A Meshfree Approach for Large Deformation Analysis in Thermal Nanoimprint

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Background

- Thermal nanoimprinting and micro hot embossing have been in industrialization stage.
- Effective method for process design (temperature, pressure, time, etc.) is required.

Current situation

- Repetitive experiments for process optimization.
- Repetitive experiments cost high!!
- Numerical simulation should help.

Final Goal

Establishment of numerical technique for thermal nanoimprint process optimization.

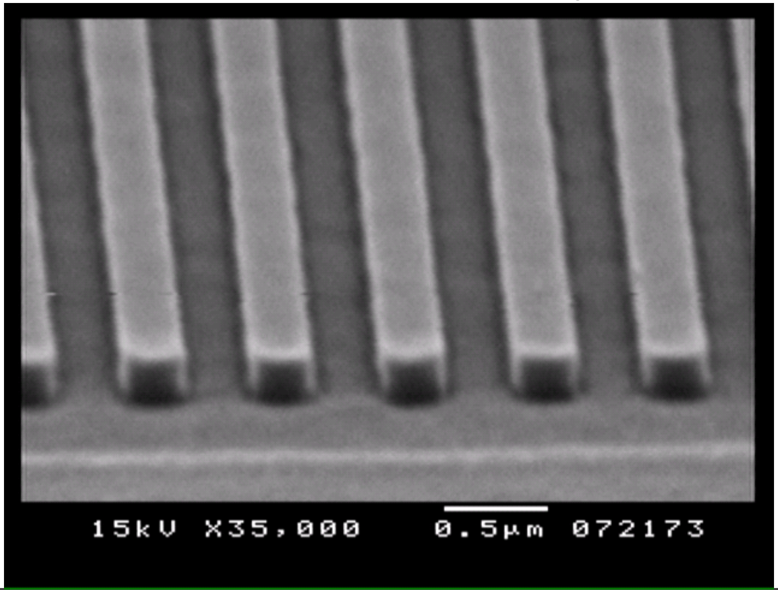
Choice of Numerical Method

- Choice1: Continuum or Molecular
  - If the target size is over several tens of nms, the number of molecules is large enough to be modeled as a continuum.
  - The problem is huge for MD.
- Choise2: Solid or Fluid
  - In thermal imprints, temperature is around *T*g at most.
  - Rheology effect can be consolidated in viscoelastic model.
- Choise3: Meshfree or Mesh
  - "Mesh"(=FEM) is usually used and has achievements.
  - "Meshfree"(=SPH, EFGM, etc.) is expected to be a good method to treat extremely large deformation, but still under development and yet has no achievements.
  - Most of the researches use FEM.

Our Previous Work (Outline)

■ Finite element Analysis

- Geometric nonlinear (Large deformation)
- Material nonlinear (thermo-viscoelastic polymer)
- Contact nonlinear
- Quasi-static analysis

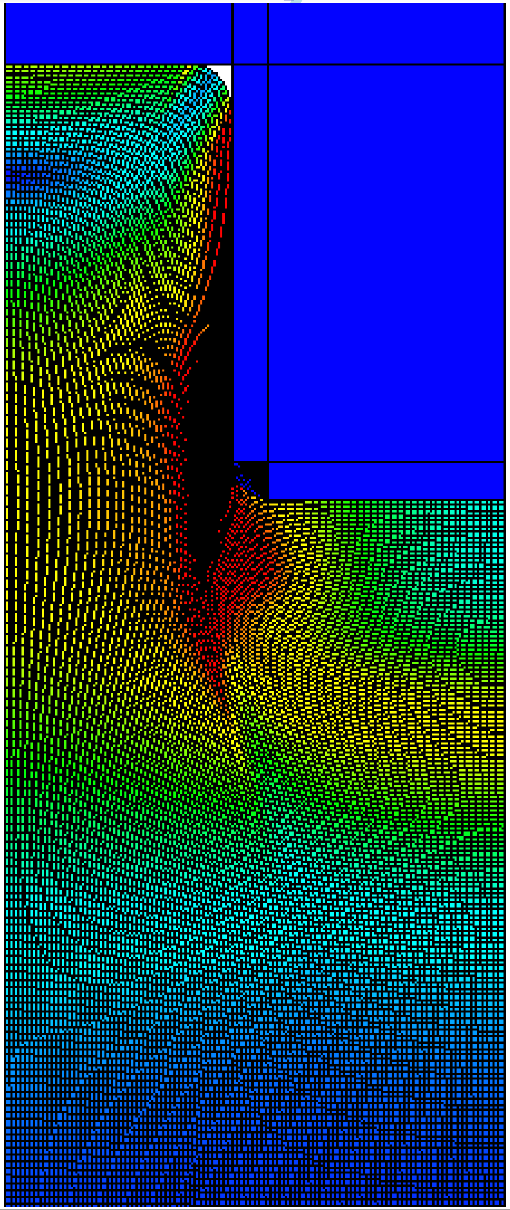


FE analyses agreed with experiments in case of line-and-space up to ***AR*=1**

Onishi et al., JVST B (2008) etc.

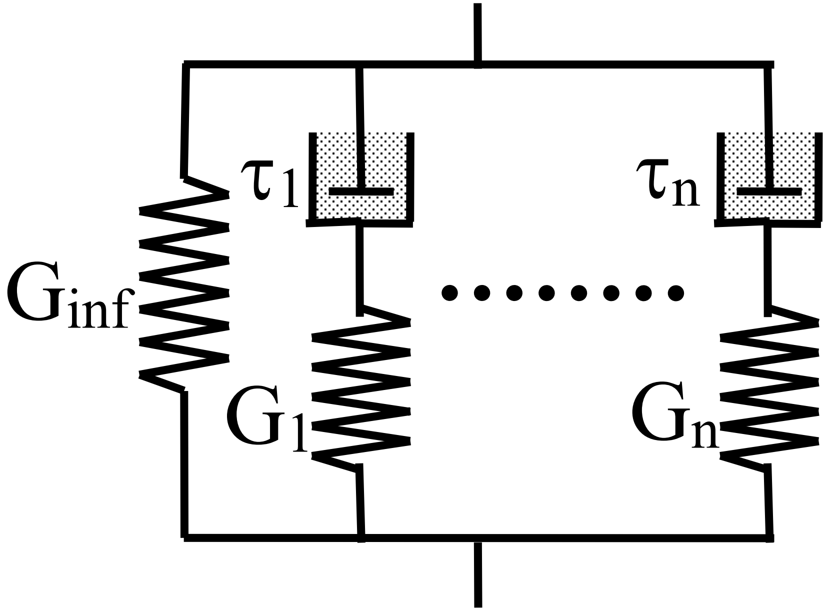
Mold (rigid)

Polymer (thermo-viscoelastic)



Our Previous Work (Viscoelastic)

■ Generalized Maxwell Model



When a forced displacement $x(t)=\sin(\omega t)$ applied at the temperature θ, reaction force f(t) become

$$f(t) = G'(\omega,\theta)\sin(\omega t) + G''(\omega,\theta)\cos(\omega t)$$

G_{inf} : Long-term shear modulus

$G_0=G_{inf}+\sum G_i$:
Instantaneous shear Modulus

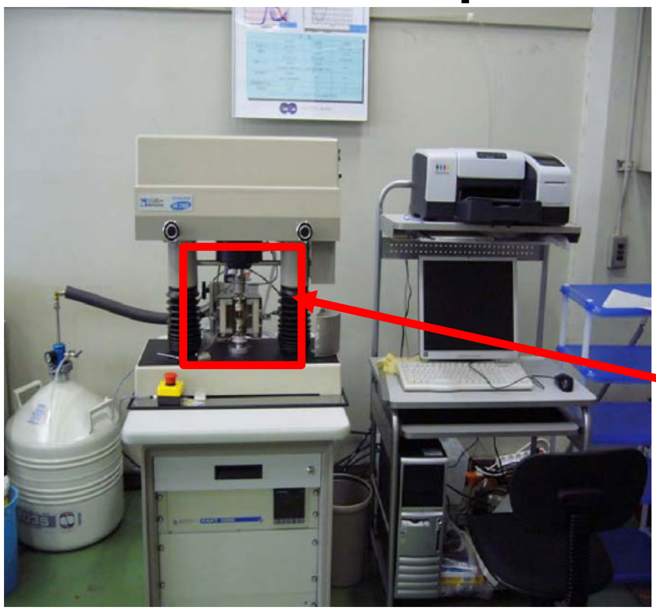
$\tau_1 \sim \tau_n$: Relaxation time

G' : Shear storage modulus (same phase)

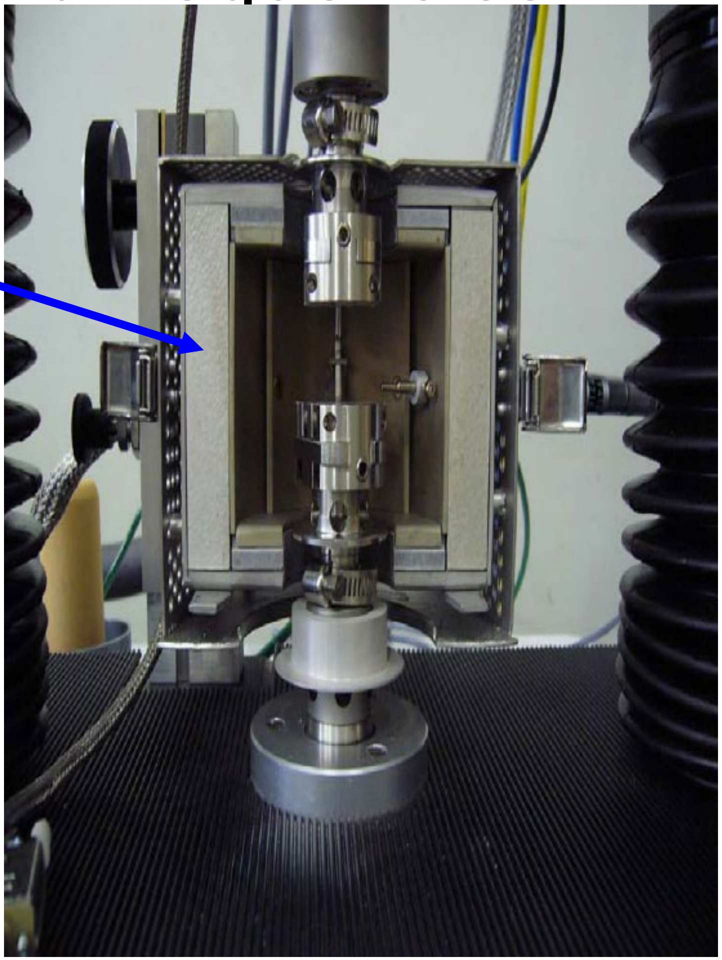
G'' : Shear loss modulus (90^o shifted)

Our Previous Work (Material Test)

- Uniaxial tension-compression tests at various temperatures and frequencies

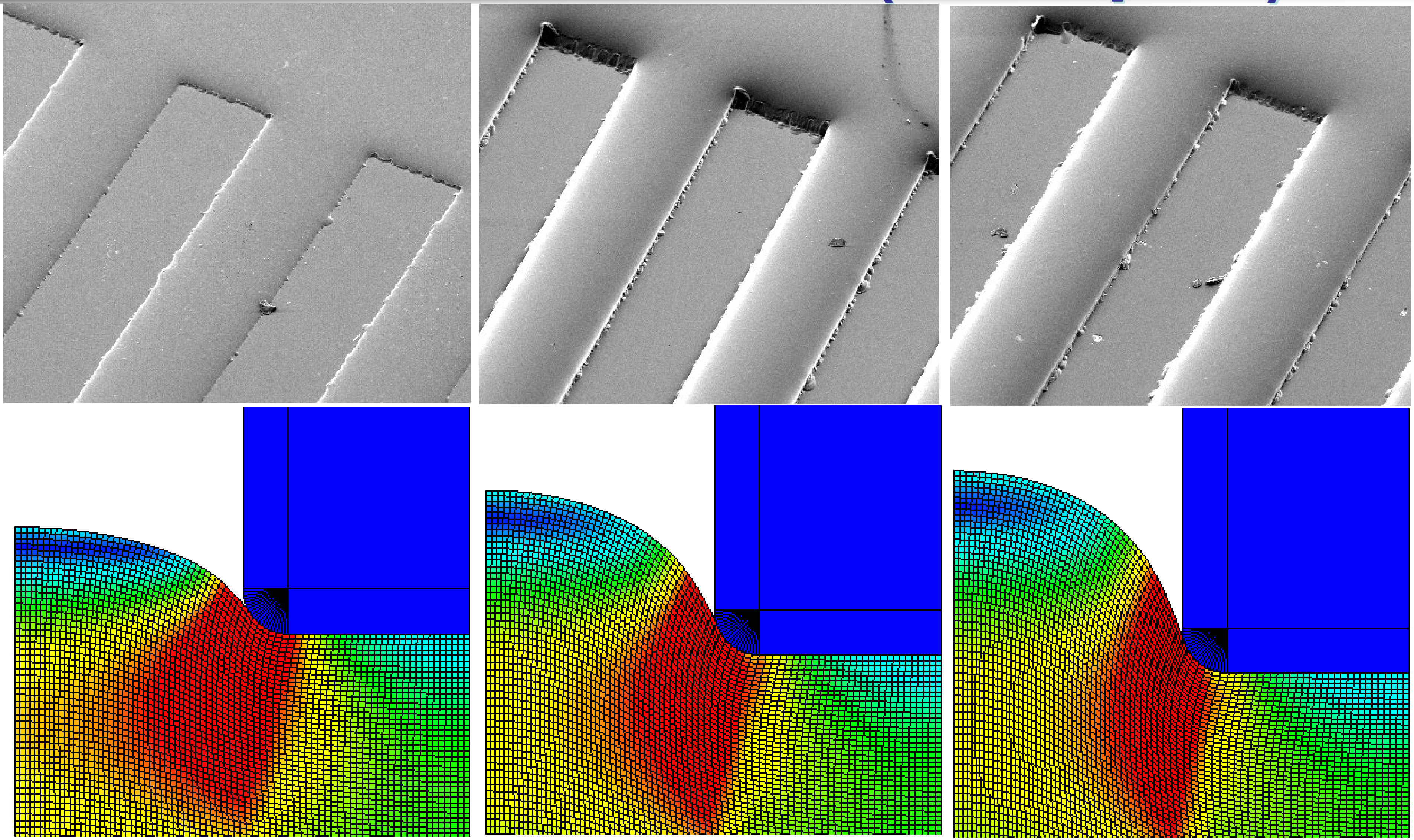


heater



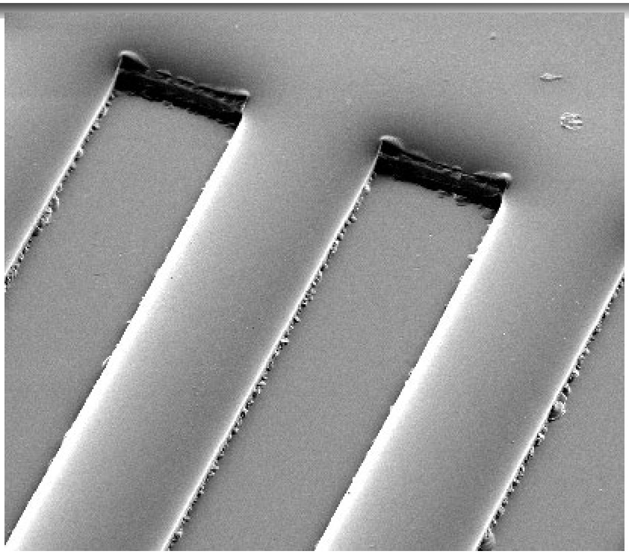
device：01dB-METRAVIB VA2000
frequency range：0.001～200(Hz)
load range：±100(N)
temperature range：-150～450(degC)

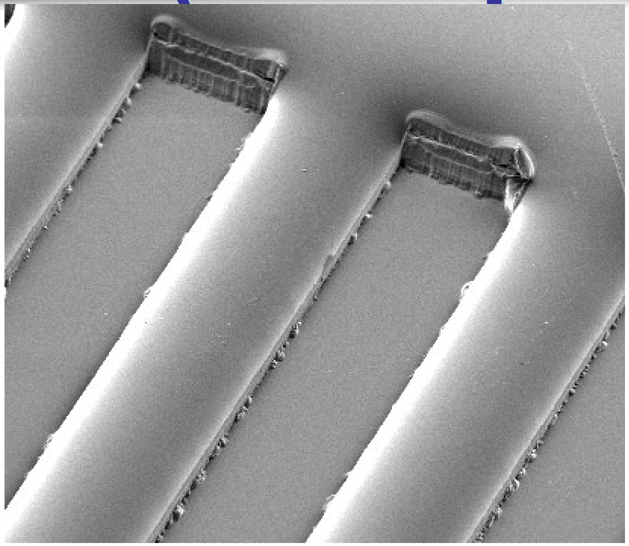
Our Previous Work (Example2)

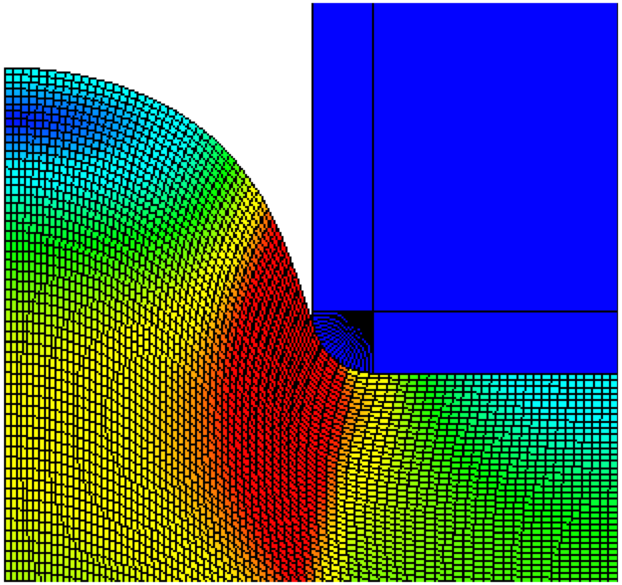


10sec　　30sec　　60sec

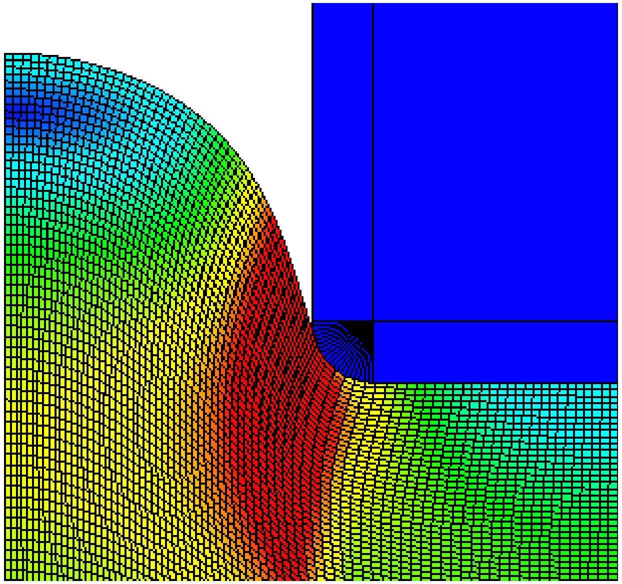
Our Previous Work (Example2)







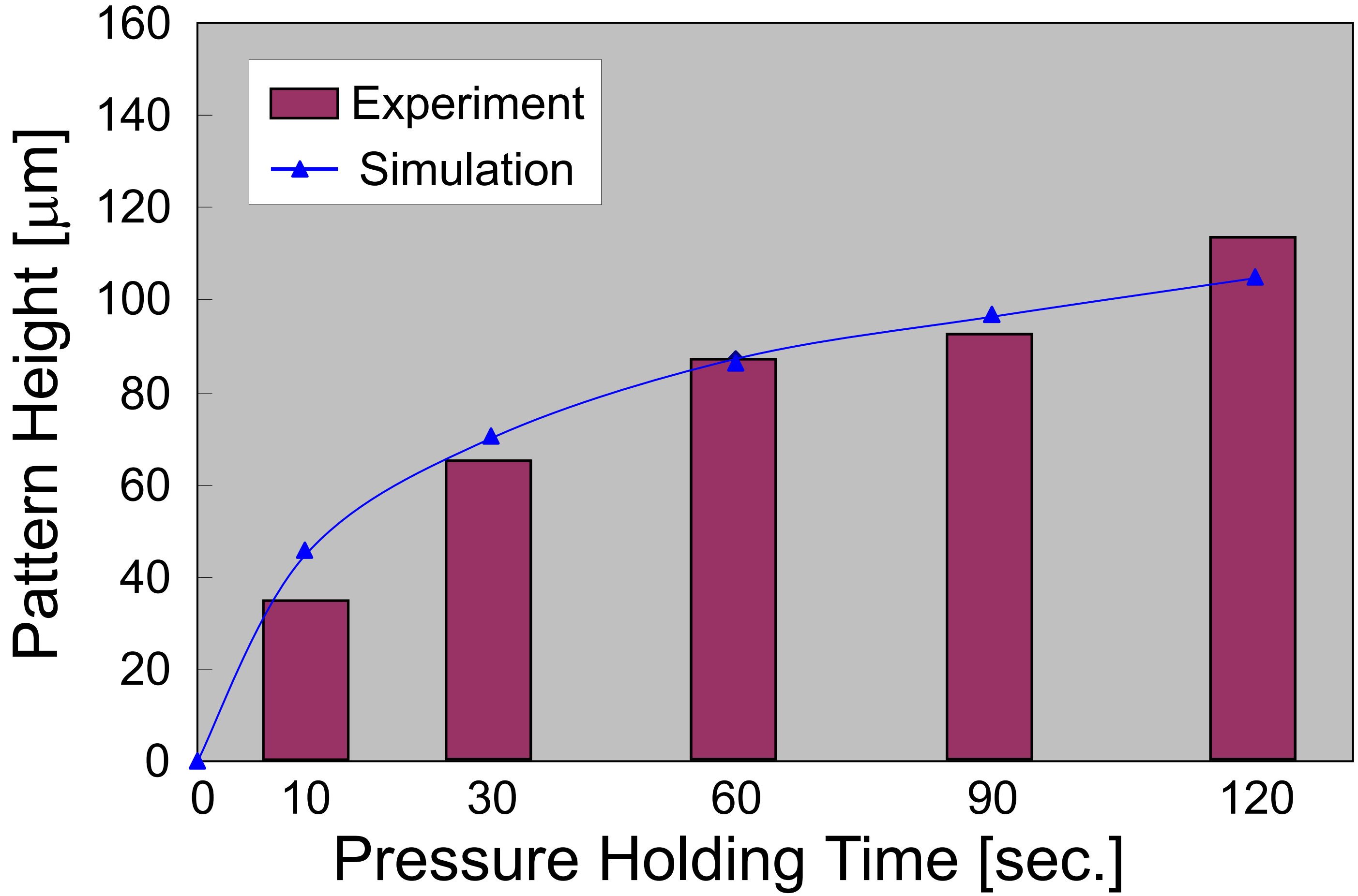
90sec



120sec

Our Previous Work (Example1)

Our Previous Work (Example2)



■ Simulated deformations of the line-and-space imprinting agreed with experiments.

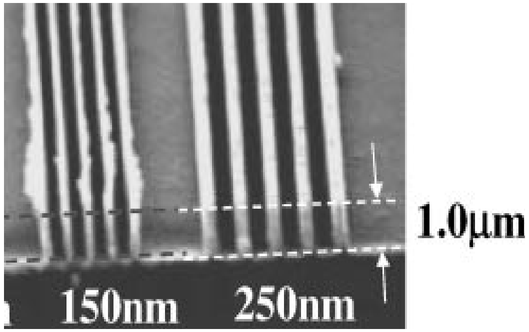
Our Previous Work (Summary)

- Time evolutional deformation behavior was successfully simulated with FEM in cases of line-and-space patterning.
- The thermo-viscoelastic constitutive model we chose was appropriate.
- It has potential to simulate any deformation in thermal nanoimprintings.

Objective

Our previous work hit the wall…

- In practical applications, AR over 1 is not uncommon. (even AR>3 is usual.)



Hiral et. al

- FEM cannot treat the extremely large deformation without adaptive meshing. (Adaptive meshing is difficult to implement.)

Objective

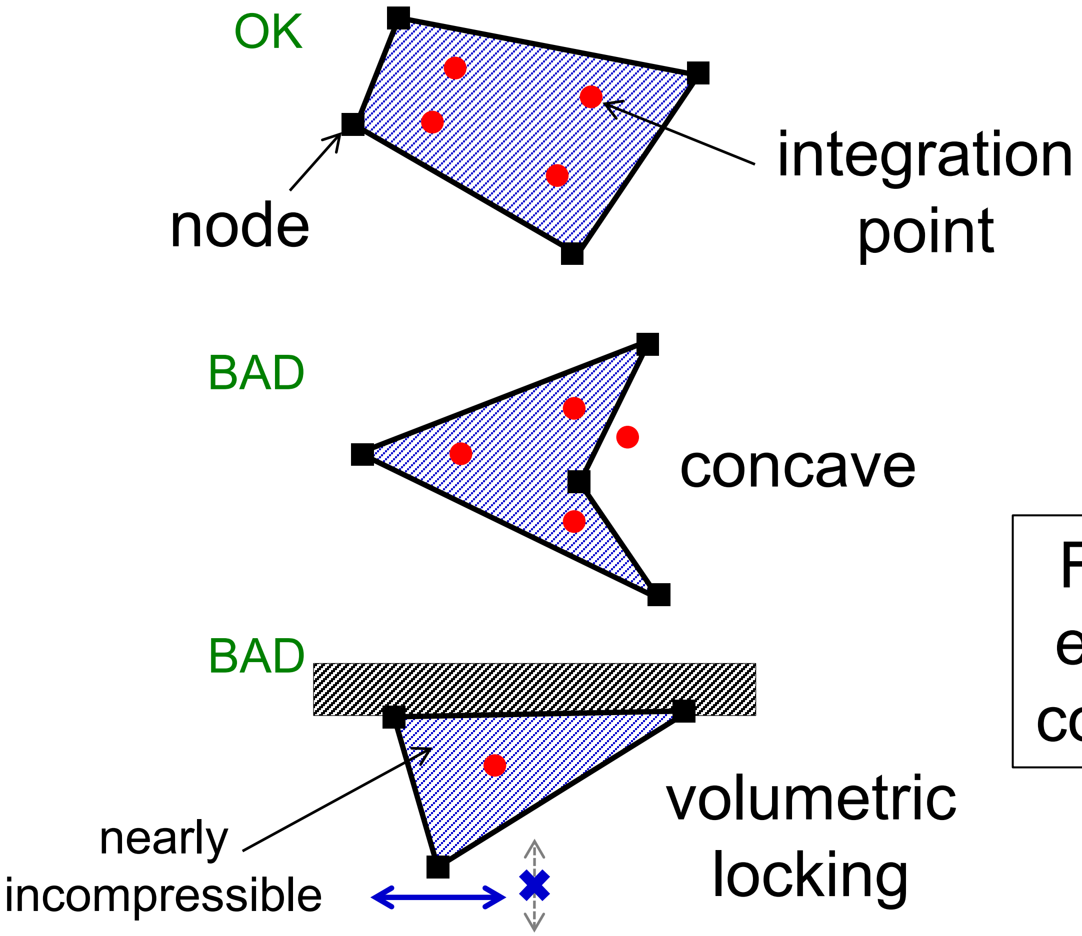
Development of a **meshfree** method for viscoelastic large deformation analysis

(utilize it for thermal nanoimprint process optimization in the future)

Difference between FEM and Meshfree

■ Way of domain integration

- FEM (element base)

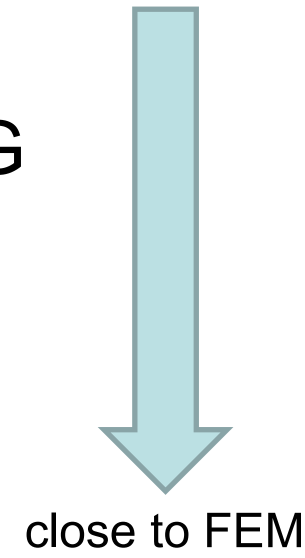


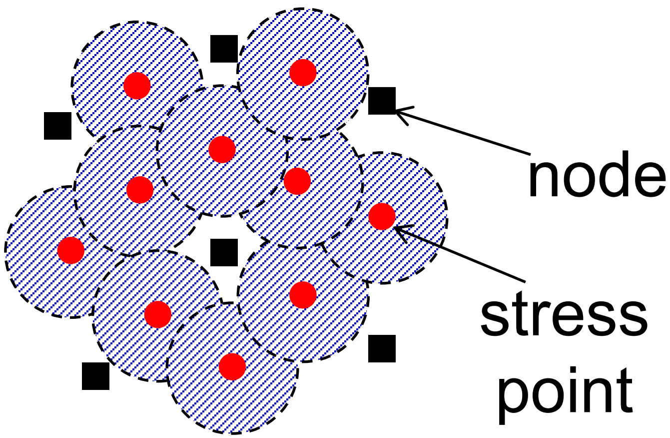
Frequently happens especially in case of compression analysis

Difference between FEM and Meshfree

■ Way of domain integration

- Meshfree (collocation type) ---- SPH
- Meshfree (Petrov-Galerkin type) ---- MLPG
- Meshfree (Galerkin type) ---- EFGM
  - ◆background cell integration
  - ◆nodal integration
  - ◆stress point integration (SPI)





(No standard formulation of SPI)

*No element

*Less locking

*Fair integration accuracy

*Requirement of stabilization

Robust MLS Approximation

Moving Least Squares (MLS) to build shape function

■ Support radius

set initial ${}^{I}R$ (small)

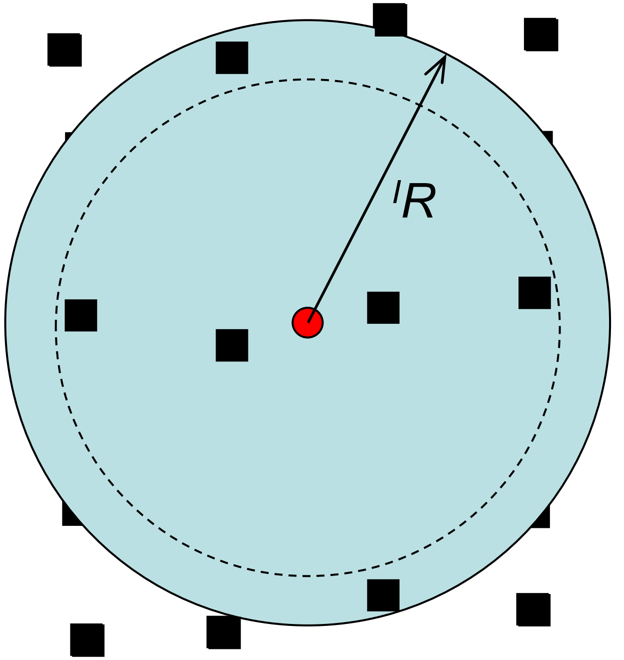
begin loop $\quad \boldsymbol{p} = \{1, x, y\}^T$

calculate $\boldsymbol{A} (= \sum_{J \in {}^{I}\mathbb{S}} {}^{I}w_J \, {}_{J}\boldsymbol{p}^T \, {}_{J}\boldsymbol{p})$

if $\mathrm{cond}(\boldsymbol{A}) < 1 \times 10^5$, break

${}^{I}R \longleftarrow 1.01 \times {}^{I}R$

end loop



■ Weight function

$$
{}^{I}w_J = \begin{cases} 1/{}^{I}d_J - 1 & (0 < {}^{I}d_J < 1) \\ 0 & (1 \le {}^{I}d_J) \end{cases} , \quad {}^{I}d_J = \frac{\|{}_{J}\boldsymbol{x} - {}^{I}\boldsymbol{x}\|}{{}^{I}R}
$$

Update of SP States

[note] ${}^{I}\boldsymbol{x}$: location of SP, ${}_{J}\boldsymbol{x}$: location of node

- Location

$$ {}^{I}\boldsymbol{x}^{\mathrm{trial}} \longleftarrow {}^{I}\boldsymbol{x} + \sum_{J \in {}^{I}\mathbb{S}} {}^{I}\phi_{J} \left({}_{J}\boldsymbol{x}^{\mathrm{trial}} - {}_{J}\boldsymbol{x} \right) $$

x: current location, S: set of nodes in the support,

ϕ: shape function

- Volume

$$ {}^{I}V^{\mathrm{trial}} \longleftarrow {}^{I}V^{\mathrm{initial}} \det({}^{I}\boldsymbol{F}^{\mathrm{trial}}) $$

V^{initial} : initial volume, $\boldsymbol{F}$: deformation gradient

Viscoelastic Material Properties

- material constants used in example analysis

instantaneous Young's modulus (E_0) : 9 GPa

instantaneous Poisson's ratio (ν_0) : 0.333・・・

instantaneous shear modulus (G_0) : 3.375 GPa

behavior at room temperature

bulk modulus (K) : 9 GPa

dimensionless shear modulus (g) : 0.9

relaxation time (τ) : 5 s

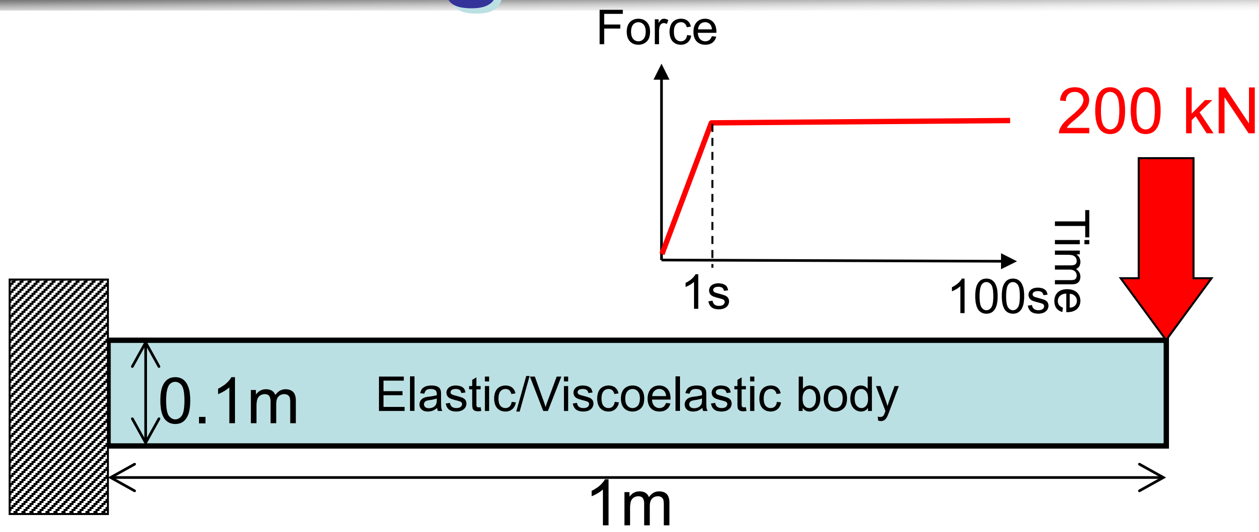
long-term Young's modulus (E_∞) : 1 GPa

long-term Poission's ratio (ν_∞) : 0.481

long-term shear modulus(G_∞): 0.3375 GPa

behavior around Tg

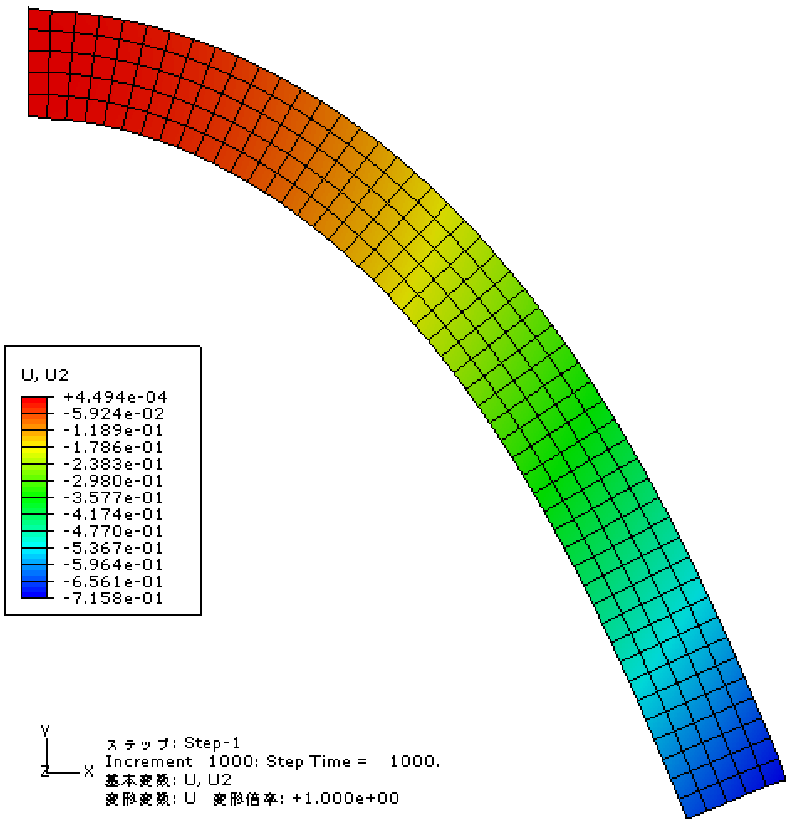
Bending of Cantilever



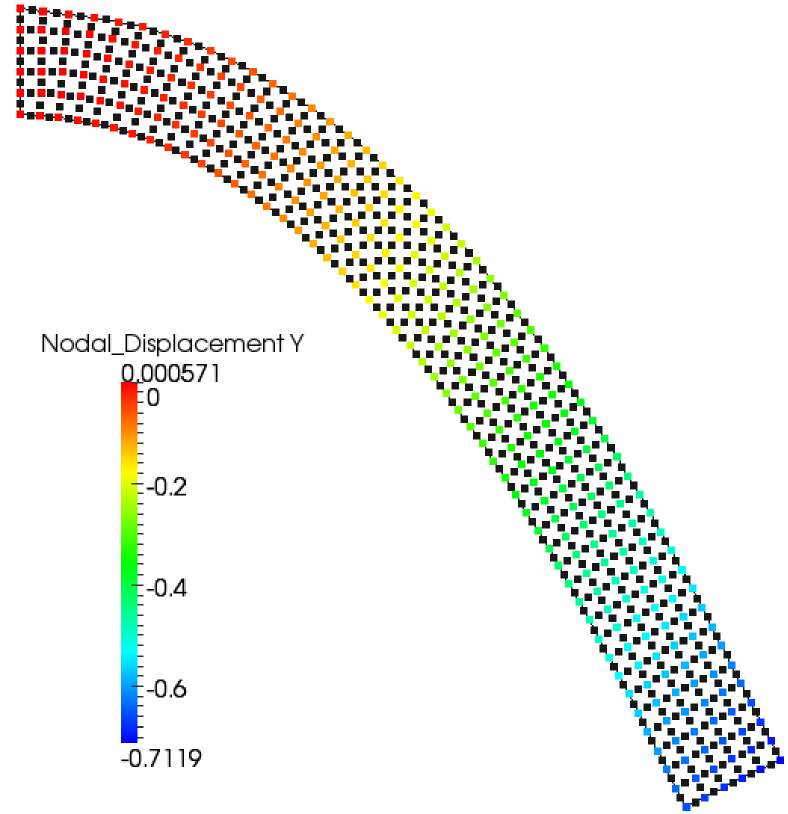
- Static/Quasi-static, Plane strain
- 50x5 structured grid nodes
- Concentrated force at right-top node
- Compared to FEM(ABAQUS/Standard) with same node arrangements and selective reduced integration quadrangle elements

Bending of Cantilever (elastic)

E=1GPa, ν=0.49



ABAQUS/Standard

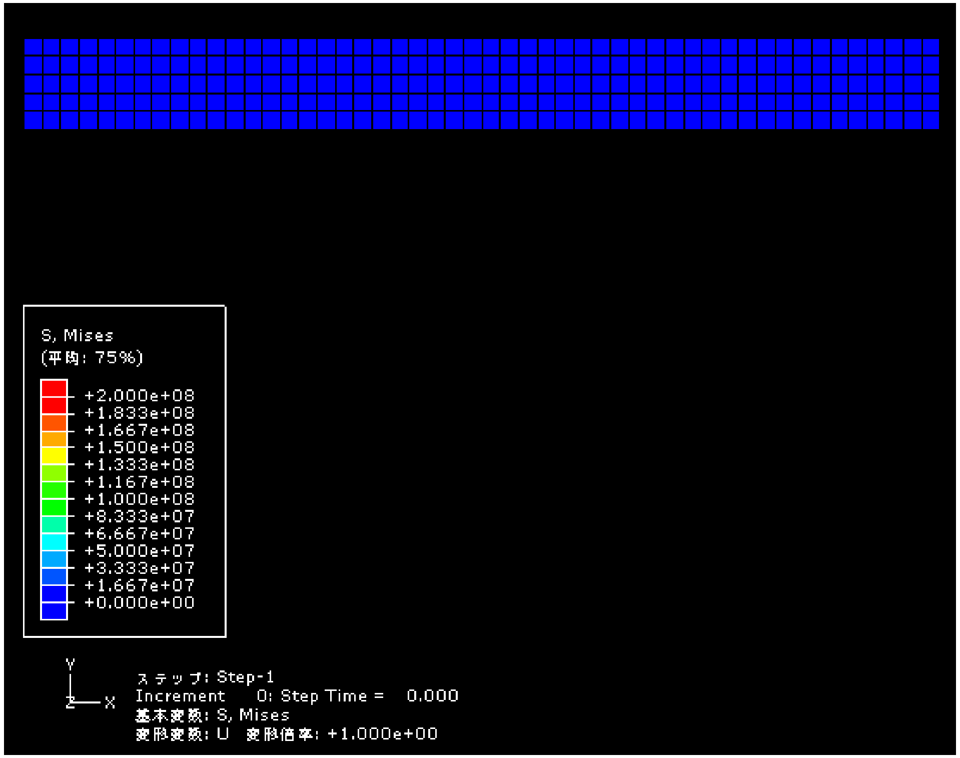


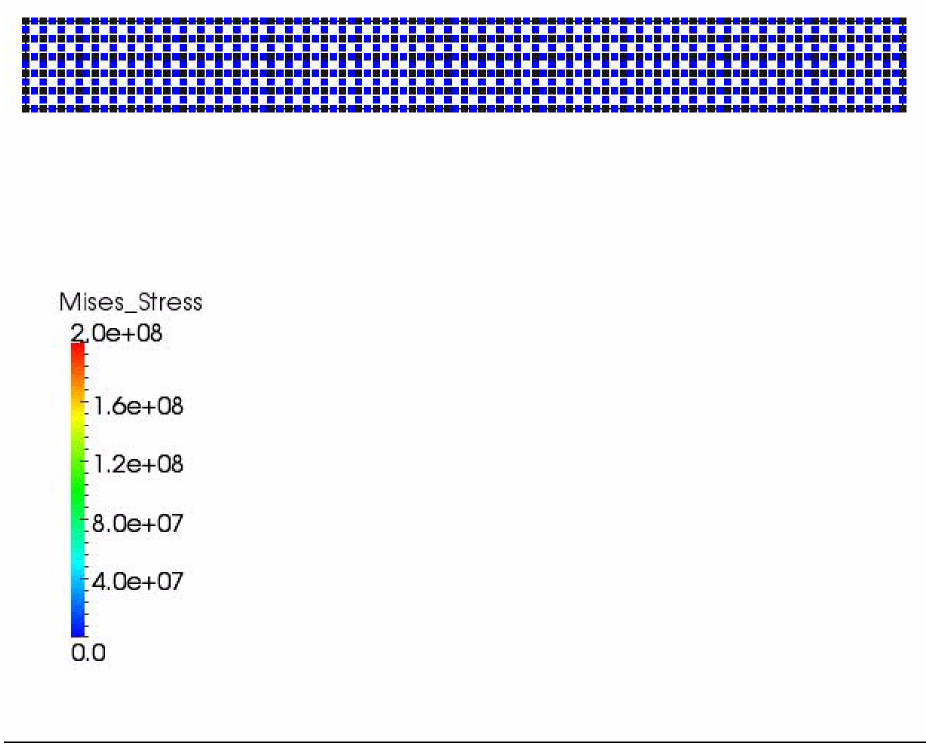
Proposed Method

- Less than 1% error of displacement
- No problem in elastic large deflection analysis

Bending of Cantilever (viscoelastic)

E_0=9GPa, ν_0=0.333, E_{inf}=1GPa, ν_{inf}=0.481

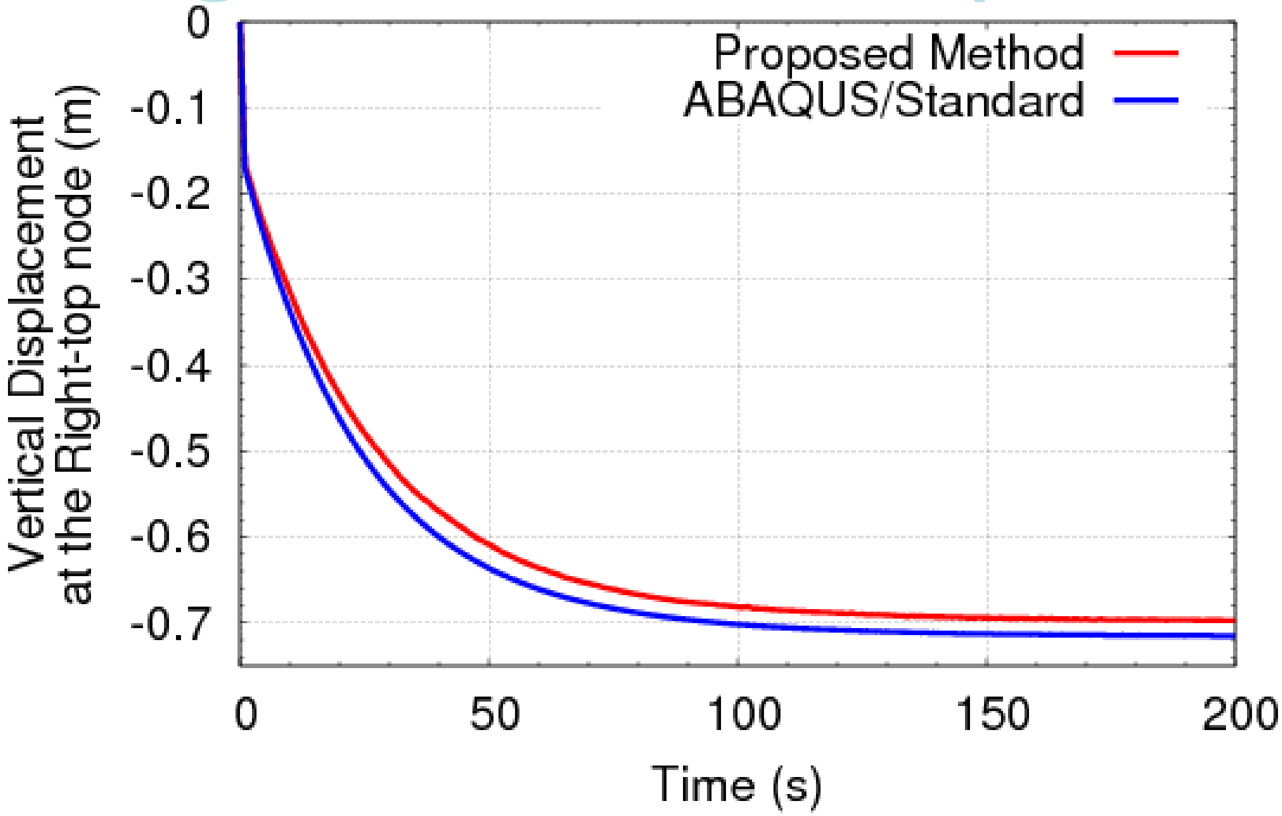




ABAQUS/Standard

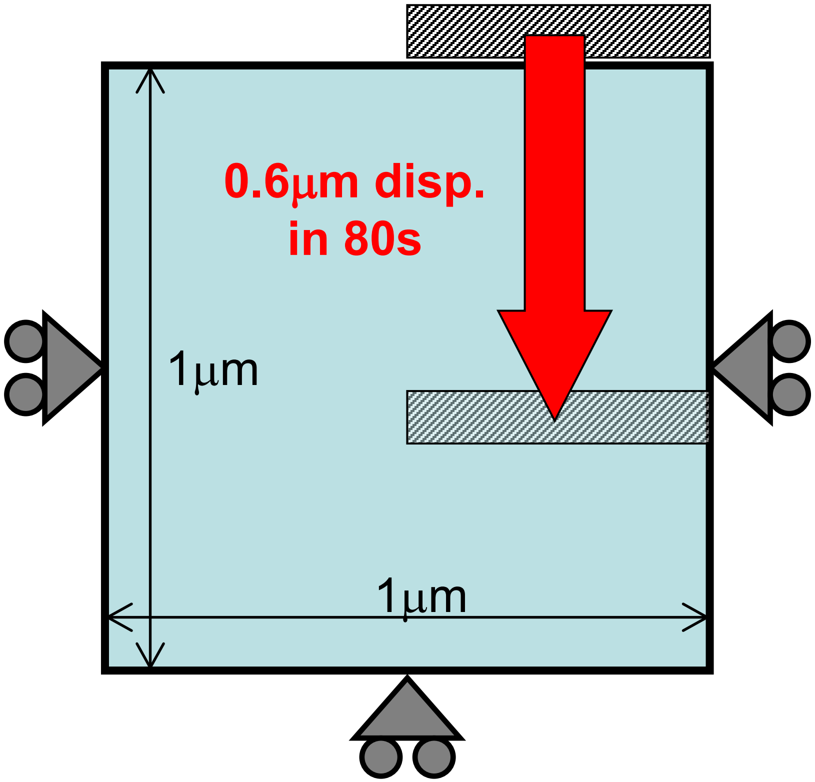
Proposed Method

Bending of Cantilever (viscoelastic)



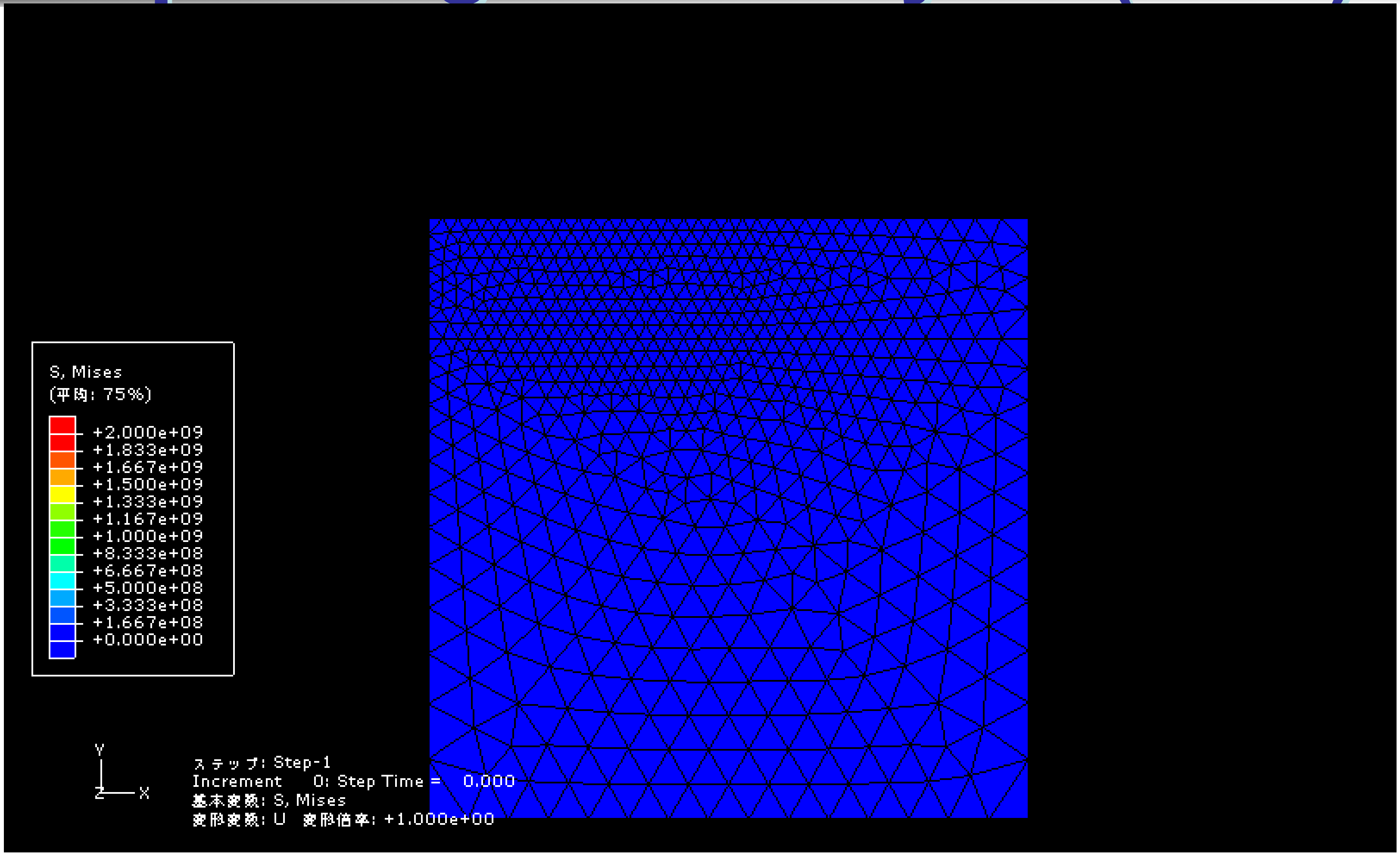
- 2.5% error of displacement
- Error decreases as d*t* decreases
- Further improvement of time-advancing scheme is necessary

Imprinting-like Analysis



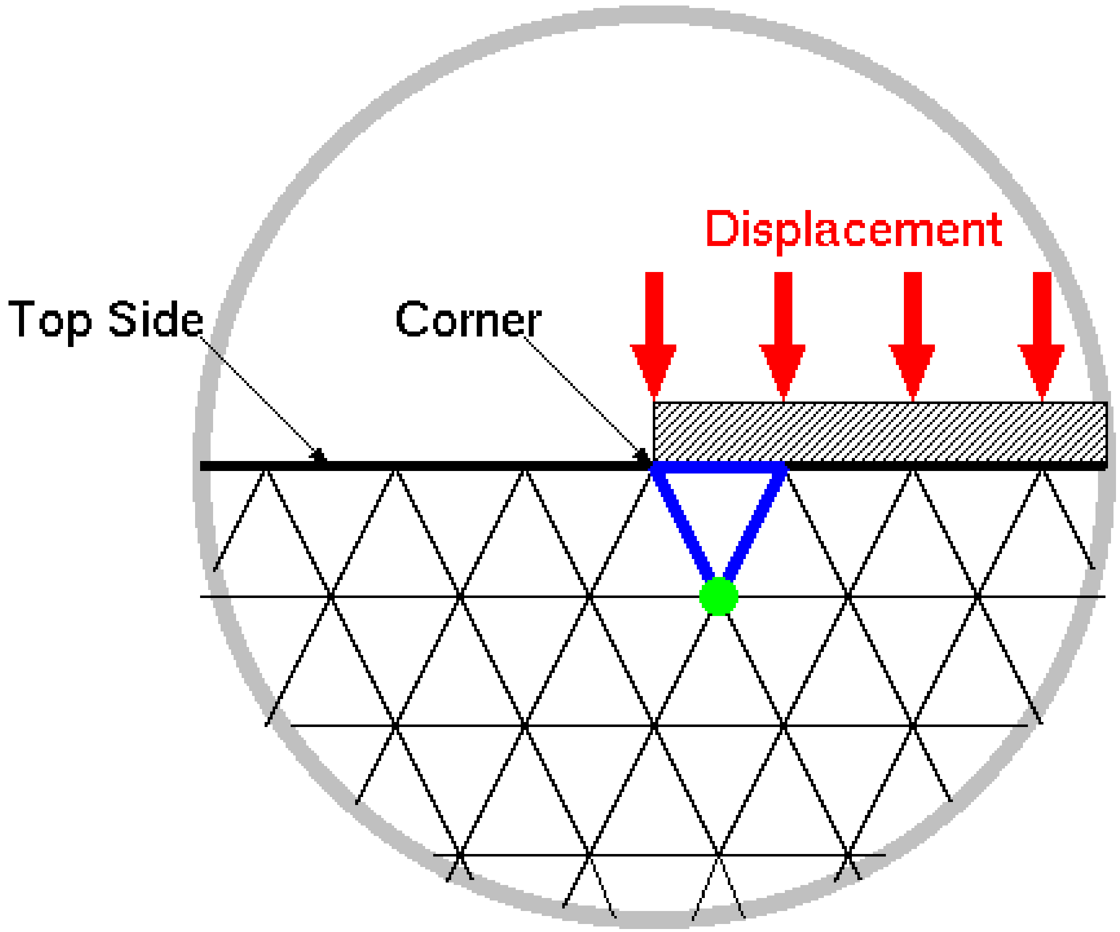
- Quasi-static, plane strain
- Horizontal bounding for left and right side
- Vertical bounding for bottom side
- Enforced displacement for right half of top side toward downward with horizontal bounding
- Unstructured grid with fineness and coarseness

Imprinting-like Analysis (FEM)

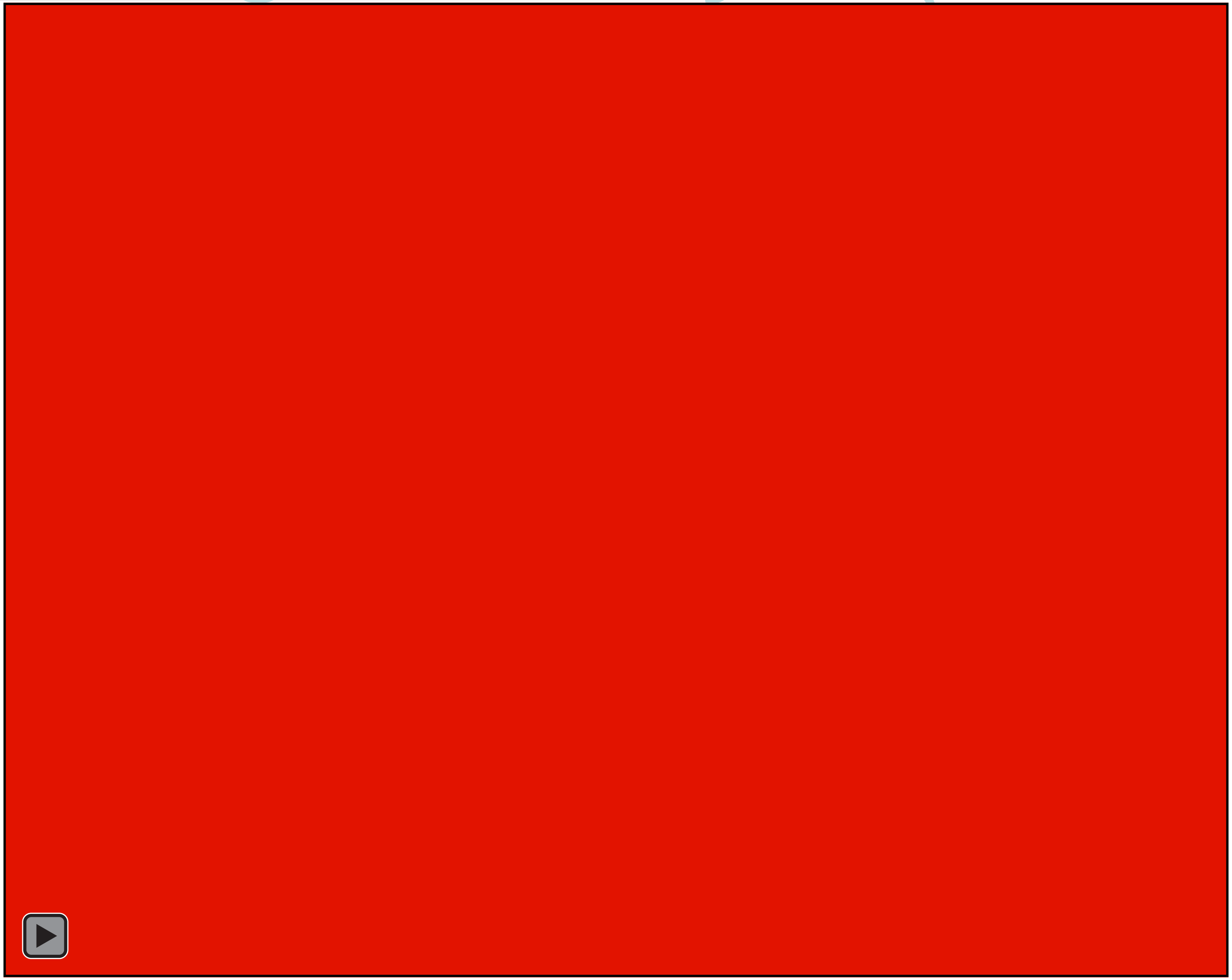


- Inappropriate deformation because of the locking under the corner

Imprinting-like Analysis (FEM)



Imprinting-like Analysis (animation)



■ An appropriate result was obtained.

Summary & Future Work

Summary

- A Meshfree formulation of large deformation of viscoelastic body was proposed.
- It has fair accuracy in large deflation analysis.
- Appropriate result is obtained in imprinting-like analysis.
- Further modification is required to apply it to thermal nanoimprint simulation.

Future work

- Improvement of time advancing scheme
- Verification with experiments or FEM with adaptive meshing
- Insertion of additional nodes and SPs during analysis
- Contact analysis
- Cooling and demolding analysis

Appendix

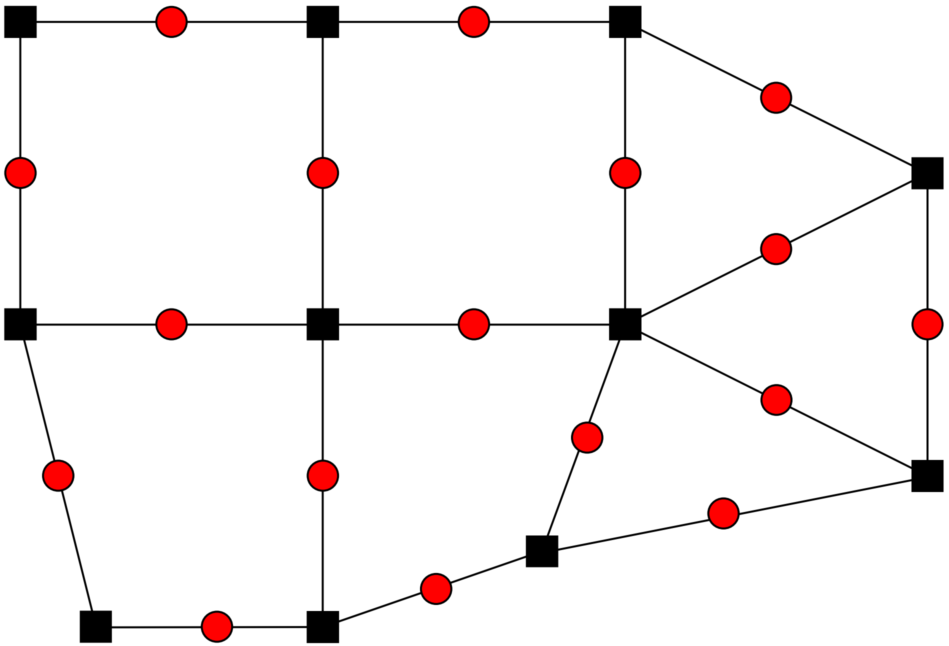
SP Integration (initialization)

- (currently) SPs are generated from FE meshes
  [Note] meshes are only for initialization!!!
- Locate every SP in the middle edges

  (Belytschko's SP integration has master and slave SPs.)
- Corresponding SP volume is calculated with meshes

■ : node
(has only ***x*** and ***u***)

● : stress point (SP)
(has ***x***, ***T***, ***E***, $\boldsymbol{E}^{v}$, etc.)



Integration Correction

- Integration constraint

$$\sum_{I\in {}_J\mathbb{S}} \nabla^I\phi_J{}^IV = \mathbf{0} \qquad \text{(for } J \text{ in interior nodes)},$$

$$\sum_{I\in {}_J\mathbb{S}} \nabla^I\phi_J{}^IV = {}_J\boldsymbol{n}_J A \qquad \text{(for } J \text{ in exterior nodes)}.$$

n: outward normal unit vector, *A*: correspoiding nodal area
$_J$S: set of SPs that include node *J* in the support

- Integration correction (IC)

$$^I\tilde{\boldsymbol{\psi}} = \begin{bmatrix} 1+{}^I\gamma_1 & 0 \\ 0 & 1+{}^I\gamma_2 \end{bmatrix} \nabla^I\phi_J$$

determine γ s so that modified ψ s satisfy reproducing constraints including integration constraint

Quasi-implicit Time Advancing

Typical fully-implicit time advancing

- Start of time increment loop
  - Start of Newton-Raphson loop
    - update support, w, ϕ, etc.
    - calc $\boldsymbol{f}^{\text{int.}}$ and $\boldsymbol{K}$
    - calc $\boldsymbol{r} = \boldsymbol{f}^{\text{int.}} - \boldsymbol{f}^{\text{ext.}}$
    - solve $\boldsymbol{K}\,\delta\boldsymbol{u} = \boldsymbol{r}$
    - update node locations
    - update SP locations
  - End of Newton-Raphson loop
- End of time increment loop

Quasi-implicit Time Advancing

- Start of time increment loop
  - update support, w, ϕ, etc.
  - renew $\boldsymbol{f}^{\text{virtual}}$
  - Start of Newton-Raphson loop
    - update support, w, ϕ, etc.
    - calc $\boldsymbol{f}^{\text{int.}}$ and $\boldsymbol{K}$
    - calc $\boldsymbol{r} = \boldsymbol{f}^{\text{int.}} - \boldsymbol{f}^{\text{ext.}} - \boldsymbol{f}^{\text{virtual}}$
    - solve $\boldsymbol{K}\,\delta\boldsymbol{u} = \boldsymbol{r}$
    - update node locations
    - update SP locations
  - End of Newton-Raphson loop
- End of time increment loop

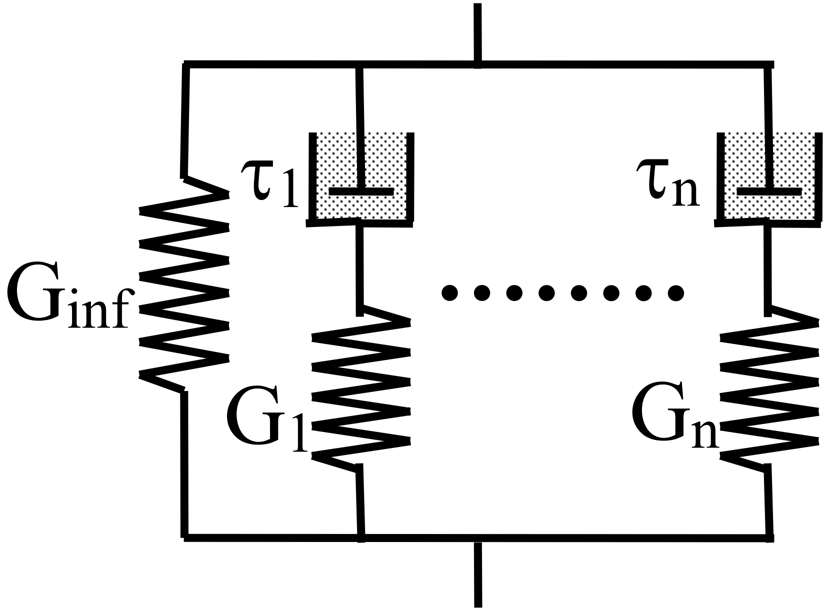
Constant shape function in each Newton-Raphson loop

Enforcement of temporal continuity of the mechanical equilibrium

- FEM
  - Integration points are pseudo-Lagrange points.
  - Elements must be convex.
  - 1st order triangular element has volumetric locking.
- Meshfree with BG cells
  - Integration points are Euler points.
  - Difficulties in treating free surfaces.
  - Difficulties in convection of state quantities.
- Meshfree without cells
  - Integration points are Lagrange points.
  - Difficulties in precise domain integration.

Shear Behavior of Polymer

■ Generalized Maxwell Model



When a forced displacement $x(t)=\sin(\omega t)$ applied at the temperature θ, reaction force f(t) become

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G_{inf} : Long-term shear modulus

$G_0 = G_{inf} + \sum G_i$: Instantaneous shear Modulus

$\tau_1 \sim \tau_n$: Relaxation time

G' : Shear storage modulus (same phase)

G'' : Shear loss modulus (90^o shifted)

Constitutive Equation of Polymer

■ Constitutive equation

1)Volumetric Behavior

$$[P] = -KE_{\mathrm{vol}}[I]$$

[P] : hydrostatic stress tensor
K : bulk modulus
Evol: volumetric strain
[I]: identity tensor

2)Shear Behavior

$$[S] = 2G_0\left([E'] - \sum_{i=1}^{n} g_i[E'_v]_i\right)$$

[S]: deviatoric stress tensor
G0: instantaneous shear modulus
(=Ginf +G1+ ... + Gn)
[E']: deviatoric strain tensor
gi: ith dimensionless shear modulus
(=Gi/G0)
[Ev']i: ith viscous strain tensor

Combining [P] and [S], We obtain stress tensor [T] as:

$$[T] = -[P] + [S] = KE_{\mathrm{vol}}[I] + 2G_0\left([E'] - \sum_{i=1}^{n} g_i[E'_v]_i\right)$$

Temperature Dependency of Polymer

- WLF law (temperature-time conversion)

WLF law

temperature increase ⇔ reduced time increase

$$\log_{10} A(\theta) = -\frac{C_1(\theta - \theta_{\mathrm{ref}})}{C_2 + (\theta - \theta_{\mathrm{ref}})}$$

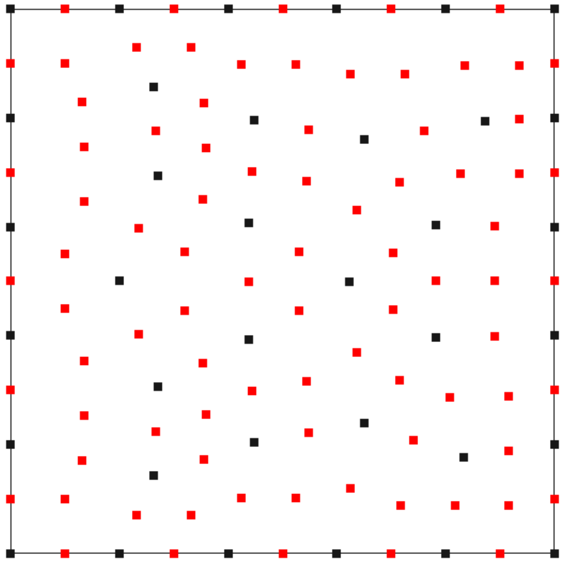
$$t' = \int_t^{t+\Delta t} \frac{1}{A(\theta)}\, dt$$

t: real time

t': reduced time

θref, C1, C2: material constants

Patch Test

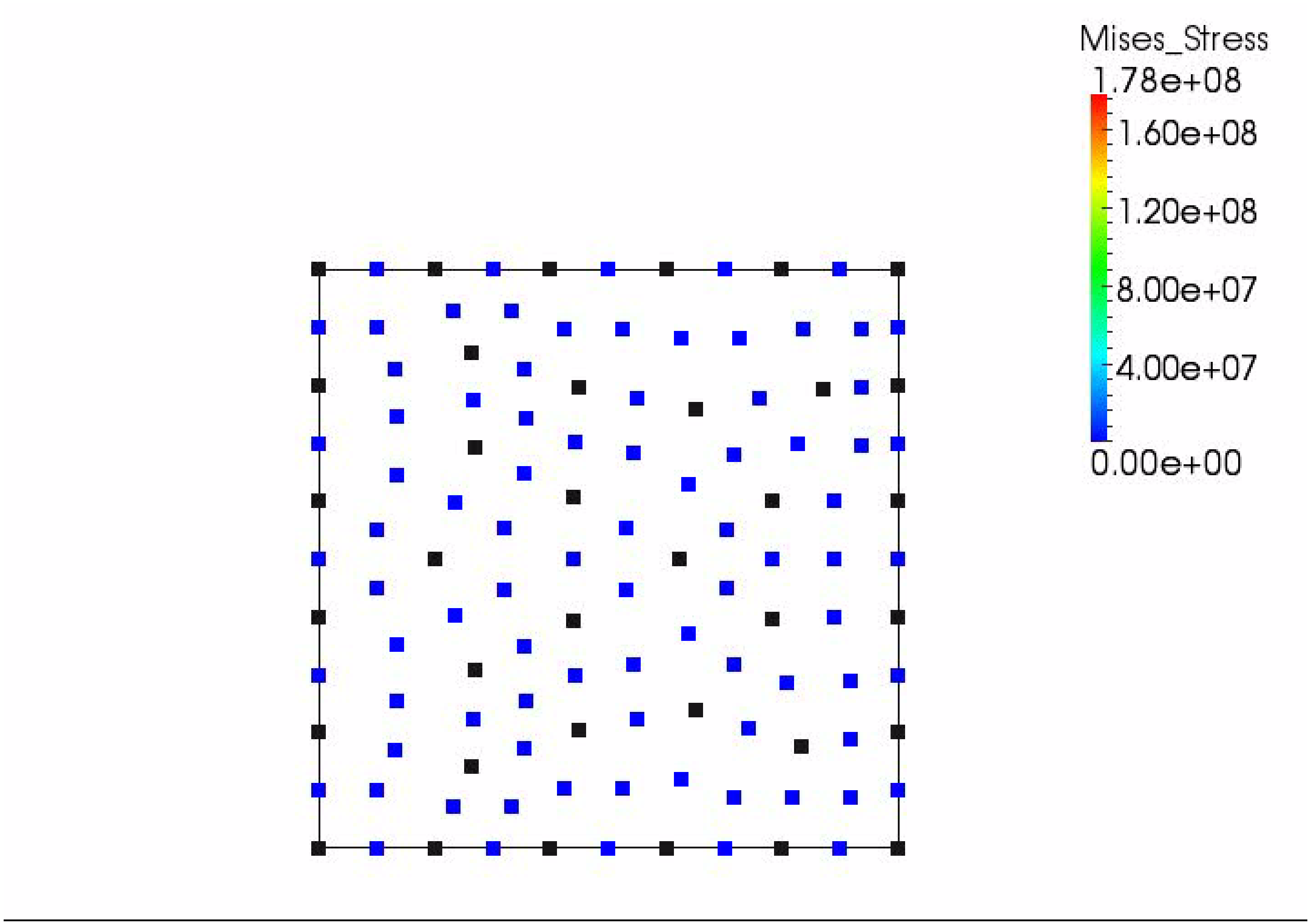


■ : node
■ : stress point (SP)

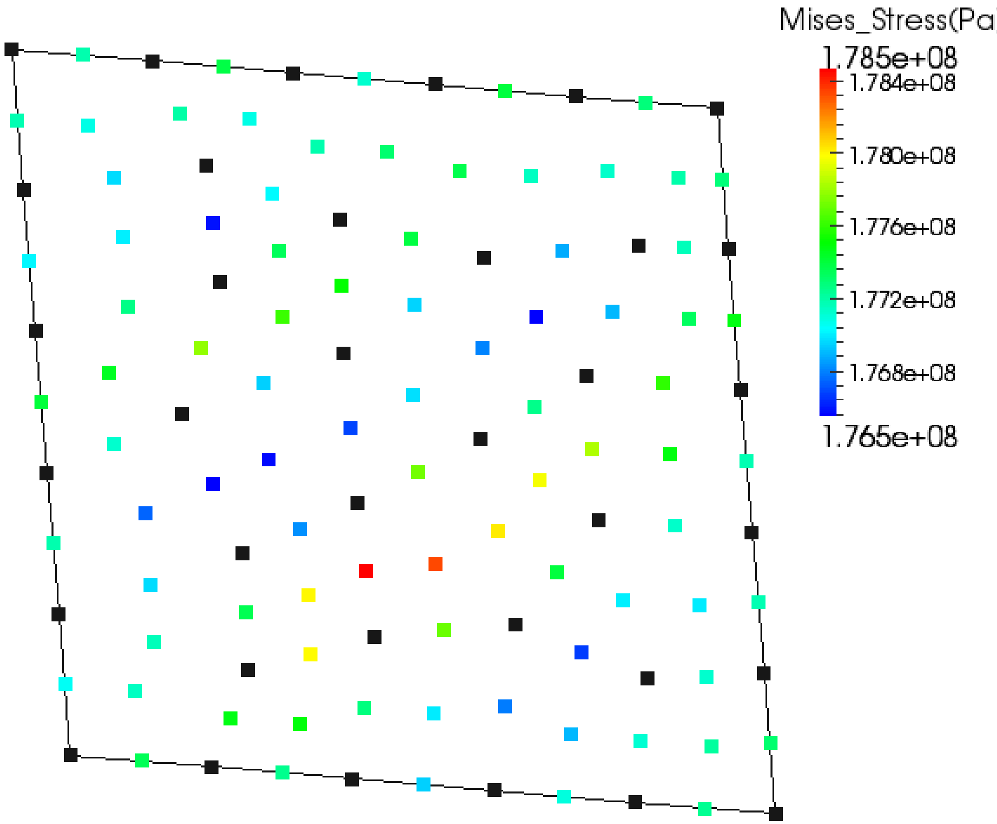
- Elastic body, Static, Plane-strain
- Irregularly-arranged nodes and SPs
- Displacement BC for every external nodes

$$\boldsymbol{u}(\boldsymbol{x}) = \begin{Bmatrix} 0.1 + 0.2x_1 - 0.1x_2 \\ 0.2 - 0.1x_1 + 0.2x_2 \end{Bmatrix}$$

Patch Test (animation)



Patch Test (result)



- within 1% error of Mises stress
- Proposed method passes the patch test