A Novel Meshfree Method for Large Deformation Analysis of Elastic and Viscoelastic Bodies without using Background Cells

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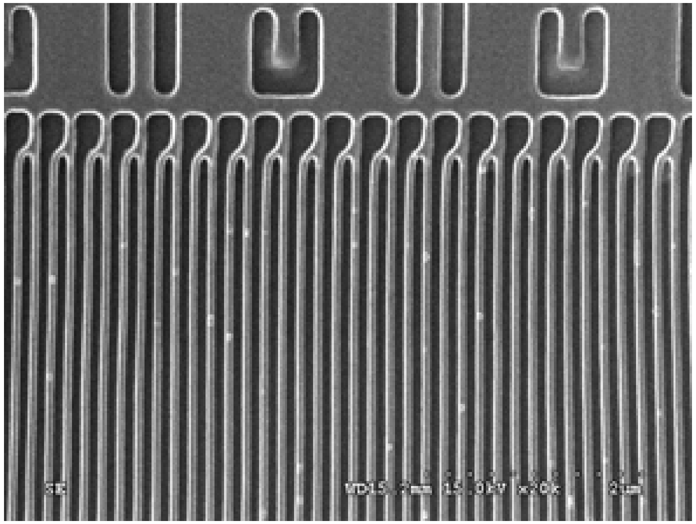
Background

- After the advent of nanoimprinting, micro hot embossing and thermal nanoimprinting have been in area of active research.
  - Pressing patterned mold onto **polymer or glass** to transcribe the pattern.
  - Better precision than photo lithography
  - A mechanical process
  - **Experiments cost high!**



J.W.Lee et al., EIPBN (2007)

- Goal

Establishment of numerical technique for thermal nanoimprint process optimization.

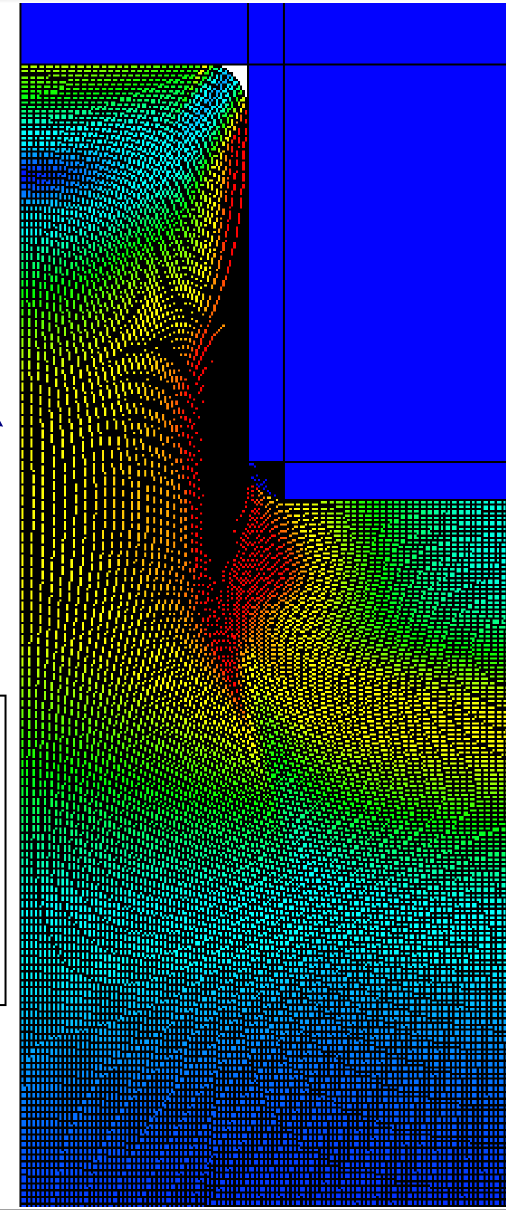
Our Previous Work

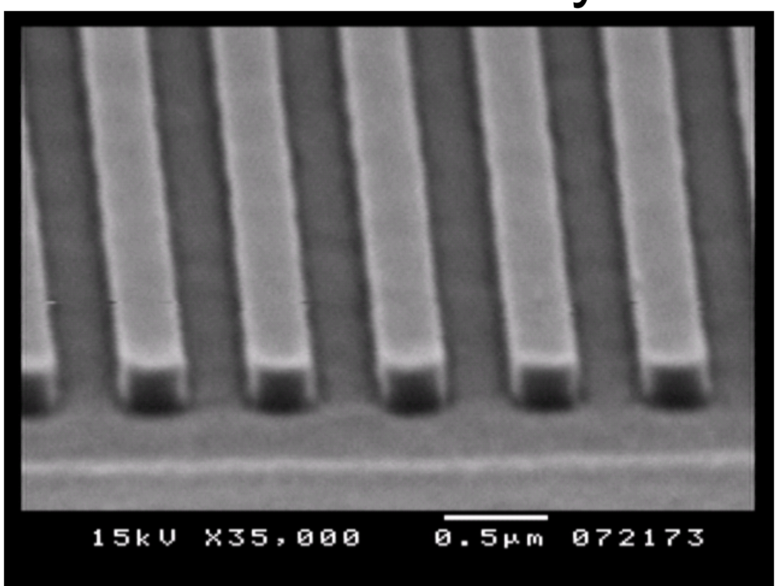
■ Finite element Analysis

- Geometric nonlinear (Large deformation)
- Material nonlinear (rigid mold and **viscoelastic** polymer)
- Contact nonlinear
- Quasi-static analysis

Mold (rigid)

Polymer (viscoelastic)

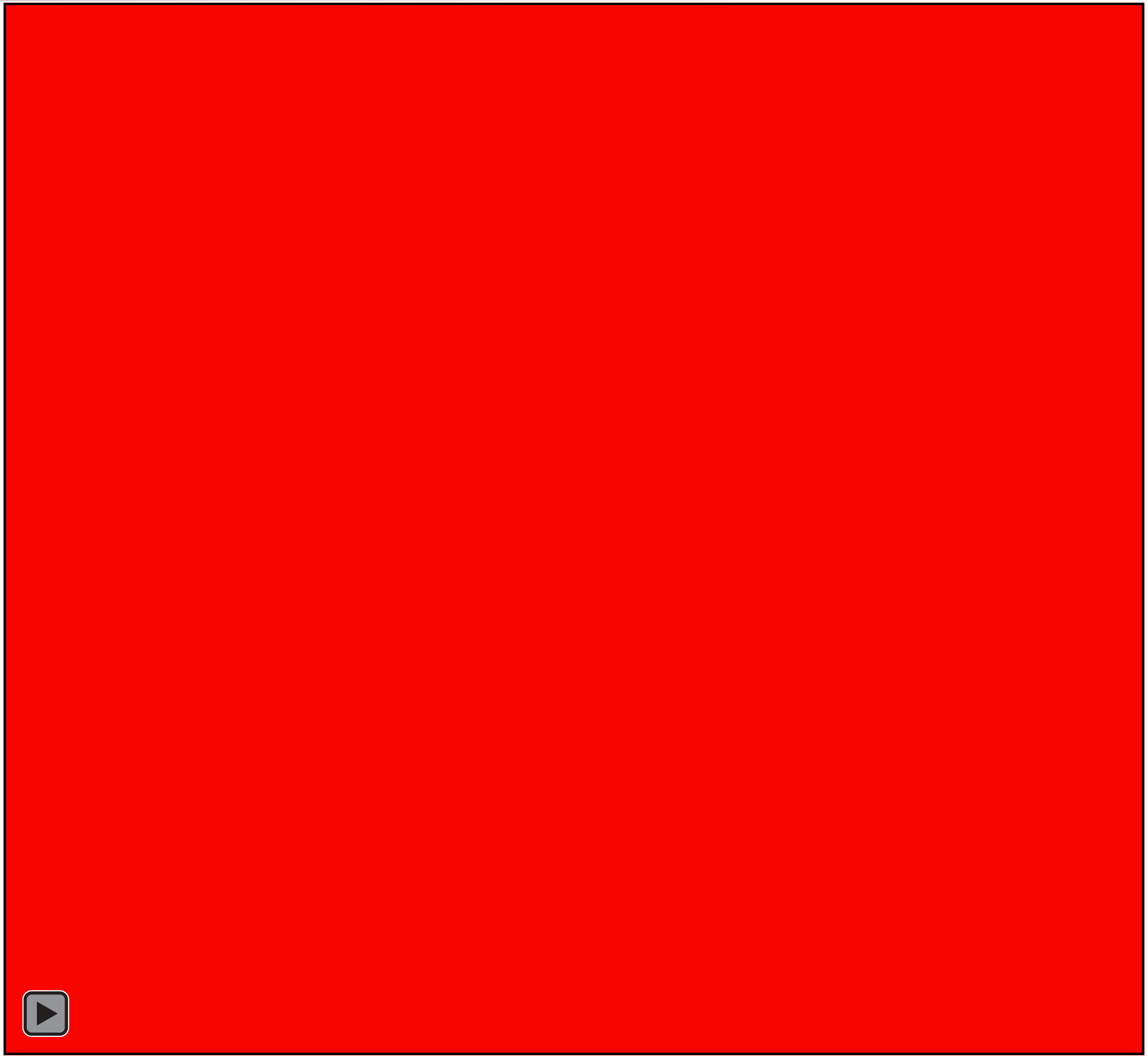




FE analyses agreed with experiments in case of line-and-space up to ***AR*=1**

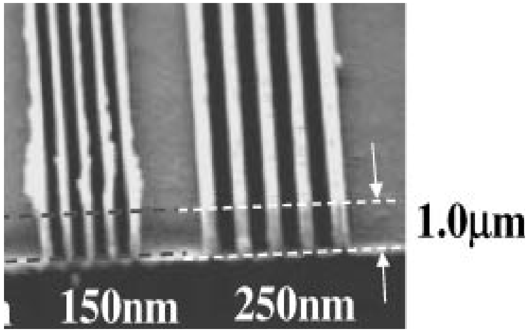
Onishi et al., JVST B (2008) etc.

Our Previous Work



Objective

Our previous work was incomplete…



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

Proposing Meshfree Formulation

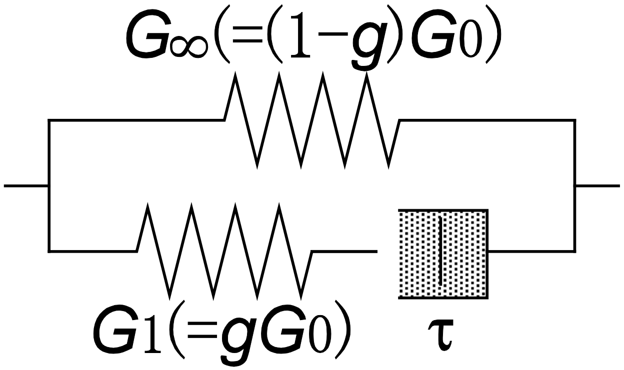
[4 Points]

1. Quasi-static analysis for viscoelastic body
2. Modified stress-point integration
3. Robust moving least squares (Robust MLS) with integration correction
4. Quasi-implicit time advancing

1. Viscoelastic Model

■ **Standard solid model** in shear
(the simplest generalized Maxwell model)

● Schematic diagram



G_∞ : long-term shear modulus
G_0 : instantaneous shear modulus
g : dimensionless shear modulus
τ : relaxation time

On the other hand, bulk modulus, *K*, is a constant.

● Constitutive equation

$$\boldsymbol{T} = K E^{\mathrm{vol}} \boldsymbol{I} + 2G_0(\boldsymbol{E}' - g\boldsymbol{E}^{\mathrm{v}\prime}).$$

$\boldsymbol{T}$: Cauchy stress, E^{vol} : logarithmic volumetric strain,
$\boldsymbol{E}'$: logarithmic deviatoric strain, $\boldsymbol{E}^{\mathrm{v}\prime}$: logarithmic viscous strain

1. Viscoelastic Model

■ 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

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

2. Modified SP Integration

Meshfree domain integration with BG cells is not suitable for large deformation.
There are 2 ways of domain integration without BG cells.

[1] Nodal integration (J. S. Chen)

merit) very simple.
generation of stress-points is not necessary.

demerit) zero-energy mode arise without **artificial stabilization**. (similar to hour-glass modes in FEM)

[2] Stress-point (SP) integration (T. Belytschko)

merit) **artificial stabilization** is not essential.

demerit) generation and translation of stress-points are required.

No practical SP integration scheme for large deformation analysis was developed so far.

→

We introduce a SP integration modified for large deformation analysis.

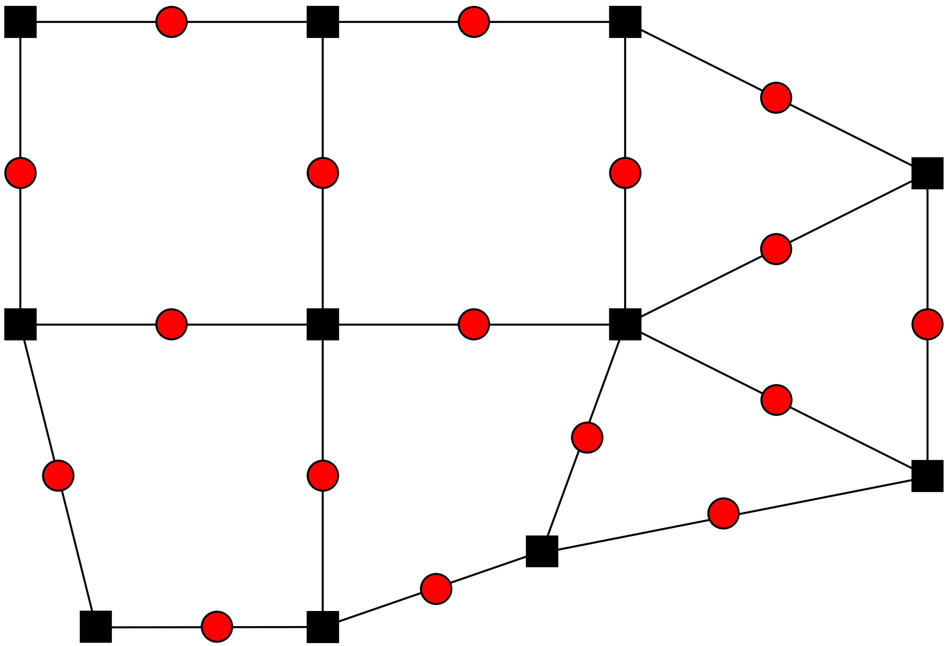
2. Modified SP Integration (initialization)

- (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***, ***E***^{v}, etc.)



2. Modified SP Integration (updates)

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

■ Location

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

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

ϕ: shape function

■ Volume

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

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

3. Robust MLS (approximation)

■ Weight function

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

not bell shape

but mountain shape

■ Support radius

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

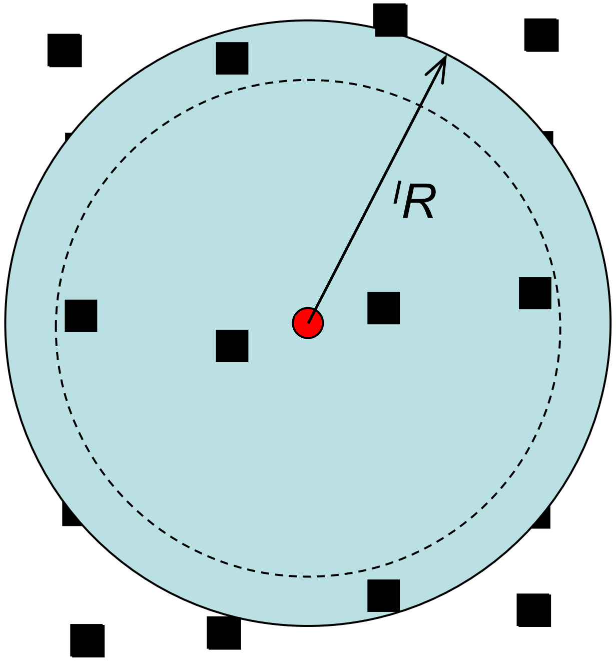
begin loop $\quad \boldsymbol{p} = \{1, x, y\}^T$

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

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

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

end loop



3. Robust MLS (integration correction)

■ Integration constraint

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

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

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 γs so that modified ψs satisfy reproducing constraints including integration constraint

4. Quasi-implicit Time Advancing

- Start of time increment loop

Typical fully-implicit
time advancing

  - 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

4. Quasi-implicit Time Advancing

■ Start of time increment loop

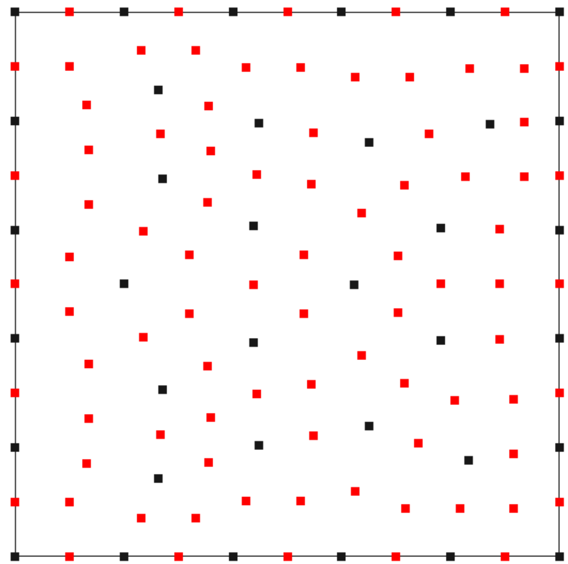
- update support, w, ϕ, etc.
- renew $\boldsymbol{f}^{\text{virtual}}$
- Start of Newton-Raphson loop
  - ◆ update support, w, ϕ, etc.
  - ◆ calc $\boldsymbol{f}^{\text{int.}}$ and $\boldsymbol{K}$
  - ◆ calc $\boldsymbol{r} = \boldsymbol{f}^{\text{int.}} - \boldsymbol{f}^{\text{ext.}} - \boldsymbol{f}^{\text{virtual}}$
  - ◆ 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

Patch Test

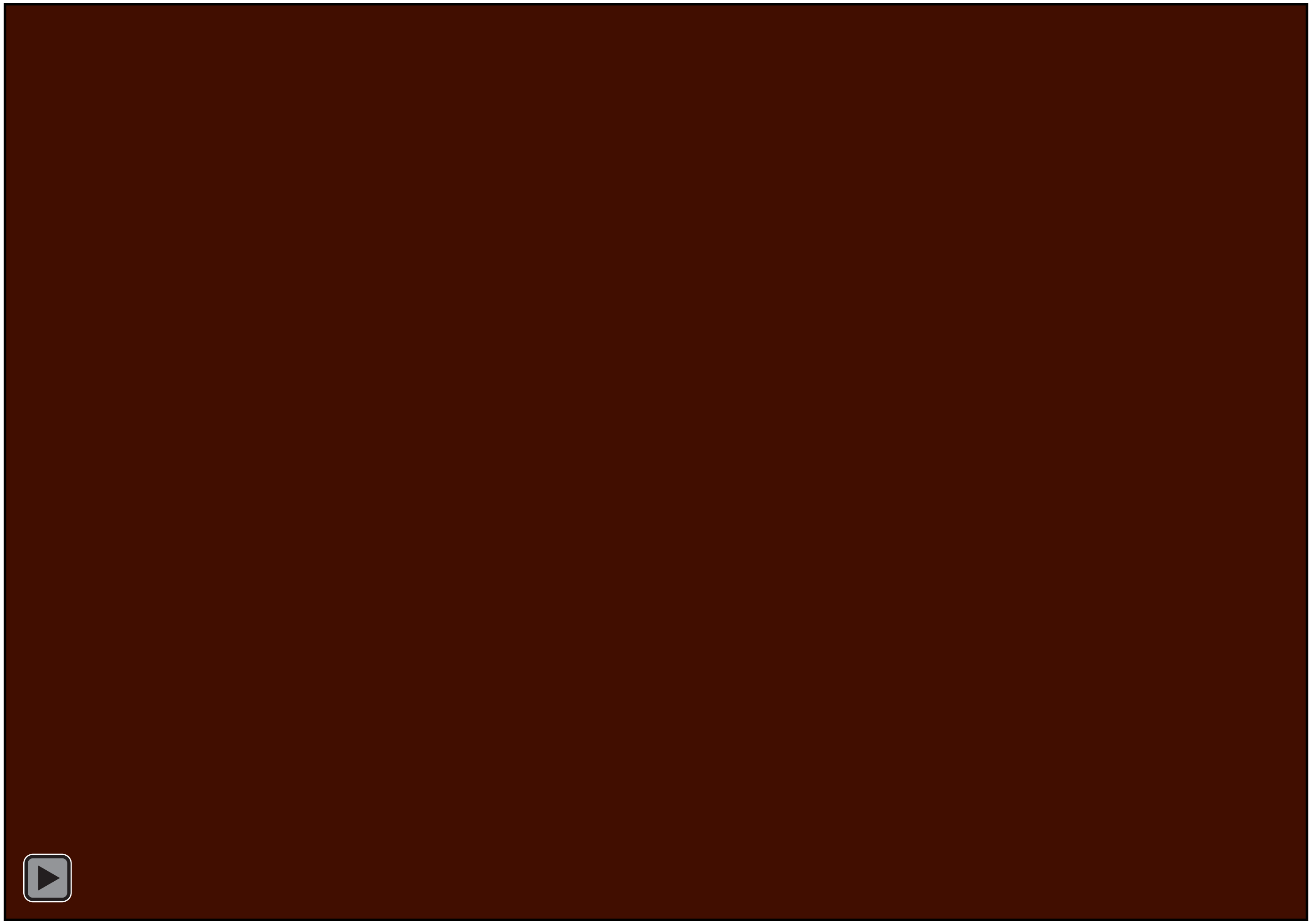


- ■ : node
- ■ : stress point (SP)

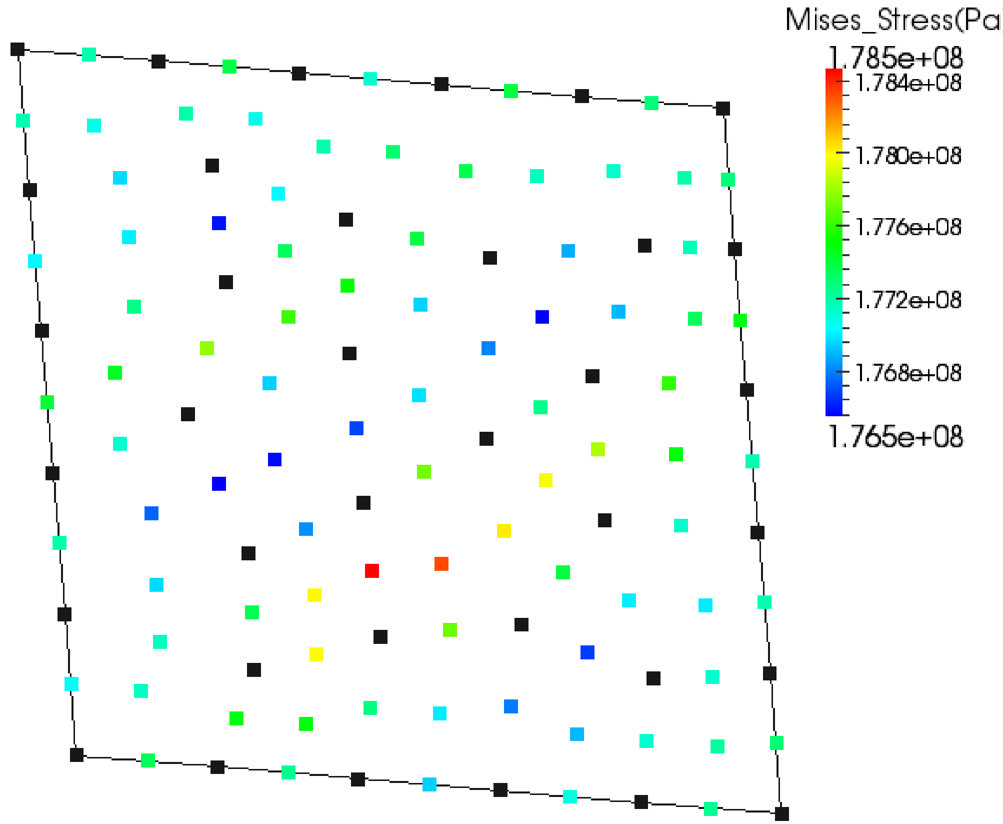
- Elastic body, Static, Plane-strain
- Irregularly-arranged nodes and SPs
- Displacement BC for every external nodes

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

Patch Test (animation)

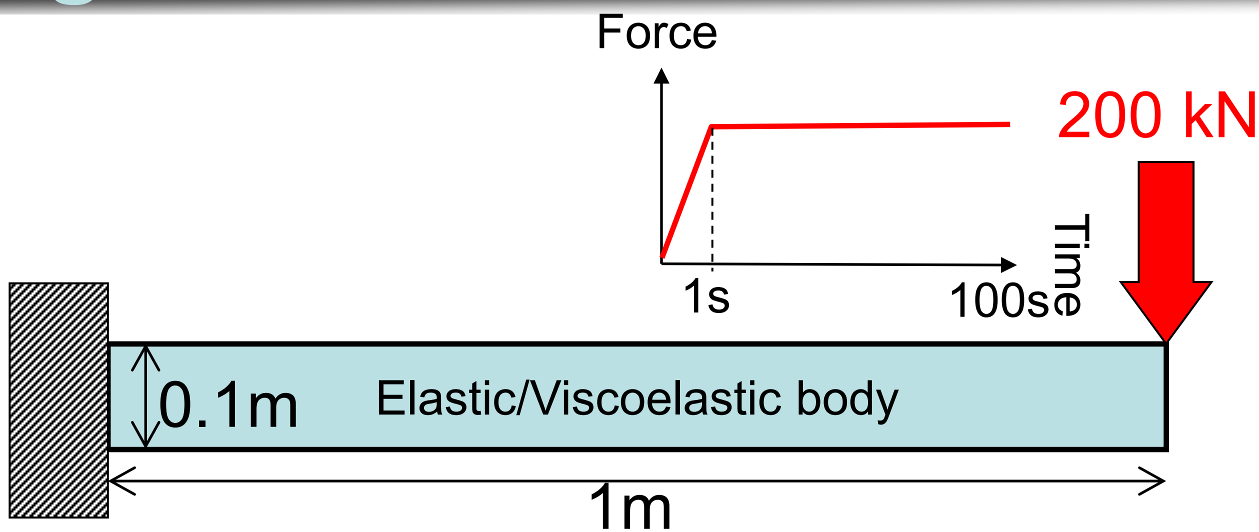


Patch Test (result)



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

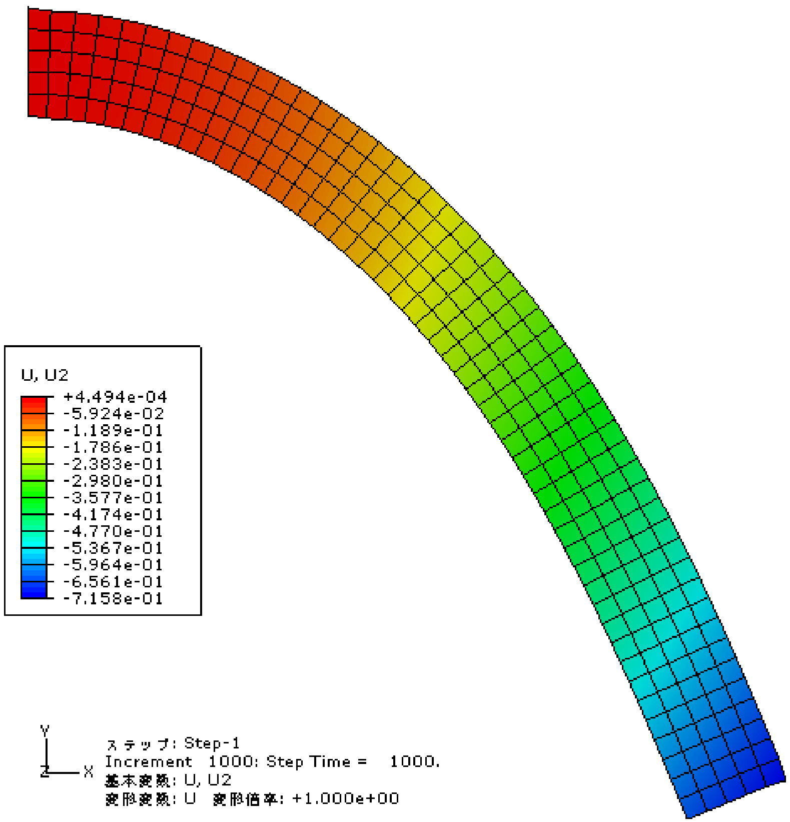
Bending of Cantilever



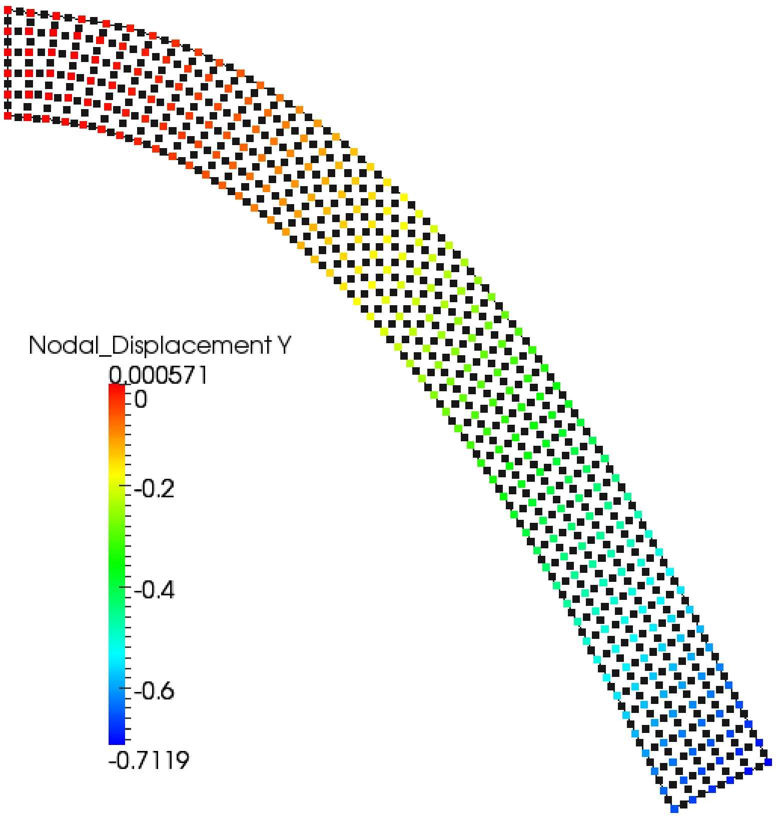
- Static/Quasi-static, Plane strain
- 50x5 structured grid nodes
- Concentrated force at right-top node
- Compared to FEM(ABAQUS/Standard) with same node arrangements and selective reduced integration quadrangle elements

Bending of Cantilever (elastic)

E=1GPa, ν=0.481



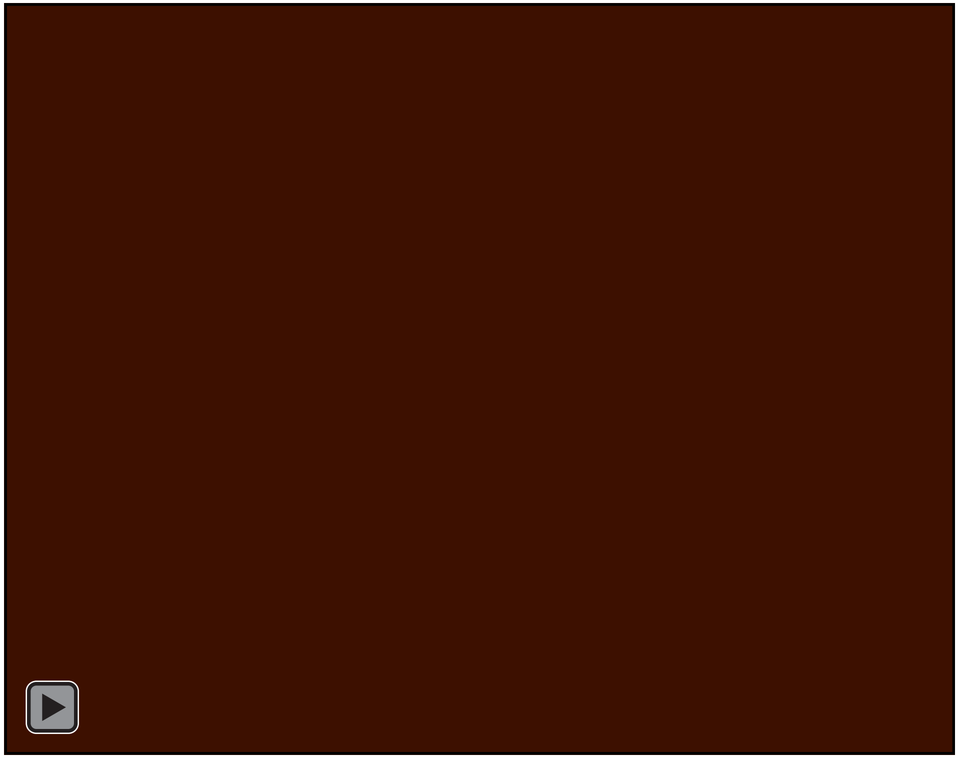
ABAQUS/Standard



Proposed Method

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

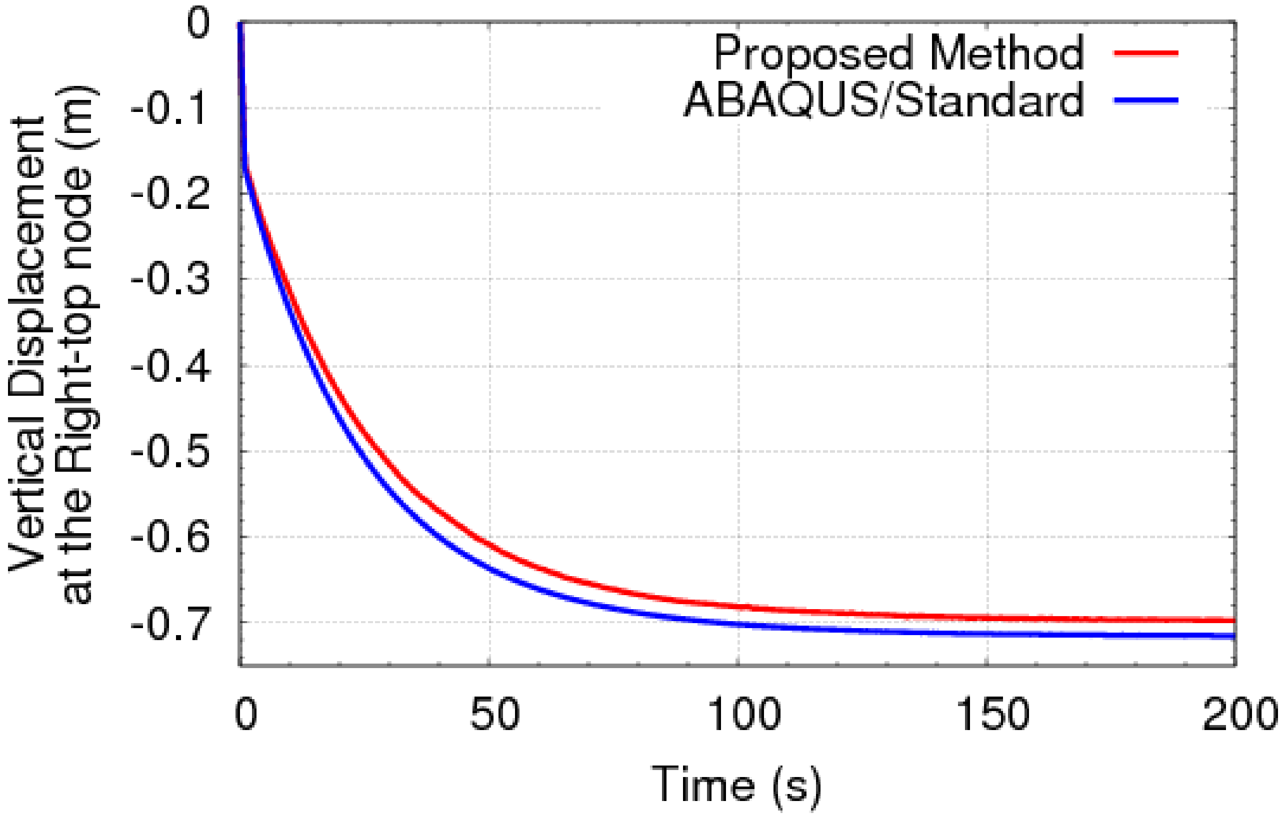
Bending of Cantilever (viscoelastic)



ABAQUS/Standard

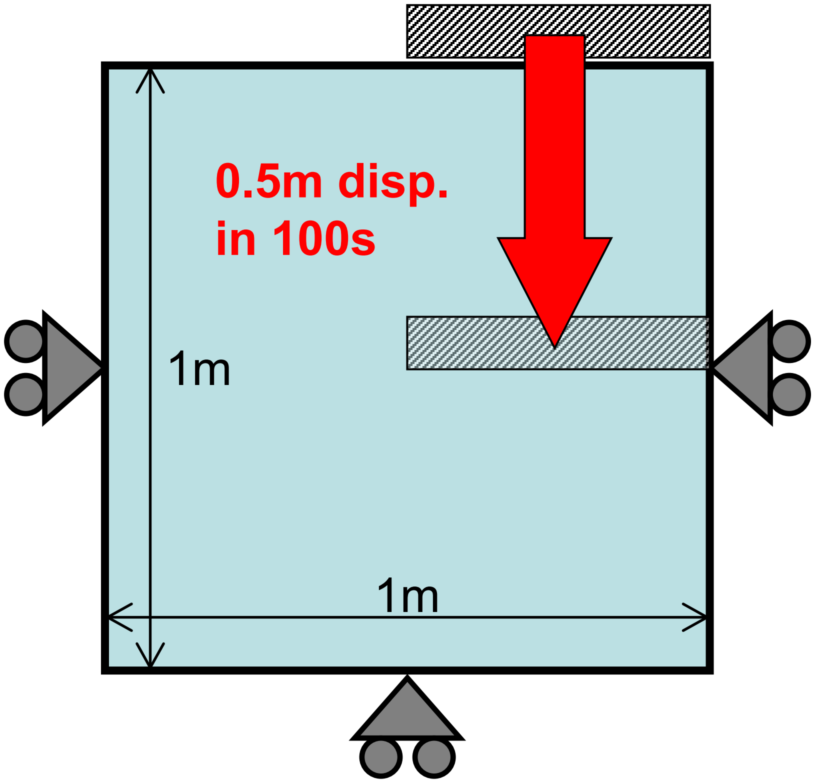
Proposed Method

Bending of Cantilever (viscoelastic)



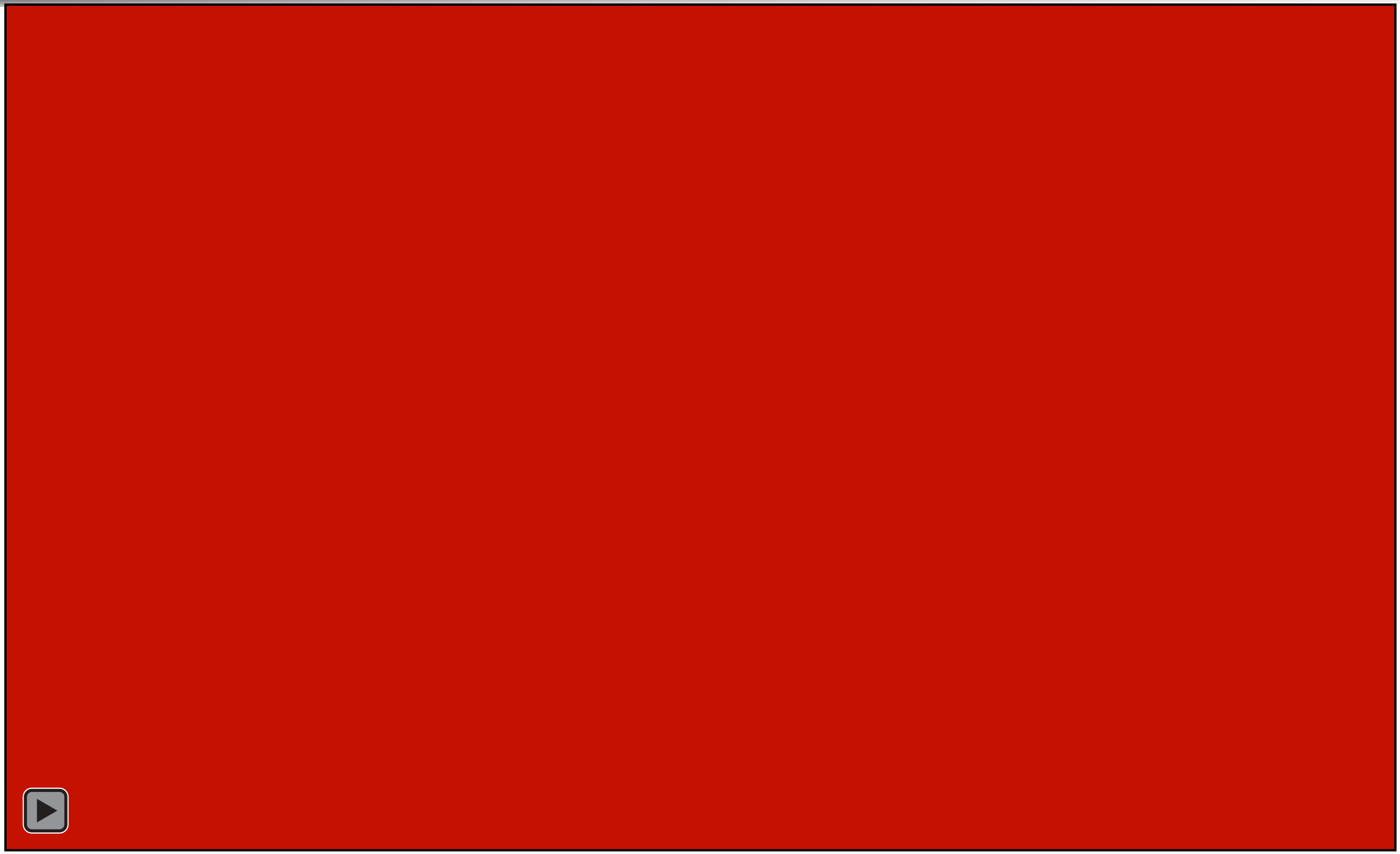
- 2.5% error of displacement
- Error decreases as d*t* decreases
- Further improvement of time-advancing scheme is necessary

Imprinting-like Analysis



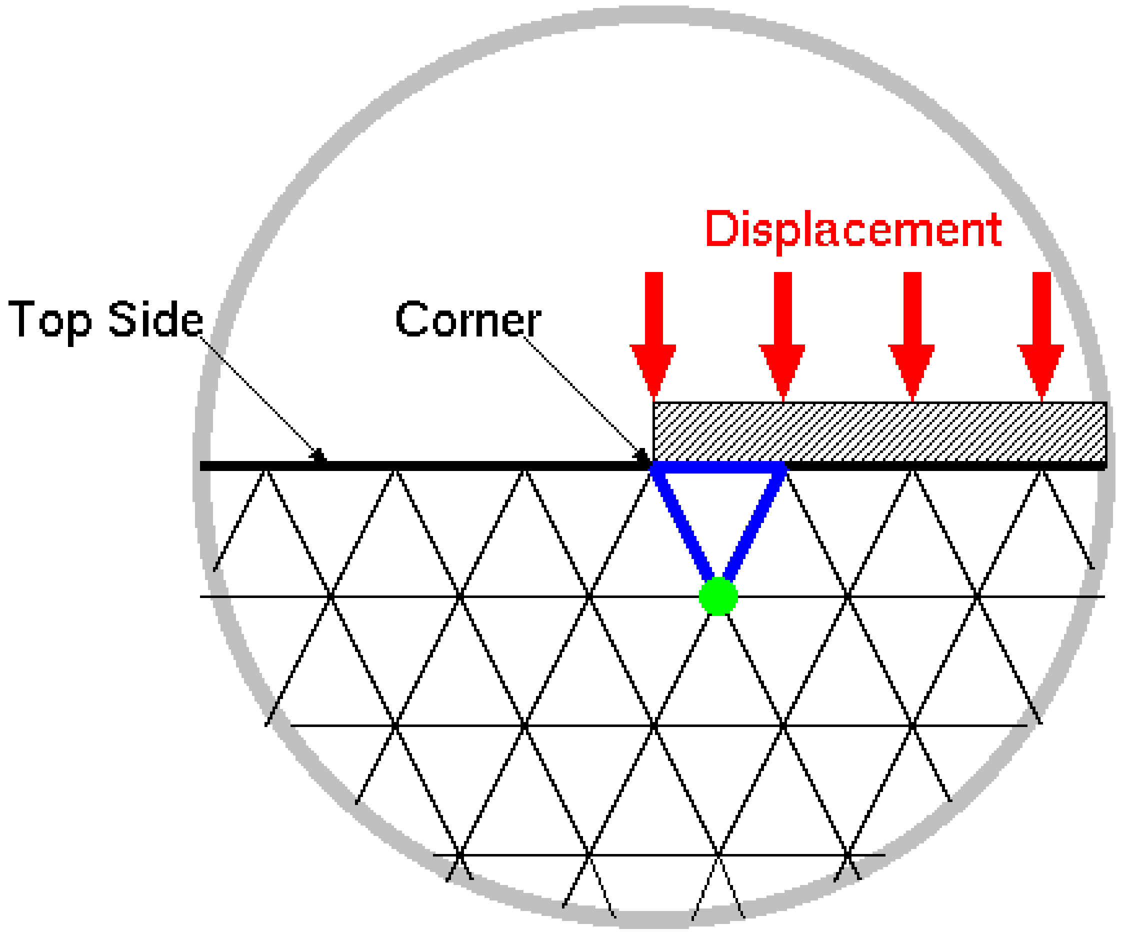
- Quasi-static, plane strain
- Horizontal bounding for left and right side
- Vertical bounding for bottom side
- Enforced displacement for right half of top side toward downward with horizontal bounding
- Unstructured grid with fineness and coarseness

Imprinting-like Analysis (FEM)

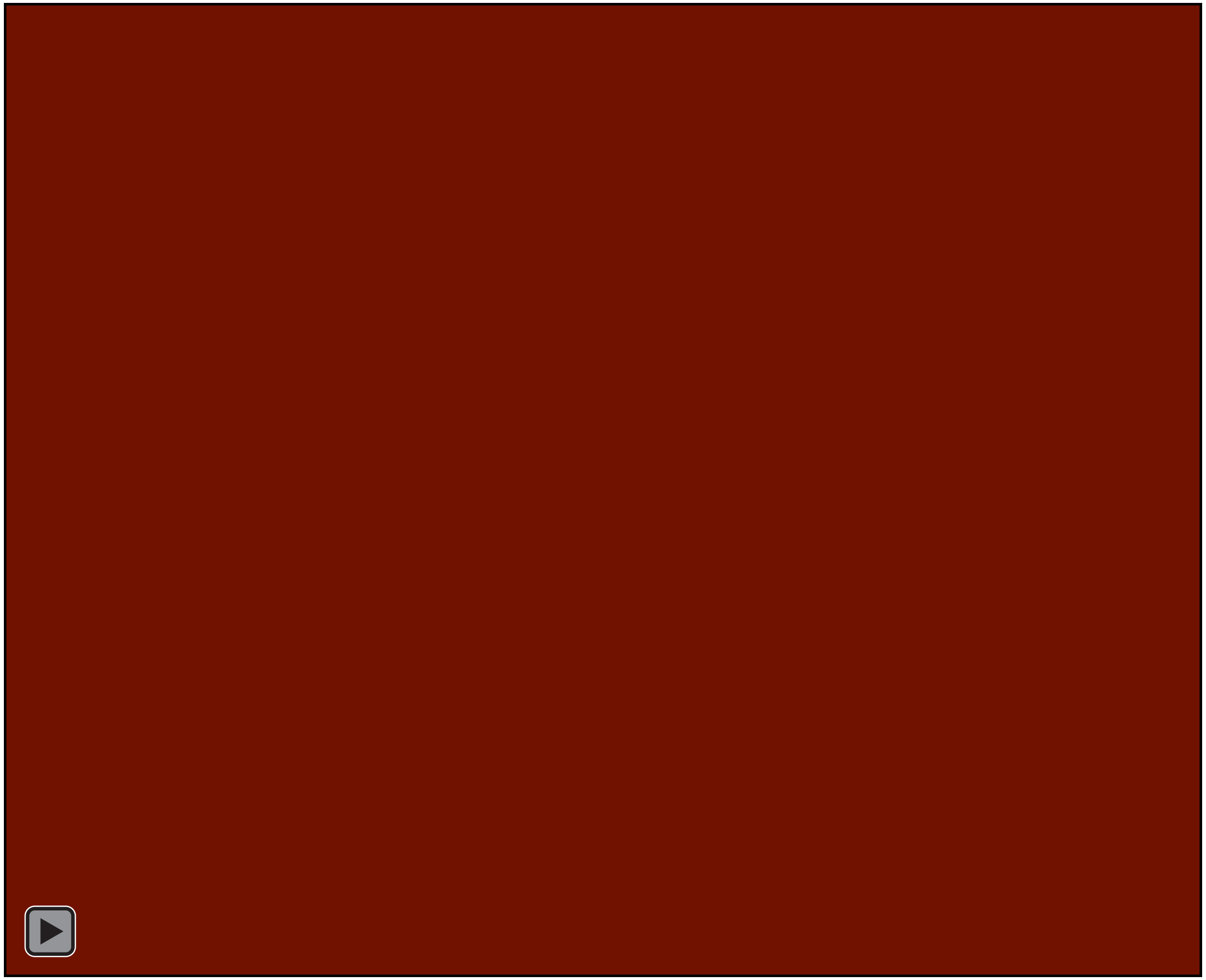


- Inappropriate deformation because of the locking under the corner

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 without BG cells was proposed.
- It passes the patch test.
- 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