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Introduction of fintie element method

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Poisson equation with mixed B.C. and a weak formulation: 1/2

$\Omega \subset \mathbb{R}^2$, $\partial\Omega = \Gamma_D \cup \Gamma_N$

$$-\triangle u = f \text{ in } \Omega,$$
$$u = g \text{ on } \Gamma_D,$$
$$\frac{\partial u}{\partial n} = h \text{ on } \Gamma_N.$$

weak formulation
V : function space, $V(g) = \{u \in V\,;\, u = g \text{ on } \Gamma_D\}$. $V = C^1(\Omega) \cap C^0(\bar{\Omega})$?
Find $u \in V(g)$ s.t.

$$\int_\Omega -\triangle u\, v dx = \int_\Omega f\, v dx \quad \forall v \in V(0)$$

Gauss-Green's formula

$u, v \in V$, $n = \begin{bmatrix} n_1 \\ n_2 \end{bmatrix}$: outer normal to $\partial\Omega$

$$\int_\Omega (\partial_i u) v\, dx = -\int_\Omega u \partial_i v\, dx + \int_{\partial\Omega} u\, n_i v\, ds\,.$$

Poisson equation with mixed B.C. and a weak formulation: 2/2

$$\int_\Omega (-\partial_1^2 - \partial_2^2) u\, v\, dx = \int_\Omega (\partial_1 u \partial_1 v + \partial_2 u \partial_2 v)\, dx - \int_{\partial\Omega} (\partial_1 u\, n_1 + \partial_2 u\, n_2) v\, ds$$

$$= \int_\Omega \nabla u \cdot \nabla v\, dx - \int_{\Gamma_D \cup \Gamma_N} \nabla u \cdot n\, v\, ds$$

$$v = 0 \text{ on } \Gamma_D \Rightarrow \quad = \int_\Omega \nabla u \cdot \nabla v\, dx - \int_{\Gamma_N} hv\, ds$$

Find $u \in V(g)$ s.t.

$$\int_\Omega \nabla u \cdot \nabla v dx = \int_\Omega f\, v dx + \int_{\Gamma_N} h\, v ds \quad \forall v \in V(0)$$

- $a(\cdot,\cdot) : V \times V \to \mathbb{R}$: bilinear form
- $F(\cdot) : V \to \mathbb{R}$: functional

Find $u \in V(g)$ s.t.

$$a(u, v) = F(v) \quad \forall v \in V(0)$$

discretization and matrix formulation : 1/2

finite element basis, span$[\varphi_1, \dots, \varphi_N] = V_h \subset V$

$u_h \in V_h \ \Rightarrow \ u_h = \sum_{1 \leq i \leq N} u_i \varphi_i$

finite element nodes $\{P_j\}_{j=1}^N$, $\varphi_i(P_j) = \delta_{i\,j}$ Lagrange element

$\Lambda_D \subset \Lambda = \{1, \dots, N\}$: index of node on the Dirichlet boundary
Dirichlet data : $u(P_k) = g(P_k) \quad P_k \in \Gamma_D$

$$V_h(g) = \{u_h \in V_h \,;\, u_h = \sum u_i \varphi_i, u_k = g_k \ (k \in \Lambda_D)\}$$

Find $u_h \in V_h(g)$ s.t.

$$a(u_h, v_h) = F(v_h) \quad \forall v_h \in V_h(0).$$

Find $\{u_j\}, u_k = g_k (k \in \Lambda_D)$ s.t.

$$a(\sum_j u_j \varphi_j, \sum_i v_i \varphi_i) = F(\sum_i v_i \varphi_i) \ \forall \{v_i\}, v_k = 0 (k \in \Lambda_D)$$

Find $\{u_j\}_{j \in \Lambda}$s.t.

$$\sum_j a(\varphi_j, \varphi_i) u_j = F(\varphi_i) \qquad \forall i \in \Lambda \setminus \Lambda_D$$

$$u_k = g_k \qquad \forall k \in \Lambda_D$$

discretization and matrix formulation : 2/2

Find $\{u_j\}_{j\in\Lambda\setminus\Lambda_D}$ s.t.

$$\sum_{j\in\Lambda\setminus\Lambda_D} a(\varphi_j,\varphi_i)u_j = F(\varphi_i) - \sum_{k\in\Lambda_D} a(\varphi_k,\varphi_i)g_k \quad \forall i\in\Lambda\setminus\Lambda_D$$

$A=\{a(\varphi_j,\varphi_i)\}_{i,j\in\Lambda\setminus\Lambda_D}$: symmetric.
$A\in\mathbb{R}^{N\times N}$, $f\in\mathbb{R}^N$, $N=\#(\Lambda\setminus\Lambda_D)$

positivity of the matrix from coercivity of the bilinear form

A : (symmetric) positive definite i.e., $(A\vec{u},\vec{u})>0\ \forall\vec{u}\neq 0$
poof

$$(A\vec{u},\vec{u}) = \sum_i\left(\sum_j a(\varphi_j,\varphi_i)u_i\right)u_j$$
$$= a(\sum_j\varphi_j u_j,\sum_i\varphi_i u_i) = a(u,u)\geq\alpha||u||_1^2$$

corecivity of blinear form $a(\cdot,\cdot)$ ensures positivity of stiffness matrix A
corecivity is obtained by the Poincare's inequality $|u|_1^2\geq c||u||_0^2$

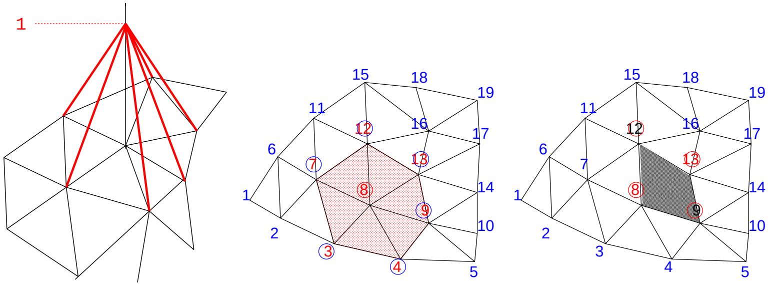
$$a(u,u)=\int_\Omega\nabla u\cdot\nabla u = ||\nabla u||_0^2 = |u|_1^2$$
$$|u|_1^2 = ((1-\beta)+\beta)|u|_1^2 \geq c\beta||u||_0^2+(1-\beta)||u||_1^2 = \frac{c}{1+c}||u||_1^2$$

P1 finite element and sparse matrix

$\mathcal{T}_h$: triangulation of a domain Ω, triangular element $K \in \mathcal{T}_h$
piecewise linear element : $\varphi_i|_K(x_1, x_2) = a_0 + a_1 x_1 + a_2 x_2$

$\varphi_i|_K(P_j) = \delta_{i\,j}$

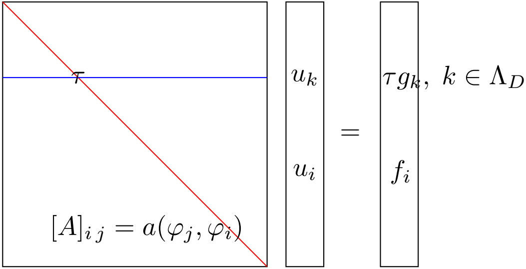
$$[A]_{i\,j} = a(\varphi_j, \varphi_i) = \int_\Omega \nabla\varphi_j \cdot \nabla\varphi_i\, dx = \sum_{K \in \mathcal{T}_h} \int_K \nabla\varphi_j \cdot \nabla\varphi_i\, dx.$$



A : sparse matrix, CRS (Compressed Row Storage) format to store

penalty method to solve inhomogeneous Dirichlet problem

modification of diagonal entries of A where index $k \in \Lambda_D$
penalization parameter $\tau = 1/\varepsilon$; `tgv`



$$\tau u_k + \sum_{j \neq k} a_{k\,j} u_j = \tau g_k \ \Leftrightarrow \ u_k - g_k = \varepsilon(-\sum_{j \neq k} a_{k\,j} u_j),$$

$$\sum_j a_{i\,j} u_j = f_i \qquad \forall i \in \{1, \ldots, N\} \setminus \Lambda_D.$$

keeping symmetry of the matrix without changing index numbering.

abstract framework

V: Hilbert space with inner product $(\cdot,\cdot)$ and norm $||\cdot||$.
bilinear form $a(\cdot,\cdot) : V \times V \to \mathbb{R}$

- coercive : $\exists \alpha > 0 \quad a(u,u) \geq \alpha ||u||^2 \ \forall u \in V$.
- continuous : $\exists \gamma > 0 \quad |a(u,v)| \leq \gamma ||u|| \, ||v|| \ \forall u,\, v \in V$.

functional $F(\cdot) : V \to \mathbb{R}$.

$$\text{find } \ u \in V \ \text{ s.t. } \ a(u,v) = F(v) \quad \forall v \in V$$

has a unique solution : Lax-Milgram's theorem

most general case on $a(\cdot,\cdot)$

- inf-sup conditions
  - $\exists \alpha_1 > 0 \qquad \sup_{v \in V, v \neq 0} \dfrac{a(u,v)}{||v||} \geq \alpha_1 ||u|| \ \forall u \in V$.
  - $\exists \alpha_2 > 0 \qquad \sup_{u \in V, u \neq 0} \dfrac{a(u,v)}{||u||} \geq \alpha_2 ||v|| \ \forall v \in V$.

find $u \in V$ s.t. $a(u,v) = F(v) \quad \forall v \in V$ has a unique solution.

error estimate : theory 1 /2

V : Hilbert space, $V_h \subset V$: finite element space.

- $u \in V$, $a(u, v) = F(v) \ \ \forall v \in V$.
- $u_h \in V_h$, $a(u_h, v_h) = F(v_h) \ \ \forall v_h \in V_h \subset V$.

$a(u, v_h) = F(v_h) \ \ \forall v_h \in V_h \subset V$. Galerkin orthogonality

$$a(u - u_h, v_h) = 0 \ \ \forall v_h \in V_h.$$

assuming coercivity and continuity of $a(\cdot, \cdot)$.

Céa's lemma $||u - u_h|| \leq \dfrac{\gamma}{\alpha} \inf_{v_h \in V_h} ||u - v_h||$.

proof: $||u - u_h|| \leq ||u - v_h|| + ||v_h - u_h||$

$$\begin{aligned}
\alpha ||u_h - v_h||^2 &\leq a(u_h - v_h, u_h - v_h) \\
&= a(u_h, u_h - v_h) - a(v_h, u_h - v_h) \\
&= a(u, u_h - v_h) - a(v_h, u_h - v_h) \\
&= a(u - v_h, u_h - v_h) \leq \gamma ||u - v_h|| ||u_h - v_h||.
\end{aligned}$$

error estimate : theory 2 /2

$\Pi_h : C(\bar{\Omega}) \to V_h, \quad \Pi_h u = \sum_{1 \le i \le N} u(P_i)\phi_i,$
span$[\{\phi_i\}_{1 \le i \le N}] = S_h$, P_k finite element basis.

interpolation error by polynomial $K \in \mathcal{T}_h$, $P_k(K) \subset H^l(K)$, $v \in H^{k+1}(\Omega)$
$\Rightarrow$
$\exists c > 0 \quad |v - \Pi_h v|_{s,K} \le c\, h_K^{k+1-s} |v|_{k+1,K} \ (0 \le s \le \min\{k+1, l\})$.

finite element error $u \in H^{k+1}$, u_h : finite element solution by P_k element.
$\Rightarrow$
$\exists c > 0 \quad ||u - u_h||_{1,\Omega} \le c\, h^k |u|_{k+1,\Omega}$

proof:

$$\begin{aligned} ||u - u_h||_{1,\Omega} &\le c \inf_{v_h \in V_h} ||u - v_h||_{1,\Omega} \\ &\le c||u - \Pi_h u||_{1,\Omega} \\ &\le c \sum_{K \in \mathcal{T}_h} (h_K^k + h_K^{(k+1)}) |u|_{k+1,K} \\ &\le c h^k |u|_{k+1,\Omega} \end{aligned}$$

Sobolev space

P1 element element space does not belong to $C^1(\Omega)$.

$$H^1(\Omega) = \{u \in L^2(\Omega)\,;\, ||u||_1^2 = (u,u) < +\infty\}$$
$$(u,v) = \int_\Omega u\,v + \nabla u \cdot \nabla v,$$
$$||u||_0^2 = \int_\Omega u\,v, \quad |u|_1^2 = \int_\Omega \nabla u \cdot \nabla v$$

$H_0^1 = \{u \in H^1(\Omega)\,;\, u = 0$ on $\partial\Omega\}$.
Poincaré's inequality $\exists C(\Omega)\ u \in H_0^1 \ \Rightarrow\ ||u||_0 \leq C(\Omega)|u|_1$.
proof for the case $\Omega \subset B = (0,s) \times (0,s)$
$v \in C_0^\infty(\Omega)$,

$$v(x_1,x_2) = v(0,x_2) + \int_0^{x_1} \partial_1 v(t,x_2)dt$$
$$|v(x_1,x_2)|^2 \leq \int_0^{x_1} 1^2 dt \int_0^{x_1} |\partial_1 v(t,x_2)|^2 dt \leq s \int_0^s |\partial_1 v(t,x_2)|^2 dt$$
$$\int_0^s |v(x_1,x_2)|^2 dx_1 \leq s^2 \int_0^s |\partial_1 v(x)|^2 dx_1$$
$$\int_\Omega |v|^2 = \int_B |v|^2 dx_1 dx_2 \leq s^2 \int_B |\partial_1 u|^2 dx_1 dx_2 = s^2 \int_\Omega |\partial_1 u|^2.$$

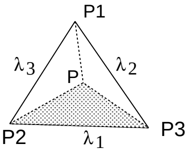
numerical integration

Numerical quadrature:
$\{P_i\}_{i\leq i\leq m}$: integration points in K, $\{\omega_i\}_{i\leq i\leq m}$: weights

$$|u-u_h|^2_{0,\Omega}=\sum_{K\in\mathcal{T}_h}\int_K|u-u_h|^2dx\sim\sum_{K\in\mathcal{T}_h}\sum_{i=1}^{m}|(u-u_h)(P_i)|^2\omega_i$$

formula : degree 5, 7 points,
P.C. Hammer, O.J. Marlowe, A.H. Stroud [1956]

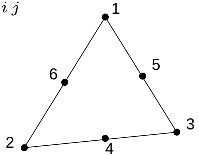
area coordinates $\{\lambda_i\}_{i=1}^3$	weight	
$(\frac{1}{3},\frac{1}{3},\frac{1}{3})$	$\frac{9}{40}\|K\|$	$\times 1$
$(\frac{6-\sqrt{15}}{21},\frac{6-\sqrt{15}}{21},\frac{9+2\sqrt{15}}{21})$	$\frac{155-\sqrt{15}}{1200}\|K\|$	$\times 3$
$(\frac{6+\sqrt{15}}{21},\frac{6+\sqrt{15}}{21},\frac{9-2\sqrt{15}}{21})$	$\frac{155+\sqrt{15}}{1200}\|K\|$	$\times 3$

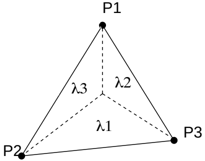


Remark
it is not good idea to use interpolation of continuous function to finite element space, for verification of convergence order.
$|\Pi_h u-u_h|_{1,\Omega}$ may be smaller (in extreme cases, super convergence)

P2 finite element

$\mathcal{T}_h$: triangulation of a domain Ω, triangular element $K \in \mathcal{T}_h$
piecewise quadratic element : 6 DOF on element K.
$\varphi_i|_K(x_1, x_2) = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_1^2 + a_4 x_1 x_2 + a_5 x_2^2$
$\varphi_i|_K(P_j) = \delta_{i\,j}$





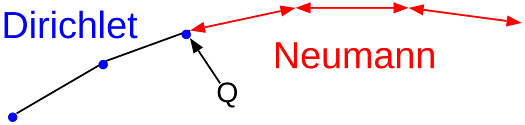
by using area coordinates $\{\lambda_1, \lambda_2, \lambda_3\}$, $\lambda_1 + \lambda_2 + \lambda_3 = 1$.

$$\begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \\ \varphi_5 \\ \varphi_6 \end{pmatrix} = \begin{pmatrix} 1 & & & & -1 & -1 \\ & 1 & & -1 & & -1 \\ & & 1 & -1 & -1 & \\ & & & 4 & & \\ & & & & 4 & \\ & & & & & 4 \end{pmatrix} \begin{pmatrix} \lambda_1^2 \\ \lambda_2^2 \\ \lambda_3^2 \\ \lambda_2\lambda_3 \\ \lambda_3\lambda_1 \\ \lambda_1\lambda_2 \end{pmatrix} = \begin{pmatrix} \lambda_1(2\lambda_1 - 1) \\ \lambda_2(2\lambda_2 - 1) \\ \lambda_3(2\lambda_3 - 1) \\ 4\lambda_2\lambda_3 \\ 4\lambda_3\lambda_1 \\ 4\lambda_1\lambda_2 \end{pmatrix}$$

treatment of Neumann data around mixed boundary

Neumann data is evaluated by line integral with FEM basis φ_i.

$$\int_{\Gamma_N} h\,\varphi_i\,ds$$



For given discrete Neumann data, h is interpolated in FEM space, $h = \sum_j h_j \varphi_j|_{\Gamma_N}$,

$$\sum_j h_j \int_{\Gamma_N} \varphi_j \varphi_i \, ds.$$

On the node $Q \in \bar{\Gamma}_D \cap \bar{\Gamma}_N$, both Dirichlet and Neumann are necessary.

advantages of finite element formulation

- weak formulation is obtained by integration by part with clear description on the boundary
- Dirichlet boundary condition is embedded in a functional space, called as essential boundary condition
- Neumann boundary condition is treated with surface/line integral by Gauss-Green's formula, called as natural boundary condition
- solvability of linear system is inherited from solvability of continuous weak formulation
- error of finite element solution is evaluated by approximation property of finite element space

linear and nonlinear solid mechanics : 1/2

a problem with the second Piola-Kirchhoff stress tensor Σ
in Ω with $\partial\Omega = \Gamma_D \cup \Gamma_N$

$$
\begin{aligned}
-\mathrm{div}\,((I+\nabla u)\Sigma(u(x))) &= f(x) \quad \text{in } \Omega,\\
u &= 0 \quad \text{on } \Gamma_D,\\
(I+\nabla u)\Sigma(u(x))n &= g(x) \quad \text{on } \Gamma_N.
\end{aligned}
$$

Green-St. Venant tensor $E(u)$

$$E(u) = \frac{1}{2}\left((\nabla u)^T + \nabla u + (\nabla u)^T(\nabla u)\right) = E_L(u) + E_{NL}(u)$$

Piola-Kirchhoff stress tensor with Lamé constants λ and μ

$$\Sigma(u) = \check{\Sigma}(E(u)) = \lambda\,(\mathrm{tr}(E(u)))\,I + 2\mu\,E(u)$$

variational problem with test function $v,\ v = 0$ on Γ_D

$$
\begin{aligned}
&-\int_\Omega \mathrm{div}(I+\nabla u)\check{\Sigma}(E(u))\cdot v = \int_\Omega f\cdot v\\
\Leftrightarrow &\int_\Omega (I+\nabla u)\check{\Sigma}(E(u)) : \nabla v = \int_\Omega f\cdot v + \int_{\Gamma_N\cup\Gamma_D}(I+\nabla u)\check{\Sigma}(E(u))n\cdot v\\
&\qquad = \int_\Omega f\cdot v + \int_{\Gamma_N} g\cdot v
\end{aligned}
$$

Dirchlet data is treated as the essential boundary condition

linear and nonlinear solid mechanics : 2/2

The variational equation is re-written as

$$\int_\Omega \check{\Sigma}(E(u)) : dE(u)[v] = \int_\Omega f \cdot v + \int_{\Gamma_N} g \cdot v\,.$$

symmetry of $\check{\Sigma}(E)$ leads to

$$\begin{aligned}(I+\nabla u)\check{\Sigma}(E(u)) : \nabla v &= \check{\Sigma}(E(u)) : (I+\nabla u)^T \nabla v \\ &= \frac{1}{2}\check{\Sigma}(E(u)) : \Big((I+\nabla u)^T\nabla v + \nabla v^T(I+\nabla u)\Big) \\ &= \frac{1}{2}\check{\Sigma}(E(u)) : \Big(\nabla v + (\nabla u)^T\nabla v + \nabla v^T + \nabla v^T\nabla u\Big) \\ &= \check{\Sigma}(E(u)) : dE(u)[v]\end{aligned}$$

tensors A, B, C $\Rightarrow$ $A\,B : C = B : A^T C$

$$\sum_{i\,j}\left(\sum_k [A]_{i\,k}[B]_{k\,j}\right)[C]_{i\,j} = \sum_{k\,j}[B]_{k\,j}\left(\sum_i [A^T]_{k\,i}[C]_{i\,j}\right)$$

- nonlinear solver by Newton iteration (linearization for iterative solver)
- linearization of the Green-St. Venant tensor $E(u)$ by $E_L(u)$

linearized elasticity

Piola-Kirchhoff stress tensor with Lamé constants λ and μ

$$\Sigma(u) = \check{\Sigma}(E(u)) = \lambda\,(\mathrm{tr}(E(u)))\,I + 2\mu\,E(u)$$

linearization of Green-St. Venant tensor $E(u)$

$$E(u) = \frac{1}{2}\left((\nabla u)^T + \nabla u + (\nabla u)^T(\nabla u)\right) \simeq \frac{1}{2}\left((\nabla u)^T + \nabla u\right) = E_L(u) = e(u)$$

$$\begin{aligned} E_L(u+v) - E_L(u) &= \frac{1}{2}\left((\nabla(u+v)^T + \nabla(u+v)\right) - \frac{1}{2}\left(((\nabla u)^T + \nabla u\right) \\ &= \frac{1}{2}\left((\nabla v)^T + \nabla v\right) = dE_L(u)[v] \\ \check{\Sigma}(E(u)) : dE_L(u)[v] &= \lambda\,(\mathrm{tr}(E(u)))\,I : E_L(v) + 2\mu\,E_L(u) : dE_L(v) \\ &= \lambda\nabla\cdot u\nabla\cdot v + 2\mu E_L(u) : E_L(v) \end{aligned}$$

variational problem of the linear elasticity with test function $v,\ v = 0$ on Γ_D

$$\int_\Omega 2\mu\,e(u)) : e(v) + \lambda\nabla\cdot u\,\nabla\cdot v = \int_\Omega f\cdot v + \int_{\Gamma_N} g\cdot v$$

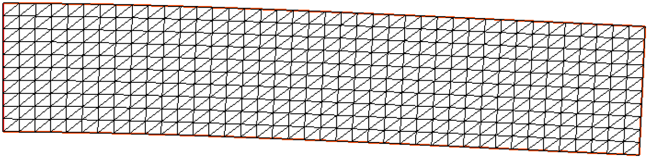
Korn's inequality $u \in H^1_1(\Omega)^3$

$$\Rightarrow \qquad \exists\alpha(\Omega)\ \int_\Omega e(u) : e(u) \geq \alpha(\Omega)\int_\Omega u\cdot u + \nabla u : \nabla u$$

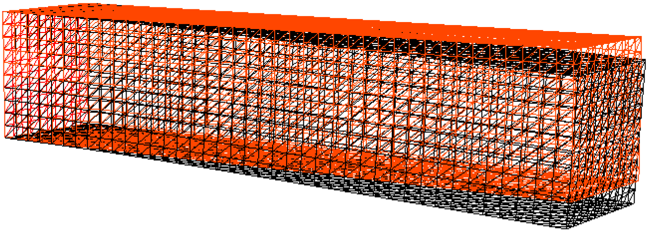
A : ternsor $\Rightarrow I : A = \mathrm{tr}(A)$, $\mathrm{tr}(e(u)) = \partial_1 u_1 + \partial_2 u_2 + \partial_3 u_3 = \nabla\cdot u$

linear elasticity problem in 3D : 4/4

2D beam : displacement on the left wall is fixed



3D beam : displacement on the left wall is fixed



solution of nonlinear problem by Newton iteration

nonlinear problem: $F : \mathbb{R}^N \to \mathbb{R}^N$, $\vec{x} \in \mathbb{R}^N$

$$\text{find } \vec{x} \; F(\vec{x}) = \vec{0}$$

Fréchet derivative of F : $F(\vec{x} + \vec{\delta x}) - F(\vec{x}) \simeq \nabla F(\vec{x})\vec{\delta x}$
Jacobian matrix $\nabla F(\vec{x}) \in \mathbb{R}^{N \times N}$
Algorithm : Newton iteration

$\vec{x}_0 \in \mathbb{R}^N$: initial guess
loop $n = 0, 1, 2, \cdots$

$$\nabla F(\vec{x}_{n-1})\vec{\delta x} = F(\vec{x}_{n-1})$$

$$\vec{x}_n = \vec{x}_{n-1} - \vec{\delta x}$$

nonlinear variational problem $f(\cdot, \cdot) : V \times V \to \mathbb{R}$

$$\text{find } x \in V(g) \; F(x, y) = 0 \; \forall y \in V(0)$$

Fréchet derivative of $F(\cdot, \cdot)$:
$F(x + \delta x, y) - F(x, y) \simeq (\nabla F(x)\delta x, y) \;\; \forall y \in V(0)$
Algorithm : Newton iteration

$x_0 \in V(g)$: initial guess
loop $n = 0, 1, 2, \cdots$

$$\text{find } \delta x \in V(0) \;\; (\nabla F(x_{n-1})\delta x, y) = F(x_{n-1}, y) \; \forall y \in V(0)$$

$$x_n = x_{n-1} - \delta x$$

nonlinear elasticity : 1/3

derivatives of Green-St. Venant tensor

- first order derivative $dE(u)[v]$

$$\begin{aligned} dE(u)[v] &= \frac{1}{2}\left((\nabla v)^T + \nabla v\right) + \frac{1}{2}\left((\nabla u)^T \nabla v + (\nabla v)^T \nabla u\right) \\ &= E_L(v) + dE_{NL}(u)[v] \end{aligned}$$

calculated from variation as

$$\begin{aligned} E(u+v) - E(u) &= E_L(u+v) + E_{NL}(u+v) - ((E_L(u) + E_{NL}(u)) \\ &= E_L(v) + \frac{1}{2}(\nabla(u+v)^T \nabla(u+v)) - E_{NL}(u) \\ &= E_L(v) + \frac{1}{2}((\nabla u)^T \nabla v + (\nabla v)^T \nabla u + (\nabla v)^T \nabla v) \end{aligned}$$

- second order derivative $d^2E(u)[v,w]$

$$d^2E(u)[v,w] = dE_{NL}(w)[v]$$

calculated from variation as

$$\begin{aligned} dE(u+w)[v] - dE(u)[v] &= E_L(v) + dE_{NL}(u+w)[v] - (E_L(v) + dE_{NL}(u)[v]) \\ &= \frac{1}{2}\left((\nabla(u+w))^T \nabla v + (\nabla v)^T \nabla(u+w)\right. \\ &\quad \left. - (\nabla u)^T \nabla v + (\nabla v)^T \nabla u\right) \\ &= \frac{1}{2}\left((\nabla w)^T \nabla v + (\nabla v)^T \nabla w\right) \end{aligned}$$

nonlinear elasticity : 2/3

The variational equation

$$\int_\Omega \check{\Sigma}(E(u)) : dE(u)[v] = \int_\Omega f \cdot v + \int_{\Gamma_N} g \cdot v \,.$$

Newton iteration of the nonlinear system u^0 : given
loop $n = 0, 1, 2, \cdots$
solve linear system to find update w,

$$\int_\Omega \check{\Sigma}(dE(u^n)[w]) : dE(u^n)[v] + \check{\Sigma}(E(u^n)) : d^2E(u^n)[v, w]$$
$$= \int_\Omega \check{\Sigma}(E(u^n)) : dE(u^n)[v] - \int_\Omega f \cdot v - \int_{\Gamma_N} g \cdot v \quad \forall v$$

update $u^{n+1} = u^n - w$

Jacobian of the variational problem is calculated as

$$\int_\Omega \check{\Sigma}(E(u^n + w)) : dE(u^n + w)[v] - \int_\Omega \check{\Sigma}(E(u^n)) : dE(u^n)[v]$$
$$\simeq \int_\Omega \check{\Sigma}\left(E(u^n) + dE(u^n)[w]\right)) : \left(dE(u^n)[v] + d^2E(u^n)[v, w]\right)$$
$$- \int_\Omega \check{\Sigma}(E(u^n)) : dE(u^n)[v]$$
$$\simeq \int_\Omega \check{\Sigma}(dE(u^n)[w]) : dE(u^n)[v] + \check{\Sigma}(E(u^n)) : d^2E(u^n)[v, w]$$

nonlinear elasticity : 3/3

Jacobian for Newton iteration

$$\int_\Omega \check{\Sigma}(dE(u^n)[w]) : dE(u^n)[v] + \check{\Sigma}(E(u^n)) : d^2E(u^n)[v,w]\,.$$

is symmetric, which is shown from

- $d^2E(u^n)[v,w] = dE_{NL}(w)[v] = \frac{1}{2}\left((\nabla w)^T\nabla v + (\nabla v)^T\nabla w\right)$ is sym.
- by recalling $I : A = \mathrm{tr}(A)$ and for symmetric tensors η and ζ

$$\begin{aligned}\check{\Sigma}(\eta) : \zeta = (\lambda\mathrm{tr}(\eta)I + 2\mu\eta) : \zeta &= \lambda\mathrm{tr}(\eta)\mathrm{tr}(\zeta) + 2\mu\eta : \zeta \\ &= \lambda\mathrm{tr}(\zeta)\mathrm{tr}(\eta) + 2\mu\zeta : \eta = \check{\Sigma}(\zeta) : \eta\end{aligned}$$

coercivity depends on previous iteration step u^n

- the first half part :
$$\int_\Omega \check{\Sigma}(dE(u^n)[w]) : dE(u^n)[w] \geq 2\int_\Omega \mu E_L(w) : E_L(w)$$
- the second half part : coercivity depends on $\check{\Sigma}(E(u^n))$

$$\begin{aligned}&\int_\Omega \check{\Sigma}(E(u^n)) : d^2E(u^n)[w,w] = \int_\Omega \check{\Sigma}(E(u^n)) : d^2E_{NL}(u^n)[w,w] \\ &= \int_\Omega \check{\Sigma}(E(u^n)) : dE_{NL}(w)[w] = \int_\Omega \check{\Sigma}(E(u^n)) : (\nabla w)^T(\nabla w) \\ &= \int_\Omega \check{\Sigma}(E(u^n))(\nabla w)^T : (\nabla w)^T\end{aligned}$$

nonlinear iteration by Newton method : 1/2

Jacobian and RHS are calculated from the previous u^n in Newton step

$$(\nabla F(u^n)w, v) = \int_\Omega \check{\Sigma}(dE(u^n)[w]) : dE(u^n)[v] + \check{\Sigma}(E(u^n)) : d^2E(u^n)[v, w] \quad \forall v$$
$$(F(u^n), v) = \int_\Omega \check{\Sigma}(E(u^n)) : dE(u^n)[v] \quad \forall v$$

initial guess of the Newton iteration by linear elasticity with small load given by inhomogeneous Dirichlet data g
solution space $V(g) := \{u \in H^1(\Omega)^3\,;\, u = g \text{ on } \Gamma_D\}$

linear elasticity problem is solved as

$$\text{to find } u^0 \in V(g) \quad \int_\Omega \check{\Sigma}(e(u^0)) : e(v) = 0 \quad \forall v \in V(0)$$

and the perform Newton iteration
loop $n = 0, 1, 2, \cdots$

find $w \in V(0)$ $\quad (\nabla F(u^n)w, v) = (F(u^n), v) \quad \forall v \in V_0$

$u^{n+1} = u^n - w$

The update w in the Newton iteration supposed to have homogeneous Dirichlet boundary condition, i.e., $w \in V(0)$.

nonlinear iteration by Newton method : 2/2

a method as incremental loading:
sequence of in homogeneous Dirichlet data whose magnitude is increasing

$$||g^{(0)}|| < ||g^{(1)}|| < \cdots < ||g^{(N)}||, \ g = g^{(N)}$$

The procedure consists of nested loops for increment and Newton iteration.

perform incremental loading::
loop $m = 0, 1, 2, \cdots, N-1$

if $m = 0$ then solve linear elasticity

$$\text{to find } u^0 \in V(g^0) \quad \int_\Omega \check{\Sigma}(e(u^0)) : e(v) = 0 \quad \forall v \in V(0)$$

otherwise set $u^{m,0} \in V(g^{(m)})$ from previous u^{m-1}.

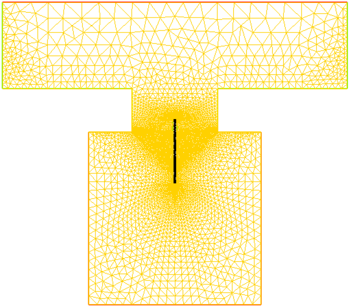
perform Newton iteration::
loop $n = 0, 1, 2, \cdots$

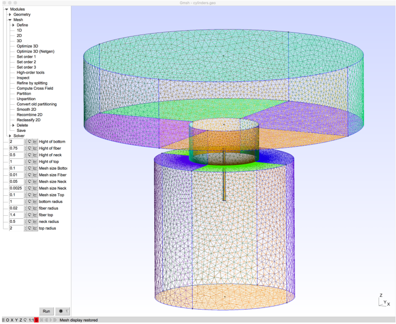
find $w \in V(0) \quad (\nabla F(u^{m,n})w, v) = (F(u^{m,n}), v) \quad \forall v \in V_0$

$u^{m,n+1} = u^{m,n} - w$

description of complex geometry

- 2D : `bamg` embedded in FreeFEM generates isotropic triangulation of the domain consisting of parameterized segments.
  By changing of the metric based on finite element solution, an-isotropic triangulation is also performed
- 3D : `Gmsh` can handle parameterized surface segments and/or treat `STEP` file by `OepnCASCADE` geometry engine. Surface mesh generator and volume mesh generator constructs isotropic tetrahedral mesh decomposition





2D geometry definition by FreeFEM

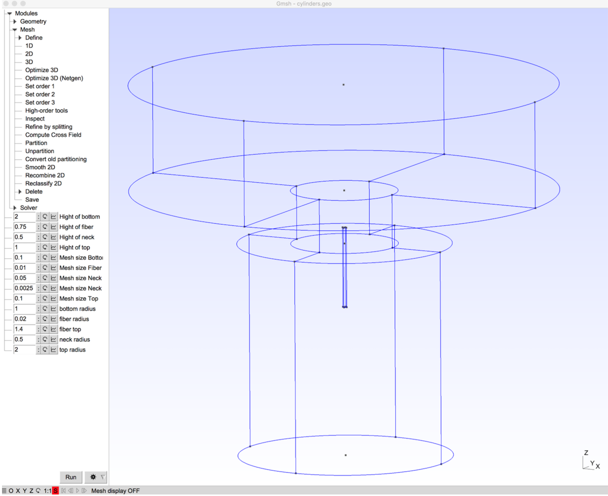
```
real rb = 1.0; real lb = 2.0; // ....
border c1(t=0,1){x=-rb + 2*rb*t; y = 0.0; label = 2;};
border c2(t=0,1){x=rb; y = lb * t; label = 3;};
border c3(t=0,1){x=(rb + (r0 - rb) * t); y = lb; label = 4;};
border c4(t=0,1){x=r0; y = lb + l0 * t*t; label = 5;};
border c5(t=0,1){x=r0 + (rc - r0) * t; y = lb+l0; label = 6;};
border c6(t=0,1){x=rc; y = lb + l0 + lc * t; label = 7;};
border c7(t=0,1){x=-rc + 2*rc * t; y = lb+l0+lc; label = 1;};
//
border c8(t=0,1){x=-rb; y = lb * t; label = 3;};
border c9(t=0,1){x=-(rb + (r0 - rb) * t); y = lb; label = 4;};
// ...
// fiber
border d1(t=0,1){x=-rd+2*rd * t + re; y = le; label = 8;};
border d2(t=0,1){x = rd+re; y = le + ld * t; label = 8; };
border d3(t=0,1){x=rd-2*rd * t + re; y = le+ld; label=8;};
border d4(t=0,1){x = -rd+re; y = le+ld * t; label = 8; };

int n = 20; int nn = 20; int nnn = 50;
mesh Th = buildmesh(c1(n) + c2(n) + c3(nn) + c4(nn)
            + c5(n) + c6(nn) + c7(-n)
            + c8(-n) + c9(-nn) + c10(-nn) + c11(-n) + c12(-nn)
            + d1(nn) + d2(nnn) + d3(nn) +d4(-nnn));
```

3D geometry definition by Gmsh : 1/4

```
pext = newp;
Point(pext+0) = {0, 0, 0, hBottom};
Point(pext+1) = {RRb, 0, 0, hBottom};
Point(pext+2) = {0, RRb, 0, hBottom};
Point(pext+3) = {-RRb, 0, 0, hBottom};
Point(pext+4) = {0, -RRb, 0, hBottom};
lext = newl;
Circle(lext+0) = {pext+1, pext+0, pext+2};
Circle(lext+4) = {pext+6, pext+5, pext+7};
Line(lext+8) = {pext+1, pext+6};
Line(lext+9) = {pext+2, pext+7};
llext = newll;
Line Loop(llext+0) = {lext+0, lext+9, -(lext+4), -(lext+8)};
// ..
sext = news;
Ruled Surface(sext+0) = {llext+0};      Side[0] = sext+0;
// ..
Physical Surface(SIDE) = {Side[],Neck[]};
// ..
sl = newsl;
Surface Loop(sl+1)={Neck[],NeckFine[],Side[],Top[],Bottom[]};
v = newv;
Volume(v+0) = {sl+1, sl+2};
```

3D geometry definition by Gmsh : 2/4

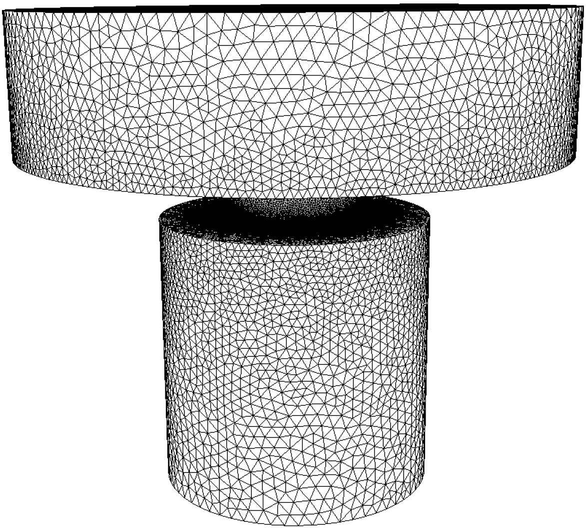
{ points } → { lines, splines } → { loops } ≃ { surfaces } → { volumes }



surface segments and generated mesh can be verified by GUI
command line option can generate mesh readable by `FreeFEM`

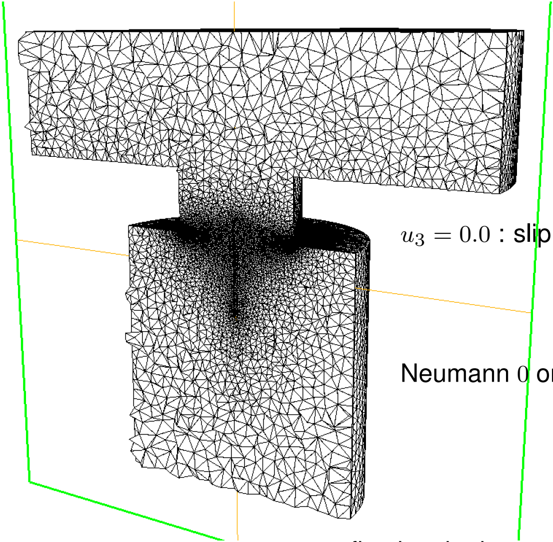
```
gmsh -3 -format msh2 -o test.msh test.geo
```

3D geometry definition by Gmsh : 3/4



3D geometry definition by Gmsh : 4/4

$u = [0, 0, 0.06]$: pulling up



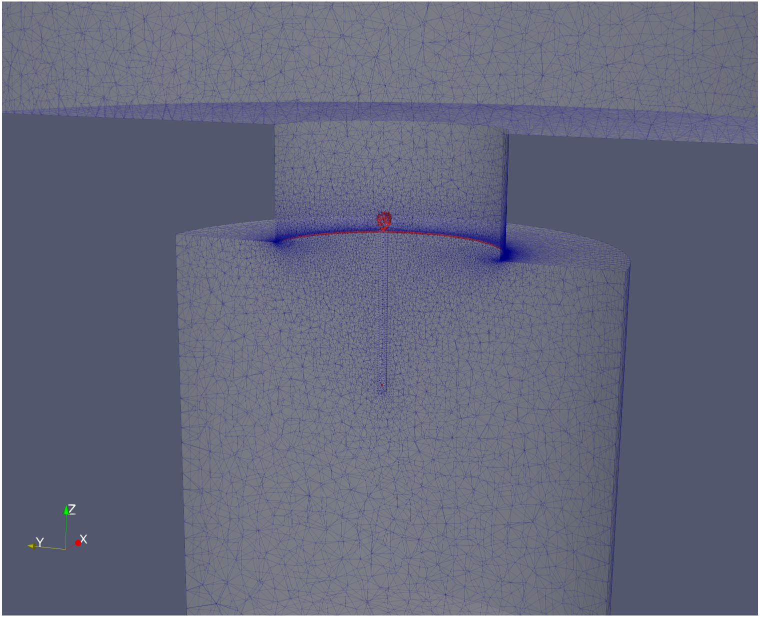
$u_3 = 0.0$: slip on xy plane

Neumann 0 on all other sides

$u = 0.0$: fixed at the bottom

- height of the domain is 2.5, radius of the top is 2, bottom 1
- internal fiber has 100 times large Lamé constants than the surround

stress concentration



$708,947$ vertexes, $2,076,809$ DOF with P1 element

References

- Finite Elements: Theory, Fast Solvers, and Applications in Elasticity Theory, 3rd ed. D. Braess Cambridge University Press, 2010
- Numerical Models for Differential Problems, 2nd ed. A. Quarteroni Springer, 2014 ISBN 978-88-470-5521-6
- Theory and Practice of Finite Elements A. Ern, J.-L. Guermond Springer, 2004 ISBN 978-1-4419-1918-2
- The Mathematical Theory of Finite Element Methods, 3rd ed. S. Brenner, R. Scott Springer, 2008 ISBN 978-0-387-75933-3
- Numerical Approximation of Partial Differential Equations A. Quartenori, A. Valli Springer, 2008
- Mathematical Elasticity: Three-Dimensional Elasticity. P. Ciarlet, SIAM Classics in Applied Mathematics, 2021