Challenges in Multi Scale Modeling

-Our Experience in the Polymer Modeling Project-

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Outline

- What is multi-scale modeling
- The polymer modeling project
  - Objective
  - The difficult part
  - Our strategy
  - Some outcomes
- Conclusion

What is Multi Scale Modeling

What is multiscale modeling?

A modeling which uses two or more models for different scale

Multiscale calculation can be done

by concurrent calculation

– e.g. Car-Pallinello method

by separate calculation

– e.g. conventional method

The core is to make consistent models by passing information among different simulation programs.

Multiscale modeling is difficult

- How to let different programs share information

Some kind of translation is needed

- How to gurantee the correctness of the translation.

Some uncertainities are unavoidable

- How to ensure sustanable development

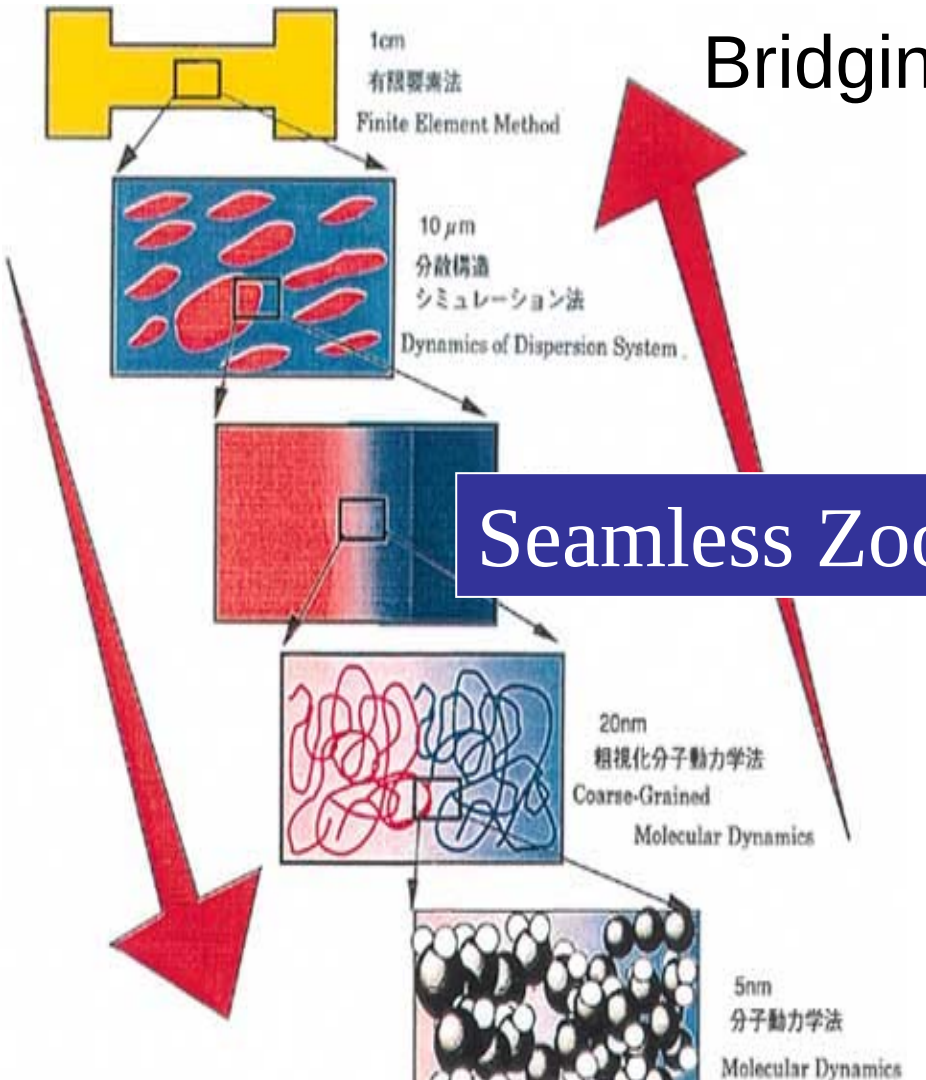
Some uncertainities are unavoidable

The Polymer Modeling Project

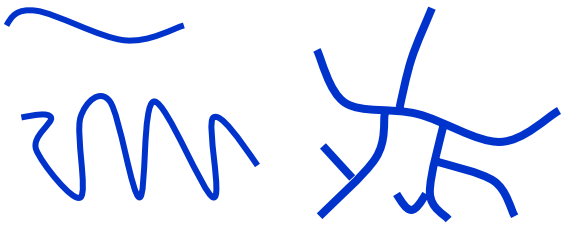
The Polymer Modeling Project

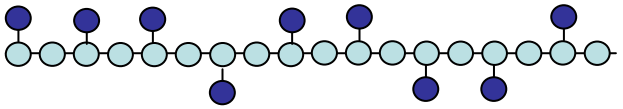
METI project from1998 to 2002

Bridging “micro” and “macro”

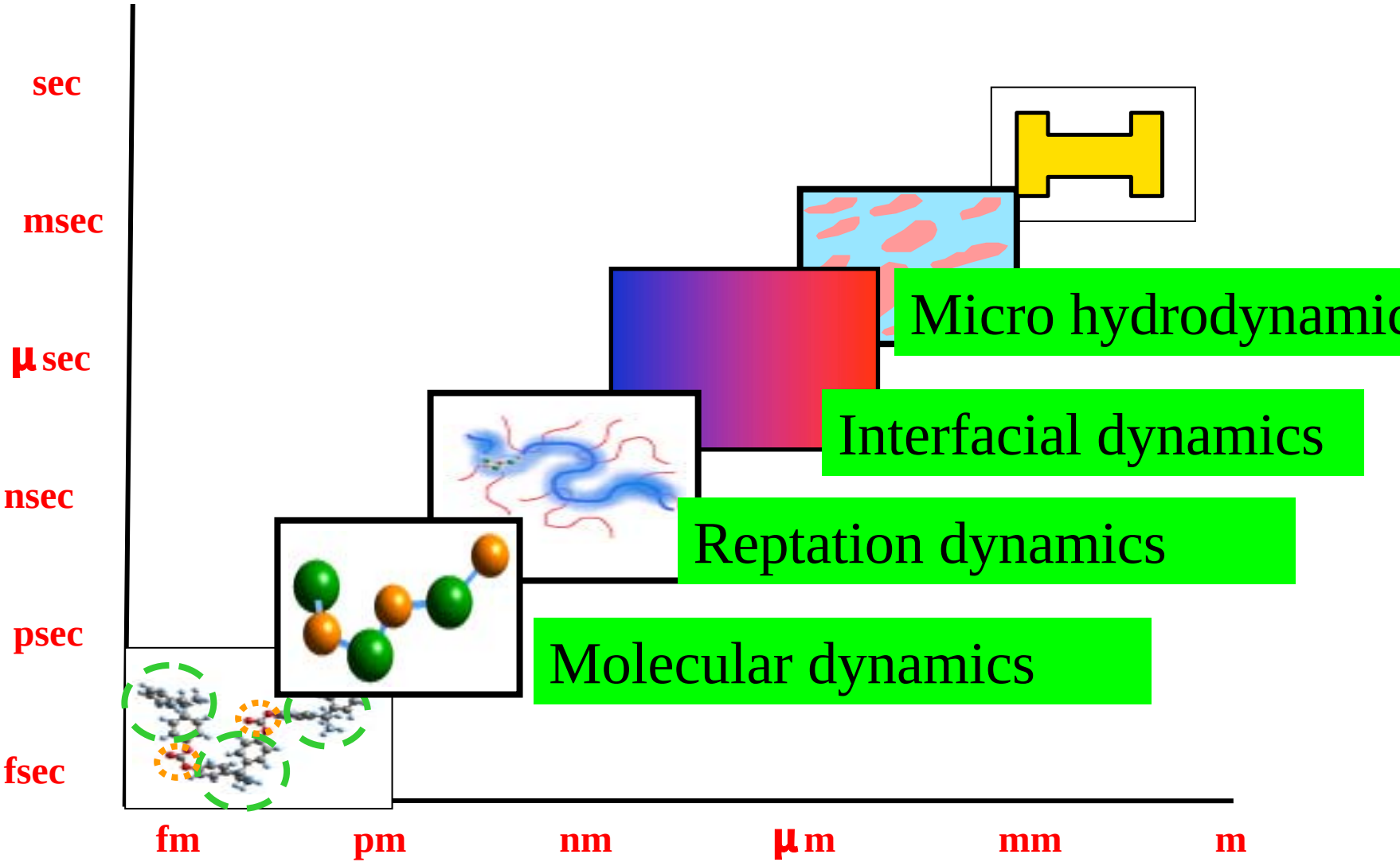


Seamless Zooming





Mesoscale Simulation Engines

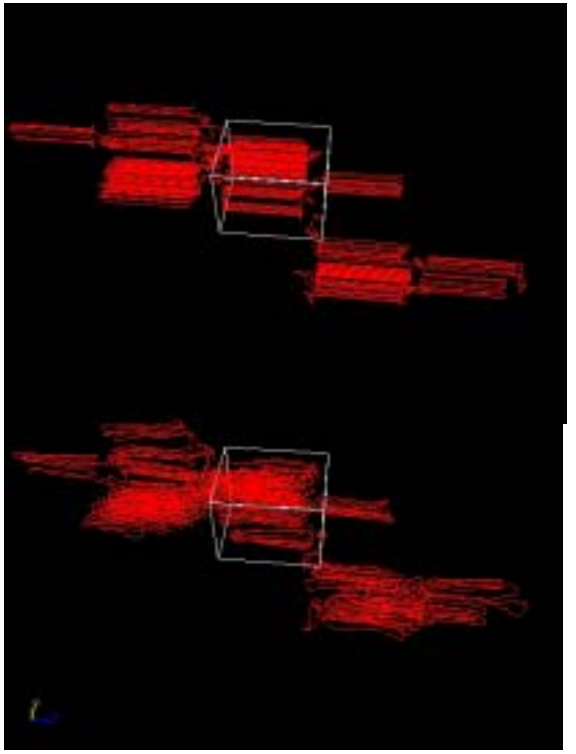


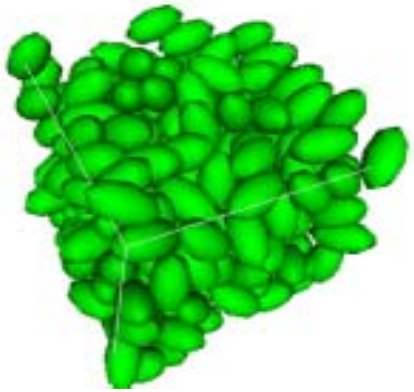
Molecular Dynamics

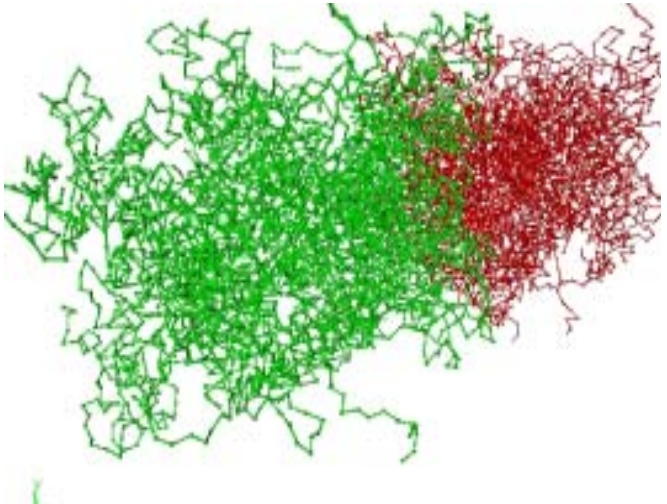
- Solve the equation of motion of particles:

$$m\frac{d^2\mathbf{r}_i}{dt^2} = -\frac{\partial U}{\partial \mathbf{r}_i}$$

Aoyagi,Sawa





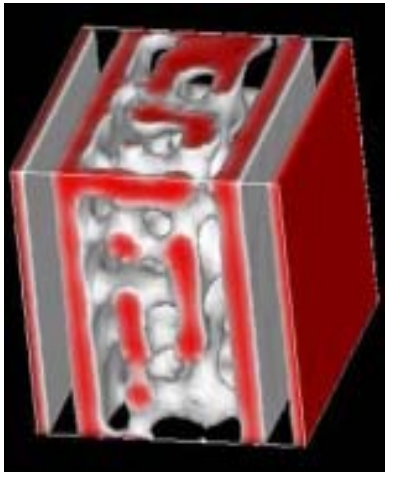


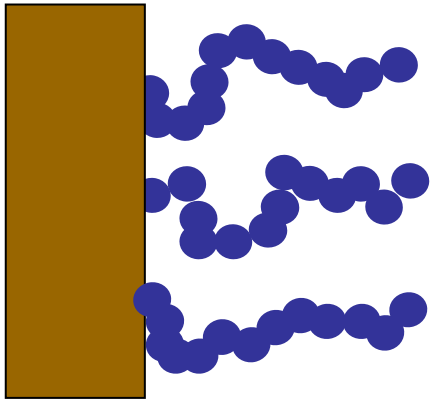
Interfacial Dynamics

Sove the Edwards equation for polymer conformation

- Structure of polymers near the interface
- Phase separation, Microphases, Micellization

Honda,Kawakatsu





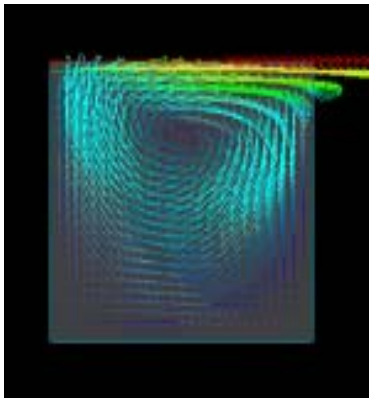
$$\frac{\partial}{\partial t}Q(n,\mathbf{r}) = \left[\frac{b^2}{6}\nabla^2 - \beta V(\mathbf{r})\right]Q(n,\mathbf{r})$$

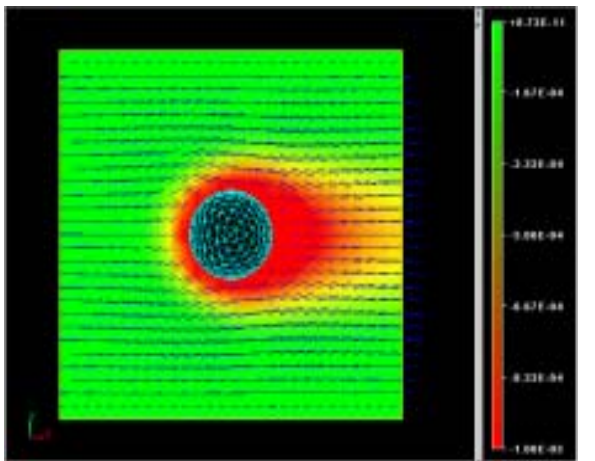
$$V(r) = V[Q(r,n)]$$

Micro Hydrodynamics

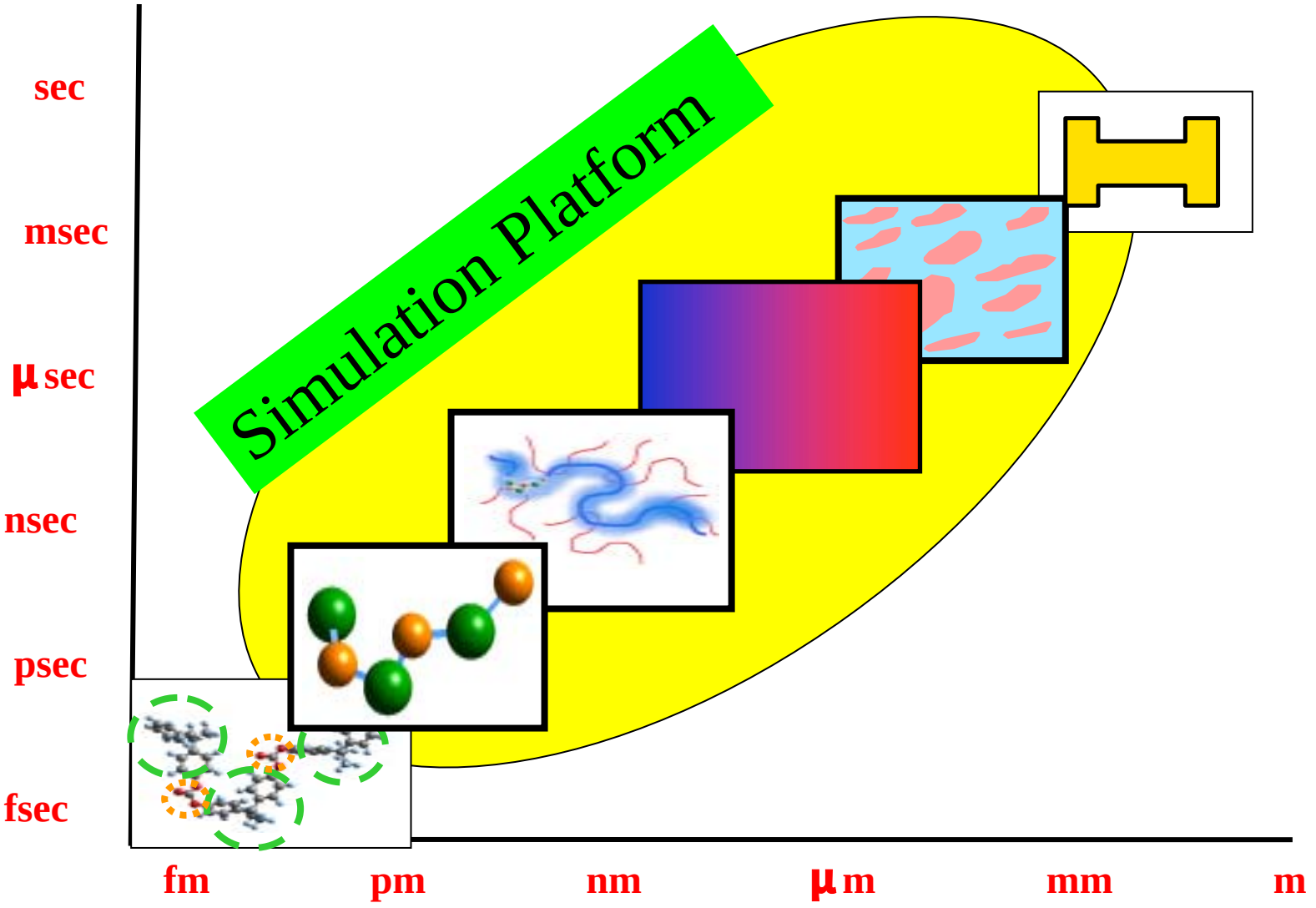
Yamaue, Taniguchi, Sasaki

- Fluid engine and solid (gel) engine.
- Solve continuum equations
  - Stokes eq. for velocity and pressure
  - Elastic eq. for displacement
  - Diffusion eq. for solute and ions
  - Poisson eq. for electric field





How to Bridge Simulation Engines



Difficulty in the design of the simulation platform

Integration of engines requires a common expression for physical data, but it is very difficult to set up such data format.

- Different engines use different physical models, and need diffirent data.
- The mesoscale engines are evolving, and the platform has to accomodate the engines which will be developed in future.

Integration of engines was very very difficult.

“Open” is the key

Multiscale modeling is a grand challenge.

- Let us try to make soft wares which will grow and expand after our project ends.
  - The system should be able to grow on its own.
  - We should not force our way of “zooming”: the basic part must be independent of it.

Our decision for the platform design

- We leave the task of defining the data structures to researchers.
- We determine a rule to express the data structure.
- The platform provides a service for engines which state the data structure following this rule.

We don’t impose zooming.
We don’t define words.

UDF (User Definable Format)

- UDF consists of two parts:
  - the data definition part
  - the data part.
- The definition part defines the type, unit and the other attributes for each item in the data.
- The data part gives the value for each item.

An example of UDF

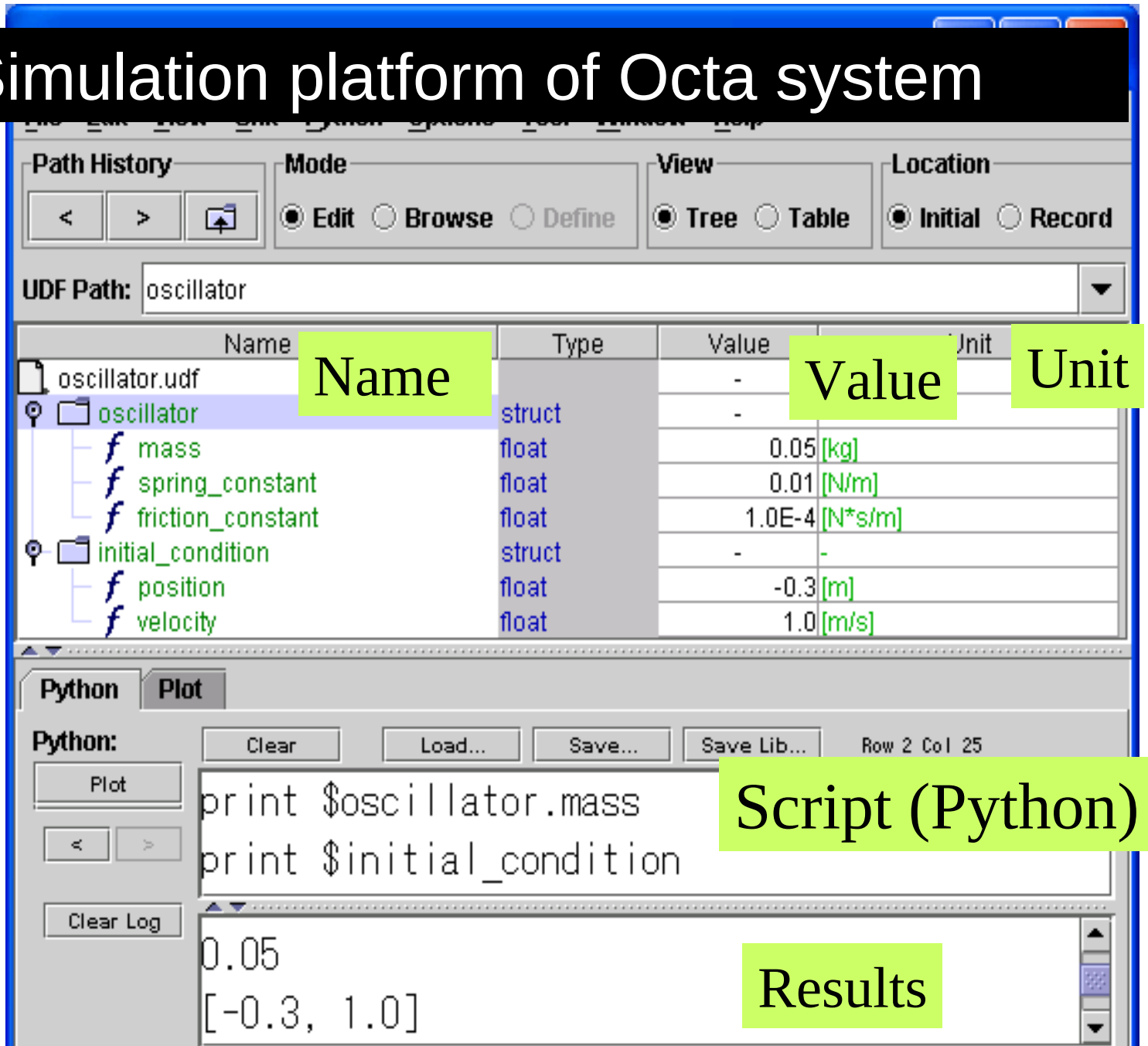
Definition of data structure

```
¥begin{def}
  oscillator: {
        mass   :   float  [kg]
        spring_constant   :   float   [N/m]
        friction_constant :   float   [N*s/m] }
  initial_condition:{
        position: float [m]
        velocity: float [m/s]  }
¥end{def}
```

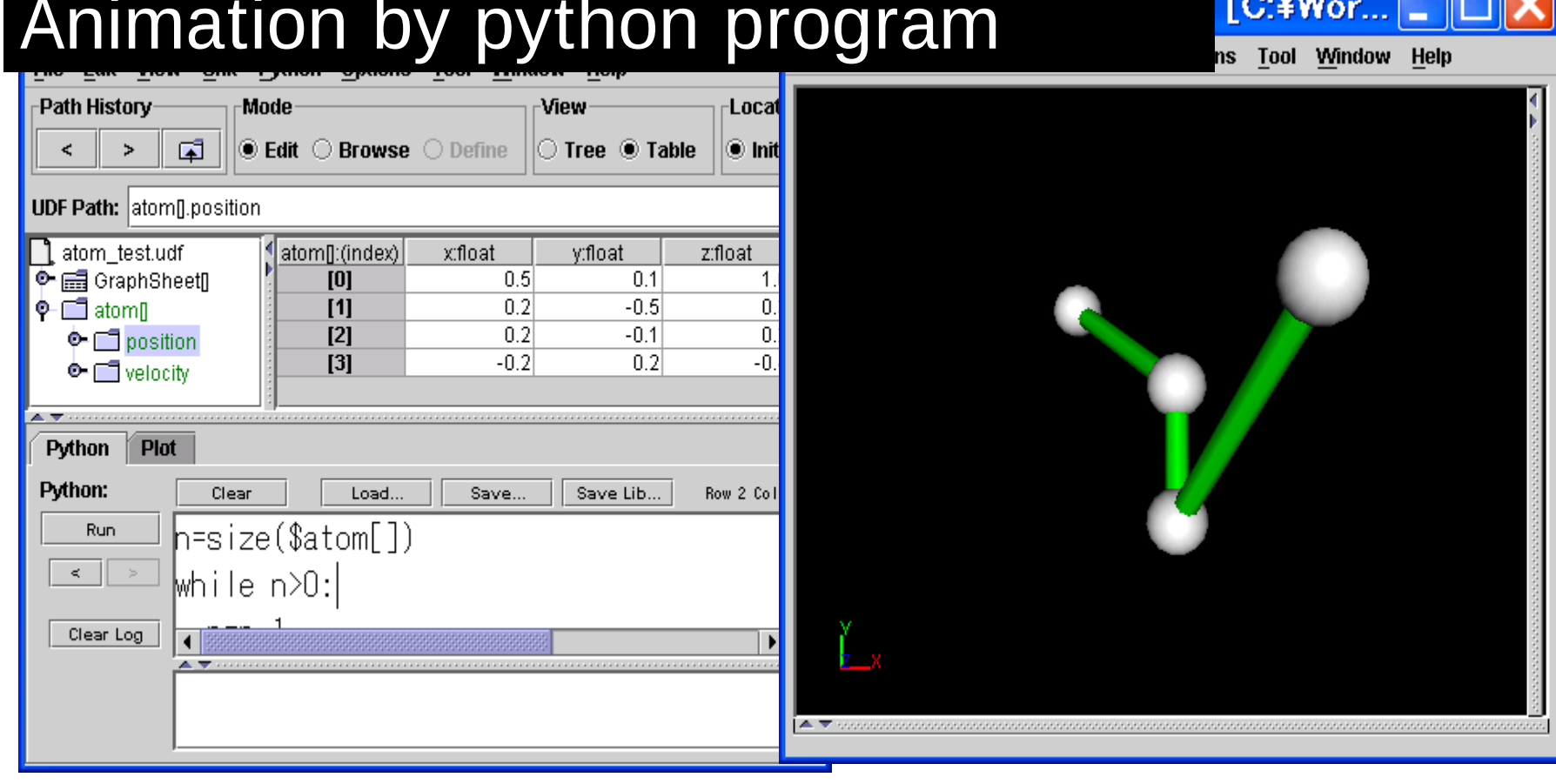
Data

```
¥begin{data}
      oscillator:{0.05, 0.01, 0.0001}
      initial_condition:{-0.3, 1.0}
¥end{data}
```

Simulation platform of Octa system



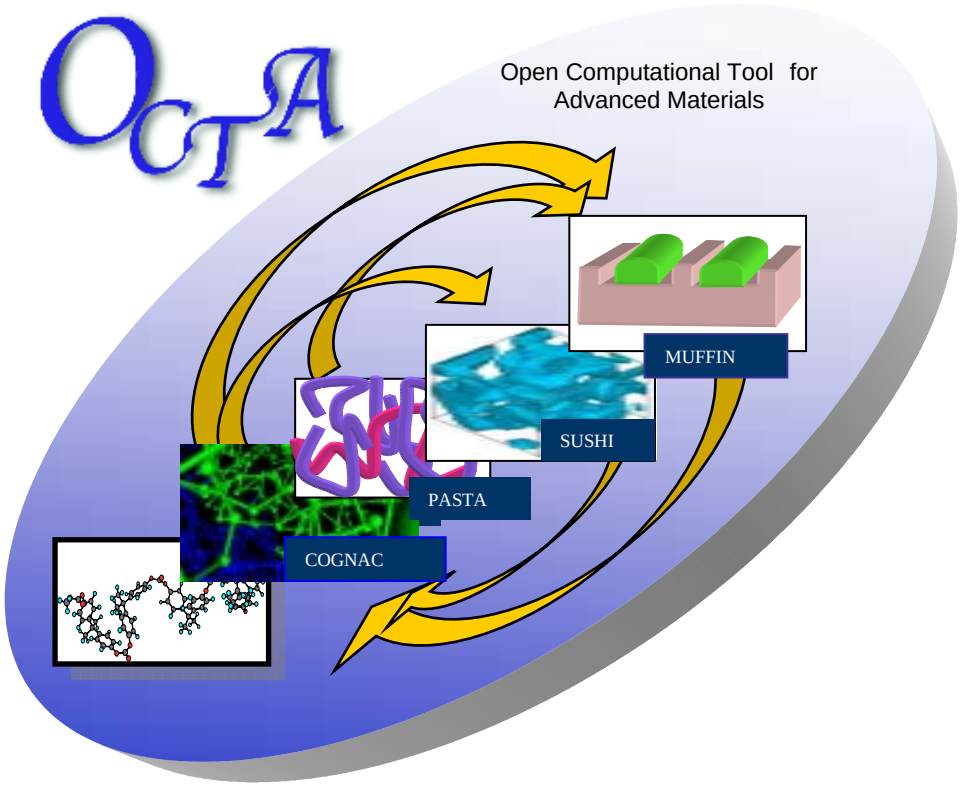
Animation by python program




```
n=size($atom[])
while n>0:
  n=n-1
  sphere($atom[n].position,0)
  if n>0:cylinder($atom[n].position, $atom[n-1].position, 2)
```

Octa system

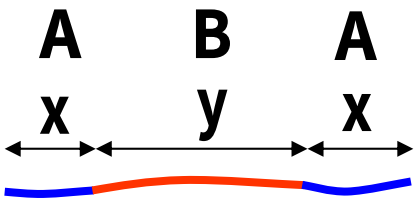
- Open
- Computational Tool for
- Advanced material technology



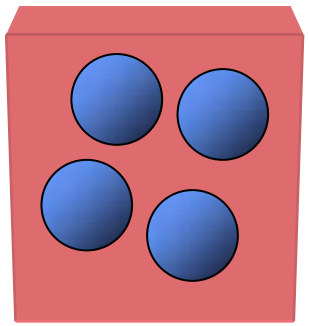
◆Open to public at http:octa.jp in 2002

◆Has been updated by voluntary group

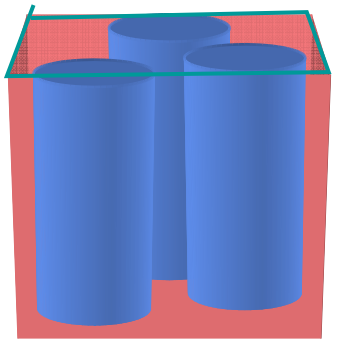
An example:study of ABA triblock copolymers



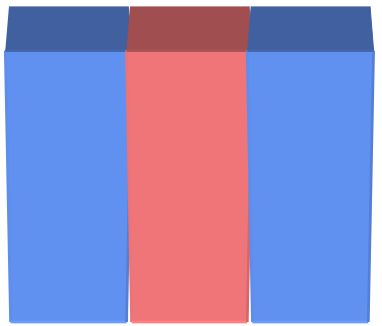
Symmetric Triblock Polymer AxByAx



Sphere



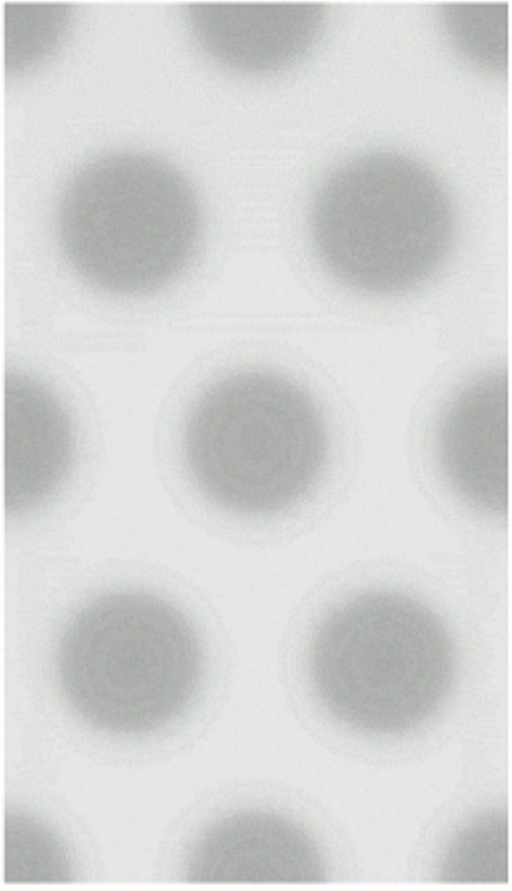
Cylinder

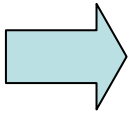


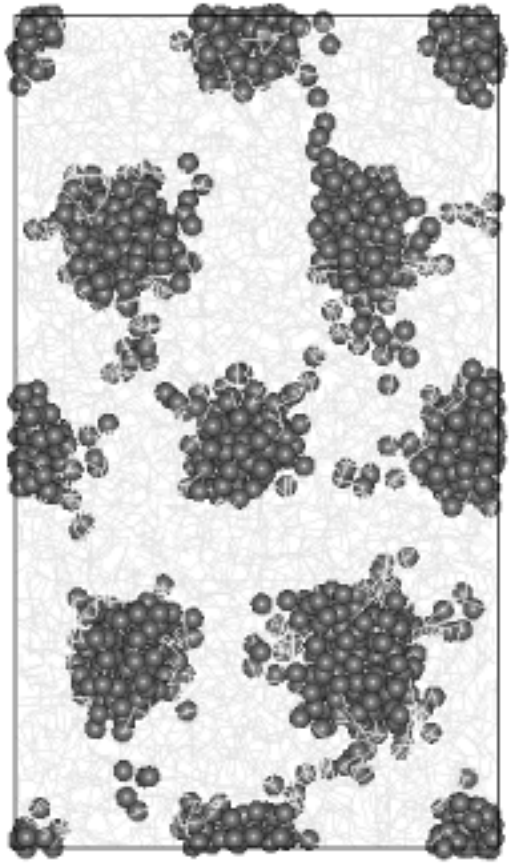
Lamella

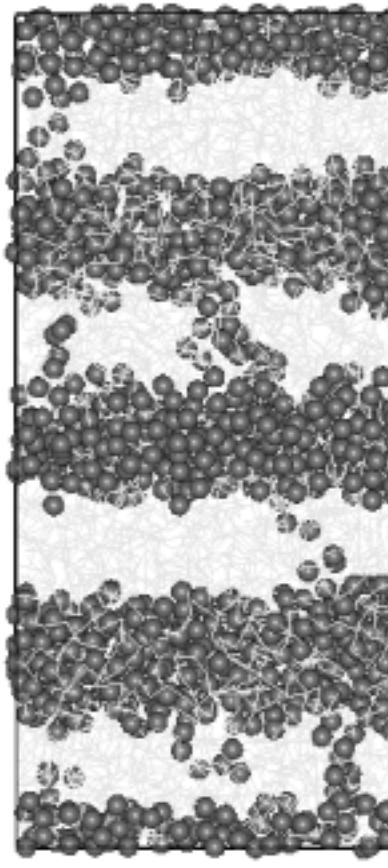
- What structure is formed for the tri-block copolymers.
- How does the bridging affects the mechanical properties.

Results of “zooming in”

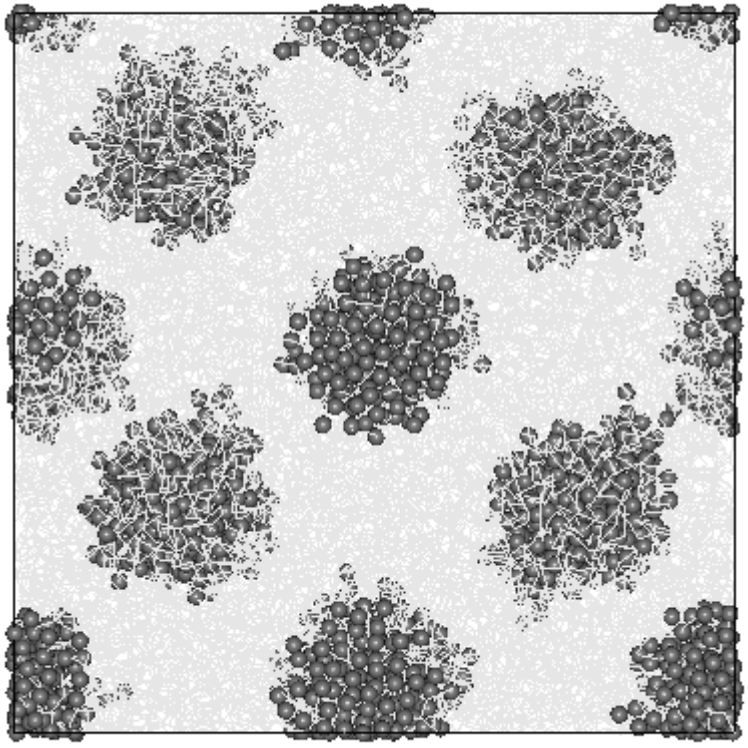








Equilibrium structure



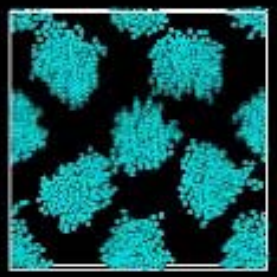
A5B73A5

$PS_{2600}IP_{20000}PS_{2600}$

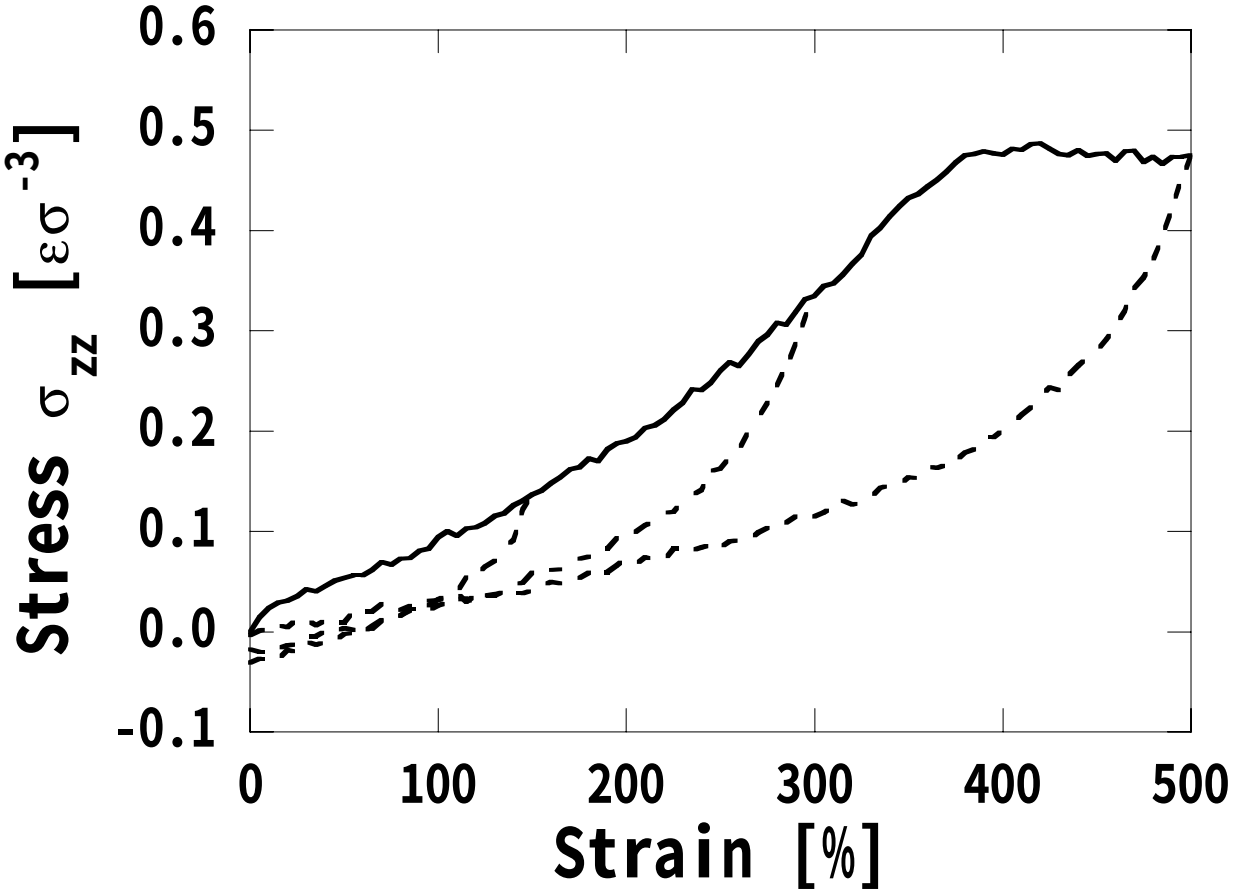
347 polymers
8 unit cell of bcc

Aoyagi et al. Fig.6

Deformation of domains

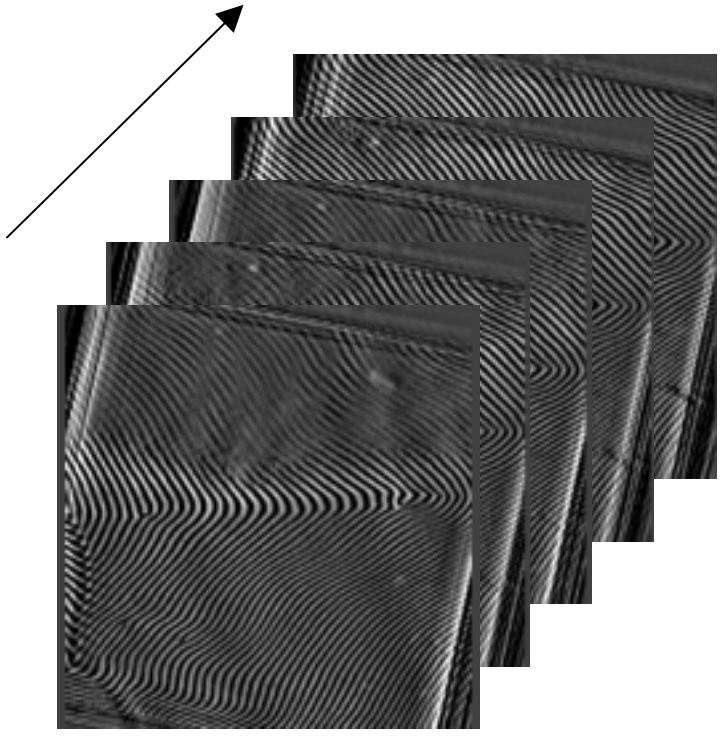


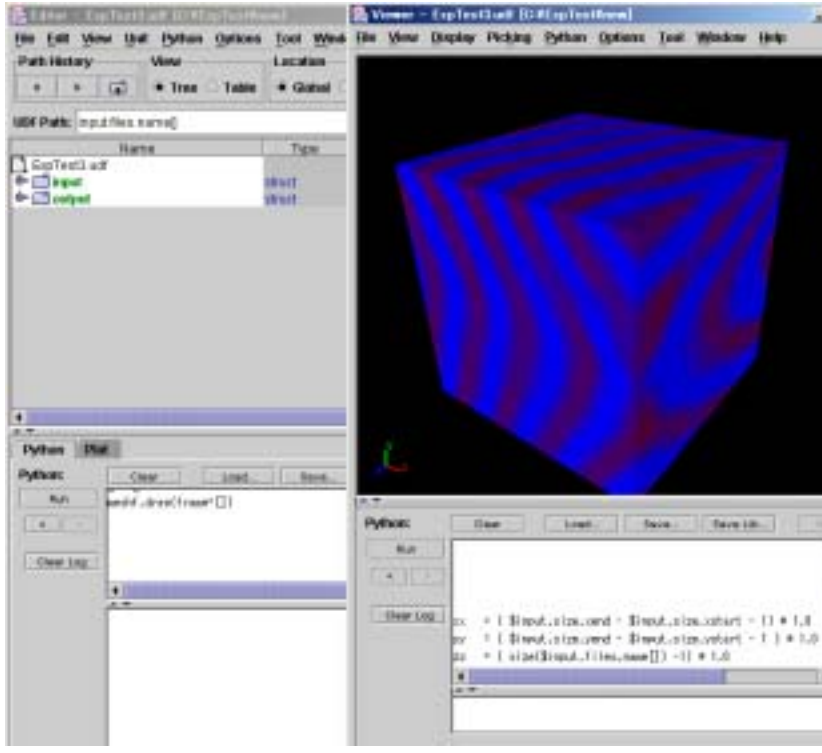
Stress- strain curve for spherical structure



Aoyagi et al. Fig.7

Fusion with experimental system

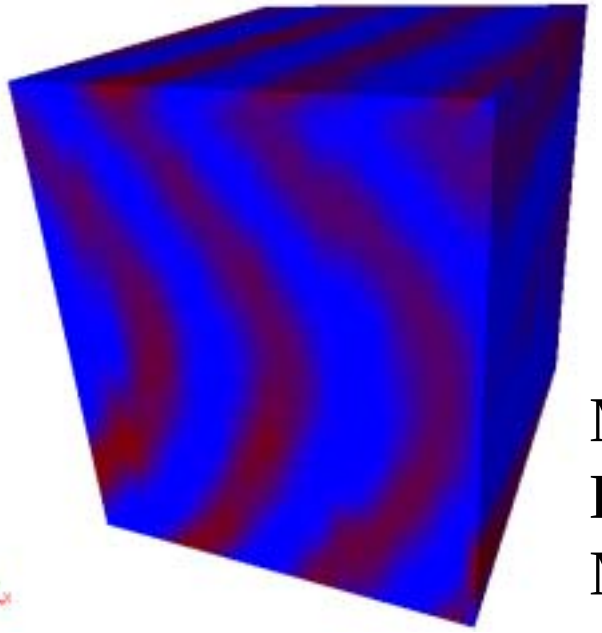




3D TEM

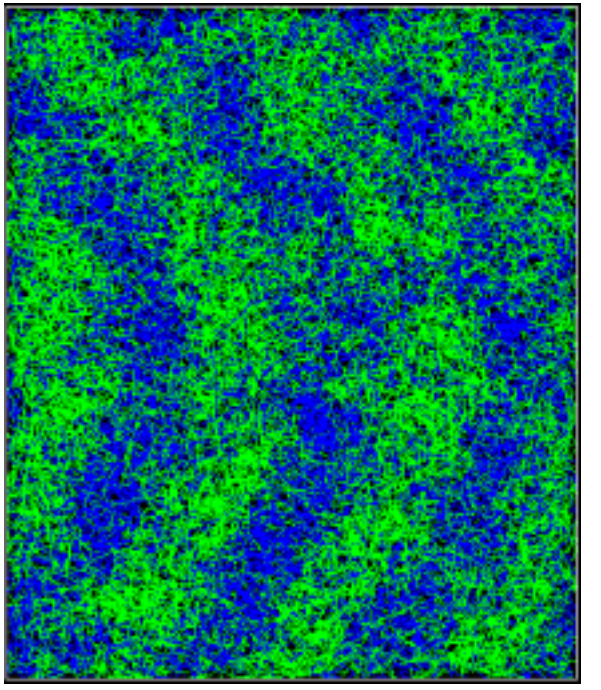
Octa

View with the aid of simulators



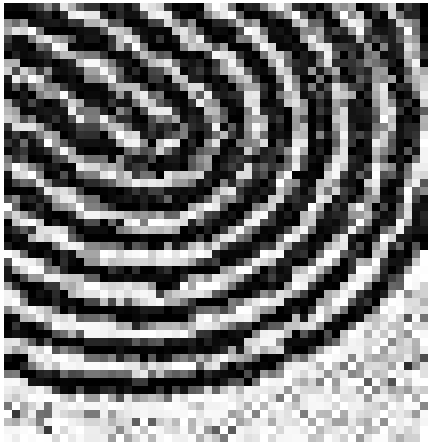
Data of 3D TEM

MD Engines
Density Biased
Monte Carlo

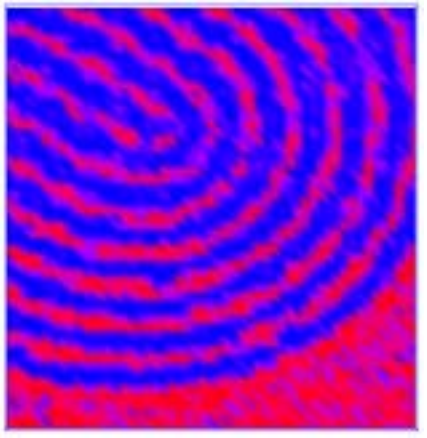


General Chains

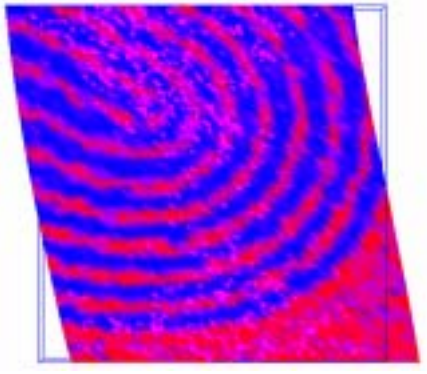
Virtual experiments



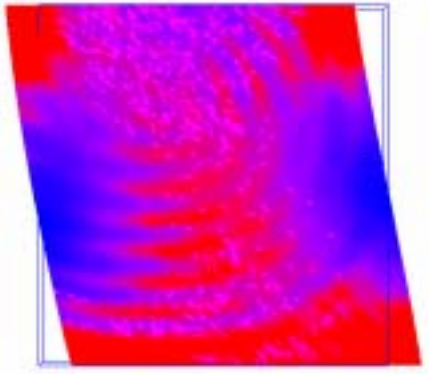
TEM



View in Octa



Virtual Experiments in Octa



Energy Distribution

Similar things can be don

- Mechanical
- Thermal
- Transport
- Optical

Conclusion

Summing up our experience

- We realized that collaboration of engines, and collaboration of human being are more important than programmed “zooming”
- We decided not to pursue automatic “zooming”.
- We focused on constructing a platform on which various simulation programs can collaborate with each other.
- This gave flexibility and expandability to Octa system.

Multi-scale modeling is a grand grand chanllenge