Hyperelasticity based Mesh-Deformation

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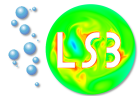
Contents



Motivation

Mesh-deformation is useful for

- complex geometries
- multi-phase flow
- FSI
- smoothening a mesh from a mesh-generator
- ...

Focus today: Outer boundary do not move

Task

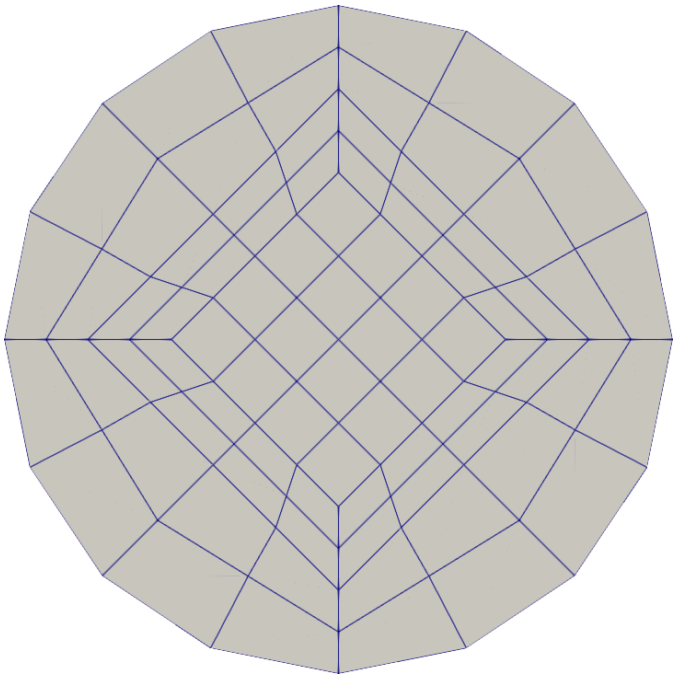


Figure: initial mesh

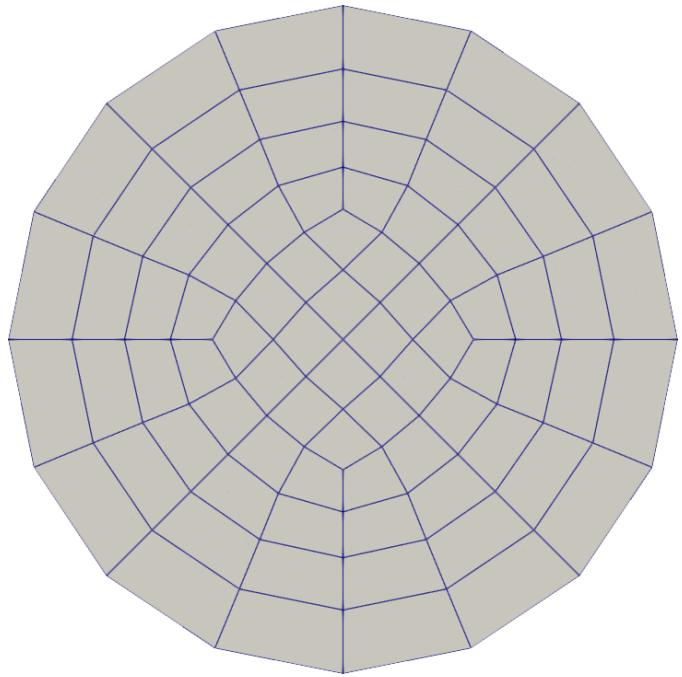


Figure: desired mesh

Link to solid mechanics

In solid mechanics

- engineers take an elastic material, for example a beam
- apply some load to it
- calculate the resulting stresses
- calculate the resulting strains
- calculate the deformed state
- and then calculate other quantities of interest

Sounds familiar!

Solid mechanics I

- Each material has an energy that models the material behaviour
- The internal energy of a material must not depend on the position in space
- All systems seek a state that minimizes the energy in the system
- There exist stable and unstable states that minimize the energy in the system

Unfortunately, the model cannot be linear!

Solid mechanics II

Let $\gamma(X)$ be the mapping between the undeformed and deformed state. It can be proven that a model that is objective must depend on $\mathbf{C} := (\nabla\gamma)^T(\nabla\gamma)$.

Definition: A material model is called Neo-Hooke-Model if it only depends linear on $\mathrm{Tr}(\mathbf{C})$, not on $\frac{1}{2}((\mathrm{Tr}(\mathbf{C}))^2 - \mathrm{Tr}((\mathbf{C})^2))$ and in some way on $\det(\mathbf{C})$.

Let Ψ be the energy functional.

- Growth condition: $\Psi(\nabla\gamma) \to \infty$ for $\det(\nabla\gamma) \to 0$
- Growth condition: $\Psi(\nabla\gamma) \to \infty$ for $\{||\nabla\gamma|| + ||\,\mathrm{cof}(\nabla\gamma)|| + \det(\nabla\gamma)\} \to \infty$

The growth conditions rule out convexity.

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Choice of energy

Neo-Hookean-Type model:
$\tilde{\Psi}(\gamma) = \frac{1}{2}\lambda(\log(\sqrt{\det(\mathbf{C})}))^2 + \frac{1}{2}\mu(\mathrm{Tr}(\mathbf{C}) - d - 2\log(\sqrt{\det(\mathbf{C})}))$
with λ and μ material parameters (Lamé-Parameters) and d the spatial dimension

Modeling

Measure how much energy is required to deform an optimal cell into a cell of the mesh. Define $\gamma : \hat{T} \to T$
Sum up all local contributions to the energy:

$$\Psi(\gamma) = \int \{\frac{1}{2}\lambda(\log(\sqrt{\det(\mathbf{C})}))^2$$

$$+ \frac{1}{2}\mu(\mathrm{Tr}(\mathbf{C}) - d - 2\log(\sqrt{\det(\mathbf{C})}))\}$$

This is the term we need to minimize $\to$ Optimization in Banach spaces

General Descent Algorithm for functions
given: $F(x)$, x_0

General Descent Algorithm

---

find searchdirection s_k
find stepsize σ_k with $F(x_k + \sigma_k s_k) < F(x_k)$
$x_{k+1} = x_k + \sigma_k s_k$

For nonlinear optimization:

- Gradient Method: $s_k = -\nabla F(x_k)$
- Newton: $F''(x_k)s_k = -\nabla F(x_k)$

We have to transfer this into banach spaces

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Existence of Solution

Based on [1]

Theorem

Let Ω be a domain in $\mathbb{R}^3$ and $\hat{W} : \Omega \times \mathbb{M}^3_+ \to \mathbb{R}$ be a stored energy function with the following properties

1. *Polyconvexity: For almost all $x \in \Omega$ there exists a convex function $\mathbb{W}(x, .) : \mathbb{M}^3 \times (0, +\infty) \to \mathbb{R}$ such that $\mathbb{W}(x, F, \det(F)) = \hat{W}(x, F) \forall F \in \mathbb{M}^3_+$*
2. $\lim_{\det F \to 0^+} \hat{W}(x, \det(F)) = +\infty$
3. *Coerciveness: There exist α, β, p, q, r such that $\alpha > 0$, $p \geq 2$, $q \geq \frac{p}{p-1}$, $r > 1$: $\hat{W}(x, F) \geq \alpha(||F||^p + (\det(F))^r) + \beta$ and $\Phi := \left\{\Psi \in W^{1,p}, \operatorname{cof} \nabla\Psi \in L^q, \det(\nabla\Psi) \in L^r\right\}$ is not empty.*

Then there exists at least one function φ such that $\varphi \in \Phi$ and $\int_\Omega \hat{W}(x, \nabla\varphi)) = \inf_{\psi \in \Phi} \int_\Omega \hat{W}(x, \nabla\psi))$

Our energy is not polyconvex and not coercive!
Convex only as long as $\det \nabla\gamma < \exp(\frac{\mu}{\lambda} + 1)$ Therefore: the energy is modified:

$$\begin{aligned}\tilde{\Psi}(\gamma) = &\frac{1}{2}\lambda(\log(\sqrt{\det(\mathbf{C})}))^2 \\ &+ \frac{1}{2}\mu(\mathrm{Tr}(\mathbf{C}) - d - 2\log(\sqrt{\det(\mathbf{C})})) \\ &+ \kappa\left(\left(\sqrt{\det(\mathbf{C})} - \exp\left(\frac{\mu}{\lambda} + 1\right)\right)_+\right)^2\end{aligned}$$

But: In practice, the last term should always be zero, so we ignore it from here on.

Fréchet-derivatives

We want to use Newton:

$$F''(\gamma)[s_k, \psi] = F'(\gamma)\psi$$

$$F'(\gamma)\varphi = \int [\lambda \log(\det(\nabla\gamma))(\nabla\gamma)^{-T} - \mu(\nabla\gamma)^{-T} + \mu\nabla\gamma] : \nabla\varphi \, \mathrm{dx}$$

$$\begin{aligned} F''(\gamma)[\varphi, \psi] = \int & \lambda[(\nabla\gamma)^{-T} : \nabla\psi][(\nabla\gamma)^{-T} : \nabla\varphi] \\ & + \lambda \log(\det(\nabla\gamma))(-(\nabla\gamma)^{-T}(\nabla\psi)^T(\nabla\gamma)^{-T}) : \nabla\varphi \\ & - \mu(-(\nabla\gamma)^{-T}(\nabla\psi)^T(\nabla\gamma)^{-T}) : \nabla\varphi \\ & + \mu\nabla\psi : \nabla\varphi \mathrm{dx} \end{aligned}$$

Problem: $F''(\gamma)[s_k, \psi]$ is not positive definite.

Quasi-Newton

$$
\begin{aligned}
H(\gamma,\alpha)[\varphi,\psi] = \int & \lambda[(\nabla\gamma)^{-T} : \nabla\psi][(\nabla\gamma)^{-T} : \nabla\varphi] \\
& + \alpha\lambda \log(\det(\nabla\gamma))(-(\nabla\gamma)^{-T}(\nabla\psi)^{T}(\nabla\gamma)^{-T}) : \nabla\varphi \\
& - \alpha\mu(-(\nabla\gamma)^{-T}(\nabla\psi)^{T}(\nabla\gamma)^{-T}) : \nabla\varphi \\
& + \mu\nabla\psi : \nabla\varphi \mathrm{dx}
\end{aligned}
$$

Dennis-Moré-Condition:

$$
\frac{||(H_k - F''(\gamma^*))s_k||}{||s_k||} \to 0
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is necessary and sufficient for superlinear convergence. Therefore, we can use any heuristic for α that guarantees $\alpha_k \to 1$ for $k \to \infty$.

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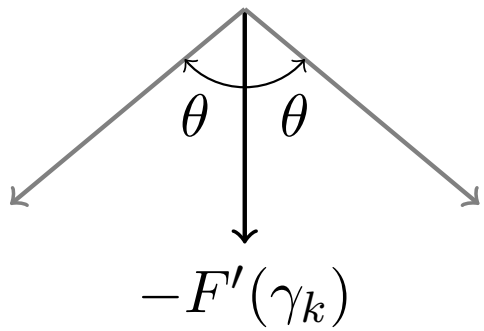
The (Quasi-)Newton-direction might be bad, so we check the angle-condition:

$$\frac{(-F'(\gamma_k), s_k)}{||F'(\gamma_k)||||s_k||} \geq \beta$$

$$\beta = |\cos(\theta)|$$



If this does not hold: Use antigradient as searchdirection.

stepsize / damping

Armijo-Scheme

given: x, searchdirection s
choose $\beta \in (0,1)$, $\gamma \in (0,1)$, $\sigma_0 > 0$, $k = 0$
while $f(x) - f(x + \sigma_k s) < -\gamma \sigma_k (\nabla f(x), s)$ **do**
  $\sigma_{k+1} = \beta \sigma_k$
  $k = k + 1$
end while

Typical values are: $\sigma_0 = 1$, $\beta = 0.5$, $\gamma = 10^{-2}$

final considerations

Problem: We need $F'(\gamma_k)$ but we only have $F'(\gamma_k)\varphi$.
Solution: Riesz-Representative: s is the Riesz-Representative of $F'(\gamma_k)$ if

$$(s, \varphi) = F'(\gamma_k)\varphi \, \forall \varphi$$

$\Rightarrow$ We have to decide on a function space for our problem and a suitable dot-product.
For the following tests and results we choose $H_0^1(\Omega)$ with

$$(\varphi, \psi) = \int_\Omega \nabla\varphi : \nabla\psi \mathrm{dx}$$

so it is only solving a Poisson problem.

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first testcase

Initial mesh: Take $[0,1]^2$, refine it one time, then move the midpoint to $(0.26, 0.26)$, then refine again 5 times. $\mu = 10$, $\lambda = 1$.
Optimal cell: A square with the volume $\frac{\#cells}{vol(\Omega)}$. Solver for both PDEs: PCG
Known optimal mesh: Refined unit-square.

Iter	Armojo-Steps	Newton-defect	$\|\|s_k\|\|$	funcvalue	angle	α	Iter Solver s_k	defect s_k	Iter Solver Antigrad	defect Antigrad
1	6	7.08E+00	1.39E+02	1.13E+00	1	0.3	-	-	92	6.94E-04
2	4	1.48E+00	8.26E+01	6.45E-02	1	0.3	-	-	93	1.45E-04
3	4	5.81E-01	9.72E+00	5.75E-03	1	0.3	-	-	98	5.19E-05
4	4	1.84E-01	2.98E+00	6.11E-04	1	0.3	-	-	97	1.64E-05
5	4	5.59E-02	8.70E-01	7.15E-05	1	0.3	-	-	98	4.90E-06
6	0	1.93E-02	2.26E-02	4.44E-06	0.979	0.422	1	1.26E-06	98	1.69E-06
7	0	4.90E-03	5.36E-03	2.71E-07	1.000	0.583	1	3.16E-07	99	4.29E-07
8	0	1.20E-03	1.15E-03	1.97E-09	1.000	0.835	1	7.96E-08	99	1.05E-07
9	0	1.02E-04	9.02E-05	1.18E-16	1.000	1.000	1	6.95E-09	99	8.96E-09
10	0	7.15E-09	6.36E-09	9.94E-17	0.964	1.000	1	5.05E-13	98	6.05E-13

Video
When to stop the Newton-Scheme? Not the focus of this work.

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For the initial problem with $\mu = 10$, $\lambda = 1$. Optimal cell: A square with the volume $\frac{\#cells}{vol(\Omega)}$. Solver for both PDEs: PCG

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3	4	1.26E+01	9.09E+00	8.42E+00	1	0.3	0	-	9	4.33E-04
4	4	1.12E+01	8.19E+00	8.05E+00	1	0.3	0	-	9	2.52E-04
5	5	1.05E+01	7.52E+00	7.15E+00	1	0.3	0	-	9	2.96E-04
6	0	1.41E+00	5.47E-02	7.14E+00	0.993	0.311	1	2.14E-05	9	6.42E-05
7	0	9.95E-01	2.73E-02	7.13E+00	0.995	0.463	1	2.28E-05	9	4.47E-05
8	0	4.40E-01	1.04E-02	7.13E+00	0.996	0.546	1	6.76E-07	9	1.56E-05
9	0	1.69E-01	3.11E-03	7.13E+00	0.996	0.728	1	1.77E-06	9	5.73E-06
10	0	3.26E-02	4.77E-04	7.13E+00	0.996	0.993	1	5.80E-07	9	1.17E-06
11	0	1.61E-04	2.28E-06	7.13E+00	0.995	1	1	4.67E-09	9	5.49E-09
12	0	4.81E-09	1.13E-10	7.13E+00	0.922	1	1	1.70E-14	9	1.14E-13

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8	0	4.40E-01	1.04E-02	7.13E+00	0.996	0.546	1	6.76E-07	9	1.56E-05
9	0	1.69E-01	3.11E-03	7.13E+00	0.996	0.728	1	1.77E-06	9	5.73E-06
10	0	3.26E-02	4.77E-04	7.13E+00	0.996	0.993	1	5.80E-07	9	1.17E-06
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Video

Adaptation

Another application: Adapt the mesh to inner boundaries.
Idea: Choose optimal cell size according to distance to the inner boundary. Do a few steps. Update the optimal cell size and calculate again. Repeat.

Initial mesh: unit square, Level 7. $\mu = 100$, $\lambda = 1$, linear solver: PCG

Video

Total: 14 cycles, 140 Newton-Iterations, 514 Armijo-Steps, 470 Iterations to solve s_k, 14463 Iterations to solve for the Antigradient

Visually, after 5 cycles / 50 Newton-Iterations not much is happening

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Another application: Adapt the mesh to inner boundaries.
Idea: Choose optimal cell size according to distance to the inner boundary. Do a few steps. Update the optimal cell size and calculate again. Repeat.
Initial mesh: unit square, Level 7. $\mu = 100$, $\lambda = 1$, linear solver: PCG
Video
Total: 14 cycles, 140 Newton-Iterations, 514 Armijo-Steps, 470 Iterations to solve s_k, 14463 Iterations to solve for the Antigradient
Visually, after 5 cycles / 50 Newton-Iterations not much is happening

Thank you for your attention!

Reference

P. G. Ciarlet, Mathematical Elasticity, no. v. 20, 27, 29 in Studies in Mathematics and Its Applications, North-Holland ; Sole distributors for the U.S.A. and Canada, Elsevier Science Pub. Co, Amsterdam ; New York : New York, N.Y., U.S.A, 1988.