General-purpose
Multi-Phase Dynamics Program

MUFFIN

\- **MU**lti**F**arious **FI**eld simulator for **N**on-equilibrium system -

Tatsuya Yamaue
JCII, Doi project

Developers of MUFFIN – WG3 Doi Project -

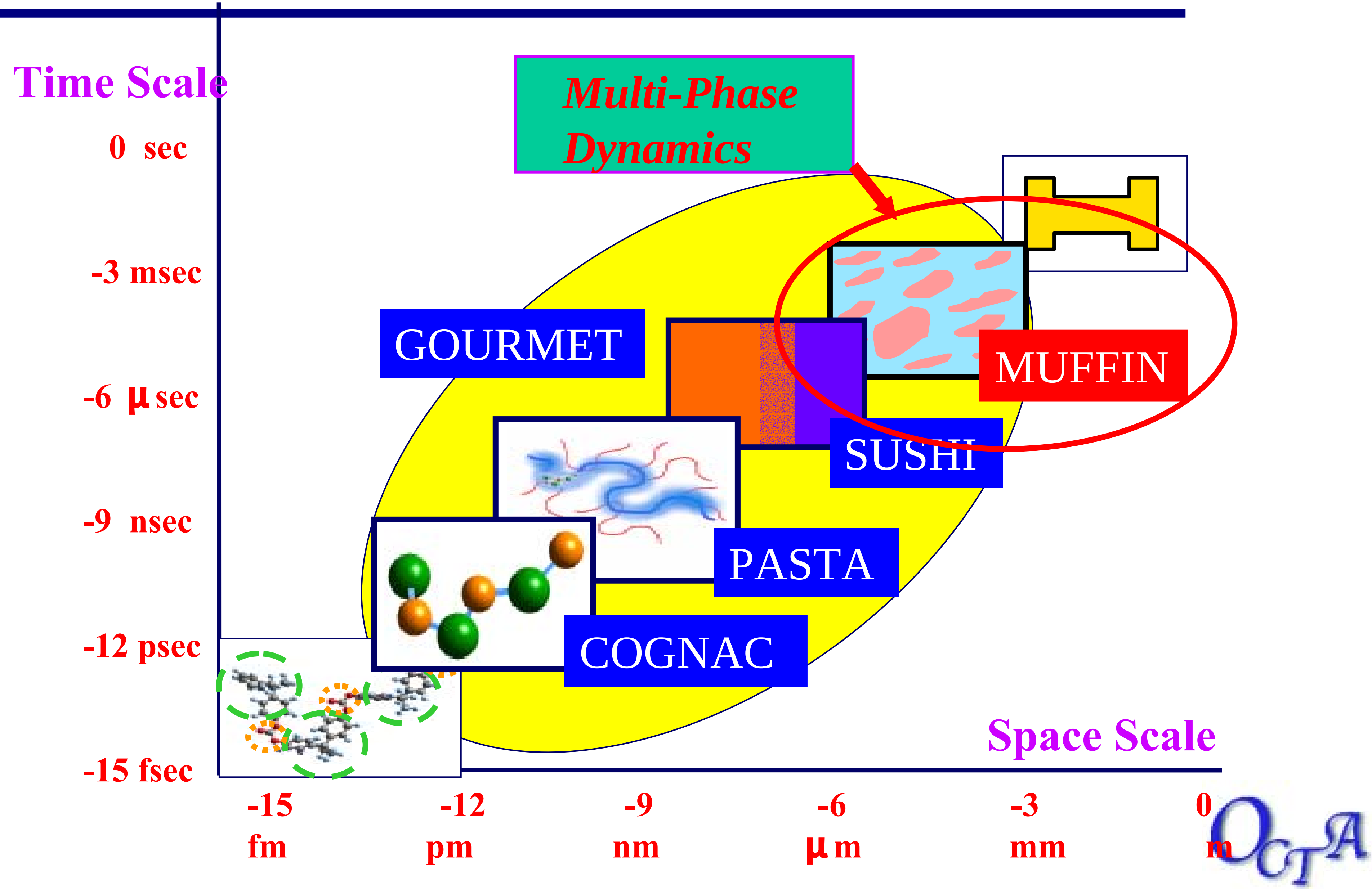
Nagoya Univ.
- **Takashi Taniguchi**

JCII, Doi project
- **Tatsuya Yamaue** (Japan Research Institute. Co.Ltd.)
- **Makoto Sasaki** (Japan Research Institute. Co.Ltd.)
- **Naoki Kobayashi** (Mitsui Chemical. Co.)
- **Masahiko Noda** (JSR. Co.)

Yamagata Univ.
- **Akiyoshi Kuroda**

Hiroshima Univ.
- **Toru Okuzono**

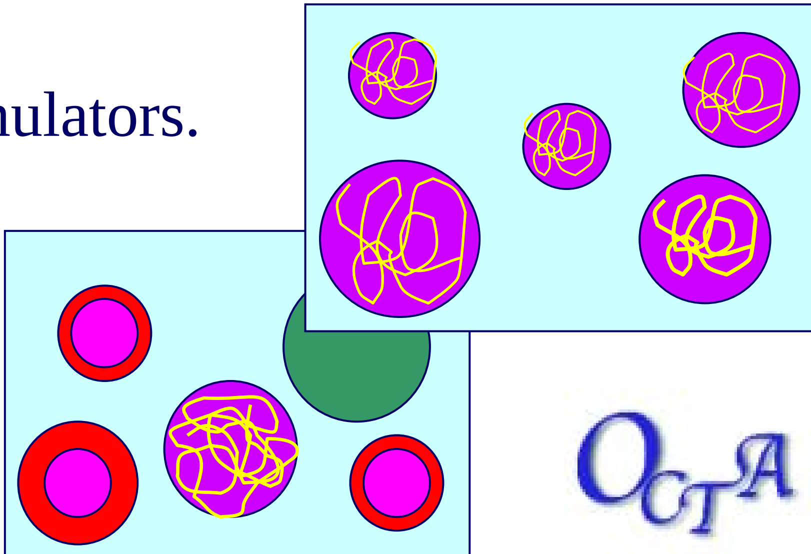
Time/Space Scales of MUFFIN



Scope of Problems handled by MUFFIN

Aim:Design and Control of Multi-Phase Structure of Polymeric Materials

- Dispersion structures.
  - Coagulation and breakup of droplets.
  - Effect of surface modification.
- Micro process control by pressure, shear, electric field, etc.
  - Micro fabrication of thin films
- Relation between stiffness and toughness, and morphology.
  - Deformation of elastic materials.
- Collaboration (zooming) with meso-simulators.
- Electrolyte fluid kinetics near eletrodes.
- Chemical reaction in narrow channels.
- Swelling and deswelling of gels.



Features of MUFFIN

Various Continuum models

◆ Various methods.

- Finite difference method (FDM) : Eulerian picture.
- Finite element method (FEM) : Eulerian and Lagrangian picture.

◆ Various Meshes.

- Structured mesh.
- Unstructured mesh (2D/3D). (Delaunay triangulation 2D/3D)

◆ Various Dynamics.

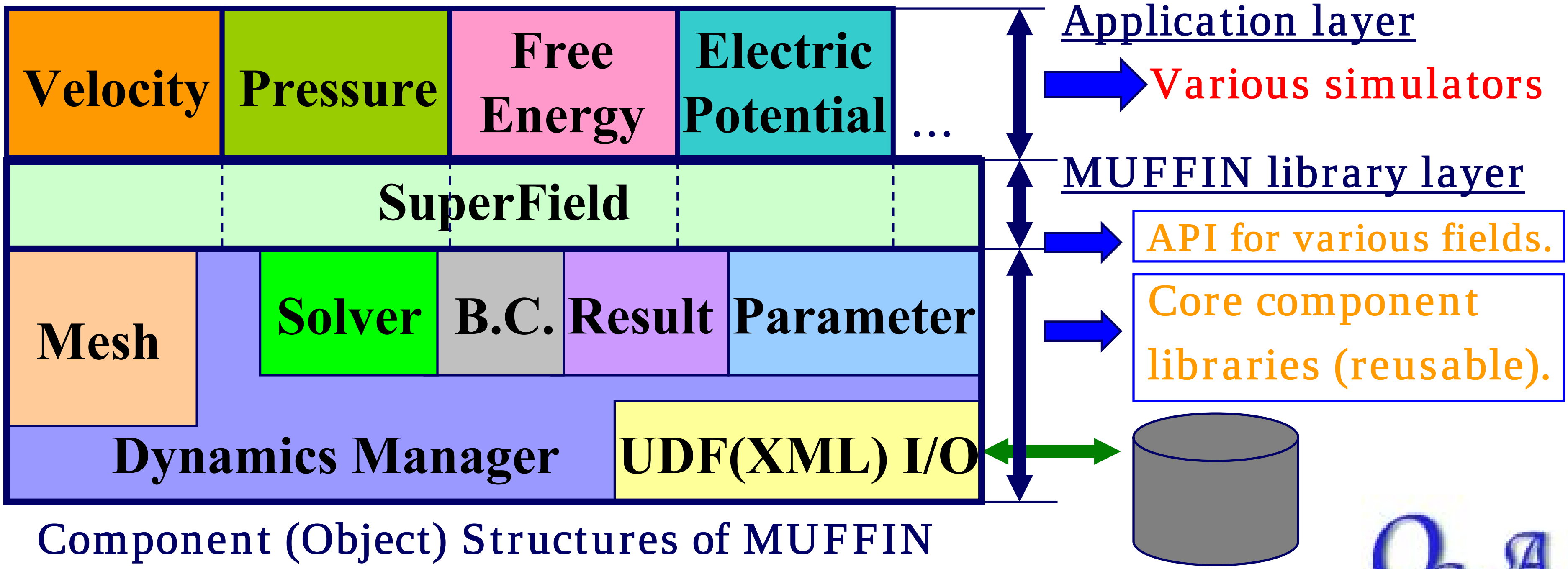
- Free energy : Flory-Huggins, Electro-Chemical, Elastic, Gels,….
- Velocity : Navier-Stokes, Stokes, Oseen, Two fluid model,…..
- Concentration : Diffusion and flow of polymer, solvent, counter ions,….
- Electric potential : Poisson, Poisson-Boltzmann, ….
- Pressure………
- Polymer Stress………
- …….

T.Yamaue
T.Taniguchi

Architecture of MUFFIN

Object-oriented designing for general multi-scale continuum fields simulation

- SuperField. (base object of physical fields)
  - Equip various methods for physical fields. Message passing between different fields.
- DynamicsManager.
  - Control I/O, construct dynamics and execute simulation for given schedule.



Velocity

Pressure

Free Energy

Electric Potential

…

SuperField

Mesh

Solver

B.C.

Result

Parameter

Dynamics Manager

UDF(XML) I/O

Application layer

Various simulators

MUFFIN library layer

API for various fields.

Core component libraries (reusable).

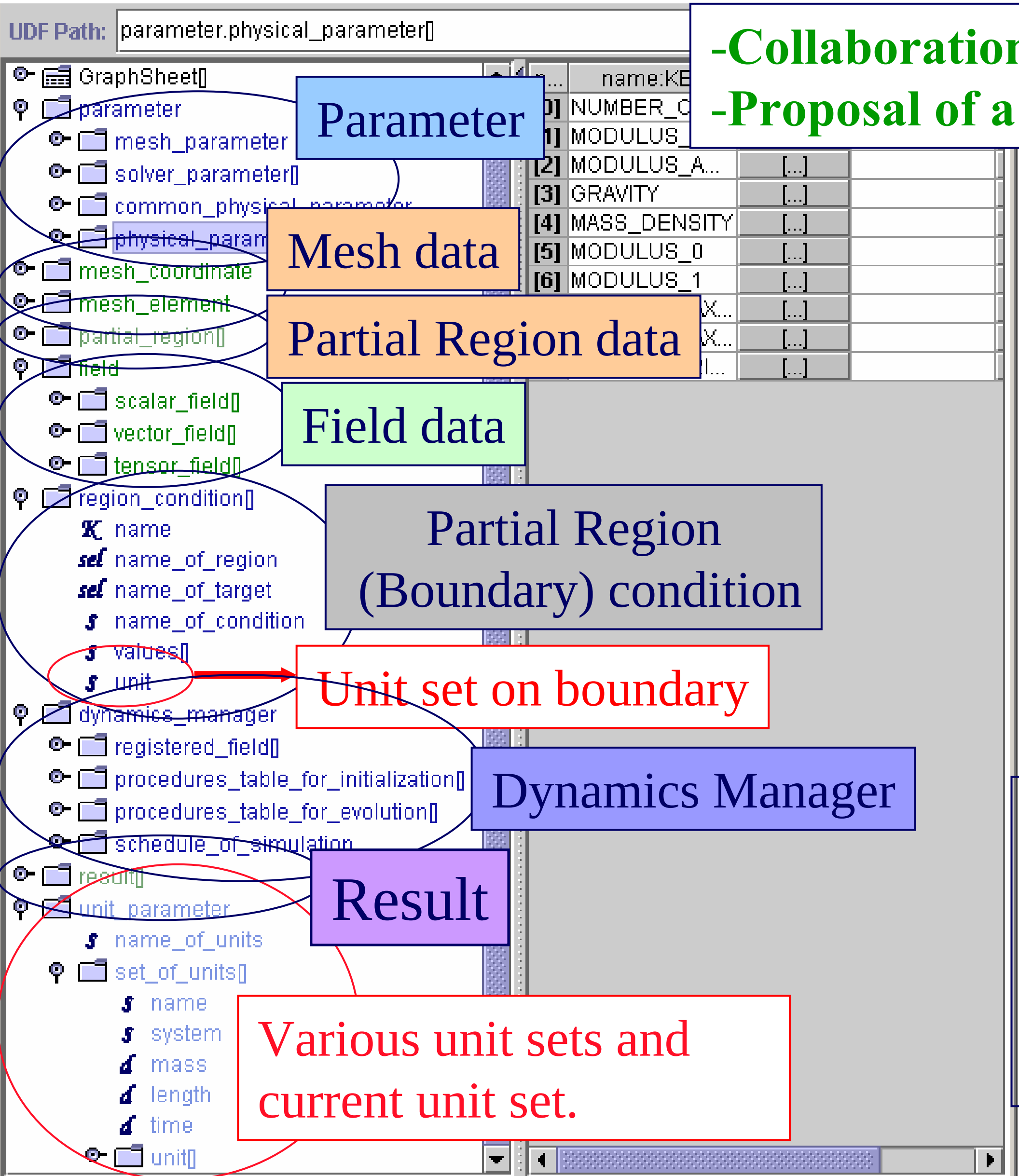
Component (Object) Structures of MUFFIN

- “MUFFIN” isn’t a name of simulator but a name of architecture. -

Structure of I/O data sheets of MUFFIN

T.Yamaue
T.Taniguchi

-Collaboration of different simulators.
-Proposal of a Front-end of multi-scale simulator.



UDF Path: parameter.physical_parameter[]

- GraphSheet[]
  - parameter
    - mesh_parameter
    - solver_parameter[]
    - common_physical_parameter
    - physical_param
  - mesh_coordinate
  - mesh_element
  - partial_region[]
  - field
    - scalar_field[]
    - vector_field[]
    - tensor_field[]
  - region_condition[]
    - name
    - name_of_region
    - name_of_target
    - name_of_condition
    - values[]
    - unit
  - dynamics_manager
    - registered_field[]
    - procedures_table_for_initialization[]
    - procedures_table_for_evolution[]
    - schedule_of_simulation
  - result[]
  - unit_parameter
    - name_of_units
    - set_of_units[]
      - name
      - system
      - mass
      - length
      - time
    - unit[]

n...	name:KE	
[0]	NUMBER_C	
[1]	MODULUS_	
[2]	MODULUS_A...	[...]
[3]	GRAVITY	[...]
[4]	MASS_DENSITY	[...]
[5]	MODULUS_0	[...]
[6]	MODULUS_1	[...]
	X...	[...]
	X...	[...]
	l...	[...]

Parameter

Mesh data

Partial Region data

Field data

Partial Region (Boundary) condition

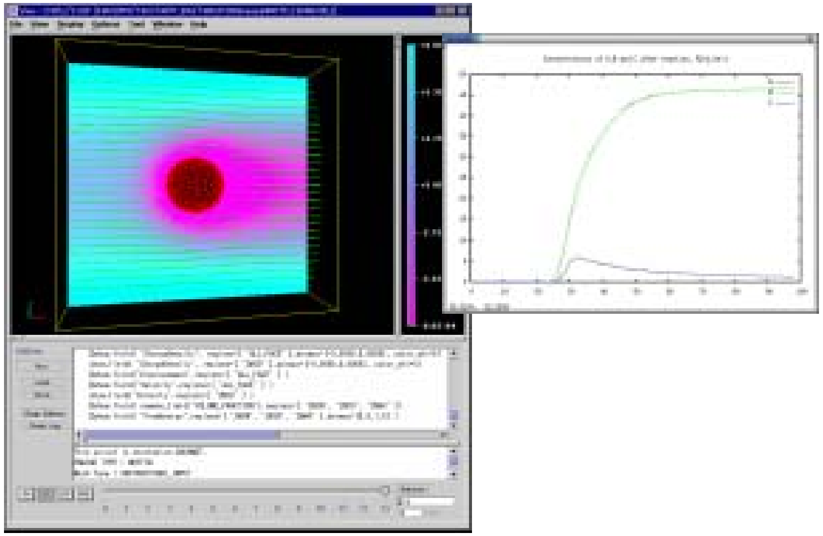
Unit set on boundary

Dynamics Manager

Result

Various unit sets and current unit set.

Visualization ***Plot***

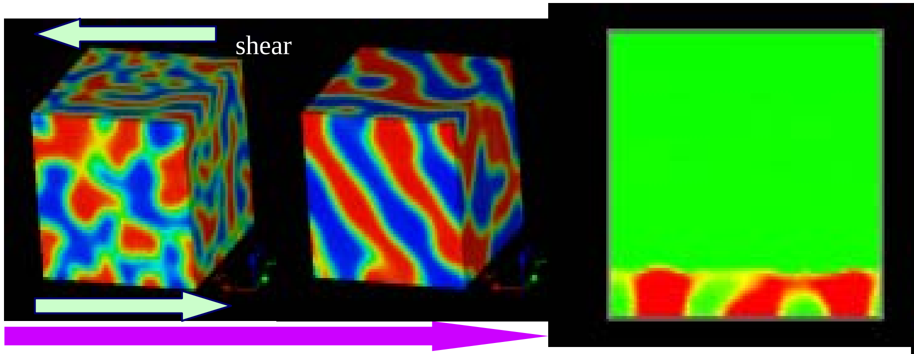


cf)
XSIL (XML Scientific Interchange)
Prof. R.Williams, CACR, Caltech.
(Center for Advanced Computing Research)

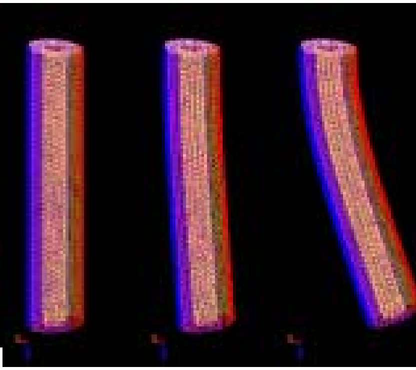
Simulation Packages of MUFFIN

Six simulation engines (three fluid simulators, two solid simulators and one optics simulator) are now on release.

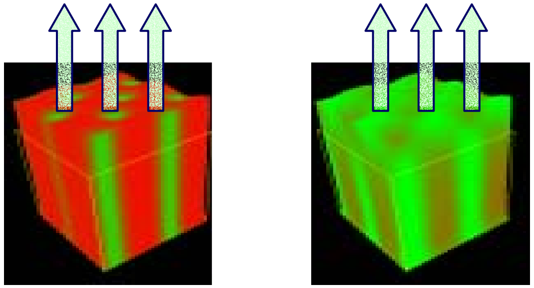
- *PhaseSeparation*
- *Electrolyte*
- *MEMFluid*
- *Elastica*
- *GelDyna*
- *TURBAN*



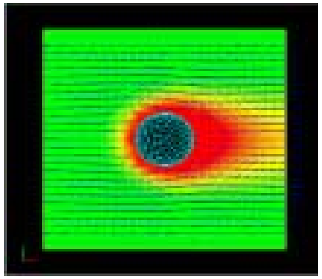
PhaseSeparation : The multi-phase dynamics simulator for polymeric fluids under the shear flow and the electric field with the hydrodynamic effect. (Fig. the phase separation dynamics of polymer blend under the shear (left), Spin coating simulation with evaporation under shear (right))



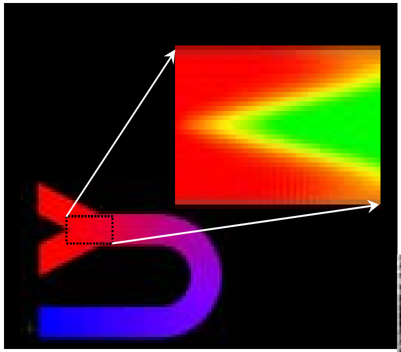
GelDyna : The large deformation dynamics simulator for multi-phase gel system by change of external stimuli, such as temperature, pH, and electric field, and external forces.



Elastica : The linear elasticity simulator for multi-phase solid system, including both isotropic and anisotropic elasticity. (Fig. the deformation (left) and strain-energy (right) of cylinder phase structure obtained by SUSHI under the external force.)



Electrolyte : The multi-component electrolyte fluid dynamics simulator under the shear flow and the electric field.



MEMFluid : The chemical reaction and extraction dynamics simulator for multi-component electrolyte fluids in the micro-fluidity chip.

TURBAN : The light transmittance simulator

Multi-Fluid Phase Dynamics Simulator "*PhaseSeparation*"

T.Taniguchi
M.Sasaki

The equations of PhaseSeparation

Basic model:

$$\frac{\partial \psi^{\alpha}}{\partial t} = -\nabla\cdot(\psi^{\alpha}\mathbf{v}) + \nabla\cdot(L_{\alpha}\nabla\mu_{\alpha})$$

$$\rho\frac{\partial \mathbf{v}}{\partial t} = -\nabla p + \nabla\left[\eta\left\{\nabla\mathbf{v} + (\nabla\mathbf{v})^{t}\right\}\right] + \mathbf{K}$$

$$\nabla\cdot\mathbf{v} = 0$$

●Flow: incompressible, slow flow (Stokes flow $\partial \mathbf{v} / \partial t = 0$)

●Chemical potential $\boldsymbol{\mu}_{\alpha}$, driving force **K** are derived from the functional of the free energy. L_{α} is the transport coefficient.

Examples of the free energy functional

- Flory-Huggins

$$F^{(FH)} = \frac{k_B T}{v_o} \int dV \Big[\sum_{\alpha=0}^{M-1} \frac{\psi_\alpha}{N_\alpha} \ln \psi_\alpha + \sum_{\alpha<\alpha'}^{M-1} \chi_{\alpha\alpha'} \psi_\alpha \psi_{\alpha'} + \frac{1}{2} \sum_{\alpha<\alpha'}^{M-1} C_{\alpha\alpha'}(\psi_\alpha, \psi_{\alpha'}) [\nabla(\psi_\alpha - \psi_{\alpha'})]^2 \Big]$$

- Multi component fluid under an electric field

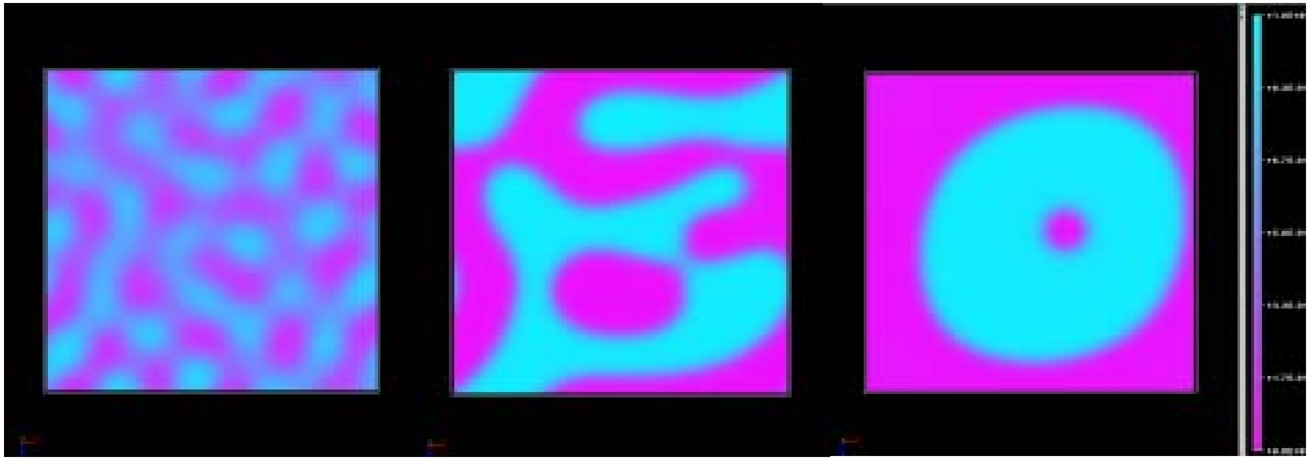
$$F = F_{mix} + \int dV \Big[-\frac{1}{2} \epsilon(\{\psi_\alpha\}, T) \boldsymbol{E}^2 + \frac{1}{2} \rho_e(\{\psi_\alpha\}) \Phi \Big]$$

$$\mu_\alpha^{(X)} = \mu_{\alpha mix}^{(X)} - \frac{1}{2}(\epsilon_\alpha - \epsilon_0) \boldsymbol{E}^2 + (\rho_{e\alpha} - \rho_{e0}) \Phi$$

$$\boldsymbol{K} = -\sum_{\alpha=1}^{M-1} \psi_\alpha \nabla \mu_\alpha$$

$$\nabla \cdot \Big[\epsilon(\boldsymbol{r}) \nabla \Phi \Big] = -\rho_e(\boldsymbol{r})$$

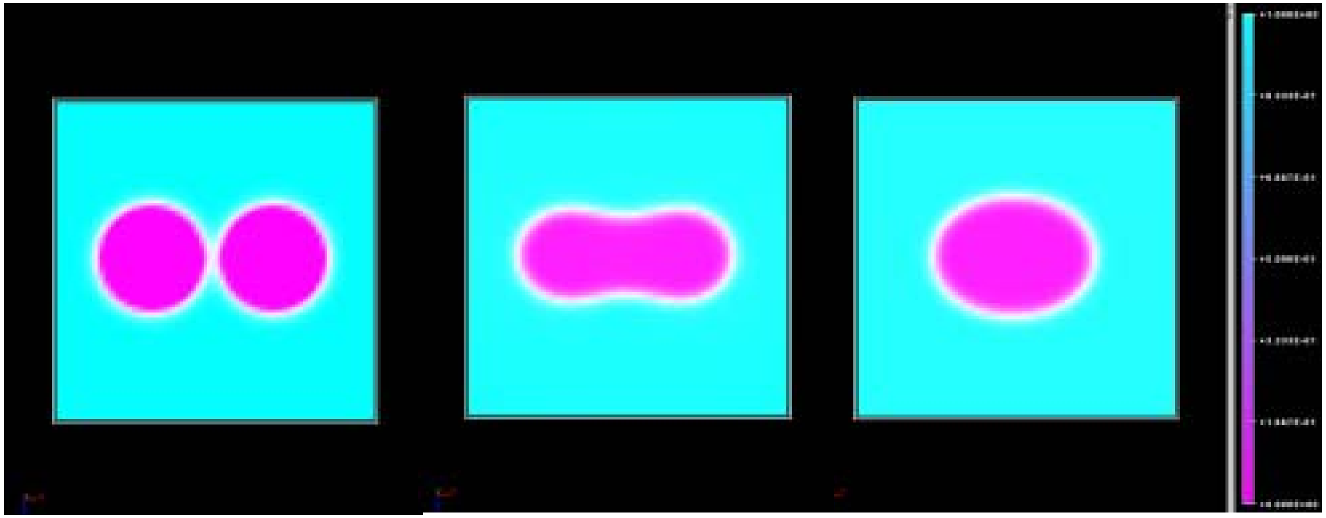
Applications of “PhaseSeparation FDM”



t=1 t=4 t=20

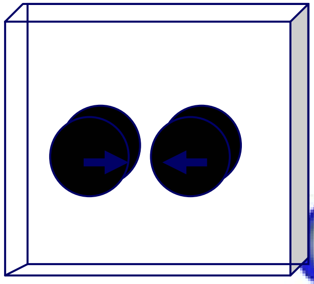
Phase separation with hydrodynamics effect.

- Flory-Huggins model. 2-dimensional, Periodic B.C.



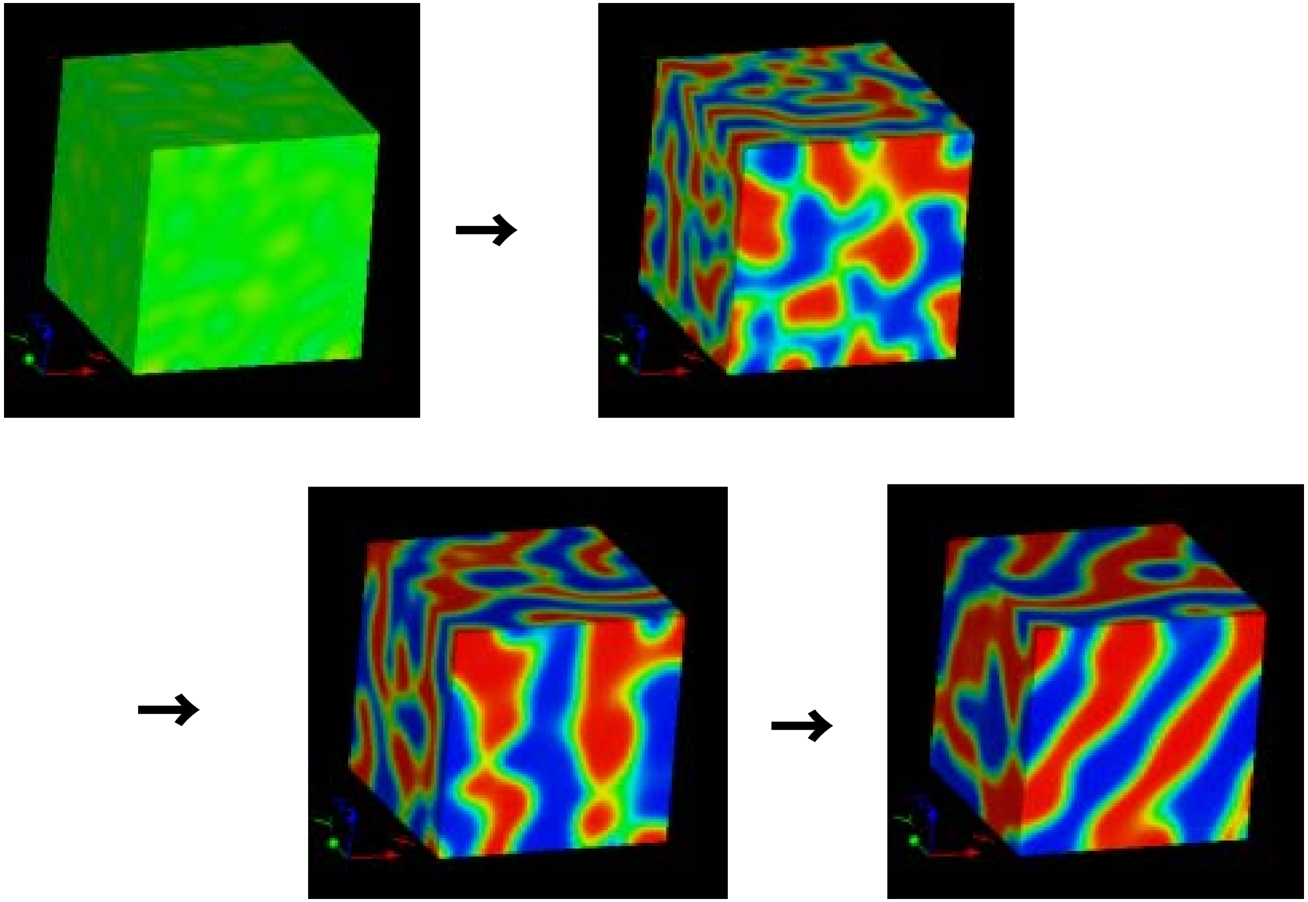
t=0 t=2 t=10

Coagulation of 2 droplets, 2-dimensional.



Application of “PhaseSeparation FDM”

Phase separation under shear



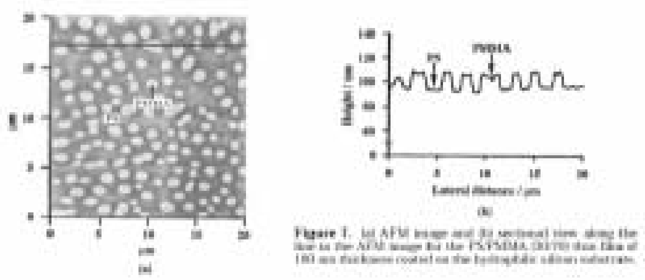
M.Noda

Simulation of Spin Coating
(An application of “PhaseSeparation FDM”)

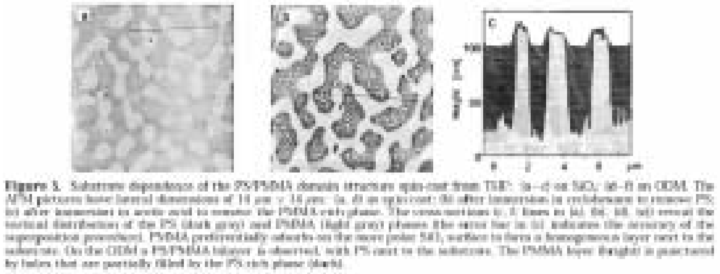
- Problems for spin coating
  - Surface roughness
  - Phase separated structure inside film

- Experimental approaches
  - Selectivity to the solvent
  - Adhesion to the substrate
  - Viscosity

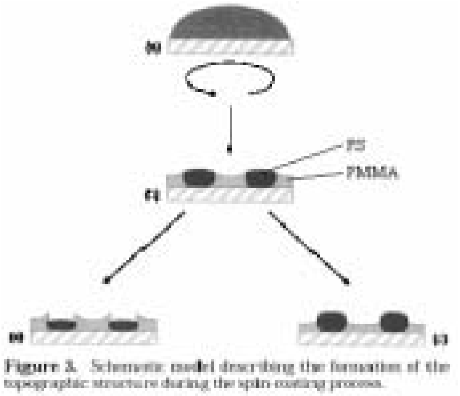
- Proposed models



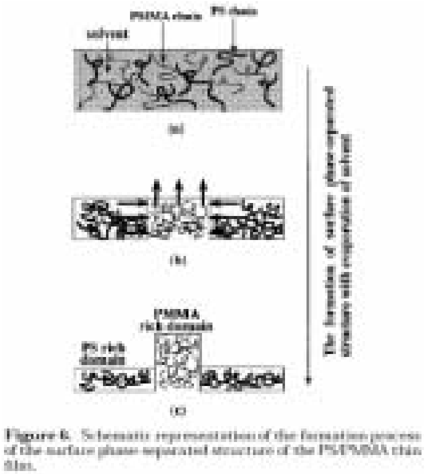
Macromolecules, 29, 3232 (1996)



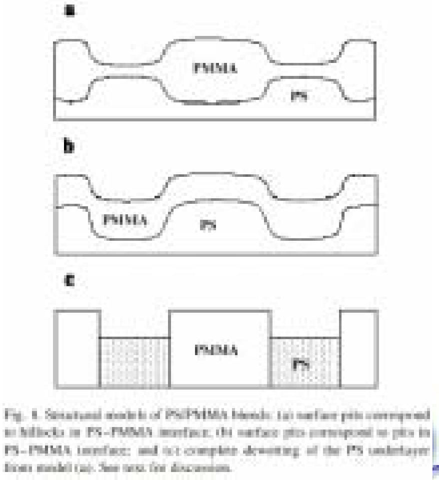
Macromolecules, 30, 4995 (1997)



Macromolecules, 30, 4995 (1997)



Macromolecules, 29, 3232 (1996)



Polymer, 42, 1121 (2001)

Spin Coating Simulation

- Evaporation of solvent
  - evaporation rate

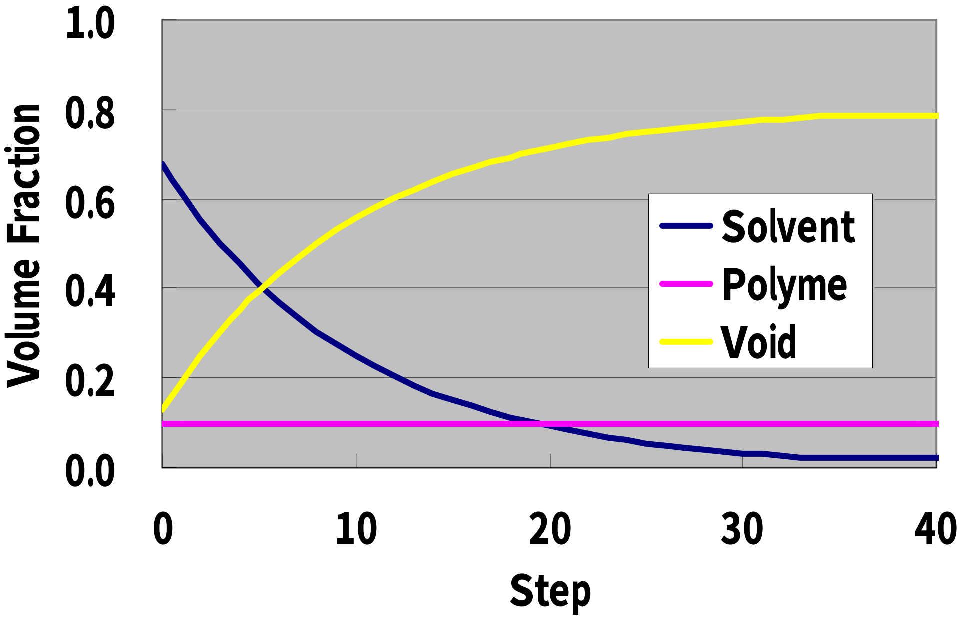
J. Electrochem. Soc., 138, 317 (1991)

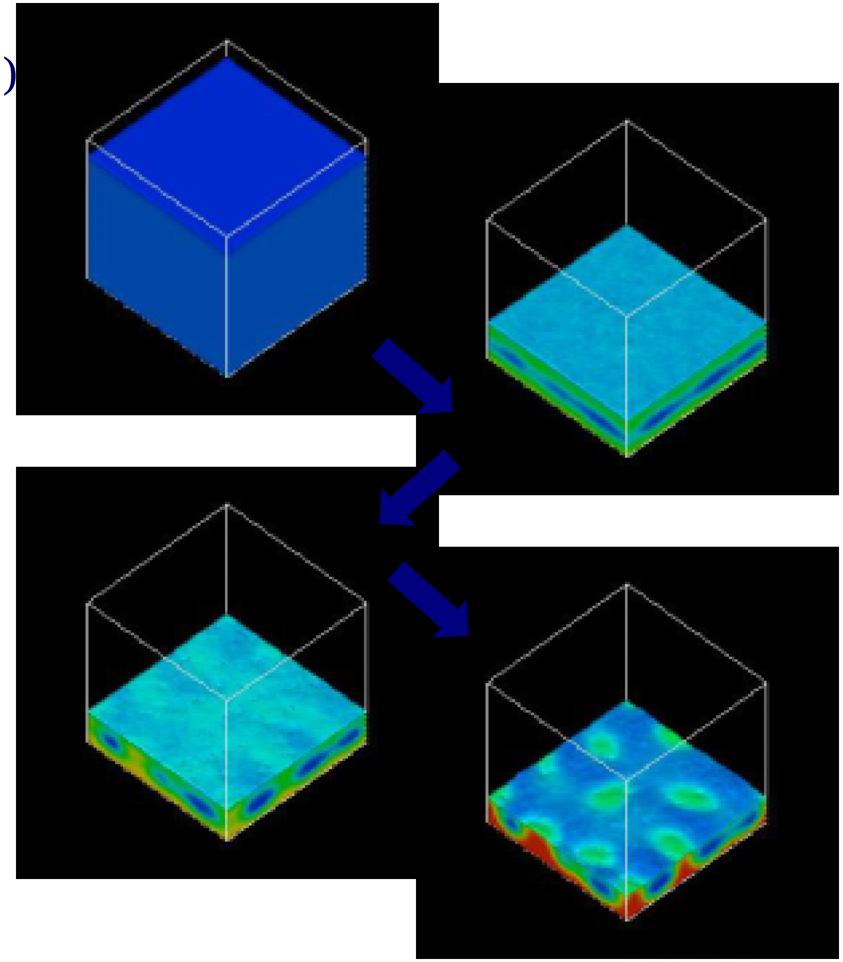
$$E = \kappa\left(x^{0}{}_{1} - x_{1\infty}\right)$$

κ: mass transfer coefficient

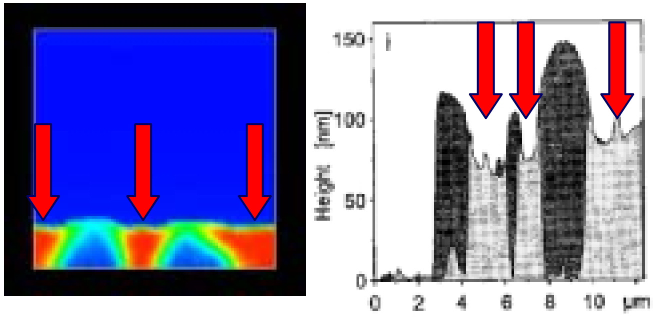
$x^{0}{}_{1}$: initial solv. fraction

$x_{1\infty}$: equilibrium solv. fraction

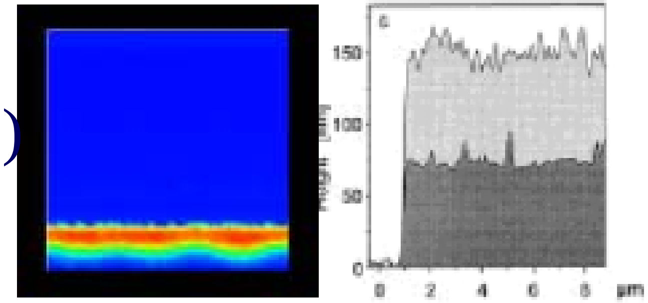




Spin Coating Simulation



- Solvent Selectivity (csolv-poly)
  - Poly1 / Poly2 / solvent (better for Poly1)
  - PMMA / PS / MEK (better for PMMA)



- Adhesion to the substrate (gS)
  - Poly1 / Poly2 /substrate (better for Poly2)
  - PMMA / PS / ODM (better for PS)

- Evaporation rate (E)
  - related to spinning rate

- Viscosity (h)
  - effect of hydrodynamic flow

Electrolyte Fluid Dynamics Simulator “*Electrolyte*”

T.Taniguchi
M.Sasaki

- Simulate ion kinetics in electrolyte solutions.
- 3-dimensional FDM and FEM simulators.
- Calculate the electro-kinetic phenomena such as electro-osmosis/electro-phoresis etc.)

The equations of Electrolyte

- Time evolution of ion density

$$\frac{\partial C_\alpha}{\partial t} = -\nabla \cdot (\boldsymbol{v} C_\alpha) - \nabla \cdot \boldsymbol{J}_\alpha.$$

$$\boldsymbol{J}_\alpha \equiv -L_\alpha \Big[\, k_B T \nabla C_\alpha + e Z_\alpha C_\alpha \nabla \Phi \,\Big].$$

- Flow field

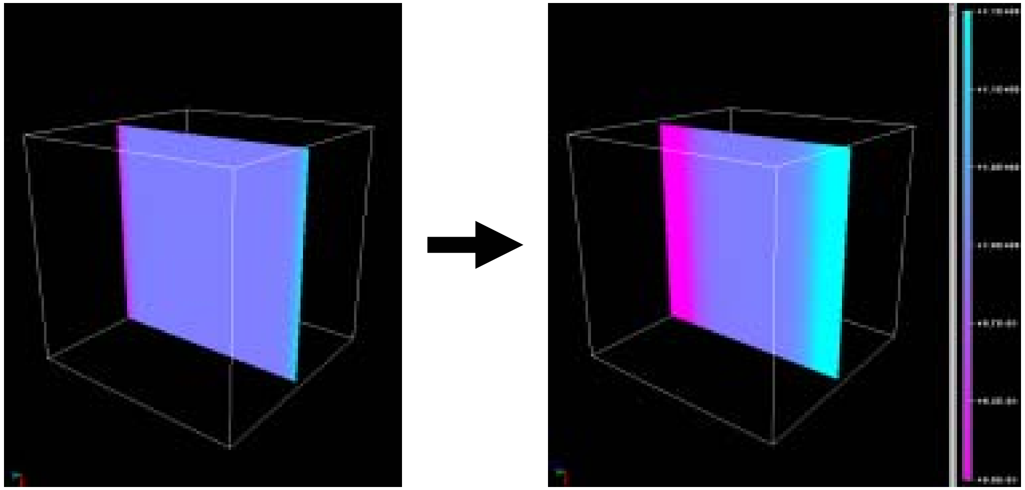
$$K = -\sum_{\alpha=0}^{N_c-1} \Big[\, k_B T \nabla C_\alpha + e Z_\alpha C_\alpha \nabla \Phi \,\Big].$$

$$-\nabla p + \eta_w \Delta \boldsymbol{v} + \boldsymbol{K} = 0$$

- Electric field

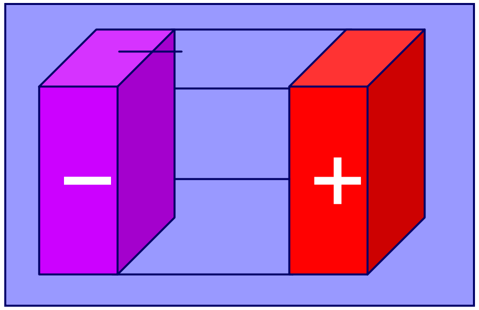
$$\Delta \Phi = -\frac{1}{\epsilon_0 \epsilon_r} \sum_\alpha e Z_\alpha C_\alpha.$$

Applications of “Electrolyte FDM”

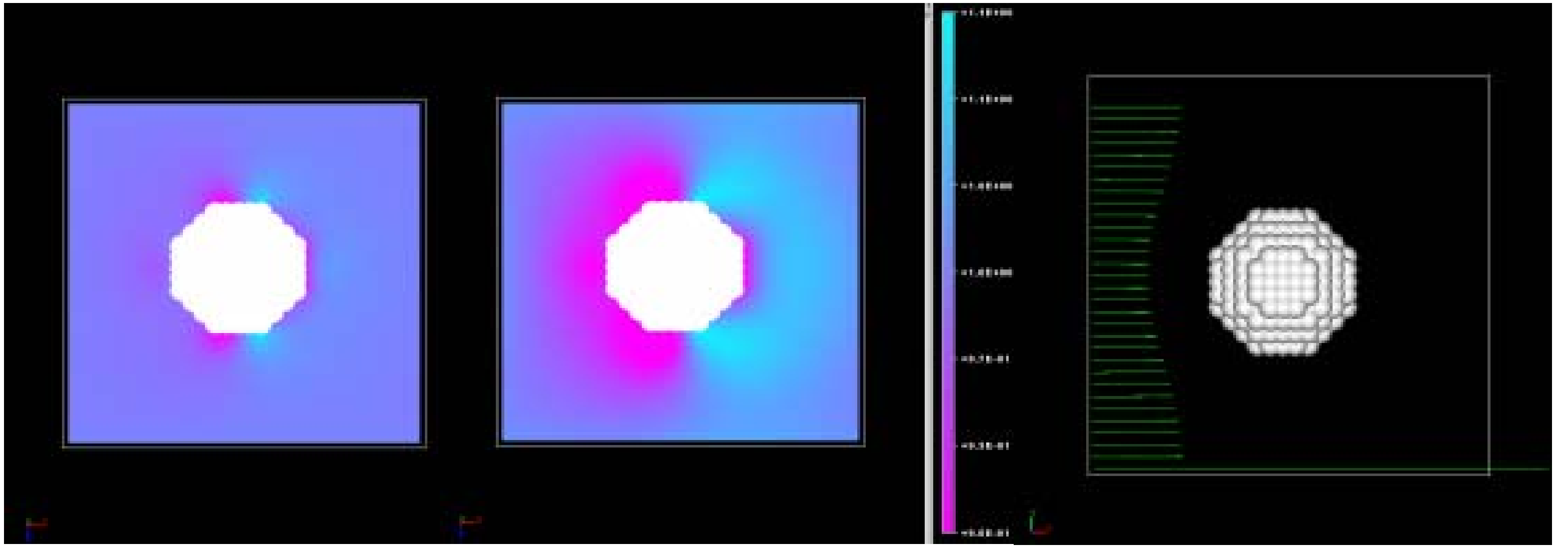


t=1 t=10

Ion density distribution



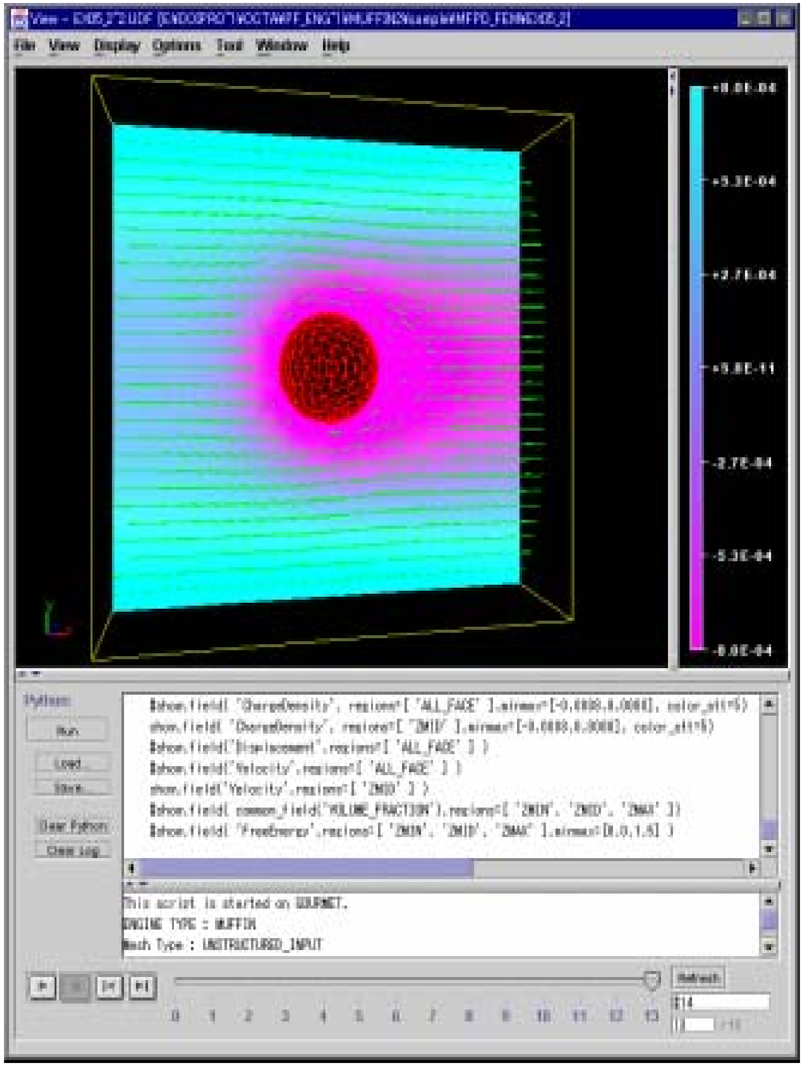
Ion distribution between electrodes under electric field



t=1 t=10 Velocity (on wall)

Flow of electrolyte around a charged particle.

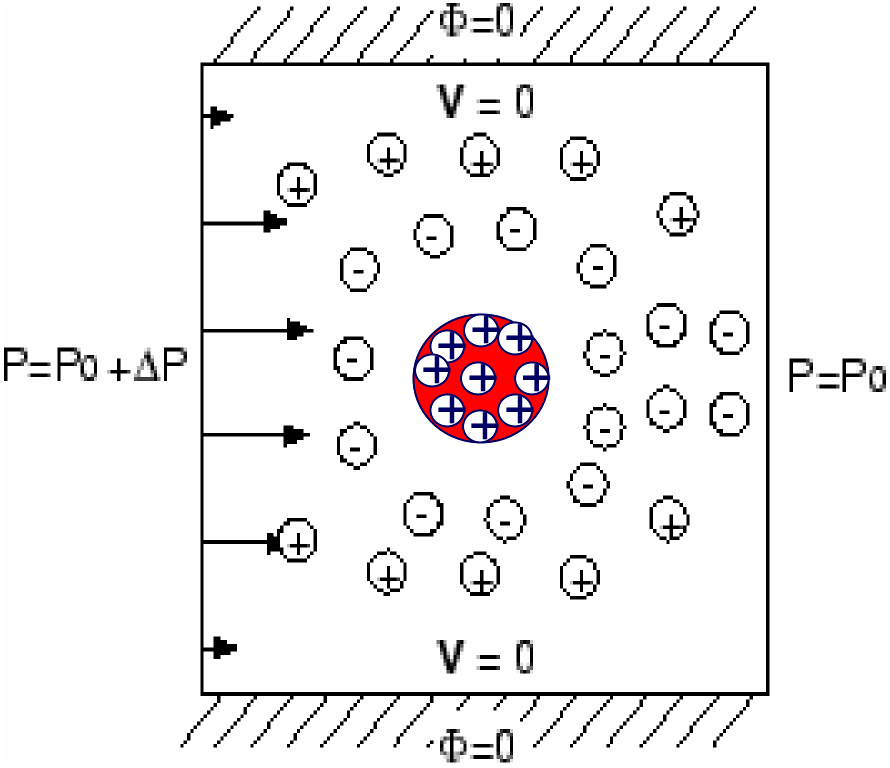
Application of “Electrolyte FEM”



```
#show.field( 'ChargeDensity', region=[ 'ALL_FACE' ],minmax=[-0.0008,0.0008], color_st=5)
show.field( 'ChargeDensity', region=[ 'ZMID' ],minmax=[-0.0008,0.0008], color_st=5)
#show.field('Displacement',region=[ 'ALL_FACE' ] )
#show.field('Velocity',region=[ 'ALL_FACE' ] )
show.field('Velocity',region=[ 'ZMID' ] )
#show.field( common_field('VOLUME_FRACTION'),region=[ 'ZMIN', 'ZMID', 'ZMAX' ])
#show.field( 'FreeEnergy',region=[ 'ZMIN', 'ZMID', 'ZMAX' ],minmax=[0.0,1.5] )
```

```
This script is started on GOURMET.
ENGINE TYPE : MUFFIN
Mesh Type : UNSTRUCTURED_INPUT
```

Ion distribution around a charged sphere moving in an electrolyte solution

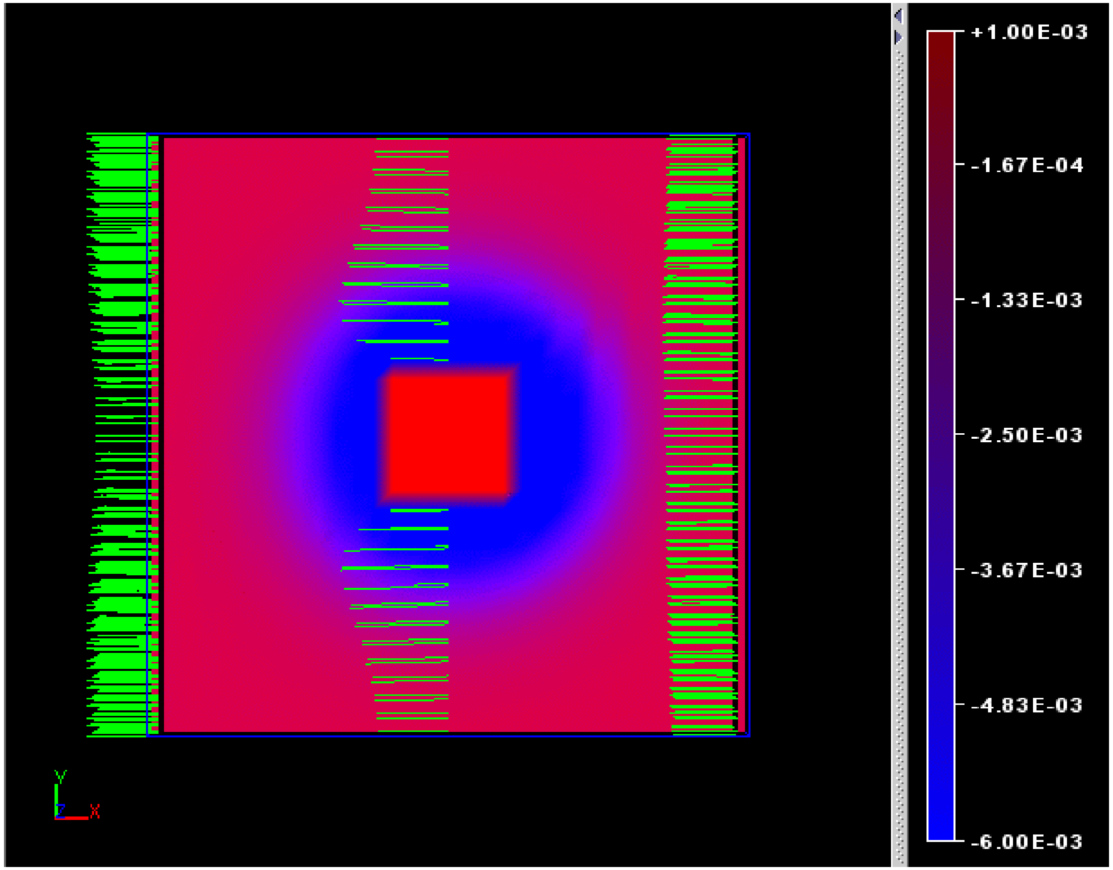


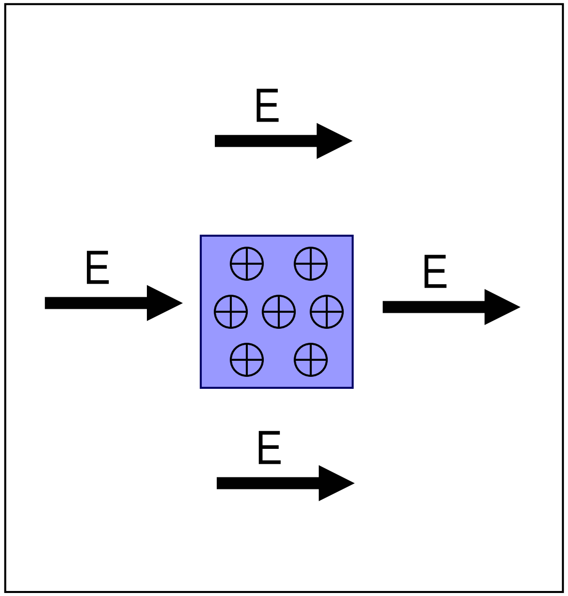
(3-dimensional Delaunay mesh)

Application of “Electrolyte FEM” : Electro osmosis and Electrophoresis

Electrolyte flow induced by electric field around a charged particle

(simulation of electro-osmosis or electro-phoresis)





T.Yamaue

Micro Fluidics Chip Simulator "*MEMFluid*"

Equations of motion.

Concentration of ions : (diffusion and reaction)

$$\frac{\partial C_\alpha}{\partial t} = -\nabla\cdot(\mathbf{v}C_\alpha) - \nabla\cdot\mathbf{j}_\alpha + \sum_{\beta} R1_{\alpha\beta}C_\beta + \sum_{\beta,\gamma} R2_{\alpha\beta\gamma}C_\beta C_\gamma$$

Flux density of ions :

$$\mathbf{j}_\alpha = -L_\alpha\left[k_BT\left\{\nabla C_\alpha + \sum_{\beta}\chi_{\alpha\beta}C_\alpha\nabla C_\beta\right\} + eZ_\alpha C_\alpha(\nabla\Phi - \mathbf{E}_0)\right]$$

Oseen equation : (laminar flow)

$$0 = -\nabla p + \nabla\left[\eta_w\left\{\nabla\mathbf{v} + (\nabla\mathbf{v})^t\right\}\right] + \mathbf{K} \qquad (\nabla\cdot\mathbf{v} = 0)$$

Volume force :

$$\mathbf{K} = -\sum_{\alpha} k_BT\left\{\nabla C_\alpha + \sum_{\beta}\chi_{\alpha\beta}C_\alpha\nabla C_\beta\right\}$$

Laplace equation :

$$\nabla^2\Phi = 0$$

In Bulk (charge neutrality)

C_α : **α**-ion concentration

$\mathbf{j}_\alpha$: Flux density of α-ion

L_α : Mobility of **α**-ion

Z_α : Charge of **α**-ion

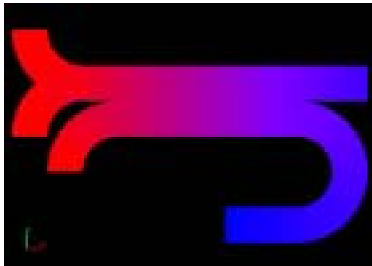
$\chi_{\alpha\beta}$: Interaction parameter between **α**-ion and **β**-ion

Φ : Electric potential

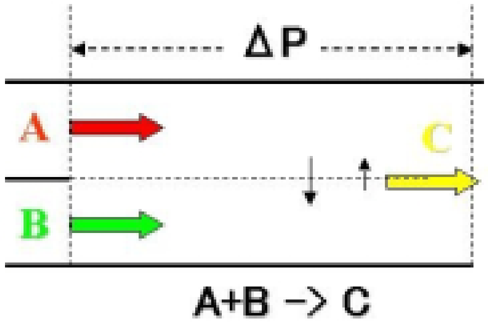
$\mathbf{E}_0$: External electric field

Applications.

- MEMS (Micro Electro Mechanical System), Lab-on-a chip.
- Micro reactor, **μ**TAS (Total Analysis System), Bio chips.

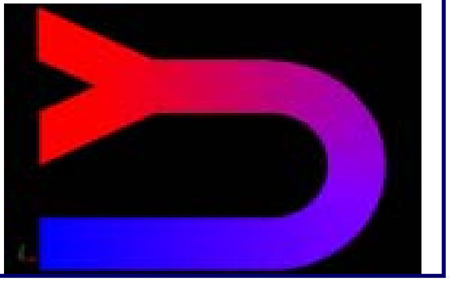


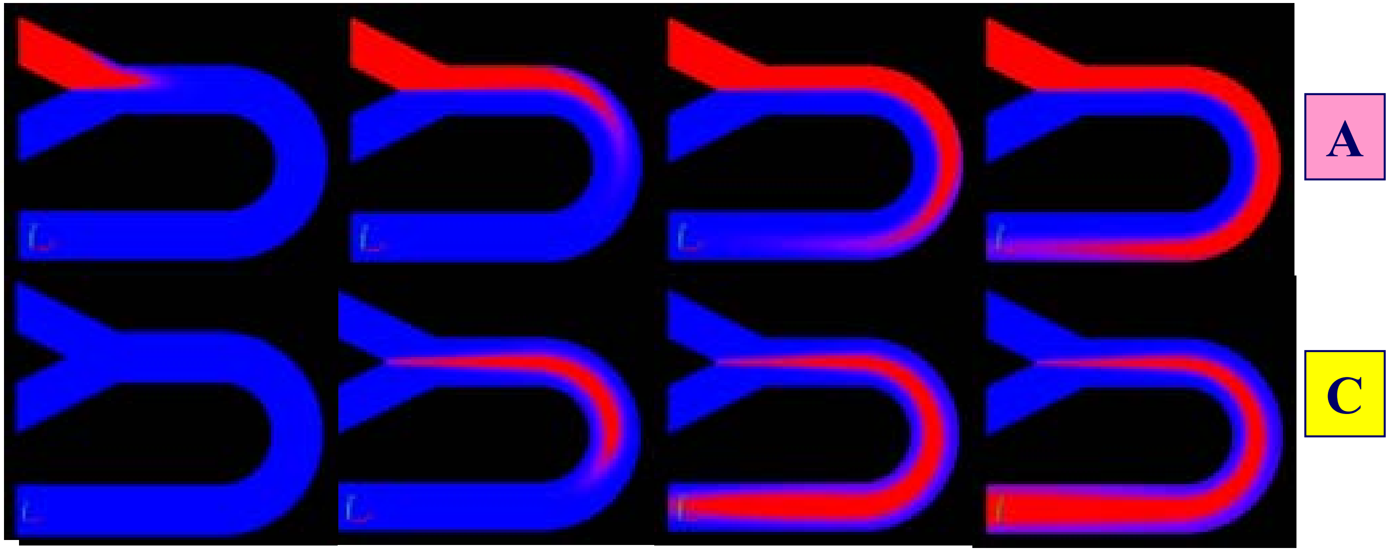
Application of “MEMFluid”:Y-shaped micro-reactor



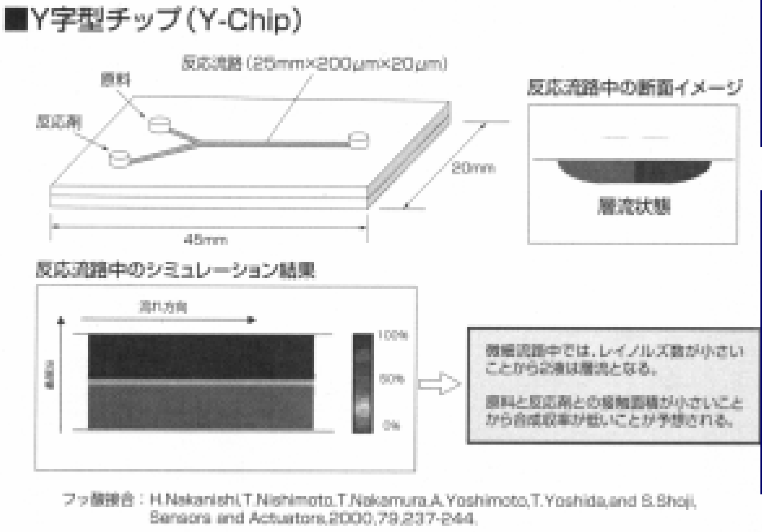
A+B -> C

Pressure field





40sec 60sec 80sec 100sec



■Y字型チップ（Y-Chip）

反応流路中のシミュレーション結果

微細流路中では、レイノルズ数が小さいことから2液は層流となる。

原料と反応剤との接触面積が小さいことから合成収率が低いことが予想される。

フッ酸接合：H.Nakanishi,T.Nishimoto,T.Nakamura,A.Yoshimoto,T.Yoshida,and S.Shoji, Sensors and Actuators,2000,79,237-244.

16cases:

ΔP=1.0,2.5,5.0,10.0

R2=1e-3,1e-2,1e-1,1.0

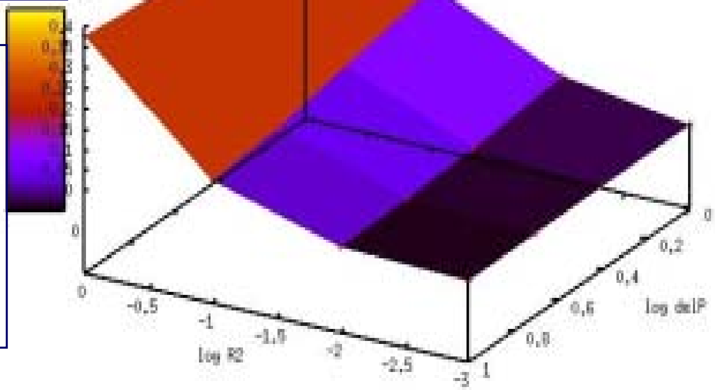
Results:

For increase Pc.

R2 > 0.4: ΔP->10.0

R2 < 0.4: ΔP->1.0

Productivity (Pc) of C-ion vs logR2 and logΔP



Application of “MEMFluid” :Electro-osmotic chip

Velocity on boundary is determined by electro-kinetics

◆ Velocity at the boundary :

$$\mathbf{v}_{eo} = \frac{\varepsilon}{\eta_w}\varsigma\mathbf{E}$$

Helmholtz-Smouluchowski eq.

◆ Calculation of **ζ** -potential on boundary:

- 1-dim Poisson-Boltzmann eq. (1-1 electrolyte)

$$\varsigma = \frac{2k_BT}{Ze}\ln\left[\frac{\sigma}{(8C\varepsilon k_BT)^{1/2}} + \left(\frac{\sigma^2}{8C\varepsilon k_BT} + 1\right)^{1/2}\right]$$

- Condenser model (linear approximation)

valid for $Ze|\varsigma|/k_BT << 1 \quad \varsigma \leq 25(mV)$

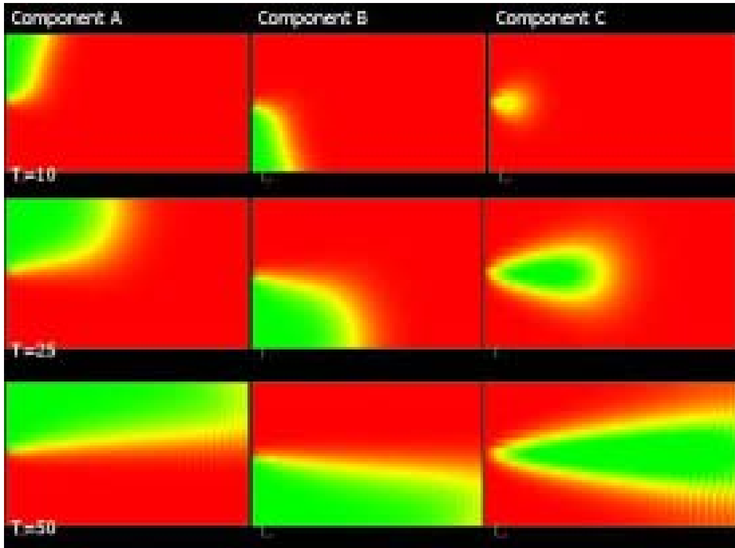
$$\begin{cases} \varsigma = \dfrac{\sigma}{\varepsilon\kappa} \\ \kappa = \left(\dfrac{\sum_\alpha Z_\alpha^2 C_\alpha e^2}{\varepsilon k_BT}\right)^{1/2} \end{cases}$$

Scaling factor: Bejurem length/System size :

$$l_b/l = e^2/(k_BT\varepsilon l) \approx 10^{-3} - 10^{-2}$$

Simulation result:

ΔP=10.0, R2=1.0



Multi-Phase Linear Elasticity Simulator “*Elastica*”

M.Sasaki

- **Basic model：linear elasticity, 3-dimensional FEM**

$$F\{u_i(\mathbf{x})\} = \int_V d^d x\{f\} - \int_V d^d x\rho(\mathbf{x}) g_i u_i(\mathbf{x}) - \int_{St} d^{d-1} x T_i u_i(\mathbf{x})$$

  - **isotropic elastic material**

$$f = G(\mathbf{x})\left(e_{ij} - \frac{1}{d}\delta_{ij} e_{ll}\right)^2 + \frac{K(\mathbf{x})}{2}(e_{ll})^2$$

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_j}\right)$$

  - **anisotropic elastic material (axissymmetric)**

$$f = D_1(e_{ii})^2 + D_2(n_i n_j e_{ij})^2 + D_3(e_{ll}\cdot n_i n_j e_{ij}) + D_4 n_l e_{il}\cdot n_k e_{ik} + D_5 e_{ij} e_{ij}$$

- **Arbitrary mixture and morphology of isotropic/anisotropic materials.**

Stiffness Matrix for Anisotropic elasticity (axissymmetric)

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} n & l & l & 0 & 0 & 0 \\ l & k+m & k-m & 0 & 0 & 0 \\ l & k-m & k+m & 0 & 0 & 0 \\ 0 & 0 & 0 & m & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{bmatrix}$$

$$f = D_1 (e_{ii})^2 + D_2 (n_i n_j e_{ij})^2 + D_3 (e_{ll} \cdot n_i n_j e_{ij}) + D_4 n_l e_{il} \cdot n_k e_{ik} + D_5 e_{ij} e_{ij}$$

$$\begin{cases} D_1 = (k-m)/2 \\ D_2 = (n+k-m)/2 - l - \mu \\ D_3 = l - k + m \\ D_4 = \mu - m \\ D_5 = m \end{cases}$$

Application of “Elastica” : Elasticity of the two phase structure calculated by SUSHI.

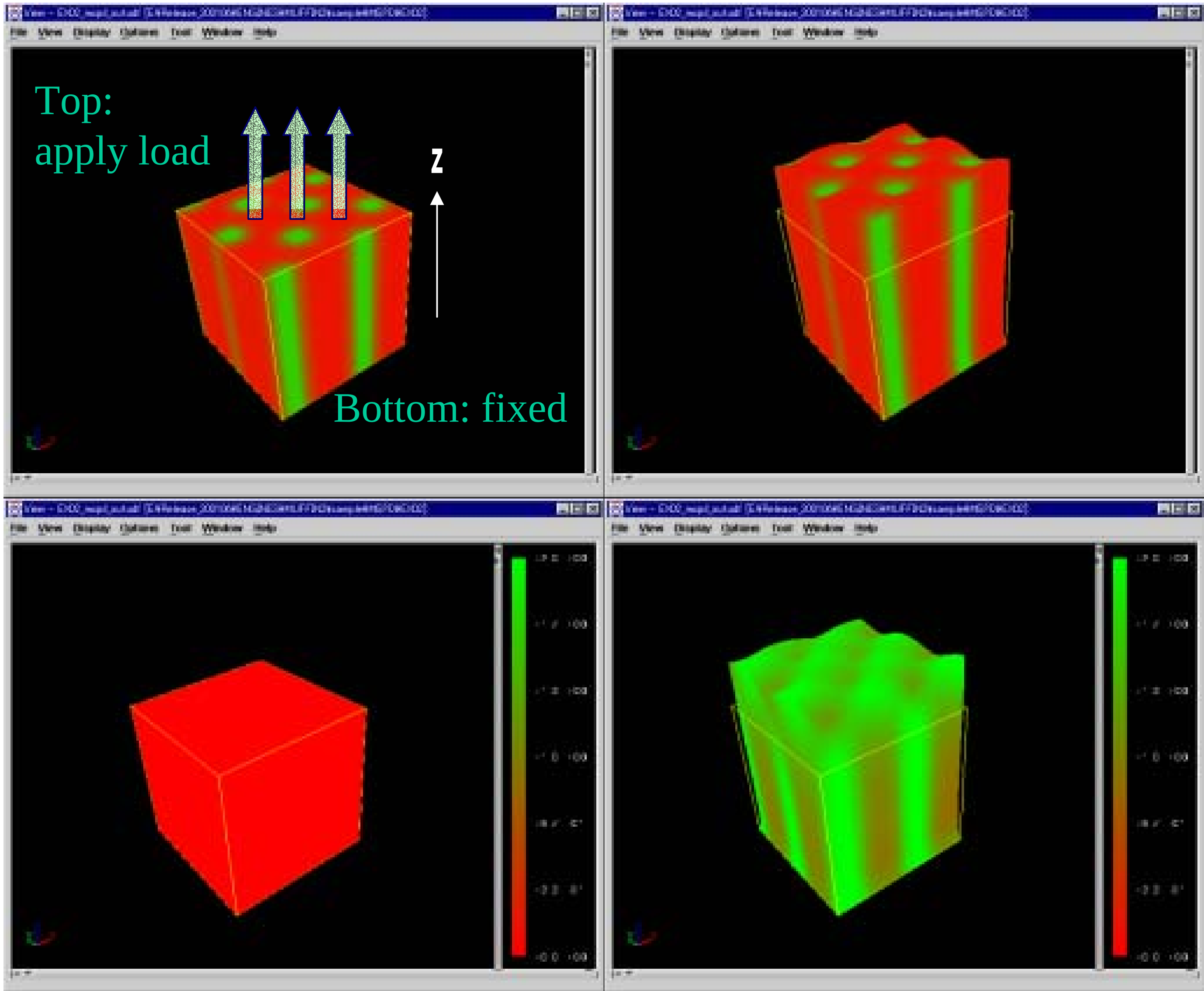
T.Yamaue
M.Sasaki

【Before deformation】 【after deformation】

【Volume fraction】

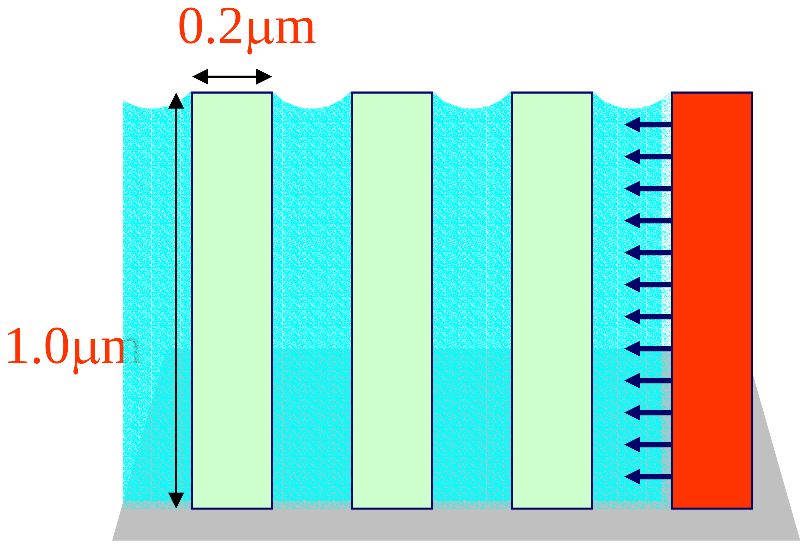
- component1(green)
  z：hard, x,y ：soft
- component2 (red)
  x,y：hard, z ：soft

【Strain energy】



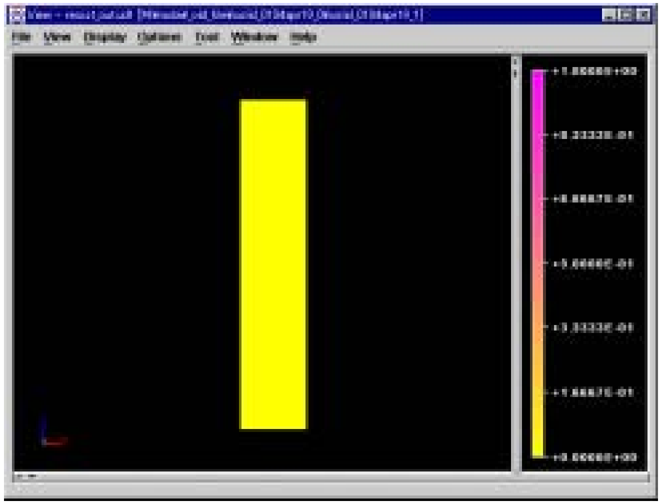
Application of “Elastica”: Deformation of photo regist pattern by capillary force

M.Noda
M.Sasaki

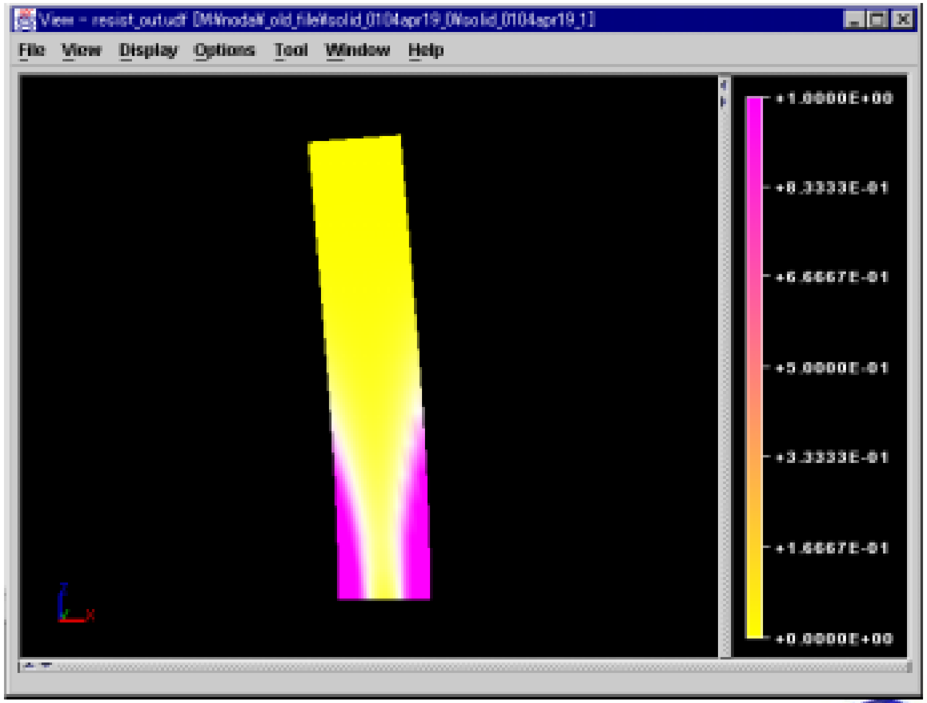


negative pressure induced by the capillary force

【before deformation】



【after deformation】 Strain energy



Application of “Elastica”:Effective modulus of two phase system for various morphology

M.Noda
M.Sasaki

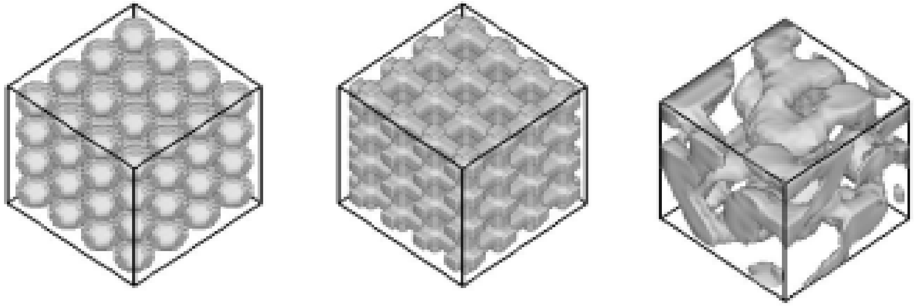
Total free energy and effective modulus

$$F = \overline{G}\sum\left\{\left(e_{ij} - \frac{1}{d}\delta_{ij}e_{ll}\right)^2\right\} + \overline{K}\sum\left(\frac{1}{2}e_{kk}{}^2\right)$$

Effective modulus is calculated by independent deformation modes

$$\overline{K} = -\frac{\sum\left\{\left(e_{ij} - \frac{1}{d}\delta_{ij}e_{ll}\right)^2\right\}}{\sum\left(\frac{1}{2}e_{kk}{}^2\right)}\overline{G} + \frac{F}{\sum\left(\frac{1}{2}e_{kk}{}^2\right)}$$

Morphology (PP + Elastomer)



(a)dispersed (b)bi-continuous (C) by SUSHI

Calculated Young’s modulus

modulus	$\overline{E}$	analytic-model
sphere	3.753	series
bi-continuous	34.67	Davies
sushi1	91.84	
sushi2	50.99	

sushi2: volume fraction is reset to 0 and 1 using a threshold value.

T.Yamaue

Gel and Elasticity Dynamics Simulator
“*GelDyna*”

Equations of motion. (Stress-Diffusion Coupling Model for Gels)

Velocity of polymer : $\varsigma(\mathbf{v}_p - \mathbf{v}_s) = -\phi\nabla \cdot p + \nabla \cdot \underline{\underline{\boldsymbol{\sigma}}}$

Velocity of solvent : $\varsigma(\mathbf{v}_s - \mathbf{v}_p) = -(1-\phi)\nabla \cdot p$

incompressibility : $\nabla \cdot [\phi \mathbf{v}_p + (1-\phi)\mathbf{v}_s] = 0$

$\mathbf{v}_p$:velocity of polymer

$\mathbf{v}_s$:velocity of solvent

ϕ : volume fraction of polymer

p :pressure

ς :friction coefficient

$\underline{\underline{\boldsymbol{\sigma}}}$: Cauchy stress tensor of polymer

Free energy of Gels.

$$F = \frac{k_B T}{v_1}\int d^d x[(1-\phi)\ln(1-\phi) + \chi\phi(1-\phi) + \frac{1}{2}\nu_0\frac{\phi}{\phi_0}(tr\,\underline{\underline{\mathbf{W}}} + 2\ln\frac{\phi}{\phi_0})]$$

Stress of polymer networks

$$\sigma_{ij} = -[\phi f_m'(\phi) - f_m(\phi)]\delta_{ij} + \nu_0\frac{\phi}{\phi_0}(W_{ij} - \delta_{ij})$$

mixing free energy (Flory-Huggins): $f_m(\phi) = (1-\phi)\ln(1-\phi) + \chi\phi(1-\phi)$

W_{ij} : finger strain tensor

ϕ_0: volume fraction of polymer in the relaxed state

χ : polymer-solvent interaction

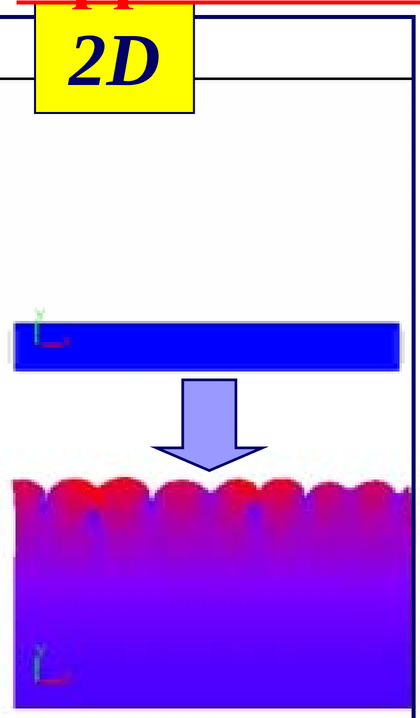
ν_0 : crosslink number density in the relaxed state

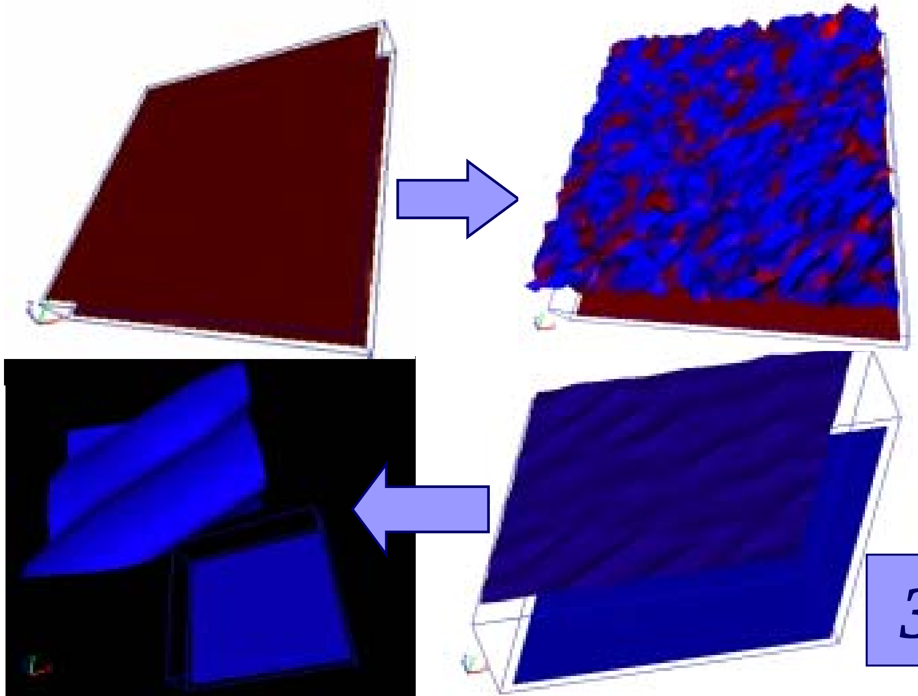
Applications of “GelDyna”

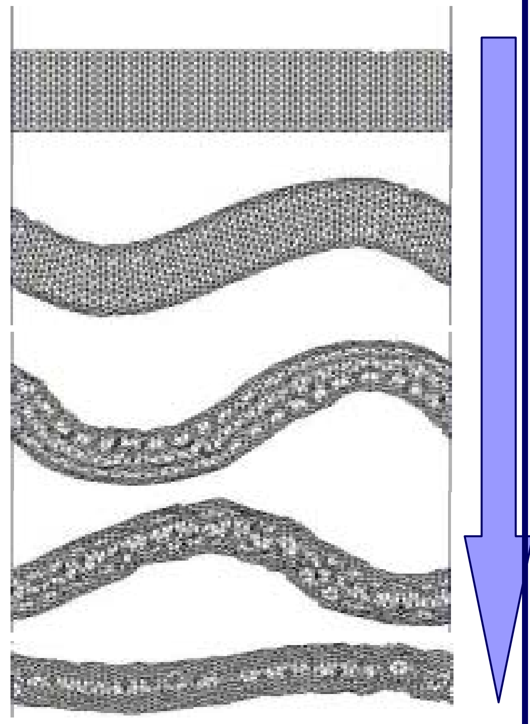
Applications.

- Super-water absorbing gels
- Temperature sensitive gels.
- Drug delivery systems (DDS)
- Actuators, sensors and switching devices.

Applications to swelling of NIPA gels.






Bending of gels in rapid deswelling process

Light Transmittance Simulator
“*TURBAN*”

N.Kobayashi

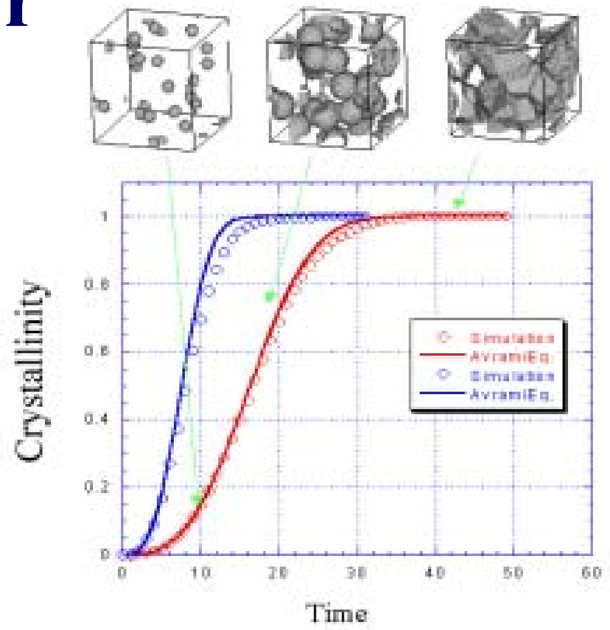
=TURBidity ANalyzer

“TURBAN” predicts the transparency of polymeric material having spherulite structures.

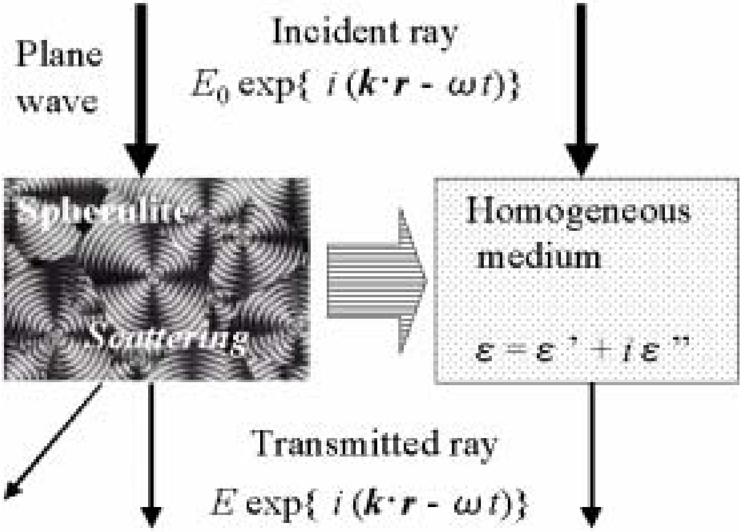
“TURBAN” consists of two parts:

(i) Calculate the spherulite growth based on Avrami models.

(ii) Calculate the light transmittance based on Maxwell equation.



The image of the spherulite growth simulator.

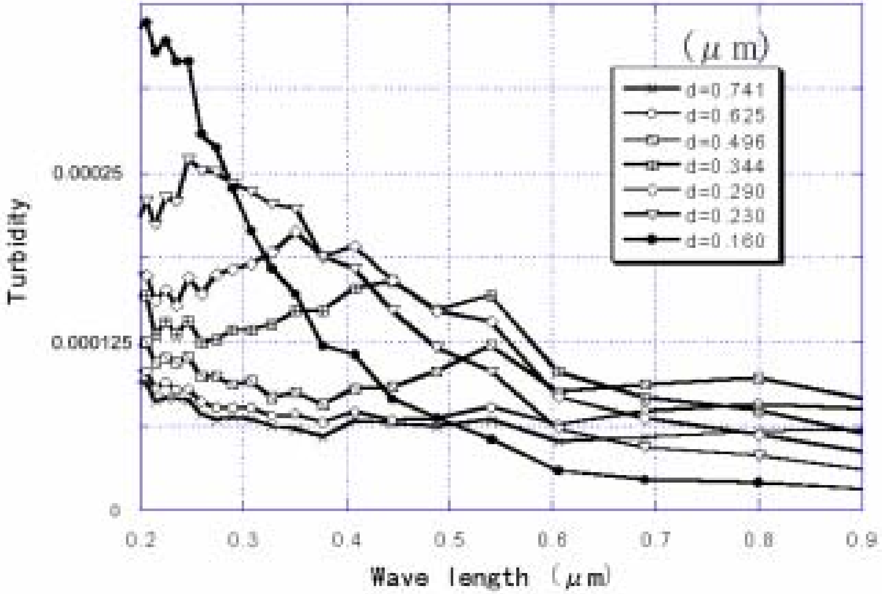


The model figure about the light which penetrates spherulite system.

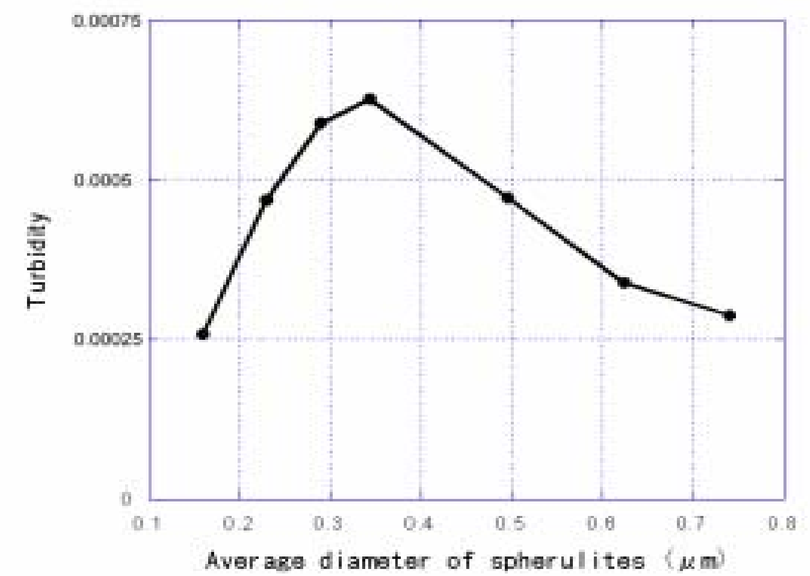
N.Kobayashi

“TURBAN” sample work

Light transmittance prediction of a PE film



The turbidity spectra for system with the various average spherulite diameters.



The turbidity integration value for the visible light in each spherulite diameter.

Simulation conditions:

- in the cubic cell of 128^3
- a visible light wavelength = 400-700nm
- non-uniform nucleation
- using known properties of PE blown film

Result:

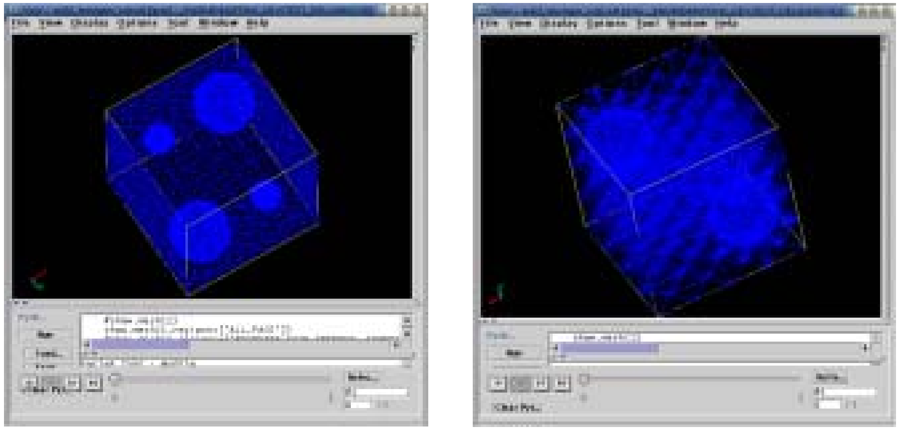
The peak of turbidity is seen near the wavelength comparable to the mean spherulite diameter.

The peak of the turbidity is in the lower range of a visible light.

These calculation are in good agreement with experiments.

Support tools of MUFFIN
”**Pre-processors**”

T.Yamaue
A.Kuroda



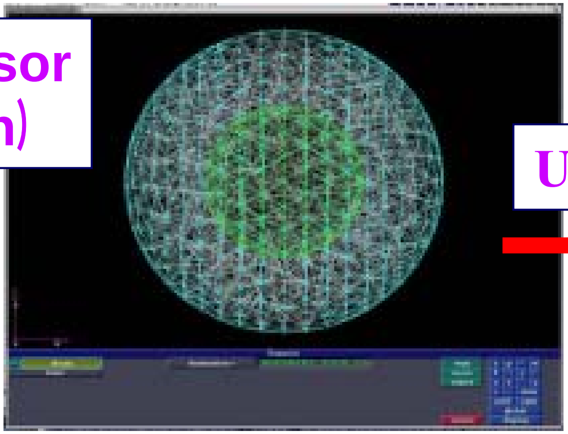
◆ “**MILK**” (Mesh Generator)

- Delaunay3D/2D auto meshing.
- Tetrahedron and Triangle.
- Internal Structures.

◆ “**NASTRAN BULK FILTER**”

- Import NASTRAN BULK mesh data to UDF mesh data.

FEM pre-processor (ex. HyperMesh)



UDF convert

GOURMET

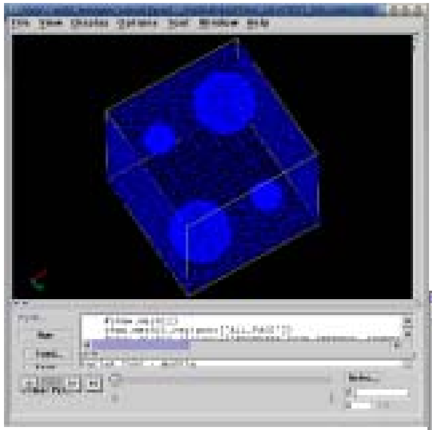
◆ “**MeshFieldConvertor (IMPORT/EXPORT_...)**”

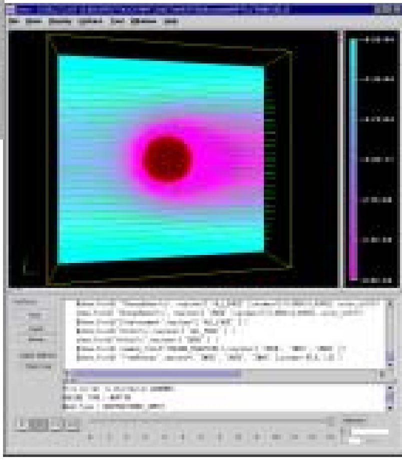
- Import/Export fields (morphology) data with SUSHI.

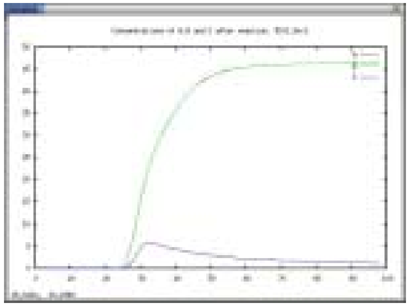
Support tools of MUFFIN
”Post-processors”

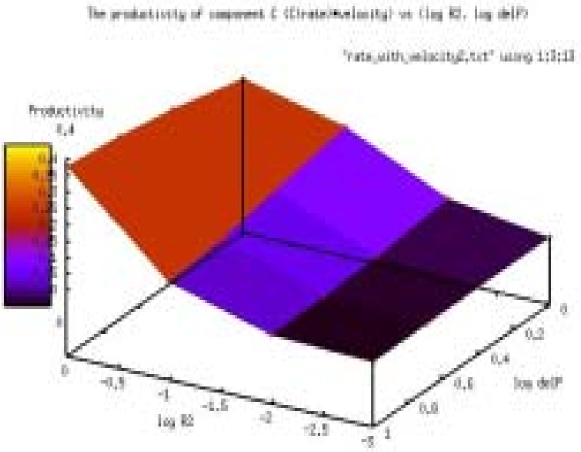
T.Yamaue
T.Taniguchi
M.Sasaki

- **“MeshFieldShow (SHOW_...)”**
  - Show mesh and field.
  - Structured and Unstructured.
  - Any cross section and Partial Regions.
- **“MeshFieldPlot (PLOT_...)”**
  - Plot field (using gnuplot).
  - Structured and Unstructured.
  - Any cross section and Partial Regions.
- **“udf2avs”**
  - Convert UDF field to AVS field.
  - Structured and Unstructured.
- **Some Support tools for each package.**
  - “ModelingSupporter”, “analyze_reactor”, ……

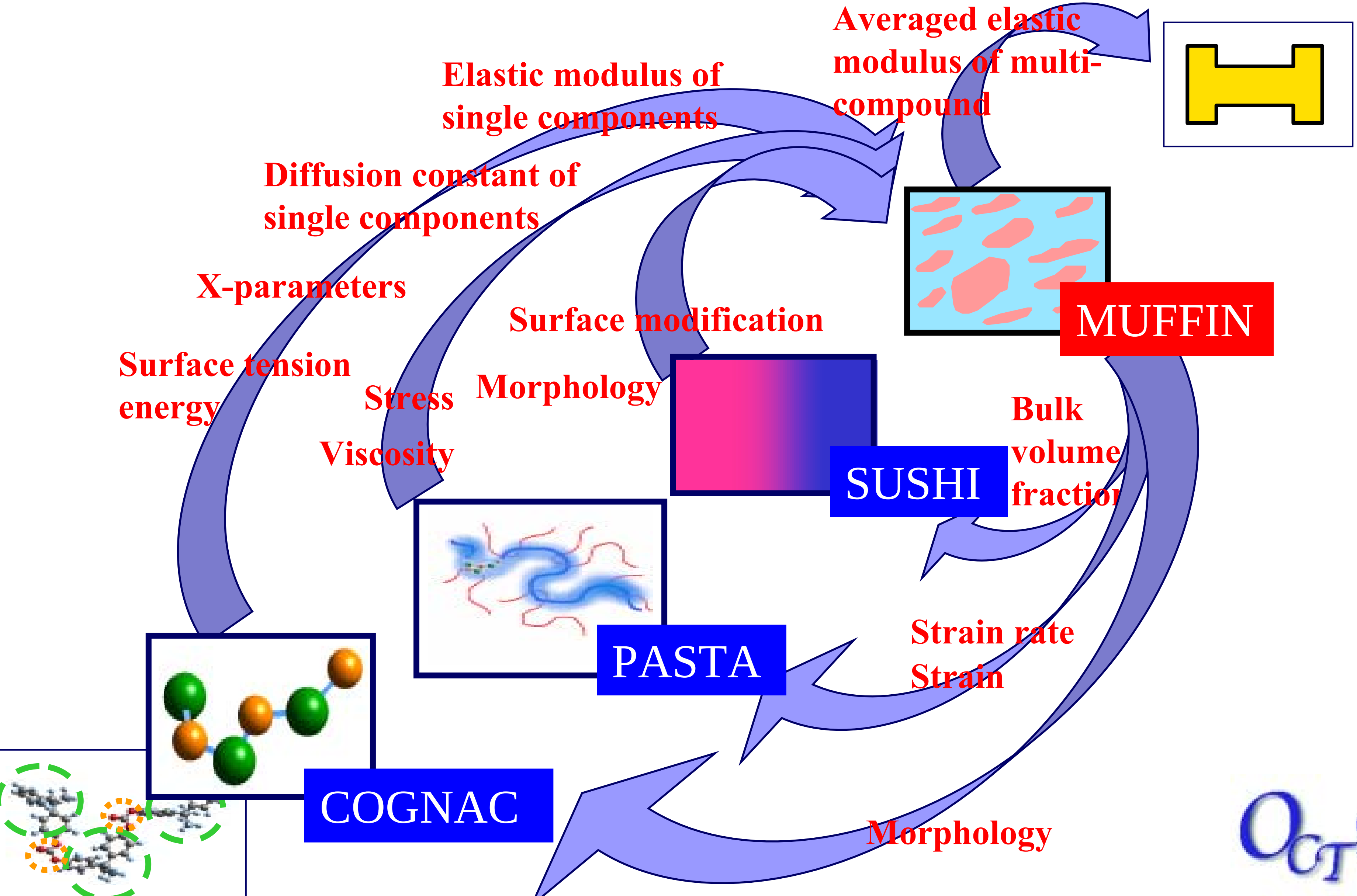








MUFFIN : Linking to other layers



Averaged elastic modulus of multi-compound

Elastic modulus of single components

Diffusion constant of single components

X-parameters

Surface modification

Surface tension energy

Stress

Morphology

Viscosity

MUFFIN

SUSHI

Bulk volume fraction

PASTA

Strain rate
Strain

COGNAC

Morphology

Summary

- MUFFIN (**MU**ltiFarious **FI**eld simulator for **N**on-equilibrium system) is an architecture for simulations of spatio-temporal behavior of multi-phase polymeric systems (～0.1 μm to 1mm, ～sec).

- Six simulation engines, “**PhaseSeparation**”, “**Electrolyte**”, “**MEMFluid**”, “**Elastica**”, “**GelDyna**” and “**TURBAN**” are implemented.

- MUFFIN is designed by the object-oriented modeling and serves various reusable components libraries, such as structured and unstructured mesh, foundation of fields, I/O routines, matrix solvers, finite elements solvers and “DynamicsManager”.

- The MUFFIN component library will be useful for you to construct your own simulator.