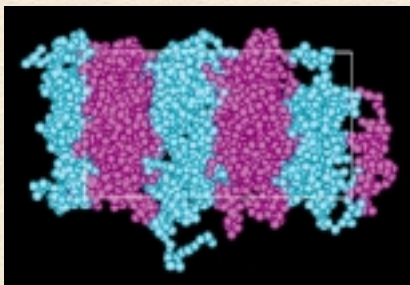


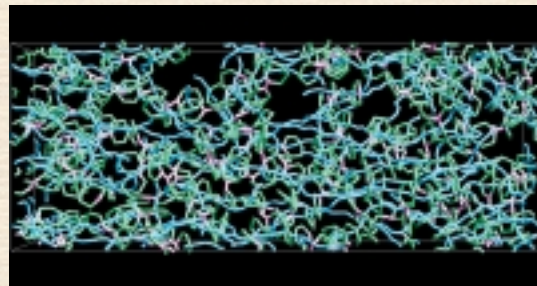
# COGNAC

(Coarse-Graigned molecular dynamics program by Nagoya Cooperation)

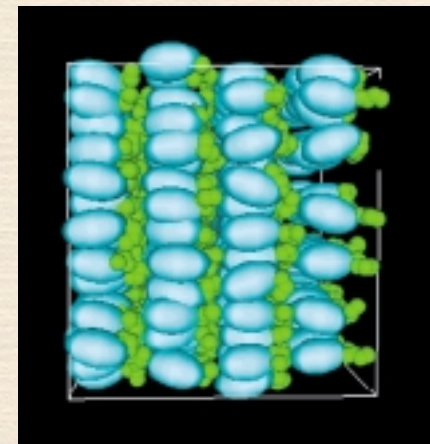
COGNAC is a general molecular dynamics simulation program which covers a large class of molecular models, ranging from full atomistic models to bead-spring models. Many potential functions used in coarse-grained models are implemented in COGNAC, such as Lennard-Jones, Gay-Berne and Coulombic potentials, and new potential functions can be added easily. COGNAC can conduct MD simulations under various conditions such as under constant temperature, under deformation (elongation and shear), and under external fields. COGNAC has a special function, called zooming, which generates the equilibrium molecular configuration for given density profile of atoms.



**Block copolymer :**  
Lamellar structure of ABA tri-block copolymer. Initial chain configuration is generated from the information obtained by SUSHI.



**Topological gel :**  
Snapshot of a topological gel under elongation. Unique elastic properties of topological gels are reproduced by COGNAC.



**Liquid crystal :**  
Snapshot of a liquid crystalline phase obtained for a molecular system consisting of rigid and flexible parts by COGNAC. The rigid part is approximated by an ellipsoid.

## Basic functions

- \* Molecular dynamics/Langevin dynamics/Energy minimization
- \* Potential : 2-4 body bonding potential  
Non-bonding interaction, e.g. LJ, GB, Coulomb  
External interaction, e.g. electric field, solid wall
- \* Ensemble : NVE/NVT/NPH/NPT and non-equilibrium dynamics
- \* Chemical reaction
- \* Initial structure generation, e.g. amorphous, helix, crystal
- \* Functions for zooming

## Examples of applications

- \* Chain conformation of phase-separated block copolymers
- \* Interfacial properties of polymer blends
- \* Properties of semi-crystalline lamellae
- \* Elastic properties of network polymers
- \* Clay-polymer nanocomposites
- \* Dynamics of confined polymer melts
- \* Phase transition of liquid crystals
- \* Ion diffusion in polyelectrolytes