

Module 19

Space Parallel Reference Frame

- Definition of twist using space parallel reference frame



Goal

- Formulate a reference frame on the rod centerline using parallel transport along the arc-length (space parallel transport)
- Compute the twist along the rod using space parallel reference frame
- At the end of this module, you should be able to compute the twisting energy of a rod given its centerline and material frame

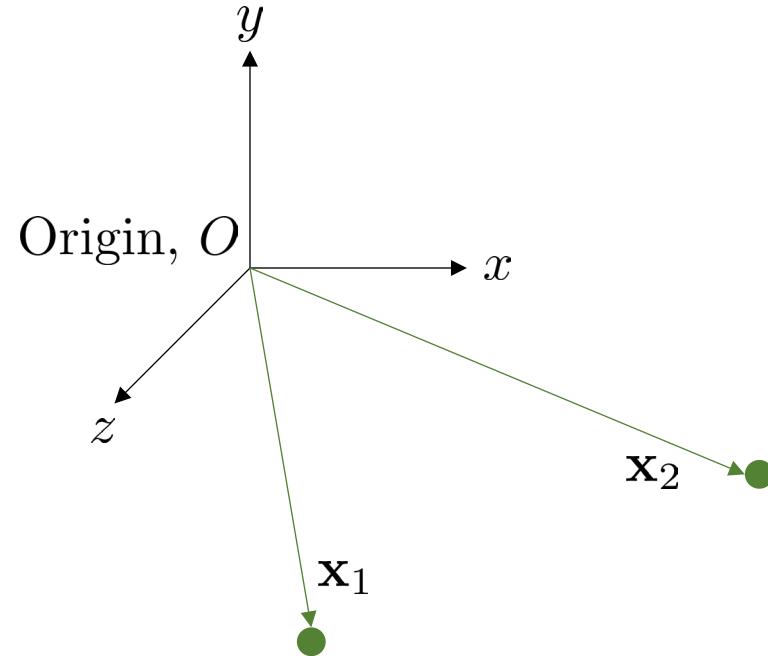


Resources

- Read “*Chapter 6: Discrete Twist*”
- Review Bergou, Miklós, et al. “Discrete elastic rods” ACM SIGGRAPH (2008) 1-12.



Relative Position



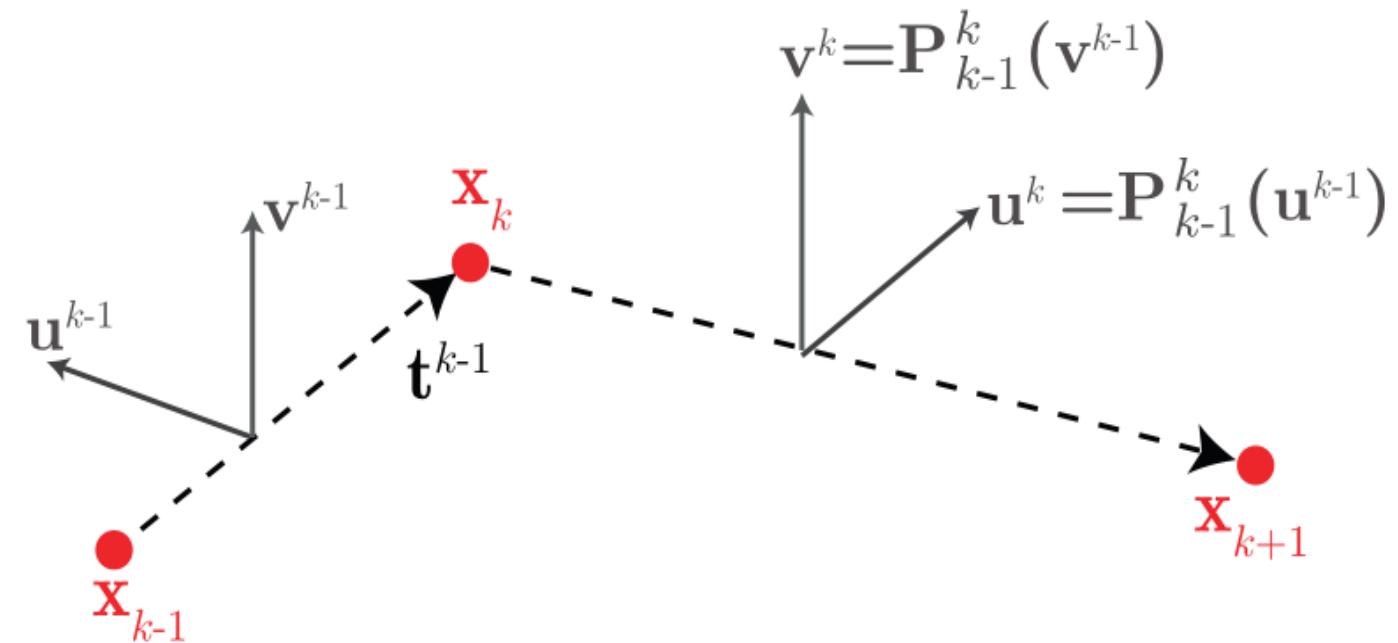
When describing the nodal coordinates, e.g. x_1 , we implicitly assume a reference frame with origin O .

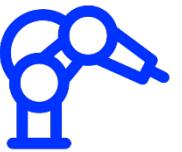


Relative Rotation - Twist

When describing the rotation of the material frame, we need a reference frame

- How to compute the reference frame, $(\mathbf{u}^k, \mathbf{v}^k, \mathbf{t}^k)$?
- Known quantities: the nodal coordinates, \mathbf{x}_k





Reference Frame

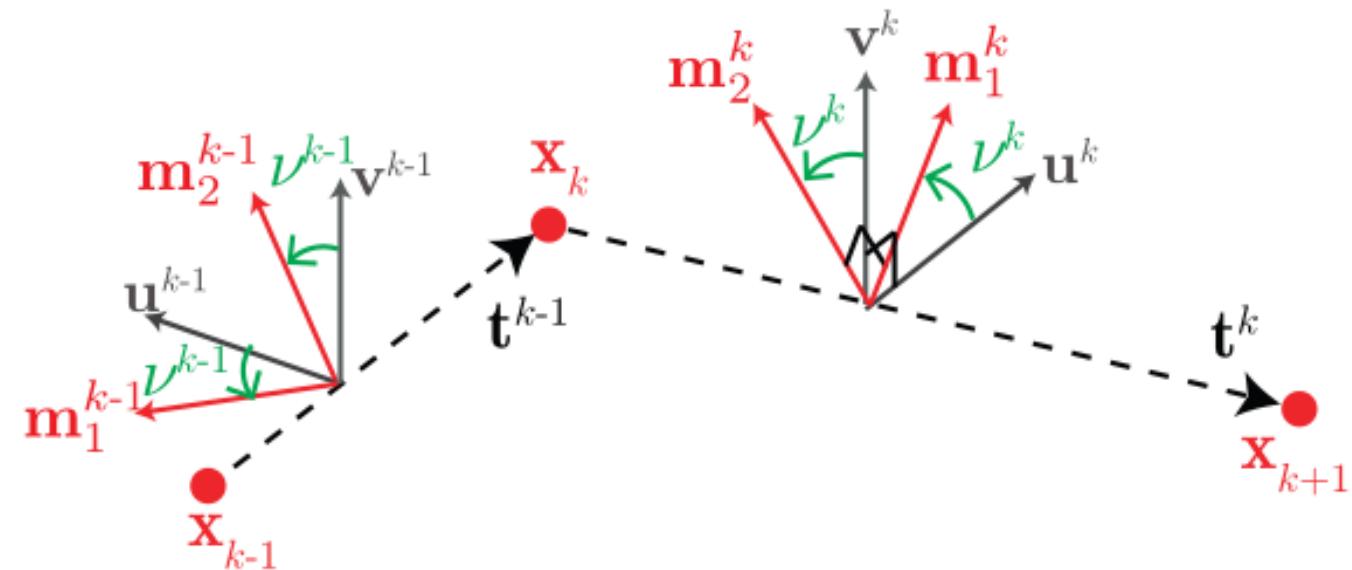
- Since the positions of the nodes are known, the tangent on each edge is known:

$$\mathbf{t}^k = \frac{\mathbf{e}^k}{\|\mathbf{e}^k\|} = \frac{\mathbf{x}_{k+1} - \mathbf{x}_k}{\|\mathbf{x}_{k+1} - \mathbf{x}_k\|}$$

- Start with an arbitrary (but adapted) orthonormal frame at the first edge, \mathbf{e}^1 . For that purpose, choose any unit vector \mathbf{u}^1 that is orthogonal to \mathbf{t}^1 . The second director is $\mathbf{v}^1 = \mathbf{t}^1 \times \mathbf{u}^1$ and the frame is $(\mathbf{u}^1, \mathbf{v}^1, \mathbf{t}^1)$.
- Sequentially compute the reference frames for the subsequent edges using $\mathbf{u}^k = P_{k-1}^k(\mathbf{u}^{k-1}) \equiv \text{parallel_transport}(\mathbf{u}^{k-1}, \mathbf{t}^{k-1}, \mathbf{t}^k)$ and $\mathbf{v}^k = \mathbf{t}^k \times \mathbf{u}^k$.

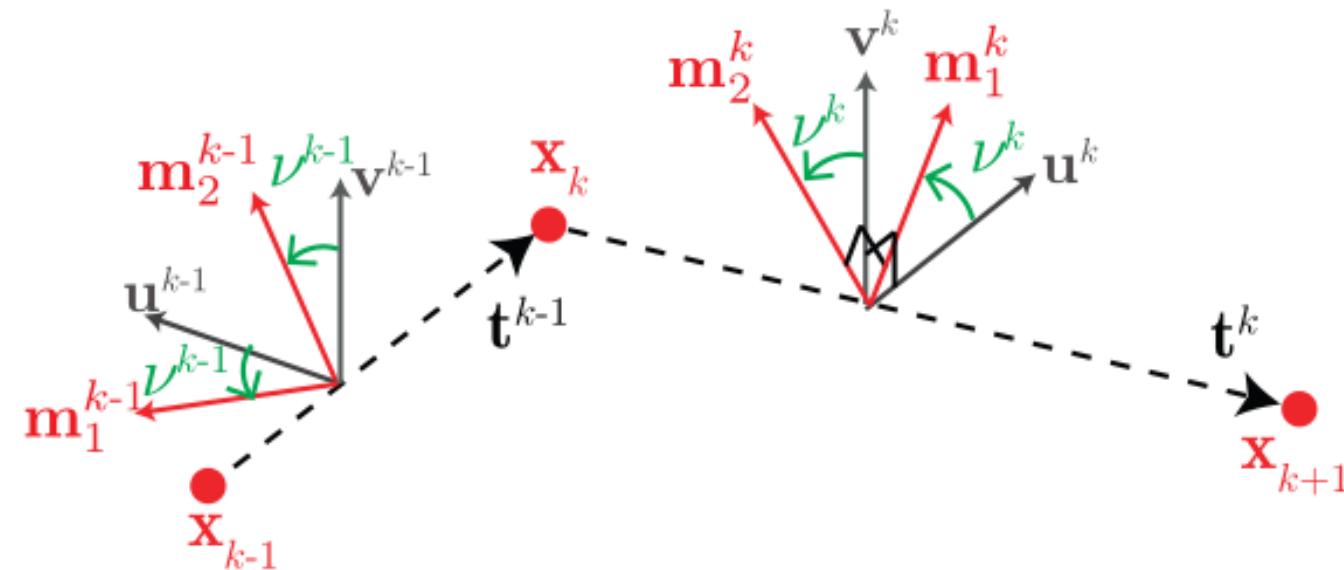
How to compute the discrete integrated twist?

- Known quantities: configuration of the rod
 - Nodal coordinates, x_k
 - Material frame on each edge, (m_1^k, m_2^k, t^k)
 - We learned how to compute the reference frame, (u^k, v^k, t^k) , using space parallel transport



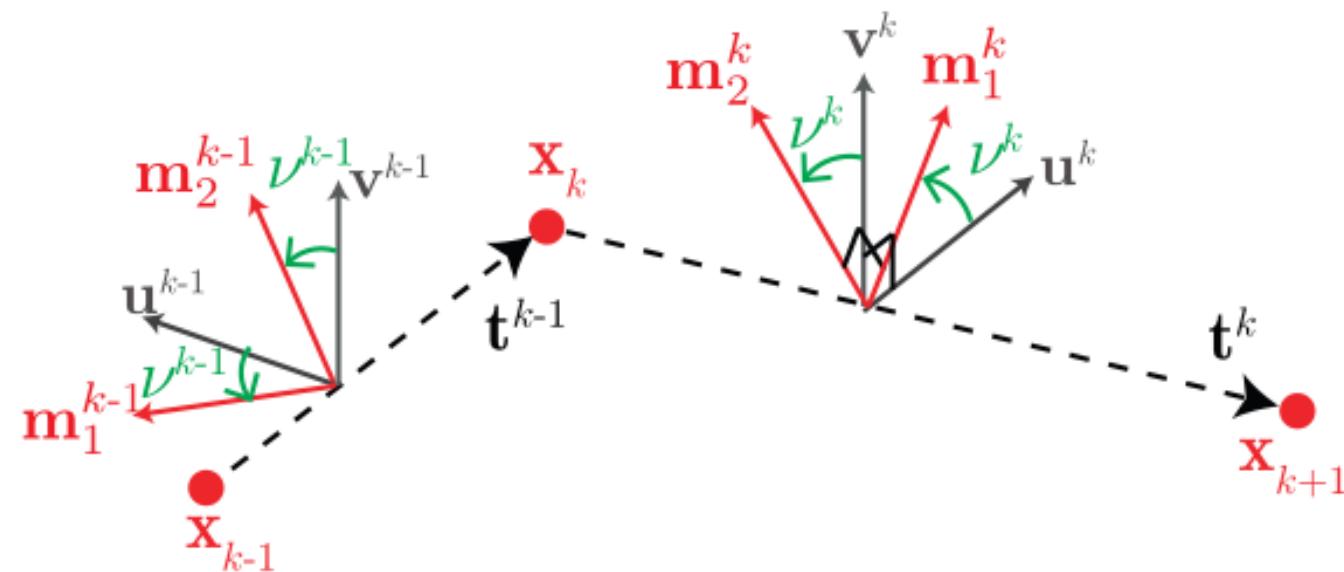
How to compute the discrete integrated twist?

- Steps to compute the twist at the node, x_k
 1. Compute the signed angles from the reference frame to the material frame, ν^k
 2. Discrete integrated twist is the difference between the signed rotation angles of two consecutive edges: $\tau_k = \nu^k - \nu^{k-1}$



Degrees of Freedom of a Rod

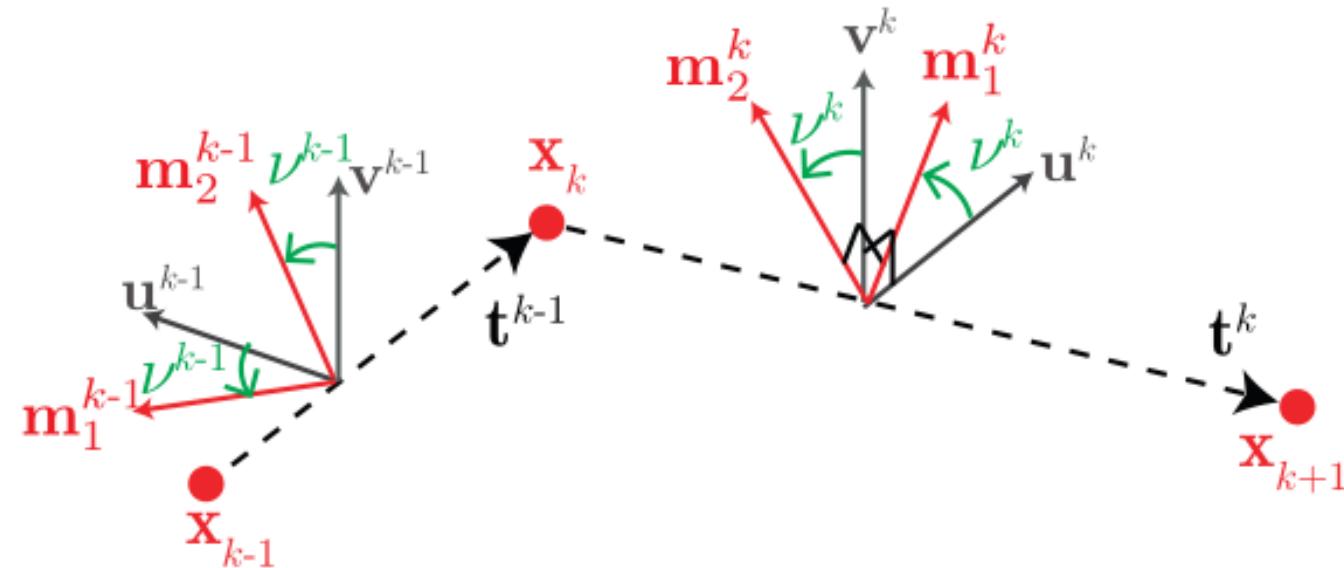
- If only the nodal coordinates, x_k , and twist angles, ν_k , are known, the complete configuration of the rod can be determined
 - First, determine the space parallel reference frame
 - Rotate the reference frame director, u^k , by an angle ν_k to get the material frame director, m_1^k . Recall that $m_2^k = t^k \times m_1^k$.





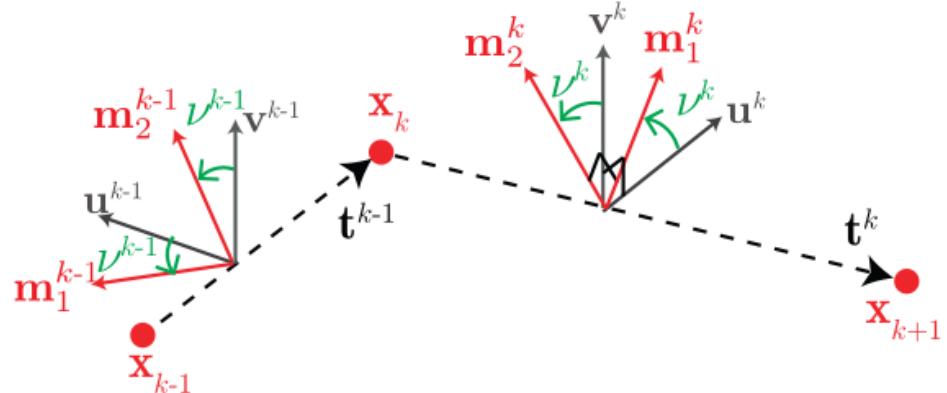
Degrees of Freedom (DOF) of a Rod

- A rod with N nodes has $(4N-1)$ DOFs
 1. $3N$ DOFs associated with the positions of N nodes, x_k ($1 \leq k \leq N$)
 2. $(N-1)$ DOFs for the twist angles of the edges, v^k ($1 \leq k \leq N - 1$)





Discrete Elastic Twisting Energy



$$E_t = \sum_{k=2}^{N-1} E_{t,k}$$

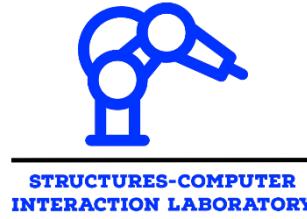
$$\text{where } E_{t,k} = \frac{1}{2} \frac{GJ}{l_k} (\tau_k)^2 = \frac{1}{2} \frac{GJ}{l_k} (\nu^k - \nu^{k-1})^2$$

- G = shear modulus = $\frac{\text{Young's modulus}}{2(1+\text{Poisson ratio})}$
- J = polar moment of area ($= \frac{\pi r_0^4}{2}$ if circular)
- τ_k = signed angle from $P_{k-1}^k(\mathbf{m}_1^{k-1})$ to \mathbf{m}_1^k about the axis \mathbf{t}^k



Future Plan

- Bergou et al. *SIGGRAPH* (2008) used space-parallel reference frame
- In 2010 (Bergou et al. *SIGGRAPH* (2010)), the authors formulated another formulation of reference frame: time-parallel reference frame
 - This leads to significant speed-up in computation
 - In this class, we will follow the formulation in the 2010 version and discuss time-parallel reference frame in next module



Module 20

Time Parallel Reference Frame

- Definition of twist using time parallel reference frame



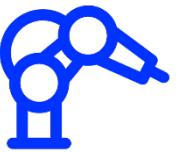
Goal

- Formulate a reference frame on the rod centerline using parallel transport along time (time parallel transport)
- Compute the twist along the rod using time parallel reference frame
- At the end of this module, you should be able to compute the twisting energy of a rod using time parallel reference frame



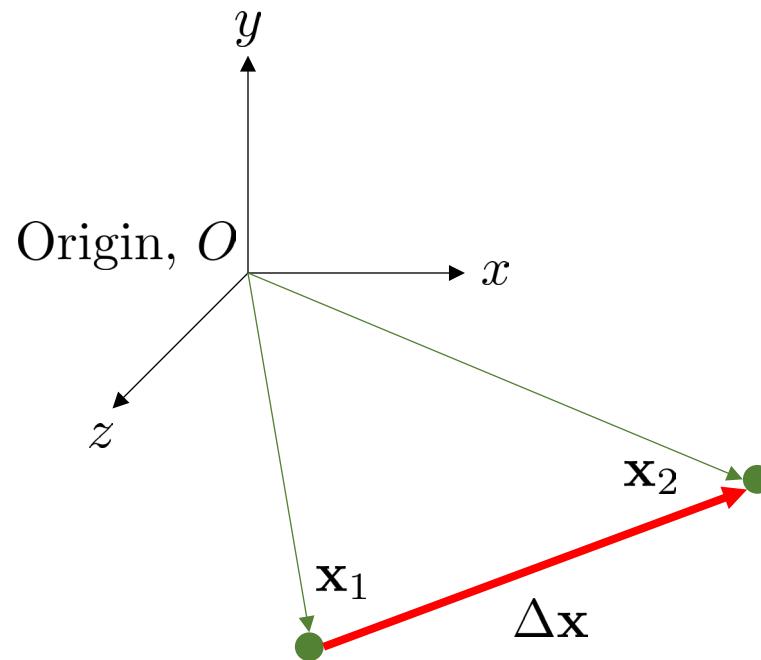
Resources

- Read “*Chapter 6: Discrete Twist*”
- Review Bergou, Miklós, et al. “Discrete viscous threads” SIGGRAPH (2010) 29(4) 1-10



Warm up: Relative Position

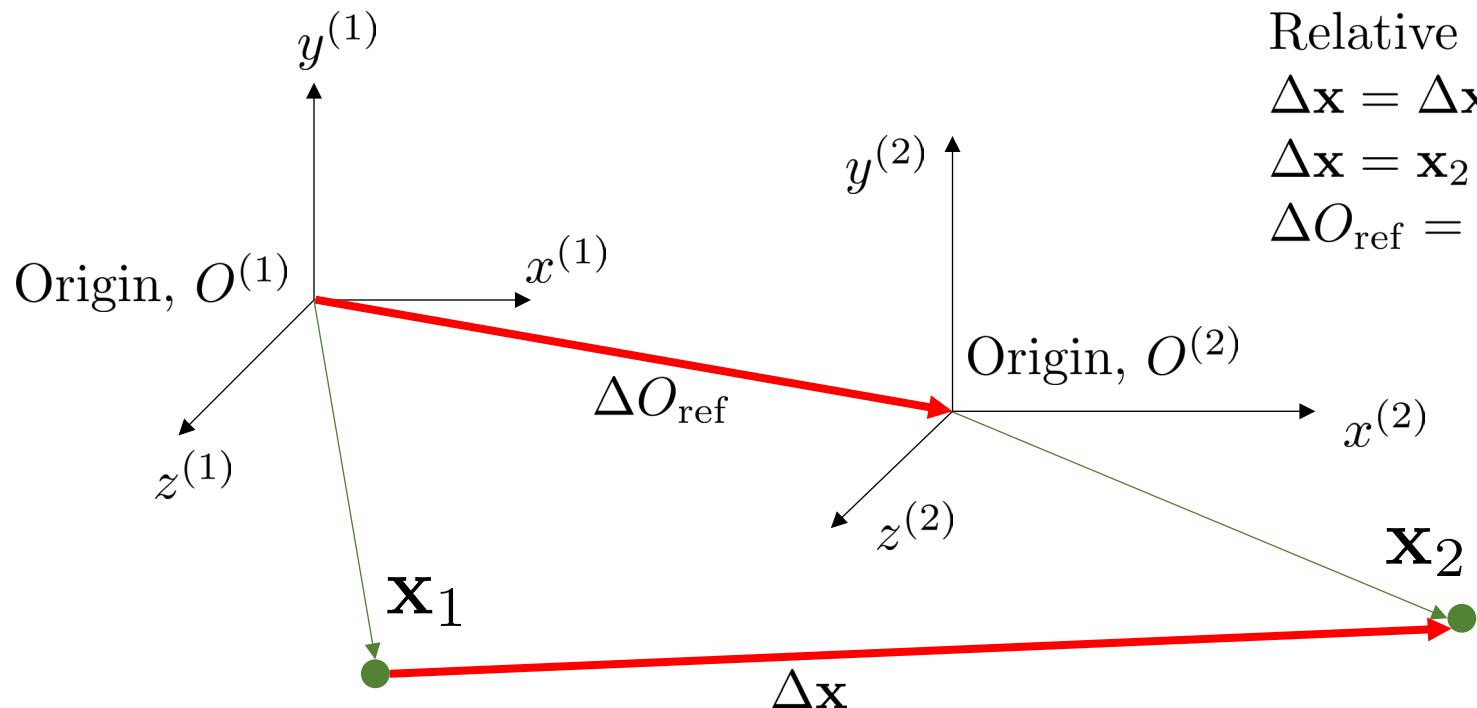
Relative position of node # 2 with respect to # 1:
 $\Delta\mathbf{x} = \mathbf{x}_2 - \mathbf{x}_1$





Warm up: Relative Position

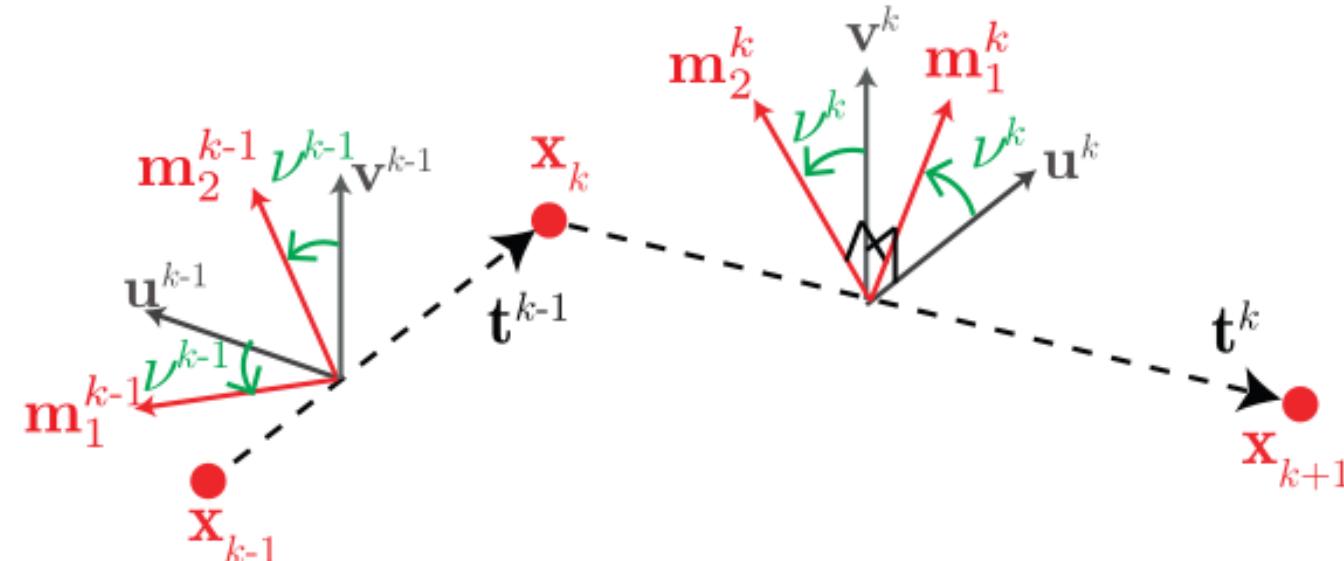
What if \mathbf{x}_1 and \mathbf{x}_2 are measured in two different Cartesian frames?



Relative position of node # 2 with respect to # 1:
 $\Delta\mathbf{x} = \mathbf{x}_2 - \mathbf{x}_1$ and
 $\Delta O_{\text{ref}} = \text{"reference" displacement}$

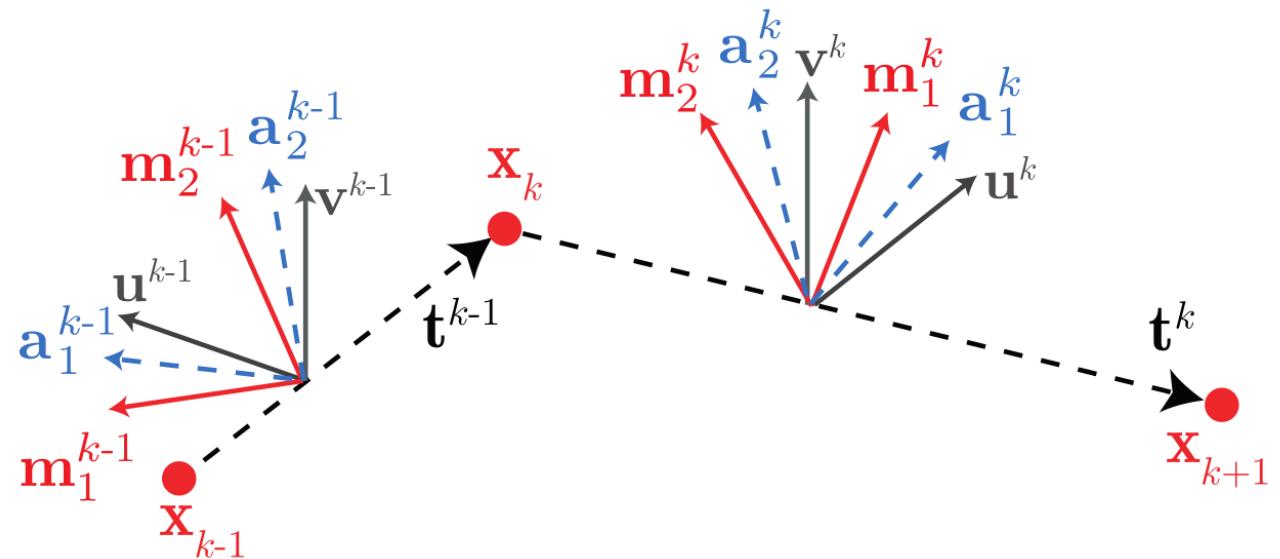
Recall: Twist using Space-Parallel Reference Frame

- The frame from the $(k - 1)$ -th edge is transported *without twist* to the k -th edge
- Twist between $(\mathbf{u}^{k-1}, \mathbf{v}^{k-1}, \mathbf{t}^{k-1})$ and $(\mathbf{u}^k, \mathbf{v}^k, \mathbf{t}^k)$ is zero (analogous to $\Delta O_{\text{ref}} = 0$)
- Discrete twist at the k -th node (\mathbf{x}_k) is $\tau_k = \nu^k - \nu^{k-1}$ (analogous to $\Delta x = \mathbf{x}_2 - \mathbf{x}_1$)



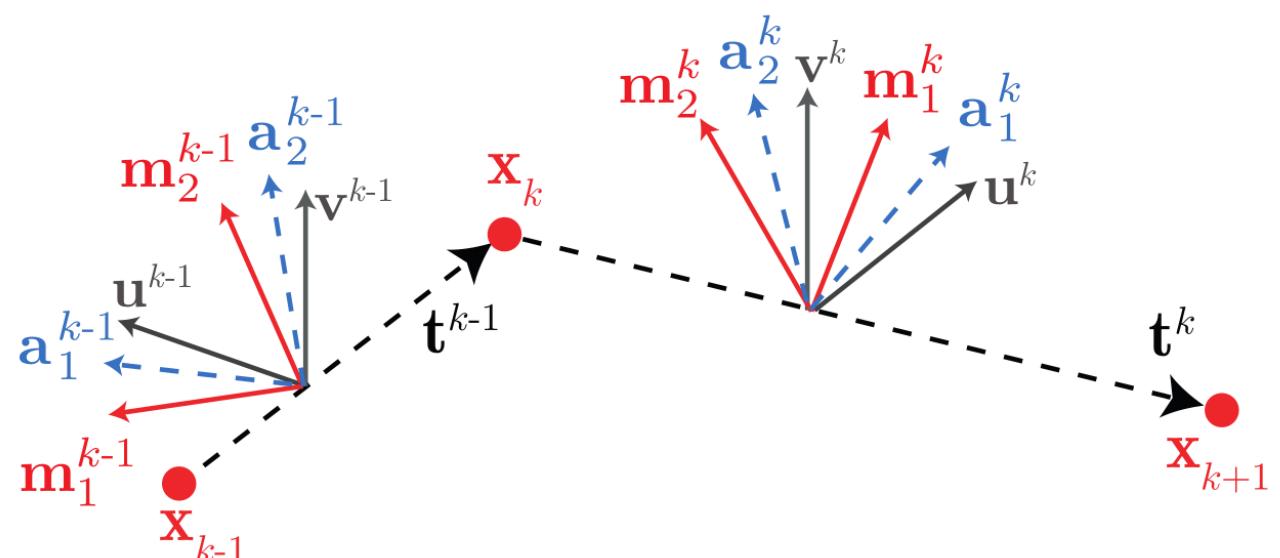
Time-Parallel Reference Frame

- At time $t = t_{j+1}$, space-parallel reference frame is
 $\mathbf{u}^k(t_{j+1}) = \text{parallel_transport}(\mathbf{u}^{k-1}(t_{j+1}), \mathbf{t}^{k-1}(t_{j+1}), \mathbf{t}^k(t_{j+1}))$ and
 $\mathbf{v}^k(t_{j+1}) = \mathbf{t}^k(t_{j+1}) \times \mathbf{u}^k(t_{j+1})$
- At time $t = t_{j+1}$, time-parallel reference frame is
 $\mathbf{a}_1^k(t_{j+1}) = \text{parallel_transport}(\mathbf{a}_1^k(t_j), \mathbf{t}^k(t_j), \mathbf{t}^k(t_{j+1}))$ and
 $\mathbf{a}_2^k(t_{j+1}) = \mathbf{t}^k(t_{j+1}) \times \mathbf{a}_1^k(t_{j+1})$



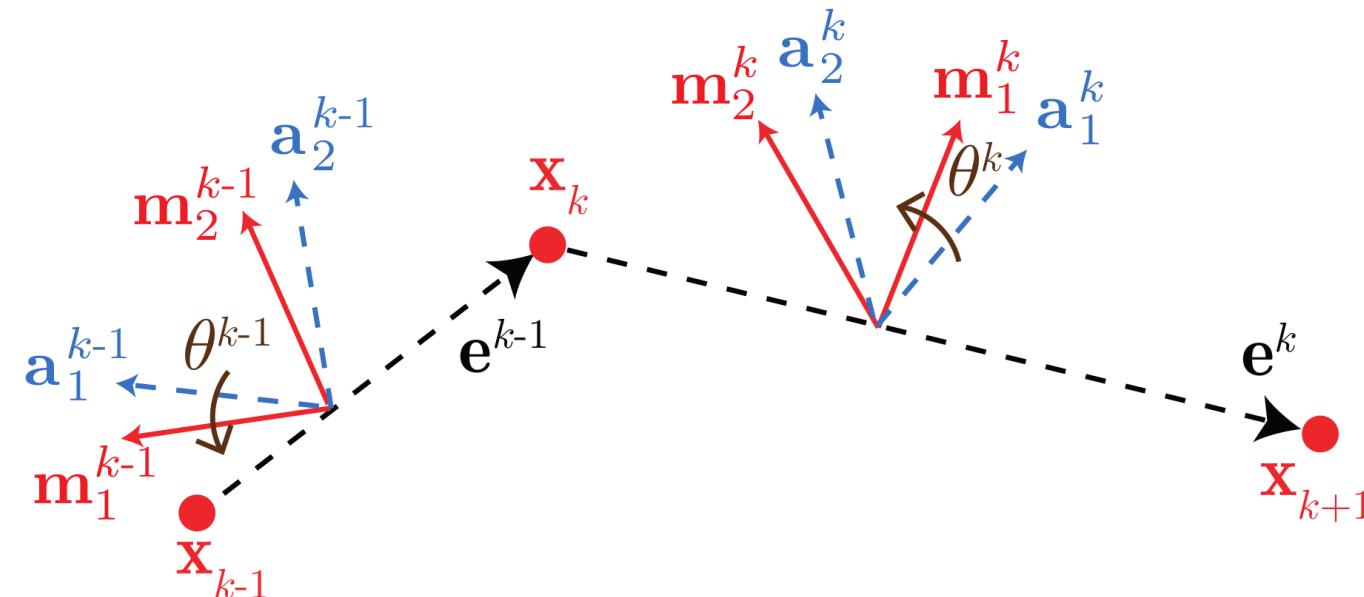
Time-Parallel Reference Frame

- Space-parallel frame $\mathbf{u}^k(t_{j+1}), \mathbf{v}^k(t_{j+1}), \mathbf{t}^k(t_{j+1})$ moves forward in *space*
- Time-parallel frame $\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1})$ moves forward in *time*
- Space-parallel frame has no *reference twist*
- Time-parallel frame may have *reference twist* (analogous to $\Delta O_{\text{ref}} \neq 0$)



New Definition of Twist Angle

- Recall: signed angle from space-parallel frame director $\mathbf{u}^k(t_{j+1})$ to the material frame director $\mathbf{m}_1^k(t_{j+1})$ is the *twist angle* ν^k
- Signed angle from time-parallel frame director $\mathbf{a}_1^k(t_{j+1})$ to the material frame director $\mathbf{m}_1^k(t_{j+1})$ is the new *twist angle* θ^k
- We will use θ^k ($1 \leq k < N$) as the DOFs of the rod

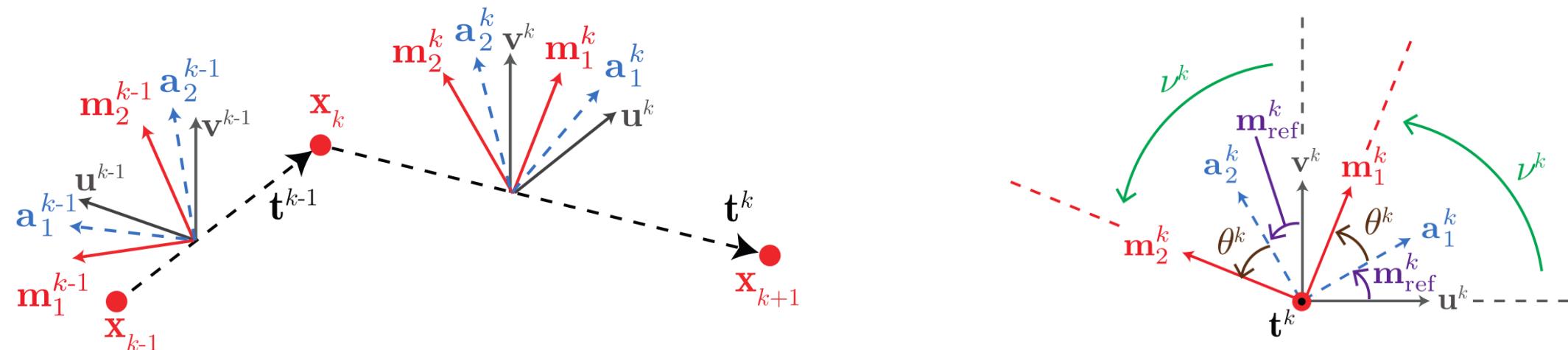


Reference Twist

- m_{ref}^k is the signed angle from space-parallel frame director, \mathbf{u}^k , to time-parallel frame director, \mathbf{a}_1^k

$$\nu^k = \theta^k + m_{\text{ref}}$$

- Reference twist at the k -th node is $\Delta m_{\text{ref}} = m_{\text{ref}}^k - m_{\text{ref}}^{k-1}$





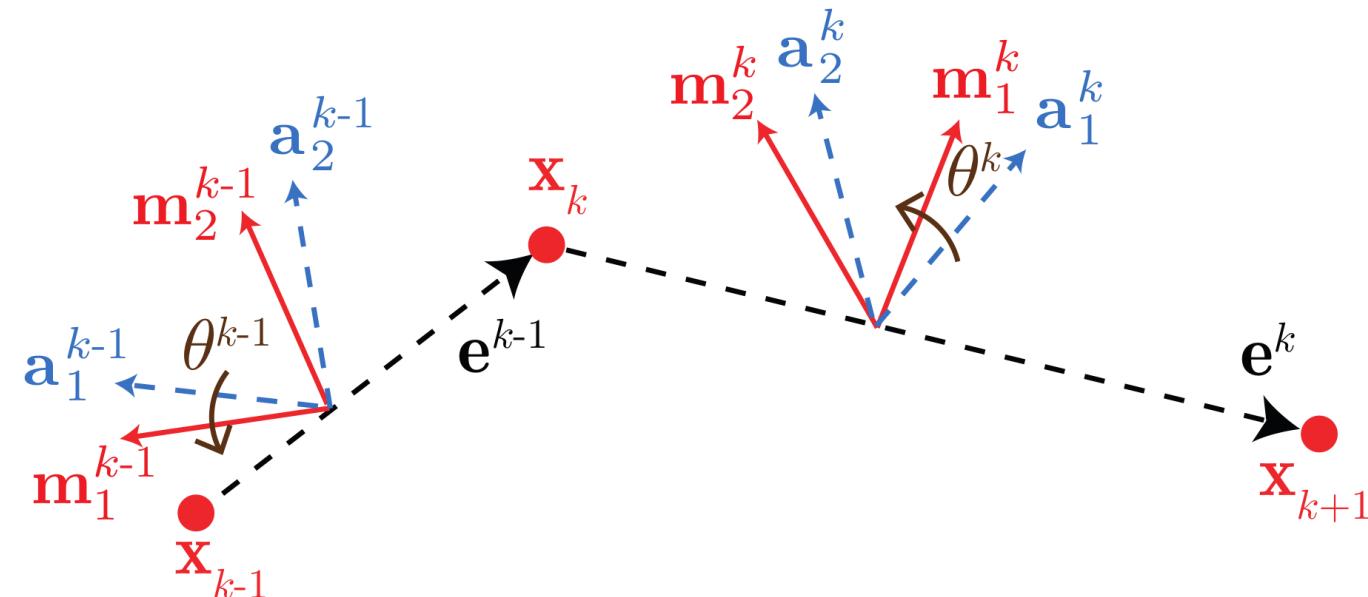
Measurement of Discrete Twist using Time-Parallel Reference Frame

Twist at the k -th node is

$$\tau_k = \nu^k - \nu^{k-1} = (\theta^k + m_{\text{ref}}^k) - (\theta^{k-1} + m_{\text{ref}}^{k-1}) = \Delta\theta_k + \Delta m_{k,\text{ref}}$$

The reference twist, $\Delta m_{k,\text{ref}}$, at node \mathbf{x}_k is the signed angle from $P_{k-1}^k(\mathbf{a}_1^{k-1}(t_{j+1}))$ to $\mathbf{a}_1^k(t_{j+1})$ about the axis $\mathbf{t}^k(t_{j+1})$, i.e.

$$\Delta m_{k,\text{ref}} = \text{signedAngle}\left(P_{k-1}^k(\mathbf{a}_1^{k-1}(t_{j+1})), \mathbf{a}_1^k(t_{j+1}), \mathbf{t}^k(t_{j+1})\right)$$



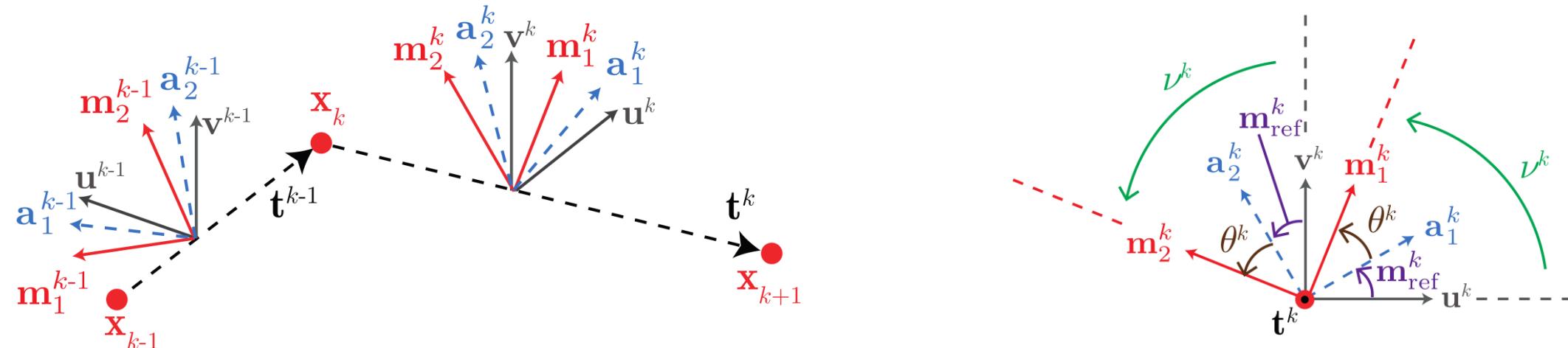


Summary: Time-Parallel Reference Frame and Twist

- At time $t = 0$, start with a space-parallel reference frame on each edge of the rod. This is also our time-parallel frame at $t = 0$
- Parallel transport the frame from previous time step ($t = t_j$) to the next time step ($t = t_{j+1}$)
- Twist at the k -th node is

$$\tau_k = \nu^k - \nu^{k-1} = (\theta^k + m_{\text{ref}}^k) - (\theta^{k-1} + m_{\text{ref}}^{k-1}) = \Delta\theta_k + \Delta m_{k,\text{ref}}$$

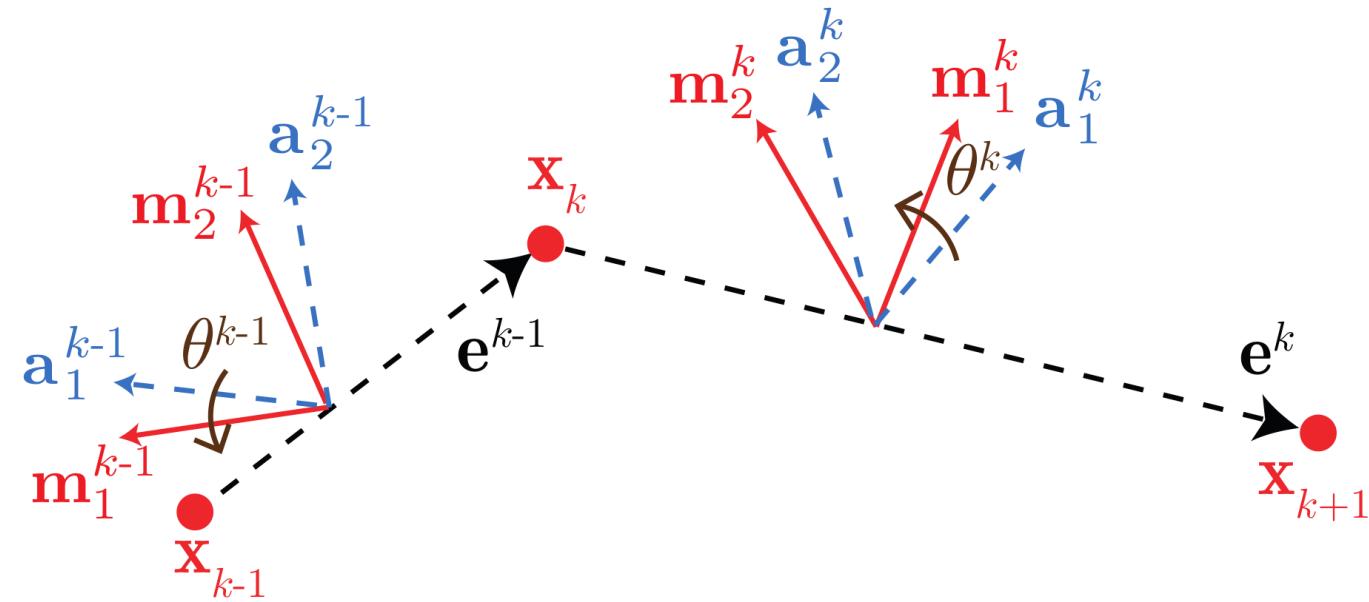
where $\Delta m_{k,\text{ref}} = \text{signedAngle}\left(P_{k-1}^k(\mathbf{a}_1^{k-1}(t_{j+1})), \mathbf{a}_1^k(t_{j+1}), \mathbf{t}^k(t_{j+1})\right)$





Degrees of Freedom (DOF) of a Rod

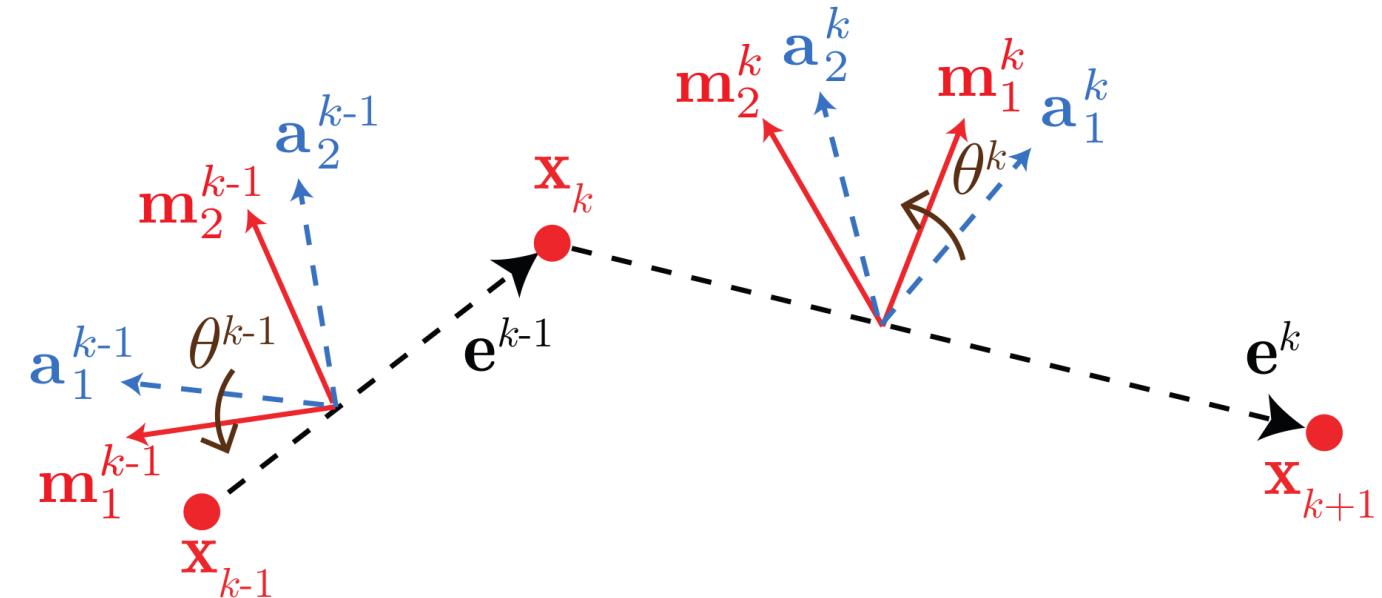
- A rod with N nodes has $(4N-1)$ DOFs
 1. $3N$ DOFs associated with the positions of N nodes, x_k ($1 \leq k \leq N$)
 2. $(N-1)$ DOFs for the twist angles of the edges, θ^k ($1 \leq k \leq N - 1$)



Discrete Elastic Twisting Energy

$$E_t = \sum_{k=2}^{N-1} E_{t,k}$$

where $E_{t,k} = \frac{1}{2} \frac{GJ}{l_k} (\tau_k)^2 = \frac{1}{2} \frac{GJ}{l_k} (\Delta\theta_k + \Delta m_{k,\text{ref}})^2$

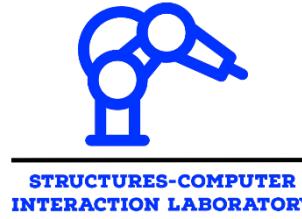


- G = shear modulus = $\frac{\text{Young's modulus}}{2(1+\text{Poisson ratio})}$
- J = polar moment of area ($= \frac{\pi r_0^4}{2}$ if circular)



Future Plan

- Follow Bergou et al. *SIGGRAPH* (2010) to formulate a discrete simulation algorithm for elastic rods



Module 21

Discrete Elastic Rods (DER) Algorithm



Goal

- Equations of motion of an elastic rod
- Programming implementation of the Discrete Elastic Rods (DER) algorithm



Resources

- Read “*Chapter 7: Discrete Elastic Rods Algorithm*”
- Review Bergou, Miklós et al. “Discrete viscous threads” SIGGRAPH (2010) 29(4) 1-10
- Review Jawed, M. K. et al. “A primer on the kinematics of discrete elastic rods” (2018)

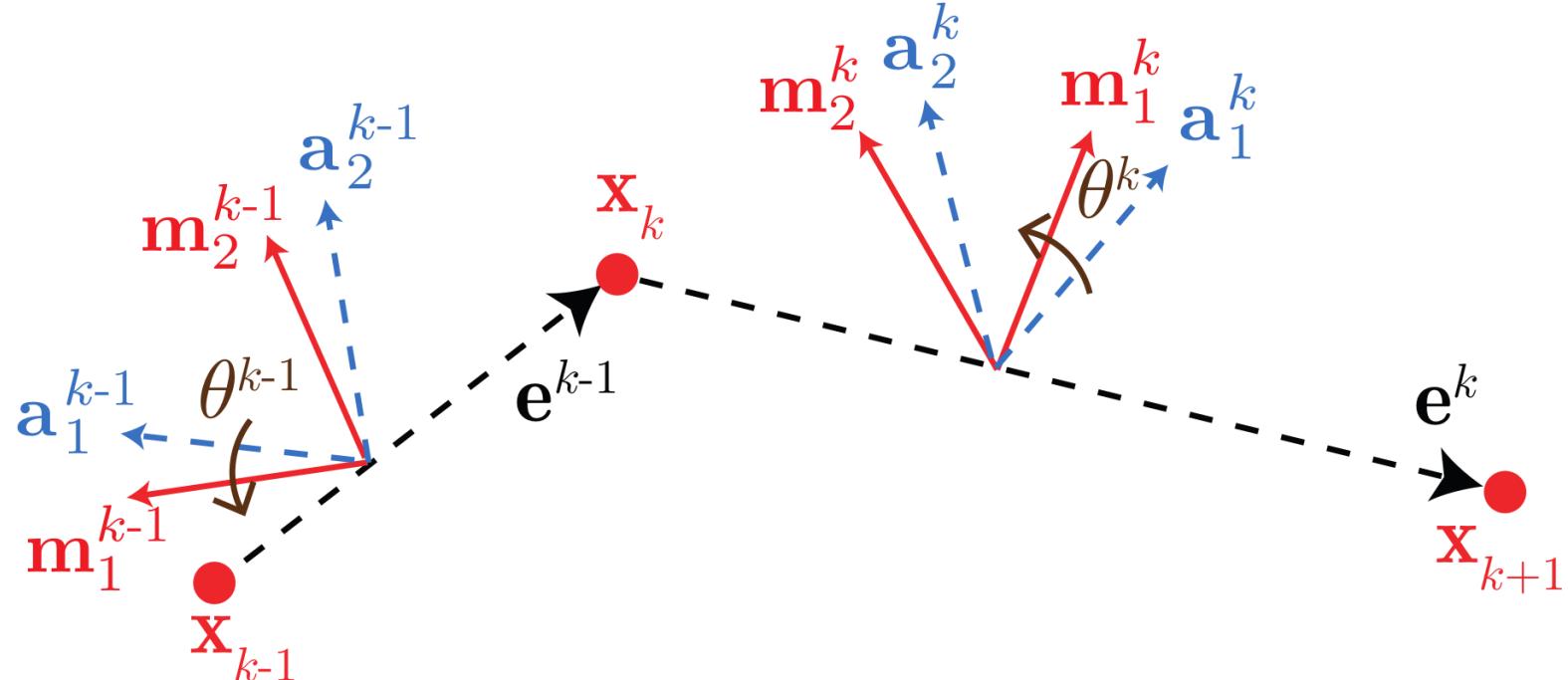


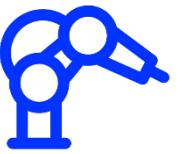
Degrees of Freedom (DOF)

$(4N - 1)$ DOF for a rod with N nodes:
 $3N$ nodal coordinates and $N - 1$ twist angles

Degrees of Freedom (DOF) vector,

$$\mathbf{q} = \begin{bmatrix} x_1 \\ y_1 \\ z_1 \\ \theta^1 \\ x_2 \\ y_2 \\ z_2 \\ \theta^2 \\ \dots \\ \dots \\ \dots \\ \dots \\ \theta^{N-1} \\ x_N \\ y_N \\ z_N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 \\ \theta^1 \\ \mathbf{x}_2 \\ \theta^2 \\ \dots \\ \dots \\ \dots \\ \dots \\ \theta^{N-1} \\ \mathbf{x}_N \end{bmatrix}$$





Discrete Equations of Motion

$$\mathbf{M} \ddot{\mathbf{q}} + \frac{\partial E_{\text{elastic}}}{\partial \mathbf{q}} - \mathbf{f}_{\text{external}} = \mathbf{0}$$

$$f_i \equiv \frac{m_i}{\Delta t} \left[\frac{q_i(t_{k+1}) - q_i(t_k)}{\Delta t} - \dot{q}_i(t_k) \right] + \frac{\partial E_{\text{elastic}}}{\partial q_i} - F_{i,\text{external}} = 0$$

$$\mathbb{J}_{ij} = \frac{\partial f_i}{\partial q_j} = \mathbb{J}_{ij}^{\text{inertia}} + \boxed{\mathbb{J}_{ij}^{\text{elastic}}} + \mathbb{J}_{ij}^{\text{external}},$$

where

$$\mathbb{J}_{ij}^{\text{inertia}} = \frac{m_i}{\Delta t^2} \delta_{ij},$$

$$\mathbb{J}_{ij}^{\text{elastic}} = \frac{\partial^2 E_{\text{elastic}}}{\partial q_i \partial q_j},$$

$$\mathbb{J}_{ij}^{\text{external}} = -\frac{\partial f_i^{\text{ext}}}{\partial q_j}.$$



Discrete Elastic Energies

$$f_i \equiv \frac{m_i}{\Delta t} \left[\frac{q_i(t_{k+1}) - q_i(t_k)}{\Delta t} - \dot{q}_i(t_k) \right] + \boxed{\frac{\partial E_{\text{elastic}}}{\partial q_i}} - F_{i,\text{external}} = 0$$

$$\mathbb{J}_{ij} = \frac{\partial f_i}{\partial q_j} = \mathbb{J}_{ij}^{\text{inertia}} + \boxed{\mathbb{J}_{ij}^{\text{elastic}}} + \mathbb{J}_{ij}^{\text{external}},$$

$$E_{\text{elastic}} = \underbrace{\sum_{k=1}^{N-1} E_k^s}_{\text{stretching energy}} + \underbrace{\sum_{k=2}^{N-1} E_k^b}_{\text{bending energy}} + \underbrace{\sum_{k=2}^{N-1} E_k^t}_{\text{twisting energy}}$$

$$\begin{aligned}\mathbb{J}_{ij}^{\text{inertia}} &= \frac{m_i}{\Delta t^2} \delta_{ij}, \\ \mathbb{J}_{ij}^{\text{elastic}} &= \frac{\partial^2 E_{\text{elastic}}}{\partial q_i \partial q_j}, \\ \mathbb{J}_{ij}^{\text{external}} &= -\frac{\partial f_i^{\text{ext}}}{\partial q_j}.\end{aligned}$$

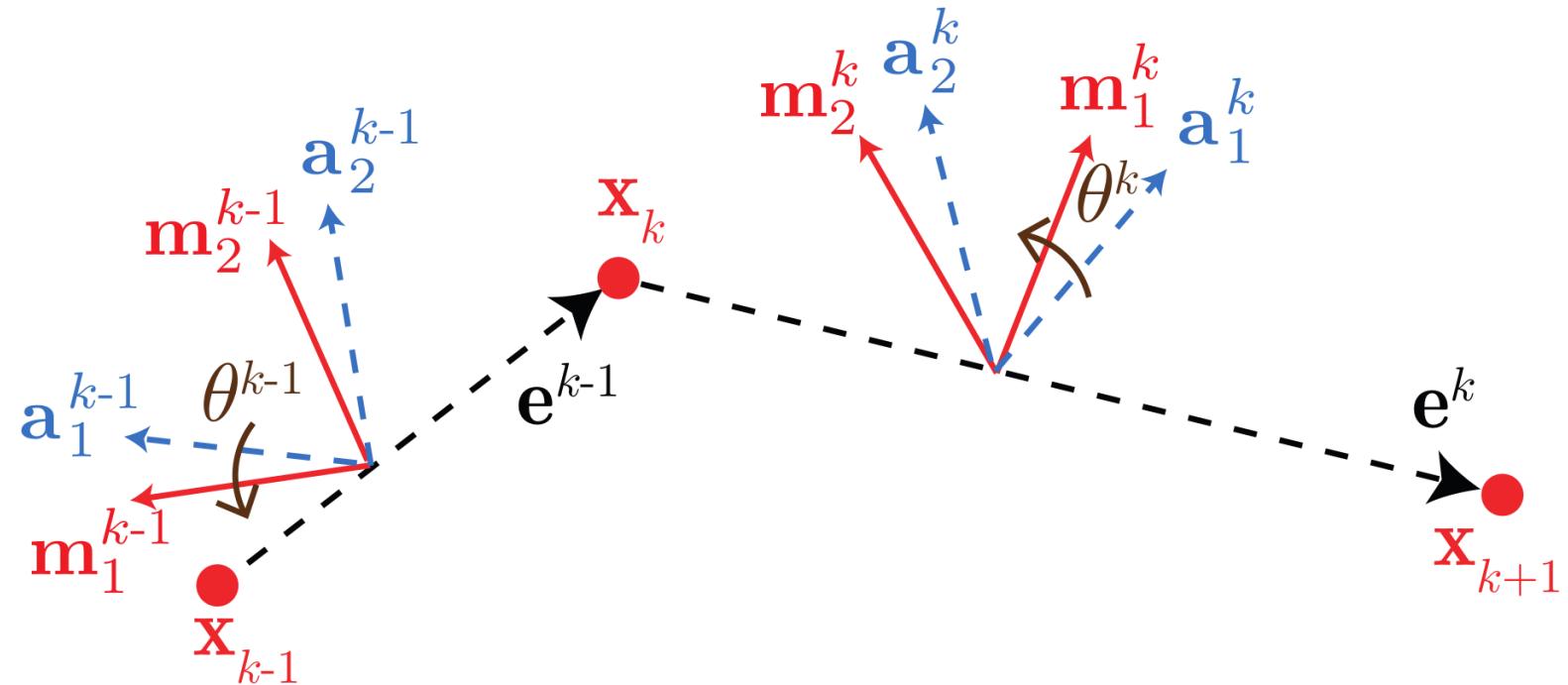
$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial}{\partial q_i} E_k^s + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$

$$\frac{\partial^2}{\partial q_i \partial q_j} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^s + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^b + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^t$$



Reminder 1: Time Parallel Reference Frame

- At every time step, we need to compute the reference frame along the rod to measure twist





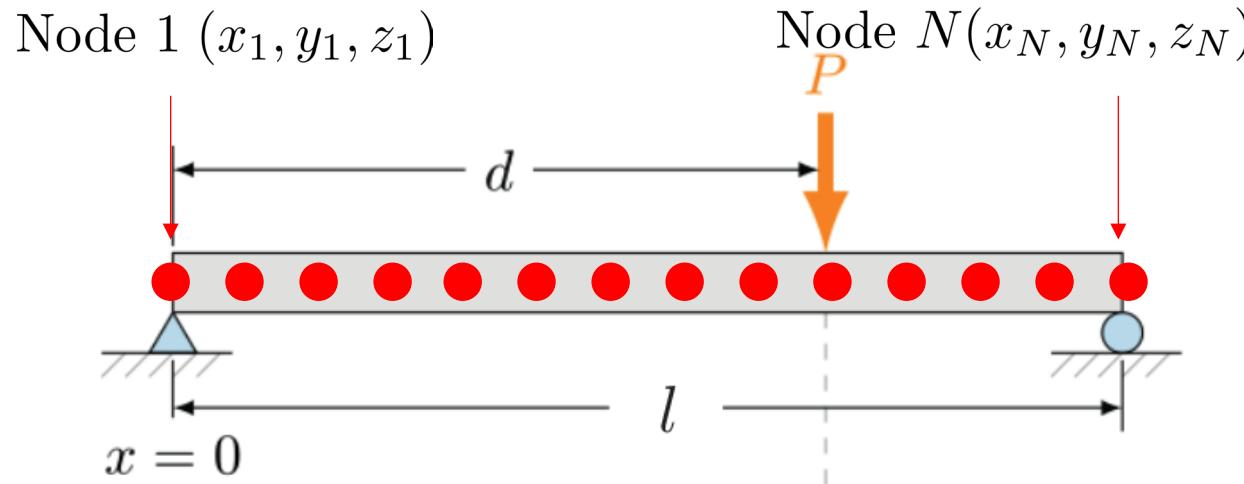
Reminder 2: Fixed and Free DOFs

- Some DOFs are fixed

fixed_index: [1, 2, 3, 4N - 2, 4N - 1]

free_index: [4, 5, ..., 4N - 3]

We will need this later.



Fixed DOF:

$$x_1 = 0$$

$$y_1 = 0$$

$$z_1 = 0$$

$$y_N = 0$$

$$z_N = 0$$



Discrete Elastic Rods (DER)

Algorithm 1 Discrete Elastic Rods

Require: $\mathbf{q}(t_j), \dot{\mathbf{q}}(t_j)$ ▷ DOFs and velocities at $t = t_j$
Require: $(\mathbf{a}_1^k(t_j), \mathbf{a}_2^k(t_j), \mathbf{t}^k(t_j))$ ▷ Reference frame at $t = t_j$
Require: `free_index` ▷ index of the free DOFs
Ensure: $\mathbf{q}(t_{j+1}), \dot{\mathbf{q}}(t_{j+1})$ ▷ DOFs and velocities at $t = t_{j+1}$
Ensure: $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$ ▷ Reference frame at $t = t_{j+1}$

Algorithm 1 Discrete Elastic Rods

Require: $\mathbf{q}(t_j), \dot{\mathbf{q}}(t_j)$ ▷ DOFs and velocities at $t = t_j$
Require: $(\mathbf{a}_1^k(t_j), \mathbf{a}_2^k(t_j), \mathbf{t}^k(t_j))$ ▷ Reference frame at $t = t_j$
Require: `free_index` ▷ index of the free DOFs
Ensure: $\mathbf{q}(t_{j+1}), \dot{\mathbf{q}}(t_{j+1})$ ▷ DOFs and velocities at $t = t_{j+1}$
Ensure: $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$ ▷ Reference frame at $t = t_{j+1}$

1: **function** DISCRETE_ELASTIC_RODS($\mathbf{q}, \dot{\mathbf{q}}(t_j), (\mathbf{a}_1^k(t_j), \mathbf{a}_2^k(t_j), \mathbf{t}^k(t_j))$)

2: **Guess:** $\mathbf{q}^{(1)}(t_{j+1}) \leftarrow \mathbf{q}(t_j)$

3: $n \leftarrow 1$

4: **while** error > tolerance **do**

Only update free DOFs

5: Compute \mathbf{f} and \mathbb{J}

6: $\mathbf{f}_{\text{free}} \leftarrow \mathbf{f}(\text{free_index})$

7: $\mathbb{J}_{\text{free}} \leftarrow \mathbb{J}(\text{free_index}, \text{free_index})$

8: $\Delta\mathbf{q}_{\text{free}} \leftarrow \mathbb{J}_{\text{free}} \backslash \mathbf{f}_{\text{free}}$

9: $\mathbf{q}^{(n+1)}(\text{free_index}) \leftarrow \mathbf{q}^{(n)}(\text{free_index}) - \Delta\mathbf{q}_{\text{free}}$

10: error $\leftarrow \text{sum}(\text{abs}(\mathbf{f}_{\text{free}}))$

11: $n \leftarrow n + 1$

12: **end while**

13: **return** $\mathbf{q}(t_{j+1}), \dot{\mathbf{q}}(t_{j+1}), (\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$

14: **end function**

Newton-Raphson

Algorithm 1 Discrete Elastic Rods

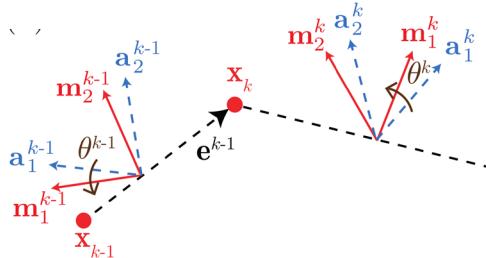
Require: $\mathbf{q}(t_j), \dot{\mathbf{q}}(t_j)$ ▷ DOFs and velocities at $t = t_j$
Require: $(\mathbf{a}_1^k(t_j), \mathbf{a}_2^k(t_j), \mathbf{t}^k(t_j))$ ▷ Reference frame at $t = t_j$
Require: `free_index` ▷ index of the free DOFs
Ensure: $\mathbf{q}(t_{j+1}), \dot{\mathbf{q}}(t_{j+1})$ ▷ DOFs and velocities at $t = t_{j+1}$
Ensure: $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$ ▷ Reference frame at $t = t_{j+1}$

```
1: function DISCRETE_ELASTIC_RODS(  $\mathbf{q}, \dot{\mathbf{q}}(t_j), (\mathbf{a}_1^k(t_j), \mathbf{a}_2^k(t_j), \mathbf{t}^k(t_j))$  )  
2:   Guess:  $\mathbf{q}^{(1)}(t_{j+1}) \leftarrow \mathbf{q}(t_j)$   
3:    $n \leftarrow 1$   
4:   while error > tolerance do  
5:     Compute  $\mathbf{f}$  and  $\mathbb{J}$   
6:      $\mathbf{f}_{\text{free}} \leftarrow \mathbf{f}$  (free_index)  
7:      $\mathbb{J}_{\text{free}} \leftarrow \mathbb{J}$  (free_index, free_index)  
8:      $\Delta\mathbf{q}_{\text{free}} \leftarrow \mathbb{J}_{\text{free}} \backslash \mathbf{f}_{\text{free}}$   
9:      $\mathbf{q}^{(n+1)}(\text{free\_index}) \leftarrow \mathbf{q}^{(n)}(\text{free\_index}) - \Delta\mathbf{q}_{\text{free}}$   
10:    error  $\leftarrow \text{sum}(\text{abs}(\mathbf{f}_{\text{free}}))$   
11:     $n \leftarrow n + 1$   
12:   end while  
13:    $\mathbf{q}(t_{j+1}) \leftarrow \mathbf{q}^{(n)}(t_{j+1})$   
14:    $\dot{\mathbf{q}}(t_{j+1}) \leftarrow \frac{\mathbf{q}(t_{j+1}) - \mathbf{q}(t_j)}{\Delta t}$   
15:    $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1})) \leftarrow (\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))^{(n)}$   
16:   return  $\mathbf{q}(t_{j+1}), \dot{\mathbf{q}}(t_{j+1}), (\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$   
17: end function
```

Return once we are below tolerance

Algorithm 1 Discrete Elastic Rods

Require: $\mathbf{q}(t_j), \dot{\mathbf{q}}(t_j)$ ▷ DOFs and velocities at $t = t_j$
Require: $(\mathbf{a}_1^k(t_j), \mathbf{a}_2^k(t_j), \mathbf{t}^k(t_j))$ ▷ Reference frame at $t = t_j$
Require: `free_index` ▷ index of the free DOFs
Ensure: $\mathbf{q}(t_{j+1}), \dot{\mathbf{q}}(t_{j+1})$ ▷ DOFs and velocities at $t = t_{j+1}$
Ensure: $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$ ▷ Reference frame at $t = t_{j+1}$



```

1: function DISCRETE_ELASTIC_RODS(  $\mathbf{q}, \dot{\mathbf{q}}(t_j), (\mathbf{a}_1^k(t_j), \mathbf{a}_2^k(t_j), \mathbf{t}^k(t_j))$  )
2:   Guess:  $\mathbf{q}^{(1)}(t_{j+1}) \leftarrow \mathbf{q}(t_j)$ 
3:    $n \leftarrow 1$ 
4:   while error > tolerance do
5:     Compute reference frame  $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))^{(n)}$ 
6:     Compute reference twist  $\Delta m_{k,\text{ref}}^{(n)}$  ( $k = 2, \dots, N - 1$ )
7:     Compute material frame  $(\mathbf{m}_1^k(t_{j+1}), \mathbf{m}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))^{(n)}$ 
8:     Compute  $\mathbf{f}$  and  $\mathbb{J}$ 
9:      $\mathbf{f}_{\text{free}} \leftarrow \mathbf{f}(\text{free\_index})$ 
10:     $\mathbb{J}_{\text{free}} \leftarrow \mathbb{J}(\text{free\_index}, \text{free\_index})$ 
11:     $\Delta \mathbf{q}_{\text{free}} \leftarrow \mathbb{J}_{\text{free}} \backslash \mathbf{f}_{\text{free}}$ 
12:     $\mathbf{q}^{(n+1)}(\text{free\_index}) \leftarrow \mathbf{q}^{(n)}(\text{free\_index}) - \Delta \mathbf{q}_{\text{free}}$ 
13:    error  $\leftarrow \text{sum}(\text{abs}(\mathbf{f}_{\text{free}}))$ 
14:     $n \leftarrow n + 1$ 
15:   end while

16:    $\mathbf{q}(t_{j+1}) \leftarrow \mathbf{q}^{(n)}(t_{j+1})$ 
17:    $\dot{\mathbf{q}}(t_{j+1}) \leftarrow \frac{\mathbf{q}(t_{j+1}) - \mathbf{q}(t_j)}{\Delta t}$ 
18:    $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1})) \leftarrow (\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))^{(n)}$ 
19:   return  $\mathbf{q}(t_{j+1}), \dot{\mathbf{q}}(t_{j+1}), (\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$ 
20: end function

```

We need the frames to compute bending and twisting energies

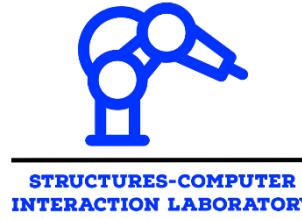


Next Step

- Programming implementation of gradient and Hessian of elastic energies

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial}{\partial q_i} E_k^s + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$

$$\frac{\partial^2}{\partial q_i \partial q_j} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^s + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^b + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^t$$



Module 22

Gradient and Hessian of Elastic Energies in Discrete Rod

- Programming Implementation



Goal

- Understand the computation of gradient and Hessian of elastic energies in Discrete Elastic Rods (DER)

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial}{\partial q_i} E_k^s + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$

$$\frac{\partial^2}{\partial q_i \partial q_j} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^s + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^b + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^t$$



Resources

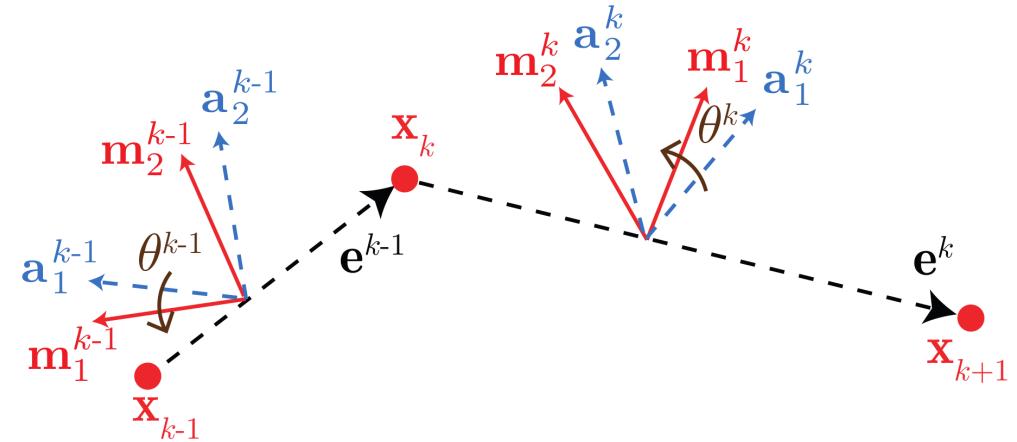
- Read “*Chapter 7: Discrete Elastic Rods Algorithm*”
- Review Bergou, Miklós et al. “Discrete viscous threads” SIGGRAPH (2010) 29(4) 1-10
- Review Jawed, M. K. et al. “A primer on the kinematics of discrete elastic rods” (2018)

Degrees of Freedom (DOF)

$(4N - 1)$ DOF for a rod with N nodes:
 $3N$ nodal coordinates and $N - 1$ twist angles

Degrees of Freedom (DOF) vector,

$$\mathbf{q} = \begin{bmatrix} x_1 \\ y_1 \\ z_1 \\ \theta^1 \\ x_2 \\ y_2 \\ z_2 \\ \theta^2 \\ \dots \\ \dots \\ \dots \\ \dots \\ \theta^{N-1} \\ x_N \\ y_N \\ z_N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 \\ \theta^1 \\ \mathbf{x}_2 \\ \theta^2 \\ \dots \\ \dots \\ \dots \\ \dots \\ \theta^{N-1} \\ \mathbf{x}_N \end{bmatrix}$$



Index of the k -th node, \mathbf{x}_k , in DOF vector:
 $4k - 3, 4k - 2, 4k - 1$, where $1 \leq k \leq N$

Index of the k -th twist angle, θ^k , in DOF vector:
 $4k$, where $1 \leq k \leq N - 1$

We will need this during programming implementation.



Discrete Elastic Energies

$$f_i \equiv \frac{m_i}{\Delta t} \left[\frac{q_i(t_{k+1}) - q_i(t_k)}{\Delta t} - \dot{q}_i(t_k) \right] + \boxed{\frac{\partial E_{\text{elastic}}}{\partial q_i}} - F_{i,\text{external}} = 0$$

$$\mathbb{J}_{ij} = \frac{\partial f_i}{\partial q_j} = \mathbb{J}_{ij}^{\text{inertia}} + \boxed{\mathbb{J}_{ij}^{\text{elastic}}} + \mathbb{J}_{ij}^{\text{viscous}},$$

$$E_{\text{elastic}} = \underbrace{\sum_{k=1}^{N-1} E_k^s}_{\text{stretching energy}} + \underbrace{\sum_{k=2}^{N-1} E_k^b}_{\text{bending energy}} + \underbrace{\sum_{k=2}^{N-1} E_k^t}_{\text{twisting energy}}$$

$$\begin{aligned}\mathbb{J}_{ij}^{\text{inertia}} &= \frac{m_i}{\Delta t^2} \delta_{ij}, \\ \mathbb{J}_{ij}^{\text{elastic}} &= \frac{\partial^2 E_{\text{elastic}}}{\partial q_i \partial q_j}, \\ \mathbb{J}_{ij}^{\text{external}} &= -\frac{\partial f_i^{\text{ext}}}{\partial q_j}.\end{aligned}$$

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial}{\partial q_i} E_k^s + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$

$$\frac{\partial^2}{\partial q_i \partial q_j} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^s + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^b + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^t$$

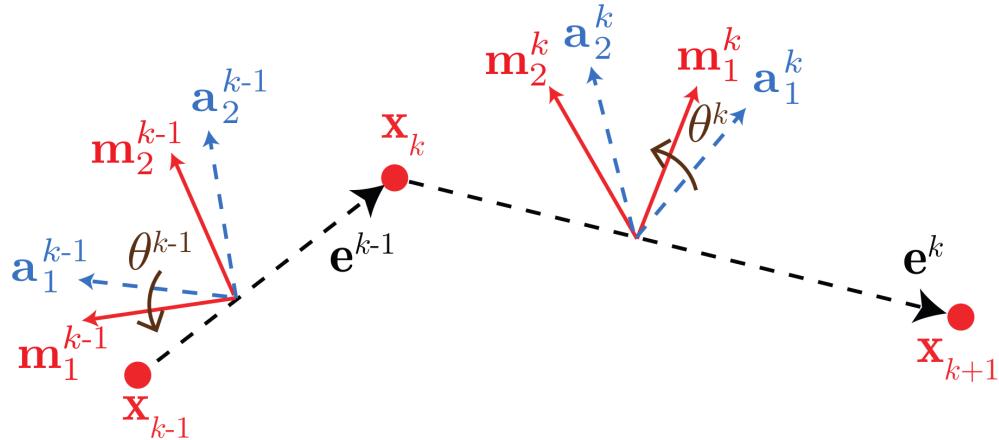


Gradient of Elastic Energy Computation

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \boxed{\frac{\partial}{\partial q_i} E_k^s} + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$

$F \equiv \frac{\partial}{\partial q_i} \rightarrow (4N - 1)$ sized vector

“Big gradient vector” F



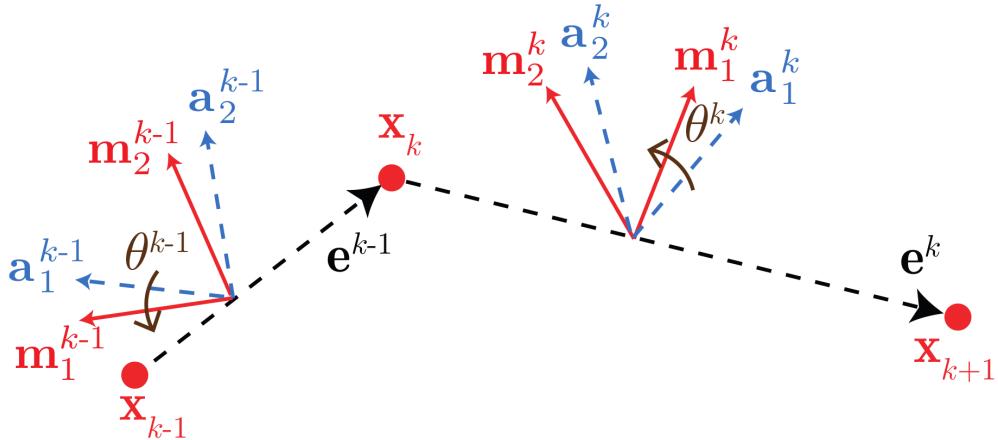


Gradient of Elastic Energy Computation

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \boxed{\frac{\partial}{\partial q_i} E_k^s} + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$

$\mathbf{F} \equiv \frac{\partial}{\partial q_i} \rightarrow (4N - 1)$ sized vector

“Big gradient vector” \mathbf{F}



Stretching energy, E_k^s , only depends on \mathbf{x}_k and \mathbf{x}_{k+1} .

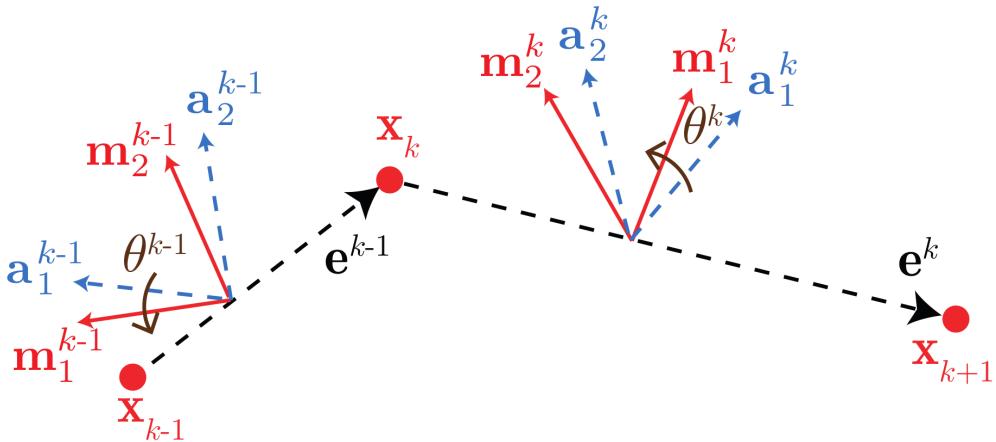
The corresponding indices in the DOF vector are:

$$\text{ind} = [4k - 3, 4k - 2, 4k - 1, 4k + 1, 4k + 2, 4k + 3]$$



Gradient of Elastic Energy Computation

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \boxed{\frac{\partial}{\partial q_i} E_k^s} + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$



Stretching energy, E_k^s , only depends on \mathbf{x}_k and \mathbf{x}_{k+1} .

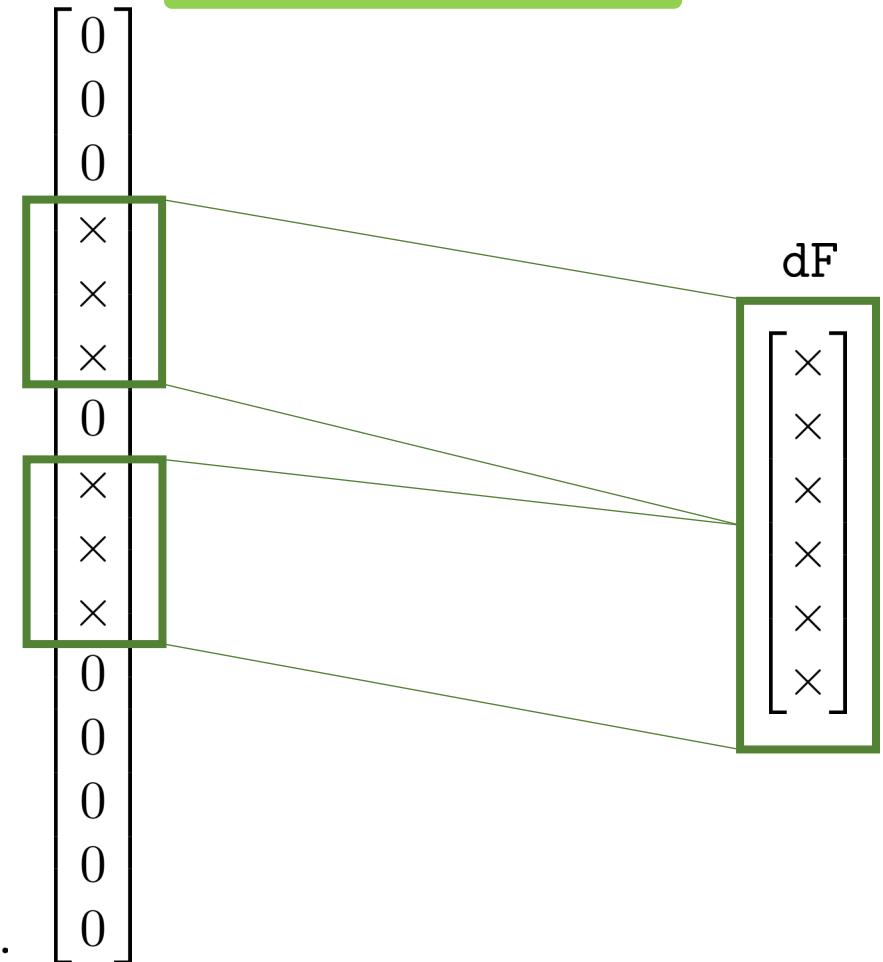
The corresponding indices in the DOF vector are:
 $\text{ind} = [4k - 3, 4k - 2, 4k - 1, 4k + 1, 4k + 2, 4k + 3]$

$\frac{\partial}{\partial q_i} E_k^s$ has 6 non-zero elements.

See Appendix for codes to compute non-zero “small” gradient, dF .

$\mathbf{F} \equiv \frac{\partial}{\partial q_i} \rightarrow (4N - 1)$ sized vector

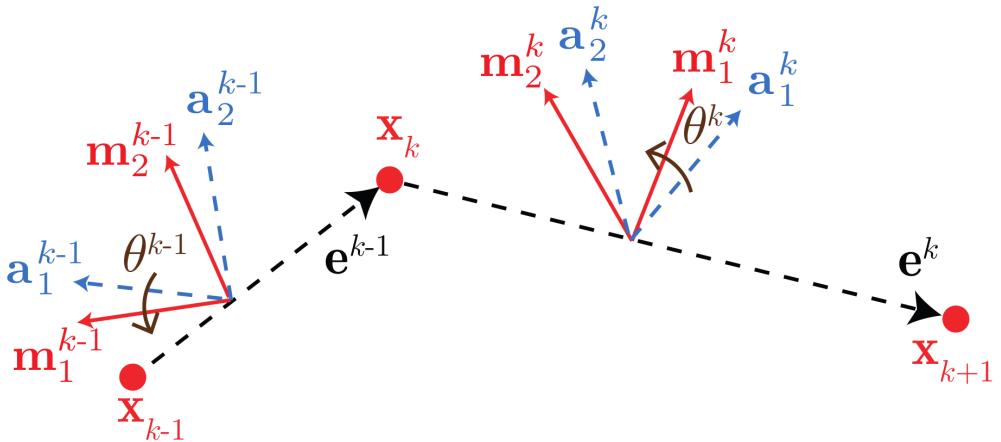
“Big gradient vector” \mathbf{F}





Gradient of Elastic Energy Computation

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \boxed{\frac{\partial}{\partial q_i} E_k^s} + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$



Stretching energy, E_k^s , only depends on \mathbf{x}_k and \mathbf{x}_{k+1} .

The corresponding indices in the DOF vector are:

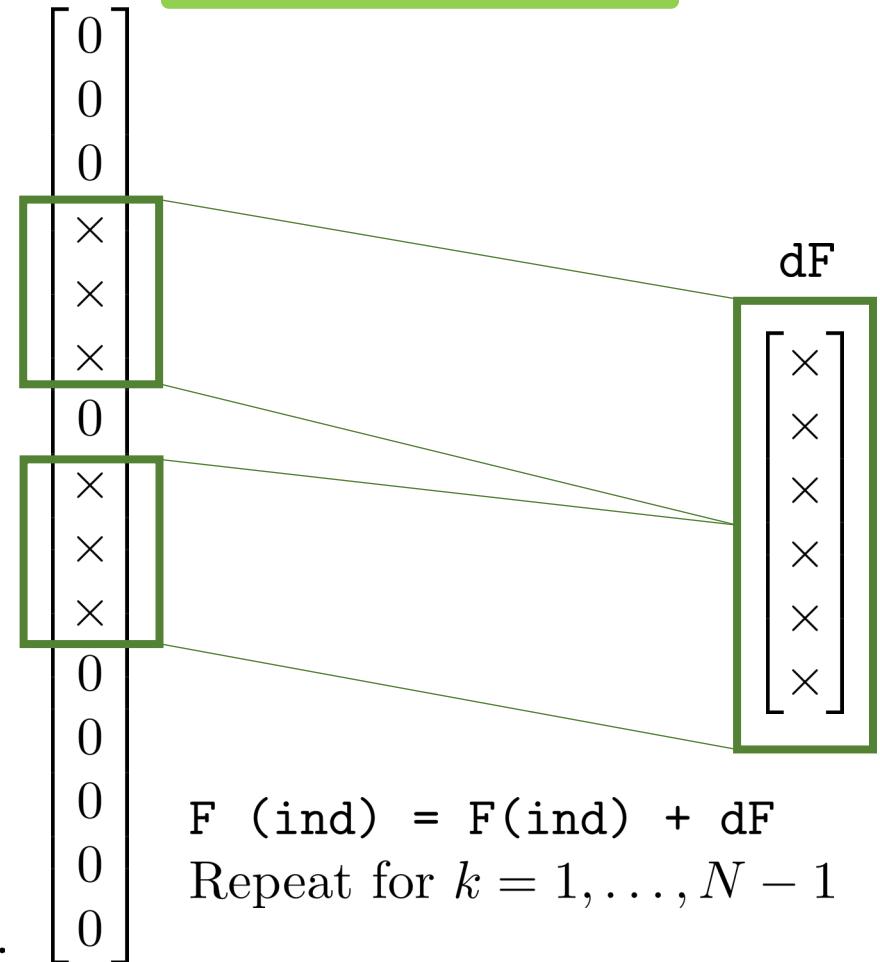
$$\text{ind} = [4k - 3, 4k - 2, 4k - 1, 4k + 1, 4k + 2, 4k + 3]$$

$\frac{\partial}{\partial q_i} E_k^s$ has 6 non-zero elements.

See Appendix for codes to compute non-zero “small” gradient, dF .

$$\mathbf{F} \equiv \frac{\partial}{\partial q_i} \rightarrow (4N - 1) \text{ sized vector}$$

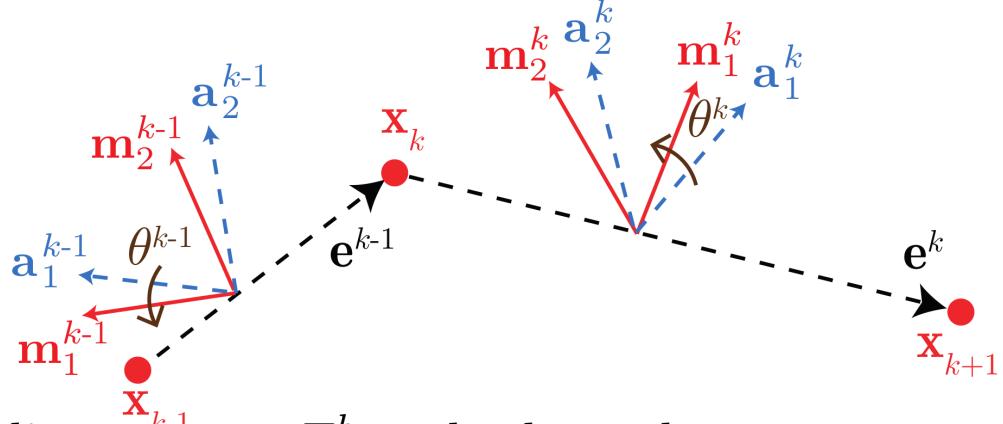
“Big gradient vector” \mathbf{F}





Gradient of Elastic Energy Computation

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial}{\partial q_i} E_k^s + \sum_{k=2}^{N-1} \boxed{\frac{\partial}{\partial q_i} E_k^b} + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$



Bending energy, E_k^b , only depends on $\mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k$, and \mathbf{x}_{k+1} .

The corresponding indices in the DOF vector are:

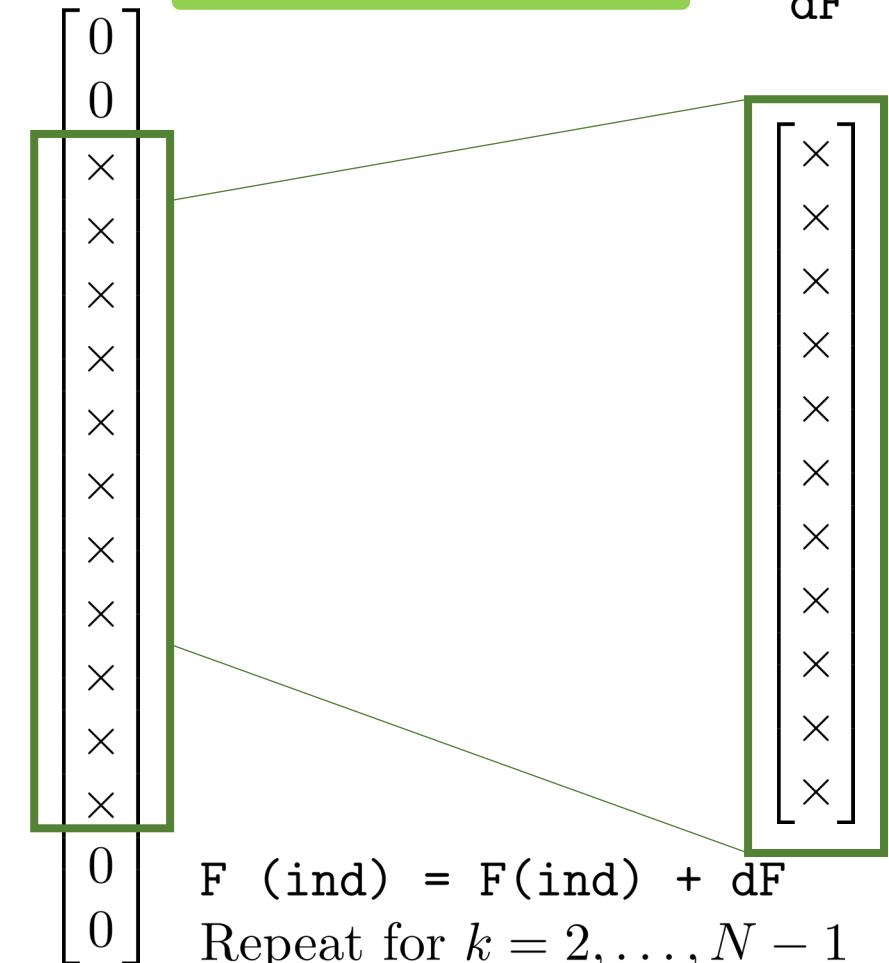
$$\text{ind} = [4k - 7, 4k - 6, 4k - 5, 4k - 4, \\ 4k - 3, 4k - 2, 4k - 1, 4k, 4k + 1, 4k + 2, 4k + 3]$$

$\frac{\partial}{\partial q_i} E_k^b$ has 11 non-zero elements.

See Appendix for codes to compute non-zero “small” gradient, dF .

$\mathbf{F} \equiv \frac{\partial}{\partial q_i} \rightarrow (4N - 1)$ sized vector

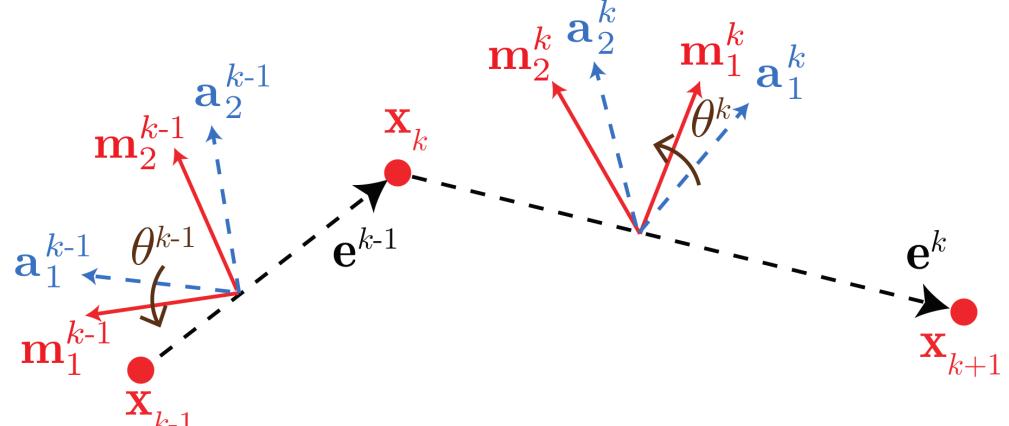
“Big gradient vector” \mathbf{F}





Gradient of Elastic Energy Computation

$$\frac{\partial}{\partial q_i} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial}{\partial q_i} E_k^s + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^b + \sum_{k=2}^{N-1} \frac{\partial}{\partial q_i} E_k^t$$



Twisting energy, E_k^t , only depends on $\mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k$, and \mathbf{x}_{k+1} .

The corresponding indices in the DOF vector are:

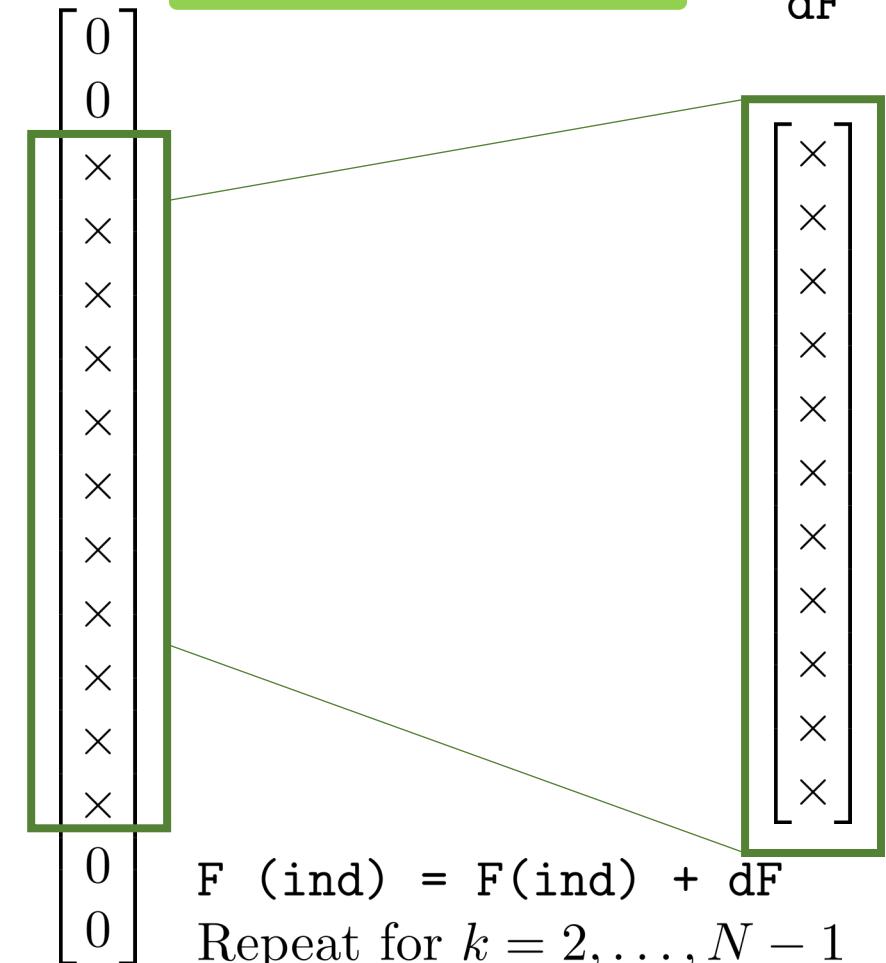
$$\text{ind} = [4k - 7, 4k - 6, 4k - 5, 4k - 4, \\ 4k - 3, 4k - 2, 4k - 1, 4k, 4k + 1, 4k + 2, 4k + 3]$$

$\frac{\partial}{\partial q_i} E_k^t$ has 11 non-zero elements.

See Appendix for codes to compute non-zero “small” gradient, dF .

$\mathbf{F} \equiv \frac{\partial}{\partial q_i} \rightarrow (4N - 1)$ sized vector

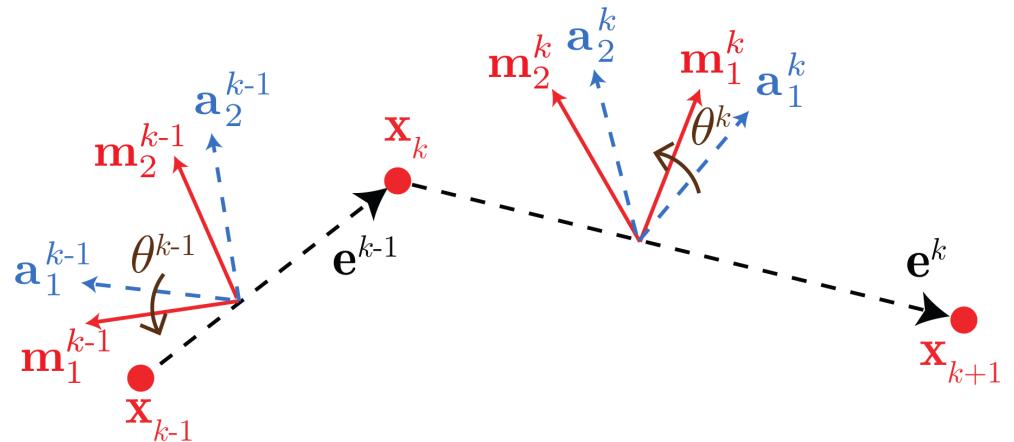
“Big gradient vector” \mathbf{F}





Hessian of Elastic Energy Computation

$$\frac{\partial^2}{\partial q_i \partial q_j} E_{\text{elastic}} = \sum_{k=1}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^s + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^b + \sum_{k=2}^{N-1} \frac{\partial^2}{\partial q_i \partial q_j} E_k^t$$



$J \equiv \frac{\partial}{\partial q_i \partial q_j} E_{\text{elastic}} \rightarrow (4N - 1) \times (4N - 1)$ sized matrix

“Big Hessian matrix” J

Non-zero component of Hessian of discrete energies
Code in Appendix of the Course Notes

$F(\text{ind}) = F(\text{ind}) + dF$

Repeat for $k = 1, \dots, N - 1$ (stretching)

Repeat for $k = 2, \dots, N - 1$ (bending and twisting)

$J(\text{ind}, \text{ind}) = J(\text{ind}, \text{ind}) + dJ$

Repeat for $k = 1, \dots, N - 1$ (stretching)

Repeat for $k = 2, \dots, N - 1$ (bending and twisting)

Pseudocode to compute gradient and Hessian

Algorithm 1 Gradient and Hessian of Elastic Energy in a Rod

Require: $\mathbf{q} = [\mathbf{x}_0, \theta^0, \mathbf{x}_1, \theta^1, \dots, \theta^{N-1}, \mathbf{x}_N]^T$ \triangleright Degrees of Freedom

Require: EA, EI, GJ

Require: \bar{l}_k ($1 \leq k \leq N$) \triangleright Undeformed Voronoi length

Require: $\bar{\mathbf{e}}^k$ ($1 \leq k < N$) \triangleright Undeformed edge length

Require: $\bar{\kappa}_k^0$ ($1 < k < N$) \triangleright Natural curvature

Require: Reference frame, $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$, where $1 \leq k < N$

Require: Reference twist, $\Delta m_{k,\text{ref}}$ ($1 \leq k < N$)

Require: Material frame, $(\mathbf{m}_1^k(t_{j+1}), \mathbf{m}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$, where $1 \leq k < N$

Ensure: \mathbf{F} \triangleright $4N - 1$ sized elastic gradient vector, $\frac{\partial E_{\text{elastic}}}{\partial \mathbf{q}}$

Ensure: \mathbf{J} \triangleright $(4N - 1) \times (4N - 1)$ sized elastic Hessian matrix, $\mathbb{J}_{\text{elastic}}$

Output of the function

```

1: function GRAD_HESS_ELASTIC_ROD(q)
2:   F  $\leftarrow$  zeros(3N, 1)
3:   J  $\leftarrow$  zeros(3N, 3N)
4:   for  $k \leftarrow 1$  to  $N - 1$  do
5:     ind  $\leftarrow$  locations of  $\mathbf{x}_k$  and  $\mathbf{x}_{k+1}$ 
6:     [dF, dJ]  $\leftarrow$  gradEs_hessEs( $\mathbf{x}_k$ ,  $\mathbf{x}_{k+1}$ )
7:     F (ind) = F (ind) + dF
8:     J (ind) = F (ind, ind) + dJ
9:   end for

```

Stretching Energy

```

10:  for  $k \leftarrow 2$  to  $N - 1$  do
11:    ind  $\leftarrow$  locations of  $\mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k$ , and  $\mathbf{x}_{k+1}$ 
12:    [dF, dJ]  $\leftarrow$  gradEb_hessEb( $\mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k, \mathbf{x}_{k+1}$ )
13:    F (ind) = F (ind) + dF
14:    J (ind) = J (ind, ind) + dJ
15:    [dF, dJ]  $\leftarrow$  gradEt_hessEt( $\mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k, \mathbf{x}_{k+1}$ )
16:    F (ind) = F (ind) + dF
17:    J (ind) = J (ind, ind) + dJ
18:  end for
19:  return F and J
20: end function

```

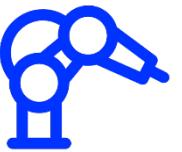
Bending and Twisting Energy

Algorithm 1 Gradient and Hessian of Elastic Energy in a Rod

Require: $\mathbf{q} = [\mathbf{x}_0, \theta^0, \mathbf{x}_1, \theta^1, \dots, \theta^{N-1}, \mathbf{x}_N]^T$ \triangleright Degrees of Freedom
Require: EA, EI, GJ
Require: \bar{l}_k ($1 \leq k \leq N$) \triangleright Undeformed Voronoi length
Require: $\bar{\mathbf{e}}^k$ ($1 \leq k < N$) \triangleright Undeformed edge length
Require: $\bar{\kappa}_k^0$ ($1 < k < N$) \triangleright Natural curvature
Require: Reference frame, $(\mathbf{a}_1^k(t_{j+1}), \mathbf{a}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$, where $1 \leq k < N$
Require: Reference twist, $\Delta m_{k,\text{ref}}$ ($1 \leq k < N$)
Require: Material frame, $(\mathbf{m}_1^k(t_{j+1}), \mathbf{m}_2^k(t_{j+1}), \mathbf{t}^k(t_{j+1}))$, where $1 \leq k < N$
Ensure: \mathbf{F} $\triangleright 4N - 1$ sized elastic gradient vector, $\frac{\partial E_{\text{elastic}}}{\partial \mathbf{q}}$
Ensure: \mathbf{J} $\triangleright (4N - 1) \times (4N - 1)$ sized elastic Hessian matrix, $\mathbb{J}_{\text{elastic}}$

```
1: function GRAD_HESS_ELASTIC_ROD( $\mathbf{q}$ )
2:    $\mathbf{F} \leftarrow \text{zeros}(3N, 1)$ 
3:    $\mathbf{J} \leftarrow \text{zeros}(3N, 3N)$ 
4:   for  $k \leftarrow 1$  to  $N - 1$  do
5:      $\text{ind} \leftarrow \text{locations of } \mathbf{x}_k \text{ and } \mathbf{x}_{k+1}$ 
6:      $[\mathbf{dF}, \mathbf{dJ}] \leftarrow \text{gradEs\_hessEs}(\mathbf{x}_k, \mathbf{x}_{k+1})$ 
7:      $\mathbf{F}(\text{ind}) = \mathbf{F}(\text{ind}) + \mathbf{dF}$ 
8:      $\mathbf{J}(\text{ind}) = \mathbf{F}(\text{ind}, \text{ind}) + \mathbf{dJ}$ 
9:   end for

10:  for  $k \leftarrow 2$  to  $N - 1$  do
11:     $\text{ind} \leftarrow \text{locations of } \mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k, \text{ and } \mathbf{x}_{k+1}$ 
12:     $[\mathbf{dF}, \mathbf{dJ}] \leftarrow \text{gradEb\_hessEb}(\mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k, \mathbf{x}_{k+1})$ 
13:     $\mathbf{F}(\text{ind}) = \mathbf{F}(\text{ind}) + \mathbf{dF}$ 
14:     $\mathbf{J}(\text{ind}) = \mathbf{J}(\text{ind}, \text{ind}) + \mathbf{dJ}$ 
15:     $[\mathbf{dF}, \mathbf{dJ}] \leftarrow \text{gradEt\_hessEt}(\mathbf{x}_{k-1}, \theta^{k-1}, \mathbf{x}_k, \theta^k, \mathbf{x}_{k+1})$ 
16:     $\mathbf{F}(\text{ind}) = \mathbf{F}(\text{ind}) + \mathbf{dF}$ 
17:     $\mathbf{J}(\text{ind}) = \mathbf{J}(\text{ind}, \text{ind}) + \mathbf{dJ}$ 
18:  end for
19:  return  $\mathbf{F}$  and  $\mathbf{J}$ 
20: end function
```



Assignments

- Complete the assignments in Chapter 6: *Discrete Twist* and Chapter 7: *Discrete Elastic Rods Algorithm*