Elasticity of one-dimensional continua and nanostructures

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Extension, torsion and bending of rods/beams

$$F = E\,A\,\epsilon$$

$$M_t = G\,J\,\frac{\Theta}{L}$$

$$M = E\,I\,\kappa$$

3D elasticity (recap of some basics)

deformation map $\underline{x} = \underline{f}(\underline{X})$

- takes a (Langrangian/material) vector/point $\underline{X}$ in the undeformed configuration
- returns a (Eulerian/spatial) vector/point $\underline{x}$ in the deformed configuration

deformation gradient $\underline{\underline{F}}(\underline{X}) = \nabla_{\underline{X}}\, \underline{f}(\underline{X})$

- takes a (Langrangian/material) vector/point $\underline{X}$ in the undeformed configuration
  $\rightarrow$ $\underline{X}$ is material point where the gradient is evaluated
- returns a second order (two-point) tensor $\underline{\underline{F}}$ that depends on $\underline{X}$ (in the general case)
- $\underline{\underline{F}}$ contains (first order accurate) information about how line elements in the material configuration are transformed into deformed (stretched and rotated) line elements in the spatial configuration by $\underline{f}(.)$
  $\rightarrow \mathrm{d}\underline{x} = \underline{\underline{F}}(\underline{X}) \cdot \mathrm{d}\underline{X} = \nabla_{\underline{X}}\, \underline{f}(\underline{X}) \cdot \mathrm{d}\underline{X}$

equations of equilibrium

- material description: $\nabla_{\underline{X}} \cdot \underline{\underline{P}} + \underline{B} = \rho_0 \cdot \underline{A}$
- spatial description: $\nabla_{\underline{x}} \cdot \underline{\underline{\sigma}} + \underline{b} = \rho \cdot \underline{a}$

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1D elasticity

we talk about **slender bodies** ($\frac{\text{Length}}{\text{Diameter}} > 10$)

we only have **one material coordinate** s along the axis of the beam

- s uniquely identifies a particular cross section along the beam axis
- model equations will be a system of ODEs in s (instead of PDE)
- equations are obtained by averaging a PDE in 3 dimensions over the cross section

kinematic quantities in the model

- **position of centerline** $\underline{r}(s)$
- **orientation/rotation of cross section** $\underline{\underline{R}}(s)$
- more accuracy $\rightarrow$ more unknowns

Outline of this course

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The Euler-Bernoulli beam (planar case)

- assumption of the model

  all cross sections remain planar

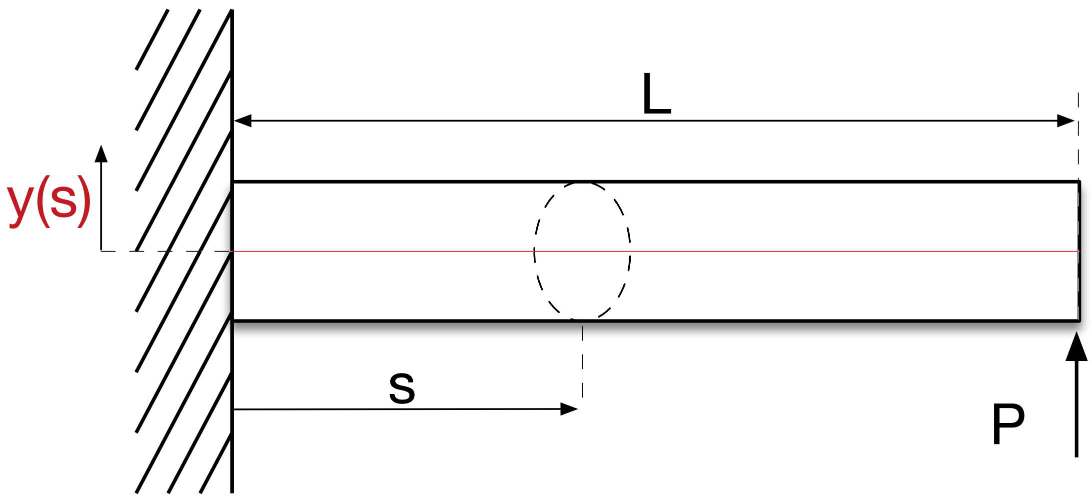
  cross section normal and centerline tangent are of same orientation φ
  $\rightarrow$ model only allows for pure bending (no shear)

- bending moment $M(s) = E\,I\,\kappa(s)$
- centerline of beam described by function $y(s)$
- curvature of centerline given by $\kappa(s) = \frac{\frac{\mathrm{d}^2 y}{\mathrm{d}s^2}(s)}{\left(1+\left(\frac{\mathrm{d}y}{\mathrm{d}s}(s)\right)^2\right)^{\frac{3}{2}}}$

  $\rightarrow$ geometric nonlinearity $\rightarrow$ non-linear ODE

- linear approximation for small deflections: $\frac{\mathrm{d}y}{\mathrm{d}s} = \tan(\varphi) \ll 1 \Rightarrow \frac{\mathrm{d}y}{\mathrm{d}s} \approx \varphi$
- Euler-Bernoulli beam equation: $M(s) = E\,I\,\frac{\mathrm{d}^2 y}{\mathrm{d}s^2}$

Example: Cantilever beam (part 1)



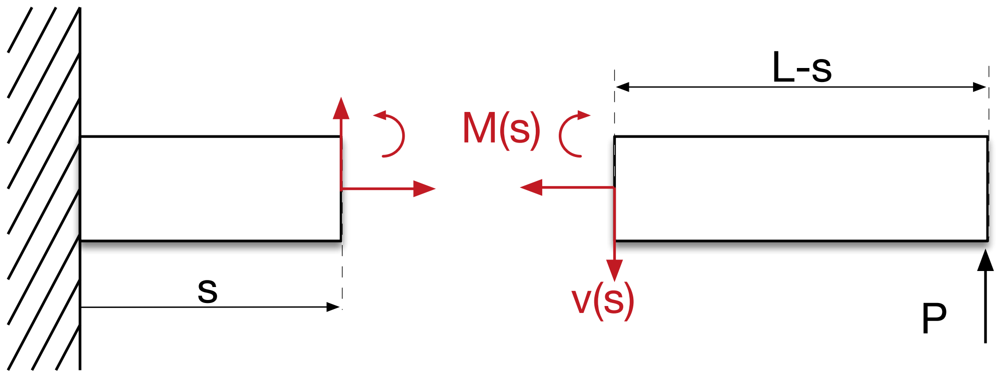
boundary conditions at $s = 0$:

- $y(0) = 0$
- $\frac{\mathrm{d}y}{\mathrm{d}s}(0) = 0$

boundary conditions at $s = L$:

- $v(L) = P$
- $M(L) = 0 \Rightarrow \frac{\mathrm{d}^2y}{\mathrm{d}s^2}(L) = 0$

Example: Cantilever beam (part 2)

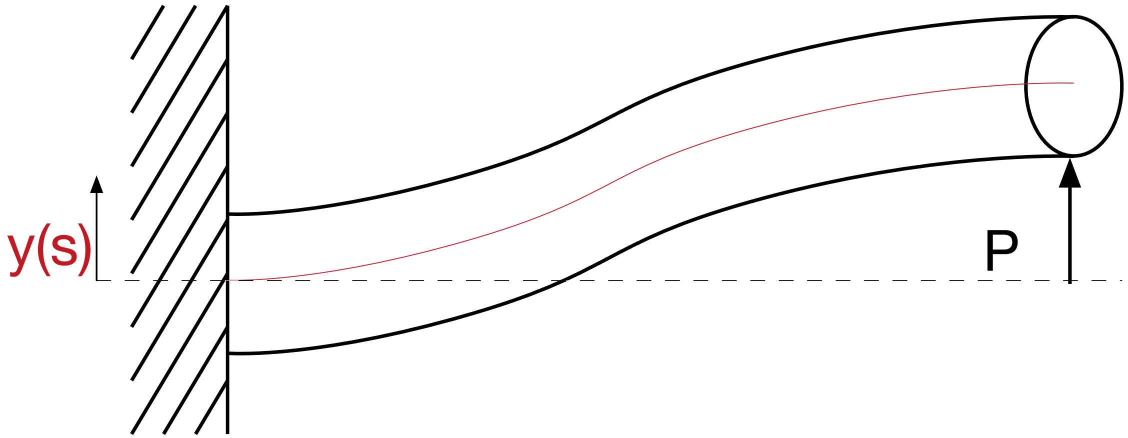


moment balance: $-M(s) + P(L-s) = 0 \quad \Rightarrow \quad M(s) = P\,(L-s)$

$$M(x) = E\,I\,\frac{\mathrm{d}^2 y}{\mathrm{d}s^2} \quad \Rightarrow \quad \frac{\mathrm{d}^2 y}{\mathrm{d}s^2} = \frac{M(s)}{E\,I} = \frac{P\,(L-s)}{E\,I}$$

$$\Rightarrow y(s) = \frac{P}{E\,I}\left(-\frac{s^3}{6} + \frac{L\,s^2}{2}\right) + \cancel{c_1}\,s + \cancel{c_2} = \frac{P\,L^3}{2\,E\,I}\left(\left(\frac{s}{L}\right)^2 - \frac{1}{3}\left(\frac{s}{L}\right)^3\right)$$

Another example of a cantilever beam



boundary conditions at $s = 0$:

- $y(0) = 0$
- $\frac{\mathrm{d}y}{\mathrm{d}s}(0) = 0$

boundary conditions at $s = L$:

- $v(L) = P$
- $\frac{\mathrm{d}y}{\mathrm{d}s}(L) = 0 \Rightarrow M(L) \neq 0$
  (rotation is restricted)

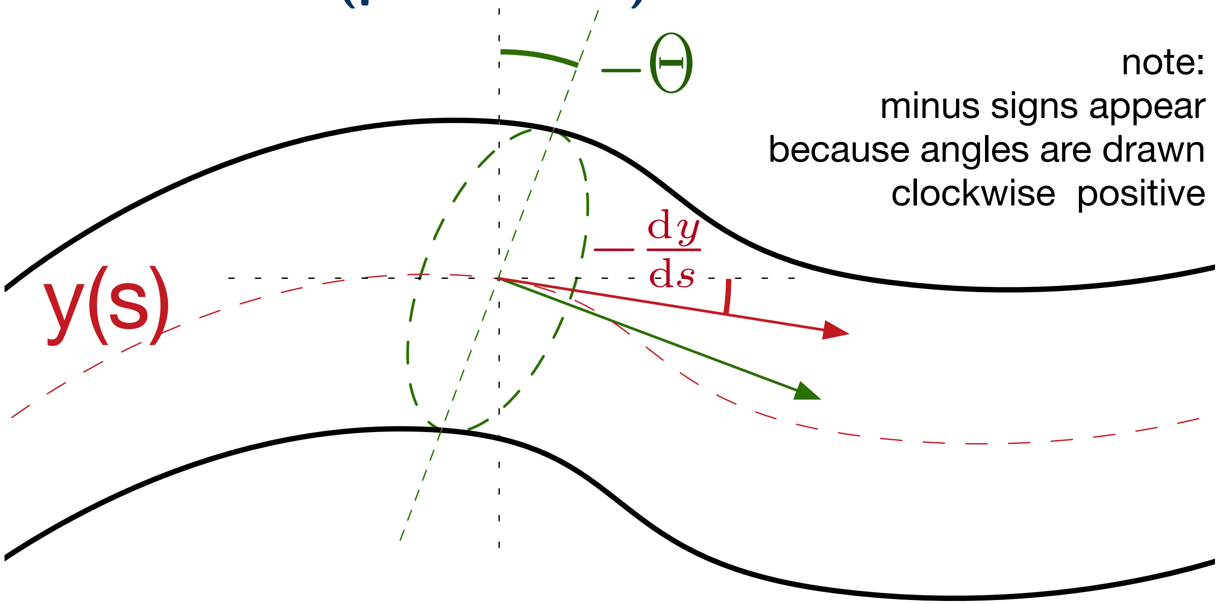
$$\Rightarrow M(s) = M(L) + P\,(L - s)$$

Boundary conditions

displacement	force
prescribed $\Rightarrow$	unknown
unknown	$\Leftarrow$ prescribed

rotation	moment
prescribed $\Rightarrow$	unknown
unknown	$\Leftarrow$ prescribed

The Timoshenko beam (planar case)



- individual cross sections still remain planar
- centerline tangent orientation (red) $\neq$ cross section normal (green)

  $-\Theta$ measures orientation of cross section

  centerline tangent $\frac{\mathrm{d}y}{\mathrm{d}s}$ influenced by **bending and shearing**
- shear strain $\gamma(s) = \frac{\mathrm{d}y}{\mathrm{d}s}(s) - \Theta(s) = \frac{v(s)}{k\,G\,A}$
- curvature $\kappa(s) = \frac{\mathrm{d}\Theta}{\mathrm{d}s}(s) = \frac{M(s)}{E\,I}$ (see next slide)

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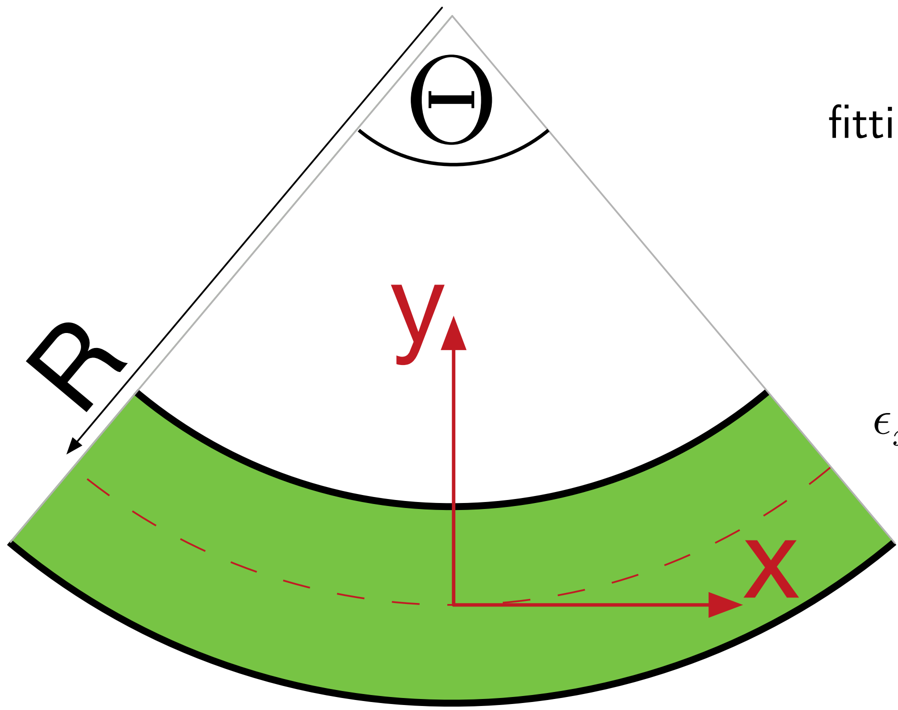
Connection between curvature and moment



$$L = R\,\Theta \quad \Rightarrow \quad \frac{1}{R} = \frac{\Theta}{L} = \frac{\mathrm{d}\Theta}{\mathrm{d}s}$$

fitting circles to the centerline locally:

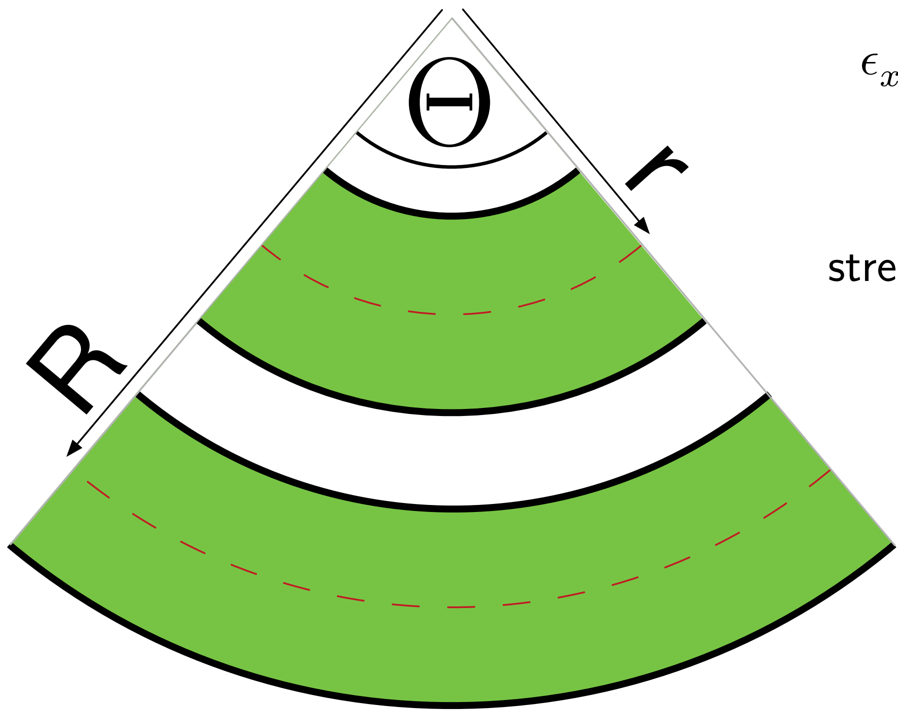
$$\kappa(s) = \frac{\mathrm{d}\Theta}{\mathrm{d}s}(s)$$

$$\epsilon_{xx} = \frac{\Delta L}{L} = \frac{(R-y)\,\Theta - R\,\Theta}{R\,\Theta} = \frac{-y}{R}$$

$$\sigma_{xx} = -E\,\frac{y}{R}$$

$$M = -\int_{\Omega} y\,\sigma_{xx}\;\mathrm{d}A = E\,I\,\frac{1}{R} = E\,I\,\kappa$$

Bending and axial compression together



because of axial forces the beam got shorter!

$$\epsilon_{xx} = \frac{(r-y)\,\Theta - R\,\Theta}{R\,\Theta} = \frac{r-R}{R} + \frac{-y}{R}$$
$$= \epsilon - \frac{y}{R}$$

stress due to axial stretch + bending:

$$\sigma_{xx} = E\left(\epsilon + \frac{-y}{R}\right)$$

$$M = -\int_\Omega y\,\sigma_{xx}\,\mathrm{d}A$$
$$= -E\,\epsilon \cancel{\int_\Omega y\,\mathrm{d}A} + \frac{E}{R}\int_\Omega y^2\,\mathrm{d}A$$
$$= E\,I\,\kappa$$

→ bending and axial stretch are independent!

Model linearity

$$\frac{\mathrm{d}y}{\mathrm{d}s} = \frac{1}{k\,G\,A} \cdot v(s) + \Theta$$

$$\frac{\mathrm{d}\Theta}{\mathrm{d}s} = \frac{1}{E\,I} \cdot M(s)$$

we obtained a linear model because we assumed...

- small slopes of the centerline (linear kinematics)

  $\frac{\mathrm{d}y}{\mathrm{d}s} = \tan\Theta \approx \Theta$

  approximation is not valid for larger deformations

- material linearity (linear constitutive law)

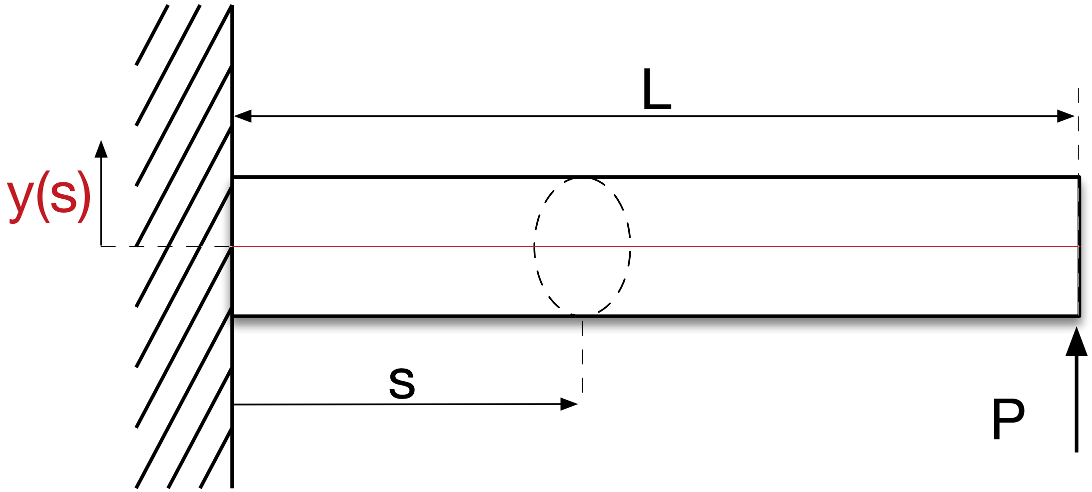
  $v(s)$, $M(s)$ get multiplied by constants

  or by functions that depend on s but not on $v(s)$, $M(s)$

  material may eg. get stiffer with increasing deformation energy

  btw. k is a correction factor, that depends on the shape of the beam's cross section

Example: Cantilever beam (part 1)



boundary conditions at $s = 0$:

- $y(0) = 0$
- $\cancel{\frac{\mathrm{d}y}{\mathrm{d}s}(0) = 0}$ (because of shear!)
- $\Theta(0) = 0$ (cross section fixed)

boundary conditions at $s = L$:

- $v(L) = P$
- $M(L) = 0$

Timoshenko beam theory

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Example: Cantilever beam (part 2)

As before with the Euler-Bernoulli cantilever beam we have

$$v(s) = P \quad \text{and} \quad M(s) = P\,(L - s)$$

We integrate the Timoshenko beam equations ...

$$\frac{\mathrm{d}\Theta}{\mathrm{d}s}(s) = \frac{M(s)}{E\,I} = \frac{P\,(L-s)}{E\,I} \quad \Rightarrow \quad \Theta(s) = \frac{P}{E\,I}\left(L\,s - \frac{s^2}{2}\right) + \cancel{c}$$

$$\frac{\mathrm{d}y}{\mathrm{d}s}(s) = \frac{v(s)}{k\,G\,A} + \Theta(s) = \frac{P}{k\,G\,A} + \frac{P}{E\,I}\left(L\,s - \frac{s^2}{2}\right)$$

$$\Rightarrow y(s) = \frac{P\,s}{k\,G\,A} + \frac{P}{E\,I}\left(L\frac{s^2}{2} - \frac{s^3}{6}\right) + \cancel{c} = \frac{P\,s}{k\,G\,A} + \frac{P\,L^3}{2\,E\,I}\left(\left(\frac{s}{L}\right)^2 - \frac{1}{3}\left(\frac{s}{L}\right)^3\right)$$

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Comparison of Euler-Bernoulli and Timoshenko cantilever beams

Euler-Bernoulli beam

$$y^{(E)}(s) = \frac{P\,L^3}{2\,E\,I}\left(\left(\frac{s}{L}\right)^2 - \frac{1}{3}\left(\frac{s}{L}\right)^3\right) \Rightarrow y^{(E)}(L) = \frac{P\,L^3}{3\,E\,I}$$

Timoshenko beam

$$y^{(T)}(s) = \frac{P\,s}{k\,G\,A} + \frac{P\,L^3}{2\,E\,I}\left(\left(\frac{s}{L}\right)^2 - \frac{1}{3}\left(\frac{s}{L}\right)^3\right) \Rightarrow y^{(T)}(L) = \frac{P\,L}{k\,G\,A} + \frac{P\,L^3}{3\,E\,I}$$

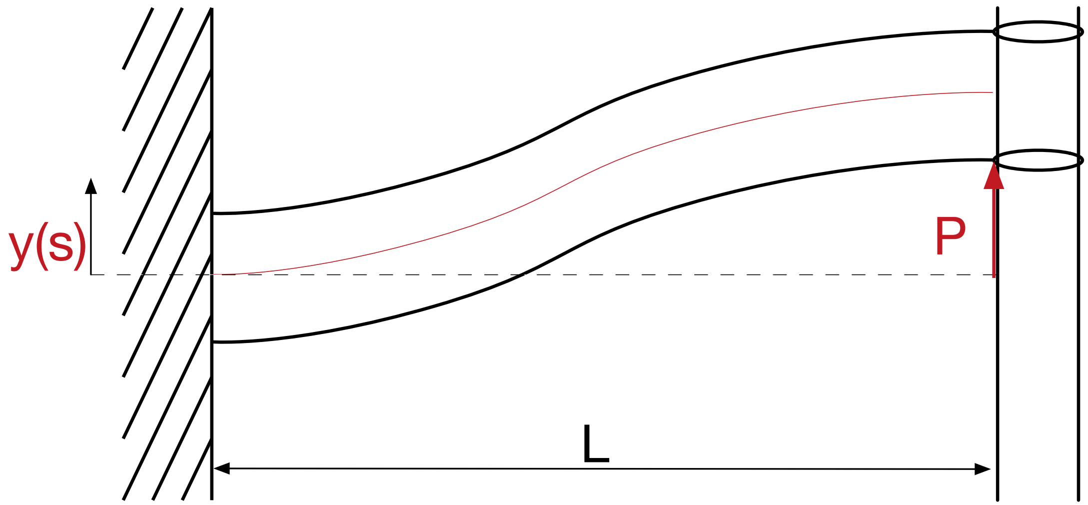
relative error (taking Euler-Bernoulli as the reference)

$$\epsilon_r = \frac{y^{(T)}(L) - y^{(E)}(L)}{y^{(E)}(L)} = \frac{\frac{P\,L}{k\,G\,A}}{\frac{P\,L^3}{3\,E\,I}} = \frac{3\,E\,I}{k\,G\,A\,L^2}$$

$$= \frac{3\,E\,b\,h^3}{k\,G\,b\,h\,L^2\,12} = \frac{1}{4}\frac{E}{k\,G}\left(\frac{h}{L}\right)^2$$

$\rightarrow$ Euler-Bernoulli beam model performs equally good as the Timoshenko model when the beam is very slender (h/L small)

Another example of a cantilever beam (part 1)



cross section at $s = L$ can not rotate or displace horizontally

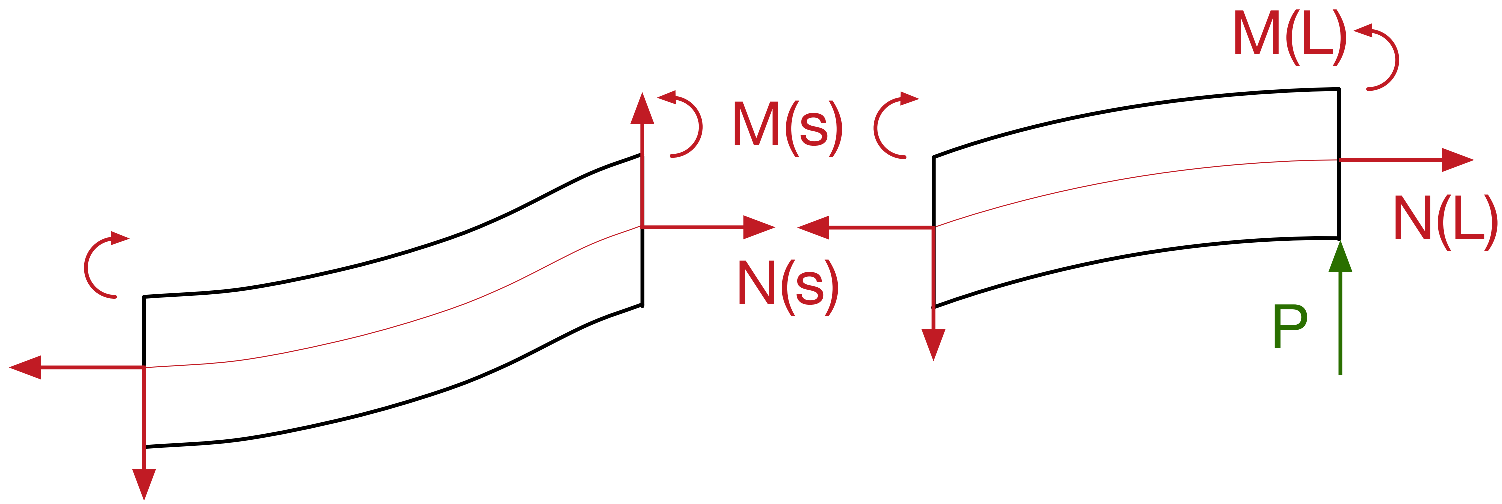
boundary conditions at $s = 0$:

- $y(0) = 0$
- $\Theta(0) = 0$

boundary conditions at $s = L$:

- $v(L) = P$
- $\Theta(L) = 0$

Another example of a cantilever beam (part 2)

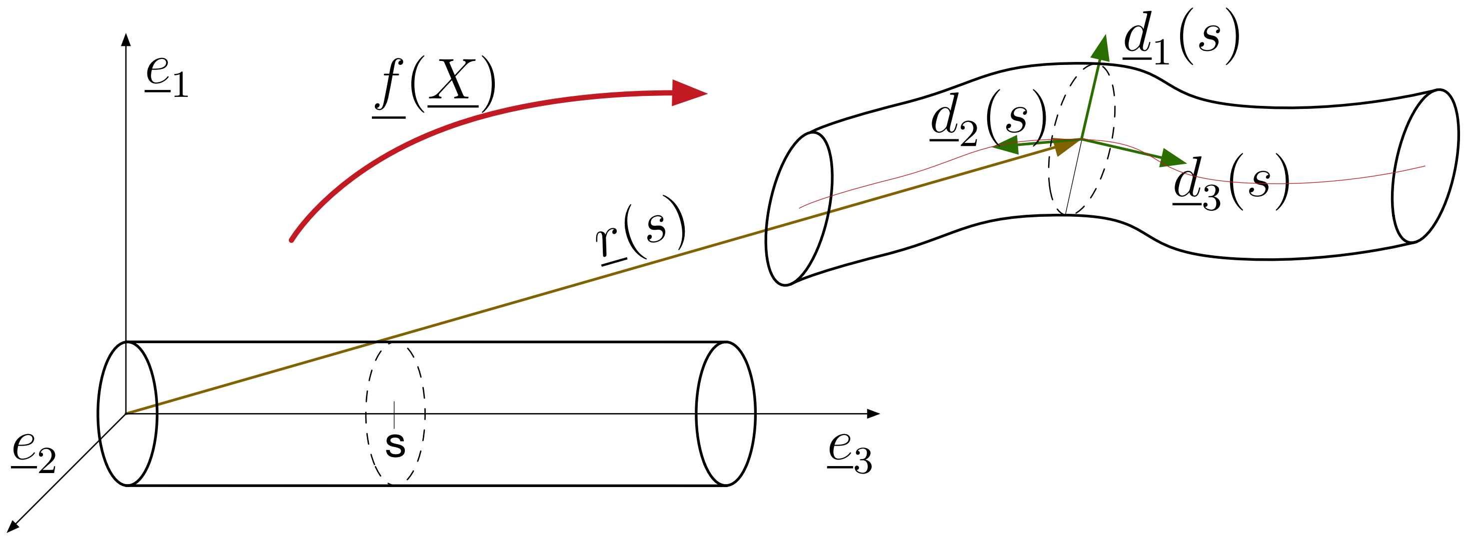


moment balance (in the deformed configuration):

$$-M(s) + M(L) + P\,(L - s) - N(y(L) - y(s))$$

$\rightarrow$ the last term results in nonlinear behavior of the model
$\rightarrow$ $M(L)$ and $N(L)$ are two extra unknowns

Introduction to ~~special~~ Cosserat rods (part 1)



remember: s is the unique identifier for a particular cross section of the beam

kinematic quantities:

- position of the deformed cross section $\underline{r}(s)$
- shearing of the deformed cross section $\underline{d}_1(s)$, $\underline{d}_2(s)$
- orientation of the deformed cross section $\underline{d}_3(s)$
  (perpendicular to $\underline{d}_1(s)$ and $\underline{d}_2(s)$ $\rightarrow$ not independent)

Introduction to ~~special~~ Cosserat rods (part 2)

constrained deformation map

$$\underline{f}(\underline{X}) = \underline{f}(X_1, X_2, X_3 = s) = \underline{r}(s) + X_\alpha \, \underline{d}_\alpha \quad \text{with } \alpha \in \{1, 2\}$$

consequences of the imposed kinematic constraints

- cross sections remain flat
- straight lines within the cross section remain straight lines
- boundary of the cross section: circles are mapped to ellipses
  (not to arbitrary curves in 2D)
- $\underline{d}_1(s)$ and $\underline{d}_2(s)$ are not perpendicular in the general case (shearing)

Kinematics of Special Cosserat rods

What makes the Special Cosserat rod special?

- $\underline{d}_1(s)$ and $\underline{d}_2(s)$ *are* perpendicular and unit-normed
- hence $\left(\underline{d}_1, \underline{d}_2, \underline{d}_3\right)$ form an orthonormal triad

consequences

$$\exists\ \underline{\underline{R}}(s) \in SO(3)\ \forall s : \Big(R : \left(\underline{e}_1, \underline{e}_2, \underline{e}_3\right) \mapsto \left(\underline{d}_1, \underline{d}_2, \underline{d}_3\right)\Big)$$

- $\left(\underline{e}_1, \underline{e}_2, \underline{e}_3\right)$ is called the global basis
- $\left(\underline{d}_1, \underline{d}_2, \underline{d}_3\right)(s)$ is called the local basis or director basis at s
- $\underline{d}_i(s) = \underline{\underline{R}}(s) \cdot \underline{e}_i \quad$ ($\underline{\underline{R}}$: rotation matrix ; $SO(3)$: special orthogonal matrix group)

constrained deformation map

$$\underline{f}(\underline{X}) = \underline{f}(X_1, X_2, X_3 = s) = \underline{r}(s) + \underline{\underline{R}}(s) \cdot (X_\alpha\, \underline{e}_\alpha) \quad \text{with } \alpha \in \{1, 2\}$$

$\rightarrow$ but the rigidity of the cross section is stiffening the beam!

Warping / relaxation of the cross section

we want to introduce warping of the cross section,
while at the same time keeping the director basis $\underline{d}_i$

modified deformation map

$$\underline{f}(\underline{X}) = \underline{f}(X_1, X_2, X_3 = s) = \underline{r}(s) + \underline{\underline{R}}(s) \cdot (X_\alpha \underline{e}_\alpha + \underline{u}) \quad \text{with } \alpha \in \{1, 2\}$$

geometric meaning of $\underline{u}$

- u_1, u_2 : in-plane shrinking
- u_3 : out-of-plane warping $\rightarrow$ cross section not planar anymore
- then $\underline{d}_1$, $\underline{d}_1$ represent the average orientation of the warped cross section

what are our kinematic unknowns?

- if $\underline{u} = \underline{u}(X_1, X_2, s)$ then we would be dealing with a 3D elasticity problem
- here we have $\underline{u}(X_1, X_2,$ local strains$)$, not a function of s
  (we will come back to this later)
- $\underline{r}(s)$ and $\underline{\underline{R}}(s)$ are the only kinematic unknowns! (6 scalar quantities)

Rotations in 3D revisited

a **rotation about *one* axis** is determined by

- axis of rotation given by $\underline{a}$ with $\|\underline{a}\| = 1$
- angle of rotation Θ

composition of rotations

$$\left(\underline{a}_1, \Theta_1\right) + \left(\underline{a}_2, \Theta_2\right) + \left(\underline{a}_3, \Theta_3\right) + \cdots = \left(\underline{a}_{eff}, \Theta_{eff}\right)$$

note: "$+$" here denotes the composition of two rotations

$$\underline{\underline{R}}_{eff} = \cdots \cdot \underline{\underline{R}}_3 \cdot \underline{\underline{R}}_2 \cdot \underline{\underline{R}}_1$$

In the general case, i.e. when $\underline{a}_i \neq \underline{a}_j$ if $i \neq j$) rotations do not commute!

example (rotation about $\underline{e}_3$):

$$\left(\underline{a} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \Theta\right) \quad \rightarrow \quad \underline{\underline{R}} = \begin{bmatrix} +\cos(\Theta) & -\sin(\Theta) & 0 \\ +\sin(\Theta) & +\cos(\Theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Axis-angle representation of rotations in 3D

from the axis-angle representation

$$\left(\underline{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \Theta\right)$$

we obtain the corresponding rotation matrix

$$\underline{\underline{R}} = \exp(\Theta \cdot \underline{\underline{a}})$$

where

$$\Theta \cdot \underline{\underline{a}} = \Theta \cdot \begin{bmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{bmatrix}$$

is a skew-symmetric matrix obtained from the definition

$$\underline{\underline{a}} = \underline{\underline{a}} \cdot \underline{\underline{I}} = \begin{bmatrix} \underline{a} \times \underline{e}_1 & \underline{a} \times \underline{e}_2 & \underline{a} \times \underline{e}_3 \end{bmatrix}$$
$$\Rightarrow \quad \underline{\underline{a}} \cdot \underline{v} = \underline{a} \times \underline{v} \quad \forall \underline{v} \in \mathbb{R}^3$$

Observe the relationship between cross products and skew-symmetric matrices:

$$\underline{a} = \text{axial}(\underline{\underline{a}}) = \text{axial}(\underline{a} \times \underline{\underline{I}}) = \text{axial}([\underline{a}]_\times)$$

Kinematics of Special Cosserat rods

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Axis-angle representation of rotations in 3D: Rodrigues' formula

$$\underline{\underline{R}} = \cos(\Theta)\,\underline{\underline{I}} + \sin(\Theta)\,\underline{\underline{a}} + (1 - \cos(\Theta))\,\underline{a} \otimes \underline{a}$$

the Rodrigues' rotation formula allows us to compute the rotation matrix $\underline{\underline{R}}$,
that corresponds to a given axis-angle representation $(\underline{a}, \Theta)$,
without actually computing the matrix exponential

computing matrix exponentials (of non-diagonal matrices) is either expensive or not precise!

example

$$\underline{v}_{\text{rotated}} = \underline{\underline{R}}\,\underline{v} = \cos(\Theta)\,\underline{v} + \sin(\Theta)\underline{a} \times \underline{v} + (1 - \cos(\Theta))\,(\underline{a} \cdot \underline{v})\,\underline{a}$$

3D rotations expressed by unit quaternions

Quaternions are a number system that extends the complex numbers. A quaternion consists of one real part and three independent imaginary parts. A unit quaternion is a quaternion of norm one and therefore has three independent components.
There exists an isomorphism between unit quaternions and rotation matrices:

$$\text{given } \underline{q} = \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} \quad \rightarrow \quad \underline{\underline{R}}(\underline{q}) = 2 \cdot \begin{bmatrix} \frac{1}{2} - (q_2^2 + q_3^2) & q_1\, q_2 - q_0\, q_3 & q_1\, q_3 + q_0\, q_2 \\ q_1\, q_2 + q_0\, q_3 & \frac{1}{2} - (q_1^2 + q_3^2) & q_2\, q_3 - q_0\, q_1 \\ q_1\, q_3 - q_0\, q_2 & q_2\, q_3 + q_0\, q_1 & \frac{1}{2} - (q_1^2 + q_2^2) \end{bmatrix}$$

$$\text{real part: } q_0 = \cos\left(\frac{\Theta}{2}\right) \text{ and imaginary part: } \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \sin\left(\frac{\Theta}{2}\right) \underline{a}$$

advantages

- quadratic polynomials are faster for computation than $\sin(.)$ and $\cos(.)$
- numeric stability: when composing rotations rounding error makes unit quaternions not unit normed but normalizing is simple ; making a slightly non-orthogonal matrix orthogonal again is much harder

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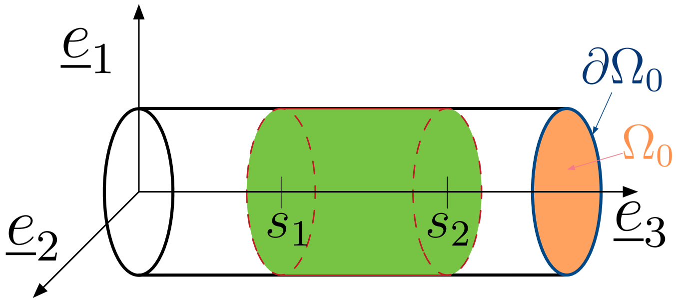
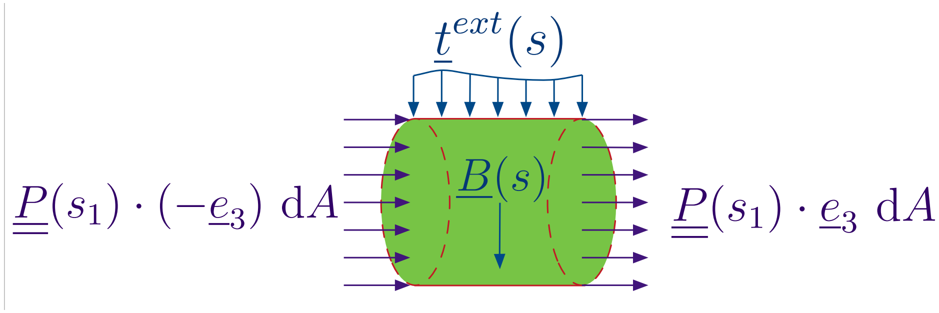
Balance of forces (part 1)





to obtain the forces and moments we integrate the pullback of the tractions / tensions acting in the deformed configuration, hence using the reference configuration as the domain of integration ...

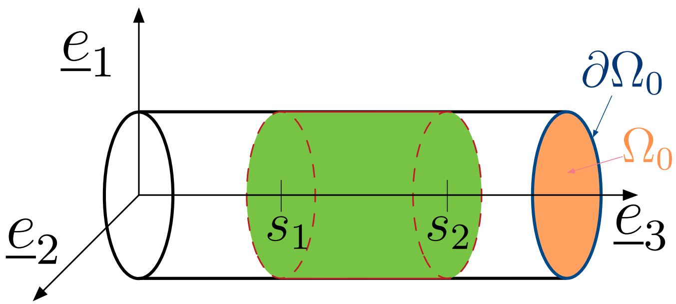
external forces: body force $\underline{B}$ and external traction $\underline{t}^{ext}$

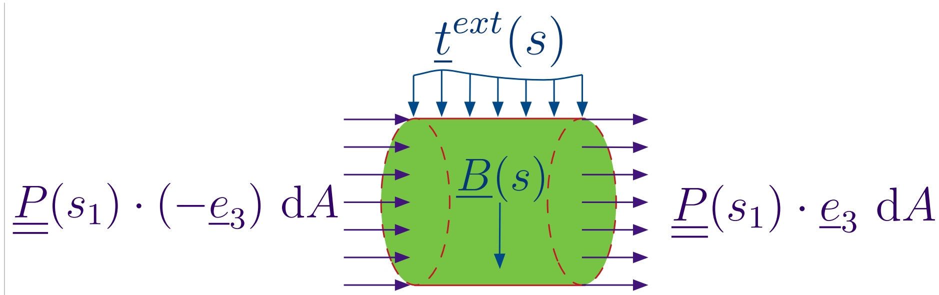
$$\int_{s_1}^{s_2} \left(\iint_{\Omega_0(s)} \underline{B}(X_1, X_2, s)\,\mathrm{d}A + \oint_{\partial\Omega_0(s)} \underline{t}^{ext}(l, s)\,\mathrm{d}l \right) \mathrm{d}s =:$$

$$=: \int_{s_1}^{s_2} \hat{\underline{n}}(s)\,\mathrm{d}s$$

$\rightarrow$ distributed external load $\hat{\underline{n}}(s)$ (force per unit of undeformed length)

Balance of forces (part 2)





internal forces

$$\iint_{\Omega_0(s)} \underline{\underline{P}} \cdot \underline{n}\, \mathrm{d}A =$$

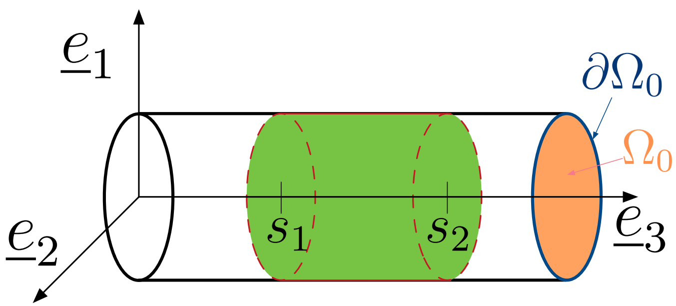
$$= \iint_{\Omega_0(s)} \underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3\, \mathrm{d}X_1\, \mathrm{d}X_2 =$$

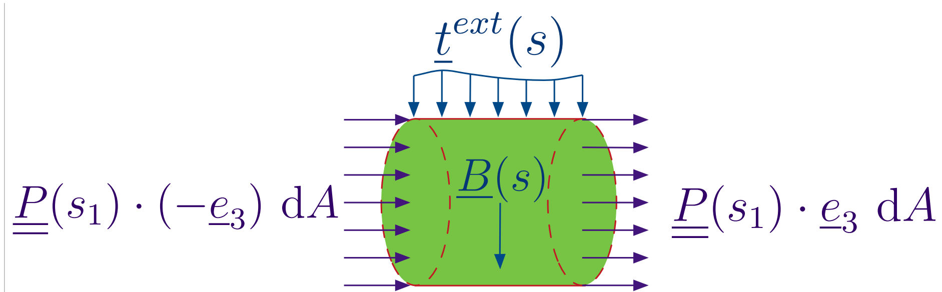
$$=: \underline{n}(s)$$

$\rightarrow$ internal contact force $\underline{n}(s)$ (force per unit of undeformed length)

Balance equations

Balance of forces (part 3)





balance of forces (statics)

$$\int_{s_1}^{s_2} \underline{\hat{n}}(s)\,\mathrm{d}s + \underline{n}(s_2) - \underline{n}(s_1) = \int_{s_1}^{s_2} \underline{\hat{n}}(s) + \underline{n}'(s)\,\mathrm{d}s = \underline{0}$$

since s_1 and s_2 are arbitrary cross sections we let $s_2 \to s_1$
and obtain the **local force balance**

$$\underline{n}'(s) + \underline{\hat{n}}(s) = \underline{0}$$

local balance of linear momentum (dynamics)

$$\underline{n}'(s) + \underline{\hat{n}}(s) = \rho_0 \cdot A \cdot \underline{\ddot{r}}(s)$$

Balance of moments (part 1)

we write the moment balance about the origin: $\underline{M} = \underline{x} \times \underline{F}$
with $\underline{x}(X_1, X_2, s) = \underline{r}(s) + \big(\underline{x}(X_1, X_2, s) - \underline{r}(s)\big)$

moment due to external loads

$$\iiint_{\text{reference volume}} \underline{x} \times \underline{B}\,\mathrm{d}V + \iint_{\text{lateral surface of reference volume}} \underline{x} \times \underline{t}^{ext}\,\mathrm{d}A =$$

$$= \int_{s_1}^{s_2} \left(\underline{r}(s) \times \iint_{\Omega_0(s)} \underline{B}(X_1, X_2, s)\,\mathrm{d}A \right) \mathrm{d}s +$$

$$+ \int_{s_1}^{s_2} \left(\iint_{\Omega_0(s)} \big(\underline{x}(X_1, X_2, s) - \underline{r}(s)\big) \times \underline{B}(X_1, X_2, s)\,\mathrm{d}A \right) \mathrm{d}s +$$

$$+ \int_{s_1}^{s_2} \left(\underline{r}(s) \times \oint_{\partial\Omega_0(s)} \underline{t}^{ext}(l, s)\,\mathrm{d}l \right) \mathrm{d}s +$$

$$+ \int_{s_1}^{s_2} \left(\oint_{\partial\Omega_0(s)} \big(\underline{x}(X_1, X_2, s) - \underline{r}(s)\big) \times \underline{t}^{ext}(l, s)\,\mathrm{d}l \right) \mathrm{d}s =$$

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Balance of moments (part 2)

$$
\begin{aligned}
&= \int_{s_1}^{s_2} \left(\underline{r}(s) \times \left(\iint_{\Omega_0} \underline{B}(X_1, X_2, s)\, \mathrm{d}A + \oint_{\partial\Omega_0(s)} \underline{t}^{ext}(s)\, \mathrm{d}l \right) \right) \mathrm{d}s + \\
&+ \int_{s_1}^{s_2} \left(\iint_{\Omega_0(s)} \big(\underline{x}(X_1, X_2, s) - \underline{r}(s) \big) \times \underline{B}(X_1, X_2, s)\, \mathrm{d}A + \right. \\
&\qquad \left. + \oint_{\partial\Omega_0} \big(\underline{x}(X_1, X_2, s) - \underline{r}(s) \big) \times \underline{t}^{ext}(l, s)\, \mathrm{d}l \right) \mathrm{d}s = \\
&=: \int_{s_1}^{s_2} \underline{r}(s) \times \underline{\hat{n}}(s)\, \mathrm{d}s + \int_{s_1}^{s_2} \underline{\hat{m}}(s)\, \mathrm{d}s
\end{aligned}
$$

Balance of moments (part 3)

moment due to internal forces

$$
\begin{aligned}
&\iint_{\Omega_0(s)} \underline{x}(X_1, X_2, s) \times \left(\underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3\right) \mathrm{d}A = \\
&= \iint_{\Omega_0(s)} \underline{r}(s) \times \left(\underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3\right) \mathrm{d}X_1 \, \mathrm{d}X_2 + \\
&+ \iint_{\Omega_0(s)} \left(\underline{x}(X_1, X_2, s) - \underline{r}(s)\right) \times \left(\underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3\right) \mathrm{d}X_1 \, \mathrm{d}X_2 = \\
&= \underline{r}(s) \times \iint_{\Omega_0(s)} \underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3 \, \mathrm{d}X_1 \, \mathrm{d}X_2 + \ldots = \\
&=: \underline{r}(s) \times \underline{n}(s) + \underline{m}(s)
\end{aligned}
$$

Balance of moments (part 4)

balance of moments (statics)

$$\int_{s_1}^{s_2} \Big(\underline{r}(s) \times \underline{\hat{n}}(s) + \underline{\hat{m}}(s)\Big)\,\mathrm{d}s +$$

$$+ \Big(\underline{r}(s_2) \times \underline{n}(s_2) + \underline{m}(s_2)\Big) - \Big(\underline{r}(s_1) \times \underline{n}(s_1) + \underline{m}(s_1)\Big) =$$

$$= \int_{s_1}^{s_2} \Big(\Big(\cancel{\underline{r}(s) \times \underline{\hat{n}}(s)} + \underline{\hat{m}}(s)\Big) + \Big(\underline{r}'(s) \times \underline{n}(s) + \cancel{\underline{r}(s) \times \underline{n}'(s)} + \underline{m}'(s)\Big)\Big)\,\mathrm{d}s =$$

$$= \int_{s_1}^{s_2} \Big(\underline{\hat{m}}(s) + \underline{r}'(s) \times \underline{n}(s) + \underline{m}'(s)\Big)\,\mathrm{d}s$$

since s_1 and s_2 are arbitrary cross sections we let $s_2 \to s_1$
and obtain the **local moment balance**

$$\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \underline{\hat{m}}(s) = \underline{0}$$

local balance of angular momentum (dynamics) (with $\underline{\underline{I}}_0$ the moment of area tensor)

$$\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \underline{\hat{m}}(s) = \rho_0 \cdot \frac{\mathrm{d}}{\mathrm{d}t}\Big(\underline{\underline{I}}_0 \cdot \underline{\omega}\Big)$$

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Review of balance equations (statics)

force balance (3 equations)

$$\underline{n}'(s) + \underline{\hat{n}}(s) = \underline{0}$$

moment balance (3 equations)

$$\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \underline{\hat{m}}(s) = \underline{0}$$

we have **6 kinematic unknowns**, $\underline{r}(s)$ and $\underline{\underline{R}}(s)$ with 3 unknowns each,

and we have **6 kinetic unknowns**

$$\underline{n}(s) = \iint_{\Omega_0(s)} \underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3 \,\mathrm{d}X_1 \,\mathrm{d}X_2$$

$$\underline{m}(s) = \iint_{\Omega_0(s)} \left(\underline{x}(X_1, X_2, s) - \underline{r}(s)\right) \times \left(\underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3\right) \mathrm{d}X_1 \,\mathrm{d}X_2$$

to close the system, we need a relationship between the kinematic and the kinetic quantities

$\rightarrow$ this relationship is called *constitutive law of the material*

Motivation of constitutive law

let's recall the **constrained deformation map** (without warping)

$$\underline{x}(X_1, X_2, s) = \underline{f}(X_1, X_2, s) = \underline{r}(s) + X_\alpha \, \underline{d}_\alpha = \underline{r}(s) + \underline{\underline{R}}(s) \cdot (X_\alpha \, \underline{e}_\alpha)$$

we compute the **deformation gradient** and obtain

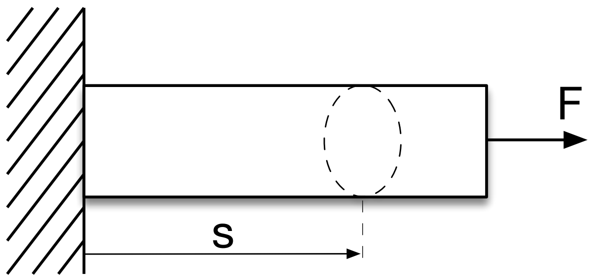
$$\begin{aligned}\underline{\underline{F}}(X_1, X_2, s) &= \underline{r}'(s) \otimes \underline{e}_3 + \underline{\underline{R}}(s) \cdot \left(\underline{e}_\alpha \otimes \underline{e}_\alpha\right) + \underline{\underline{R}}'(s) \cdot \left(X_\alpha \underline{e}_\alpha\right) \otimes \underline{e}_3 = \\ &= \underline{\underline{R}}(s) \cdot \left(\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{r}'(s) \otimes \underline{e}_3 + \underline{e}_\alpha \otimes \underline{e}_\alpha + \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\underline{R}}'(s) \cdot \left(X_\alpha \underline{e}_\alpha\right) \otimes \underline{e}_3\right)\end{aligned}$$

we then obtain an expression of the form

$$\underline{\underline{P}}(X_1, X_2, s) = \mathrm{function}\Big(\underline{\underline{F}}(X_1, X_2, s)\Big) \, ,$$

from the 3-dimensional constitutive law of the material

Example with constrained deformation map: stretching of a bar



we have the **deformed configuration**

$$\underline{r}(s) = \lambda\, s\, \underline{e}_3 \quad \text{with } \lambda \in \mathbb{R}^+$$
$$\underline{\underline{R}}(s) = \underline{\underline{I}}$$

therefore the **deformation map** is

$$\underline{x}(X_1, X_2, s)\underline{x}(s) = \lambda\, s\, \underline{e}_3 + \underline{\underline{I}} \cdot (X_\alpha\, \underline{e}_\alpha)$$

and its **deformation gradient** is given by

$$\underline{\underline{F}}(X_1, X_2, s) = \underline{\underline{F}}(s) = \lambda\, \underline{e}_3 \otimes \underline{e}_3 + \underline{e}_\alpha \otimes \underline{e}_\alpha = (\lambda - 1)\underline{e}_3 \otimes \underline{e}_3 + \underline{\underline{I}}$$

but the **axial force**

$$\underline{n}(s) = \iint_{\Omega_0(s)} \underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3\, \mathrm{d}X_1\, \mathrm{d}X_2$$
$$\neq E\, A\, (\lambda - 1)$$

because the deformation map violates the traction-free boundary condition
$\rightarrow$ the cross section must be able to shrink when the bar is stretched!

Constitutive equation for a hyperelastic rod

- a hyperelastic material is a model for reversible elasticity $\rightarrow$ stress-strain relationship derives from a potential function, i.e. the strain energy density of the material
- in general a hyperelastic material has a nonlinear stress-strain relationship
- well known hyperelastic material models are the Neo-Hookean and Mooney-Rivlin solids

strain energy per unit of undeformed length

$$\phi = \phi\Big(\underline{r}(s), \underline{\underline{R}}(s), \underline{r}'(s), \underline{\underline{R}}'(s)\Big)$$

strain energy per unit of undeformed volume

$$W\Big(\cancel{\underline{f}(s)}, \underline{\underline{F}}(s), \cancel{\nabla\underline{\underline{F}}(s)}\Big) = W\Big(\underline{\underline{F}}(s)\Big)$$

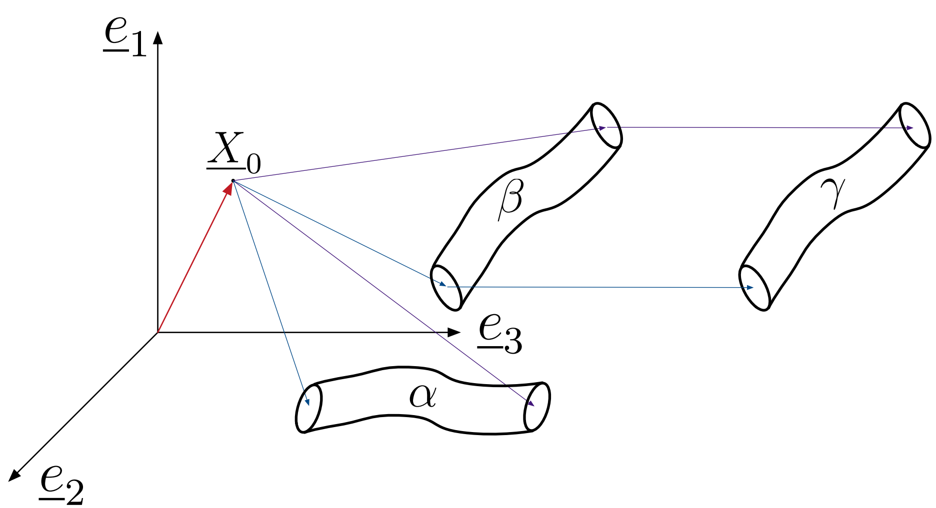
- $\underline{f}(s)$ canceled because of principle of frame-indifference
- $\nabla\underline{\underline{F}}(s)$ canceled because we will not consider higher order derivatives of the deformation map in classical elasticity (compared to higher gradient elasticity theory)

Principle of material frame-indifference (part 1)

- constitutive laws should be invariant with regard to the external frame of reference, i.e. the coordinate system ($\rightarrow$ observer objectivity)
- $\Rightarrow$ rigid body motions do not affect the internally stored energy in the system, (i.e. the mechanical/deformation energy)
- $\rightarrow$ we want to identify a set of strain measures which is invariant to rigid body motions!

to that end we set up a simple **thought experiment**

- perform two rigid body motions: one rotation followed by one translation
- equate the internal mechanical energy potentials: $\phi\big|_{\alpha} = \phi\big|_{\beta} = \phi\big|_{\gamma}$



Principle of material frame-indifference (part 2)

1. initial configuration α
   - centerline given by $\underline{r}^{\alpha}(s)$
   - cross section orientation given by $\underline{\underline{R}}^{\alpha}(s)$
   - energy potential given by $\phi\big|_{\beta}(s) = \phi\Big(\underline{r}^{\alpha}\alpha(s),\, \underline{\underline{R}}^{\alpha}(s),\, \underline{r}^{\alpha\prime}(s),\, \underline{\underline{R}}^{\alpha\prime}(s)\Big)$
2. configuration β after rigid body rotation by some $\underline{\underline{Q}} \in SO(3)$ about some $\underline{X}_0 \in \mathbb{R}^3$
   - $\underline{r}^{\beta}(s) = \underline{X}_0 + \underline{\underline{Q}}\left(\underline{r}^{\alpha}(s) - \underline{X}_0\right) \quad \Rightarrow \quad \underline{r}^{\beta\prime}(s) = \underline{\underline{Q}}\,\underline{r}^{\alpha\prime}(s)$
     (shift coordinate system s.t. rotation's fix-point $\hat{=}$ origin; rotate; undo shift)
   - $\underline{\underline{R}}^{\beta}(s) = \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}(s) \quad \Rightarrow \quad \underline{\underline{R}}^{\beta\prime}(s) = \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}(s)$
   - $\phi\big|_{\beta}(s) = \phi\Big(\underline{X}_0 + \underline{\underline{Q}}\left(\underline{r}^{\alpha}(s) - \underline{X}_0\right),\, \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}(s),\, \underline{\underline{Q}}\,\underline{r}^{\alpha\prime}(s),\, \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}(s)\Big)$
3. configuration γ after rigid body translation by some $\underline{t} \in \mathbb{R}^3$
   - $\underline{r}^{\gamma}(s) = \underline{X}_0 + \underline{\underline{Q}}\left(\underline{r}^{\alpha}(s) - \underline{X}_0\right) + \underline{t} \quad \Rightarrow \quad \underline{r}^{\gamma\prime}(s) = \underline{r}^{\beta\prime}(s) = \underline{\underline{Q}}\,\underline{r}^{\alpha\prime}(s)$
   - $\underline{\underline{R}}^{\gamma}(s) = \underline{\underline{I}}\,\underline{\underline{R}}^{\beta}(s) = \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}(s) \quad \Rightarrow \quad \underline{\underline{R}}^{\gamma\prime}(s) = \underline{\underline{R}}^{\beta\prime}(s) = \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}(s)$
   - $\phi\big|_{\gamma}(s) = \phi\Big(\underline{X}_0 + \underline{\underline{Q}}\left(\underline{r}^{\alpha}(s) - \underline{X}_0\right) + \underline{t},\, \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}(s),\, \underline{\underline{Q}}\,\underline{r}^{\alpha\prime}(s),\, \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}(s)\Big)$

Principle of material frame-indifference (part 3)

comparing $\phi\big|_{\beta}(s) \overset{!}{=} \phi\big|_{\gamma}(s)$ gives

$$\phi\Big(\underline{X}_0 + \underline{\underline{Q}}\left(\underline{r}^{\alpha}(s) - \underline{X}_0\right), \quad \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}(s), \underline{\underline{Q}}\,\underline{r}^{\alpha\prime}(s), \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}(s)\Big) =$$
$$\phi\Big(\underline{X}_0 + \underline{\underline{Q}}\left(\underline{r}^{\alpha}(s) - \underline{X}_0\right) + \underline{t}, \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}(s), \underline{\underline{Q}}\,\underline{r}^{\alpha\prime}(s), \underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}(s)\Big) \Rightarrow$$

$\Rightarrow$ ϕ is independent of $\underline{r}(s)$, i.e. the first argument can be omitted

without loss of generality we can set the arbitrarily chosen rotation matrix $\underline{\underline{Q}} := \underline{\underline{R}}^{\mathrm{T}}$

$$\phi(s) = \phi\Big(., \underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{\underline{R}}(s), \underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{r}'(s), \underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{\underline{R}}'(s)\Big)$$

we define a new version of ϕ that depends only on the invariants

$$\psi(s) := \psi\Big(\underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{r}'(s), \underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{\underline{R}}'(s)\Big)$$

Invariant strain measures (part 1)

we can verify that $\underline{\underline{R}}^{\mathrm{T}}\,\underline{r}'$ and $\underline{\underline{R}}^{\mathrm{T}}\,\underline{\underline{R}}'$ are truly invariant strain measures:

we get

$$\underline{\underline{R}}^{\gamma\mathrm{T}}\,\underline{r}^{\gamma\prime} = \left(\underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}\right)^{\mathrm{T}}\left(\underline{\underline{Q}}\,\underline{r}^{\alpha\prime}\right) = \left(\underline{\underline{R}}^{\alpha\mathrm{T}}\,\underline{\underline{Q}}^{\mathrm{T}}\right)\left(\underline{\underline{Q}}\,\underline{r}^{\alpha\prime}\right) = \underline{\underline{R}}^{\alpha\mathrm{T}}\,\underline{r}^{\alpha\prime}$$

and

$$\underline{\underline{R}}^{\gamma\mathrm{T}}\,\underline{\underline{R}}^{\gamma\prime} = \left(\underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha}\right)^{\mathrm{T}}\left(\underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}\right) = \left(\underline{\underline{R}}^{\alpha\mathrm{T}}\,\underline{\underline{Q}}^{\mathrm{T}}\right)\left(\underline{\underline{Q}}\,\underline{\underline{R}}^{\alpha\prime}\right) = \underline{\underline{R}}^{\alpha\mathrm{T}}\,\underline{\underline{R}}^{\alpha\prime}$$

Constitutive laws

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Invariant strain measures (part 2)

we define $\underline{v}$ as the shorthand for the first invariant

$$\underline{v} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = v_i \, \underline{e}_i := \underline{\underline{R}}^{\mathrm{T}} \underline{r}' \quad \Rightarrow \quad \underline{r}' = \underline{\underline{R}} \, \underline{v} = v_i \, \underline{\underline{R}} \, \underline{e}_i = v_i \, \underline{d}_i$$

and from orthogonality of the director basis ($\underline{d}_i \cdot \underline{d}_j = \delta_{ij}$) it follows that $v_i = \underline{r}' \cdot \underline{d}_i$

$\rightarrow \underline{v} = \underline{\underline{R}}^{\mathrm{T}} \underline{r}'$ is the centerline tangent vector resolved in the local director basis!

more specifically we have ...

- $v_1 = \underline{r}' \, \underline{d}_1$: rate of transverse shift $\hat{=}$ shear along $\underline{d}_1$
- $v_2 = \underline{r}' \, \underline{d}_2$: shear along $\underline{d}_2$
- $v_3 = \underline{r}' \, \underline{d}_3$: rate of axial shift $\hat{=}$ axial stretch

Invariant strain measures (part 3)

we define $\underline{\underline{K}}$ as the shorthand for the second invariant

$$\underline{\underline{K}} = K_{ij}\, \underline{e}_i \otimes \underline{e}_j := \underline{\underline{R}}^{\mathrm{T}}\, \underline{\underline{R}}'$$

proof that $\underline{\underline{K}}$ is *skew-symmetric* $(K_{ij} = -K_{ji})$

$$\underline{\underline{R}}^{\mathrm{T}}\, \underline{\underline{R}} = \underline{\underline{I}} \quad \Rightarrow \quad \underline{\underline{R}}^{\mathrm{T}}\, \underline{\underline{R}}' + \underline{\underline{R}}'^{\mathrm{T}}\, \underline{\underline{R}} = \underline{\underline{0}} \quad \Rightarrow \quad \underline{\underline{K}} = -\underline{\underline{K}}^{\mathrm{T}}$$

we therefore can write

$$\underline{\underline{K}} = \begin{bmatrix} 0 & -k_3 & k_2 \\ k_3 & 0 & -k_1 \\ -k_2 & k_1 & 0 \end{bmatrix}$$

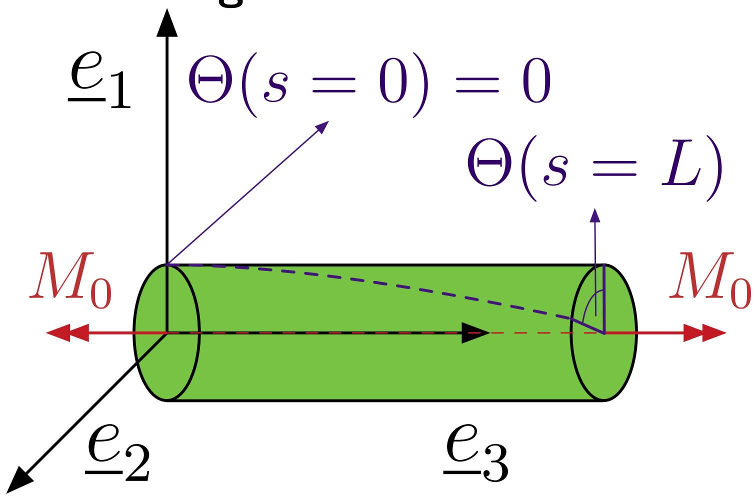
and we recall that $\underline{\underline{K}}\, \underline{a} = \underline{k} \times \underline{a}\ \forall \underline{a} \in \mathbb{R}^3$ with $\underline{k} = \mathrm{axial}(\underline{\underline{K}}) = k_i\, \underline{e}_i$

$\rightarrow$ with $(\underline{v}, \underline{k})$ we have the 6 strain measures given in the frame of the director basis!
$\rightarrow \psi = \psi\big(\underline{v}, \underline{\underline{K}}\big) =: \hat{\psi}\big(\underline{v}, \underline{k}\big)$ (for easy notation we will drop the $\hat{.}$ in the sequel)

Invariant strain measures (part 4)

to better understand the physical meaning of $\underline{k}$ we have a look at two examples ...

pure twisting of a rod



- rotation of cross sections around $\underline{e}_3$-axis
- angle of rotation for the cross section at s given by $\Theta(s) = \Theta' \cdot s$ with $\Theta' = const.$ because external moments act only at $s=0$ and $s=L$

$$\underline{r}(s) = s \cdot \underline{e}_3 \;\Rightarrow\; \underline{r}'(s) = \underline{e}_3$$

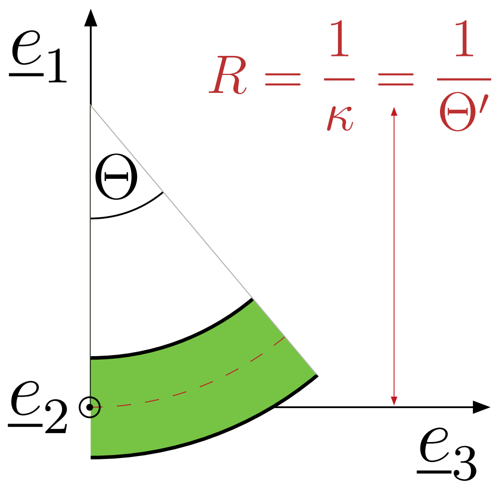
$$\Rightarrow\; \underline{v} = \underline{\underline{R}}^{\mathrm{T}} \underline{r}' = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}^{\mathrm{T}} \;\Rightarrow\; v_3 = 1$$

$$\underline{\underline{R}}(s) = \begin{bmatrix} +\cos(\Theta(s)) & -\sin(\Theta(s)) & 0 \\ +\sin(\Theta(s)) & +\cos(\Theta(s)) & 0 \\ 0 & 0 & 1 \end{bmatrix} \Rightarrow \underline{\underline{R}}'(s) = \Theta' \cdot \begin{bmatrix} -\sin(\Theta(s)) & -\cos(\Theta(s)) & 0 \\ +\cos(\Theta(s)) & -\sin(\Theta(s)) & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\underline{\underline{K}}(s) = \underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{\underline{R}}'(s) = \begin{bmatrix} 0 & -\Theta' & 0 \\ +\Theta' & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \;\Rightarrow\; \underline{k} = \begin{bmatrix} 0 \\ 0 \\ \Theta' \end{bmatrix} \;\Rightarrow\; k_3 = \Theta'$$

Invariant strain measures (part 5)

pure bending of a rod



- rotation of cross sections around $\underline{e}_2$-axis
- angle of rotation for the cross section at s given by $\Theta(s) = \Theta' \cdot s = \kappa \cdot s$ with $\Theta' = \kappa = const.$ because external moments act only at $s = 0$ and $s = L$

$$\underline{r}(s) = s \cdot \underline{e}_3 \;\Rightarrow\; \underline{r}'(s) = \underline{e}_3$$

$$\Rightarrow\; \underline{v} = \underline{\underline{R}}^{\mathrm{T}}\,\underline{r}' = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}^{\mathrm{T}} \;\Rightarrow\; v_3 = 1$$

$$\underline{\underline{R}}(s) = \begin{bmatrix} +\cos(\Theta(s)) & 0 & +\sin(\Theta(s)) \\ 0 & 1 & 0 \\ -\sin(\Theta(s)) & 0 & +\cos(\Theta(s)) \end{bmatrix} \Rightarrow \underline{\underline{R}}'(s) = \Theta' \cdot \begin{bmatrix} -\sin(\Theta(s)) & 0 & +\cos(\Theta(s)) \\ 0 & 0 & 0 \\ -\cos(\Theta(s)) & 0 & -\sin(\Theta(s)) \end{bmatrix}$$

$$\underline{\underline{K}}(s) = \underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{\underline{R}}'(s) = \begin{bmatrix} 0 & 0 & +\Theta' \\ 0 & 0 & 0 \\ -\Theta' & 0 & 0 \end{bmatrix} \;\Rightarrow\; \underline{k} = \begin{bmatrix} 0 \\ \Theta' \\ 0 \end{bmatrix} \;\Rightarrow\; k_2 = \Theta'$$

Constitutive laws

Recap of what we have so far

balance equations (in terms of nominal stresses in the reference configuration)

$$\underline{n}' + \hat{\underline{n}} = \underline{0} \quad \text{and} \quad \underline{m}' + \underline{r}' \times \underline{n} + \hat{\underline{m}} = \underline{0}$$

kinematic quantities $\underline{v}$, $\underline{k}$

$\rightarrow$ local strain measures

- v_1, v_2, v_3 : shear along d_1, shear along d_2, and stretch along d_3, respectively
- k_1, k_2, k_3 : curvature about d_1-, curvature about d_2-, and twist about d_3-axis,

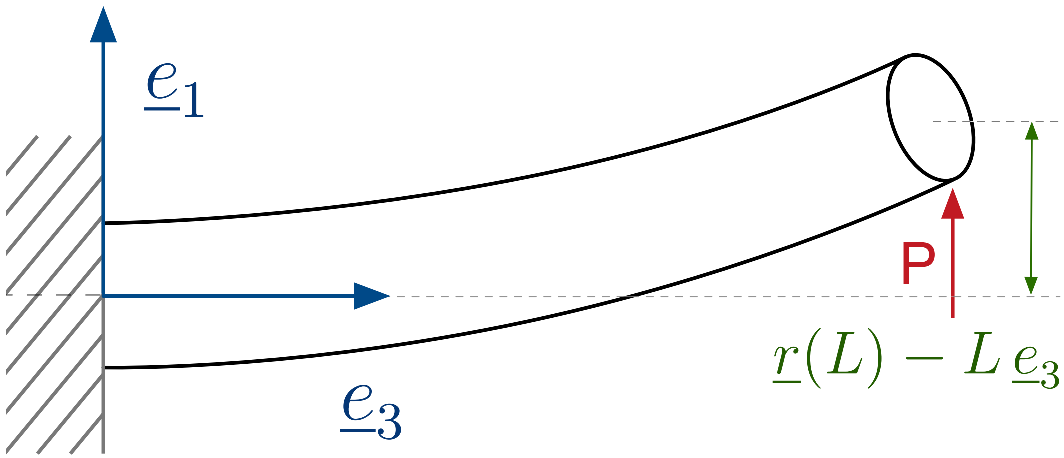
deformation energy per unit of undeformed length

$$\psi\left(\underline{\underline{R}}^{\mathrm{T}}\underline{r}', \underline{\underline{R}}^{\mathrm{T}}\underline{\underline{R}}'\right) = \psi\left(\underline{v}, \underline{\underline{K}}\right) = \psi\left(\underline{v}, \underline{k}\right)$$

$\rightarrow$ the derivatives of ψ with respect to the strains $\underline{v}$, $\underline{k}$ are the stress measures resolved in the local director basis

Minimum potential energy method (part 1)

we consider a system consisting of a beam with and an external load P at $s = L$



the **total energy of the closed system** is given by

$$\Pi\left(\underline{r},\,\underline{\underline{R}}\right) = \int_0^L \psi\left(\underline{v},\,\underline{k}\right)\mathrm{d}s - P\,\underline{e}_1 \cdot \underline{r}(L)$$

note regarding minus sign: load performs work on the beam,
thereby lowering the load's potential and also the potential of the closed system

$\rightarrow$ we now want to identify the **conditions for a minimum of** Π

Minimum potential energy method (part 2)

perturbed versions of $\underline{r}$ and $\underline{\underline{R}}$

$$\underline{r}_\epsilon(s) = \underline{r}(s) + \epsilon \cdot \delta\underline{r}(s)$$

$$\underline{\underline{R}}_\epsilon(s) = \underbrace{\cancel{\underline{\underline{R}}(s) + \epsilon \cdot \delta\underline{\underline{R}}(s)}}_{\notin SO(3)} = \underbrace{\exp\Big(\epsilon \cdot \delta\underline{\underline{\Theta}}(s)\Big)}_{\in SO(3)} \underline{\underline{R}}(s) \quad \text{with} \quad \delta\underline{\Theta} := \operatorname{axial}\Big(\delta\underline{\underline{\Theta}}\Big)$$

perturbed version of total energy

$$\Pi\Big(\underline{r}_\epsilon, \underline{\underline{R}}_\epsilon\Big) = \int_0^L \psi\Big(\underline{v}_\epsilon, \underline{k}_\epsilon\Big)\,\mathrm{d}s - P\,\underline{e}_1 \cdot \underline{r}_\epsilon(L) \stackrel{!}{=} \Pi\Big(\underline{r}, \underline{\underline{R}}\Big) + \epsilon \cdot \delta\Pi\Big(\underline{r}, \underline{\underline{R}}\Big) + o(\epsilon)$$

first variation of total energy

$$\delta\Pi = \frac{\mathrm{d}\Pi}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} = \int_0^L \left(\frac{\partial\psi}{\partial\underline{v}}(s) \cdot \underbrace{\frac{\mathrm{d}\underline{v}_\epsilon}{\mathrm{d}\epsilon}(s)\bigg|_{\epsilon=0}}_{\delta\underline{v}(s)} + \frac{\partial\psi}{\partial\underline{k}}(s) \cdot \underbrace{\frac{\mathrm{d}\underline{k}_\epsilon}{\mathrm{d}\epsilon}(s)\bigg|_{\epsilon=0}}_{\delta\underline{k}(s)} \right) \mathrm{d}s - P\,\underline{e}_1 \cdot \frac{\mathrm{d}\underline{r}_\epsilon}{\mathrm{d}\epsilon}(L)\bigg|_{\epsilon=0}$$

in the sequel we will work on the terms $\delta\underline{v}(s)$ and $\delta\underline{k}(s)$

Minimum potential energy method (part 3)

perturbed version of $\underline{v}$

$$\underline{v}_\epsilon(s) = \underline{\underline{R}}_\epsilon^{\mathrm{T}}(s) \cdot \underline{r}_\epsilon'(s) = \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \left(\exp\left(\epsilon \cdot \delta\underline{\underline{\Theta}}(s)\right)\right)^{\mathrm{T}} \cdot \left(\underline{r}'(s) + \epsilon \cdot \delta\underline{r}'(s)\right)$$

first variation of $\underline{v}$

$$\delta\underline{v}(s) = \frac{\mathrm{d}\underline{v}_\epsilon}{\mathrm{d}\epsilon}(s)\bigg|_{\epsilon=0} = \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\exp\left(\epsilon \cdot \delta\underline{\underline{\Theta}}(s)\right)\right)^{\mathrm{T}}\bigg|_{\epsilon=0} \cdot \underline{r}'(s) + \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \delta\underline{r}'(s)$$

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\exp\left(\epsilon \cdot \delta\underline{\underline{\Theta}}(s)\right)\right)^{\mathrm{T}}\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\underline{\underline{I}} + \epsilon \cdot \delta\underline{\underline{\Theta}} + \frac{\epsilon^2}{2} \cdot \delta\underline{\underline{\Theta}}^2 + \dots\right)^{\mathrm{T}}\bigg|_{\epsilon=0} = \left(\delta\underline{\underline{\Theta}}\right)^{\mathrm{T}} = -\delta\underline{\underline{\Theta}}$$

$$\Rightarrow \delta\underline{v}(s) = \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \left(-\delta\underline{\underline{\Theta}}(s) \cdot \underline{r}'(s) + \delta\underline{r}'(s)\right)$$

Minimum potential energy method (part 4)

perturbed version of $\underline{\underline{K}}$, respectively $\underline{k}$

$$\underline{\underline{K}}_\epsilon(s) = \underline{\underline{R}}^{\mathrm{T}}_\epsilon(s) \cdot \underline{\underline{R}}'_\epsilon(s) \quad \text{and} \quad \underline{k}_\epsilon(s) = \operatorname{axial}\Big(\underline{\underline{K}}_\epsilon(s)\Big)$$

first variation of $\underline{k}$

$$\delta\underline{k}(s) = \frac{\mathrm{d}\underline{k}_\epsilon}{\mathrm{d}\epsilon}(s)\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg(\operatorname{axial}\Big(\underline{\underline{R}}^{\mathrm{T}}_\epsilon(s) \cdot \underline{\underline{R}}'_\epsilon(s)\Big)\bigg)\bigg|_{\epsilon=0} =$$

$$= \operatorname{axial}\bigg(\frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big(\underline{\underline{R}}^{\mathrm{T}}_\epsilon(s) \cdot \underline{\underline{R}}'_\epsilon(s)\Big)\bigg|_{\epsilon=0}\bigg) \overset{(1)}{=} \operatorname{axial}\Big(\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \delta\underline{\underline{\Theta}}'(s) \cdot \underline{\underline{R}}\Big) \overset{(2)}{=} \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \delta\underline{\Theta}'(s)$$

regarding equality (2) we have ...

$$\Big(\underline{\underline{R}}^{\mathrm{T}} \cdot \delta\underline{\underline{\Theta}}' \cdot \underline{\underline{R}}\Big) \cdot \underline{a} = \underline{\underline{R}}^{\mathrm{T}} \cdot \delta\underline{\underline{\Theta}}' \cdot \Big(\underline{\underline{R}} \cdot \underline{a}\Big) = \underline{\underline{R}}^{\mathrm{T}} \cdot \bigg(\delta\underline{\Theta}' \times \Big(\underline{\underline{R}} \cdot \underline{a}\Big)\bigg) = \Big(\underline{\underline{R}}^{\mathrm{T}} \cdot \delta\underline{\Theta}'\Big) \times \underline{a}$$

Minimum potential energy method (part 5)

and regarding equality (1) we have ...

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\underline{\underline{R}}^{\mathrm{T}}_{\epsilon}(s)\cdot\underline{\underline{R}}'_{\epsilon}(s)\right)\bigg|_{\epsilon=0} =$$

$$= \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left[\underline{\underline{R}}^{\mathrm{T}}\cdot\Big(\exp\big(\epsilon\cdot\delta\underline{\underline{\Theta}}\big)\Big)^{\mathrm{T}}\cdot\bigg(\Big(\exp\big(\epsilon\cdot\delta\underline{\underline{\Theta}}\big)\Big)'\cdot\underline{\underline{R}}+\exp\big(\epsilon\cdot\delta\underline{\underline{\Theta}}\big)\cdot\underline{\underline{R}}'\bigg)\right]\bigg|_{\epsilon=0} =$$

$$= \left[\cancel{-\underline{\underline{R}}^{\mathrm{T}}\cdot\delta\underline{\underline{\Theta}}\cdot\underline{\underline{R}}'}+\underline{\underline{R}}^{\mathrm{T}}\cdot\Big(\delta\underline{\underline{\Theta}}'\cdot\underline{\underline{R}}+\cancel{\delta\underline{\underline{\Theta}}\cdot\underline{\underline{R}}'}\Big)\right] = \underline{\underline{R}}^{\mathrm{T}}\cdot\delta\underline{\underline{\Theta}}'\cdot\underline{\underline{R}}$$

... where we used ...

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big(\exp\big(\epsilon\cdot\delta\underline{\underline{\Theta}}(s)\big)\Big)'\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big(\underline{\underline{I}}+\epsilon\cdot\delta\underline{\underline{\Theta}}+\frac{\epsilon^2}{2}\cdot\delta\underline{\underline{\Theta}}^2+\ldots\Big)'\bigg|_{\epsilon=0} =$$

$$= \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big(\epsilon\cdot\delta\underline{\underline{\Theta}}'+\frac{\epsilon^2}{2}\cdot\delta\underline{\underline{\Theta}}'^2+\ldots\Big)'\bigg|_{\epsilon=0} = \delta\underline{\underline{\Theta}}'$$

Minimum potential energy method (part 6)

plugging back into the **first variation of total energy** we get ...

$$\delta\Pi = \int_0^L \left(\frac{\partial\psi}{\partial \underline{v}}(s) \cdot \left(\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \left(-\delta\underline{\Theta}(s) \cdot \underline{r}'(s) + \delta\underline{r}'(s) \right) \right) + \right.$$

$$\left. + \frac{\partial\psi}{\partial \underline{k}}(s) \cdot \left(\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \delta\underline{\Theta}'(s) \right) \right) \mathrm{d}s - P\,\underline{e}_1 \cdot \delta\underline{r}(L) =$$

$$= \int_0^L \left(\left(\underline{\underline{R}} \cdot \frac{\partial\psi}{\partial \underline{v}}(s) \right) \cdot \left(\delta\underline{r}'(s) + \underline{r}'(s) \times \delta\underline{\Theta}(s) \right) + \right.$$

$$\left. + \left(\underline{\underline{R}} \cdot \frac{\partial\psi}{\partial \underline{k}}(s) \right) \cdot \delta\underline{\Theta}'(s) \right) \mathrm{d}s - P\,\underline{e}_1 \cdot \delta\underline{r}(L) \overset{\text{IBP}}{=}$$

$$= \left[\underline{\underline{R}}(s) \cdot \frac{\partial\psi}{\partial \underline{v}}(s) \cdot \delta\underline{r}(s) \right]_0^L - \int_0^L \left(\left(\underline{\underline{R}}(s) \cdot \frac{\partial\psi}{\partial \underline{v}}(s) \right)' \cdot \delta\underline{r}(s) \right) \mathrm{d}s - P\,\underline{e}_1 \cdot \delta\underline{r}(L) +$$

$$+ \left[\underline{\underline{R}}(s) \cdot \frac{\partial\psi}{\partial \underline{k}}(s) \cdot \delta\underline{\Theta}(s) \right]_0^L - \int_0^L \left(\left(\left(\underline{\underline{R}}(s) \cdot \frac{\partial\psi}{\partial \underline{k}}(s) \right)' + \underline{r}'(s) \times \left(\underline{\underline{R}}(s) \cdot \frac{\partial\psi}{\partial \underline{v}}(s) \right) \right) \cdot \delta\underline{\Theta}(s) \right) \mathrm{d}s$$

IBP : integration by parts

Minimum potential energy method (part 7)

to finally obtain the conditions for a minimum of the potential energy we set $\delta \mathit{\Pi} = 0$

the integrals must each be 0 regardless of the variations $\delta \underline{r}$ and $\delta \underline{\mathit{\Theta}}$
this gives us the conditions

$$\left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s) \right)' = \underline{0}$$

$$\left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s) \right)' + \underline{r}'(s) \times \left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s) \right) = \underline{0}$$

which must be satisfied for $s \in [0, L]$ in a point-wise manner

at the boundary $s = 0$ the cross section is fixed $\Rightarrow \delta \underline{r}(0) \overset{!}{=} \underline{0}$ and $\delta \underline{\mathit{\Theta}}(0) \overset{!}{=} \underline{0}$
at the boundary $s = L$ we get the condition

$$\left(\underline{\underline{R}}(L) \cdot \frac{\partial \psi}{\partial \underline{v}}(L) - P\, \underline{e}_1 \right) \cdot \delta \underline{r}(L) + \underline{\underline{R}}(L) \cdot \frac{\partial \psi}{\partial \underline{k}}(L) \cdot \delta \underline{\mathit{\Theta}}(L) = \underline{0}$$

because $\delta \underline{r}(L)$ and $\delta \underline{\mathit{\Theta}}(L)$ are independent we get

$$\underline{\underline{R}}(L) \cdot \frac{\partial \psi}{\partial \underline{v}}(L) = P\, \underline{e}_1 \quad \text{and} \quad \underline{\underline{R}}(L) \cdot \frac{\partial \psi}{\partial \underline{k}}(L) = \underline{0}$$

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Minimum potential energy method (part 8)

inside the domain $s \in [0, L]$ we obtained the conditions

$$\left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s)\right)' = \underline{0}$$

$$\left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s)\right)' + \underline{r}'(s) \times \left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s)\right) = \underline{0}$$

balance of linear / angular momentum gives

$$\underline{n}'(s) + \cancel{\hat{\underline{n}}(s)} = \underline{0}$$

$$\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \cancel{\hat{\underline{m}}(s)} = \underline{0}$$

note: there are no distributed loads in the example

we identify the relations

$$\underline{n}(s) = \underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s)$$

$$\underline{m}(s) = \underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s)$$

Relationship between potential energy and kinetic quantities

$$\underline{n}(s) = \underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s) = n_i \, \underline{e}_i = N_i \, \underline{d}_i$$

$$\underline{m}(s) = \underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s) = m_i \, \underline{e}_i = M_i \, \underline{d}_i$$

with $\underline{d}_i(s) = \underline{\underline{R}}(s) \cdot \underline{e}_i$; it follows that

$$N_i(s) = \frac{\partial \psi}{\partial v_i}(s)$$

$$M_i(s) = \frac{\partial \psi}{\partial k_i}(s)$$

- N_1, N_2 are the shear forces in direction $\underline{d}_1$, $\underline{d}_2$, respectively
- N_3 is the axial force (in direction d_3)
- M_1, M_2 are the bending moments about the $\underline{d}_1$-, $\underline{d}_2$-axis, respectively
- M_3 is the twisting moment about the d_3-axis

Constitutive laws

Energy potential for isotropic circular beams

$$\psi\big(\underline{v},\,\underline{k}\big) = \frac{1}{2}\mathcal{C}\,v_1^2 + \frac{1}{2}\mathcal{C}\,v_2^2 + \frac{1}{2}\mathcal{D}\,(v_3-1)^2 + \frac{1}{2}\mathcal{A}\,k_1^2 + \frac{1}{2}\mathcal{A}\,k_2^2 + \frac{1}{2}\mathcal{B}\,k_3^2$$

- shearing stiffness
  $$N_1(s) = \frac{\partial\psi}{\partial v_1}(s) = \mathcal{C}\,v_1(s) \overset{!}{=} k\,G\,A\,v_1(s) \;\Rightarrow\; \mathcal{C} = k\,G\,A$$
- stretching stiffness
  $$N_3(s) = \frac{\partial\psi}{\partial v_3}(s) = \mathcal{D}\,(v_3(s)-1) \overset{!}{=} E\,A\,(v_3(s)-1) \;\Rightarrow\; \mathcal{D} = E\,A$$
- bending stiffness
  $$M_1(s) = \frac{\partial\psi}{\partial k_1}(s) = \mathcal{A}\,k_1(s) \overset{!}{=} E\,I\,k_1(s) \;\Rightarrow\; \mathcal{A} = E\,I$$
- twisting stiffness
  $$M_3(s) = \frac{\partial\psi}{\partial k_3}(s) = \mathcal{B}\,k_3(s) \overset{!}{=} G\,J\,k_3(s) \;\Rightarrow\; \mathcal{B} = G\,J$$

similarly in 3D-elasticity we have as a constitutive law

$$\underline{\underline{P}} = \frac{\partial W(\underline{\underline{F}})}{\partial \underline{\underline{F}}}$$

Model equations

force balance with constitutive law

$$\left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s)\right)' + \underline{\hat{n}}(s) = \underline{\underline{R}}'(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s) + \underline{\underline{R}}(s) \cdot \left(\frac{\partial \psi}{\partial \underline{v}}(s)\right)' + \underline{\hat{n}}(s) = \underline{0}$$

moment balance with constitutive law

$$\left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s)\right)' + \underline{r}'(s) \times \left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s)\right) + \underline{\hat{m}}(s) =$$

$$= \underline{\underline{R}}'(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s) + \underline{\underline{R}}(s) \cdot \left(\frac{\partial \psi}{\partial \underline{k}}(s)\right)' + \underline{r}'(s) \times \left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s)\right) + \underline{\hat{m}}(s) = \underline{0}$$

we now want to write the equations in terms of $\underline{v}$ and $\underline{k}$ ...

Force balance

multiplying with $\underline{\underline{R}}^{\mathrm{T}}$ on the left we get ...

$$\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\underline{R}}'(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s) + \left(\frac{\partial \psi}{\partial \underline{v}}(s)\right)' + \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\hat{n}}(s) =$$

$$= \underline{k}(s) \times \frac{\partial \psi}{\partial \underline{v}}(s) + \frac{\partial^2 \psi}{\partial \underline{v}^2}(s) \cdot \underline{v}'(s) + \frac{\partial^2 \psi}{\partial \underline{v} \partial \underline{k}}(s) \cdot \underline{k}'(s) + \underline{\tilde{n}}(s) = \underline{0}$$

with

$$\underline{\tilde{n}}(s) := \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\hat{n}}(s)$$

Moment balance

again multiplying with $\underline{\underline{R}}^{\mathrm{T}}$ on the left we get ...

$$
\begin{aligned}
&\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\underline{R}}'(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s) + \left(\frac{\partial \psi}{\partial \underline{k}}(s)\right)' + \\
&+\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \left(\underline{r}'(s) \times \left(\underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s)\right)\right) + \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\hat{m}}(s) = \\
&= \underline{k}(s) \times \frac{\partial \psi}{\partial \underline{k}}(s) + \frac{\partial^2 \psi}{\partial \underline{v} \partial \underline{k}}(s) \cdot \underline{v}'(s) + \frac{\partial^2 \psi}{\partial \underline{k}^2}(s) \cdot \underline{k}'(s) + \\
&+\underline{v}(s) \times \frac{\partial \psi}{\partial \underline{v}}(s) + \underline{\tilde{m}}(s) = \underline{0}
\end{aligned}
$$

with

$$
\underline{\tilde{m}}(s) := \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\hat{m}}(s)
$$

Combined model

Model equations

force balance

$$\underline{k}(s) \times \frac{\partial \psi}{\partial \underline{v}}(s) + \frac{\partial^2 \psi}{\partial \underline{v}^2}(s) \cdot \underline{v}'(s) + \frac{\partial^2 \psi}{\partial \underline{v} \partial \underline{k}}(s) \cdot \underline{k}'(s) + \underline{\tilde{n}}(s) = \underline{0}$$

and **moment balance**

$$\underline{k}(s) \times \frac{\partial \psi}{\partial \underline{k}}(s) + \frac{\partial^2 \psi}{\partial \underline{v} \partial \underline{k}}(s) \cdot \underline{v}'(s) + \frac{\partial^2 \psi}{\partial \underline{k}^2}(s) \cdot \underline{k}'(s) +$$

$$+ \underline{v}(s) \times \frac{\partial \psi}{\partial \underline{v}}(s) + \underline{\tilde{m}}(s) = \underline{0}$$

expressed in terms of the **strains** (in the director basis)

$$\underline{v}(s) = \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{r}'(s) \quad ; \quad \underline{k}(s) = \operatorname{axial}\left(\underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\underline{R}}'(s)\right)$$

given the **distributed external loads** (resolved in the director basis)

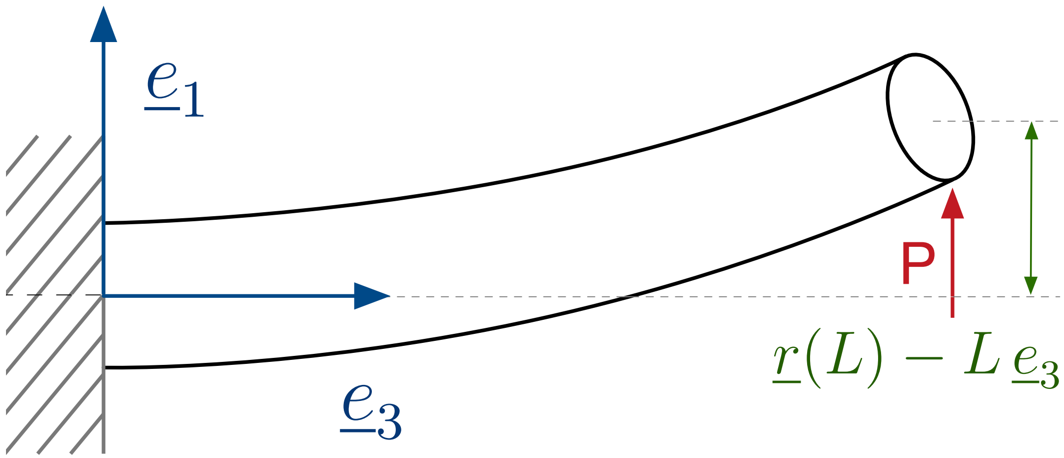
$$\underline{\tilde{n}}(s) = \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\hat{n}}(s) \quad ; \quad \underline{\tilde{m}}(s) = \underline{\underline{R}}^{\mathrm{T}}(s) \cdot \underline{\hat{m}}(s)$$

$\rightarrow$ system of 6 equations ; 1^{st} order in $\underline{v}$, $\underline{k}$ but 2^{nd} order in $\underline{r}$, $\underline{\underline{R}}$

$\rightarrow$ 12 boundary conditions required

Combined model

Example with boundary conditions



we have 12 boundary conditions:

boundary conditions at $s = 0$:

- $\underline{r}(0) = \underline{0}$
- $\underline{\underline{R}}(0) = \underline{\underline{I}} = \exp \underline{\underline{\Theta}} \iff \underline{\Theta} = \underline{0}$

boundary conditions at $s = L$:

- $\underline{\underline{R}} \cdot \frac{\partial \psi}{\partial \underline{v}}(L) = P \cdot \underline{e}_1$
- $\frac{\partial \psi}{\partial \underline{k}}(L) = \underline{0} \iff M_i = 0 \; (i \in 1, 2, 3)$

note that the boundary conditions are not stated in our unknown variables $\underline{v}$, $\underline{k}$

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Model as a system of first order equations (part 1)

boundary conditions for forces and moments can be written in terms of strains ; this is not possible with the boundary conditions for displacements and rotations ; therefore the system is not closed

to *close the system*, we will rewrite the model as 12 first order equations, by including 6 extra equations relating strain quantities to displacement quantities:

$$\underline{v} = \underline{\underline{R}}^{\mathrm{T}} \cdot \underline{r}' \Rightarrow \underline{r}' = \underline{\underline{R}} \cdot \underline{v}$$

$$\underline{\underline{K}} = \underline{\underline{R}}^{\mathrm{T}} \cdot \underline{\underline{R}}' \Rightarrow \underline{\underline{R}}' = \underline{\underline{R}} \cdot \underline{\underline{K}}$$

we already noticed, that using unit quaternions to encode $SO(3)$ matrices has some great advantages for computation. therefore we chose to replace the matrix differential equation in $\underline{\underline{R}}$ by a matrix differential equation in terms of unit quaternions $\underline{q} \in \mathbb{R}^4$

$$\underline{q}' = \underline{\underline{E}}(\underline{q}) \cdot \underline{k} = \frac{1}{2} \cdot \begin{bmatrix} -q_1 & -q_2 & -q_3 \\ +q_0 & -q_3 & +q_2 \\ +q_3 & +q_0 & -q_1 \\ -q_2 & +q_1 & +q_0 \end{bmatrix} \cdot \underline{k}$$

Model as a system of first order equations (part 2)

we have the same 6 equations as before here expressed in matrix form

$$\underbrace{\begin{bmatrix} \frac{\partial^2 \psi}{\partial \underline{v}^2} & \frac{\partial^2 \psi}{\partial \underline{v} \partial \underline{k}} \\ \frac{\partial^2 \psi}{\partial \underline{k} \partial \underline{v}} & \frac{\partial^2 \psi}{\partial \underline{k}^2} \end{bmatrix}}_{=:\underline{\underline{C}}} \cdot \begin{bmatrix} \underline{v}' \\ \underline{k}' \end{bmatrix} = \begin{bmatrix} -\underline{k} \times \frac{\partial \psi}{\partial \underline{v}} \\ -\underline{k} \times \frac{\partial \psi}{\partial \underline{k}} - \underline{v} \times \frac{\partial \psi}{\partial \underline{v}} \end{bmatrix} - \begin{bmatrix} \underline{\underline{R}}^{\mathrm{T}} \underline{\hat{n}} \\ \underline{\underline{R}}^{\mathrm{T}} \underline{\hat{m}} \end{bmatrix}$$

$\underline{\underline{C}}$ is the (positive definite) elasticity tensor matrix

we close the system by adding the seven extra first order equations (relating derivatives of displacements to strains)

$$\underline{r}' = \underline{\underline{R}} \cdot \underline{v}$$

$$\underline{q}' = \underline{\underline{E}}(\underline{q}) \cdot \underline{k}$$

$\rightarrow$ this gives us a system of 13 coupled nonlinear ODEs

Extra constraint for unit quaternions

using unit quaternions to encode rotations leads to a system of 13 equations instead of just 12 ; this extra equation is contained within

$$\underline{q}' = \underline{\underline{E}}(\underline{q}) \cdot \underline{k} \quad (\star)$$

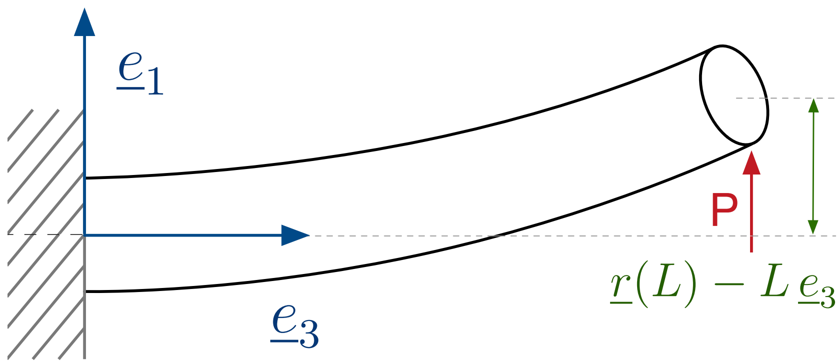
since rotations are encoded by *unit* quaternions the constraint $\left\|\underline{q}\right\|_2 \overset{!}{=} 1$ must be satisfied

from the constraint we obtain a necessary condition: $\underline{q} \cdot \underline{q} \overset{!}{=} 1 \;\Rightarrow\; \underline{q} \cdot \underline{q}' \overset{!}{=} 0$, which is automatically satisfied by $(\star)$: dotting $(\star)$ with $\underline{q}$ gives ...

$$\underline{q}' \cdot \underline{q} = \left(\underline{\underline{E}}(\underline{q}) \cdot \underline{k}\right) \cdot \underline{q} = \underline{k} \cdot \left(\underline{\underline{E}}^{\mathrm{T}} \cdot \underline{q}\right) = \underline{k} \cdot \left(\begin{bmatrix} -q_1 & +q_0 & +q_3 & -q_2 \\ -q_2 & -q_3 & +q_0 & +q_1 \\ -q_3 & +q_2 & -q_1 & +q_0 \end{bmatrix} \cdot \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} \right) = \underline{k} \cdot \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = 0$$

adding one (13^{th}) boundary condition for $\underline{q}$ (either $\left\|\underline{q}\right\|_2 \Big|_{s=0} = 1$ or $\left\|\underline{q}\right\|_2 \Big|_{s=L} = 1$) is (in combination with the automatically satisfied necessary condition) sufficient to satisfy the constraint for all s

Example with boundary conditions (revisited)



we have 13 boundary conditions:

boundary conditions at $s = 0$:

- $\underline{r}(0) = \underline{0}$
- $\underline{q}(0) = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^{\mathrm{T}}$ because

$$q_0 = \cos\left(\frac{\Theta}{2}\right) = 1 \text{ and}$$

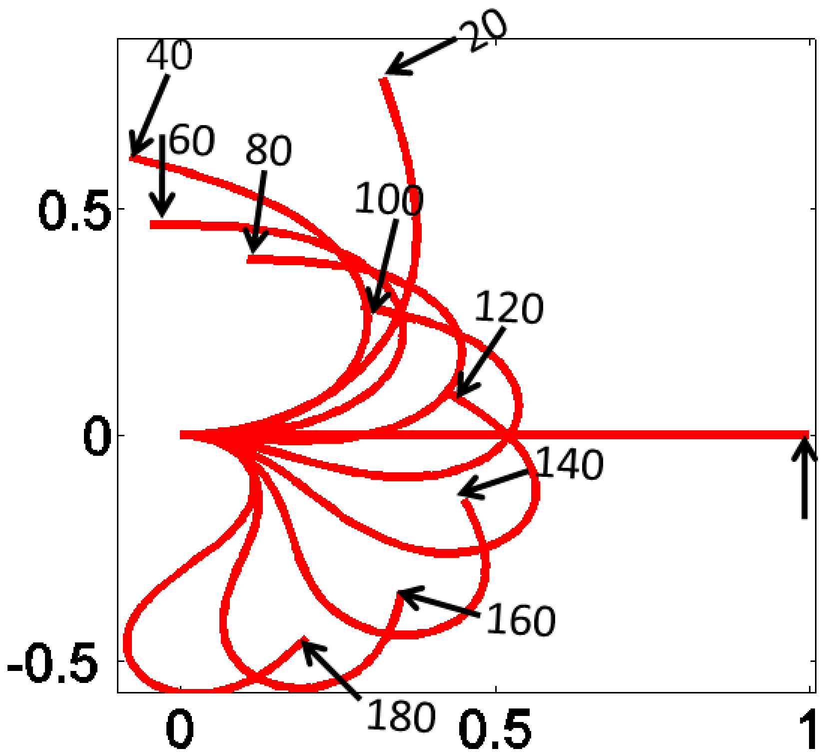
$$\begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \sin\left(\frac{\Theta}{2}\right) \cdot \underline{a} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

boundary conditions at $s = L$:

- $\underline{\underline{R}} \cdot \frac{\partial \psi}{\partial \underline{v}}(L) = P \cdot \underline{e}_1$
- $\frac{\partial \psi}{\partial \underline{k}}(L) = \underline{0} \iff$

$$M_i(L) = 0 \; (i \in 1, 2, 3)$$

Another example with boundary conditions: follower load problem



boundary conditions at $s = 0$:

- $\underline{r}(0) = \underline{0}$

- $\underline{q}(0) = \begin{bmatrix}1 & 0 & 0 & 0\end{bmatrix}^{\mathrm{T}}$ because

$$q_0 = \cos\left(\frac{\Theta}{2}\right) = 1 \text{ and}$$

$$\begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \sin\left(\frac{\Theta}{2}\right) \cdot \underline{a} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

boundary conditions at $s = L$:

- $\underline{\underline{R}} \cdot \frac{\partial \psi}{\partial \underline{v}}(L) = P \cdot \underline{d}_1 = \underline{\underline{R}} \cdot P \cdot \underline{e}_1 \Rightarrow$

$$\frac{\partial \psi}{\partial v_1}(L) = P$$

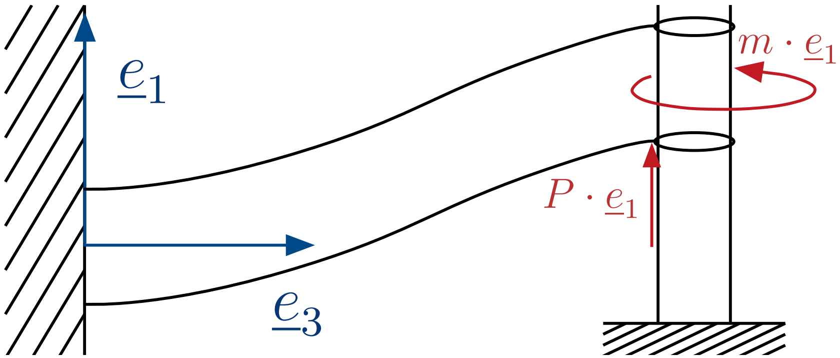
$$\frac{\partial \psi}{\partial v_2}(L) = 0$$

$$\frac{\partial \psi}{\partial v_3}(L) = 0$$

- $\frac{\partial \psi}{\partial \underline{k}}(L) = \underline{0} \iff$

$$M_i(L) = 0 \; (i \in 1, 2, 3)$$

Yet another example with boundary conditions



boundary conditions at $s = 0$:

- $\underline{r}(0) = \underline{0}$
- $\underline{q}(0) = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^{\mathrm{T}}$ because

$$q_0 = \cos\left(\frac{\Theta}{2}\right) = 1 \text{ and}$$

$$\begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \sin\left(\frac{\Theta}{2}\right) \cdot \underline{a} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

boundary conditions at $s = L$:

- $n_1(L) = P$

$$\underline{\underline{R}} \cdot \frac{\partial \psi}{\partial \underline{v}}(L) = P \cdot \underline{e}_1 \Rightarrow$$

$$\left(\underline{\underline{R}} \cdot \frac{\partial \psi}{\partial \underline{v}}(L)\right) \cdot \underline{e}_1 = P \wedge \underline{e}_1 = \underline{d}_1(L) \Rightarrow$$

$$\frac{\partial \psi}{\partial v_1}(L) = P$$

- $r_2(L) = 0$
- $r_3(L) = L$
- $\dfrac{\partial \psi}{\partial k_1}(L) = m$
- $\begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \sin\left(\frac{\Theta}{2}\right) \cdot \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \Rightarrow q_2 = 0,\ q_3 = 0$

Constitutive laws (part 2)

Material symmetry in 3D elasticity

$$W\left(\underline{\underline{F}}\right) \overset{\star}{=} W\left(\underline{\underline{U}}\right) \overset{\diamond}{=} W\left(I_1,\, I_2,\, I_3\right)$$

- $\star$: principle of frame-indifference
- $\underline{\underline{U}}$: from polar decomposition $\underline{\underline{F}} = \underline{\underline{\tilde{R}}} \cdot \underline{\underline{U}}$
- $\diamond$: isotropy: material law is the same for all directions in the material
- $I_1,\, I_2,\, I_3$: strain-invariants
- in case of an orthotropic material law, there would simply result a few more invariants ; othotropy here means that the material behavior in s direction differs from the behavior in $X_1,\, X_2$ directions

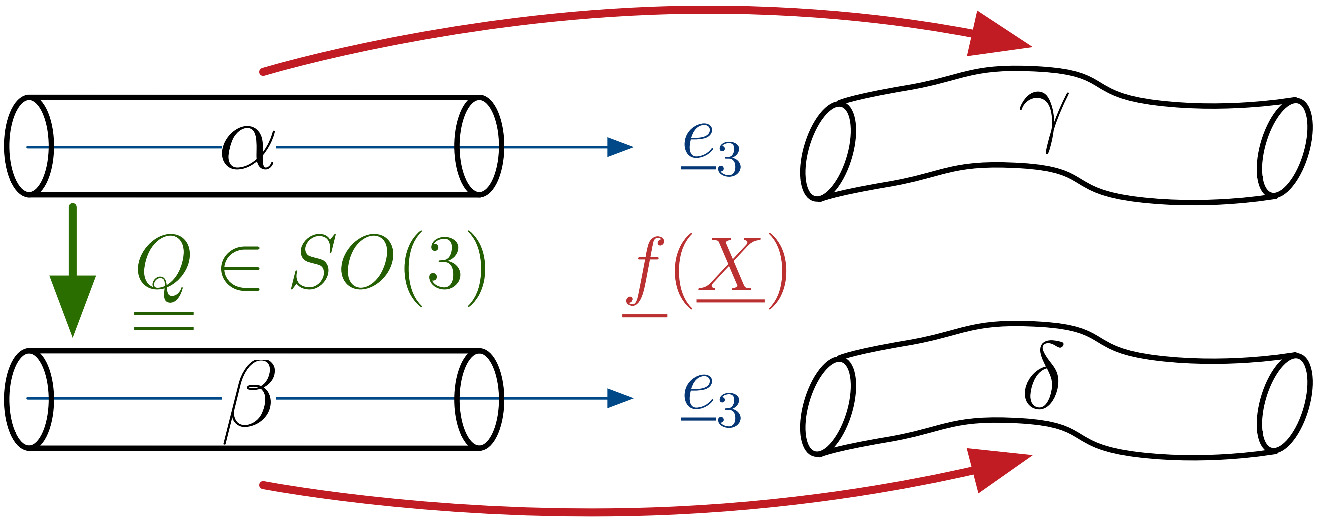
how to obtain the specific form of the energy potential function?
remember for example the already postulated function

$$\psi\left(\underline{v},\, \underline{k}\right) = \frac{1}{2}\mathcal{C}\, v_1^2 + \frac{1}{2}\mathcal{C}\, v_2^2 + \frac{1}{2}\mathcal{D}\,(v_3 - 1)^2 + \frac{1}{2}\mathcal{A}\, k_1^2 + \frac{1}{2}\mathcal{A}\, k_2^2 + \frac{1}{2}\mathcal{B}\, k_3^2$$

$\rightarrow$ how to identify the strain invariants?

Material symmetry in elastic rods (part 1)

to get a better understanding of the concept of material symmetry,
we set up **another thought experiment**



- we start with the reference configuration α
- we rotate α by $\underline{\underline{Q}}$ to get β (a rotated reference configuration)
- $\underline{f}(.)$ maps $\alpha \mapsto \gamma$ and $\beta \mapsto \delta$

if $\underline{\underline{Q}}$ is in the symmetry group $\mathcal{G}$ then then we have $\psi\big|_{\gamma} = \psi\big|_{\delta}$

Material symmetry in elastic rods (part 2)

1. configuration γ (image of reference configuration α)
   - $\underline{r}^{\gamma}(s)$
   - $\underline{\underline{R}}^{\gamma}(s)$
2. configuration δ (image of rotated reference configuration β)
   - $\underline{r}^{\delta}(s) = \underline{r}^{\gamma}(s)$
   - $\underline{\underline{R}}^{\delta}(s) = \underline{\underline{R}}^{\gamma}(s) \cdot \underline{\underline{Q}}$
   - $\underline{v}^{\delta}(s) = \underline{\underline{R}}^{\gamma\mathrm{T}}(s) \cdot \underline{r}^{\gamma\prime}(s) = \underline{\underline{Q}}^{\mathrm{T}} \cdot \underline{\underline{R}}^{\gamma\mathrm{T}}(s) \cdot \underline{r}^{\gamma\prime}(s) = \underline{\underline{Q}}^{\mathrm{T}} \cdot \underline{v}^{\gamma}(s)$
   - $\underline{k}^{\delta} = \mathrm{axial}\left(\underline{\underline{R}}^{\delta\mathrm{T}} \cdot \underline{\underline{R}}^{\delta\prime}\right) = \mathrm{axial}\left(\underline{\underline{Q}}^{\mathrm{T}} \cdot \underline{\underline{R}}^{\gamma\mathrm{T}} \cdot \underline{\underline{R}}^{\gamma\prime} \cdot \underline{\underline{Q}}\right) = \underline{\underline{Q}}^{\mathrm{T}} \cdot \mathrm{axial}\left(\underline{\underline{R}}^{\gamma\mathrm{T}} \cdot \underline{\underline{R}}^{\gamma\prime}\right) = \underline{\underline{Q}}^{\mathrm{T}} \cdot \underline{k}^{\gamma}$

$$\Rightarrow \psi\left(\underline{\underline{Q}}^{\mathrm{T}} \cdot \underline{v}^{\gamma}, \underline{\underline{Q}}^{\mathrm{T}} \cdot \underline{k}^{\gamma}\right) \overset{!}{=} \psi\left(\underline{v}^{\gamma}, \underline{k}^{\gamma}\right) \, \forall \underline{\underline{Q}} \in \mathcal{G}$$

- the symmetry group $\mathcal{G}$ depends on geometry and on the material of the beam
- $\mathcal{G} \equiv SO(2)$ (all rotations about $\underline{e}_3$-axis), if beam has circular cross section and isotropic material ; also the case for circular ropes with continuous helicity

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Material symmetry in elastic rods (part 3)

with $\mathcal{G} \equiv SO(2)$ we had ...

$$\underline{\underline{Q}} = \begin{bmatrix} +\cos(\Theta) & -\sin(\Theta) & 0 \\ +\sin(\Theta) & +\cos(\Theta) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \forall\, \Theta \in [0, 2\,\pi]$$

$$\underline{v}^{\delta} = \underline{\underline{Q}}^{\mathrm{T}} \cdot \underline{v}^{\gamma} = \begin{bmatrix} \begin{bmatrix} +\cos(\Theta) & +\sin(\Theta) \\ -\sin(\Theta) & +\cos(\Theta) \end{bmatrix} \cdot \begin{bmatrix} v_1^{\gamma} \\ v_2^{\gamma} \end{bmatrix} \\ v_3^{\gamma} \end{bmatrix} \quad ; \quad \underline{v}^{\delta} = \ldots \text{(replace } v \text{ by } k\text{)}$$

we introduce some abbreviations ...

$$\underline{v}^{\delta} = \begin{bmatrix} \hat{\underline{\underline{Q}}}^{\mathrm{T}} \cdot \hat{\underline{v}}^{\gamma} \\ v_3^{\gamma} \end{bmatrix} \text{ with } \hat{\underline{v}}^{\gamma} = \begin{bmatrix} v_1^{\gamma} \\ v_2^{\gamma} \end{bmatrix} \text{ and } \hat{\underline{\underline{Q}}} = \begin{bmatrix} +\cos(\Theta) & -\sin(\Theta) \\ +\sin(\Theta) & +\cos(\Theta) \end{bmatrix}$$

we observe the following **invariants** under all such transformations $\underline{\underline{Q}} \in \mathcal{G}$

- angle between and magnitude of $\hat{\underline{v}}$, $\hat{\underline{k}}$ $\quad \rightarrow \quad \|\hat{\underline{v}}\|\,,\|\hat{\underline{k}}\|\,,\ \hat{\underline{v}} \cdot \hat{\underline{k}}\ ,\ \left(\hat{\underline{v}} \times \hat{\underline{k}}\right) \cdot \underline{e}_3$
- v_3, k_3

$$\Rightarrow \psi = \psi\Big(\underbrace{v_1^2 + v_2^2}_{I_1},\ \underbrace{k_1^2 + k_2^2}_{I_2},\ \underbrace{v_1 \cdot k_1 + v_2 \cdot k_2}_{I_3},\ \underbrace{v_1 \cdot k_2 - v_2 \cdot k_1}_{I_4},\ \underbrace{v_3}_{I_5},\ \underbrace{k_3}_{I_6}\Big)$$

Material symmetry in elastic rods (part 4)

to derive the concrete form of the energy potential function,
we do a Taylor-expansion of ψ about $\left(\underline{v}_0, \underline{k}_0\right) = \left(\begin{bmatrix}0 & 0 & 1\end{bmatrix}^{\mathrm{T}}, \begin{bmatrix}0 & 0 & 0\end{bmatrix}^{\mathrm{T}}\right)$

$$\psi\left(\underline{v}, \underline{k}\right) = \cancelto{0}{\psi\left(\underline{v}_0, \underline{k}_0\right)} + \cancelto{0}{\tfrac{\partial \psi}{\partial \underline{v}}\left(\underline{v}_0, \underline{k}_0\right)} \cdot \left(\underline{v} - \underline{v}_0\right) + \cancelto{0}{\tfrac{\partial \psi}{\partial \underline{k}}\left(\underline{v}_0, \underline{k}_0\right)} \cdot \left(\underline{k} - \underline{k}_0\right) +$$

$$+\frac{1}{2}\Bigg(\left(\frac{\partial^2 \psi}{\partial \underline{v}^2} \cdot \left(\underline{v} - \underline{v}_0\right)\right) \cdot \left(\underline{v} - \underline{v}_0\right) + \left(\frac{\partial^2 \psi}{\partial \underline{k}^2} \cdot \left(\underline{k} - \underline{k}_0\right)\right) \cdot \left(\underline{k} - \underline{k}_0\right) +$$

$$+2 \cdot \left(\frac{\partial^2 \psi}{\partial \underline{v} \partial \underline{k}} \cdot \left(\underline{k} - \underline{k}_0\right)\right) \cdot \left(\underline{v} - \underline{v}_0\right)\Bigg) + \text{HOT}$$

from the Taylor expansion consider for example the term

$$\frac{\partial^2 \psi}{\partial \underline{v}^2} = \frac{\partial}{\partial \underline{v}}\left(\frac{\partial \psi}{\partial \underline{v}}\right) = \frac{\partial}{\partial \underline{v}}\left(\frac{\partial \psi}{\partial I_1} \cdot \frac{\partial I_1}{\partial \underline{v}} + \dots + \frac{\partial \psi}{\partial I_6} \cdot \frac{\partial I_6}{\partial \underline{v}}\right) = \dots$$

$\frac{\partial \psi}{\partial I_j}$ are unknowns that must be obtained from experiments / 3D elasticity, whereas $\frac{\partial I_j}{\partial \underline{v}}$ can easily be computed from kinematics ($j = 1, \dots, 6$)

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Material symmetry in elastic rods (part 5)

doing the computations and grouping terms in a way to get a polynomial in the strains we obtain

$$\psi = \frac{1}{2}\Big(\mathcal{A}\cdot\left(k_1^2+k_2^2\right)+\mathcal{B}\cdot k_3^2+\mathcal{C}\cdot\left(v_1^2+v_2^2\right)+\mathcal{D}\cdot\left(k_3-1\right)^2\Big)+$$
$$+\cdot\mathcal{E}\cdot\left(v_3-1\right)\cdot k_3+\cdot\mathcal{F}\cdot\left(v_1\cdot k_1+v_2\cdot k_2\right)+\text{HOT}$$

as **another experiment** consider now a reflection of the beam about the $\underline{e}_1$-$\underline{e}_2$-plane

- reflections are in the group $O(2)$
- reflections are not in the symmetry group $\mathcal{G}\equiv SO(2)$ of a pre-twisted rod
- $O(2)$ is the symmetry group for rods without helicity of fibers in the undeformed configuration ; for such rods $\mathcal{E}=\mathcal{F}=0$

Relaxation of cross section

Recap: kinematics

- s identifies a certain cross section of the rod
- $\underline{r}(s)$ describes the position of the cross section centroid for the cross section at s

  $\rightarrow$ describes the centerline of the rod
- $\underline{\underline{R}}(s)$ describes the (average) orientation of the cross section at s

  $\rightarrow$ $\underline{d}_i(s) = \underline{\underline{R}}(s) \cdot \underline{e}_i$ is the local director basis

deformation map with warping of the cross section

$$\underline{f}(\underline{X}) = \underline{f}(X_1, X_2, X_3 = s) = \underline{r}(s) + \underline{\underline{R}}(s) \cdot (X_\alpha \, \underline{e}_\alpha + \underline{u}) \quad \text{with } \alpha \in \{1, 2\}$$

note that so far we did not use any deformation map in the derivations!

local **strain measures**

- $\underline{v} = \underline{\underline{R}}^{\mathrm{T}} \cdot \underline{r}' = \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}^{\mathrm{T}}$

  v_1 : shear along $\underline{d}_1$

  v_2 : shear along $\underline{d}_2$

  v_3 : axial stretch (along $\underline{d}_3$)
- $\underline{k} = \mathrm{axial}\left(\underline{\underline{R}}^{\mathrm{T}} \cdot \underline{\underline{R}}'\right) = \begin{bmatrix} k_1 & k_2 & k_3 \end{bmatrix}^{\mathrm{T}}$

  k_1 : curvature about $\underline{d}_1$-axis

  k_2 : curvature about $\underline{d}_2$-axis

  k_3 : twist about $\underline{d}_3$-axis

Relaxation of cross section

Recap: balance laws

balance of linear momentum

$$\underline{n}'(s) + \hat{\underline{n}}(s) = \rho_0 \cdot A \cdot \ddot{\underline{r}}(s)$$

balance of angular momentum

$$\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \hat{\underline{m}}(s) = \rho_0 \cdot \frac{\mathrm{d}}{\mathrm{d}t}\left(\underline{\underline{I}}_0 \cdot \underline{\omega}\right)$$

equations are in terms of the **internal contact force** and **internal moment**

$$\underline{n}(s) = \iint_{\Omega_0(s)} \underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3 \,\mathrm{d}X_1 \,\mathrm{d}X_2$$

$$\underline{m}(s) = \iint_{\Omega_0(s)} \Big(\underline{x}(X_1, X_2, s) - \underline{r}(s)\Big) \times \Big(\underline{\underline{P}}(X_1, X_2, s) \cdot \underline{e}_3\Big) \,\mathrm{d}X_1 \,\mathrm{d}X_2$$

with **external loads**

$$\hat{\underline{n}}(s) = \iint_{\Omega_0(s)} \underline{B}(X_1, X_2, s) \,\mathrm{d}A + \oint_{\partial\Omega_0(s)} \underline{t}^{ext}(l, s) \,\mathrm{d}l$$

$$\hat{\underline{m}}(s) = \iint_{\Omega_0(s)} \Big(\underline{x}(.,.,s) - \underline{r}(s)\Big) \times \underline{B}(s) \,\mathrm{d}A + \oint_{\partial\Omega_0} \Big(\underline{x}(.,.,s) - \underline{r}(s)\Big) \times \underline{t}^{ext}(s) \,\mathrm{d}l\Big)$$

Relaxation of cross section

Recap: constitutive laws

strain energy per unit of undeformed length

$$\phi\Big(\underline{r}(s), \underline{\underline{R}}(s), \underline{r}'(s), \underline{\underline{R}}'(s)\Big) \stackrel{\star}{=} \psi\Big(\underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{r}'(s),\ \underline{\underline{R}}^{\mathrm{T}}(s)\,\underline{\underline{R}}'(s)\Big) = \psi\Big(\underline{v}(s), \underline{k}(s)\Big)$$

$\star$: principle of frame-indifference

relationship between potential energy and kinetic quantities

$$\underline{n}(s) = \underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{v}}(s) \quad ; \quad \underline{m}(s) = \underline{\underline{R}}(s) \cdot \frac{\partial \psi}{\partial \underline{k}}(s)$$

material symmetry in elastic rods

$$\psi\Big(\underline{v}(s), \underline{k}(s)\Big) \stackrel{\mathcal{G}\equiv SO(2)}{=} \psi\Big(v_1^2 + v_2^2,\ k_1^2 + k_2^2,\ v_1 \cdot k_1 + v_2 \cdot k_2,\ v_1 \cdot k_2 - v_2 \cdot k_1,\ v_3, k_3\Big)$$

$$\approx \frac{1}{2}\Big(\mathcal{A}\Big(k_1^2 + k_2^2\Big) + \mathcal{B} \cdot k_3^2 + \mathcal{C} \cdot \Big(v_1^2 + v_2^2\Big) + \mathcal{D} \cdot \Big(k_3 - 1\Big)^2\Big) +$$

$$+ \cdot \mathcal{E} \cdot \Big(v_3 - 1\Big) \cdot k_3 + \cdot \mathcal{F} \cdot \Big(v_1 \cdot k_1 + v_2 \cdot k_2\Big)$$

if fibers of the rod are not pre-twisted we have $\mathcal{G} \equiv O(2) \ \Rightarrow\ \mathcal{E} = \mathcal{F} = 0$

Relaxation of cross section

Motivation for relaxation / warping of the cross section

the model that we have so far is too stiff because every cross section is assumed to be rigid!

we therefore already introduced a modified deformation map, that allows for warping / relaxation of the cross section:

$$\underline{f}(X_1, X_2, s) = \underline{r}(s) + \underline{\underline{R}}(s) \cdot \left(X_\alpha \, \underline{e}_\alpha + \underline{u} \right)$$

it has already been stated that we do not want to have $\underline{u}$ as a function of s, because that would imply solving the expensive 3D problem

strategy for 1D theory

- we consider the rod in a configuration where $\left(\underline{v}(s), \underline{k}(s)\right) = \left(\underline{v}^\star, \underline{k}^\star\right)$ constant $\forall\, s$
- in the sequel we call this configuration the $\star$-problem
- then we compute $\underline{u}^\star(X_1, X_2)$

  $\rightarrow$ because of uniformity in s this is a 2D elasticity problem
- in the context of a finite element discretization, one such 2D problem is solved for every quadrature point within an element to approximate the average warping $\underline{u}^\star(X_1, X_2)$ of the cross sections within that element ; $\left(\underline{v}^\star, \underline{k}^\star\right)$ are the strains at the quadrature points

Relaxation of cross section

Uniformly strained rod

- we have a rod with the same $\left(\underline{v}^\star, \underline{k}^\star\right)$ for every s
- all its cross sections warp / relax in exactly the same way

  $\rightarrow$ we must consider just one cross section, i.e. we have a 2D problem
- this cross section is completely relaxed
- the deformation map of this relaxed configuration is
  $\underline{f}^\star(X_1, X_2, s) = \underline{r}^\star(s) + \underline{\underline{R}}^\star(s) \cdot \left(X_\alpha\, \underline{e}_\alpha + \underline{u}^\star(X_1, X_2)\right)$

accuracy of the approximation

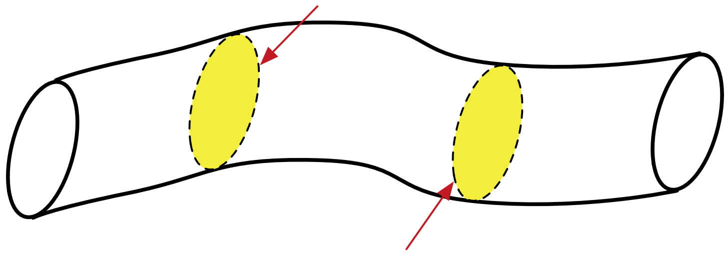
- consider an arbitrary rod in a deformed configuration and one particular cross section $s^\star$
- set $\left(\underline{v}^\star, \underline{k}^\star\right) := \left(\underline{v}(s^\star), \underline{k}(s^\star)\right)$
- consider the same rod but in the configuration with $\left(\underline{v}(s), \underline{k}(s)\right) = \left(\underline{v}^\star, \underline{k}^\star\right) \forall\, s$,
  i.e. the particular $\star$-problem at $s = s^\star$
- if in the arbitrarily deformed configuration $\left(\underline{v}(s), \underline{k}(s)\right)$ change slowly with s in some neighborhood of $s^\star$, then $\underline{u}^\star(X_1, X_2)$, obtained from the $\star$-problem, is a good *local* approximation for $\underline{u}(X_1, X_2, s = s^\star)$, obtained from 3D theory

Strain energy of a cross section

the warping of the cross section will be determined by a minimization of strain energy

$$\psi\big(\underline{v},\, \underline{k}\,;\, \underline{u}(\underline{v},\, \underline{k})\big) = \lim_{s_2 \to s_1} \frac{1}{s_2 - s_1} \int_{s_1}^{s_2} \left(\iint_{\Omega_0(s)} W\big(\underline{\underline{F}}\big)\, \mathrm{d}\Omega_0 \right) \mathrm{d}s = \iint_{\Omega_0(s)} W\big(\underline{\underline{F}}\big)\, \mathrm{d}\Omega_0$$

$$\psi_1 = \psi\big(\underline{v}_1, \underline{k}_1\big) = \psi\big(\underline{v}(s_1), \underline{k}(s_1)\big)$$



$$\psi_2 = \psi\big(\underline{v}_2, \underline{k}_2\big) = \psi\big(\underline{v}(s_2), \underline{k}(s_2)\big)$$

in order to compute the strain energy ψ, considering relaxation of the cross section, we require a material model $W(.)$ from 3D elasticity, such as the Neo-Hookean solid or the Mooney-Rivlin solid

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Deformation gradient of the star-problem

starting with the deformation map of the $\star$-problem

$$\underline{f}^\star(X_1, X_2, s) = \underline{r}^\star(s) + \underline{\underline{R}}^\star(s) \cdot \Big(\underbrace{X_\alpha\, \underline{e}_\alpha + \underline{u}^\star(X_1, X_2)}_{\underline{x}_0^\star(X_1,X_2)}\Big)$$

we compute its deformation gradient

$$\underline{\underline{F}}^\star(X_1, X_2, s) =$$

$$= \underline{r}^{\star\prime}(s) \otimes \underline{e}_3 + \underline{\underline{R}}^\star(s) \cdot \left(\underline{e}_\alpha \otimes \underline{e}_\alpha + \frac{\partial \underline{u}^\star}{\partial X_\alpha} \otimes \underline{e}_\alpha\right) + \underline{\underline{R}}^{\star\prime}(s) \cdot \Big(X_\alpha \underline{e}_\alpha + \underline{u}^\star(X_1, X_2)\Big) \otimes \underline{e}_3 =$$

$$= \underline{\underline{R}}^\star(s) \cdot \left(\underline{v}^\star\cancel{(s)} \otimes \underline{e}_3 + \underline{e}_\alpha \otimes \underline{e}_\alpha + \frac{\partial \underline{u}^\star}{\partial X_\alpha} \otimes \underline{e}_\alpha + \underline{\underline{K}}^\star\cancel{(s)} \cdot \Big(X_\alpha \underline{e}_\alpha + \underline{u}^\star(X_1, X_2)\Big) \otimes \underline{e}_3\right) =$$

$$= \underline{\underline{R}}^\star(s) \cdot \left(\underline{v}^\star \otimes \underline{e}_3 + \underline{e}_\alpha \otimes \underline{e}_\alpha + \frac{\partial \underline{u}^\star}{\partial X_\alpha} \otimes \underline{e}_\alpha + \underline{k}^\star \times \Big(X_\alpha \underline{e}_\alpha + \underline{u}^\star(X_1, X_2)\Big) \otimes \underline{e}_3\right) =$$

$$=: \underline{\underline{R}}^\star(s) \cdot \underline{\underline{\tilde{F}}}^\star(X_1, X_2, s)$$

Relaxation of cross section

Warping of the cross section in the star-problem

without loss of generality ...

- we consider the cross section at $s = 0$
- we prescribe $\underline{\underline{R}}^\star(s=0) = \underline{\underline{R}}_0^\star = \underline{\underline{I}}$ (rigid body rotation)
- we prescribe $\underline{r}^\star(s=0) = \underline{r}_0^\star = \underline{0}$ (rigid body translation)

minimization of energy

$$\underline{u}^\star(X_1, X_2) = \underset{\underline{u}(X_1,X_2)}{\arg\min}\ \psi\big(\underline{v}^\star,\, \underline{k}^\star\,;\, \underline{u}\big) = \underset{\underline{u}(X_1,X_2)}{\arg\min} \iint_{\Omega_0} W\Big(\underline{\underline{\tilde{F}}}^\star(X_1, X_2, s=0)\Big)\, \mathrm{d}\Omega_0$$

- here $\underline{\underline{\tilde{F}}}^\star$ is the deformation gradient we just computed *but* we consider $\underline{u}(X_1, X_2)$ as a free variable, for which we optimize, i.e. $\underline{\underline{\tilde{F}}}^\star = \underline{\underline{\tilde{F}}}^\star(X_1, X_2, s=0\,;\,\underline{u})$
- the minimization is carried out subject to constraints:
  (mass) center and orientation of the cross section must be preserved

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Displacements in the star-problem (part 1)

rotation / orientation of cross section

$$\underline{\underline{R}}^{\star\mathrm{T}}(s) \cdot \underline{\underline{R}}^{\star\prime}(s) = \underline{\underline{K}}^{\star} \text{ (const.) } \Rightarrow \underline{\underline{R}}^{\star\prime}(s) = \underline{\underline{R}}^{\star}(s) \cdot \underline{\underline{K}}^{\star}$$

$$\Rightarrow \underline{\underline{R}}^{\star}(s) = \underline{\underline{R}}^{\star}_{0} \cdot \exp\Big(\underline{\underline{K}}^{\star} \cdot s\Big) = \exp\Big(\underline{\underline{K}}^{\star} \cdot s\Big)$$

translation / displacement of cross section

$$\underline{\underline{R}}^{\star\mathrm{T}}(s) \cdot \underline{r}^{\star\prime}(s) = \underline{v}^{\star} \text{ (const.) } \Rightarrow \underline{r}^{\star\prime}(s) = \underline{\underline{R}}^{\star}(s) \cdot \underline{v}^{\star} = \exp\Big(\underline{\underline{K}}^{\star} \cdot s\Big) \cdot \underline{v}^{\star}$$

$$\underline{r}^{\star}(s) = \cancel{\underline{r}^{\star}_{0}} + \left(\int_0^s \exp\Big(\underline{\underline{K}}^{\star} \cdot l\Big)\, \mathrm{d}l\right) \cdot \underline{v}^{\star}$$

Displacements in the star-problem (part 2)

decomposition of $\underline{v}^\star$

we split $\underline{v}^\star$ in a part that is parallel to $\underline{k}^\star$ and a part that is perpendicular to $\underline{k}^\star$

$$\underline{v}^\star = \left(\cos(\phi) \cdot \underline{\widehat{k}} + \sin(\phi) \cdot \underline{\widehat{k}}^\perp\right) \cdot \|\underline{v}^\star\|$$

- ϕ is the angle between $\underline{v}^\star$ and $\underline{k}^\star$, i.e. $\phi = \arcsin\left(\frac{\underline{v}^\star \cdot \underline{k}^\star}{\|\underline{v}^\star\| \cdot \|\underline{k}^\star\|}\right)$
- $\underline{\widehat{k}}$ is the unit vector along $\underline{k}^\star$, i.e. $\underline{\widehat{k}} = \frac{\underline{k}^\star}{\|\underline{k}^\star\|}$
- $\underline{\widehat{k}}^\perp$ is a unit vector perpendicular to $\underline{\widehat{k}}$

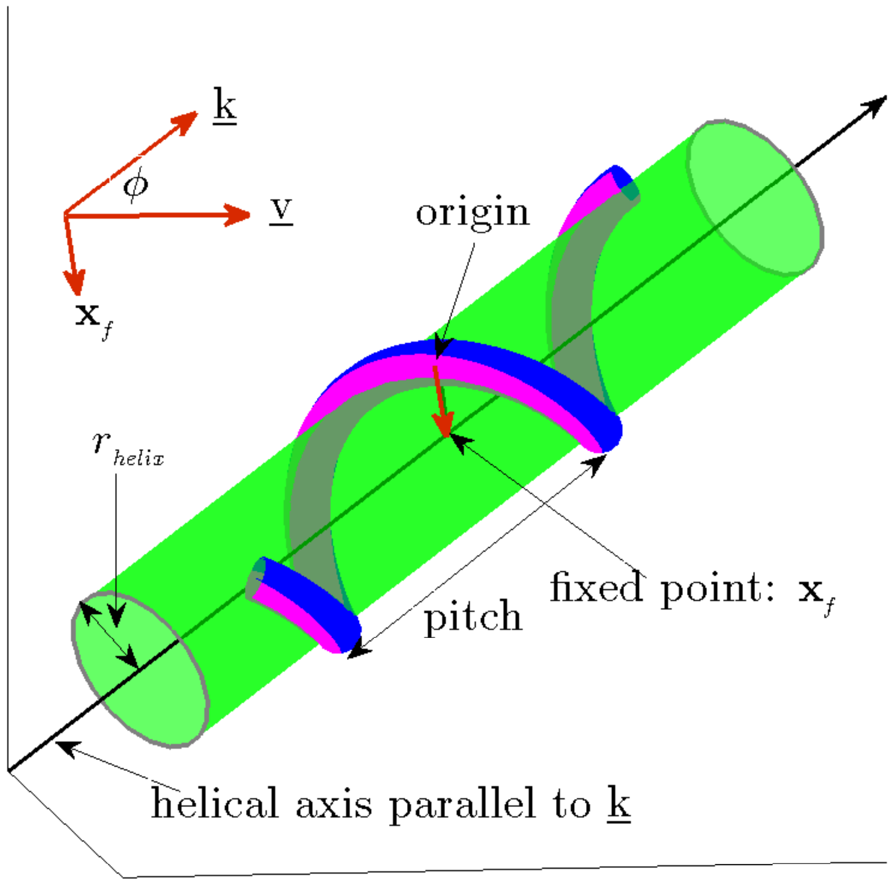
translation / displacement of cross section (revisited)

$$\underline{r}^\star(s) = \left(\underbrace{\cos(\phi) \cdot \int_0^s \overbrace{\exp\left(\underline{\underline{K}}^\star \cdot l\right) \cdot \underline{\widehat{k}}}^{\underline{\widehat{k}}} \, \mathrm{d}l}_{\text{straight line along } \underline{\widehat{k}}} + \underbrace{\sin(\phi) \cdot \int_0^s \exp\left(\underline{\underline{K}}^\star \cdot l\right) \cdot \underline{\widehat{k}}^\perp \, \mathrm{d}l}_{\text{circle with normal along } \underline{\widehat{k}}}\right) \cdot \|\underline{v}^\star\|$$

Relaxation of cross section

The centerline turns into a helix

$$\underline{r}^{\star}(s) = \left(\cos(\phi) \cdot \underline{\hat{k}} \cdot s + \sin(\phi) \cdot \int_0^s \exp\left(\underline{\underline{K}}^{\star} \cdot l\right) \cdot \underline{\hat{k}}^{\perp} \, \mathrm{d}l \right) \cdot \left\| \underline{v}^{\star} \right\|$$



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Helix equation

rewriting the equation we get ...

$$\underline{r}^{\star}(s) = \left\|\underline{v}^{\star}\right\| \cdot \left(\cos(\phi) \cdot \underline{\hat{k}} \cdot s + \sin(\phi) \cdot \frac{1}{\left\|\underline{k}^{\star}\right\|} \cdot \left(\underline{\underline{I}} - \exp\left(\underline{\underline{K}}^{\star} \cdot s\right)\right) \cdot \underline{\hat{k}} \times \underline{\hat{k}}^{\perp}\right)$$

we introduce the abbreviations

- $\tau = \left\|\underline{v}^{\star}\right\| \cdot \cos(\phi)$
- $\underline{x}_f = \frac{\sin(\phi) \cdot \underline{\hat{k}} \times \underline{\hat{k}}^{\perp}}{\|\underline{k}^{\star}\|} = \frac{\underline{v}^{\star} \times \underline{k}^{\star}}{\|\underline{k}^{\star}\|^2}$ (fixed point of the helix)

and get ...

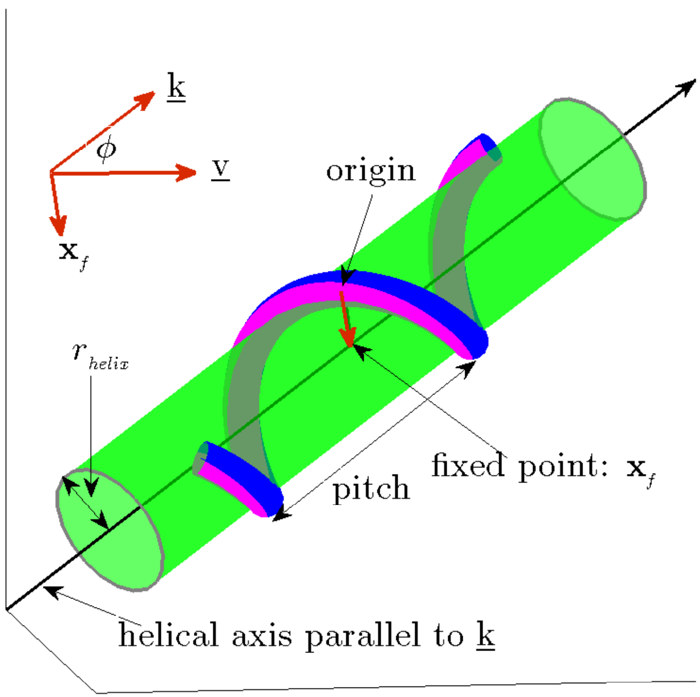
$$\underline{r}^{\star}(s) = s \cdot \tau \cdot \underline{\hat{k}} + \left(\underline{\underline{I}} - \exp\left(\underline{\underline{K}}^{\star} \cdot s\right)\right) \cdot \underline{x}_f = s \cdot \tau \cdot \underline{\hat{k}} + \underbrace{\underline{x}_f + \underline{\underline{R}}^{\star}(s) \cdot \left(\underline{r}_0^{\star} - \underline{x}_f\right)}_{\text{rotation of the origin about } \underline{x}_f}$$

examples

- $\underline{v}^{\star} \parallel \underline{k}^{\star}$: centerline degenerates into a straight line (e.g. combined extension & torsion)
- $\underline{v}^{\star} \perp \underline{k}^{\star}$: centerline degenerates into a circle (e.g. pure bending)

Helix

$$\underline{r}^{\star}(s) =$$
$$s \cdot \tau \cdot \hat{\underline{k}} + \underline{x}_f + \exp\left(\underline{\underline{K}}^{\star} \cdot s\right) \cdot \left(\underline{r}_0^{\star} - \underline{x}_f\right)$$



pitch

for one full turn of the helix we have

$$\left\|\underline{k}^{\star}\right\| \cdot \overset{\circ}{s} \overset{!}{=} 2 \cdot \pi$$

plugging $\overset{\circ}{s}$ into the part of the helix equation that generates the axial motion we obtain the pitch of the helix as

$$\overset{\circ}{s} \cdot \tau = \frac{2\,\pi}{\left\|\underline{k}^{\star}\right\|} \cdot \left\|\underline{v}^{\star}\right\| \cdot \cos(\phi)$$

radius

$$\left\|\underline{r}_0^{\star} - \underline{x}_f\right\| = \left\|\underline{x}_f\right\|$$

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Deformation map and deformation gradient of the star-problem

we rewrite the **deformation map** of the $\star$-problem, using the helix equation ...

$$\underline{f}^{\star}(X_1,X_2,s)=\underline{r}^{\star}(s)+\underline{\underline{R}}^{\star}(s)\cdot\Big(X_\alpha\,\underline{e}_\alpha+\underline{u}^{\star}(X_1,X_2)\Big)=\underline{r}^{\star}(s)+\underline{\underline{R}}^{\star}(s)\cdot\underline{x}_0^{\star}(X_1,X_2)=$$

$$=s\cdot\tau\cdot\underline{\hat{k}}+\underline{x}_f+\underline{\underline{R}}^{\star}(s)\cdot\Big(\underline{x}_0^{\star}(X_1,X_2)-\underline{x}_f\Big)$$

$\rightarrow$ rotating $\underline{r}^{\star}=\underline{0}$ about $\underline{x}_f$ creates centerline ; rotating $\underline{x}_0^{\star}$ about $\underline{x}_f$ creates entire rod

and then we compute its **deformation gradient** ...

$$\underline{\underline{F}}^{\star}(X_1,X_2,s)=\underline{r}^{\star\prime}(s)\otimes\underline{e}_3+\underline{\underline{R}}^{\star\prime}(s)\cdot\underline{x}_0^{\star}(X_1,X_2)\otimes\underline{e}_3+\underline{\underline{R}}^{\star}(s)\cdot\frac{\partial\underline{x}_0^{\star}}{\partial X_\alpha}\otimes\underline{e}_\alpha=$$

$$=\underline{\underline{R}}^{\star}(s)\cdot\Big(\underline{\underline{R}}^{\star\mathrm{T}}(s)\cdot\underline{r}^{\star\prime}(s)\otimes\underline{e}_3+\underline{\underline{R}}^{\star\mathrm{T}}(s)\cdot\underline{\underline{R}}^{\star\prime}(s)\cdot\underline{x}_0^{\star}(X_1,X_2)\otimes\underline{e}_3+\frac{\partial\underline{x}_0^{\star}}{\partial X_\alpha}\otimes\underline{e}_\alpha\Big)=$$

$$=\underline{\underline{R}}^{\star}(s)\cdot\Big(\underline{v}^{\star}\otimes\underline{e}_3+\Big(\underline{k}^{\star}\times\underline{x}_0^{\star}(X_1,X_2)\Big)\otimes\underline{e}_3+\frac{\partial\underline{x}_0^{\star}}{\partial X_\alpha}\otimes\underline{e}_\alpha\Big)$$

Relaxation of cross section

2D minimization problem (part 1)

$$\min_{\underline{x}_0^\star} \iint_{\Omega_0} W\Big(\tilde{\underline{\underline{F}}}^\star(X_1, X_2, s=0)\Big)\,\mathrm{d}\Omega_0$$

such that ...

∘ the center(line) remains at the origin or more precisely that the mass center of the cross section remains in the origin, i.e.

$$\iint_{\Omega_0} \rho_0 \cdot \underline{x}_0^\star\,\mathrm{d}\Omega_0 = \underline{0}$$

∘ and such that orientation of the cross section remains in the $\underline{e}_1$-$\underline{e}_2$-plane or more precisely that the principal axis of the inertia tensor remains aligned with the $\underline{e}_3$-axis ; this is the same as saying that the mixed moments of inertia must vanish

$$\iint_{\Omega_0} \underbrace{\rho_0 \cdot \begin{bmatrix} x_2 \cdot x_3 \\ x_1 \cdot x_3 \\ x_1 \cdot x_2 \end{bmatrix}}_{=:\underline{M}}\,\mathrm{d}\Omega_0 = \underline{0}$$

with x_i the components of $\underline{x}_0^\star$

2D minimization problem (part 2)

minimization problem with augmented Langrangian

$$\min_{\underline{x}_0^\star, \underline{\lambda}, \underline{\mu}} \iint_{\Omega_0} \Big(W\big(\underline{\underline{\tilde{F}}}^\star(X_1, X_2, s=0)\big) + \underline{\lambda} \cdot \rho_0 \cdot \underline{x}_0^\star + \underline{\mu} \cdot \underline{M} \Big) \, \mathrm{d}\Omega_0$$

perturbed version of $\underline{x}_0^\star$

$$\underline{x}_0^\epsilon(X_1, X_2) = \underline{x}_0^\star(X_1, X_2) + \epsilon \cdot \delta \underline{x}_0^\star(X_1, X_2)$$

perturbed version of the cross section energy

$$\psi_\epsilon = \iint_{\Omega_0} \Big(W\big(\underline{\underline{\tilde{F}}}^\epsilon(X_1, X_2, s=0)\big) + \underline{\lambda} \cdot \rho_0 \cdot \underline{x}_0^\epsilon(X_1, X_2) + \underline{\mu} \cdot \underline{M}^\epsilon(X_1, X_2) \Big) \, \mathrm{d}\Omega_0$$

first variation of the cross section energy

$$\delta\psi = \left.\frac{\mathrm{d}\psi_\epsilon}{\mathrm{d}\epsilon}\right|_{\epsilon=0} = \iint_{\Omega_0} \Big(\underbrace{\frac{\partial W}{\partial \underline{\underline{F}}}}_{\underline{\underline{P}}} : \left.\frac{\mathrm{d}\underline{\underline{\tilde{F}}}^\epsilon}{\mathrm{d}\epsilon}\right|_{\epsilon=0} + \underline{\lambda} \cdot \rho_0 \cdot \left.\frac{\mathrm{d}\underline{x}_0^\epsilon}{\mathrm{d}\epsilon}\right|_{\epsilon=0} + \underline{\mu} \cdot \left.\frac{\mathrm{d}\underline{M}^\epsilon}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \Big) \, \mathrm{d}\Omega_0$$

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2D minimization problem (part 3)

from

$$\underline{\underline{F}}^{\epsilon}(X_1, X_2, s) = \underline{\underline{R}}^{\star}(s) \cdot \left(\underline{v}^{\star} \otimes \underline{e}_3 + \left(\underline{k}^{\star} \times \underline{x}_0^{\epsilon}(X_1, X_2)\right) \otimes \underline{e}_3 + \frac{\partial \underline{x}_0^{\epsilon}}{\partial X_\alpha} \otimes \underline{e}_\alpha\right)$$

it follows that

$$\left.\frac{\mathrm{d}\underline{\underline{\tilde{F}}}^{\epsilon}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} = \left(\underline{k}^{\star} \times \delta\underline{x}_0^{\star}(X_1, X_2)\right) \otimes \underline{e}_3 + \frac{\partial \delta\underline{x}_0^{\star}}{\partial X_\alpha} \otimes \underline{e}_\alpha$$

and from

$$\underline{M}^{\epsilon} = \rho_0 \cdot \begin{bmatrix} x_2^{\epsilon} \cdot x_3^{\epsilon} \\ x_1^{\epsilon} \cdot x_3^{\epsilon} \\ x_1^{\epsilon} \cdot x_2^{\epsilon} \end{bmatrix} = \rho_0 \cdot \begin{bmatrix} (x_2 + \epsilon \cdot \delta x_2) \cdot (x_3 + \epsilon \cdot \delta x_3) \\ (x_1 + \epsilon \cdot \delta x_1) \cdot (x_3 + \epsilon \cdot \delta x_3) \\ (x_1 + \epsilon \cdot \delta x_1) \cdot (x_2 + \epsilon \cdot \delta x_2) \end{bmatrix}$$

it follows that

$$\left.\frac{\mathrm{d}\underline{M}^{\epsilon}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} = \rho_0 \cdot \begin{bmatrix} x_2 \cdot \delta x_3 + x_3 \cdot \delta x_2 \\ x_1 \cdot \delta x_3 + x_3 \cdot \delta x_1 \\ x_1 \cdot \delta x_2 + x_2 \cdot \delta x_1 \end{bmatrix} = \underbrace{\rho_0 \cdot \begin{bmatrix} 0 & x_3 & x_2 \\ x_3 & 0 & x_1 \\ x_2 & x_1 & 0 \end{bmatrix}}_{=:\underline{\underline{M}}(X_1, X_2)} \cdot \delta\underline{x}_0^{\star}(X_1, X_2)$$

2D minimization problem (part 4)

note that

$$\underline{\underline{P}} : \left(\underline{a} \otimes \underline{b}\right) \mathrel{\hat{=}} P_{ij}\, a_i\, b_j = P_{ij}\, b_j\, a_i \mathrel{\hat{=}} \left(\underline{\underline{P}} \cdot \underline{b}\right) \cdot \underline{a}$$

and that

$$\underline{a} \cdot \left(\underline{b} \times \underline{c}\right) = \underline{b} \cdot \left(\underline{c} \times \underline{a}\right) = \underline{c} \cdot \left(\underline{a} \times \underline{b}\right)$$

first variation of the cross section energy

$$\delta\psi = \iint_{\Omega_0} \left(\underline{\underline{P}} : \left(\left(\underline{k}^\star \times \delta\underline{x}_0^\star \right) \otimes \underline{e}_3 + \frac{\partial \delta \underline{x}_0^\star}{\partial X_\alpha} \otimes \underline{e}_\alpha \right) + \underline{\lambda} \cdot \left(\rho_0 \cdot \delta\underline{x}_0^\star \right) + \underline{\mu} \cdot \left(\underline{\underline{M}} \cdot \delta\underline{x}_0^\star \right) \right) \mathrm{d}\Omega_0 =$$

$$= \iint_{\Omega_0} \left(\left(\underline{\underline{P}} \cdot \underline{e}_3 \right) \cdot \left(\underline{k}^\star \times \delta\underline{x}_0^\star \right) + \overbrace{\left(\underline{\underline{P}} \cdot \underline{e}_\alpha \right) \cdot \frac{\partial \delta\underline{x}_0^\star}{\partial X_\alpha}}^{\to \text{IBP}} + \left(\rho_0 \cdot \underline{\lambda} + \underline{\underline{M}} \cdot \underline{\mu} \right) \cdot \delta\underline{x}_0^\star \right) \mathrm{d}X_1\, \mathrm{d}X_2 =$$

$$= \iint_{\Omega_0} \left(\left(\left(\underline{\underline{P}} \cdot \underline{e}_3 \right) \times \underline{k}^\star \right) \cdot \delta\underline{x}_0^\star + \frac{\partial}{\partial X_\alpha} \left(\left(\underline{\underline{P}} \cdot \underline{e}_\alpha \right) \cdot \delta\underline{x}_0^\star \right) - \frac{\partial}{\partial X_\alpha} \left(\underline{\underline{P}} \cdot \underline{e}_\alpha \right) \cdot \delta\underline{x}_0^\star + \right.$$

$$\left. + \left(\rho_0 \cdot \underline{\lambda} + \underline{\underline{M}} \cdot \underline{\mu} \right) \cdot \delta\underline{x}_0^\star \right) \mathrm{d}\Omega_0 = \ldots$$

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2D minimization problem (part 5)

$$\delta\psi = \iint_{\Omega_0} \Bigg(\bigg(\big(\underline{\underline{P}} \cdot \underline{e}_3 \big) \times \underline{k}^\star \bigg) \cdot \delta\underline{x}_0^\star + \frac{\partial}{\partial X_\alpha} \bigg(\big(\underline{\underline{P}} \cdot \underline{e}_\alpha \big) \cdot \delta\underline{x}_0^\star \bigg) - \frac{\partial}{\partial X_\alpha} \bigg(\underline{\underline{P}} \cdot \underline{e}_\alpha \bigg) \cdot \delta\underline{x}_0^\star + $$
$$+ \big(\rho_0 \cdot \underline{\lambda} + \underline{\underline{M}} \cdot \underline{\mu} \big) \cdot \delta\underline{x}_0^\star \Bigg) \,\mathrm{d}\Omega_0 =$$
$$= \iint_{\Omega_0} - \Bigg(\frac{\partial}{\partial X_\alpha} \bigg(\underline{\underline{P}} \cdot \underline{e}_\alpha \bigg) + \underline{k}^\star \times \big(\underline{\underline{P}} \cdot \underline{e}_3 \big) - \big(\rho_0 \cdot \underline{\lambda} + \underline{\underline{M}} \cdot \underline{\mu} \big) \Bigg) \cdot \delta\underline{x}_0^\star \,\mathrm{d}\Omega_0 +$$
$$+ \iint_{\Omega_0} \frac{\partial}{\partial X_\alpha} \bigg(\big(\underline{\underline{P}} \cdot \underline{e}_\alpha \big) \cdot \delta\underline{x}_0^\star \bigg) \,\mathrm{d}\Omega_0$$

2D minimization problem (part 6)

for the second integral we can use the divergence theorem ...

$$\iint_{\Omega_0} \frac{\partial}{\partial X_\alpha}\left(\left(\underline{\underline{P}}\cdot\underline{e}_\alpha\right)\cdot\delta\underline{x}_0^\star\right)\mathrm{d}\Omega_0 = \iint_{\Omega_0} \frac{\partial}{\partial X_\alpha}\left(\left(\underline{\underline{P}}^{\mathrm{T}}\cdot\delta\underline{x}_0^\star\right)\cdot\underline{e}_\alpha\right)\mathrm{d}\Omega_0 =$$

$$= \iint_{\Omega_0} \underline{\nabla}\cdot\left(\underline{\underline{P}}^{\mathrm{T}}\cdot\delta\underline{x}_0^\star\right)\mathrm{d}\Omega_0 = \int_{\partial\Omega_0}\left(\underline{\underline{P}}^{\mathrm{T}}\cdot\delta\underline{x}_0^\star\right)\cdot\underline{n}_0\,\mathrm{d}l = \int_{\partial\Omega_0}\left(\underline{\underline{P}}\cdot\underline{n}_0\right)\cdot\delta\underline{x}_0^\star\,\mathrm{d}l$$

with $\underline{n}_0$ the unit normal of the cross section boundary

setting $\delta\psi = 0$ gives us the **Euler-Lagrange equations** of the $\star$-problem

$$\underline{\nabla}_\alpha\cdot\underline{\underline{P}} + \underline{k}^\star\times\left(\underline{\underline{P}}\cdot\underline{e}_3\right) = \rho_0\cdot\underline{\lambda} + \underline{\underline{M}}\cdot\underline{\mu} \quad \text{in } \Omega_0$$

$$\underline{\underline{P}}\cdot\underline{n}_0 = \underline{0} \quad \text{on } \partial\Omega_0 \quad \text{(traction free boundary condition)}$$

together with the constraints

$$\iint_{\Omega_0}\rho_0\cdot\underline{x}_0^\star\,\mathrm{d}\Omega_0 = \underline{0} \quad \text{and} \quad \iint_{\Omega_0}\underline{\underline{M}}\,\mathrm{d}\Omega_0 = \underline{0}$$

the Euler-Lagrange equations are the (necessary) conditions for a minimum of the cross section energy ; $\underline{x}_0^\star(X_1, X_2)$, $\underline{\lambda}$ and $\underline{\mu}$ are the unknowns of the problem

Recap

strain energy density function (per unit of undeformed length)

$$\psi\Big(\underline{v},\, \underline{k}\,;\, \underline{u}(\underline{v},\, \underline{k})\Big) = \iint_{\Omega_0} W\Big(\underline{\underline{F}}\Big)\,\mathrm{d}\Omega_0$$

deformation gradient of the $\star$-problem

$$\underline{\underline{F}}^\star(X_1, X_2, s) = \underline{\underline{R}}^\star(s)\cdot\left(\underline{v}^\star\otimes\underline{e}_3 + \Big(\underline{k}^\star\times\underbrace{\underline{x}_0^\star(X_1, X_2)}_{\text{warping function}}\Big)\otimes\underline{e}_3 + \frac{\partial\underline{x}_0^\star}{\partial X_\alpha}\otimes\underline{e}_\alpha\right)$$

in order to find $\underline{x}_0^\star(X_1, X_2)$ we must find a solution to the **Euler-Lagrange equations** of the $\star$-problem

$$\underline{\nabla}_\alpha\cdot\underline{\underline{P}} + \underline{k}^\star\times\Big(\underline{\underline{P}}\cdot\underline{e}_3\Big) = \rho_0\cdot\underline{\lambda} + \underline{\underline{M}}\cdot\underline{\mu}\ \text{ in } \Omega_0$$

$$\underline{\underline{P}}\cdot\underline{n}_0 = \underline{0}\ \text{ on } \partial\Omega_0\ \text{ (traction free boundary condition)}$$

that also respects the **kinematic constraints**

$$\iint_{\Omega_0}\rho_0\cdot\underline{x}_0^\star\,\mathrm{d}\Omega_0 = \underline{0}\quad\text{and}\quad\iint_{\Omega_0}\underline{\underline{M}}\,\mathrm{d}\Omega_0 = \underline{0}$$

Modeling of continuum and nanorods using molecular approaches

- what is the form of $W\left(\underline{\underline{F}}\right)$?

  either obtain it from experiments ...

  or use theory $\rightarrow$ molecular approach called *Cauchy Born rule*
- if the radius of the rod is at the nanoscale surface effects become also important, i.e.

$$\psi\left(\underline{v},\, \underline{k}\right) = \underbrace{\iint_{\Omega_0} W\left(\underline{\underline{F}}\right) \mathrm{d}\Omega_0}_{\text{bulk energy}} + \underbrace{\int_{\partial\Omega_0} \psi^S\left(\underline{\underline{E}}^S\right) \mathrm{d}l}_{\text{surface energy}}$$

  $\rightarrow$ extension of the approach called *Surface Cauchy Born rule*
- hollow tube at nanoscale (SWCNT $=$ single wall carbon nanotube)

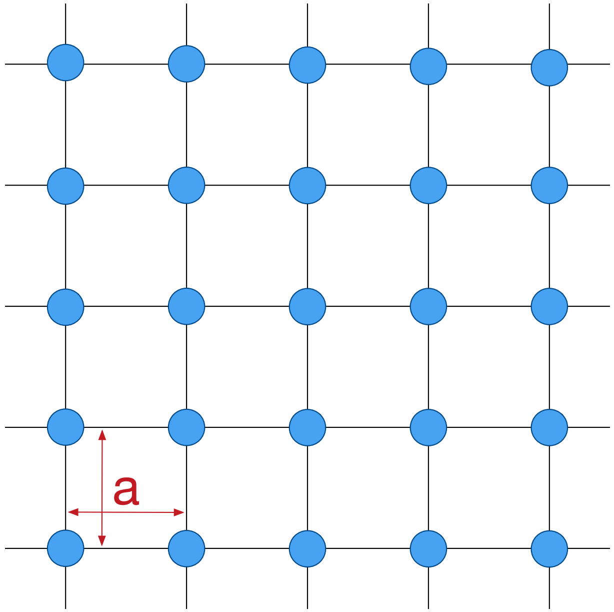
  can not be thought of as a 3D continuum anymore!

  $\psi\left(\underline{v},\, \underline{k}\right) \rightarrow$ direct approach called *Helical Cauchy Born rule*

Arrangement of atoms in crystalline materials (part 1)

crystals have a regular arrangement of atoms: translational periodicity

consider for example a simple 2D crystal:



to generate any crystal we need

- lattice vectors: $\left(\underline{A}_1,\, \underline{A}_2,\, \underline{A}_3\right)$
- basis atoms: $\underline{X}_{0,j}$ with $j = 1, \ldots, M$

  M the number of atoms per unit cell ;

  the zero index indicates the unit cell

in this 2D example we have

- $\left(\underline{A}_1,\, \underline{A}_2\right) = \left(a \cdot \underline{e}_1,\, a \cdot \underline{e}_2\right)$
- $\underline{X}_{\underline{0},1} = \left(0,\, 0\right) \quad ;\, M = 1$

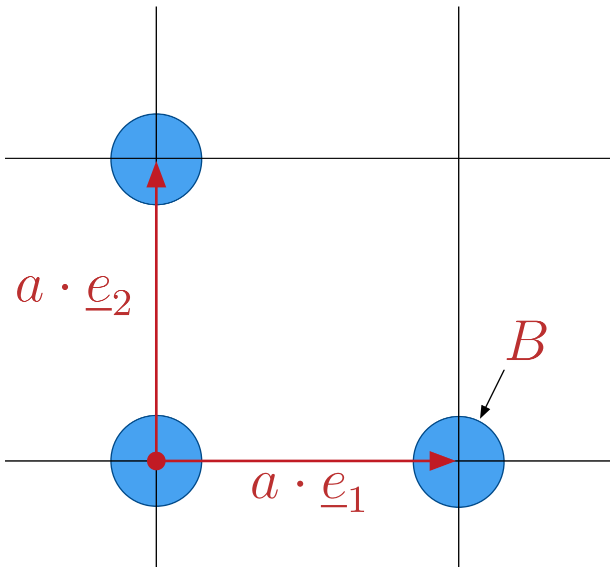
Arrangement of atoms in crystalline materials (part 2)

generators of a crystal

$$\underline{X}_{(n_1,n_2,n_3,j)} = n_i \cdot \underline{A}_i + \left(\underline{X}_j\right)_{j=1,\dots,M} = \underbrace{n_1 \cdot \underline{A}_1 + n_2 \cdot \underline{A}_2 + n_3 \cdot \underline{A}_3}_{\text{generates lattice}} + \underbrace{\left(\underline{X}_j\right)_{j=1,\dots,M}}_{\text{puts atoms on lattice}}$$

$n_1,\ n_2,\ n_3 \in \mathbb{Z}$ gives the translation of the unit cell and
$j = 1, \dots, M$ represents the different atoms that are present within the unit cell

2D example from last slide



atom B is generated by

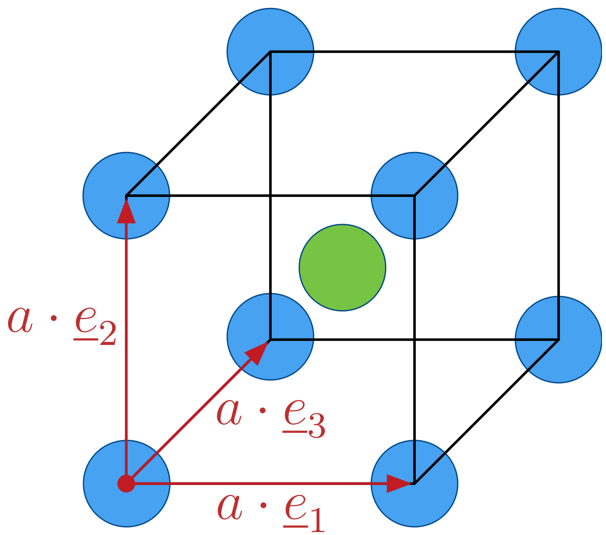
$$\underline{X}_B = \underline{X}_{(1,0,1)} =$$

$$= \underbrace{1}_{n_1} \cdot \underbrace{(a \cdot \underline{e}_1)}_{\underline{A}_1} + \underbrace{0}_{n_2} \cdot \underbrace{(a \cdot \underline{e}_2)}_{\underline{A}_2} + 0 \cdot \underline{e}_1 + 0 \cdot \underline{e}_2$$

Arrangement of atoms in crystalline materials (part 3)

another example: BCC crystal (body centered cubic)

unit cell with two atoms

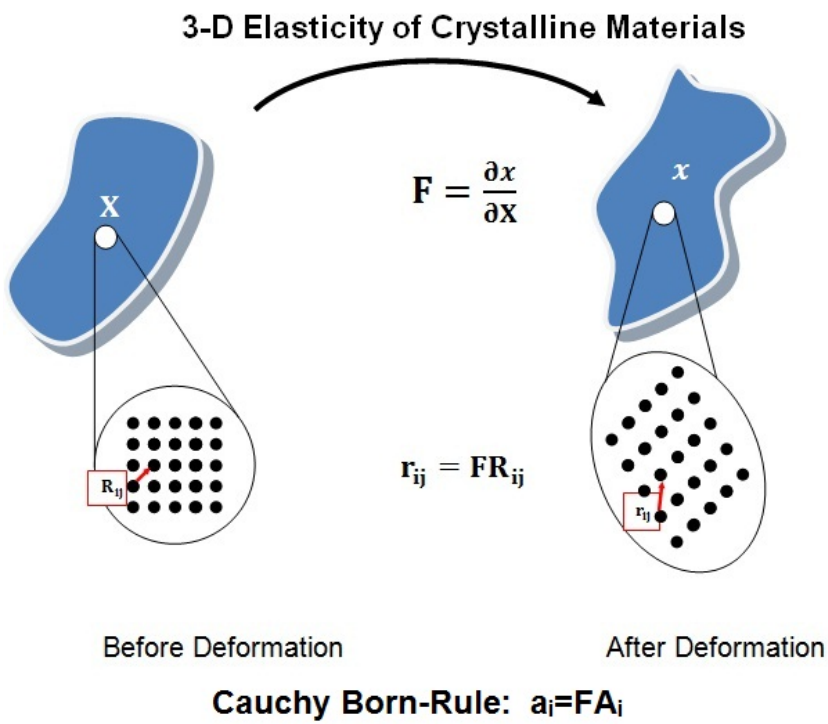


the 7 blue atoms, that are not at the origin, actually belong to the neighboring unit cells!

- lattice vectors:
  $\left(\underline{A}_1,\, \underline{A}_2,\, \underline{A}_3\right) = \left(a \cdot \underline{e}_1,\, a \cdot \underline{e}_2,\, a \cdot \underline{e}_3\right)$
- basis atoms:
  $\underline{X}_{0,1} = \left(0,\, 0,\, 0\right)$
  $\underline{X}_{0,2} = \frac{a}{2} \cdot \left(\underline{e}_1 + \underline{e}_2 + \underline{e}_3\right) \quad ;\, M = 2$

Cauchy Born rule (part 1)

- at the continuum level : straining a rod
- at the molecular level : the atoms are moving
- the movement of atoms is determined by the bond energy between the atoms
- assumption: periodicity is maintained by slowly varying deformations



Cauchy Born rule (part 2)

as an example consider the homogeneous deformation map

$$x_1 = X_1$$
$$x_2 = X_2$$
$$x_3 = \lambda \cdot X_3 \quad \Rightarrow \quad \underline{a}_3 = \lambda \cdot \underline{A}_3$$

if the continuum deformation map is also valid at the atomic level, we have $\underline{a}_3 = \lambda \cdot \underline{A}_3$ or more generally the Cauchy Born rule

$$\underline{a}_i = \underline{\underline{F}} \cdot \underline{A}_i$$

- bridges the continuum and the atomistic viewpoint
- the crystal lattice deforms like the continuum
- the positions of the atoms are still unknown
  (they are not dictated by the macroscopic deformation gradient)

the position of *any* atom in the deformed configuration is given by

$$\underline{x}_{(n_1,n_2,n_3,j)} = n_i \cdot \underline{\underline{F}} \cdot \underline{A}_i + \underline{x}_{\underline{0},j}$$

where $\underline{x}_{\underline{0},j}$ are the positions of the basis atoms within the unit cell
$\rightarrow$ unknowns : can be determined by minimizing the energy of the unit cell

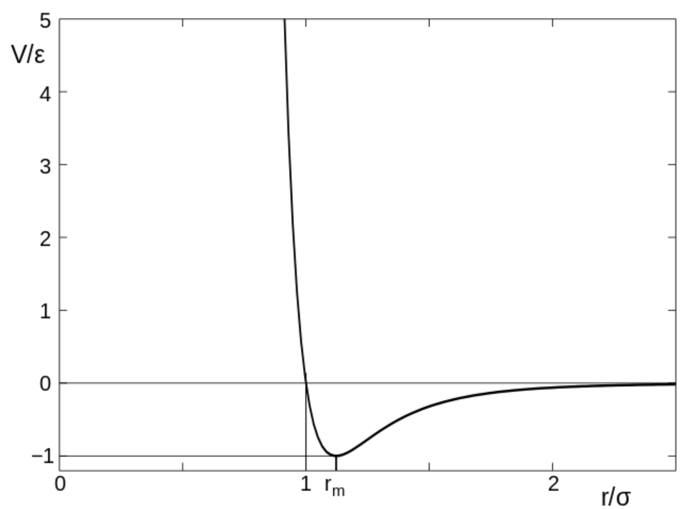
Minimizing the energy of the unit cell (part 1)

average strain energy density of the unit cell

$$W\left(\underline{\underline{F}}\right) = \min_{\left(\underline{x}_{0,1},\dots,\underline{x}_{0,M}\right)} \frac{E\left(\underline{x}_{0,1},\, \underline{x}_{0,2},\, \dots,\, \underline{x}_{0,M};\, \underline{\underline{F}}\right) - E\left(\underline{X}_{0,1},\, \underline{X}_{0,2},\, \dots,\, \underline{X}_{0,M};\, \underline{\underline{I}}\right)}{\left(\underline{A}_1 \times \underline{A}_2\right) \cdot \underline{A}_3}$$

where E is a measure of the interatomic energy of the unit cell

a **interatomic potential** determines the energy due to atomic bonds
in the simplest case this is a pair potential, i.e. the energy that is present within an individual bond between two atoms or molecules



the **Lennard-Jones potential** models the interaction between two atoms or molecules that are neutral and have no chemical bonds between them

← potential energy as a function of the distance between the two atoms or molecules

$$V(r) = 4 \cdot \epsilon \cdot \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right)$$

Minimizing the energy of the unit cell (part 2)

unit cell energy

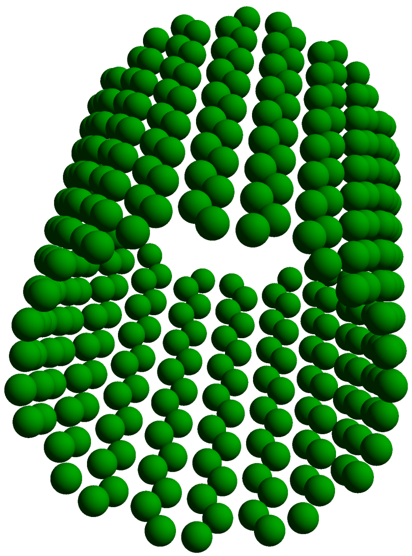
$$E = \frac{1}{2} \sum_{\alpha} \sum_{\beta} V(r_{\alpha,\beta})$$

- α iterates over the basis atoms of the unit cell
- β iterates over all neighbors of α (also within the neighboring unit cells)
- a cutoff-radius defines the size of this neighborhood
- the factor $1/2$ comes from the fact that every bond appears twice: $(\alpha, \beta) \leftrightarrow (\beta, \alpha)$
- bonds that cross the boundary of the unit cell have a part inside and a part outside of the unit cell ; this symmetry implies that for every such bond only the part inside the unit cell is taken into account because the inside part of (α, β) equals exactly the outside part of (β, α) ; this works out regardless of the energy potential model V, i.e. also for models that are not pair-potentials

Direct molecular approach (part 1)

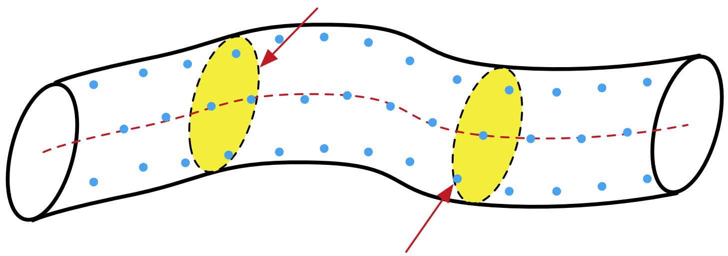
- for larger deformations of a rod / nanotube the translational periodicity of the crystalline material is not preserved
  $\rightarrow$ standard Cauchy Born rule cannot be used to compute the energy of a unit cell
- the idea is to *directly* obtain $\psi\left(\underline{v},\, \underline{k}\right)$, i.e. without first computing $W\left(\underline{\underline{F}}\right)$
- the direct molecular approach takes care of surface effects
- and it can still be used whenever the rod cannot be thought of as a 3D continuum, because e.g. the rod consists only of a wall with a thickness of one atom (SWCNT)

schematic of a SWCNT:

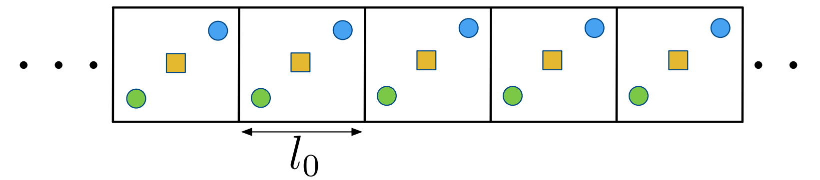


Direct molecular approach (part 2)

$$\psi_1 = \psi\big(\underline{v}_1, \underline{k}_1\big) = \psi\big(\underline{v}(s_1), \underline{k}(s_1)\big)$$



$$\psi_2 = \psi\big(\underline{v}_2, \underline{k}_2\big) = \psi\big(\underline{v}(s_2), \underline{k}(s_2)\big)$$



$\rightarrow$ the nanorod can be thought of as a 1D crystal, i.e. it has a unit cell that repeats only along $\underline{e}_3$-axis ; this repeating unit is sometimes also called fundamental domain

$\rightarrow$ we will again subject the rod to constant $\big(\underline{v}, \underline{k}\big)\ \forall s$ to obtain $\psi\big(\underline{v}, \underline{k}\big)$

$\rightarrow$ all unit cells deform in the same way for constant $\big(\underline{v}, \underline{k}\big)\forall s$

Direct molecular approach (part 3)

deformation map for the repeating unit cells

the reference state is given by $\underline{X}_{i,j}$

- i is an integer that indicates a particular unit cell (analog to the continuous scalar s)
- j is an integer that indicates a particular basis atom within the unit cell (analog to the continuous scalars X_1, X_2)

we want to determine $\underline{x}_{i,j}$ for a nanorod subjected to constant $\left(\underline{v},\, \underline{k}\right) \forall s$

the idea is to find a discrete analog of the 3D deformation map

$$\underline{x}(X_1, X_2, s) = \underbrace{\underline{x}_f + \exp\left(s \cdot \underline{\underline{K}}\right) \cdot \left(\underline{x}_0(X_1, X_2) - \underline{x}_f\right)}_{\text{rotate cross section } s=0} + \underbrace{s \cdot \tau \cdot \underline{\hat{k}}}_{\text{translate cross section}}$$

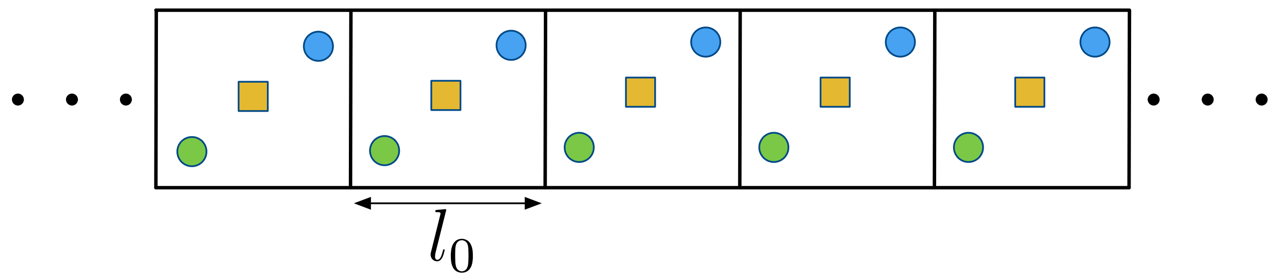
with $s \rightarrow i \cdot l_0$ we get

$$\underline{x}_{i,j} = \underbrace{\underline{x}_f + \exp\left(i \cdot l_0 \cdot \underline{\underline{K}}\right) \cdot \left(\underline{x}_{0,j} - \underline{x}_f\right)}_{\text{rotate unit cell } i=0} + \underbrace{i \cdot l_0 \cdot \tau \cdot \underline{\hat{k}}}_{\text{translate unit cell}}$$

$\rightarrow$ the atomic positions $\underline{x}_{0,j}$ in the unit cell $i = 0$ are the unknowns we have to solve for

Direct molecular approach (part 4)

short recap



- unit cells are the analogs of cross sections: $s \to i \cdot l_0$ with $i = 0, \dots,$
- the atomic positions in the unit cell $i = 0$ are given by $\left(\underline{x}_{0,j}\right)_{j=0,\dots,M}$ with the number of basis atoms $M = 3$ in the example picture above
- for constant $\left(\underline{v},\, \underline{k}\right) \forall s$ we get the discrete deformation map

$$\underline{x}_{i,j} = \underline{x}_f + \exp\left(i \cdot l_0 \cdot \underline{\underline{K}}\right) \cdot \left(\underline{x}_{0,j} - \underline{x}_f\right) + i \cdot l_0 \cdot \tau \cdot \hat{\underline{k}}$$

- $\left(\underline{x}_{0,j}\right)_{j=1,\dots,M}$ are not functions as in the continuous case (no dependence on X_1, X_2)

Direct molecular approach (part 5)

- reference state of the unit cell at $i = 0$ given by $\left(\underline{X}_{0,j}\right)_{j=1,\dots,M}$
- reference state of entire crystal given by $\underline{X}_{0,j} = i \cdot l_0 \cdot \underline{e}_3 + \underline{X}_{0,j}$
- we apply a deformation such that the strains $\underline{v}$, $\underline{k}$ are constant for all s
- we obtain the unknown $\underline{x}_{0,j}$ by minimizing the unit cell energy:

$$\underline{x}_{0,j} = \underset{(\underline{x}_{0,j})}{\arg\min}\, E\left(\underline{x}_{0,1}, \dots, \underline{x}_{0,M}\, ; \, \underline{v}, \underline{k}\right)$$

- the minimization is carried out subject to constraints:
  (mass) center and orientation of the unit cell must be preserved, i.e.

$$\sum_{j=1}^{M} m_j \cdot \underline{x}_{0,j} = \underline{0}$$

  and

$$\sum_{j=1}^{M} \underbrace{m_j \cdot \begin{bmatrix} x_2 \cdot x_3 \\ x_1 \cdot x_3 \\ x_1 \cdot x_2 \end{bmatrix}}_{=:\underline{M}_j} = \underline{0}$$

  with x_1, x_2, x_3 the components of $\underline{x}_{0,j}$

Direct molecular approach (part 6)

minimization of energy under constraints

$$\min_{(\underline{x}_{0,j}\,;\,\underline{\lambda},\,\underline{\mu})} E\Big(\underline{x}_{0,1},\,\dots,\,\underline{x}_{0,M}\,;\,\underline{v},\,\underline{k}\Big) + \underline{\lambda}\cdot\sum_{j=1}^{M} m_j\cdot\underline{x}_{0,j} + \underline{\mu}\cdot\sum_{j=1}^{M}\underline{M}_j$$

setting the **first derivative** to zero we obtain

$$\frac{\partial E}{\partial \underline{x}_{0,j}} + m_j\cdot\underline{\lambda} + \underbrace{m_j\cdot\begin{bmatrix}0 & x_3 & x_2\\ x_3 & 0 & x_1\\ x_2 & x_1 & 0\end{bmatrix}}_{=:\underline{\underline{M}}_j}\cdot\underline{\mu} = \underline{0} \quad \forall j = 1,\dots,M$$

together with the 2 constraint equations this gives a system of $3\,M+6$ algebraic equations

Direct molecular approach (part 7)

$$-\frac{\partial E}{\partial \underline{x}_{0,j}} = m_j \cdot \underline{\lambda} + \underline{\underline{M}}_j \cdot \underline{\mu} \quad \forall j = 1, \ldots, M$$

physical meaning:

- $-\frac{\partial E}{\partial \underline{x}_{0,j}}$ is the force on basis atom j (due to its bond interactions with all other atoms)
- $\left(m_j \cdot \underline{\lambda} + \underline{\underline{M}}_j \cdot \underline{\mu}\right)$ is the external force on basis atom j that is required to keep the nanorod in the uniform configuration $\left(\underline{v}, \underline{k}\right)$

in the case of pure bending or combined extension & torsion the extra constraint forces $\left(m_j \cdot \underline{\lambda} + \underline{\underline{M}}_j \cdot \underline{\mu}\right)$ are zero, i.e. no such forces are required to hold the beam in that configuration

Direct molecular approach (part 8)

the **strain energy density of the nanorod** is then given by

$$\psi\big(\underline{v},\, \underline{k}\big) = \frac{1}{l_0} \cdot E\Big(\underline{\hat{x}}_{0,1}(\underline{v}, \underline{k}),\; \dots,\; \underline{\hat{x}}_{0,M}(\underline{v}, \underline{k})\,;\, \underline{v},\, \underline{k}\Big)$$

with

$$\Big(\underline{\hat{x}}_{0,j}(\underline{v}, \underline{k})\Big)_{j=1,\dots,M} = \underset{(\underline{x}_{0,j})_{j=1,\dots,M}}{\arg\min}\; E\Big(\underline{x}_{0,1},\; \dots,\; \underline{x}_{0,M}\,;\, \underline{v},\, \underline{k}\Big)$$

such that the kinematic constraints are satisfied

for further information on this topic please consider reading the paper “A Helical Cauchy-Born Rule for Special Cosserat Rod Modeling of Nano and Continuum Rods” by Kumar et al. in Journal of Elasticity 124, June 2016

Weak form of the equations (part 1)

by multiplying the **strong form** of the equations

$$\underline{n}'(s) + \hat{\underline{n}}(s) = \rho_0 \cdot A \cdot \ddot{\underline{r}}(s)$$

$$\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \hat{\underline{m}}(s) = \rho_0 \cdot \frac{\mathrm{d}}{\mathrm{d}t}\big(\underline{\underline{I}}_0 \cdot \underline{\omega}\big)$$

with test functions $\delta\underline{r}(s)$ and $\delta\underline{\Theta}(s)$ respectivly and integrating over the length of the rod we get a weak form of the equations ...

$$\int_0^L \Big(\underline{n}'(s) + \hat{\underline{n}}(s)\Big) \cdot \delta\underline{r}(s) \;\mathrm{d}s = \int_0^L \rho_0 \cdot A \cdot \ddot{\underline{r}}(s) \cdot \delta\underline{r}(s) \;\mathrm{d}s$$

$$\int_0^L \Big(\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \hat{\underline{m}}(s)\Big) \cdot \delta\underline{\Theta}(s) \;\mathrm{d}s = \int_0^L \rho_0 \cdot \frac{\mathrm{d}}{\mathrm{d}t}\big(\underline{\underline{I}}_0 \cdot \underline{\omega}\big) \cdot \delta\underline{\Theta}(s) \;\mathrm{d}s$$

where $\underline{\underline{I}}_0$ is the moment of area tensor

Weak form of the equations (part 2)

by adding both equations together we obtain the **weak form**

$$G = \underbrace{\int_0^L \left(\rho_0 \cdot A \cdot \ddot{\underline{r}}(s) \cdot \delta \underline{r}(s) + \rho_0 \cdot \tfrac{\mathrm{d}}{\mathrm{d}t}\left(\underline{\underline{I}}_0 \cdot \underline{\omega} \right) \cdot \delta \underline{\Theta}(s) \right) \, \mathrm{d}s}_{=:G_{\mathsf{dyn}}}$$

$$\underbrace{- \int_0^L \left(\underline{n}'(s) + \hat{\underline{n}}(s) \right) \cdot \delta \underline{r}(s) \, \mathrm{d}s - \int_0^L \left(\underline{m}'(s) + \underline{r}'(s) \times \underline{n}(s) + \hat{\underline{m}}(s) \right) \cdot \delta \underline{\Theta}(s) \, \mathrm{d}s}_{=:G_{\mathsf{stat}}}$$

since the internal contact force $\underline{n}(s)$ and the internal moment $\underline{m}(s)$ depend on the strains $\underline{v}(s)$ and $\underline{k}(s)$ they are of first order in the kinematic variables $\underline{r}(s)$ and $\underline{\Theta}(s)$
with $\underline{\underline{R}}(s) = \exp\left(\underline{\underline{\Theta}}(s) \right) = \exp\left([\underline{\Theta}]_\times \right)$

$\rightarrow$ $\underline{n}'(s)$ and $\underline{m}'(s)$ are therefore of second order in the kinematic variables

FEM discretization

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TECHNISCHE FAKULTÄT

Weak form of the equations (part 3)

we can relax the regularity requirements for a solution by transferring one order of the derivatives onto the test functions via integration by parts ...

$$G_{\text{stat}} = -\int_0^L \Big(\big(\underline{n}(s)\cdot\delta\underline{r}(s)\big)' - \underline{n}(s)\cdot\delta\underline{r}'(s) + \big(\underline{m}(s)\cdot\delta\underline{\Theta}(s)\big)' - \underline{m}(s)\cdot\delta\underline{\Theta}'(s) +$$

$$+\,\hat{\underline{n}}(s)\cdot\delta\underline{r}(s) + \hat{\underline{m}}(s)\cdot\delta\underline{\Theta}(s) + \big(\underline{r}'(s)\times\underline{n}(s)\big)\cdot\delta\underline{\Theta}(s)\Big)\,\mathrm{d}s =$$

$$= \overbrace{\int_0^L \Big(\underline{n}(s)\cdot\delta\underline{r}'(s) + \underline{m}(s)\cdot\delta\underline{\Theta}'(s) + \big(\underline{n}(s)\times\underline{r}'(s)\big)\cdot\delta\underline{\Theta}(s)\Big)\,\mathrm{d}s}^{\text{internal response}} +$$

$$\overbrace{-\int_0^L \Big(\hat{\underline{n}}(s)\cdot\delta\underline{r}(s) + \hat{\underline{m}}(s)\cdot\delta\underline{\Theta}(s)\Big)\,\mathrm{d}s}^{\text{external distributed loads}}\ \overbrace{-\Big(\underline{n}_p(s)\cdot\delta\underline{r}(s) + \underline{m}_p(s)\cdot\delta\underline{\Theta}(s)\Big)\Big|_0^L}^{\text{external loads at boundaries}}$$

with $\underline{n}_p$ and $\underline{m}_p$ as prescribed quantities at the boundary
whereas $\underline{n}(s)$ and $\underline{m}(s)$ are obtained from constitutive law

Weak form of the equations (part 4)

changing the order of the scalar triple product gives ...

$$G_{\mathsf{stat}} = \overbrace{\int_0^L \Big(\underline{n}(s) \cdot \delta \underline{r}'(s) + \underline{m}(s) \cdot \delta \underline{\Theta}'(s) + \underline{n}(s) \cdot \big(\underline{r}'(s) \times \delta \underline{\Theta}(s) \big) \Big) \, \mathrm{d}s}^{\text{internal response}} +$$

$$\overbrace{- \int_0^L \Big(\hat{\underline{n}}(s) \cdot \delta \underline{r}(s) + \hat{\underline{m}}(s) \cdot \delta \underline{\Theta}(s) \Big) \, \mathrm{d}s}^{\text{external distributed loads}} \overbrace{- \Big(\underline{n}_p(s) \cdot \delta \underline{r}(s) + \underline{m}_p(s) \cdot \delta \underline{\Theta}(s) \Big) \Big|_0^L}^{\text{external loads at boundaries}}$$

we can write the internal part in a more compact form by introducing the operator

$$\underline{\underline{E}}^{\mathrm{T}}(s) = \begin{bmatrix} \underline{\underline{I}} \frac{\mathrm{d}}{\mathrm{d}s} & [\underline{r}'(s)]_\times \\ \underline{\underline{0}} & \underline{\underline{I}} \frac{\mathrm{d}}{\mathrm{d}s} \end{bmatrix}$$

$$G_{\mathsf{stat}} = \overbrace{\int_0^L \begin{bmatrix} \underline{n} \\ \underline{m} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}}(s) \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \mathrm{d}s}^{\text{internal response}} \overbrace{- \int_0^L \begin{bmatrix} \hat{\underline{n}} \\ \hat{\underline{m}} \end{bmatrix} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \mathrm{d}s}^{\text{external distributed loads}} \overbrace{- \begin{bmatrix} \underline{n}_p \\ \underline{m}_p \end{bmatrix} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \Bigg|_0^L}^{\text{external loads at boundaries}}$$

Weak form of the equations (part 5)

the weak form of the problem is

$$G = G_{\text{dyn}} + G_{\text{stat}} = 0 \quad \forall \big(\delta \underline{r},\, \delta \underline{\Theta}\big) \text{ admissible}$$

admissible means that the test functions must satisfy the kinematic boundary conditions

in the sequel we will work with the **static problem**, i.e. we assume $G_{\text{dyn}} \equiv 0$

the weak form $G_{\text{stat}}\big(\underline{r},\, \underline{\Theta}\,;\, \delta\underline{r},\, \delta\underline{\Theta}\big)$ is

- nonlinear in the unknowns $\big(\underline{r},\, \underline{\Theta}\big)$
- and linear in the test functions $\big(\delta\underline{r},\, \delta\underline{\Theta}\big)$

in order to find a solution we must linearize the weak form and solve iteratively ...

Linearization of the weak form (part 1)

we introduce **perturbed versions of the unknowns**

$$\underline{r}_{\epsilon}(s) = \underline{r}(s) + \epsilon \cdot \Delta\underline{r}(s) \quad \text{and} \quad \underline{\underline{R}}_{\epsilon}(s) = \exp\Big(\epsilon \cdot \Delta\underline{\underline{\Theta}}(s)\Big) \cdot \exp\Big(\underline{\underline{\Theta}}(s)\Big)$$

with $\Delta\underline{r}$ the increment in $\underline{r}$ and $\Delta\underline{\Theta} = \mathrm{axial}\Big(\Delta\underline{\underline{\Theta}}\Big)$ the increment in $\underline{\Theta}$

we then obtain the **linearized weak form** by truncating the Taylor expansion of $G_{\text{stat}}\Big(\underline{r}_{\epsilon},\, \underline{\Theta}_{\epsilon}\,;\, \delta\underline{r},\, \delta\underline{\Theta}\Big)$ in ϵ after the linear term

$$\underbrace{G_{\text{stat}}\Big(\underline{r}_{\epsilon},\, \underline{\Theta}_{\epsilon}\,;\, \delta\underline{r},\, \delta\underline{\Theta}\Big)}_{\text{should equal } 0} \approx \underbrace{G_{\text{stat}}\Big(\underline{r},\, \underline{\Theta}\,;\, \delta\underline{r},\, \delta\underline{\Theta}\Big) + \frac{\mathrm{d}}{\mathrm{d}\epsilon} G_{\text{stat}}\Big(\underline{r}_{\epsilon},\, \underline{\Theta}_{\epsilon}\,;\, \delta\underline{r},\, \delta\underline{\Theta}\Big)\bigg|_{\epsilon=0} \cdot \epsilon}_{\text{linearized weak form}} + \cancel{\text{HOT}}$$

Linearization of the weak form (part 2)

for simplicity we now assume $\hat{\underline{n}}(s) \equiv 0$, $\hat{\underline{m}}(s) \equiv 0$ and we also ignore the boundary terms so we only have

$$G_{\text{stat}} = \int_0^L \begin{bmatrix} \underline{n}(s) \\ \underline{m}(s) \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}}(s) \cdot \begin{bmatrix} \delta\underline{r}(s) \\ \delta\underline{\Theta}(s) \end{bmatrix} \, \mathrm{d}s$$

we introduce the perturbed version of G_{stat}

$$G^{\epsilon}_{\text{stat}} = \int_0^L \begin{bmatrix} \underline{n}_{\epsilon}(s) \\ \underline{m}_{\epsilon}(s) \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}}_{\epsilon}(s) \cdot \begin{bmatrix} \delta\underline{r}(s) \\ \delta\underline{\Theta}(s) \end{bmatrix} \, \mathrm{d}s$$

and compute the first derivative at $\epsilon = 0$

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon} G^{\epsilon}_{\text{stat}} \bigg|_{\epsilon=0} = \int_0^L \frac{\mathrm{d}}{\mathrm{d}\epsilon} \begin{bmatrix} \underline{n}_{\epsilon} \\ \underline{m}_{\epsilon} \end{bmatrix} \bigg|_{\epsilon=0} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \, \mathrm{d}s + \int_0^L \begin{bmatrix} \underline{n} \\ \underline{m} \end{bmatrix} \cdot \frac{\mathrm{d}}{\mathrm{d}\epsilon} \underline{\underline{E}}^{\mathrm{T}}_{\epsilon} \bigg|_{\epsilon=0} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \, \mathrm{d}s$$

in the sequel we will compute the individual terms of the first derivative step by step and then recompile the results

Linearization of the weak form (part 3)

the linearization of the internal contact force is

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\underline{n}_\epsilon\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\underline{\underline{R}}_\epsilon\cdot\frac{\partial\psi}{\partial\underline{v}}\big(\underline{v}_\epsilon,\,\underline{k}_\epsilon\big)\right)\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\underline{\underline{R}}_\epsilon\bigg|_{\epsilon=0}\cdot\frac{\partial\psi}{\partial\underline{v}}\big(\underline{v},\,\underline{k}\big)+\underline{\underline{R}}\cdot\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\frac{\partial\psi}{\partial\underline{v}}\big(\underline{v}_\epsilon,\,\underline{k}_\epsilon\big)\right)\bigg|_{\epsilon=0}$$

with

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\underline{\underline{R}}_\epsilon\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\exp\big(\epsilon\cdot\mathit{\Delta}\underline{\underline{\mathit{\Theta}}}\big)\cdot\underline{\underline{R}}\right)\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\exp\big(\epsilon\cdot\mathit{\Delta}\underline{\underline{\mathit{\Theta}}}\big)\bigg|_{\epsilon=0}\cdot\underline{\underline{R}} = \mathit{\Delta}\underline{\underline{\mathit{\Theta}}}\cdot\underline{\underline{R}}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\frac{\partial\psi}{\partial\underline{v}}\big(\underline{v}_\epsilon,\,\underline{k}_\epsilon\big)\right)\bigg|_{\epsilon=0} = \frac{\partial^2\psi}{\partial\underline{v}^2}\cdot\frac{\mathrm{d}\underline{v}_\epsilon}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} + \frac{\partial^2\psi}{\partial\underline{v}\partial\underline{k}}\cdot\frac{\mathrm{d}\underline{k}_\epsilon}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}$$

and the linearized strains (cf. pages 50 and 51)

$$\frac{\mathrm{d}\underline{v}_\epsilon}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\underline{\underline{R}}_\epsilon^{\mathrm{T}}\cdot\underline{r}'_\epsilon\right)\bigg|_{\epsilon=0} = \underline{\underline{R}}^{\mathrm{T}}\cdot\left(\mathit{\Delta}\underline{r}'+\underline{r}'\times\mathit{\Delta}\underline{\mathit{\Theta}}\right) \quad \text{and} \quad \frac{\mathrm{d}\underline{k}_\epsilon}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} = \underline{\underline{R}}^{\mathrm{T}}\cdot\mathit{\Delta}\underline{\mathit{\Theta}}'$$

Linearization of the weak form (part 4)

plugging back in gives ...

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\underline{n}_\epsilon\bigg|_{\epsilon=0} = \Delta\underline{\underline{\Theta}} \cdot \underline{\underline{R}} \cdot \frac{\partial\psi}{\partial\underline{v}} + \underline{\underline{R}} \cdot \begin{bmatrix} \frac{\partial^2\psi}{\partial\underline{v}^2} & \frac{\partial^2\psi}{\partial\underline{v}\partial\underline{k}} \end{bmatrix} \cdot \begin{bmatrix} \underline{\underline{R}}^{\mathrm{T}} \cdot \left(\Delta\underline{r}' + \underline{r}' \times \Delta\underline{\Theta}\right) \\ \underline{\underline{R}}^{\mathrm{T}} \cdot \Delta\underline{\Theta}' = \end{bmatrix}$$

$$= -\underline{n} \times \Delta\underline{\Theta} + \underline{\underline{R}} \cdot \begin{bmatrix} \frac{\partial^2\psi}{\partial\underline{v}^2} & \frac{\partial^2\psi}{\partial\underline{v}\partial\underline{k}} \end{bmatrix} \cdot \begin{bmatrix} \underline{\underline{R}}^{\mathrm{T}} \cdot \left(\Delta\underline{r}' + \underline{r}' \times \Delta\underline{\Theta}\right) \\ \underline{\underline{R}}^{\mathrm{T}} \cdot \Delta\underline{\Theta}' = \end{bmatrix}$$

likewise the linearization of the internal moment is

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\underline{m}_\epsilon\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\underline{\underline{R}}_\epsilon \cdot \frac{\partial\psi}{\partial\underline{k}}\left(\underline{v}_\epsilon, \underline{k}_\epsilon\right)\right)\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\underline{\underline{R}}_\epsilon\bigg|_{\epsilon=0} \cdot \frac{\partial\psi}{\partial\underline{k}}\left(\underline{v}, \underline{k}\right) + \underline{\underline{R}} \cdot \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\frac{\partial\psi}{\partial\underline{k}}\left(\underline{v}_\epsilon, \underline{k}_\epsilon\right)\right)\bigg|_{\epsilon=0}$$

with the first term already computed above and with

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\frac{\partial\psi}{\partial\underline{k}}\left(\underline{v}_\epsilon, \underline{k}_\epsilon\right)\right)\bigg|_{\epsilon=0} = \frac{\partial^2\psi}{\partial\underline{k}\partial\underline{v}} \cdot \frac{\mathrm{d}\underline{v}_\epsilon}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} + \frac{\partial^2\psi}{\partial\underline{k}^2} \cdot \frac{\mathrm{d}\underline{k}_\epsilon}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0}$$

Linearization of the weak form (part 5)

plugging back in gives ...

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\underline{m}_{\epsilon}\bigg|_{\epsilon=0} = \Delta\underline{\underline{\Theta}} \cdot \underline{\underline{R}} \cdot \frac{\partial \psi}{\partial \underline{k}} + \underline{\underline{R}} \cdot \begin{bmatrix} \frac{\partial^2 \psi}{\partial \underline{k} \partial \underline{v}} & \frac{\partial^2 \psi}{\partial \underline{k}^2} \end{bmatrix} \cdot \begin{bmatrix} \underline{\underline{R}}^{\mathrm{T}} \cdot \left(\Delta \underline{r}' + \underline{r}' \times \Delta \underline{\Theta} \right) \\ \underline{\underline{R}}^{\mathrm{T}} \cdot \Delta \underline{\Theta}' = \end{bmatrix} =$$

$$= -\underline{m} \times \Delta\underline{\Theta} + \underline{\underline{R}} \cdot \begin{bmatrix} \frac{\partial^2 \psi}{\partial \underline{k} \partial \underline{v}} & \frac{\partial^2 \psi}{\partial \underline{k}^2} \end{bmatrix} \cdot \begin{bmatrix} \underline{\underline{R}}^{\mathrm{T}} \cdot \left(\Delta \underline{r}' + \underline{r}' \times \Delta \underline{\Theta} \right) \\ \underline{\underline{R}}^{\mathrm{T}} \cdot \Delta \underline{\Theta}' = \end{bmatrix}$$

we also linearize the introduced operator matrix ...

$$\underline{\underline{E}}_{\epsilon}^{\mathrm{T}}(s) = \begin{bmatrix} \underline{\underline{I}} \frac{\mathrm{d}}{\mathrm{d}s} & [\underline{r}_{\epsilon}'(s)]_{\times} \\ \underline{\underline{0}} & \underline{\underline{I}} \frac{\mathrm{d}}{\mathrm{d}s} \end{bmatrix} \quad \Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}\epsilon} \underline{\underline{E}}_{\epsilon}^{\mathrm{T}}\bigg|_{\epsilon=0} = \begin{bmatrix} \underline{\underline{0}} & [\Delta \underline{r}'(s)]_{\times} \\ \underline{\underline{0}} & \underline{\underline{0}} \end{bmatrix}$$

Linearization of the weak form (part 6)

finally we obtain the linearized weak form ...

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\epsilon} G^{\epsilon}_{\text{stat}}\Big|_{\epsilon=0} &= \int_0^L \left(\begin{bmatrix} \underline{\underline{0}} & -[\underline{n}]_\times \\ \underline{\underline{0}} & -[\underline{m}]_\times \end{bmatrix} \cdot \begin{bmatrix} \Delta \underline{r} \\ \Delta \underline{\Theta} \end{bmatrix} + \right. \\
&\left. + \underbrace{\begin{bmatrix} \underline{\underline{R}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{R}} \end{bmatrix}}_{=:\underline{\underline{\pi}}} \cdot \underbrace{\begin{bmatrix} \frac{\partial^2 \psi}{\partial \underline{v}^2} & \frac{\partial^2 \psi}{\partial \underline{v} \partial \underline{k}} \\ \frac{\partial^2 \psi}{\partial \underline{k} \partial \underline{v}} & \frac{\partial^2 \psi}{\partial \underline{k}^2} \end{bmatrix}}_{=:\underline{\underline{H}}} \cdot \begin{bmatrix} \underline{\underline{R}}^{\mathrm{T}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{R}}^{\mathrm{T}} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \Delta \underline{r} \\ \Delta \underline{\Theta} \end{bmatrix} \right) \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \mathrm{d}s + \\
&+ \int_0^L \underbrace{\begin{bmatrix} \underline{n} \\ \underline{m} \end{bmatrix} \cdot \begin{bmatrix} \underline{\underline{0}} & [\Delta \underline{r}']_\times \\ \underline{\underline{0}} & \underline{\underline{0}} \end{bmatrix} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix}}_{\underline{n} \cdot \left(\Delta \underline{r}' \times \delta \underline{\Theta} \right)} \mathrm{d}s = \\
&= \int_0^L \begin{bmatrix} \underline{\underline{0}} & -[\underline{n}]_\times \\ \underline{\underline{0}} & -[\underline{m}]_\times \end{bmatrix} \cdot \begin{bmatrix} \Delta \underline{r} \\ \Delta \underline{\Theta} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \mathrm{d}s + \int_0^L \underline{\underline{\pi}} \cdot \underline{\underline{H}} \cdot \underline{\underline{\pi}}^{\mathrm{T}} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \Delta \underline{r} \\ \Delta \underline{\Theta} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \mathrm{d}s + \\
&+ \int_0^L [\underline{n}]_\times \cdot \Delta \underline{r}' \cdot \delta \underline{\Theta} \ \mathrm{d}s
\end{aligned}
$$

FEM discretization

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Linearization of the weak form (recap)

$$\overbrace{G_{\mathsf{stat}}\left(\underline{r}_{\epsilon},\,\underline{\Theta}_{\epsilon}\,;\,\delta\underline{r},\,\delta\underline{\Theta}\right)}^{\text{nonlinear weak form}} \equiv G_{\mathsf{stat}}\left(\Delta\underline{r},\,\Delta\underline{\Theta}\,;\,\underline{r},\,\underline{\Theta}\,;\,\delta\underline{r},\,\delta\underline{\Theta}\right) \approx$$

$$\approx \underbrace{G_{\mathsf{stat}}\left(\underline{r},\,\underline{\Theta}\,;\,\delta\underline{r},\,\delta\underline{\Theta}\right) + DG_{\mathsf{stat}}\left(\Delta\underline{r},\,\Delta\underline{\Theta}\,;\,\underline{r},\,\underline{\Theta}\,;\,\delta\underline{r},\,\delta\underline{\Theta}\right)}_{\text{linearized weak form}}$$

with the nonlinear weak form

$$G_{\mathsf{stat}} = \int_0^L \begin{bmatrix} \underline{n} \\ \underline{m} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}}(s) \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \,\mathrm{d}s - \int_0^L \begin{bmatrix} \hat{\underline{n}} \\ \hat{\underline{m}} \end{bmatrix} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \,\mathrm{d}s - \begin{bmatrix} \underline{n}_p \\ \underline{m}_p \end{bmatrix} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \Bigg|_0^L$$

and the first order term from its Taylor expansion

$$DG_{\mathsf{stat}} = \int_0^L \begin{bmatrix} \underline{\underline{0}} & -[\underline{n}]_\times \\ \underline{\underline{0}} & -[\underline{m}]_\times \end{bmatrix} \cdot \begin{bmatrix} \Delta\underline{r} \\ \Delta\underline{\Theta} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \,\mathrm{d}s + \int_0^L \underline{\underline{\pi}} \cdot \underline{\underline{H}} \cdot \underline{\underline{\pi}}^{\mathrm{T}} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \Delta\underline{r} \\ \Delta\underline{\Theta} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \,\mathrm{d}s +$$

$$+ \int_0^L [\underline{n}]_\times \cdot \Delta\underline{r}' \cdot \delta\underline{\Theta} \,\mathrm{d}s + \ldots \text{(first order terms of distributed load and boundary terms)}$$

Iteratively solving the nonlinear problem

note that $DG_{\text{stat}}\big(\Delta\underline{r},\, \Delta\underline{\Theta}\,;\, \underline{r},\, \underline{\Theta}\,;\, \delta\underline{r},\, \delta\underline{\Theta}\big)$ is

- linear in $\big(\Delta\underline{r},\, \Delta\underline{\Theta}\big)$
- nonlinear in $\big(\underline{r},\, \underline{\Theta}\big)$
- and linear in $\big(\delta\underline{r},\, \delta\underline{\Theta}\big)$

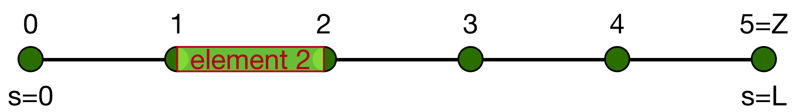
Newton-Rhapson method for solving the nonlinear problem

$$G_{\text{stat}}\big(\underline{r}_\epsilon,\, \underline{\Theta}_\epsilon\,;\, \delta\underline{r},\, \delta\underline{\Theta}\big) = 0$$

- in first iteration guess initial $\underline{r}(s)$ and $\underline{\Theta}(s)$
- linearize the weak form about $\underline{r}(s)$ and $\underline{\Theta}(s)$
- obtain $\Delta\underline{r}(s)$ and $\Delta\underline{\Theta}(s)$ by solving the linearized problem
- update: $\underline{r}(s) \leftarrow \underline{r}(s) + \Delta\underline{r}(s)$ and $\underline{\Theta}(s) \leftarrow \dots$ (a bit more tricky)
- check if updated $\underline{r}(s)$ and $\underline{\Theta}(s)$ solve the nonlinear problem
  with a small enough error (an error bound needs to be defined)
- if the error is too large then reiterate by linearizing about the updated $\underline{r}(s)$ and $\underline{\Theta}(s)$ ...

Discretization of the weak form (part 1)

we discretize a rod of length L



with Z elements and $Z+1$ nodes

we discretize the displacements by

$$\Delta \underline{r}(s) \approx \Delta \underline{r}_i \cdot N_i(s)$$

$$\Delta \underline{\Theta}(s) \approx \Delta \underline{\Theta}_i \cdot N_i(s)$$

and the test functions by

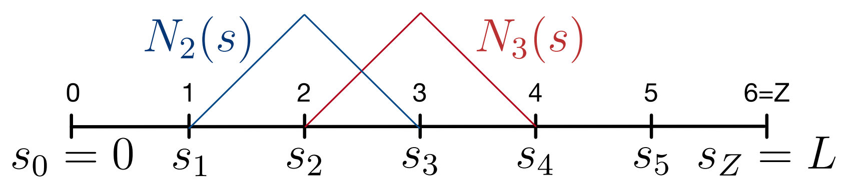
$$\delta \underline{r}(s) \approx \delta \underline{r}_i \cdot N_i(s)$$

$$\delta \underline{\Theta}(s) \approx \delta \underline{\Theta}_i \cdot N_i(s)$$

with shape functions $N_i(s)$ such that

$$N_i(s) = \begin{cases} 1 & \text{at node } i \\ 0 & \text{at every other node} \end{cases}$$

example with linear shape functions:



meaning of $\Delta \underline{r}_i$, $\Delta \underline{\Theta}_i$:

$$\Delta \underline{r}(s_j) \approx \Delta \underline{r}_i \cdot N_i(s_j) = \Delta \underline{r}_i \cdot \delta_{ij} = \underline{r}_j$$

$\rightarrow$ approximated displacements at the nodes

$\rightarrow$ interpolation of displacements via shape functions between the nodes

FEM discretization

Discretization of the weak form (part 2)

recall the nonlinear weak form

$$G_{\text{stat}} = \int_0^L \begin{bmatrix} \underline{n} \\ \underline{m} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}}(s) \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \,\mathrm{d}s - \int_0^L \begin{bmatrix} \underline{\hat{n}} \\ \underline{\hat{m}} \end{bmatrix} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \,\mathrm{d}s - \begin{bmatrix} \underline{n}_p \\ \underline{m}_p \end{bmatrix} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} \Bigg|_0^L$$

we plug in the discrete approximations of the test functions

$$\delta \underline{r}(s) \approx \delta \underline{r}_i \cdot N_i(s) \quad \text{and} \quad \delta \underline{\Theta}(s) \approx \delta \underline{\Theta}_i \cdot N_i(s)$$

- we take notice that $\underline{n}(s)$, $\underline{m}(s)$ depend on the current state $\left(\underline{r},\, \underline{\Theta}\right)$
- then we work out the next part ...

$$\underline{\underline{E}}^{\mathrm{T}}(s) \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} = \begin{bmatrix} \underline{\underline{I}}\,\frac{\mathrm{d}}{\mathrm{d}s} & [\underline{r}'(s)]_\times \\ \underline{\underline{0}} & \underline{\underline{I}}\,\frac{\mathrm{d}}{\mathrm{d}s} \end{bmatrix} \cdot \begin{bmatrix} \delta \underline{r} \\ \delta \underline{\Theta} \end{bmatrix} = \begin{bmatrix} \delta \underline{r}' + \underline{r}' \times \delta \underline{\Theta} \\ \delta \underline{\Theta}' \end{bmatrix} \approx$$

$$\approx \begin{bmatrix} \delta \underline{r}_i \cdot N_i'(s) + \underline{r}' \times \left(N_i(s) \cdot \delta \underline{\Theta}_i\right) \\ \delta \underline{\Theta}_i \cdot N_i'(s) \end{bmatrix} = \underbrace{\begin{bmatrix} N_i'(s) \cdot \underline{\underline{I}} & N_i(s) \cdot [\underline{r}'(s)]_\times \\ \underline{\underline{0}} & N_i' \cdot \underline{\underline{I}} \end{bmatrix}}_{=:\underline{\underline{E}}_i^{\mathrm{T}}(s)} \cdot \begin{bmatrix} \delta \underline{r}_i \\ \delta \underline{\Theta}_i \end{bmatrix}$$

note that $\underline{\underline{E}}_i^{\mathrm{T}}$ is a regular matrix instead of being an operator written in matrix form

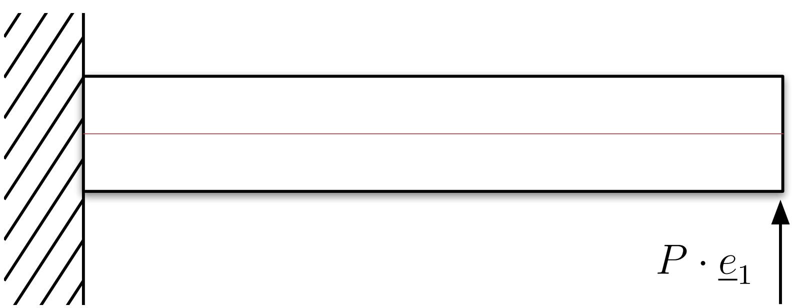
Discretization of the weak form (part 3)

- the term for the distributed forces is straightforward: we just dot the forces with the approximated test functions
- the boundary term can be simplified: e.g. at $s = L$ we have $\delta\underline{r}(L) \approx N_i(L) \cdot \delta\underline{r}_i = N_Z(L) \cdot \delta\underline{r}_Z = \delta\underline{r}_Z$

we obtain $G^h_{\text{stat}}\left(\underline{r},\, \underline{\Theta}\,;\, \delta\underline{r},\, \delta\underline{\Theta}\right) =$

$$\int_0^L \begin{bmatrix} \underline{n} \\ \underline{m} \end{bmatrix} \cdot \underline{\underline{E}}_i^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r}_i \\ \delta\underline{\Theta}_i \end{bmatrix} \mathrm{d}s - \int_0^L \begin{bmatrix} \hat{\underline{n}} \\ \hat{\underline{m}} \end{bmatrix} \cdot N_i \cdot \begin{bmatrix} \delta\underline{r}_i \\ \delta\underline{\Theta}_i \end{bmatrix} \mathrm{d}s - \begin{bmatrix} \underline{n}_p(L) \\ \underline{m}_p(L) \end{bmatrix} \cdot \begin{bmatrix} \delta\underline{r}_Z \\ \delta\underline{\Theta}_Z \end{bmatrix} + \begin{bmatrix} \underline{n}_p(0) \\ \underline{m}_p(0) \end{bmatrix} \cdot \begin{bmatrix} \delta\underline{r}_0 \\ \delta\underline{\Theta}_0 \end{bmatrix}$$

for a cantilever problem



we have

- $\underline{n}_p(L) = P \cdot \underline{e}_1$ and $\underline{m}_p(L) = 0$
- and on the clamped end the boundary term vanishes since $\delta\underline{r}_0 = \delta\underline{\Theta}_0 = 0$ (admissibility)

Discretization of the weak form (part 4)

we can rewrite the discretized weak form using a global **residual vector** $\underline{R}$

$$G^h_{\mathsf{stat}}\Big(\underline{r},\,\underline{\Theta}\,;\,\delta\underline{r},\,\delta\underline{\Theta}\Big) = \underbrace{\begin{bmatrix} \begin{bmatrix} \underline{R}_0 \\ \\ \end{bmatrix} \\ \\ \begin{bmatrix} \underline{R}_1 \\ \\ \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \underline{R}_Z \\ \\ \end{bmatrix} \end{bmatrix}}_{=:\underline{R}} \cdot \underbrace{\begin{bmatrix} \begin{bmatrix} \delta\underline{r}_0 \\ \delta\underline{\Theta}_0 \end{bmatrix} \\ \\ \begin{bmatrix} \delta\underline{r}_1 \\ \delta\underline{\Theta}_1 \end{bmatrix} \\ \vdots \\ \begin{bmatrix} \delta\underline{r}_Z \\ \delta\underline{\Theta}_Z \end{bmatrix} \end{bmatrix}}_{=:\underline{\delta}}$$

with $Z+1$ blocks / 6 dimensional subvectors of $\underline{R}$ defined as

$$\underline{R}_i = \int_0^L \underline{\underline{E}}_i(s) \cdot \begin{bmatrix} \underline{n}(s) \\ \underline{m}(s) \end{bmatrix} \,\mathrm{d}s - \int_0^L N_i(s) \begin{bmatrix} \underline{\hat{n}}(s) \\ \underline{\hat{m}}(s) \end{bmatrix} \,\mathrm{d}s$$

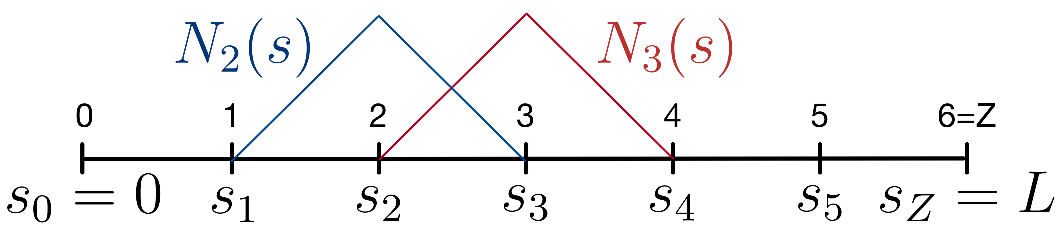
the boundary terms are added to $\underline{R}_0$ and $\underline{R}_Z$

Assembly of the residual vector (part 1)

for each of the $Z+1$ subvectors we integrate from $s=0$ to $s=L$
the integration domain can be divided into the Z elements

$$\underline{R}_i = \sum_{e=1}^{Z} \left(\int_{s_{e-1}}^{s_e} \underline{\underline{E}}_i(s) \cdot \begin{bmatrix} \underline{n}(s) \\ \underline{m}(s) \end{bmatrix} \, \mathrm{d}s - \int_{s_{e-1}}^{s_e} N_i(s) \begin{bmatrix} \underline{\hat{n}}(s) \\ \underline{\hat{m}}(s) \end{bmatrix} \, \mathrm{d}s \right)$$

now we benefit from the compact support of the shape functions,
i.e. a shape function can only be non-zero within a bounded region



in the 1D case every element has two adjacent nodes
$\rightarrow$ there are two shape functions that can contribute to each integral

example: for element $e=3$ only $N_{e-1} = N_2$ and $N_e = N_3$ need to be considered

Assembly of the residual vector (part 2)

we can assemble $\underline{R}$ with a for-loop over the elements

for $e = 1: Z$

$$\underline{R}_{e-1} \mathrel{+}= \int_{s_{e-2}}^{s_{e-1}} \underline{\underline{E}}_{e-1}(s) \cdot \begin{bmatrix} \underline{n}(s) \\ \underline{m}(s) \end{bmatrix} \, \mathrm{d}s - \int_{s_{e-2}}^{s_{e-1}} N_{e-1}(s) \begin{bmatrix} \hat{\underline{n}}(s) \\ \hat{\underline{m}}(s) \end{bmatrix} \, \mathrm{d}s$$

$$\underline{R}_{e} \mathrel{+}= \int_{s_{e-1}}^{s_{e}} \underline{\underline{E}}_{e}(s) \cdot \begin{bmatrix} \underline{n}(s) \\ \underline{m}(s) \end{bmatrix} \, \mathrm{d}s - \int_{s_{e-1}}^{s_{e}} N_{e}(s) \begin{bmatrix} \hat{\underline{n}}(s) \\ \hat{\underline{m}}(s) \end{bmatrix} \, \mathrm{d}s$$

end

remarks:

- after the loop, contributions of the boundary terms at the first and last node are added
- the integration within the elements is done with a numerical integration scheme

Discretization of the linearized weak form (part 1)

recall the increment DG_{stat} of G_{stat} that is linear in $\Delta\underline{r}$, $\Delta\underline{\Theta}$

$$DG_{\text{stat}} = \int_0^L \begin{bmatrix} \underline{\underline{0}} & -[\underline{n}]_\times \\ \underline{\underline{0}} & -[\underline{m}]_\times \end{bmatrix} \cdot \begin{bmatrix} \Delta\underline{r} \\ \Delta\underline{\Theta} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \mathrm{d}s + \int_0^L \underline{\underline{\pi}} \cdot \underline{\underline{H}} \cdot \underline{\underline{\pi}}^{\mathrm{T}} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \Delta\underline{r} \\ \Delta\underline{\Theta} \end{bmatrix} \cdot \underline{\underline{E}}^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r} \\ \delta\underline{\Theta} \end{bmatrix} \mathrm{d}s +$$

$$+ \int_0^L [\underline{n}]_\times \cdot \Delta\underline{r}' \cdot \delta\underline{\Theta}\ \mathrm{d}s + \ldots \text{(first order terms of distributed load and boundary terms)}$$

remarks regarding the missing terms:

- in the case that distributed loads act independently of the configuration we have $\underline{\hat{n}}_\epsilon = \underline{\hat{n}}$ and therefore $\frac{\mathrm{d}\underline{\hat{n}}_\epsilon}{\mathrm{d}\epsilon} = 0$, $\rightarrow$ no contribution to DG_{stat}
- likewise for the cantilever with $\underline{n}_p(L) = P \cdot \underline{e}_1$ there is no contribution to DG_{stat}
- on the other hand, for a follower load with $\underline{n}_p(L) = P \cdot \underline{d}_1 = P \cdot \underline{\underline{R}} \cdot \underline{e}_1$ there will be a contribution to DG_{stat}
- for now we will forget about these extra contributions

Discretization of the linearized weak form (part 2)

we plug the discrete approximations of the test functions into DG_{stat}

$$\delta\underline{r}(s) \approx \delta\underline{r}_i \cdot N_i(s) \quad \text{and} \quad \delta\underline{\Theta}(s) \approx \delta\underline{\Theta}_i \cdot N_i(s)$$

and also the discrete approximations of the increments

$$\Delta\underline{r}(s) \approx \Delta\underline{r}_j \cdot N_j(s) \quad \text{and} \quad \Delta\underline{\Theta}(s) \approx \Delta\underline{\Theta}_j \cdot N_j(s)$$

we obtain $DG^h_{\text{stat}}\left(\Delta\underline{r}_j,\, \Delta\underline{\Theta}_j;\, \underline{r},\, \underline{\Theta};\, \delta\underline{r}_i,\, \delta\underline{\Theta}_i\right) =$

$$\int_0^L \begin{bmatrix} \underline{\underline{0}} & -[\underline{n}]_\times \\ \underline{\underline{0}} & -[\underline{m}]_\times \end{bmatrix} \cdot N_j \cdot \begin{bmatrix} \Delta\underline{r}_j \\ \Delta\underline{\Theta}_j \end{bmatrix} \cdot \underline{\underline{E}}_i^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r}_i \\ \delta\underline{\Theta}_i \end{bmatrix} \mathrm{d}s + \int_0^L \underline{\underline{\pi}} \cdot \underline{\underline{H}} \cdot \underline{\underline{\pi}}^{\mathrm{T}} \cdot \underline{\underline{E}}_j^{\mathrm{T}} \cdot \begin{bmatrix} \Delta\underline{r}_j \\ \Delta\underline{\Theta}_j \end{bmatrix} \cdot \underline{\underline{E}}_i^{\mathrm{T}} \cdot \begin{bmatrix} \delta\underline{r}_i \\ \delta\underline{\Theta}_i \end{bmatrix} \mathrm{d}s +$$

$$+ \int_0^L N_i \cdot N_j' \cdot \left(\underline{n} \times \Delta\underline{r}_j\right) \cdot \delta\underline{\Theta}_i \, \mathrm{d}s + \ldots \text{ (first order terms of distributed load and boundary terms)}$$

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Discretization of the linearized weak form (part 3)

we want to rewrite DG^h_{stat} in the form

$$DG^h_{\text{stat}}\left(\underline{\Delta}\,;\,\underline{r},\,\underline{\Theta}\,;\,\underline{\delta}\right) = \left(\underline{\underline{K}}\cdot\underline{\Delta}\right)\cdot\underline{\delta} = \left(\underline{\underline{K}}_{ij}\cdot\underline{\Delta}_j\right)\cdot\underline{\delta}_i = \left(\underline{\underline{K}}_{ij}\cdot\begin{bmatrix}\Delta\underline{r}_j\\ \Delta\underline{\Theta}_j\end{bmatrix}\right)\cdot\begin{bmatrix}\delta\underline{r}_i\\ \delta\underline{\Theta}_i\end{bmatrix}$$

- where $\underline{\underline{K}}$ is the stiffness matrix and $\underline{\underline{K}}_{ij}$ refers to the 6×6 submatrices of $\underline{\underline{K}}$
- $\underline{\Delta}$ and $\underline{\delta}$ are the vectors that contain the discrete approximations of the increments and test functions, respectively
- note that $\underline{\delta}$ was already defined (cf. page 128) ; $\underline{\Delta}$ is of the same structure

we get

$$\underline{\underline{K}}_{ij} = \int_0^L \underbrace{\underline{\underline{E}}_i\cdot\underline{\underline{\pi}}\cdot\underline{\underline{H}}\cdot\underline{\underline{\pi}}^{\mathrm{T}}\cdot\underline{\underline{E}}_j^{\mathrm{T}}}_{\text{material stiffness matrix}}\,\mathrm{d}s + \int_0^L \underbrace{N_j\cdot\underline{\underline{E}}_i\cdot\begin{bmatrix}\underline{\underline{0}} & -[\underline{n}]_\times\\ \underline{\underline{0}} & -[\underline{m}]_\times\end{bmatrix} + N_i\cdot N_j'\cdot\begin{bmatrix}\underline{\underline{0}} & \underline{\underline{0}}\\ [\underline{n}]_\times & \underline{\underline{0}}\end{bmatrix}}_{\text{geometric stiffness matrix}}\,\mathrm{d}s$$

- the material stiffness matrix is symmetric
- the geometric stiffness matrix is not symmetric ; but it becomes symmetric for the configuration that corresponds to static equilibrium (cf. Simo & Vu-Quoc 1986)

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Iteratively solving the nonlinear problem (revisited, part 1)

recall the truncated Taylor expansion of the weak form about the configuration $\big(\underline{r},\, \underline{\Theta}\big)$

$$\underbrace{G_{\text{stat}}\Big(\underline{r} + \Delta\underline{r},\, \exp\big(\Delta\underline{\underline{\Theta}}\big) \cdot \exp\big(\underline{\underline{\Theta}}\big)\,;\, \delta\underline{r},\, \delta\underline{\Theta}\Big)}_{\text{nonlinear weak form } \overset{!}{=} 0 \text{ but intractable problem}} \approx$$

$$\approx \underbrace{G_{\text{stat}}\Big(\underline{r},\, \exp\big(\underline{\underline{\Theta}}\big)\,;\, \delta\underline{r},\, \delta\underline{\Theta}\Big) + DG_{\text{stat}}\Big(\Delta\underline{r},\, \Delta\underline{\Theta}\,;\, \underline{r},\, \exp\big(\underline{\underline{\Theta}}\big)\,;\, \delta\underline{r},\, \delta\underline{\Theta}\Big)}_{\text{linearized weak form}} \approx$$

$$\approx \underbrace{\underline{R} \cdot \underline{\delta} + \big(\underline{\underline{K}} \cdot \underline{\Delta}\big) \cdot \underline{\delta} = \big(\underline{R} + \underline{\underline{K}} \cdot \underline{\Delta}\big) \cdot \underline{\delta}}_{\text{discretized linearized weak form}} \overset{!}{=} 0 \;\; \forall \underline{\delta} \;\; \text{(admissible)}$$

$$\Rightarrow \underline{R} + \underline{\underline{K}} \cdot \underline{\Delta} = \underline{0} \qquad \Rightarrow \underline{\Delta} = -\underline{\underline{K}}^{-1} \cdot \underline{R}$$

Iteratively solving the nonlinear problem (revisited, part 2)

- by solving the linearized (about some configuration) and discrete version of the underlying nonlinear problem we obtain an updated configuration (via $\underline{\Delta}$), that is a better solution of the nonlinear problem than the configuration we started with
- the updated configuration is given by

$$\underline{r} \leftarrow \underline{r} + \Delta r$$

$$\underline{\Theta} \leftarrow \Theta\Big(\exp\big(\Delta\underline{\underline{\Theta}}\big) \cdot \exp\big(\underline{\underline{\Theta}}\big)\Big)$$

  where $\Theta\big(\,.\,\big)$ means extraction of $\underline{\Theta}$ from $\underline{\underline{R}}$
- a solution/configuration needs to be guessed to start the Newton-Rhapson iteration
- this guess converges to the true solution with each iteration
- we stop to iterate if the solution is close enough to 0
  (theoretical limit: machine precision)

Iteratively solving the nonlinear problem (revisited, part 3)

- to obtain $\underline{\underline{K}}_{ij}$ in each iteration we use numerical integration
- therefore we need the strains at the quadrature points
  but displacements are given at the nodes
- within element e we have

$$\underline{r}(s) = \underline{r}_i \cdot N_i(s) = \underline{r}_{e-1} \cdot N_{e-1}(s) + \underline{r}_e \cdot N_e(s)$$

$$\underline{\Theta}(s) = \underline{\Theta}_i \cdot N_i(s) = \underline{\Theta}_{e-1} \cdot N_{e-1}(s) + \underline{\Theta}_e \cdot N_e(s)$$

- from this we compute the updated strains

$$\underline{v}_{\text{new}} = \underline{\underline{R}}^{\mathrm{T}}_{\text{new}} \cdot \underline{r}'_{\text{new}} \quad \text{and} \quad \underline{k}_{\text{new}} = \operatorname{axial}\left(\underline{\underline{R}}^{\mathrm{T}}_{\text{new}} \cdot \underline{\underline{R}}'_{\text{new}}\right)$$

  but it is not trivial to obtain $\underline{\underline{R}}'_{\text{new}}$ at the quadrature points
  because an interpolation like $\cancel{\underline{\underline{R}} = \underline{\underline{R}}_i \cdot N_i}$ is nonsense ; luckily, Simo has worked out an update formula:

$$\underline{k}_{\text{new}} = \underline{k}_{\text{old}} + \underline{\underline{R}}'_{\text{new}} \cdot \underline{\beta}$$

  with $\underline{\beta} = \ldots$ (next slide)

Iteratively solving the nonlinear problem (revisited, part 4)

$$\underline{\beta} = \frac{\sin\|\Delta\underline{\Theta}\|}{\|\Delta\underline{\Theta}\|} \cdot \Delta\underline{\Theta}' + \left(1 - \frac{\sin\|\Delta\underline{\Theta}\|}{\|\Delta\underline{\Theta}\|}\right) \cdot \left(\frac{\Delta\underline{\Theta} \cdot \Delta\underline{\Theta}'}{\|\Delta\underline{\Theta}\|}\right) \cdot \frac{\Delta\underline{\Theta}}{\|\Delta\underline{\Theta}\|} + \\ + \frac{1}{2} \cdot \left(\frac{\sin\left(\frac{1}{2} \cdot \|\Delta\underline{\Theta}\|\right)}{\frac{1}{2} \cdot \|\Delta\underline{\Theta}\|}\right)^2 \cdot \Delta\underline{\Theta} \times \Delta\underline{\Theta}'$$

where we evaluate $\Delta\underline{\Theta}$ at the quadrature points

for $\Delta\underline{\Theta} \approx \underline{0}$ we have $\underline{\beta} \approx \Delta\underline{\Theta}'$