamics simulation of micell formation in water

- Expected results
  - Modylas will simulate all atomic calculation of virus (10 million atoms including solvent) and long-time calculation of liposome (several hundred thousand atoms).
  - Modylas will describe molecular science of viruses and nano-process of drug delivery systems at the atomic level based on computational science in order to obtain important knowledge for human beings.
- Reference
  - http://simulo.ims.ac.jp/index.html