General-purpose Coarse-grained

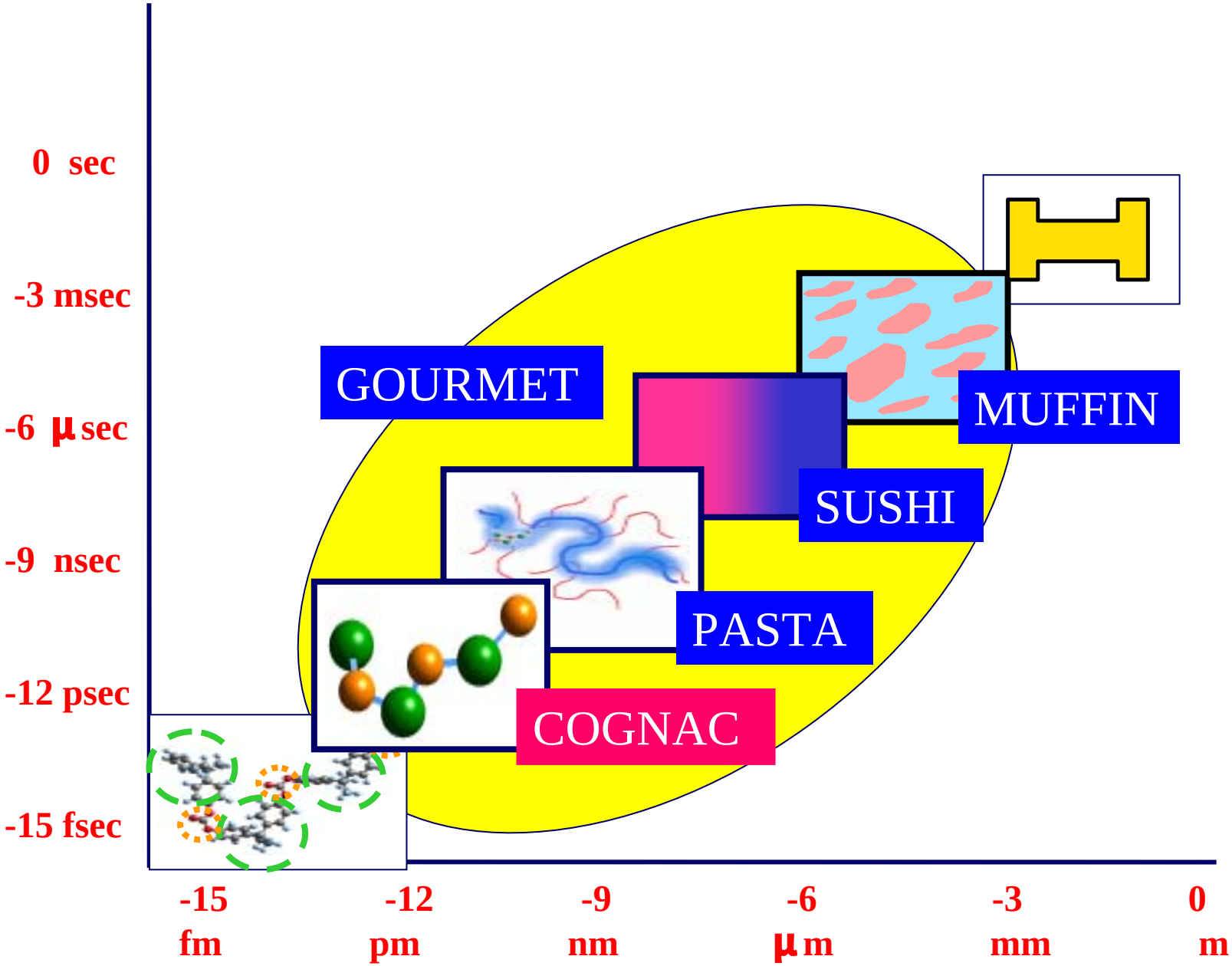
Molecular Dynamics Program

COGNAC

(COarse-Grained molecular dynamics program by NAgoya Cooperation)

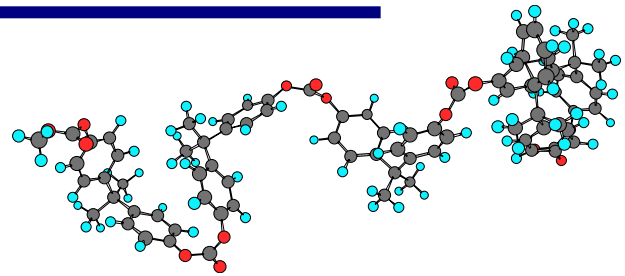
Takeshi Aoyagi

JCII, Doi project

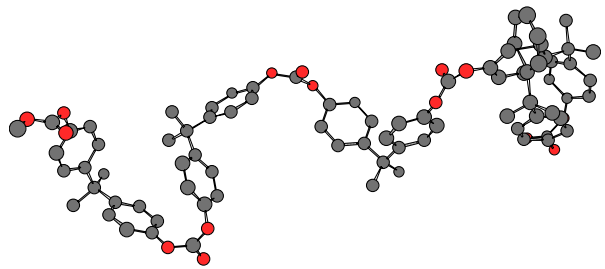

0 sec
-3 msec
-6 μsec
-9 nsec
-12 psec
-15 fsec
GOURMET
MUFFIN
SUSHI
PASTA
COGNAC
-15 fm
-12 pm
-9 nm
-6 μm
-3 mm
0 m

Coarse-grained model

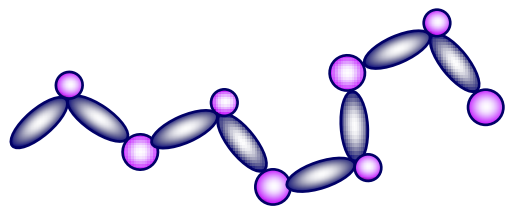
A set of atoms are represented by one dynamical unit



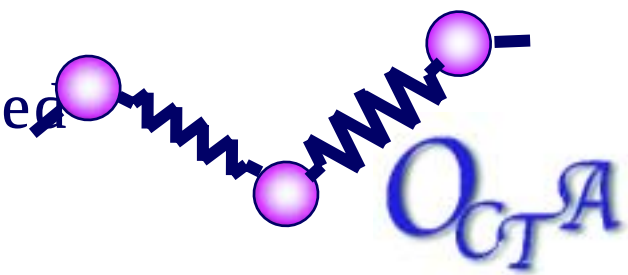
- United atom model
  - A methylene (CH_2) unit is represented by single mass point



- Gay-Berne potential model
  - A rigid part of molecule is represented by single ellipsoid



- Bead-spring model
  - Several monomer units are represented by single bead (mass point)



General-purpose

- General computational models and potential functions
- General objectives

  < Features and functions of COGNAC >
- Basic function of molecular dynamics/mechanics
- Potential functions for coarse-grained model
- Flexible modeling
- Extended functions and tools for analysis
- New functions for zooming
- Extensibility of the program
- User interface

Molecular Dynamics/Molecular Mechanics

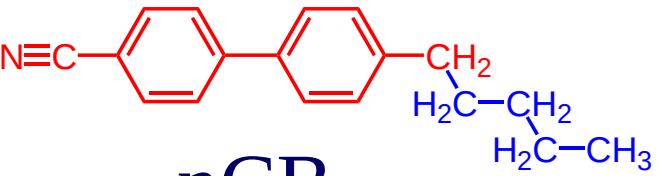
- Molecular dynamics (MD)
  - Ensembles
    - » NVE
    - » NVT,NPH,NPT
      (loose-coupling / extended Hamiltonian methods)
- Langevin dynamics
- Molecular mechanics (MM)
  - Steepest descent / conjugate gradient methods

Potential Functions for Coarse-grained Models

- Bonding
  - 2-body(bond):Harmonic,Morse,FENE,Gaussian, Polynomial,Table
  - 3-body(angle):Theta harmonic,Cosine harmonic Theta polynomial,Table
  - 4-body(torsion):Cosine polynomial,Table
- Non-bonding pair interaction
  - Lennard-Jones,Gay-Berne,LJ-GB, Table
- Electrostatic
  - Coulomb interaction(Ewald,Reaction field)
  - Dipole-dipole interaction (Reaction field)

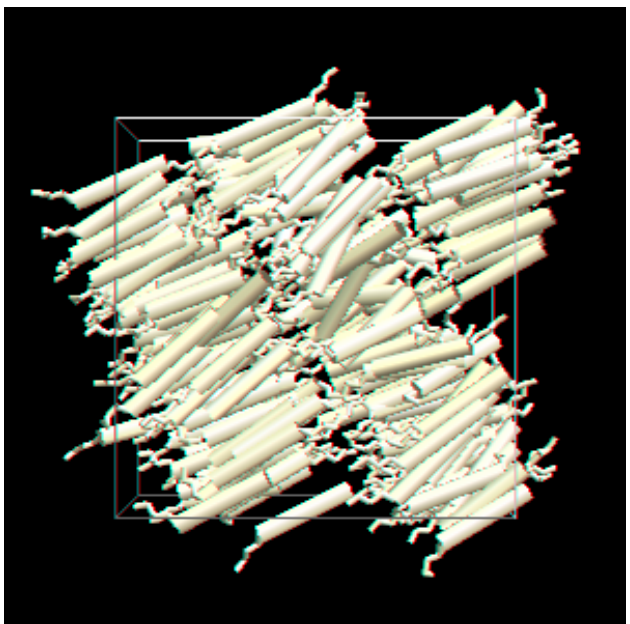
OCTA

Example of Application:
Gay-Berne - Lennard-Jones hybrid potential

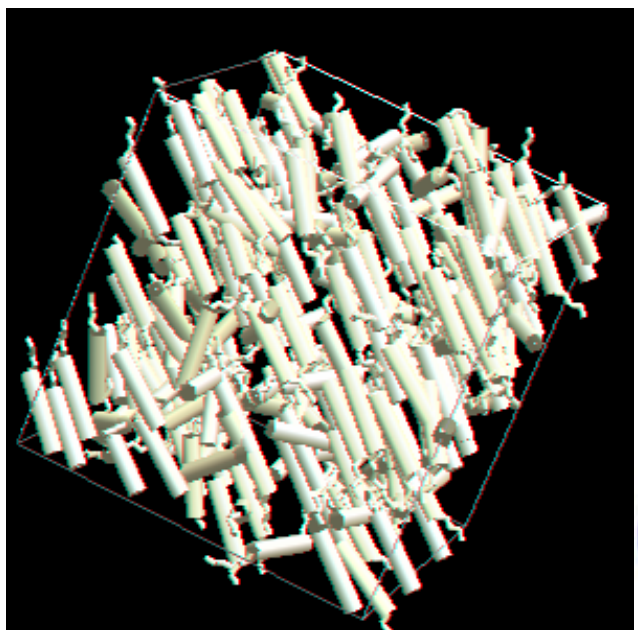


nCB
(4-methyl-4'-cyanobiphenyl)

Smectic phase(non-polar model)



Nematic phase(polar model)



Modeling molecular architectures using SILK (1)

- SILK is a tool to generate molecular architectures for COGNAC
- SILK is written in Python and used on GOURMET
- SILK has basic functions and template functions.
  - Basic functions define atoms, bonds, angles, torsions. They are used to generate molecules with complex architectures
  - Template functions are used to generate simple polymer molecules such as homopolymers and blockcopolymers

Modeling molecular architectures using SILK (2)

- An example of the usage of the basic functions

```
name="mol"
  numMol=10
  self.engine.createMolecule(name)
  for i in range(0, 4):
     self.engine.addAtoms(name, "UA", "UA_PE")
  for i in range(0, 3):
     self.engine.addBonds(name,  i, i+1, "BOND_PE")
  for i in range(0, 2):
     self.engine.addAngles(name, i, i+1, i+2, "ANGLE_PE")
  for i in range(0, 1):
     self.engine.addTorsions(name, i, i+1, i+2, i+3, "TORSION_PE")
  for i in range(0, 4):
     self.engine.addInteractionSites(name, [i], "NB_PE", "PAIR")
  self.engine.setSystem(name, numMol)
```

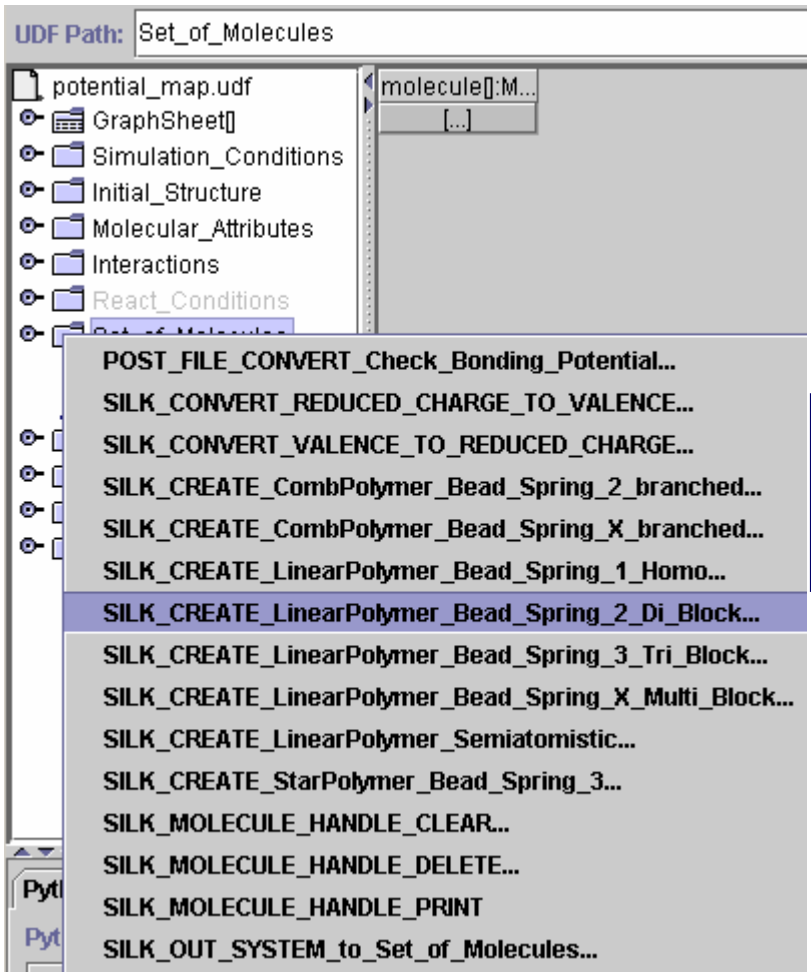
Modeling molecular architectures using SILK (3)

- An example of the usage of the template functions

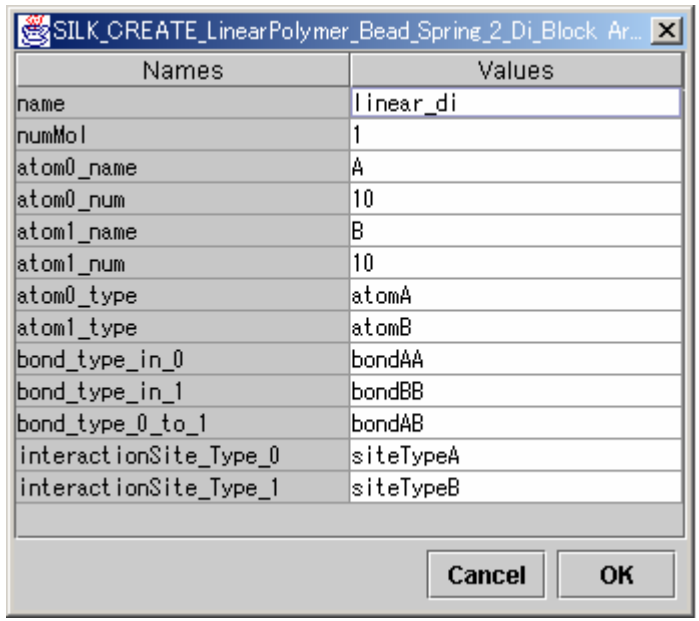
```
name="A20B40A20"
numMol=50
key="LINEAR"
sequence=[("A",20),("B",40),("A",20)]
atomType={"A":"atom1", "B":"atom2"}
bondType={"A_A":"bond1", "A_B":"bond3", "B_B":"bond2"}
interactionSiteType={"A":"siteType1", "B":"siteType2"}
self.engine.makeBeadSpringPolym(name, numMol, key, sequence, atomType,
                                bondType, interactionSiteType)
```

Modeling molecular architectures using “Action” SILK

- Running SILK by “Action” on GOUMET



Selection of diblock



Notes: This function is released as a gift without documents

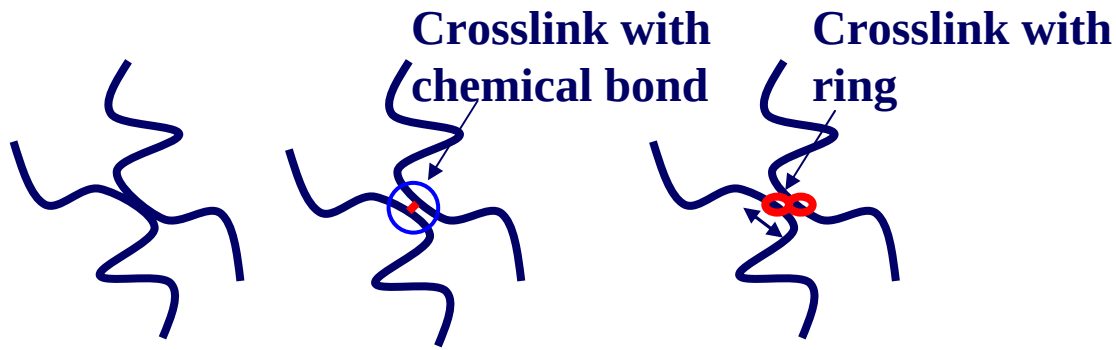
Analysis tools

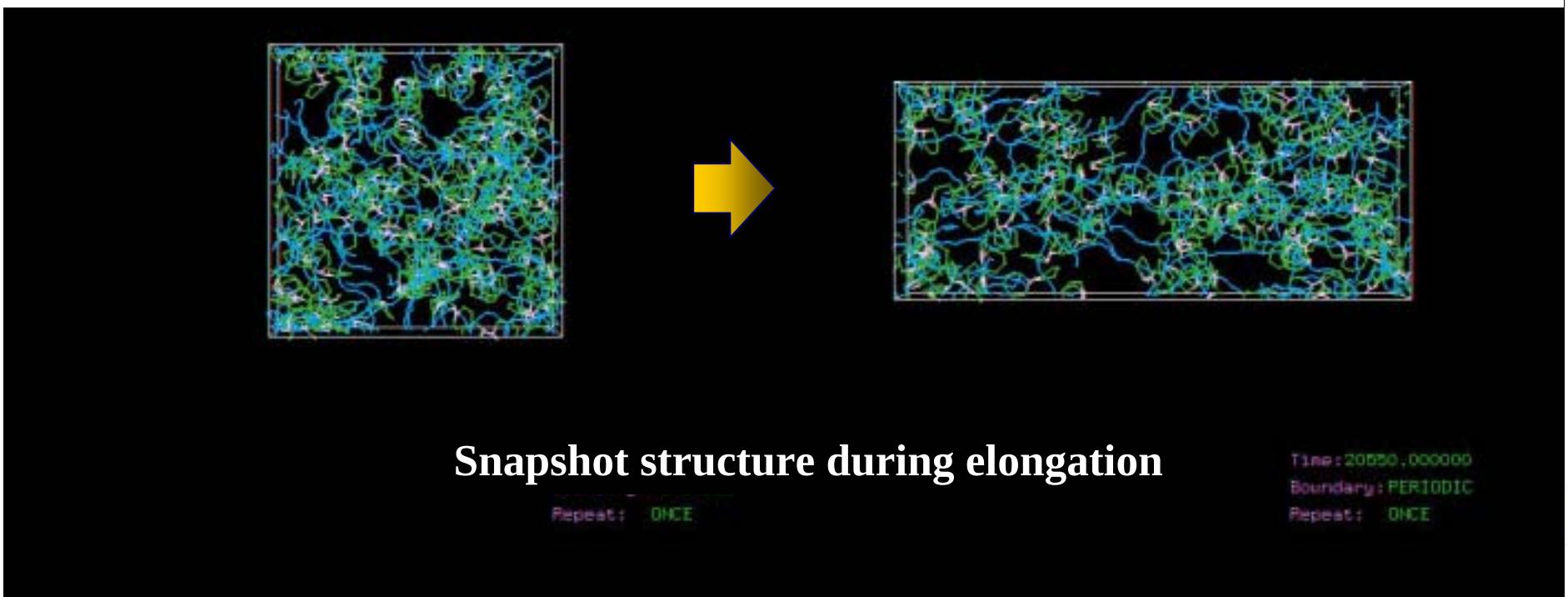
- Python scripts for the analysis of COGNAC output
  - Basic analysis
    - » Distance, angle, torsion
    - » Radius of gyration, etc.
  - Geometry analysis
    - » Pair distribution functions
    - » Orientation order parameters etc.
  - Trajectory analysis
    - » Mean square displacements
    - » Correlation function of normal coordinates etc.

Example of Application：Topological gel

Feature of topological gel

- **High degree of swelling**
- **High elasticity**
- **High clarity**



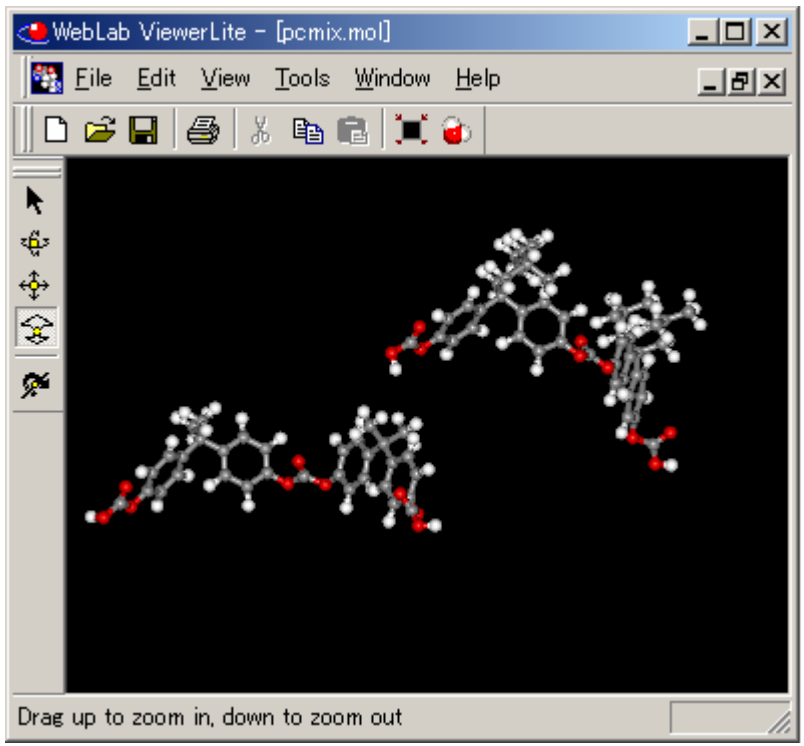


Generation of initial coordinates

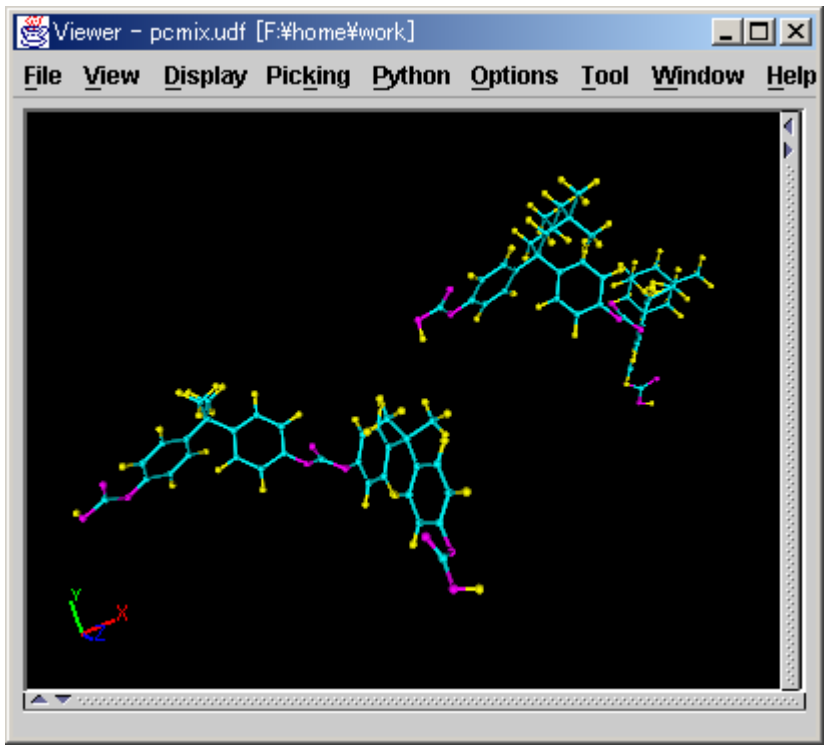
- Generation by COGNAC
  - Random: Amorphous like structures
  - Helix: Helical structures at regular lattice points
  - Crystal: Crystal structures defined by crystal data, i.e. unit lattice, symmetric operation and fractional coordinates
  - Semi-crystalline lamella: Semi-crystalline lamella structures consisting of a crystal phase and an amorphous phase
  - Multi phase structure: Micro/macro phase-separeted structures of block copolymer/polymer blend obtained by SUSHI

Data conversion of molecular structure from other file formats

- Conversion from mol/PDB format file to UDF file



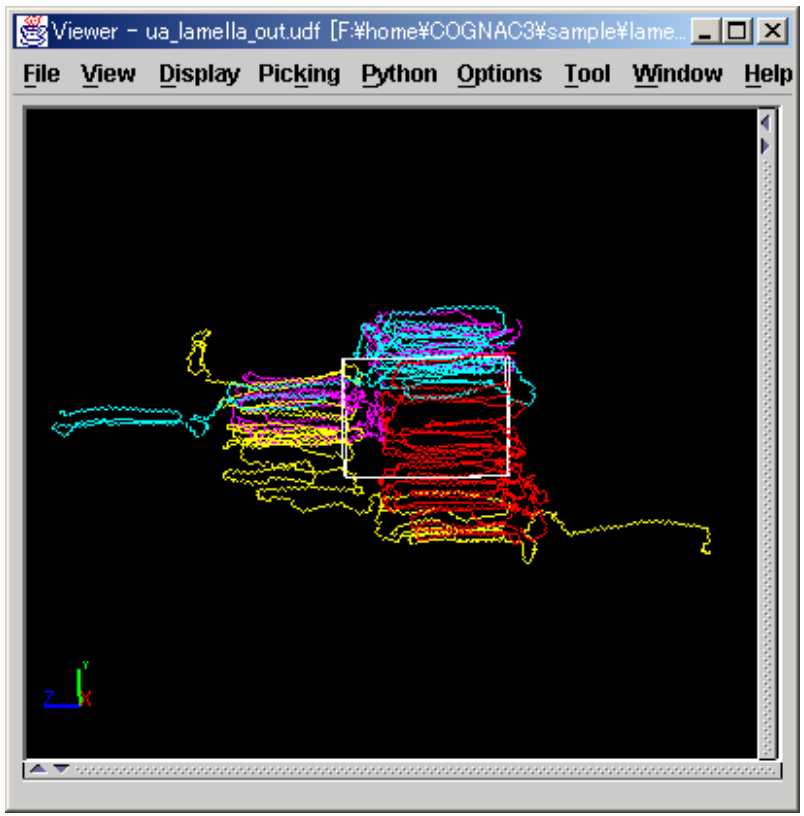
mol format file displayed
by WebLab ViewerLite(TM)

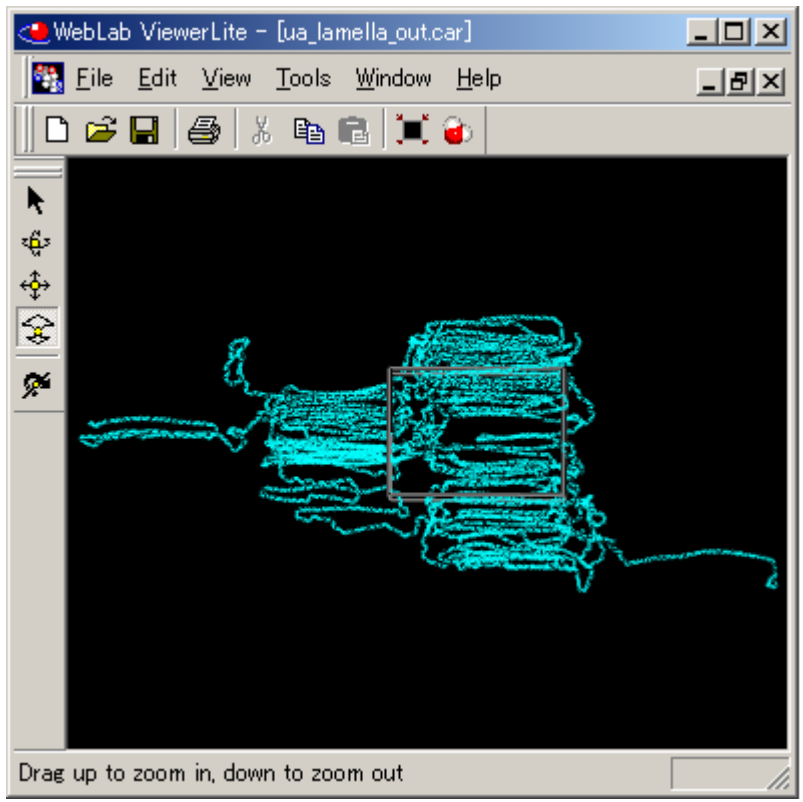


Converted data to UDF displayed
by GOURMET

Data conversion of molecular structure to other file formats

- Conversion from UDF file to PDB/car/XYZ format file





UDF file displayed by GOURMET

car format file displayed by WebLab ViewerLite(TM)

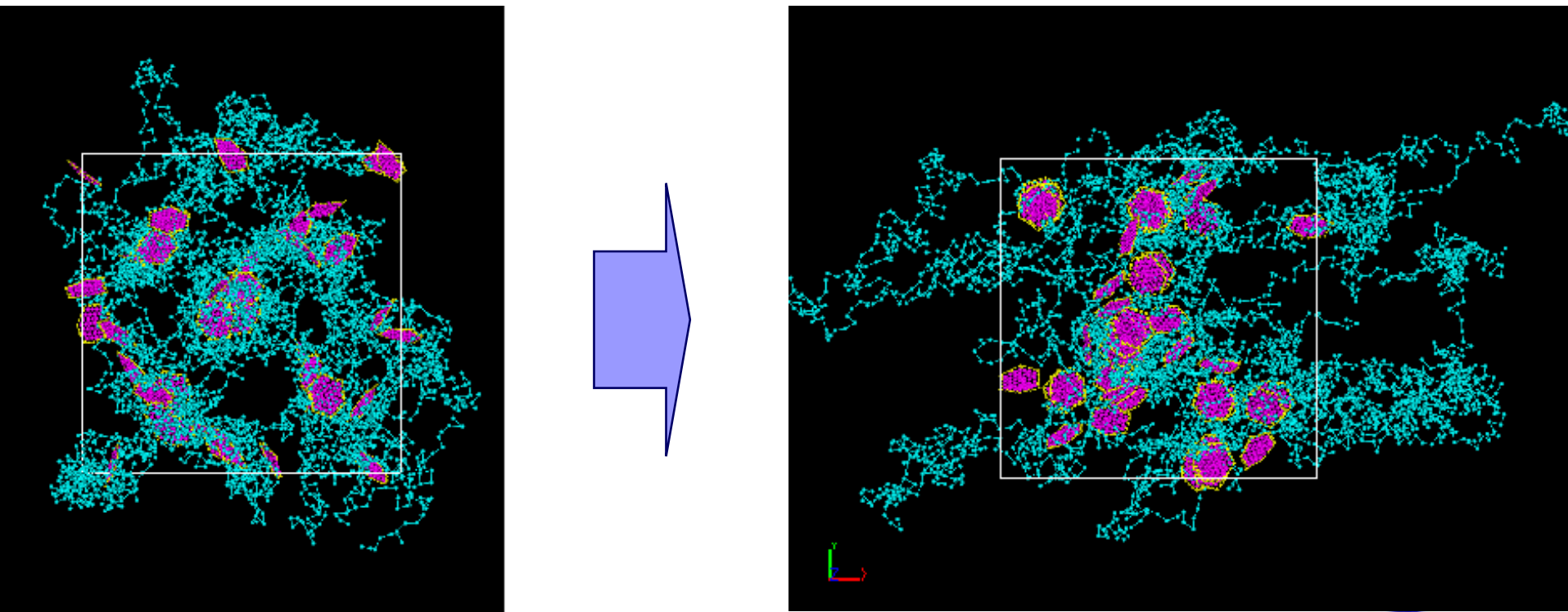
Additional functions for studying mechanical properties of materials

- External field and deformation
  - Homogeneous field, e.g. electric fields
  - Shear flow by the Lees-Edwards boundary conditions
  - Unit cell deformation
- Solid wall
  - Flat wall
  - Structured wall
- Bond creation/scission
  - Simple model for chemical reaction

Example of Application : Clay(laponite) - Polymer(PEO) composite

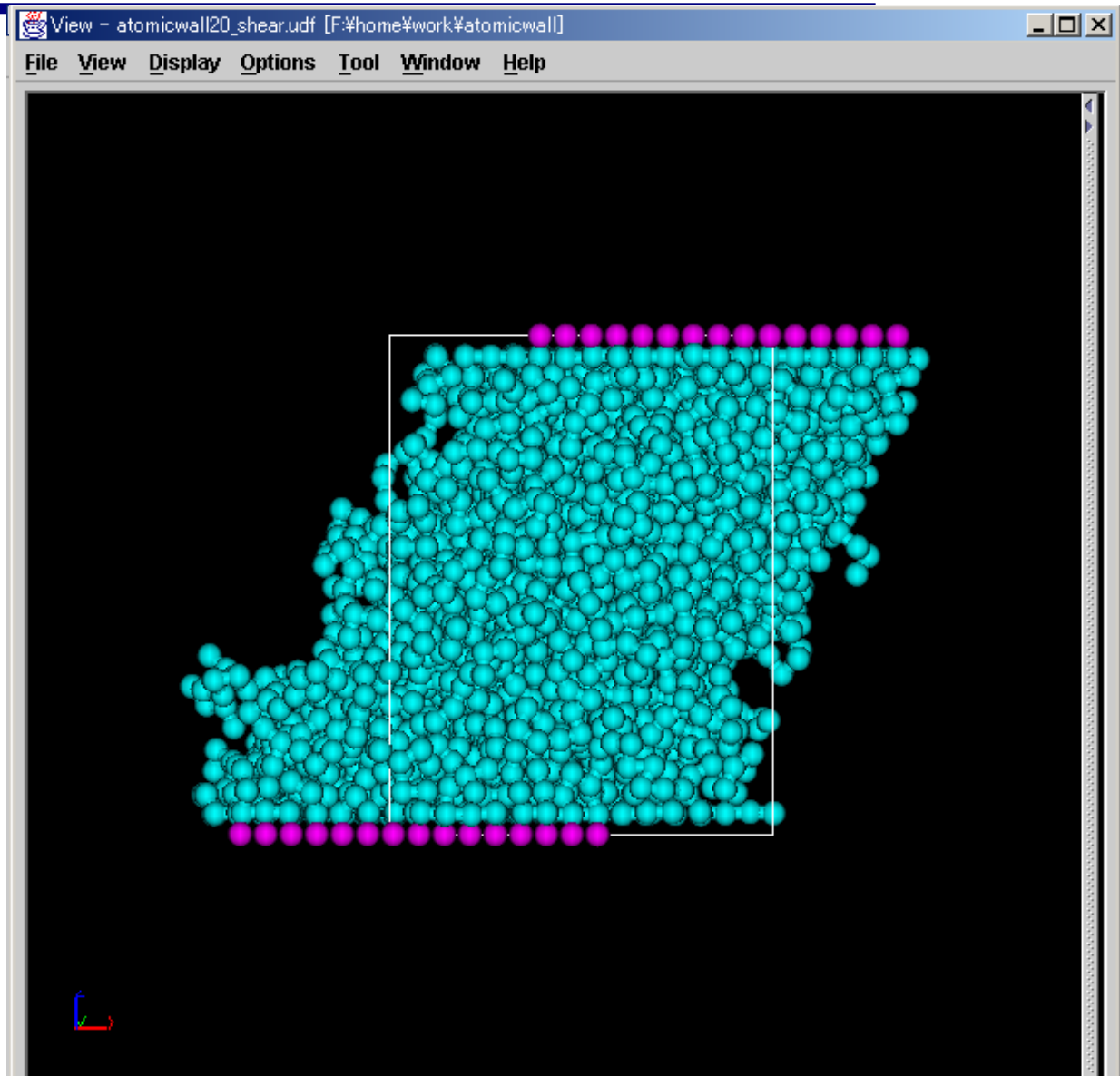
Network structure of clay-polymer is observed in water.

Clay plates order under shear flow.

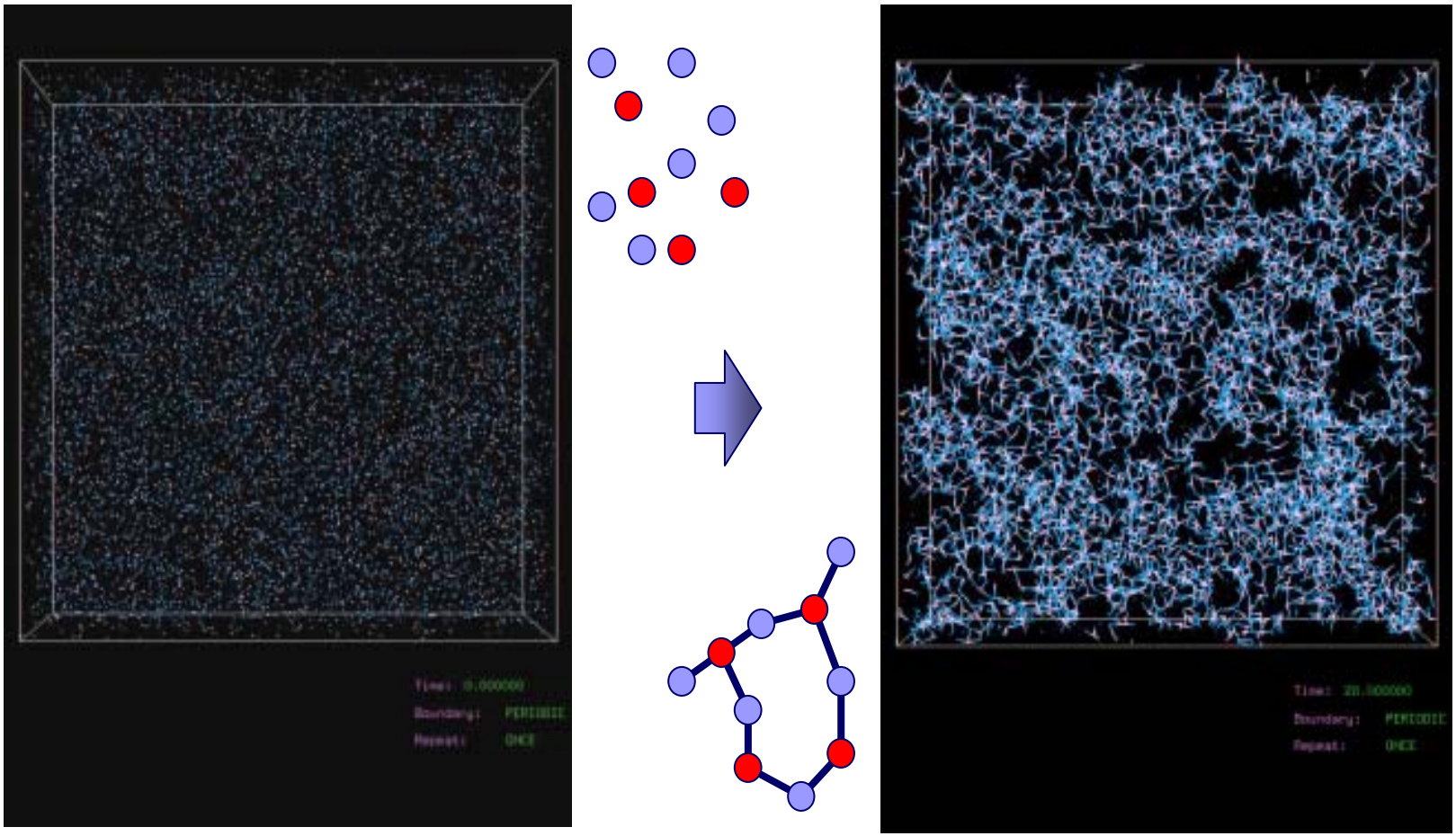


Example of Application: Confined polymer melts under shear flow

Polymer melts confined between walls. Apply shear flow by sliding the walls.



Example of Application: Network formation



Reaction among two and
three functional monomers

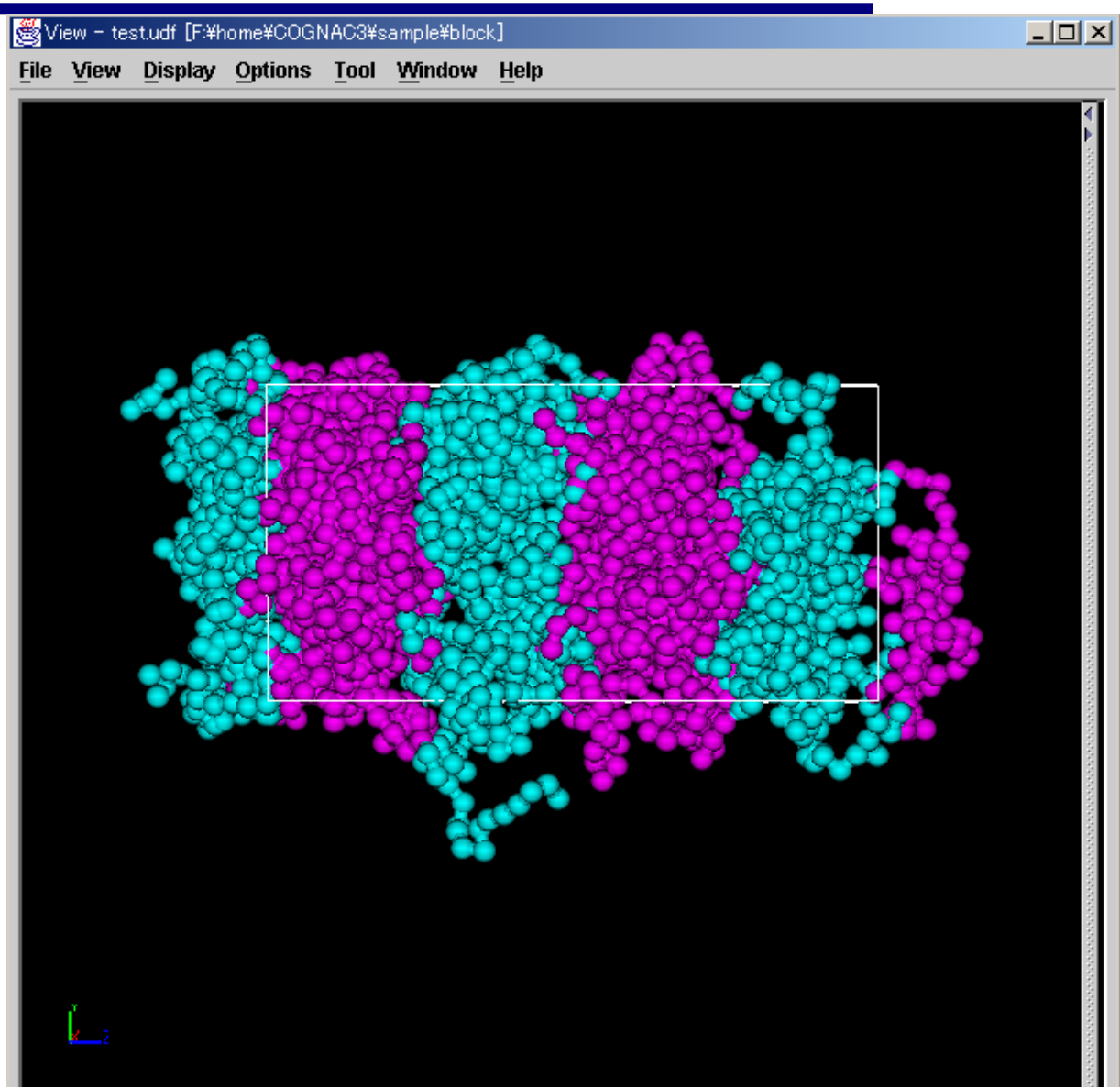
New Functions for Zooming

- Density biased Monte Carlo (DBMC)
- Density biased potential (DBP)
  - Embedding polymer chain into multiphase structures obtained by SUSHI
- Staggered reflective boundary condition (SRBC)
  - Boundary conditions for simulating interfacial structure of polymer blends
- Lamella builder
  - Generation of semi-crystalline lamella structures

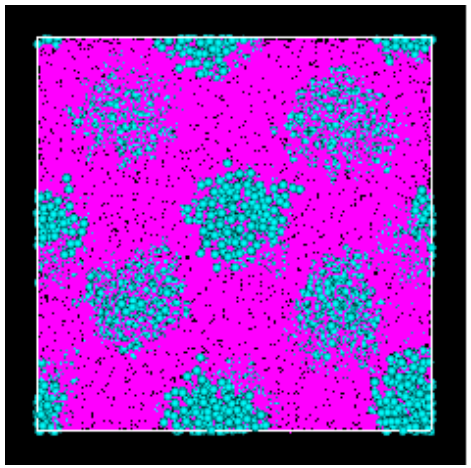
Example of Application: ABA triblock copolymer

A lamella structure of ABA triblock copolymer.

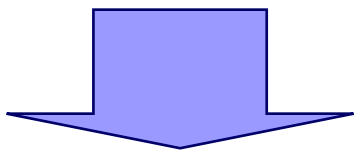
Loop/bridge ratio obtained by the SCF calculation(SUSHI) is reproduced.

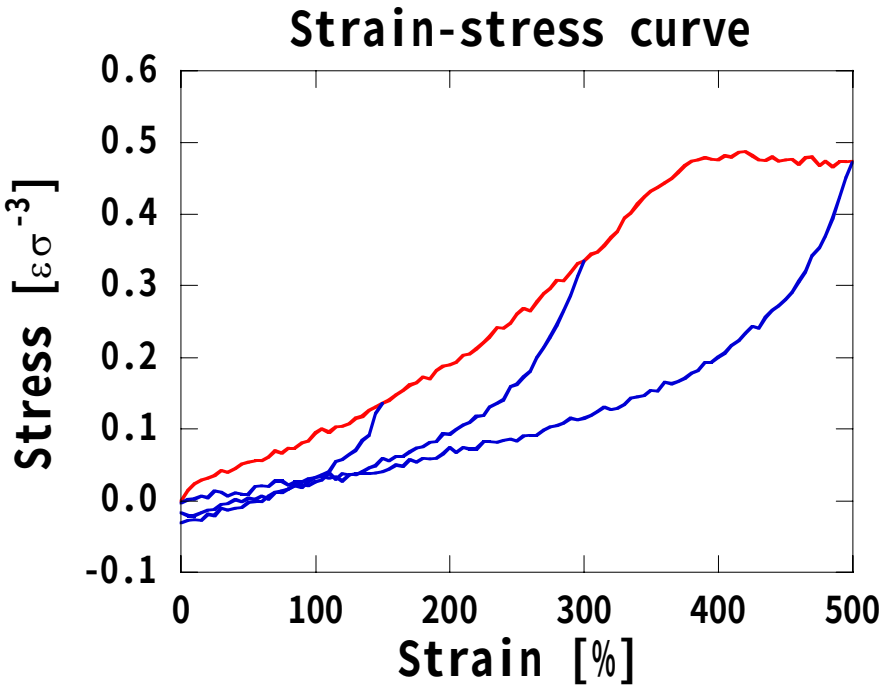


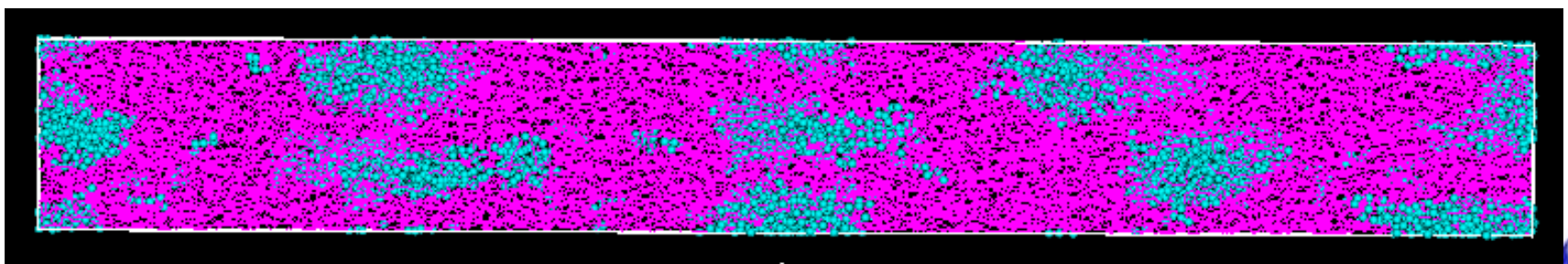
Example of Application:
Elastic behavior of ABA triblock copolymer



BCC sphere phase



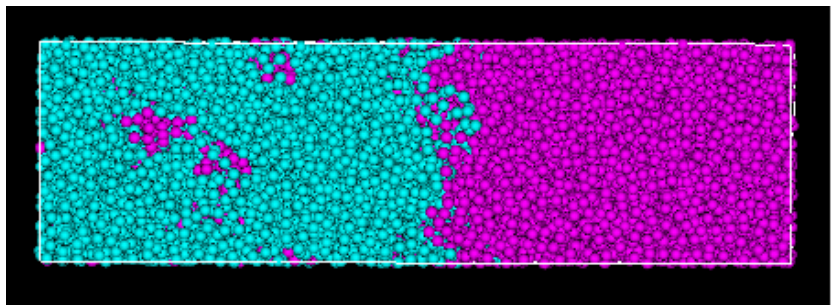




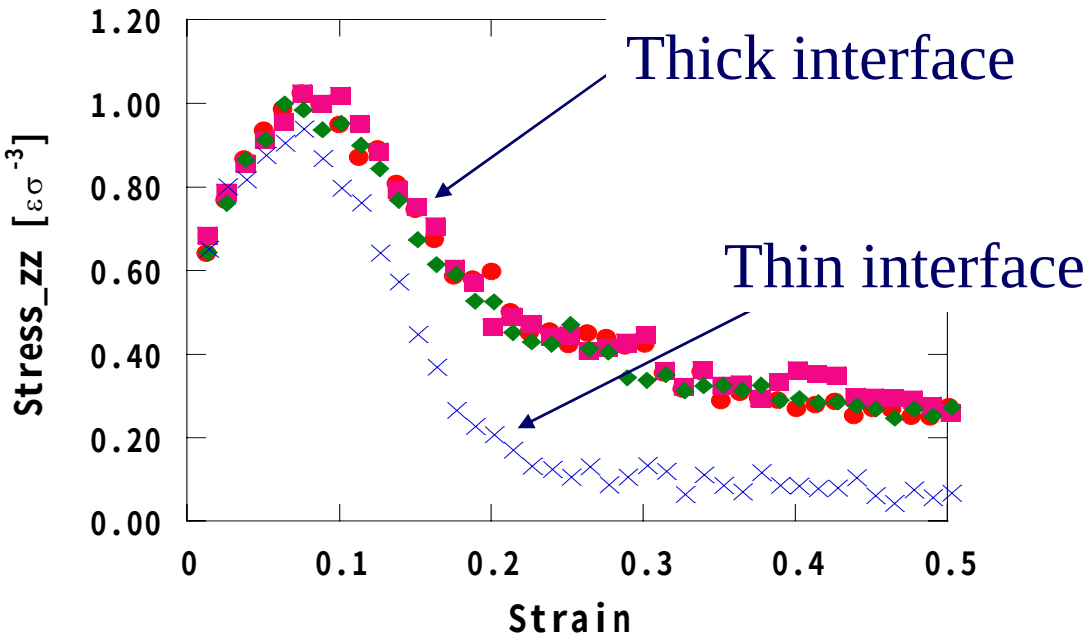
300% Strain

Example of Application: Interface of Polymer Blend

Interfacial structure of A/B polymer blend

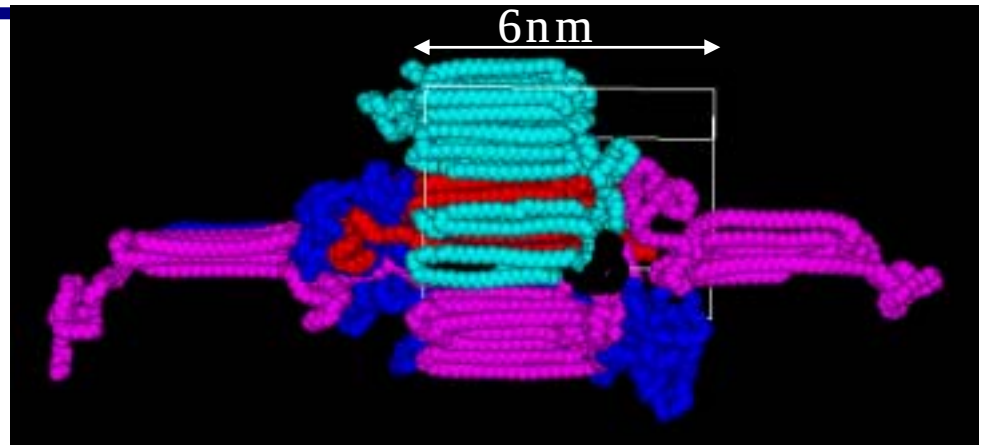


Elongation by deforming the unit cell



Example of Application: Semi-crystalline lamella

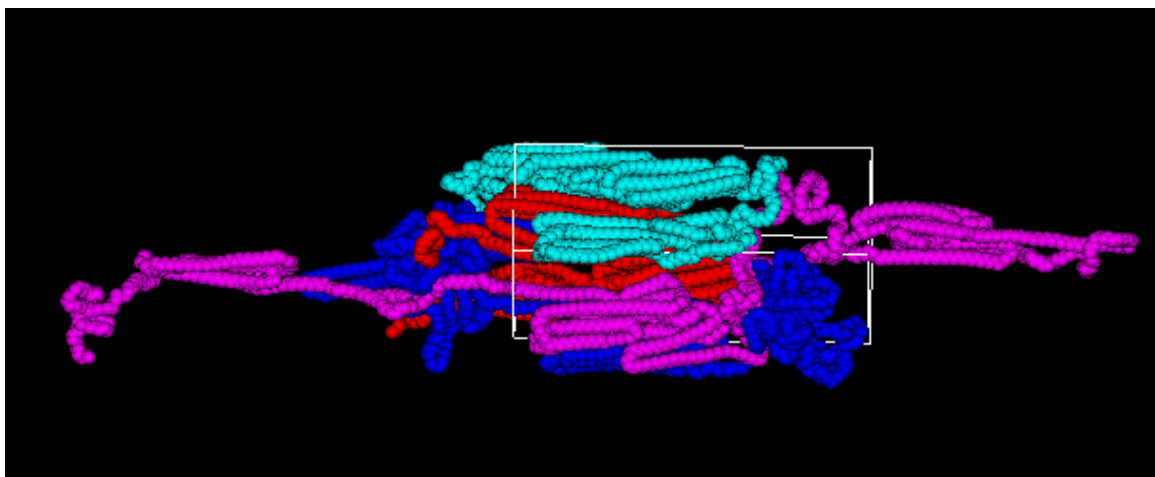
A semi-crystalline lamella structure of the united atom model of alkane



The distribution of the length and loop/bridge ratio in amorphous phase are determined by mean field theory

elongation

A snapshot during elongation



User defined potential functions

- COGNAC is written in C++
- COGNAC has classes for the templates of user defined potentials

- Users can define a functional form and parameters in a template function

```
#include "userbond1.h"
double UserBond1::calcforce(const Vector3d& dr,
                                    Vector3d& ftmp)
{
   double r,delR,ene,tmp;

   r=dr.length();
   delR=r-r0;
   tmp=kconst*delR;
   ftmp=dr*(tmp/r);
   ene=0.5*tmp*delR;
   return ene;
}
```

Example of user defined dynamics and potential functions: DPD

- Equations of motion and potential functions of dissipative particle dynamics (DPD)

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i$$

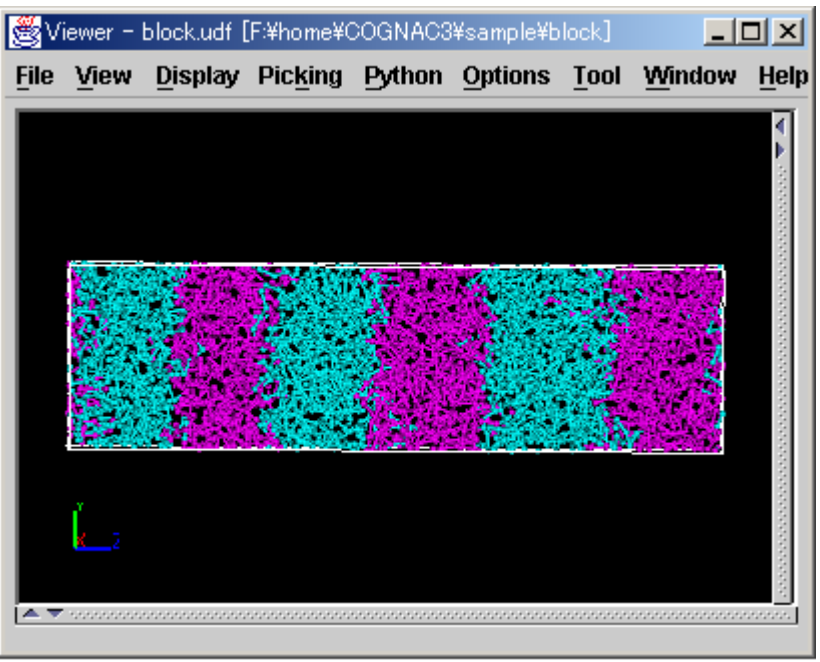
$$\mathbf{f}_i = \sum_{i \neq j} \left(\mathbf{F}_{ij}^{\mathrm{C}} + \mathbf{F}_{ij}^{\mathrm{D}} + \mathbf{F}_{ij}^{\mathrm{R}} \right)$$

$$\mathbf{F}_{ij}^{\mathrm{C}} = \begin{cases} a_{ij}\left(1 - r_{ij}\right)\hat{\mathbf{r}}_{ij} & \left(r_{ij} < 1\right), \\ 0 & \left(r_{ij} \geq 1\right) \end{cases}$$

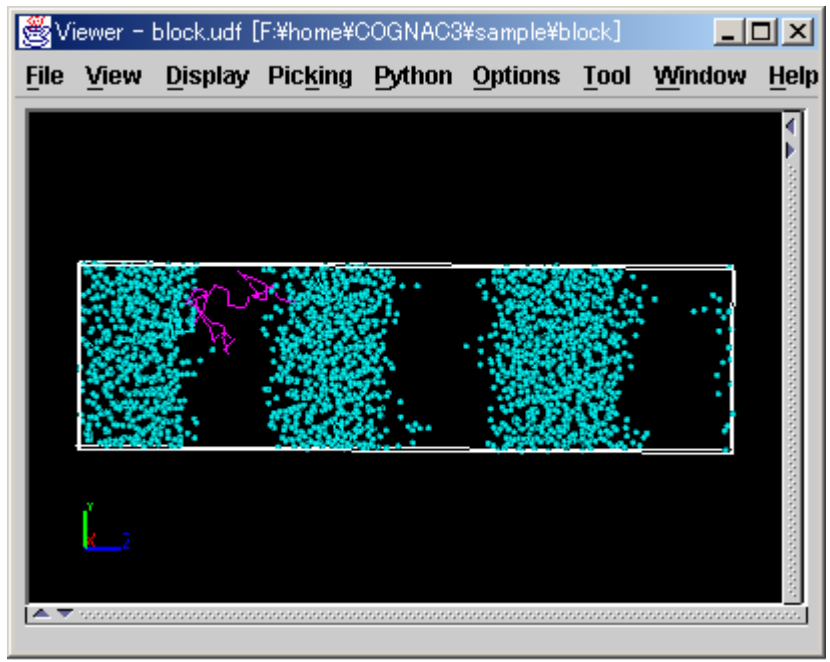
$$\mathbf{F}_{ij}^{\mathrm{D}} = -\gamma w^{\mathrm{D}}\left(r_{ij}\right)\left(\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}\right)\hat{\mathbf{r}}_{ij}, \quad \mathbf{F}_{ij}^{\mathrm{R}} = \sigma w^{\mathrm{R}}\left(r_{ij}\right)\theta_{ij}\hat{\mathbf{r}}_{ij}$$

Display of molecular structures

- Molecuar structures can be displayed by using “Action” tools or Python scripts
  - Arbitrary set of molecules/atoms/bonds can be displayed



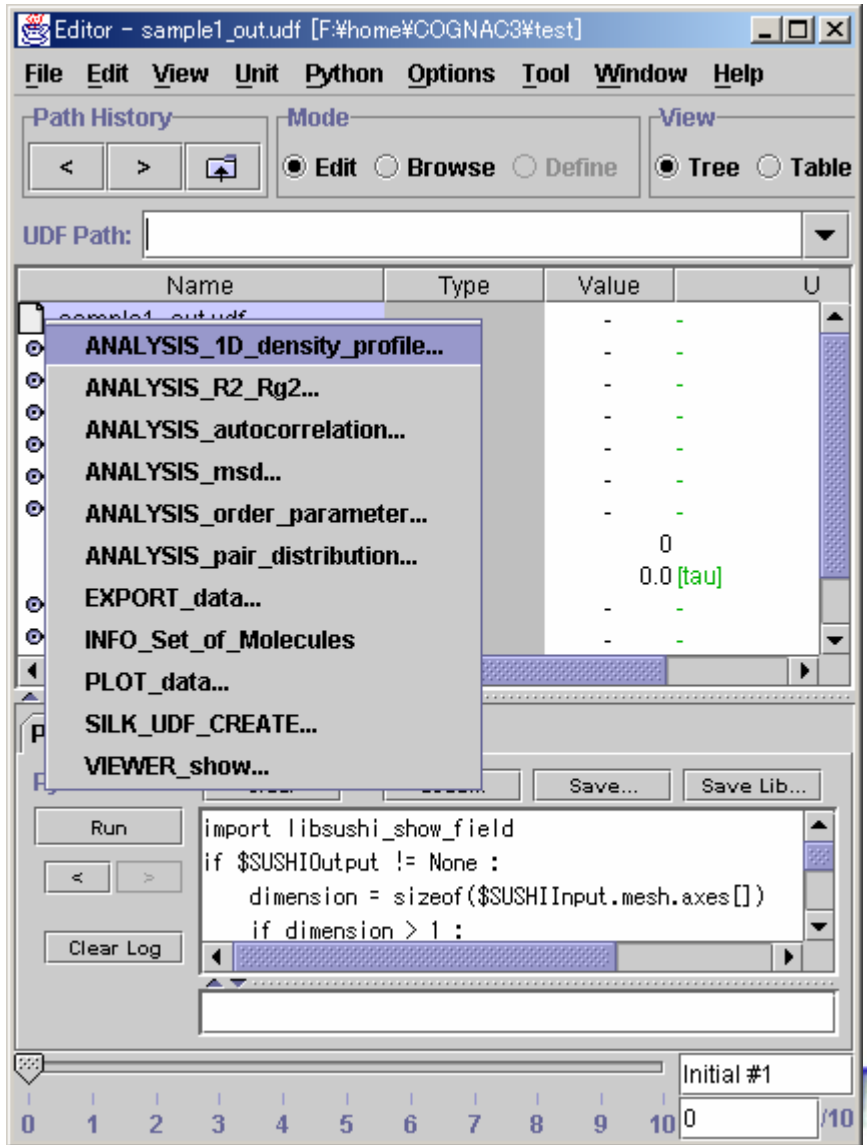
Displaying all molecules of ABA triblock copolymers in a lamella phase



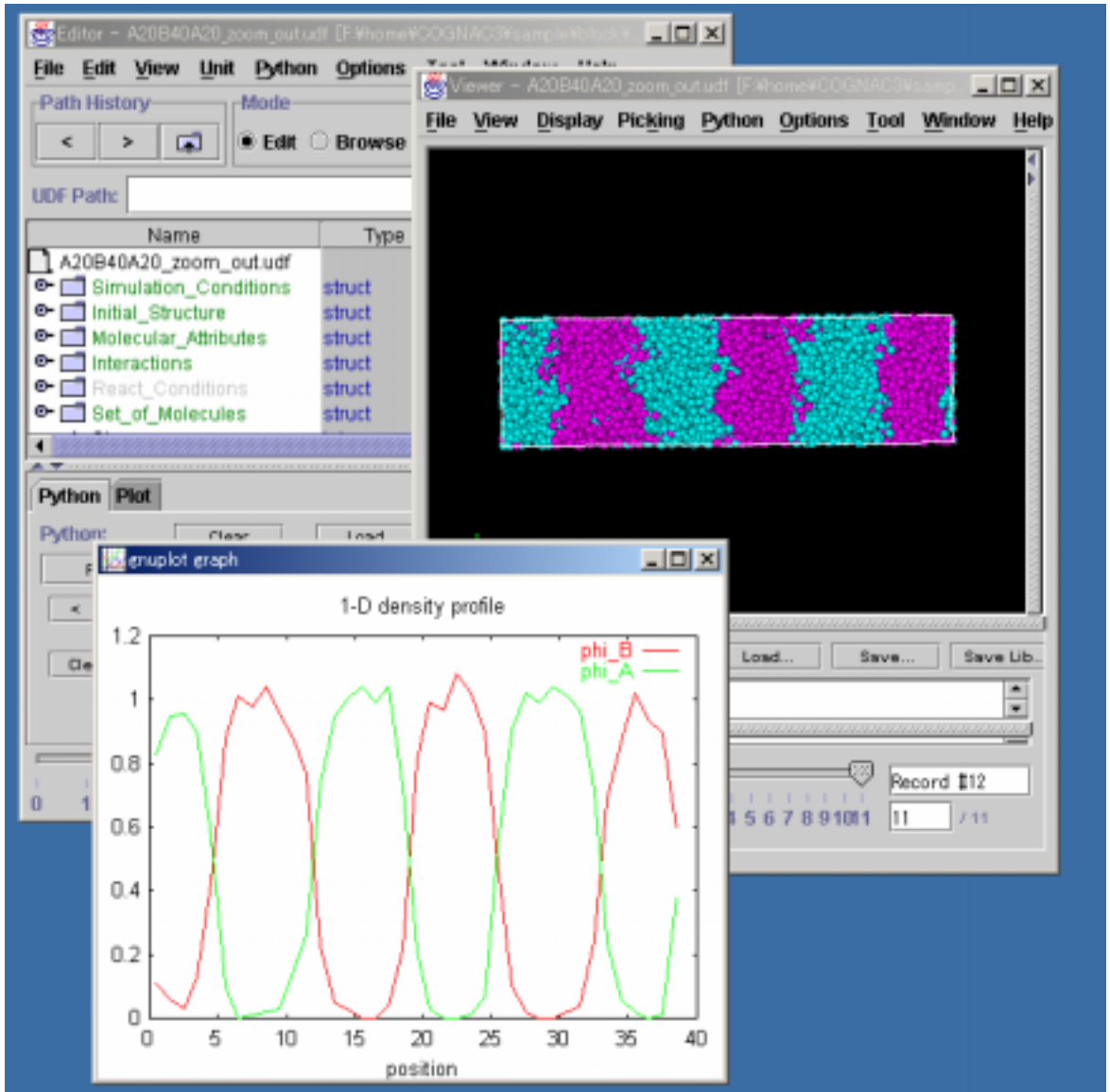
Displaying only A type atoms and single bridge chain.

Analysis using “Action” on GOURMET

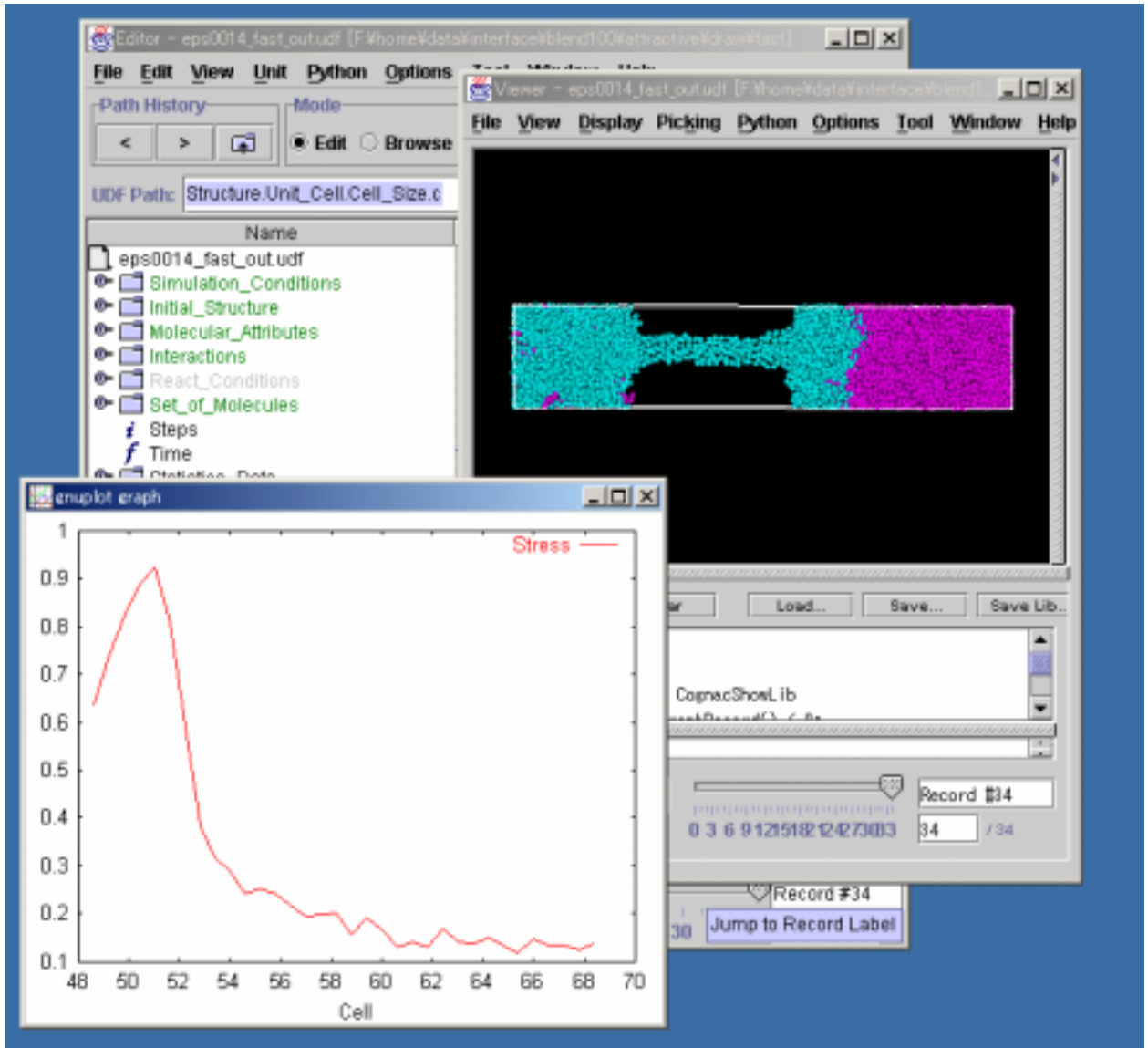
- Some of the analysis tools can be launched by “Action” on GOURMET



Plot of the results : Density profiles

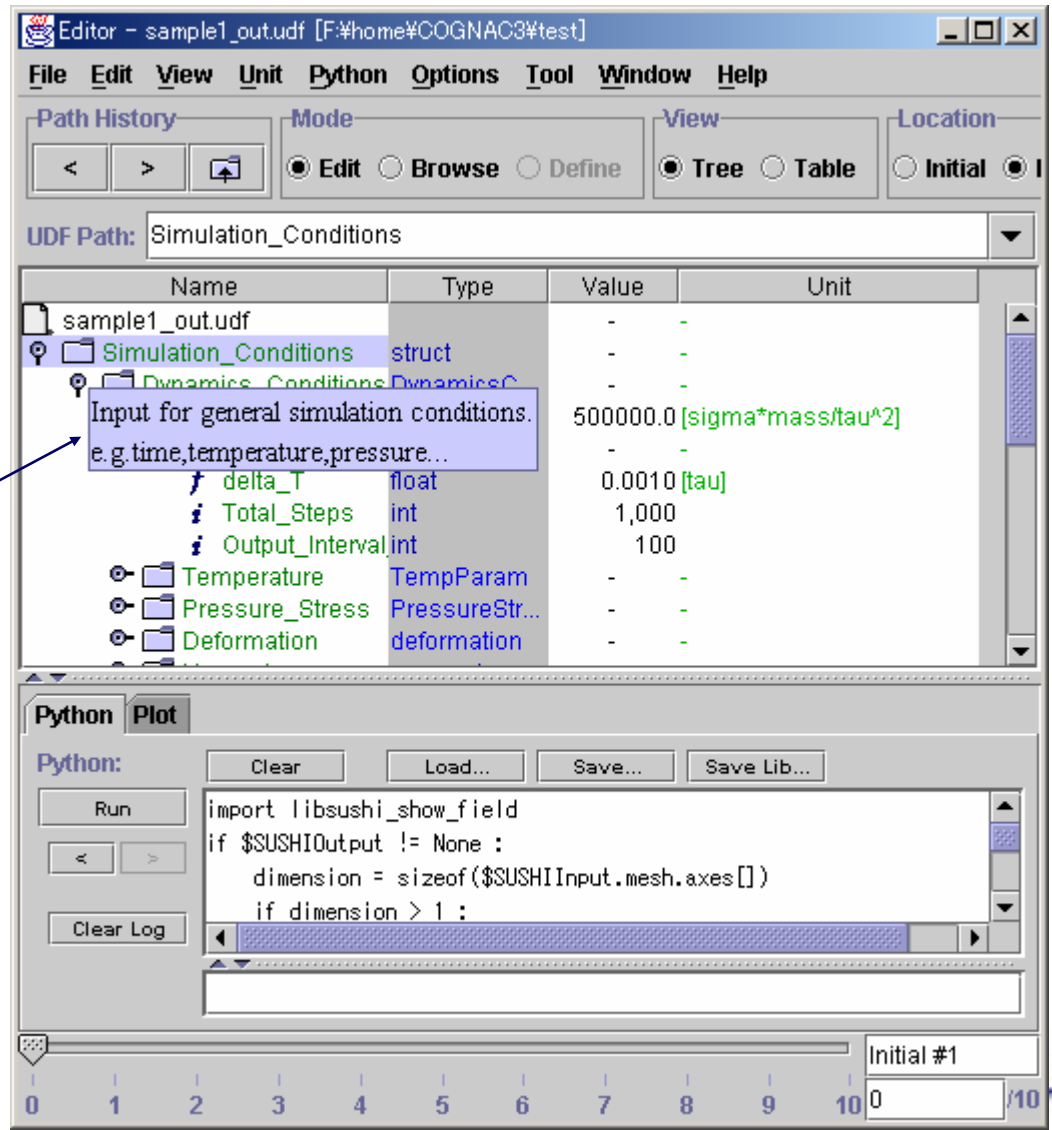


Plot of the results : Stress-strain curve



Help

- Brief comments on each UDF structure and parameter are displayed



HELP

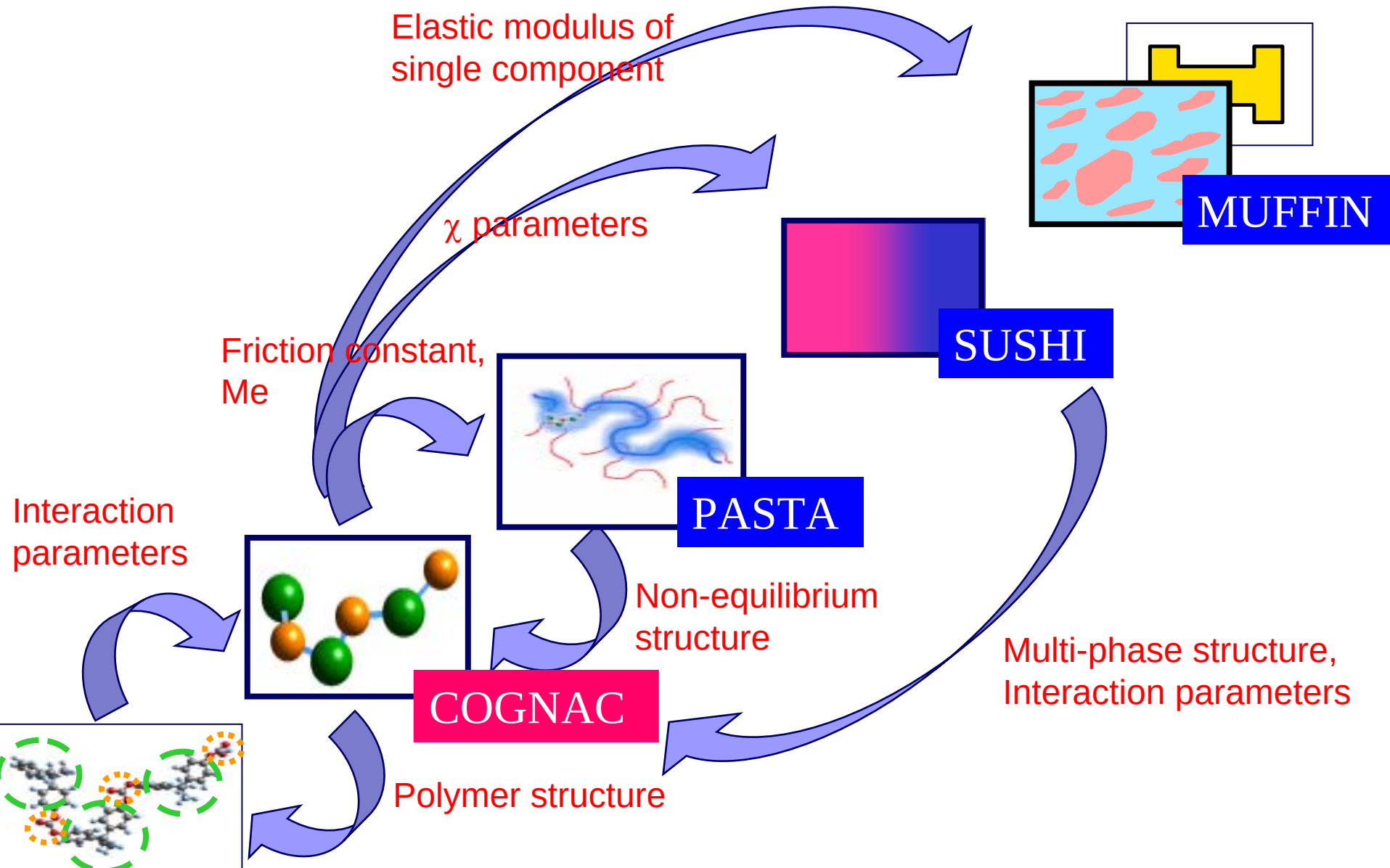
Unit conversion

- Unit of each parameter can be converted to arbitrary units
- if COGNAC UDF has unit parameters,
  i.e.
  reduced mass in [amu]
  reduced energy in [kJ/mol]
  reduced length in [nm].

Name	Type	Value	Unit
pentane50_out.udf		-	-
Simulation_Conditions	struct	-	-
Dynamics_Conditions	Dynamics...	-	-
Max_Force	float	10000.0	[sigma*mass/tau^2]
Time	time	-	-
delta_T	float	0.0010	[tau]
Total_Steps	int	2,000	
Output_Interval_Steps	int	20	
Temperature	TempParam	-	-
Temperature	float	3.0	[T]
Interval_of_Scale_Tem	int	10,000,000	
Pressure_Stress	PressureSt...	-	-
Pressure	float	1.0	[P]
Stress	SymMat3x3	-	-

Name	Type	Value	Unit
pentane50_out.udf		-	-
Simulation_Conditions	struct	-	-
Dynamics_Conditions	Dynamics...	-	-
Max_Force	float	2.1849212...	[N]
Time	time	-	-
delta_T	float	2.0107708	[fs]
Total_Steps	int	2,000	
Output_Interval_Steps	int	20	
Temperature	TempParam	-	-
Temperature	float	180.4075	[K]
Interval_of_Scale_Tem	int	10,000,000	
Pressure_Stress	PressureSt...	-	-
Pressure	float	15.131034	[MPa]
Stress	SymMat3x3	-	-

COGNAC:Linking to other layers



Summary

- COGNAC has following functions:
  - Basic functions for MD/MM
  - Versatile functions for molecular modeling
  - Various potential functions and ensembles for coarse-grained models
  - Various functions and tools for material design
  - New functions for zooming
  - Extensibility of program

- Developers of COGNAC
  - T.Aoyagi, F.Sawa, T.Shoji, H.Fukunaga (JCII, Doi project)
  - Prof. J.Takimoto (Nagoya Univ.)