Coarse-Grained Molecular Dynamics Calculation

- Program name: Octa
- Developer
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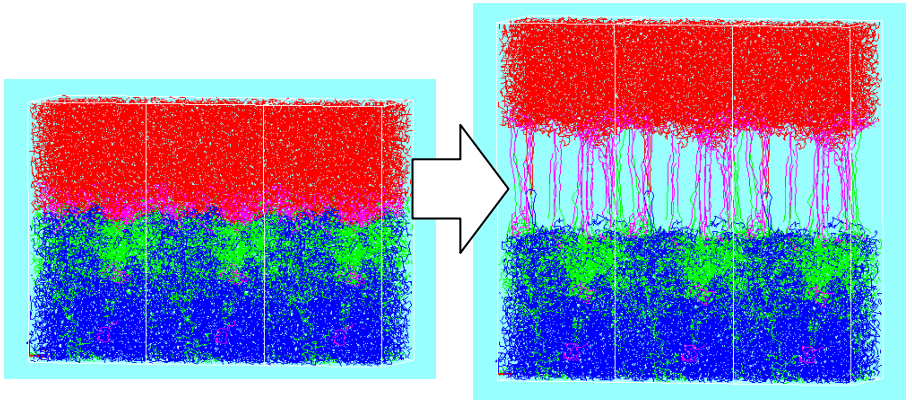
- Abstract
  - Design of high polymers, soft materials and nano-hybrid materials.
  - Multi-scale simulation in combination with other simulators (originally developed as one of the engines of the Octa system).
- Algorithm
  - NVT, NPT, NVE, and other ensembles.
  - Simulations of arbitrary chain structure.
  - Simulation of non equilibrium state under stretching and shearing.
  - Adapted to other coarse-grained dynamics such as the dissipative particle dynamics.
- Current computation size
  - 0.1 million particles on a PC.
  - 1 million particles on a supercomputer.
- Future computation size in 2010
  - 100 million particles.



Peeling of a bonded surface in a polymer material

- Expected results
  - Bridging the molecular description, meso scale description and the macro scale description of polymer materials
  - Real-time simulation of structure formation of nano materials.
  - Property estimation and material design of polymeric materials with nano structures.
- Reference
  - http://octa.jp