Build your own 2D simulator

2D Hyperelastic materials using the Finite Volume Method

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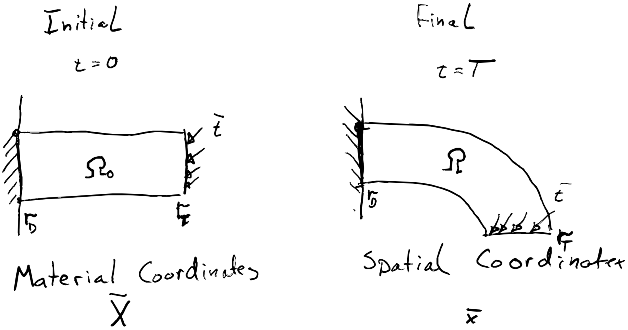
The Problem


Initial
t = 0
Ω0
Γ_D
Γ_T
Material Coordinates
X
Final
t = T
Ω
Γ_D
t
Γ_T
Spatial Coordinates
x

The Idealization Process (1/2)

We have the Cauchy equation (motion of equation).

$$\rho_0 \ddot{\mathbf{x}} = \mathbf{b}_0 + \nabla_{\mathbf{X}} \cdot \mathbf{P}, \quad \forall \mathbf{X} \in \Omega_0 \,.$$

Subscript 0 means the physical quantity is given in material coordinate spaces, $\mathbf{X}$. Spatial coordinates are written as $\mathbf{x}$ and not $\mathbf{X}$.

We will apply boundary conditions for a known traction field $\mathbf{t}$ on the boundary, Γ_T,

$$\mathbf{PN} = \mathbf{t}, \quad \forall \mathbf{X} \in \Gamma_T$$

As well as Dirichlet conditions to keep a subset of the boundary fixed, Γ_D,

$$\mathbf{x} = \text{const}, \quad \forall \mathbf{X} \in \Gamma_D$$

The Idealization Process (2/2)

We use a constitutive equation between 2nd Piola–Kirchhoff stress tensor and Green strain tensor

$$\mathbf{S} = \lambda \mathrm{tr}\left(\mathbf{E}\right)\mathbf{I} + 2\mu\mathbf{E}$$

which is related to the 1st Piola Kirchhoff stress tensor

$$\mathbf{P} = \mathbf{F}\mathbf{S}$$

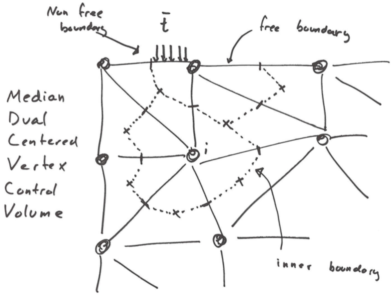
and the Green strain is by definition given as

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I})$$

Discretization Choices That is Given

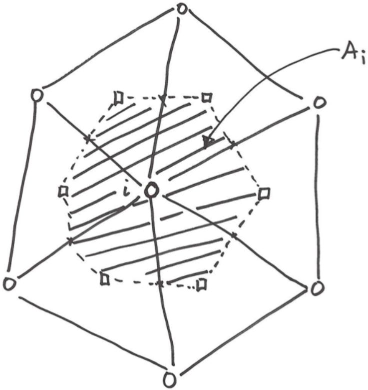
- We will use a finite volume method.
- We will use a 2D triangular computational domain.
- We will use median dual vertex centered control volume.
- We will assume that deformation gradients are constant over triangular elements.
- We will use simple first-order forward finite difference approximations in time.

The Computational Mesh

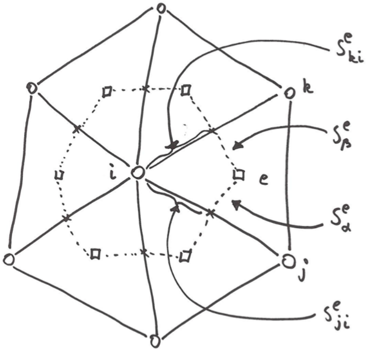


Observe we have three types of ”real” boundaries, Γ_T and Γ_D are both non-free kinds of boundaries, and the third is the ”free” boundary. The inner boundary is not a real boundary, it is just the interface between the computational cells.

The Cell Notation



The Boundary Notation



We use $\gamma \in \{\alpha, \beta, ji, ki\}$ as index in summations so S^e_γ means S^e_α, S^e_β, S^e_{ji}, and S^e_{ki}.

Write up Volume Integrals

Let A_i denote the control volume of the i^{th} vertex

$$\int_{A_i} \rho_0 \ddot{\mathbf{x}}_i dA = \int_{A_i} \mathbf{b}_0 dA + \int_{A_i} \nabla_{\mathbf{X}} \cdot \mathbf{P} dA$$

With some hard work using Leibniz rule, Piecewise continuity of integrals, Midpoint approximation rule, and Gauss–Divergence Theorem. One derives

$$m_i \ddot{\mathbf{x}}_i = \underbrace{A_i \mathbf{b}_0}_{\equiv \mathbf{f}_i^{\text{ext}}} + \sum_e \sum_\gamma \int_{S_\gamma^e} \mathbf{P}\mathbf{N} dS$$

where γ runs over all boundary surfaces, ie. it can be α, β or some ji, ki. The nodal mass is $m_i = A_i \rho_0$. The superscript on $\mathbf{f}^{\text{ext}}$ indicates this force term is an external force on the system.

The Boundary Conditions

If S_γ^e is on the boundary of the domain we can apply the boundary condition $\mathbf{t} = \mathbf{PN}$.

- On the "free" boundary we have $\mathbf{t} = 0$ so

$$\int_{S_\gamma^e} \mathbf{PN} dS = 0$$

- For non-free we have prescribed known constant traction $\mathbf{t}$ so

$$\int_{S_\gamma^e} \mathbf{PN} dS = \mathbf{t} l_\gamma^e$$

  where l_γ^e is the length of piece wise linear boundary S_γ^e.

Meaning we can restrict the boundary summation to internal boundaries only.

The Traction Forces

Thus,

- We split out the terms from non-free boundaries

$$m_i \ddot{\mathbf{x}}_i = \mathbf{f}_i^{\text{ext}} + \mathbf{f}_i^t + \sum_\gamma \int_{S_\gamma^e} \mathbf{P}\mathbf{N} dS$$

  Now γ is only running over internal boundary edges (α or β for each e) and δ over external boundaries

$$\mathbf{f}_i^t \equiv \sum_\delta \mathbf{t} l_\delta^e$$

- The vector $\mathbf{f}_i^t$ is termed the “nodal” traction force to distinguish it from the traction field $\mathbf{t}$.

Computing the Deformation Gradient

Consider the e^{th} triangle consisting of nodes i, j and k. Recall

$$d\mathbf{x} = \mathbf{F}d\mathbf{X}$$

Define $\mathbf{g}^e_{ji} = \mathbf{x}_j - \mathbf{x}_i$ and $\mathbf{G}^e_{ji} = \mathbf{X}_j - \mathbf{X}_i$ and so on. Now

$$\mathbf{g}^e_{ji} = \mathbf{F}^e\mathbf{G}^e_{ji} \text{ and } \mathbf{g}^e_{ki} = \mathbf{F}^e\mathbf{G}^e_{ki}$$

Putting it together

$$\underbrace{\begin{bmatrix}\mathbf{g}^e_{ji} & \mathbf{g}^e_{ki}\end{bmatrix}}_{\mathbf{D}^e} = \mathbf{F}^e \underbrace{\begin{bmatrix}\mathbf{G}^e_{ji} & \mathbf{G}^e_{ki}\end{bmatrix}}_{\mathbf{D}^e_0}$$

Now we can compute the deformation gradient as $\mathbf{F}^e = \mathbf{D}^e \left(\mathbf{D}^e_0\right)^{-1}$.

Computing the Stress and Strain Tensors

As $\mathbf{F}^e$ is known and constant over e then we may compute the Green strain tensor

$$\mathbf{E}^e = \frac{1}{2}\left(\left(\mathbf{F}^e\right)^T \mathbf{F}^e - \mathbf{I}\right)$$

and the 2nd Piola–Kirchhoff tensor

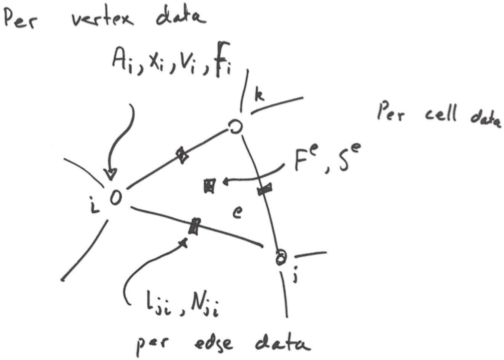
$$\mathbf{S}^e = \lambda \operatorname{tr}\left(\mathbf{E}^e\right)\mathbf{I} + 2\mu\mathbf{E}^e$$

and finally 1st Piola–Kirchhoff tensor

$$\mathbf{P}^e = \mathbf{F}^e\mathbf{S}^e$$

Observe that since $\mathbf{F}^e$ is constant per triangle so will $\mathbf{S}^e$ and $\mathbf{P}^e$ be.

The Grid Layout



Observe that $\mathbf{P}^e$ and $\mathbf{E}^e$ are also stored at face centers.

Computing Boundary Integrals $\int_{S_\gamma^e} \mathbf{P}\mathbf{N} dS$

In the usual FVM approach one would apply the midpoint approximation rule, hence

$$\int_{S_\gamma^e} \mathbf{P}\mathbf{N} dS \approx \mathbf{P}^e \mathbf{N}_\gamma^e l_\gamma^e$$

Second thoughts

- $\mathbf{P}^e$ is constant over the entire triangle so we know its value at the midpoint
- We need to pre-compute $\mathbf{N}_\gamma^e$ and l_γ^e.

As our control volume looks a bit “complex” the last parts can be a bit “difficult” to implement.

The “Clever” Approach (1/2)

Observation: The closed surface integral over a constant tensor field is always zero

$$\oint_S \mathbf{P}\mathbf{N} dS = 0$$

For e^{th} triangle we make the “imaginary” closed surface integral

$$\int_{S^e_{ji}} \mathbf{P}^e \mathbf{N} dS + \int_{S^e_{jk}} \mathbf{P}^e \mathbf{N} dS + \int_{S^e_{\alpha}} \mathbf{P}^e \mathbf{N} dS + \int_{S^e_{\beta}} \mathbf{P}^e \mathbf{N} dS = 0$$

We then slightly rewrite this into

$$\int_{S^e_{\alpha}} \mathbf{P}^e \mathbf{N} dS + \int_{S^e_{\beta}} \mathbf{P}^e \mathbf{N} dS = -\int_{S^e_{ji}} \mathbf{P}^e \mathbf{N} dS - \int_{S^e_{jk}} \mathbf{P}^e \mathbf{N} dS$$

The “Clever” Approach (2/2)

We have found the equivalence relation from the fact that we have constant stress tensors,

$$\int_{S^e_\alpha} \mathbf{P}^e \mathbf{N} dS + \int_{S^e_\beta} \mathbf{P}^e \mathbf{N} dS = -\int_{S^e_{ji}} \mathbf{P}^e \mathbf{N} dS - \int_{S^e_{jk}} \mathbf{P}^e \mathbf{N} dS$$

This means in computations we can now replace the sum of the surface integrals S^e_α and S^e_β with the negative sum of the surface integrals S^e_{ji} and S^e_{jk}. The numerical values will be equivalent.

Having done the replacement we are now ready to apply the midpoint approximation rule

The Midpoint Approximation Rule

After the replacement of the equivalent surface integrals we have,

$$\mathbf{f}_i^e \equiv -\int_{S_{ji}^e} \mathbf{P}^e \mathbf{N} dS - \int_{S_{jk}^e} \mathbf{P}^e \mathbf{N} dS$$

Using midpoint approximation rule and observing that $\mathbf{l}_{ji} = \| \mathbf{X}_j - \mathbf{X}_i \|$, we have,

$$\mathbf{f}_i^e \equiv -\frac{1}{2} \mathbf{P}^e \mathbf{N}_{ji}^e \mathbf{l}_{ji} - \frac{1}{2} \mathbf{P}^e \mathbf{N}_{ki}^e \mathbf{l}_{ki}$$

Thus, we have

$$m_i \ddot{\mathbf{x}}_i = \mathbf{f}_i^{\text{ext}} + \mathbf{f}_i^t + \sum_e f_i^e$$

Time Discretization

We have

$$m_i \ddot{\mathbf{x}}_i = \underbrace{\mathbf{f}_i^{\text{ext}} + \mathbf{f}_i^{t} + \sum_e f_i^e}_{\equiv \mathbf{f}_i^{\text{total}}}$$

From nodal velocity $\mathbf{v}_i = \dot{\mathbf{x}}_i$ we have coupled first order ODEs

$$\dot{\mathbf{v}}_i = \frac{1}{m_i}\mathbf{f}_i^{\text{total}}$$

$$\dot{\mathbf{x}}_i = \mathbf{v}_i$$

Apply first-order finite difference approximations

$$\mathbf{v}_i^{t+\Delta t} = \mathbf{v}_i^{t} + \frac{\Delta t}{m_i}\mathbf{f}_i^{\text{total}}$$

$$\mathbf{x}_i^{t+\Delta t} = \mathbf{x}_i^{t} + \Delta t \mathbf{v}_i^{t+\Delta t}$$

Notice that the velocity update is explicit whereas the position update is implicit.

The Final Numerical Method

A single simulation step:

- Step 1 Compute deformation gradients $\mathbf{F}^e$ for all e
- Step 2 Compute Green strain tensors $\mathbf{E}^e$ for all e
- Step 3 Compute 2nd Piola–Kirchhoff stress tensor $\mathbf{S}^e$ for all e
- Step 4 Compute 1st Piola–Kirchhoff stress tensor $\mathbf{P}^e$ for all e
- Step 5 Compute elastic forces $\sum_e \mathbf{f}_i^e$ for all i
- Step 6 Compute total forces $\mathbf{f}_i^{\text{total}}$ for all i
- Step 7 Compute velocity update $\mathbf{v}_i^{t+\Delta t}$ for all i
- Step 8 Compute position update $\mathbf{x}_i^{t+\Delta t}$ for all i
- Step 9 Increment time $t \leftarrow t + \Delta t$

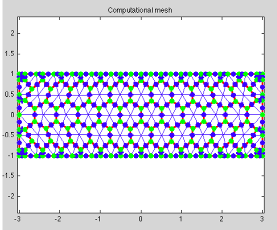
The Input Parameters

- The triangle mesh
- The surface traction field $\mathbf{t}$ (if any)
- The material density field ρ_0
- The body force density field $\mathbf{b}_0$
- The Lamé parameters λ and μ
- The time step size Δt

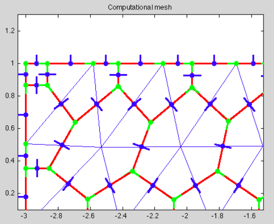
Tip: Getting A Computational Mesh for Free

Code reusability is good:

- FVM handout has meshing tool for centroid dual vertex centered control volume



Computational Mesh



Zoomed View

This can be modified to a median dual vertex-centered control volume.

The Model Collapse

Assume compression/extension in the x-axis then

$$\mathbf{x} = \begin{bmatrix} a & 0 \\ 0 & 1 \end{bmatrix} \mathbf{X}$$

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \begin{bmatrix} a & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} = \begin{bmatrix} a^2 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{E} = \frac{1}{2} \left(\mathbf{C} - \mathbf{I} \right) = \begin{bmatrix} \frac{1}{2}\left(a^2 - 1\right) & 0 \\ 0 & 0 \end{bmatrix}$$

$$\mathbf{S} = \lambda \operatorname{tr}\left(\mathbf{E}\right) \mathbf{I} + 2\mu \mathbf{E} = \begin{bmatrix} \left(\mu + \frac{\lambda}{2}\right)\left(a^2 - 1\right) & 0 \\ 0 & \frac{\lambda}{2}\left(a^2 - 1\right) \end{bmatrix}$$

The Model Collapse

Rewrite stress tensor

$$\mathbf{S} = \begin{bmatrix} \left(\mu + \frac{\lambda}{2}\right)\left(a^2 - 1\right) & 0 \\ 0 & \frac{\lambda}{2}\left(a^2 - 1\right) \end{bmatrix}$$

$$\mathbf{P} = \mathbf{FS} = \begin{bmatrix} a & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \left(\mu + \frac{\lambda}{2}\right)\left(a^2 - 1\right) & 0 \\ 0 & \frac{\lambda}{2}\left(a^2 - 1\right) \end{bmatrix}$$

$$= \begin{bmatrix} \left(\mu + \frac{\lambda}{2}\right)\left(a^3 - a\right) & 0 \\ 0 & \frac{\lambda}{2}\left(a^2 - 1\right) \end{bmatrix}$$

The Model Collapse

Let $\alpha = \left(\mu + \frac{\lambda}{2}\right)$, $\beta = \frac{\lambda}{2}$ then

$$\mathbf{P} = \begin{bmatrix} \alpha\left(a^3 - a\right) & 0 \\ 0 & \beta\left(a^2 - 1\right) \end{bmatrix}$$

We can consider $\alpha > 0$ as Lamé first parameter λ is always positive and the second μ is positive for most materials too.

The Model Collapse

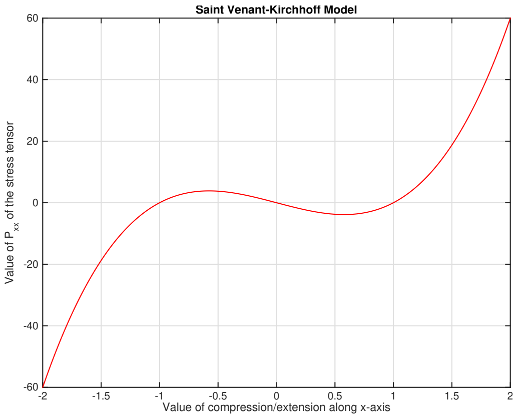
From

$$\mathbf{P}_{xx} = \alpha \left(a^3 - a \right)$$

We make the plot on the right.

Observe, no response for $a = 0$ and $a \pm 1$.

For $|a| < \frac{1}{\sqrt{3}} \approx 0.57$ material no longer resists compression.



Assignment

- Show all the steps from the initial volume integral on top of Page 9 to the discrete form at the bottom that only contains the piece-wise linear surface integrals.
- Observe that we wrote the Cauchy equation using "material" space as the domain rather than the usual "spatial" setting given as

$$\rho\ddot{\mathbf{x}} = \mathbf{b} + \nabla \cdot \sigma$$

Note that in the material setting we have $\mathbf{x}(\mathbf{X})$ whereas in the spatial setting we simply have $\mathbf{x}$. Show how to get from the spatial setting to the material setting[1]?

Assignment

- Discuss computational benefits of $\mathbf{F}^e = \mathbf{D}^e \left(\mathbf{D}_0^e\right)^{-1}$ on Page 12 Hint: What can be pre-computed?
- Discuss mesh properties needed to make sure $\mathbf{D}_0^e$ is invertible.

Assignment

- Assume a FEM approach with the local linear shape functions

$$w_i^e(\mathbf{X}) = \frac{A(\mathbf{X}_j, \mathbf{X}_k, \mathbf{X})}{A(\mathbf{X}_i, \mathbf{X}_j, \mathbf{X}_k)}$$

  where the A's are areas of respective triangles. For any point $\mathbf{X}$ inside the triangle e

$$\mathbf{x}(\mathbf{X}) \approx \sum_{a \in \{i,j,k\}} w_a^e(\mathbf{X})\mathbf{x}_a$$

  Compute $\mathbf{F}(\mathbf{X}) = \frac{\partial \mathbf{x}(\mathbf{X})}{\partial \mathbf{X}}$

- Compare the FEM formula for $\mathbf{F}$ against our formula from Page 12, what are the differences?

Assignment

The constitutive equation on Page 13 needs material parameters λ and μ.

- Find parameter values for the Lamé parameters λ and μ for real known materials. Make a table of the values that you find.

Remark: It is beneficial to use cartoon-like parameter values at first when implementing and debugging a simulator. Stiff materials can make one fight ill-conditioned systems rather than finding the real bugs in the code. For instance, Young Modulus of 1000000.0 Pa, Poisson ratio of 0.3, and mass density of 1000 Kg$/m^3$, and $\Delta t = 0.001$ s.

Assignment

Consider the theory covered from Page 15 to Page 18.

- Why is the formula

$$\mathbf{f}_i^e \equiv -\frac{1}{2}\mathbf{P}^e\mathbf{N}_{ji}^e\mathbf{l}_{ji} - \frac{1}{2}\mathbf{P}^e\mathbf{N}_{ki}^e\mathbf{l}_{ki}$$

  more "convenient" than

$$\mathbf{f}_i^e \equiv \mathbf{P}^e\mathbf{N}_\alpha^e l_\alpha^e + \mathbf{P}^e\mathbf{N}_\beta^e l_\beta^e$$

  Hint: consider whether you actually have to build the CV and whether the summation order has any importance.

Assignment

- Analyze each input parameter on Page 21 – decide upon what its “value” should be and why
- Make hypotheses about how each input parameter affects a simulation
- Conduct experiments to verify your hypotheses

Some Inspiration

- Examine the quality of triangle meshes
- Examine volume, momentum, mechanical energy conservation
- Examine stability depending on Lamé parameters and Δt
- Examine symmetry behavior
- Examine robustness in relation to setting $\mathbf{t}$
- ...

Assignment

- From where was the value $\frac{1}{\sqrt{3}}$ on Page 26 derived? Hint: Inflection points have slope zero.