

DEPARTMENT OF MATHEMATICS

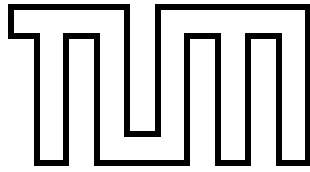
TECHNISCHE UNIVERSITÄT MÜNCHEN

Bachelor Thesis in Mathematics

Discrete Elastic Rods

Andreas Kirsch





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Author: Andreas Kirsch
Supervisor: Prof Dr Springborn
Advisor: Prof Dr Schröder
Date: March 19, 2012



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Munich, March 19, 2012

Andreas Kirsch

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¹in particular Armin and Andy, Henrik, Ben and Max

Abstract

This Bachelor Thesis expands upon the paper “Discrete Elastic Rods” by Miklós Bergou et al, which offers a novel treatment of the simulation of inextensible rods by using discrete differential geometry.

The thesis presents different ways to model a rod in the continuous setting. It describes the discretization and simulation of one model after transferring concepts from differential geometry into a discrete setting and developing a coherent theory therein.

Zusammenfassung

Diese Bachelorarbeit betrachtet das Paper "Discrete Elastic Rods" von Miklós Bergou et al im Detail, welches einen neuen Ansatz bei der Simulation elastischer Stäbe, die nicht dehnbar sind, verfolgt. Dafür wird diskrete Differentialgeometrie verwendet.

Die Arbeit stellt verschieden Arten vor um Stäbe im Kontinuierlichen zu modellieren, und beschreibt dann die Diskretisierung und Simulation eines der Modelle. Hierbei werden Konzepte aus der Differentialgeometrie ins Diskrete übertragen und eine zusammenhängende Theorie daraus entwickelt.

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Introduction

Rods make for fascinating problems: they have captured the minds of many great mathematicians. Even though their geometry is evidently simple to describe and model, they are still in the focus of on-going research in many different areas of science—maybe this is what makes them enticing.

They have accompanied the rise of natural sciences with Galileo, Bernoulli and Euler as elastica problems: the analysis of thin strips which are only bent and not twisted¹. And while rods have mainly been of interest to engineers and physicists in the last century or so, in the last decades they have seen a renaissance in computer science².

The advancements in modern computer technology allow us to calculate and simulate many physical phenomena that are impossible, or impossibly obnoxious, to analyze by hand. Or were unthinkable half a century ago. Statics software analyzes the response of bridges and buildings made out of steel rods to catastrophic events, and animated movies show off millions of strands of rendered, virtual hair, which realistically move around or flow in the (virtual) wind.

The last example is of particular interest to me. This new entertainment branch of rod simulation is a hot topic in computer graphics at the moment, and in 2008 Miklós Bergou and his co-authors released a paper called ‘Discrete Elastic Rods’ ([BWR⁺08]), which discretizes the rod problem in an elegant manner using concepts from Discrete Differential Geometry.

This thesis I am going to present the content of their research in this thesis, and I will explain the mathematical background in more detail than they could in their short paper.

As they did, I try to deal with this geometric topic in a geometric fashion and use intuitive concepts where possible.

The paper makes use of some more abstract and advanced concepts to prove certain properties and formulas, but I am going to stay basic, and try to be self-contained, while I will touch many different topics in my search to tie continuous and discrete geometry together.

Layout I alternate between the presentation of generic mathematical concepts which I need and specific explanations that concern the modeling or simulation of continuous and discrete rods.

¹see [Lev08]

²see [AP10]

You will find some proofs in the appendix, because I think that understanding them does not help you understand the rest of this thesis. But they are included for completeness' sake nevertheless—and as reference.

Mathematical foundations

2.1 Preliminaries

Notation 2.1. $\mathbf{a} \cdot \mathbf{b}$ is the **dot/scalar/inner product** of two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$: $\mathbf{a} \cdot \mathbf{b} := \mathbf{a}^T \mathbf{b}$, and $\mathbf{a}^2 = \mathbf{a} \cdot \mathbf{a} = \|\mathbf{a}\|^2$.

Remark 2.2. The identity $(S\mathbf{a}) \cdot \mathbf{b} = \mathbf{a}^T S^T \mathbf{b} = \mathbf{a}^T S^{-1} \mathbf{b} = \mathbf{a} \cdot (S^{-1} \mathbf{b})$ for $S \in O(3)$ is important. I also use the identity $\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos \angle(\mathbf{a}, \mathbf{b})$.

Notation 2.3. The standard unit vectors in \mathbb{R}^3 are denoted by $\mathbf{e}_1, \mathbf{e}_2$ and \mathbf{e}_3 .

Notation 2.4. $f' := \frac{d}{ds} f$ and $\dot{f} := \frac{d}{dt} f$.

Notation 2.5. When \mathbf{a} and \mathbf{b} are colinear, ie equal up to a scalar factor, I write $\mathbf{a} \sim \mathbf{b}$ or $\mathbf{a} \parallel \mathbf{b}$.

Notation 2.6. I is always an interval in \mathbb{R} .

2.2 Cross product and skew-symmetric matrices

Motivation The cross product is usually only quickly introduced in Linear Algebra lectures without giving many details or useful properties for calculations. The cross product and skew-symmetric matrices are important for the formulation of the derivative of a rotation matrix, that is a matrix $\in SO(3)$, and thus for working with frames later.

Definition 2.7. The cross product $\times : \mathbb{R}^3 \times \mathbb{R}^3$ of two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$ is defined as

$$\mathbf{a} \times \mathbf{b} = \begin{pmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{pmatrix}. \quad (2.7.1)$$

Proposition 2.8. The map $\mathbb{R}^3 \rightarrow \mathbb{R}^3 : \mathbf{w} \mapsto \mathbf{v} \times \mathbf{w}$ is linear:

$$\mathbf{v} \times \mathbf{w} = [\mathbf{v}] \mathbf{w} \text{ with } [\mathbf{v}] := \begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix} \quad (2.8.1)$$

Proof. This is verified by direct calculation. □

Definition 2.9. $so(3) := \{A \in \mathbb{R}^{3 \times 3} : A + A^T = 0\}$

Proposition 2.10. *The map $\mathbb{R}^3 \rightarrow so(3)$, $v \mapsto [v]$ is an isomorphism and $\mathbb{R}^3 \cong so(3)$.*

Proof from [Arn89]. The map is obviously linear. We have $\dim [\mathbb{R}^3] = 3 = \dim so(3)$, as you can see by inserting the unit vectors into the map. Hence the map is bijective, an isomorphism, and $[\mathbb{R}^3] = so(3)$. \square

Remark 2.11. The following calculation rules follow from the last lemma and its proof. I state them explicitly here, because I will use $[\cdot]$ a lot: $[v] + [w] = [v + w]$, $\alpha[v] = [\alpha v]$, $[v] = [w] \Leftrightarrow v = w$

Theorem 2.12. *Some useful properties of the cross product are (for $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d} \in \mathbb{R}^3$; $M \in GL(3)$; $R \in SO(3)$):*

- (a) $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \det \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} \end{pmatrix}$;
- (b) $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})$;
- (c) $\mathbf{a} \cdot (\mathbf{a} \times \mathbf{b}) = 0$ and $\mathbf{b} \cdot (\mathbf{a} \times \mathbf{b}) = 0$;
- (d) $(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c}) \cdot (\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d}) \cdot (\mathbf{b} \cdot \mathbf{c})$;
- (e) $\mathbf{a} \parallel \mathbf{b} \iff \mathbf{a} \times \mathbf{b} = 0$;
- (f) $M\mathbf{a} \times M\mathbf{b} = (\det M) M^{-T} (\mathbf{a} \times \mathbf{b})$;
- (g) $R\mathbf{a} \times R\mathbf{b} = R(\mathbf{a} \times \mathbf{b})$; and
- (h) $\mathbf{a} \parallel \mathbf{b} \times \mathbf{c} \iff \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \|\mathbf{a}\| \|\mathbf{b}\| \|\mathbf{c}\| \sin \angle^{\circ \mathbf{a}}(\mathbf{b}, \mathbf{c})$,

where $\angle^{\circ \mathbf{a}}(\mathbf{b}, \mathbf{c})$ is the angle between \mathbf{b} and \mathbf{c} with sense of rotation determined by \mathbf{a} .

Proof. (a) and (d) are verified by direct calculation¹. (b) follows from (a) and column swapping. (c) follows directly from (a).

For (e), the “ \Rightarrow ” part is trivial. For “ \Leftarrow ”, we use (a), respectively (b), and notice that from $\forall \mathbf{c} \in \mathbb{R}^3 : 0 = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}) = \det \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} \end{pmatrix}$ implies that \mathbf{a} and \mathbf{b} must already be linear dependent, ie colinear.

For (f) we set $\mathbf{c} = M\mathbf{a} \times M\mathbf{b}$. Assuming $\mathbf{a} \neq \mathbf{b}$ we have:

$$\begin{aligned} \mathbf{c} \cdot M\mathbf{a} = 0 \wedge \mathbf{c} \cdot M\mathbf{b} = 0 &\iff M^T \mathbf{c} \cdot \mathbf{a} = 0 \wedge M^T \mathbf{c} \cdot \mathbf{b} = 0 \implies M^T \mathbf{c} \parallel \mathbf{a} \times \mathbf{b} \\ &\implies \exists \lambda \in \mathbb{R} : M^T \mathbf{c} = \lambda (\mathbf{a} \times \mathbf{b}) \\ &\implies M^T \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}) = \lambda (\mathbf{a} \times \mathbf{b})^2 \end{aligned} \quad (2.12.1)$$

$$\begin{aligned} M^T \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}) &= M^T (M\mathbf{a} \times M\mathbf{b}) \cdot (\mathbf{a} \times \mathbf{b}) = (M\mathbf{a} \times M\mathbf{b}) \cdot M(\mathbf{a} \times \mathbf{b}) \\ &= \det \begin{pmatrix} M(\mathbf{a} \times \mathbf{b}) & M\mathbf{a} & M\mathbf{b} \end{pmatrix} \\ &= \det M \det \begin{pmatrix} \mathbf{a} \times \mathbf{b} & \mathbf{a} & \mathbf{b} \end{pmatrix} = \det M (\mathbf{a} \times \mathbf{b})^2 \end{aligned} \quad (2.12.2)$$

$$\implies \lambda = \det M \implies M^T \mathbf{c} = \det M (\mathbf{a} \times \mathbf{b}) \iff \mathbf{c} = (\det M) M^{-T} (\mathbf{a} \times \mathbf{b}) \quad (2.12.3)$$

(g) follows directly from (f). And for (h), see [Len11]. \square

Corollary 2.13. *For $R \in SO(3)$; $\mathbf{a} \in \mathbb{R}^3$: $[R\mathbf{a}] = R[\mathbf{a}]R^{-1}$*

Proof. $\forall \mathbf{b} \in \mathbb{R}^3 : [R\mathbf{a}]\mathbf{b} = R\mathbf{a} \times \mathbf{b} = R\mathbf{a} \times RR^{-1}\mathbf{b} = R(\mathbf{a} \times R^{-1}\mathbf{b}) = R([\mathbf{a}]R^{-1}\mathbf{b})$ \square

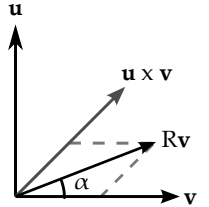
¹for (a) you can also check that the left-hand side is a determinant function and $\mathbf{e}_1 \cdot (\mathbf{e}_2 \times \mathbf{e}_3) = 1$ and since the determinant is uniquely identified the statement follows.

2.3 Rotation matrices and $SO(3)$

Motivation Rotation matrices and some basic properties of $SO(3)$ will be used throughout the text. I give a short introduction, see [Fis10] for more details.

Definition 2.14. A *rotation* $R = R_{\mathbf{u}, \alpha}$ is determined by a *rotation axis* $\mathbf{u} \in S^2$ (ie $\|\mathbf{u}\| = 1$) and a *rotation angle* α . It is a linear map $R \in SO(3)$ which maps \mathbf{u} to itself: $R\mathbf{u} = \mathbf{u}$; and a vector \mathbf{v} perpendicular to \mathbf{u} , $\mathbf{v} \perp \mathbf{u}$, to

$$R\mathbf{v} = \mathbf{v} \cos \alpha + (\mathbf{u} \times \mathbf{v}) \sin \alpha. \quad (2.14.1)$$



Remark 2.15. For $0 \neq \mathbf{u} \notin S^2$, $R_{\mathbf{u}, \alpha} := R_{\frac{\mathbf{u}}{\|\mathbf{u}\|}, \alpha}$; and $R_{0, \alpha} := \text{Id}_3$.

Remark 2.16. This definition is not one-to-one. You can quickly check this by verifying $R_{\mathbf{u}, \alpha + 2k\pi} = R_{\mathbf{u}, \alpha} = R_{-\mathbf{u}, -\alpha}$.

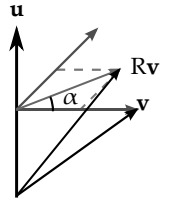
Remark 2.17. $\mathbf{v} \perp \mathbf{u} \implies R\mathbf{v} \perp \mathbf{u}$

Remark 2.18. Rotations around the same axis are additive: $R_{\mathbf{u}, \alpha} R_{\mathbf{u}, \beta} = R_{\mathbf{u}, \alpha + \beta}$. You can verify this by symbolically calculating $R_{\mathbf{u}, \alpha} R_{\mathbf{u}, \beta} \mathbf{v}$ and using the trigonometric addition identities to obtain $R_{\mathbf{u}, \alpha + \beta} \mathbf{v}$.

Remark 2.19. $R_{\mathbf{u}, \alpha} R_{\mathbf{u}, -\alpha} = R_{\mathbf{u}, 0} = \text{Id}_3$ and $R^{-1} = R_{\mathbf{u}, -\alpha}$.

Remark 2.20. From the definition we can infer the rotation of arbitrary \mathbf{v} :

$$\begin{aligned} R\mathbf{v} &= (\mathbf{v} \cdot \mathbf{u}) \mathbf{u} + (\mathbf{v} - (\mathbf{v} \cdot \mathbf{u}) \mathbf{u}) \cos \alpha + (\mathbf{u} \times (\mathbf{v} - (\mathbf{v} \cdot \mathbf{u}) \mathbf{u})) \sin \alpha \\ &= (\mathbf{v} \cdot \mathbf{u}) \mathbf{u} + (\mathbf{v} - (\mathbf{v} \cdot \mathbf{u}) \mathbf{u}) \cos \alpha + (\mathbf{u} \times \mathbf{v}) \sin \alpha \\ &= \cos \alpha \mathbf{v} + (1 - \cos \alpha) (\mathbf{v} \cdot \mathbf{u}) \mathbf{u} + \sin \alpha (\mathbf{u} \times \mathbf{v}). \end{aligned} \quad (2.20.1)$$



Theorem 2.21. $R \in SO(3)$, if and only if R is a rotation.

Proof. See [Fis10] or [MR99, chapter 9.2]. □

Corollary 2.22. $SO(3) \cong \{\mathbf{u} \in \mathbb{R}^3 : \|\mathbf{u}\| \leq \pi\}$ with antipodal points identified. $\mathbf{u} \mapsto R_{\frac{\mathbf{u}}{\|\mathbf{u}\|}, \|\mathbf{u}\|}$ is the corresponding isomorphism.

Proof. See [Fra12, p 18]. □

Remark 2.23. This means that all rotations—with the exception of rotations by π and the identity rotation—uniquely determine their rotation axis $\mathbf{u} \in S^2$ and their rotation angle $\alpha \in (0, \pi)$. A rotation by π can only have rotation axes \mathbf{u} or $-\mathbf{u}$, and the identity rotation is only ambiguous because of my definition which separates direction and angle.

Proposition 2.24 (Rotation from axis and two points). A rotation $R = R_{\mathbf{u}, \alpha}$ is uniquely identified by its rotation axis \mathbf{u} ($\|\mathbf{u}\| = 1$) and the image $R\mathbf{v}$ of a single vector \mathbf{v} that does not lie on the rotation axis ($\mathbf{v} \nparallel \mathbf{u} \iff \mathbf{v} \times \mathbf{u} \neq 0$).

If additionally $\mathbf{v} \perp \mathbf{u}$, then $\alpha = \angle^{\circ \mathbf{u}}(\mathbf{v}, R\mathbf{v})$.

Proof. Applying $\cdot (\mathbf{u} \times \mathbf{v})$ on both sides of (2.20.1), we obtain

$$R\mathbf{v} \cdot (\mathbf{u} \times \mathbf{v}) = 0 + 0 + \sin \alpha \|\mathbf{u} \times \mathbf{v}\|^2 = \sin \alpha \|\mathbf{u} \times \mathbf{v}\|^2. \quad (2.24.1)$$

Since $\mathbf{u} \times \mathbf{v} \neq 0$, we can solve for $\sin \alpha$ with $\alpha \in [0, 2\pi)$. To discern $\alpha = 0$ and $\alpha = \pi$, we only have to check whether $R\mathbf{v} = \mathbf{v}$ or not. Then $R = R_{\mathbf{u}, \alpha}$.

Now let $\mathbf{v} \perp \mathbf{u}$. Then $\mathbf{u} \parallel \mathbf{v} \times R\mathbf{v}$ because $\mathbf{v} \perp \mathbf{u}$ and $R\mathbf{v} \perp \mathbf{u}$, and we have

$$\sin \alpha = \frac{R\mathbf{v} \cdot (\mathbf{u} \times \mathbf{v})}{\|\mathbf{u} \times \mathbf{v}\|^2} = \frac{\mathbf{u} \cdot (\mathbf{v} \times R\mathbf{v})}{\|\mathbf{u}\|^2 \|\mathbf{v}\|^2} = \frac{\|\mathbf{v}\| \|R\mathbf{v}\| \sin \angle(\mathbf{v}, R\mathbf{v})}{\|\mathbf{v}\|^2} = \sin \angle^{\circ \mathbf{u}}(\mathbf{v}, R\mathbf{v}). \quad (2.24.2) \quad \square$$

Proposition 2.25 (Rotation axis characterization). *If $R\mathbf{v} = \mathbf{v}$ holds for a rotation $R \in SO(3)$ and a vector $\mathbf{v} \in \mathbb{R}^3$, \mathbf{v} lies on the rotation axis or R is the identity map.*

Proof. Assuming $R \neq \text{Id}_3$, $R = R_{\mathbf{u}, \alpha}$ for some $\mathbf{u} \in S^2$ and $\alpha \in (0, \pi]$, we obtain from

$$\mathbf{v} = \cos \alpha \mathbf{v} + (1 - \cos \alpha) (\mathbf{v} \cdot \mathbf{u}) \mathbf{u} + \sin \alpha (\mathbf{u} \times \mathbf{v}) \quad (2.25.1)$$

that

$$0 = \mathbf{v} \cdot (\mathbf{u} \times \mathbf{v}) = 0 + 0 + \sin \alpha (\mathbf{u} \times \mathbf{v}) \cdot (\mathbf{u} \times \mathbf{v}) = \sin \alpha \|\mathbf{u} \times \mathbf{v}\|^2 \quad (2.25.2)$$

for $\alpha \neq \pi$. Hence we have $\sin \alpha \neq 0$, and thus $\mathbf{u} \times \mathbf{v} = 0$ must hold, that is $\mathbf{u} \parallel \mathbf{v}$. For $\alpha = \pi$, we obtain that $\mathbf{v} = -\mathbf{v} + 2(\mathbf{v} \cdot \mathbf{u})\mathbf{u} + 0 \iff 2\mathbf{v} = 2(\mathbf{v} \cdot \mathbf{u})\mathbf{u} \implies \mathbf{v} \parallel \mathbf{u}$. \square

Proposition 2.26 (Rotation axes plane). *If $R\mathbf{v} = \mathbf{w}$ holds for a rotation $R = R_{\mathbf{u}, \alpha} \in SO(3)$, then $\mathbf{u} \perp \mathbf{w} - \mathbf{v}$, ie $(\mathbf{w} - \mathbf{v}) \cdot \mathbf{u} = 0$.*

Proof. With $R\mathbf{u} = \mathbf{u} \iff \mathbf{u} = R^{-1}\mathbf{u}$:

$$(\mathbf{w} - \mathbf{v}) \cdot \mathbf{u} = \mathbf{w} \cdot \mathbf{u} - \mathbf{v} \cdot \mathbf{u} = \mathbf{w} \cdot \mathbf{u} - \mathbf{v} \cdot R^{-1}\mathbf{u} = \mathbf{w} \cdot \mathbf{u} - R\mathbf{v} \cdot \mathbf{u} = \mathbf{w} \cdot \mathbf{u} - \mathbf{w} \cdot \mathbf{u} = 0 \quad (2.26.1) \quad \square$$

2.3.1 Continuous rotations

Definition 2.27. *A continuous rotation R is a sufficiently smooth function $R : I \rightarrow SO(3)$, $t \mapsto R(t)$.*

Theorem 2.28. *The derivative \dot{R} of a continuous rotation can be expressed as*

$$\dot{R} = [\boldsymbol{\omega}] R. \quad (2.28.1)$$

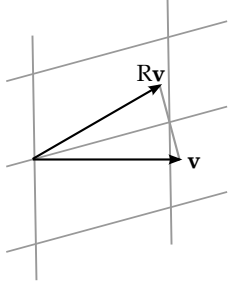
$\boldsymbol{\omega}$ is called the **angular velocity** of R and is uniquely determined by this equation.

Proof. See [Arn89, p 126/127]. \square

Remark 2.29. When I take the spatial derivative R' of a continuous rotation $R(l)$, I write

$$R' = [\mathbf{u}] R. \quad (2.29.1)$$

\mathbf{u} is called the **Darboux vector**. The Darboux vector is the spatial equivalent of the (temporal) angular velocity. I am making this distinction here in line with [BWR⁺08], [ST07] and [BAV⁺10].



The angular velocity ω describes the instantaneous rotation in *global* coordinates. We can express it using local coordinates, too—that is in the coordinate system defined by R :

Corollary 2.30.

$$\dot{R} = R[\hat{\omega}] \text{ with } \hat{\omega} := R^{-1}\omega \iff \omega = R\hat{\omega}. \quad (2.30.1)$$

Proof.

$$\dot{R} = [\omega]R = RR^{-1}[\omega]R = R[R^{-1}\omega] \quad (2.30.2)$$

□

Remark 2.31. If we write $R = \begin{pmatrix} r_0 & r_1 & r_2 \end{pmatrix}$, we can see that the components $\hat{\omega}_k$ describe the angular velocity of infinitesimal rotations around the axes r_i . I call $\hat{\omega}$ the **local angular velocity**.

Remark 2.32. The same holds for Darboux vectors u and **local Darboux vectors** \hat{u} , too.

Theorem 2.33. *If R is a continuous rotation with angular velocity ω , then the derivative of the inverse rotation R^{-1} is*

$$\dot{R}^{-1} = [\alpha]R^{-1} = R^{-1}[\hat{\alpha}] \text{ with } \alpha := -R^{-1}\omega \text{ and } \hat{\alpha} = -\omega \quad (2.33.1)$$

Proof. From $R^{-1}R = \text{Id}_3$ we obtain $\dot{R}^{-1}R + R^{-1}\dot{R} = 0$. With $\dot{R} = [\omega]R$ this becomes

$$\dot{R}^{-1}R + R^{-1}[\omega]R = 0 \iff \dot{R}^{-1}R = -[R^{-1}\omega] \iff \dot{R}^{-1} = [-R^{-1}\omega]R^{-1}. \quad (2.33.2)$$

We compare with $\dot{R}^{-1} = [\alpha]R^{-1}$ and conclude $\alpha = -R^{-1}\omega$.

For $\hat{\alpha}$ we obtain $\hat{\alpha} = (R^{-1})^{-1}\alpha = -RR^{-1}\omega = -\omega$. □

Theorem 2.34. *The derivative of the uniform rotation $R : \mathbb{R} \rightarrow SO(3), t \mapsto R_{u,\alpha t}$ is*

$$\dot{R} = [\alpha u]R = R[\alpha u] \quad (2.34.1)$$

Proof sketch.

$$\begin{aligned} \dot{R}(t)R^{-1}(t)v &= \lim_{\epsilon \rightarrow 0} \frac{R(t+\epsilon) - R(t)}{\epsilon} R^{-1}(t)v = \lim_{\epsilon \rightarrow 0} \frac{R(\epsilon) - \text{Id}_3}{\epsilon} v = \dots = \alpha(u \times v) = [\alpha u]v \\ \iff \dot{R}(t) &= [\alpha u]R(t) = R(t)[R^{-1}(t)\alpha u] = R(t)[\alpha u] \end{aligned} \quad \square$$

Remark 2.35 (Chain rule). $\frac{d}{dt}(R_{u,\alpha(t)}) = \frac{d}{dt}(R_{u,\bullet} \circ \alpha) = R_{u,\alpha(t)}[u]\dot{\alpha}(t)$

Remark 2.36 (Uniqueness). $R : \mathbb{R} \rightarrow SO(3), t \mapsto R_{u,\alpha t}$ with $u \in S^2$ is the unique solution of the ODE $R' = [\alpha u]R$, $R(0) = \text{Id}_3$

Corollary 2.37. *For $R_{u,\alpha}, T \in SO(3): TR_{u,\alpha}T^{-1} = R_{Tu,\alpha}$.*

Proof. Look at the uniform rotation $R : \mathbb{R} \rightarrow SO(3), t \mapsto R_{u,\alpha t}$. Then $R(1) = R_{u,\alpha}$. The derivative of TRT^{-1} is

$$\frac{d}{dt}(TRT^{-1}) = T[\alpha u]RT^{-1} = T[\alpha u]T^{-1}TRT^{-1} \stackrel{(2.13)}{=} [\alpha Tu](TRT^{-1}). \quad (2.37.1)$$

With $(TRT^{-1})(0) = \text{Id}_3$ and $Tu \in S^2$, remark 2.36 implies $TRT^{-1} = R_{Tu,\alpha}$. And thus $R_{Tu,\alpha} = TR_{u,\alpha}T^{-1} = (TRT^{-1})(1) = TR_{u,\alpha}T^{-1}$. □

2.3.2 Rotations using the Cayley transform

Theorem 2.38 (Cayley transform). For $\mathbf{u} \in S^2$, $\alpha \in (-\pi, \pi)$:

$$\tilde{\mathbf{u}} := \tan \frac{\alpha}{2} \mathbf{u} \quad (2.38.1)$$

$$(\text{Id}_3 - [\tilde{\mathbf{u}}])^{-1} (\text{Id}_3 + [\tilde{\mathbf{u}}]) = R_{\mathbf{u}, \alpha} \quad (2.38.2)$$

Proof. See appendix A.1 on page 47 for the proof. \square

Notation 2.39. For $\tilde{\mathbf{u}} \in \mathbb{R}^3$, the **Cayley rotation** $R_{\tilde{\mathbf{u}}}$ for $\tilde{\mathbf{u}}$ is

$$R_{\tilde{\mathbf{u}}} := \left(\text{Id}_3 - \frac{1}{2} [\tilde{\mathbf{u}}] \right)^{-1} \left(\text{Id}_3 + \frac{1}{2} [\tilde{\mathbf{u}}] \right) \quad (2.39.1)$$

Remark 2.40. Note that I have inserted $\frac{1}{2}$ in front of the skew-symmetric matrices. This simplifies the formulas in the discrete model later on.

Corollary 2.41. For $\mathbf{u} \in S^2$, $\alpha \in \mathbb{R} \setminus \pi(2\mathbb{Z} + 1)$

$$R_{\mathbf{u}, \alpha} = R_{2 \tan \frac{\alpha}{2} \mathbf{u}}. \quad (2.41.1)$$

Corollary 2.42. For $T \in SO(3)$:

1. $R_{\tilde{\mathbf{u}}}^{-1} = R_{-\tilde{\mathbf{u}}}$
2. $TR_{\tilde{\mathbf{u}}}T^{-1} = R_{T\tilde{\mathbf{u}}}$

2.4 Quaternions

Motivation Rotations can be expressed through quaternions. See [Ebe10, chapter 10] and [Hof09] for an introduction. I am only going to cover their basic properties and how to use them to express rotations.

Definition 2.43. An *associative normed division algebra* over \mathbb{R} is a normed vector space with the following properties:

1. it has a bilinear and associative (outer) vector product \cdot ; and
2. it has unique inverses for the vector product (except for the zero element); and
3. the norm and the outer product are compatible, ie $\|\mathbf{p} \cdot \mathbf{q}\| = \|\mathbf{p}\mathbf{q}\| = \|\mathbf{p}\| \|\mathbf{q}\|$

Remark 2.44. You can see from the vector space axioms that the vector product is also automatically distributive.

Definition 2.45. The set of *quaternions* \mathbb{H} can be identified with \mathbb{R}^4 . For $\mathbf{q} \in \mathbb{H}$, I write $\mathbf{q} = \begin{pmatrix} s_q \\ \mathbf{v}_q \end{pmatrix} = s_q + \mathbf{v}_q$ with $s_q \in \mathbb{R}$ and $\mathbf{v}_q \in \mathbb{R}^3$.

Remark 2.46. I identify vectors $\mathbf{v} \in \mathbb{R}^3$ with quaternions $\mathbf{v} = 0 + \mathbf{v}$ when needed.

Theorem 2.47. \mathbb{H} forms an associative normed division algebra with the following operations (for $\mathbf{p}, \mathbf{q} \in \mathbb{H}; \lambda \in \mathbb{R}$):

1. component-wise addition and scalar multiplication

$$\mathbf{p} + \mathbf{q} := (a + \mathbf{v}) + (b + \mathbf{w}) = (a + b) + (\mathbf{v} + \mathbf{w}) = \begin{pmatrix} a + b \\ \mathbf{v} + \mathbf{w} \end{pmatrix} \quad (2.47.1)$$

$$\lambda \mathbf{p} := \lambda a + \lambda \mathbf{v} \quad (2.47.2)$$

2. an outer product

$$\mathbf{p}\mathbf{q} = (a + \mathbf{v})(b + \mathbf{w}) := ab - \mathbf{v} \cdot \mathbf{w} + a\mathbf{w} + b\mathbf{v} + \mathbf{v} \times \mathbf{w} \quad (2.47.3)$$

3. the Euclidean norm on \mathbb{R}^4

$$\|\mathbf{p}\|^2 := a^2 + \mathbf{v}^2 \quad (2.47.4)$$

4. the inverse \mathbf{p}^{-1} and the **conjugate** \mathbf{p}^* (for $\mathbf{p} \neq 0$)

$$\mathbf{p}^* = (a + \mathbf{v})^* = \begin{pmatrix} a \\ \mathbf{v} \end{pmatrix}^* := \begin{pmatrix} a \\ -\mathbf{v} \end{pmatrix} = a - \mathbf{v} \quad (2.47.5)$$

$$\mathbf{p}^{-1} := \frac{\mathbf{p}^*}{\|\mathbf{p}\|^2} \quad (2.47.6)$$

Proof sketch. \mathbb{H} obviously forms a vector space with this addition and scalar multiplication. You can easily check that the outer product is distributive, associative and non-commutative. \square

Remark 2.48. Now it is clear that \mathbb{H} can be identified with \mathbb{R}^4 by choosing an appropriate basis and \mathbb{R}^3 is isomorph to a subspace of \mathbb{H} .

Theorem 2.49. Every (rotation) $R \in SO(3)$ can be described by a conjugate multiplication with a unit quaternion \mathbf{q} . Let R be a rotation around the rotation axis $\mathbf{u} \in S^2$ and the amount of rotation (in radians) be α . With

$$\mathbf{q} = \cos\left(\frac{\alpha}{2}\right) + \sin\left(\frac{\alpha}{2}\right) \mathbf{u} \quad (2.49.1)$$

we have a different formula to rotate vectors \mathbf{v} by R :

$$R\mathbf{v} = \mathbf{q}\mathbf{v}\mathbf{q}^{-1} = \mathbf{q}\mathbf{v}\mathbf{q}^* \quad (2.49.2)$$

with $\mathbf{q}^{-1} = \mathbf{q}^*$, because \mathbf{q} is a unit quaternion.

Proof. See [Ebe10] for the proof. \square

Corollary 2.50. A rotation around $\mathbf{u} \in S^2$ by α radians, can also be written with a vector $\tilde{\mathbf{u}}$

$$\tilde{\mathbf{u}} := 2 \tan \frac{\alpha}{2} \mathbf{u} \quad (2.50.1)$$

using

$$R\mathbf{v} = \left(1 + \frac{\tilde{\mathbf{u}}}{2}\right) \mathbf{v} \left(1 + \frac{\tilde{\mathbf{u}}}{2}\right)^{-1} \quad (2.50.2)$$

Proof. $1 + \frac{\tilde{\mathbf{u}}}{2} = 1 + \tan \frac{\alpha}{2} \mathbf{u} = \cos \frac{\alpha}{2} \left(\cos \frac{\alpha}{2} + \sin \frac{\alpha}{2} \mathbf{u} \right) = \cos \frac{\alpha}{2} \mathbf{q}$ The rest follows by substituting the right-hand side into (2.50.2). \square

Remark 2.51. Note the similarity to the Cayley transform (theorem 2.38 on page 8).

Proposition 2.52 (conjugation calculus). For $p, q \in \mathbb{H}; \alpha \in \mathbb{R}$, conjugation:

1. is linear:

$$(p + q)^* = p^* + q^* \quad (2.52.1)$$

$$(\alpha p)^* = \alpha p^* \quad (2.52.2)$$

2. reverses order of products: $(pq)^* = q^* p^*$

3. preserves the norm: $\|p^*\| = \|p\|$

Proof. This follows directly from the definitions. □

2.5 Curves

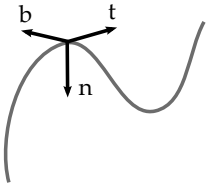
Motivation Before I introduce frames and models for rods, I need to clarify what a curve is. See [Hof11] for more details.

Definition 2.53. A *curve* γ is defined as $\gamma \in C^2(I; \mathbb{R}^3)$ with $I := [0, L]$.

Definition 2.54. A curve γ is called *regular*, when $\gamma' \neq 0$ everywhere. If furthermore $\|\gamma'\| = 1$ everywhere, the curve is called *arc-length parameterized*.

Remark 2.55. Obviously, an arc-length parameterized curve is regular.

Remark 2.56. The length of an arc-length parameterized curve is L .



Definition 2.57. For an arc-length parameterized curve γ , $\mathbf{t}_\gamma := \gamma'$ is called the **tangent** of a curve γ ; $\kappa_\gamma := \|\mathbf{t}_\gamma'\| = \|\gamma''\|$ is called the **curvature** of γ ; and $(\kappa \mathbf{b})_\gamma := \mathbf{t}_\gamma \times \mathbf{t}_\gamma'$ is called the **curvature binormal** of γ . If $\kappa_\gamma \neq 0$: $\mathbf{n}_\gamma := \frac{\mathbf{t}_\gamma'}{\kappa_\gamma}$ is called the **normal** of γ ; and $\mathbf{b}_\gamma = \mathbf{t}_\gamma \times \mathbf{n}_\gamma$ is called the **binormal** of γ .

Remark 2.58. $(\kappa \mathbf{b})_\gamma$ is suggestive: in fact $(\kappa \mathbf{b})_\gamma = \mathbf{t}_\gamma \times \mathbf{t}_\gamma' = \mathbf{t}_\gamma \times \kappa_\gamma \mathbf{n}_\gamma = \kappa_\gamma (\mathbf{t}_\gamma \times \mathbf{n}_\gamma) = \kappa_\gamma \mathbf{b}_\gamma$.

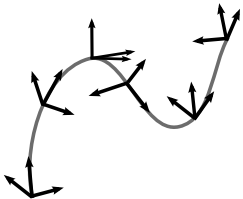
Remark 2.59. When it is clear, which curve I'm referring to, I'm going to leave out the ' γ '.

2.6 Frames and parallel transport along curves

Motivation A frame defines a local coordinate system along a curve. In fact, it is a continuous rotation that is aligned to the tangent vector. We will use a frame to model the twisting of the rod. Frames, specifically parallel frames, are connected to parallel transport which will be an important concept later, too. See [BWR⁺08], [Hof11], [LS96] and [Bis75].

Definition 2.60. An (adapted) **frame** F for an arc-length parameterized curve $\gamma : I \rightarrow \mathbb{R}^3$ is a map $F \in C^1(I; SO(3))$, $F(s) := (\mathbf{t}(s) \quad \mathbf{v}(s) \quad \mathbf{w}(s))$ with the usual $\mathbf{t} = \gamma'$.

Remark 2.61. \mathbf{t} , \mathbf{v} and \mathbf{w} are the coordinate axes of the local coordinate system spanned by F .



Remark 2.62 (Frenet equations). F is a continuous rotation by definition and thus we already know that we can write its derivative as

$$F' = [\mathbf{u}] F = F [\hat{\mathbf{u}}] \text{ with } \hat{\mathbf{u}} := \begin{pmatrix} \tau \\ k_2 \\ k_1 \end{pmatrix} \text{ and } \mathbf{u} = \tau \mathbf{t} + k_2 \mathbf{v} + k_1 \mathbf{w}. \quad (2.62.1)$$

When we expand this, we get the “Frenet equations”:

$$F' = F \begin{pmatrix} 0 & -k_1 & k_2 \\ k_1 & 0 & -\tau \\ -k_2 & \tau & 0 \end{pmatrix} \iff \begin{matrix} \mathbf{t}' = k_1 \mathbf{v} - k_2 \mathbf{w} & \mathbf{t}' = \mathbf{u} \times \mathbf{t} \\ \mathbf{v}' = -k_1 \mathbf{t} + \tau \mathbf{w} & \mathbf{v}' = \mathbf{u} \times \mathbf{v} \\ \mathbf{w}' = k_2 \mathbf{t} - \tau \mathbf{v} & \mathbf{w}' = \mathbf{u} \times \mathbf{w} \end{matrix} \quad (2.62.2)$$

We can associate k_1 and k_2 with the curvature κ of the curve γ :

$$\kappa^2 = \|\gamma''\|^2 = \|\mathbf{t}'\|^2 = \underbrace{\|k_1 \mathbf{v} - k_2 \mathbf{w}\|^2}_{\substack{\mathbf{v} \perp \mathbf{w} \\ \mathbf{v}, \mathbf{w} \in S^2}} = k_1^2 + k_2^2 \quad (2.62.3)$$

Thus we obtain:

Proposition 2.63.

$$\kappa = \sqrt{k_1^2 + k_2^2} \quad (2.63.1)$$

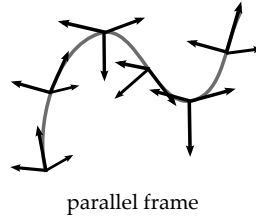
Definition 2.64. τ is called the *twist* of the frame.

Definition 2.65. A *parallel frame* is a frame with $\tau = 0$. A *Frenet frame* is a frame with $k_2 = 0$.

Remark 2.66. Thus $\kappa = |k_1|$ holds for Frenet frames.

Remark 2.67. Each axis of a parallel frame is a parallel field, as defined in [Hof11] or [Bis75]. Parallel fields are uniquely defined by a single image, that is two different parallel fields do not intersect. Moreover, the angle between two parallel fields stays constant.

Consequently if two parallel frames are equal at one point, they are equal everywhere.



Theorem 2.68. Parallel frames along a curve γ all have the same Darboux vector \mathbf{u} .

Proof. Let F be a parallel frame. Then we have $F' = [\mathbf{u}] F$. Let G be another parallel frame with $G' = [\mathbf{r}] G$. Define $R := F^{-1}(s_0)G(s_0)$ for an arbitrary but fixed $s_0 \in I$. Then $R \mathbf{e}_1 = F^{-1}(s_0)G(s_0) \mathbf{e}_1 = F^{-1}(s_0) \mathbf{t}(s_0) = \mathbf{e}_1$ and with proposition 2.25 on page 6 we conclude that R rotates around \mathbf{e}_1 . $\hat{F} := FR$ is a parallel frame, too, because its Darboux vector is \mathbf{u} : $\hat{F}' = F'R = [\mathbf{u}] FR = [\mathbf{u}] \hat{F}$ and $\hat{F} \mathbf{e}_1 = FR \mathbf{e}_1 = F \mathbf{e}_1 = \mathbf{t}$.

Finally we have $\hat{F}(s_0) = F(s_0)R = F(s_0) = F^{-1}(s_0)G(s_0) = G(s_0)$. Thus the two parallel frames are equal at s_0 and remark 2.67 implies $\hat{F} = G$ and hence $\mathbf{u} = \mathbf{r}$. \square

We can even say what the Darboux vector \mathbf{u} exactly is:

Theorem 2.69. A frame F is a parallel frame, if and only if its Darboux vector \mathbf{u} is the curvature binormal vector²:

$$\tau = 0 \iff \mathbf{u} = \mathbf{t} \times \mathbf{t}' = \kappa \mathbf{b}. \quad (2.69.1)$$

²see definition 2.53 on the preceding page

Proof. If F is a parallel frame, we have

$$\kappa \mathbf{b} = \mathbf{t} \times \mathbf{t}' \stackrel{(2.62.2)}{=} \mathbf{t} \times (k_1 \mathbf{v} - k_2 \mathbf{w}) = k_1 \underbrace{\mathbf{t} \times \mathbf{v}}_{=\mathbf{w}} - k_2 \underbrace{\mathbf{t} \times \mathbf{w}}_{=-\mathbf{v}} = k_2 \mathbf{v} + k_1 \mathbf{w} = \mathbf{u}. \quad (2.69.2)$$

If $\mathbf{u} = \kappa \mathbf{b}$, we have

$$\tau = \hat{\mathbf{u}} \cdot \mathbf{e}_1 = F^{-1} \mathbf{u} \cdot \mathbf{e}_1 = \mathbf{u} \cdot F \mathbf{e}_1 = (\mathbf{t} \times \mathbf{t}') \cdot \mathbf{t} = 0. \quad (2.69.3)$$

□

Remark 2.70. This provides another, simpler proof for the independence of the Darboux vector of the particular parallel frame: $\kappa \mathbf{b}$ only depends on the curve—not on the parallel frame.

2.6.1 (Continuous) parallel transport

Motivation For straight lines we intuitively identify parallel vectors through parallel shifts. For curves we can generalize this by the means of parallel transport which transports vectors along the curve without rotating them “more than needed”.

Definition 2.71. The *parallel transport* along the curve γ of a vector \mathbf{v} fixed at $\gamma(s_0)$ is defined as

$$P_{\mathbf{v}} : I \rightarrow \mathbb{R}^3, s \mapsto P(s)P^{-1}(s_0), \quad (2.71.1)$$

where P is an arbitrary parallel frame for γ .

Remark 2.72. This is well-defined because $P_{\mathbf{v}}$ is the unique solution of the ODE

$$P'_{\mathbf{v}} = P'(s)P^{-1}(s_0)\mathbf{v} = [\kappa \mathbf{b}] P(s)P^{-1}(s_0)\mathbf{v} = [\kappa \mathbf{b}] P_{\mathbf{v}} \text{ with } P_{\mathbf{v}}(s_0) = \mathbf{v}, \quad (2.72.1)$$

and $\kappa \mathbf{b}$ is independent of the actual parallel frame P that was chosen.

Remark 2.73. A **parallel field** along a curve γ is the parallel transport of any point on it along the curve.

2.6.2 Twisting of parallel frames under deformation

Motivation A parallel frame of a time-varying, arc-length parameterized curve can twist over time, even though it does not twist along the curve. It is possible to calculate the twist speed using only local properties of the curve.

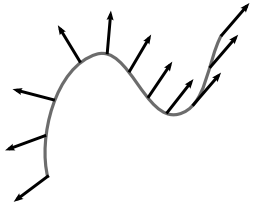
This next result is important for the calculation of internal twist forces and uses all the tools we have looked at so far.

Definition 2.74. A *time-varying curve* γ is a map $\gamma \in C^2(I \times J; \mathbb{R}^3)$ with an interval $J, 0 \in J \subset \mathbb{R}$. I write $\gamma(s, t)$. A *frame F for a time-varying curve γ* is a map $F \in C^1(I \times J; SO(3))$, such that $F(\bullet, t)$ is a frame for $\gamma(\bullet, t)$ for any fixed t .

Remark 2.75. For a time-varying curve, **parallel transport in time** can be defined similarly to the definition above. Only that the parallel frame P is **time-parallel**, that is a map $P : J \rightarrow SO(3)$ which is aligned with the curve at a fixed point and changes in time: $P(t) \mathbf{e}_1 = \gamma'(s_0, t)$, and parallel in the sense that its angular velocity has no twist.

Remark 2.76. As before I use:

- ω for the angular velocity of P , ie $\dot{P}(\bullet, 0) = [\omega] P$;



- \mathbf{u} for the Darboux vector of P , ie $P' = [\mathbf{u}] P$;
- $P = \begin{pmatrix} \mathbf{t} & \mathbf{v} & \mathbf{w} \end{pmatrix}$ for the axes of P ;
- σ for the twist of \dot{P} , ie $\omega \cdot \mathbf{t}$; and
- $\hat{\mathbf{u}} = \begin{pmatrix} 0 & k_2 & k_1 \end{pmatrix}^T$ for the components of the local Darboux vector of P .

Theorem 2.77. For a time-varying curve γ and a frame F for it, the following holds:

$$\sigma' = -\kappa \mathbf{b} \cdot \dot{\mathbf{t}} \tag{2.77.1}$$

$$\sigma(b) - \sigma(a) = - \int_a^b \kappa \mathbf{b} \cdot \dot{\mathbf{t}} ds \tag{2.77.2}$$

Proof using elementary operations. We write ω as $\omega = \sigma \mathbf{t} + \perp \dot{\mathbf{t}}$, then

$$\omega \times \mathbf{v} = \sigma (\mathbf{t} \times \mathbf{v}) + \perp \dot{\mathbf{t}} \times \mathbf{v} \tag{2.77.3}$$

and applying $\mathbf{t} \times \mathbf{v}$ in a dot product again, only

$$\underbrace{(\omega \times \mathbf{v})}_{=\dot{\mathbf{v}}} \cdot \underbrace{(\mathbf{t} \times \mathbf{v})}_{=\mathbf{w}} = \sigma (\mathbf{t} \times \mathbf{v})^2 = \sigma \mathbf{w}^2 = \sigma \tag{2.77.4}$$

remains. We need to calculate $\dot{\mathbf{v}} \cdot \mathbf{w}$. For this we look at its derivative:

$$\frac{\partial}{\partial s} (\dot{\mathbf{v}} \cdot \mathbf{w}) = \underbrace{\dot{\mathbf{v}}'}_{=\frac{\partial}{\partial t} \mathbf{v}'} \cdot \mathbf{w} + \dot{\mathbf{v}} \cdot \mathbf{w}' = \frac{\partial}{\partial t} (-k_1 \mathbf{t}) \cdot \mathbf{w} + \dot{\mathbf{v}} \cdot (k_2 \mathbf{t}) = -k_1 \dot{\mathbf{t}} \cdot \mathbf{w} + k_2 \dot{\mathbf{v}} \cdot \mathbf{t}, \tag{2.77.5}$$

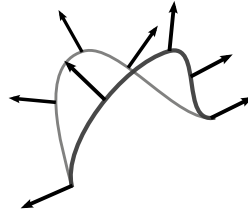
where I have used that $\frac{\partial}{\partial t} (-k_1 \mathbf{t}) = -\dot{k}_1 \mathbf{t} - k_1 \dot{\mathbf{t}} \cdot \mathbf{w} = -k_1 \dot{\mathbf{t}} \cdot \mathbf{w}$, because $\mathbf{t} \cdot \mathbf{w} = 0$. Now we use $0 = \frac{\partial}{\partial t} (\mathbf{v} \cdot \mathbf{t}) = \dot{\mathbf{v}} \cdot \mathbf{t} + \mathbf{v} \cdot \dot{\mathbf{t}}$, which follows from $\mathbf{v} \cdot \mathbf{t} = 0$, and substitute $-\mathbf{v} \cdot \dot{\mathbf{t}}$ for $\dot{\mathbf{v}} \cdot \mathbf{t}$:

$$\sigma' = \frac{\partial}{\partial s} (\dot{\mathbf{v}} \cdot \mathbf{w}) = - (k_1 \dot{\mathbf{t}} \cdot \mathbf{w} + k_2 \mathbf{v} \cdot \dot{\mathbf{t}}) = - (k_2 \mathbf{v} + k_1 \mathbf{w}) \cdot \dot{\mathbf{t}} \stackrel{(2.62.1)}{=} -\mathbf{u} \cdot \dot{\mathbf{t}} \stackrel{(2.69.1)}{=} -\kappa \mathbf{b} \cdot \dot{\mathbf{t}}. \tag{2.77.6}$$

Finally we use the fundamental theorem of calculus to obtain

$$- \int_a^b \kappa \mathbf{b} \cdot \dot{\mathbf{t}} ds = \int_a^b \frac{\partial}{\partial s} (\dot{\mathbf{v}} \cdot \mathbf{w}) ds = \int_a^b \frac{\partial}{\partial s} \sigma' ds = \sigma(b) - \sigma(a). \tag{2.77.7}$$

□



[BWR⁺08]’s argument

[BWR⁺08] uses a different argument which I want to sketch. It makes use of the linking number, total twist and writhe of (open) curves, which I am not defining here. The proof sketch is in the appendix A.2 on page 48.

Continuous models for rods

3.1 What do I mean by “rod”?

Motivation Usually when you talk about rods, you refer to seemingly inextensible, elastic, thin and long objects. However, for a more rigorous treatment I will explicitly define what properties a rod has and develop some basic consequences of these properties.

Properties As in [BWR⁺08] when I speak of a “rod”, I mean a rod that is (a) inextensible, (b) elastic, (c) infinitesimally thin, and (d) surrounded by a very thin material with uniform cross section.

Implications Because the rod is elastic, we can bend it by applying forces to it.

I assume that the rod is straight if no stress is applied to it, and that its bending response is isotropic, ie the same in every (normal) direction.

Because of the infinitesimally thin material surrounding the rod, we can twist it. Moreover, the propagation speed of twist waves is inversely proportional to the diameter of the rod. Which is tending towards zero. Hence we can assume that the twist waves propagate instantly. The rods have a **quasistatic material frame**; see [BWR⁺08, Quasistatic material frame postulation].

3.2 Cosserat curve model

Sources The following definitions are a combination of the ones used in [BWR⁺08], [ST07] and [AP10].

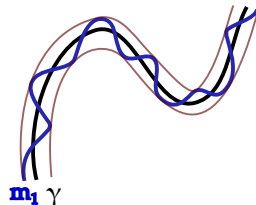
Definition 3.1. A *static Cosserat curve* Γ is a pair $(\gamma, M) \in C^2([0, L]; \mathbb{R}^3) \times C^1([0, L]; SO(3))$ consisting of a *centerline curve* γ and a *material frame* M :

$$\gamma : I \rightarrow \mathbb{R}^3, s \mapsto \gamma(s); M : I \rightarrow SO(3), s \mapsto M(s) = \begin{pmatrix} \mathbf{m}_0(s) & \mathbf{m}_1(s) & \mathbf{m}_2(s) \end{pmatrix} \quad (3.1.1)$$

with $I := [0, L]$, $\|\gamma'\| = 1$ and $\mathbf{m}_0 = \gamma'$.

Remark 3.2. γ is arc-length parameterized.

Remark 3.3. The material frame is used to model the twisting of the rod. Actually a single normal vector field along the curve suffices to model the twist. But by having a whole frame available we can also model bending at the same time.



Twisting and bending are inherently local properties of the geometry of the rod. We can measure both using the Darboux vector of the material frame: $M' = [\mathbf{u}] M$.

Definition 3.4. The *strain rates/material strains* \hat{u}_k are the components of $\hat{\mathbf{u}} = M^{-1}\mathbf{u}$: $\hat{u}_k = \mathbf{m}_k \cdot \mathbf{u}$

Remark 3.5. The strain rates measure the deformation of the rod along the material frame axes. Specifically, \hat{u}_0 measures the angle of the infinitesimal rotation¹ around the $\mathbf{m}_0 = \gamma'$ axis, ie the **twist** $\tau = \hat{u}_0$. And \hat{u}_1 and \hat{u}_2 measure the curvature κ of the centerline²: $\kappa = \sqrt{\hat{u}_1^2 + \hat{u}_2^2}$.

3.3 Cosserat rod energy

Motivation Now that I have specified a straightforward model for a rod, I present the formulas for its potential energy. They are needed to calculate the forces on the rod.

Sources [BWR⁺08] does not discuss the physical meaning of the material constants it uses³. [ST07] covers the physical interpretation and I transfer it to our model. See [AP10] for a thorough treatment.

Definition 3.6. The *potential energy* of a rod Γ is

$$E_{pot}(\Gamma) := \frac{1}{2} \int_{\gamma} \hat{\mathbf{u}}^T K \hat{\mathbf{u}} ds. \quad (3.6.1)$$

K is the **stiffness tensor**. For rods with uniform cross-section, as in our case, K can be written as diagonal matrix with regard to the material strains:

$$\hat{\mathbf{u}}^T K \hat{\mathbf{u}} = \begin{pmatrix} \hat{u}_0 & \hat{u}_1 & \hat{u}_2 \end{pmatrix} \begin{pmatrix} \beta & & \\ & \alpha & \\ & & \alpha \end{pmatrix} \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \hat{u}_2 \end{pmatrix} \text{ with } \alpha := E \frac{\pi r^4}{4}, \beta := G \frac{\pi r^4}{2}. \quad (3.6.2)$$

E is **Young's modulus**, G is the **shear modulus** and r is the radius of the rod's cross-section (which we assume to be very small compared to its length).

Remark 3.7. [ST07] actually uses $\alpha = E \frac{\pi r^2}{4}$, $\beta = G \frac{\pi r^2}{2}$. This is wrong: compare with [AP10, p 71, 78 and 81], [GHSS05] or [Bow10].

Corollary 3.8. The potential energy can be split into

$$E_{pot}(\Gamma) = E_{twist}(\Gamma) + E_{bend}(\Gamma) \quad (3.8.1)$$

$$E_{bend}(\Gamma) := \frac{1}{2} \int_{\gamma} \alpha \kappa^2 ds \quad (3.8.2)$$

$$E_{twist}(\Gamma) := \frac{1}{2} \int_{\gamma} \beta \tau^2 ds \quad (3.8.3)$$

3.4 Curve-angle model

Motivation The static model described above can be reduced to a more concise form with fewer parameters.

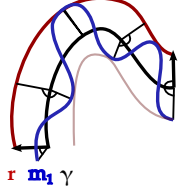
¹see remark 2.31 on page 7

²see proposition 2.63 on page 11

³ α for the bending response in the isotropic and \bar{B} in the anisotropic case; and β for the twisting response

Sources See [Sin08], [LS96] and [BWR⁺08].

Definition 3.9. A *static curve-angle model* of a rod given by its Cosserat curve $\Gamma = (\gamma, M)$ is a tuple $\hat{\Gamma} = (\gamma, \theta, \mathbf{r}) \in C^2(I; \mathbb{R}^3) \times C^1(I; \mathbb{R}) \times \mathbb{R}^3$. \mathbf{r} is the **rail vector** at $s = 0$. It is perpendicular to $\gamma(0)$, ie $\mathbf{r} \perp \gamma'(0)$. It is parallel transported along γ with the parallel transport P_r . And $\theta : I \rightarrow \mathbb{R}$, $\theta(s) := \angle^{\circ t(s)}(P_r(s), \mathbf{m}_1(s))$ is the **material frame angle**. It measures the (directed) angle between the transported rail vector and \mathbf{m}_1 along the tangent.



Remark 3.10. \mathbf{r} could have been just as well defined for a different point on the curve $\gamma(\hat{s})$. $\hat{s} = 0$ is the simplest choice.

Remark 3.11. If we choose $\mathbf{r} := \mathbf{m}_1(0)$ and $\theta(0) = 0$, θ will directly measure the deviation of the material frame from the “natural” parallel frame.

Proposition 3.12. A static curve-angle model $\hat{\Gamma} = (\gamma, \theta, \mathbf{r})$ is uniquely determined up to 2π -shifts of θ by a static Cosserat curve $\Gamma = (\gamma, M)$ and the initial rail vector \mathbf{r} , and vice-versa.

Proof. “ \implies ”: γ and \mathbf{r} uniquely determine a parallel field P_r along γ . We can construct a parallel frame based on P_r : $P = \begin{pmatrix} \gamma' & P_r & \gamma' \times P_r \end{pmatrix}$. Then M is fixed by a rotation around the curve’s tangent: $M := PR_{e_1, \theta}$.

“ \impliedby ”: We again construct P_r and P from the rail vector. Then $R(s) := P^{-1}(s)M(s) \in SO(3)$; $R(s) = R_{e_1, \alpha(s)}$ because $R\gamma' = \gamma'$ and proposition 2.25 and corollary 2.22 on page 5 and on page 6.

We can then find a smooth function⁴ θ with $\theta \cong \alpha \pmod{2\pi}$. □

An important observation is that we can link the derivative of θ with the twist τ of the material frame:

Theorem 3.13. For a given rod that is described by a curve-angle model $\hat{\Gamma} = (\gamma, \theta, \mathbf{r})$ and a static Cosserat curve $\Gamma = (\gamma, M)$, we have $\tau = \theta'$.

Proof. We start with $M = PR_{e_1, \theta}$ as defined on the current page.

$$\begin{aligned} [\mathbf{u}]M &= M' = P'R_{e_1, \theta} + PR'_{e_1, \theta} = [\mathbf{u}_P] \underbrace{PR_{e_1, \theta}}_{=M} + PR_{e_1, \theta} \underbrace{[e_1] \theta'}_{\text{from remark 2.35 on page 7}} \\ &= [\mathbf{u}_P]M + M[\theta' e_1] = [\mathbf{u}_P]M + \underbrace{M[\theta' e_1]M^{-1}M}_{=[\theta' M e_1]} = [\mathbf{u}_P]M + [\theta' \mathbf{m}_0]M \\ &= [\mathbf{u}_P + \theta' \mathbf{m}_0]M \end{aligned} \tag{3.13.1}$$

And thus: $\tau = \mathbf{u} \cdot \mathbf{m}_0 = \underbrace{\mathbf{u}_P \cdot \mathbf{m}_0}_{=0, \text{ since P is a parallel frame}} + \theta' \mathbf{m}_0^2 = \theta'$. □

Remark 3.14. This is well-defined because \mathbf{u}_P is independent of \mathbf{r} , and θ' is independent of shifts of 2π .

Remark 3.15. See [Bis75], [BWR⁺08] and [Sin08] for a trigonometric proof.

⁴ α does not have to be continuous, even though it is piecewise smooth. There will always be jumps, when α traverses the $0 \leftrightarrow 2\pi$ boundary

Corollary 3.16. *The potential energy of a rod given by a curve-angle model $\hat{\Gamma} = (\gamma, \theta, \mathbf{r})$ is:*

$$E_{pot}(\Gamma) = E_{twist}(\Gamma) + E_{bend}(\Gamma) \quad (3.16.1)$$

$$E_{bend}(\Gamma) := \frac{1}{2} \int_{\gamma} \alpha \gamma''^2 ds \quad (3.16.2)$$

$$E_{twist}(\Gamma) := \frac{1}{2} \int_{\gamma} \beta \theta'^2 ds \quad (3.16.3)$$

Remark 3.17. The potential energy is independent of $\theta(0)$ and \mathbf{r} .

We can simplify the representation of a rod even more:

Definition 3.18. *The **static curve-twist model** of a rod is a tuple $\bar{\Gamma} = (\gamma, \tau, \mathbf{r}) \in C^2(I; \mathbb{R}^3) \times C(I; \mathbb{R}) \times \mathbb{R}^3$. γ is the smooth arclength-parameterized centerline. \mathbf{r} is the rail vector. $\tau : I \rightarrow \mathbb{R}$ is the smooth map that measures the material twist of the centerline.*

Remark 3.19. If we set $\mathbf{r} = \mathbf{m}_1(0)$ we can reconstruct the curve-angle model (and then the Cosserat curve) by integrating τ and using $\theta(0) = 0$.

3.5 Dynamic models

Motivation We are interested in the motion of rods and for this we need to include a time variable in our model. Each static model can be extended to a dynamic one by adding a time parameter and requiring continuous differentiability in time, too:

Definition 3.20 (dynamic models). *For a time interval $0 \in T \subset \mathbb{R}$:*

- a **(dynamic) Cosserat curve** Γ is a pair $(\gamma, M) \in C^2([0, L] \times T; SO(3)) \times C^1([0, L] \times T; SO(3))$;
- a **(dynamic) curve-angle model** $\hat{\Gamma}$ is a tuple $\hat{\Gamma} = (\gamma, \theta, \mathbf{r}) \in C^2(I \times T; \mathbb{R}^3) \times C^1(I \times T; \mathbb{R}) \times C(I \times T; \mathbb{R}^3)$; and
- a **(dynamic) curve-twist model** is a tuple $\bar{\Gamma} = (\gamma, \tau, \mathbf{r}) \in C^2(I \times T; \mathbb{R}^3) \times C(I \times T; \mathbb{R}) \times C(I \times T; \mathbb{R}^3)$.

The rail vector is a parallel field along $\gamma(0, \bullet)$.

Remark 3.21. The only important change to the static case is that the rail vector is a time-parallel field. This is the same as saying that the rail vector at time 0 is parallel transported along the start of the curve in time.

Remark 3.22. Parallel transporting the rail vector in time has the benefit that angular twist⁵ of P_r vanishes: $\sigma(0, \bullet) = 0$. This is useful when calculating the twist forces.

For dynamic rods [ST07] gives an equation for the kinetic energy of the centerline:

Definition 3.23. *The kinetic energy of the centerline γ is*

$$E_{kinetic}(\gamma) = \frac{1}{2} \int \rho \pi r^2 \dot{\gamma}^2 ds \quad (3.23.1)$$

with the **material density** ρ and radius r .

Remark 3.24. There is no rotational energy in our model because of the quasistatic material frame. Since twist waves are propagated instantaneously, the material frame is always in the state of a static equilibrium and the rotational energy vanishes.

Before I go into more details, I want to talk about possible boundary conditions.

⁵see section 2.6.2 on page 12

3.6 Boundary conditions

Definition 3.25. *There are two kinds of boundary conditions:*

- *centerline boundary conditions, and*
- *material frame boundary conditions.*

Centerline conditions are of the form $\gamma(0) = \mathbf{x}_0$ and $\gamma(L) = \mathbf{x}_L$. Material frame conditions are of the form:

- *$M(0) = M_0$ and $M(L) = M_L$ for Cosserat curves;*
- *$\mathbf{r} = \mathbf{r}_0$, $\theta(0) = \theta_0$ and $\theta(L) = \theta_L$ for curve-angle models; and*
- *$\mathbf{r} = \mathbf{r}_0$ and $\int_0^L \tau ds = \theta_L - \theta_0$ for curve-twist models.*

Remark 3.26. The material frame boundary conditions for Cosserat curves are not as expressive as the other ones. If you only specify the material frames at the beginning and end, the material frame is only determined up to arbitrarily many full twists in-between. The curve-angle and curve-twist models don't have this issue, since the number of full twists can be determined with $\lfloor \frac{\theta_L - \theta_0}{2\pi} \rfloor$.

In the dynamic case the problem generally only exists for the initial configuration, as the material frame can only change continuously—even in the quasistatic case—and thus full twists will not be lost.

See [vdHPR07] and [AA83]⁶ for more details.

3.7 Quasistatic material frames

A quasistatic material frame always extremizes the energy of the rod because it immediately assumes the state of equilibrium. See [Sin08] and also remark 3.24 on the preceding page.

This means that

$$\frac{\partial E(\hat{\Gamma})}{\partial \theta} = 0. \quad (3.26.1)$$

[LS96] shows that in the case of an isotropic rod τ is constant and specifically $\tau = 0$ for free ends, ie rods without material frame boundary conditions. This makes [BWR⁺08]'s quasistatic material frame postulation well-defined in terms of the continuous dynamic rod definitions above when the boundary conditions change continuously.

3.8 Summary

I have introduced three simple models for representing a rod. They are mostly equivalent. But which model is preferable?

Preferred Model [BWR⁺08] prefers the curve-angle model. The reason is that it is more concise than the Cosserat curve and still preserves all information of it. The curve-twist model on the other hand contains all necessary information to calculate the potential energy but boundary conditions cannot be stated as easily as we have seen above.

⁶The ambiguous twist of Love' is a beautiful title.

Discretization of geometric concepts

The first part of the following chapter describes how continuous concepts can be discretized. The second part looks at how the continuous curve-angle model can be discretized in an elegant and coherent fashion.

4.1 Discrete curves and the difference operator

Motivation Curves, frames and parallel transport haven been used to model continuous rods. For a discrete rod model, we need discrete versions of these concepts. The following definitions are based on [Hof09].

Definition 4.1. A *discrete interval* \check{I} is $\check{I} := \{\min \check{I}, \dots, \max \check{I}\} \subset \mathbb{Z}$.

Definition 4.2. A *discrete curve* $\check{\gamma}$ is a map $\check{\gamma} : \check{I} \rightarrow \mathbb{R}^3$, $\check{\gamma}(i) := \check{\gamma}_i$ with $\check{I} := \{0, \dots, L\}$. $\check{\gamma}_i$ are the *vertices* of the discrete curve. $\check{\gamma}$ has $L + 1$ vertices in total. These vertices describe an (open) polygon with L edges.

Vertex and edge quantities We can define edge tangents as difference between vertices. Edge tangents can be described as a map from edge indices to edge tangent vectors. This map differs from the map of the discrete curve which maps point indices to vertex position vectors. Using the notation of [BWR⁺08], I call $\check{\gamma}$ a **vertex quantity** and index it using lower indices $\check{\gamma}_i$; and I call the latter an **edge quantity** and index it using upper indices, eg¹ $\check{e}^i := \check{\gamma}_{i+1} - \check{\gamma}_i$.

To distinguish between vertex and edge quantities, I use \mathcal{V} for the set of vertex quantities, eg $\check{\gamma} \in \mathcal{V}(\check{I}; \mathbb{R}^3)$, and \mathcal{E} for the set of edge quantities, eg $\check{e}^i \in \mathcal{E}$. If the domain and range are understood, I leave them out.

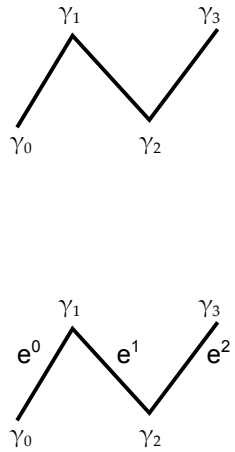
To simplify the definition of discrete edges and normal vectors and to introduce more interesting notation, we make use of the difference operator Δ :

Notation 4.3. Given a discrete set \check{I} , I write \check{I}_b^a for the **adapted set** $\check{I}_b^a := \{\min \check{I} + a, \dots, \max \check{I} + b\}$.

Definition 4.4. Given a group (G, \circ) , that is not necessarily commutative, the **difference operator** Δ is defined for both vertex and edge quantities:

$$\Delta : \mathcal{V}(\check{J}; G) \rightarrow \mathcal{E}(\check{J}_0^{-1}; G), \quad i \mapsto \Delta \alpha^i := \alpha_{i+1} \circ (\alpha_i)^{-1} \quad (4.4.1)$$

$$\Delta : \mathcal{E}(\check{J}; G) \rightarrow \mathcal{V}(\check{J}_{+1}^0; G), \quad i \mapsto \Delta \beta_i := \beta^i \circ (\beta^{i-1})^{-1}. \quad (4.4.2)$$



¹I am not going to use e^i in this meaning after this example, even though [BWR⁺08] does.

The local difference operator $\hat{\Delta}$ is defined as

$$\hat{\Delta} : \mathcal{V}(\check{J}; G) \rightarrow \mathcal{E}(\check{J}_0^{-1}; G), \quad i \mapsto \hat{\Delta}\alpha^i := (\alpha_i)^{-1} \circ \alpha_{i+1} \quad (4.4.3)$$

$$\hat{\Delta} : \mathcal{E}(\check{J}; G) \rightarrow \mathcal{V}(\check{J}_{+1}^0; G), \quad i \mapsto \hat{\Delta}\beta_i := (\beta^{i-1})^{-1} \circ \beta^i \quad (4.4.4)$$

Remark 4.5. The definition of $\hat{\Delta}$ only makes sense for non-commutative groups G . For commutative G it is redundant, as $\hat{\Delta} = \Delta$ in that case.

Example 4.6. For $G = \mathbb{R}^3$ with addition as canonical group operation, this becomes

$$\Delta\alpha^i := \alpha_{i+1} - \alpha_i \quad (4.6.1)$$

$$\Delta\beta_i := \beta^i - \beta^{i-1}. \quad (4.6.2)$$

For $G = SO(3)$ with matrix multiplication as canonical group operation, this becomes

$$\Delta\alpha^i := \alpha_{i+1} (\alpha_i)^{-1} \quad (4.6.3)$$

$$\Delta\beta_i := \beta^i (\beta^{i-1})^{-1} \quad (4.6.4)$$

$$\hat{\Delta}\alpha^i := (\alpha_i)^{-1} \alpha_{i+1} \quad (4.6.5)$$

$$\hat{\Delta}\beta_i := (\beta^{i-1})^{-1} \beta^i. \quad (4.6.6)$$

Remark 4.7. Every time the difference operator is applied the domain of the resulting map gets smaller by one element, if the domain is finite in the beginning. This is necessary since the i th element accesses either its left or right neighbor, which has to be defined. The definitions for vertex and edge quantities are different in order to keep the solution conceptually “centered” with the corresponding vertex or edge of the curve.

Notation 4.8. To keep equations concise I am using the shorter notation $\Delta^2\check{\gamma}$ for $\Delta\Delta\check{\gamma}$. I also leave out the index i , eg $\check{\gamma}_i$ becomes $\check{\gamma}$. Moreover I write $\check{\gamma}_{\underline{k}}$ for $\check{\gamma}_{i+k}$, and $\check{\gamma}_{\overline{k}}$ for $\check{\gamma}_{i-k}$; and $\Delta\check{\gamma}^{\underline{k}}$ for $\Delta\check{\gamma}^{i+k}$, and $\Delta\check{\gamma}^{\overline{k}}$ for $\Delta\check{\gamma}^{i-k}$. I use an underbar for + and an overbar for -.

For example $\check{\gamma}_{+1}$ becomes $\check{\gamma}_{\underline{1}}$ and $\Delta\check{\gamma}^{-1}$ becomes $\Delta\check{\gamma}^{\overline{1}}$. These two examples are practically all use cases: $\underline{\quad}$ for vertex quantities and $\overline{\quad}$ for edge quantities.

Nonetheless here is a full example set: $\check{\gamma}$, $\check{\gamma}_{\underline{1}}$, $\check{\gamma}_{\overline{1}}$ for $\check{\gamma}_i$, $\check{\gamma}_{i+1}$, $\check{\gamma}_{i-1}$, and $\Delta\check{\gamma}$, $\Delta\check{\gamma}^{\underline{1}}$, $\Delta\check{\gamma}^{\overline{1}}$ for $\Delta\check{\gamma}^i$, $\Delta\check{\gamma}^{i+1}$, $\Delta\check{\gamma}^{i-1}$.

I apply the same notation to adapted sets: $\check{I}^{\overline{1}} = \check{I}_0^{-1}$ and $\check{I}_{\underline{1}} = \check{I}_1^0$.

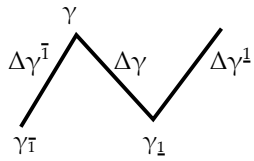
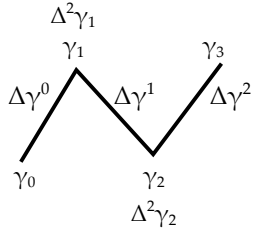
Example 4.9. With the new notation we have $\Delta\check{\gamma} = \check{\gamma}_{\underline{1}} - \check{\gamma} \in \mathcal{E}(\check{I}^{\overline{1}}) = \mathcal{E}(\{0, \dots, L-1\})$ and $\Delta^2\check{\gamma} = \Delta\check{\gamma} - \Delta\check{\gamma}^{\overline{1}} \in \mathcal{V}(\check{I}_{\underline{1}}^{\overline{1}}) = \mathcal{V}(\{1, \dots, L-1\})$.

Remark 4.10. The local difference operator $\hat{\Delta}$ can be expressed in terms of the difference operator Δ using

$$\hat{\Delta}\alpha = (\alpha_{\underline{1}})^{-1} \circ \Delta\alpha \circ \alpha_{\underline{1}} \quad (4.10.1)$$

$$\hat{\Delta}\beta = (\beta^{\overline{1}})^{-1} \circ \Delta\beta \circ \beta^{\overline{1}} \quad (4.10.2)$$

with $\alpha \in \mathcal{V}$, $\beta \in \mathcal{E}$.



We can sum up the differences to get back the original quantity:

Proposition 4.11. For $\alpha \in \mathcal{V}(\mathbb{R}^3)$, $\beta \in \mathcal{E}(\mathbb{R}^3)$:

$$\alpha_b - \alpha_a = \sum_{i=a}^{b-1} \Delta \alpha^i \quad (4.11.1)$$

$$\beta^b - \beta^a = \sum_{i=a+1}^b \Delta \beta_i \quad (4.11.2)$$

Definition 4.12. A discrete curve $\tilde{\gamma}$ is called *arc-length parameterized*, if $|\Delta \tilde{\gamma}| := \|\Delta \tilde{\gamma}\| = \text{const} \neq 0$. It is called *strictly arc-length parameterized*, if $|\Delta \tilde{\gamma}| = 1$.

Remark 4.13. From now on discrete curves, especially $\tilde{\gamma}$, will always be assumed to be parameterized by arc-length.

Remark 4.14. The discrete definition is more lenient than the continuous one. We will see that for many results it is only necessary that all edges have the same length.

Definition 4.15. The *edge tangent* $\check{\mathbf{t}} \in \mathcal{E}(\check{I}_1^{\check{I}})$ of a discrete curve $\tilde{\gamma}$ is defined as $\check{\mathbf{t}} := \frac{\Delta \tilde{\gamma}}{|\Delta \tilde{\gamma}|}$.

Definition 4.16. $\check{\phi} \in \mathcal{V}(\check{I}_1^{\check{I}})$ is the angle between two adjacent edges: $\check{\phi} := \angle_{\circlearrowleft}^{\check{\mathbf{t}}^{\check{I}} \times \check{\mathbf{t}}^{\check{I}}}(\check{\mathbf{t}}^{\check{I}}, \check{\mathbf{t}}) \in (-\pi, \pi]$.

Remark 4.17. Thus we can write:

$$\check{\mathbf{t}}^{\check{I}} \cdot \check{\mathbf{t}} = \cos \check{\phi} \quad (4.17.1)$$

$$\|\check{\mathbf{t}}^{\check{I}} \times \check{\mathbf{t}}\| = |\sin \check{\phi}| \quad (4.17.2)$$

Definition 4.18. A discrete curve $\tilde{\gamma}$ is called *regular* if any three successive vertices are pairwise disjoint.

Remark 4.19. This means, in particular, that no neighboring edges are overlapping. This is equivalent to $\check{\phi} \neq \pi$.

Remark 4.20. From now on discrete curves, especially $\tilde{\gamma}$, will always be assumed to be regular.

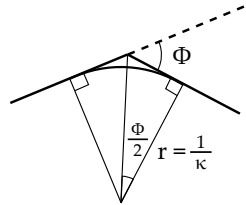
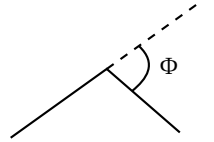
4.2 Discrete curvature and discrete binormals

Motivation There are several different ways to define discrete curvature. They all make sense one way or the other. For arc-length parameterized curves there is a natural definition though. See [Hof09, p 14–19].

Definition 4.21. The *discrete curvature* $\check{\kappa} \in \mathcal{V}(\check{I}_1^{\check{I}})$ of a discrete curve $\tilde{\gamma}$ is $\check{\kappa} := 2 \left| \tan \frac{\check{\phi}}{2} \right|$.

Remark 4.22. This discrete curvature is particularly nice because it tends to infinity as $\check{\phi} \rightarrow \pm\pi$ (compare this to other possible discrete curvatures like $\sin \check{\phi}$ or $\check{\phi}$).

Proposition 4.23. $\check{\kappa} = 2 \frac{|\sin \check{\phi}|}{1 + \cos \check{\phi}}$



Proof. First we note that

$$\cos \alpha + \imath \sin \alpha = e^{\imath \alpha} = \left(e^{\imath \frac{\alpha}{2}} \right)^2 = \cos^2 \frac{\alpha}{2} - \sin^2 \frac{\alpha}{2} + \imath 2 \cos \frac{\alpha}{2} \sin \frac{\alpha}{2}. \quad (4.23.1)$$

This implies

$$\cos \alpha = \cos^2 \frac{\alpha}{2} - \sin^2 \frac{\alpha}{2} = 2 \cos^2 \frac{\alpha}{2} - 1 \iff \cos \alpha + 1 = 2 \cos^2 \frac{\alpha}{2} \quad (4.23.2)$$

and

$$\sin \alpha = 2 \cos \frac{\alpha}{2} \sin \frac{\alpha}{2}. \quad (4.23.3)$$

Substituting and noting that $\cos \frac{\check{\phi}}{2} \geq 0$, since $\frac{\check{\phi}}{2} \in \left(-\frac{\pi}{2}, \frac{\pi}{2} \right]$,

$$\left| \tan \frac{\check{\phi}}{2} \right| = \frac{|\sin \frac{\check{\phi}}{2}|}{\cos \frac{\check{\phi}}{2}} = \frac{2 \cos \frac{\check{\phi}}{2} |\sin \frac{\check{\phi}}{2}|}{2 \cos^2 \frac{\check{\phi}}{2}} = \frac{|2 \cos \frac{\check{\phi}}{2} \sin \frac{\check{\phi}}{2}|}{2 \cos^2 \frac{\check{\phi}}{2}} = \frac{|\sin \check{\phi}|}{\cos \check{\phi} + 1}. \quad (4.23.4) \quad \square$$

Definition 4.24. The *discrete binormal* $\check{\mathbf{b}} \in \mathcal{V}(\check{I}_1^{\bar{}})$ is $\check{\mathbf{b}} := \frac{\check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}}{\|\check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}\|}$ for $\check{\mathbf{t}}^{\bar{}} \not\parallel \check{\mathbf{t}}$, and $\check{\mathbf{b}} := \frac{\mathbf{v}}{\|\mathbf{v}\|}$ for any $0 \neq \mathbf{v} \perp \check{\mathbf{t}}$ otherwise.

Remark 4.25. With eq. (4.17.2) on the preceding page we obtain $\check{\mathbf{b}} = \frac{\check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}}{|\sin \check{\phi}|}$.

Definition 4.26. The *discrete curvature binormal* $\check{\kappa} \mathbf{b} \in \mathcal{V}(\check{I}_1^{\bar{}})$ is $\check{\kappa} \mathbf{b} := 2 \frac{\check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}}{1 + \check{\mathbf{t}}^{\bar{}} \cdot \check{\mathbf{t}}}$.

Remark 4.27. This is exactly the curvature binormal used in [BWR⁺08].

Proposition 4.28. $\check{\kappa} \mathbf{b} = \check{\kappa} \check{\mathbf{b}} = 2 \left| \tan \frac{\check{\phi}}{2} \right| \frac{\check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}}{\|\check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}\|}$.

Proof. For $\check{\mathbf{t}}^{\bar{}} \not\parallel \check{\mathbf{t}}$, ie $\check{\phi} \notin \{0, \pi\}$, $\check{\kappa} \check{\mathbf{b}} = 2 \frac{|\sin \check{\phi}|}{1 + \cos \check{\phi}} \frac{\check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}}{|\sin \check{\phi}|} = \frac{2 \check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}}{1 + \cos \check{\phi}} = \frac{2 \check{\mathbf{t}}^{\bar{}} \times \check{\mathbf{t}}}{1 + \check{\mathbf{t}}^{\bar{}} \cdot \check{\mathbf{t}}}$. For $\check{\mathbf{t}}^{\bar{}} \parallel \check{\mathbf{t}}$, $\check{\kappa} \check{\mathbf{b}} = 0$ and $\check{\kappa} = 0$, and $\check{\kappa} \mathbf{b} = 0$ independent of $\check{\mathbf{b}}$. \square

4.3 Discrete normals and vertex tangents

Motivation A definition for a discrete normal vector (in the sense of 2.5) is still missing. Furthermore, edge tangents $\check{\mathbf{t}}$ are an edge quantity, but curvature binormals $\check{\kappa} \mathbf{b}$ and $\Delta^2 \check{\gamma}$ are vertex quantities. For a consistent model it is reasonable to expect a vertex tangent vector, too. You will see: it will fit it in nicely.

Proposition 4.29. $\check{\mathbf{t}}^{\bar{}} + \check{\mathbf{t}} \perp \Delta \check{\mathbf{t}} \sim \Delta^2 \check{\gamma}$

Proof. We verify $(\check{\mathbf{t}}^{\bar{}} + \check{\mathbf{t}}) \cdot \Delta \check{\mathbf{t}} = (\check{\mathbf{t}}^{\bar{}} + \check{\mathbf{t}}) \cdot (\check{\mathbf{t}} - \check{\mathbf{t}}^{\bar{}}) = \check{\mathbf{t}}^2 - (\check{\mathbf{t}}^{\bar{}})^2 = 1 - 1 = 0$. \square

Definition 4.30. The *discrete vertex tangent* $\check{\mathbf{t}}^{\vee} \in \mathcal{V}(\check{I}_1^{\bar{}})$ is $\check{\mathbf{t}}^{\vee} := \frac{1}{2} (\check{\mathbf{t}}^{\bar{}} + \check{\mathbf{t}})$.

Remark 4.31. $\check{t}^\vee \perp \Delta\check{t}$ (from proposition 4.29)

Proposition 4.32. $\Delta\check{t} = \kappa\check{b} \times \check{t}^\vee$

Proof.

$$\begin{aligned}
\kappa\check{b} \times \check{t}^\vee &= 2 \frac{\check{t}^\vee \times \check{t}}{1 + \check{t}^\vee \cdot \check{t}} \times \frac{1}{2} (\check{t}^\vee + \check{t}) = \frac{(\check{t}^\vee \times \check{t}) \times (\check{t}^\vee + \check{t})}{1 + \check{t}^\vee \cdot \check{t}} \\
&= \frac{(\check{t}^\vee \times \check{t}) \times \check{t}^\vee - (\check{t} \times \check{t}^\vee) \times \check{t}}{1 + \check{t}^\vee \cdot \check{t}} = \frac{(\check{t}^\vee)^2 \check{t} - (\check{t}^\vee \cdot \check{t}) \check{t}^\vee - \check{t}^2 \check{t}^\vee + (\check{t}^\vee \cdot \check{t}) \check{t}}{1 + \check{t}^\vee \cdot \check{t}} \\
&= \frac{(\check{t} - \check{t}^\vee) (1 + \check{t}^\vee \cdot \check{t})}{1 + \check{t}^\vee \cdot \check{t}} = \check{t} - \check{t}^\vee = \Delta\check{t}
\end{aligned} \tag{4.32.1}$$

Remark 4.33. Compare this to the continuous equation $t' = \kappa b \times t$ (from eq. (2.62.2) on page 11).

Remark 4.34. We have three perpendicular vertex quantities now: \check{t}^\vee , $\Delta\check{t}$, and $\kappa\check{b}$.

Definition 4.35. The *discrete normal* $\check{n} \in \mathcal{V}(\check{I}_1^\vee)$ is $\check{n} := \check{b} \times \frac{\check{t}^\vee}{\|\check{t}^\vee\|}$.

Remark 4.36. If for some vertex $\Delta\check{t} \neq 0$, $\check{n} = \check{b} \times \frac{\check{t}^\vee}{\|\check{t}^\vee\|} = \frac{\check{b} \times \check{t}^\vee}{\|\check{b} \times \check{t}^\vee\|} = \frac{\kappa\check{b} \times \check{t}^\vee}{\|\kappa\check{b} \times \check{t}^\vee\|} = \frac{\Delta\check{t}}{\|\Delta\check{t}\|}$.

This follows from proposition 4.32, $\Delta\check{t} \neq 0 \implies \kappa \neq 0$ and remark 4.34.

4.4 Discrete frames and parallel transport

Definition 4.37. A *discrete frame* \check{F} is a map $\check{F} \in \mathcal{E}(\check{I}_1^\vee; SO(3))$ with $\check{F}e_1 = \check{t}$.

Remark 4.38. $\Delta\check{F} = \check{F}(\check{F}^\vee)^{-1} \in SO(3)$, so $\check{F} = \Delta\check{F}\check{F}^\vee$. See example 4.6 on page 22.

Remark 4.39 (Tangent chain). $\check{t} = \Delta\check{F}\check{t}^\vee \iff \check{t} = \check{F}(\check{F}^\vee)^{-1}\check{t}^\vee \iff \check{t} = \check{F}e_1$

Definition 4.40. The *discrete Darboux vector* is the unique vector quantity $\check{u} \in \mathcal{V}(\check{I}_1^\vee)$ that satisfies $\Delta\check{F} = R_{\check{u}}$. The *discrete local Darboux vector* is the unique vector quantity $\check{u}_l \in \mathcal{V}(\check{I}_1^\vee)$ that satisfies $\hat{\Delta}\check{F} = R_{\check{u}_l}$.

Proposition 4.41. $\check{u}_l = (\check{F}^\vee)^{-1}\check{u}$

Proof. Remark 4.10 on page 22 yields $R_{\check{u}_l} = (\check{F}^\vee)^{-1}R_{\check{u}}\check{F}^\vee = R_{(\check{F}^\vee)^{-1}\check{u}}$. \square

Definition 4.42. A *discrete parallel frame* \check{P} is a discrete frame with $\check{u} = \kappa\check{b}$, ie $\Delta\check{P} = R_{\kappa\check{b}} = R_{\check{b}, \check{\phi}}$.

Remark 4.43. This is well-defined because $R_{\check{\kappa}\check{b}}$ maps $\check{\mathbf{t}}^{\bar{1}}$ onto $\check{\mathbf{t}}$. This follows from proposition 2.24 on page 5 and the fact that $\check{\kappa}\check{b}$ is perpendicular to $\check{\mathbf{t}}^{\bar{1}}$ and $\check{\mathbf{t}}$.

Remark 4.44. Moreover $\Delta\check{P}$ does not rotate along the tangents, ie rotations around $\check{\mathbf{t}}$ are preserved: $\Delta\check{P}R_{\check{\mathbf{t}}^{\bar{1}},\alpha} = R_{\check{\mathbf{t}},\alpha}\Delta\check{P}$. This follows from

$$R_{\check{\kappa}\check{b}}R_{\check{\mathbf{t}}^{\bar{1}},\alpha} = R_{\check{\kappa}\check{b}}R_{\check{\mathbf{t}}^{\bar{1}},\alpha}R_{\check{\kappa}\check{b}}^{-1}R_{\check{\kappa}\check{b}} = R_{R_{\check{\kappa}\check{b}}\check{\mathbf{t}}^{\bar{1}},\alpha}R_{\check{\kappa}\check{b}} = R_{\check{\mathbf{t}},\alpha}R_{\check{\kappa}\check{b}}. \quad (4.44.1)$$

Remark 4.45. $\Delta\check{P}$ rotates around $\check{\mathbf{b}}$ by $\check{\phi}$ radians. This is analogous to the continuous definition: For a parallel frame P we have $P' = [\check{\kappa}\check{b}]P$ —see theorem 2.69 on page 11. $[\check{\kappa}\check{b}]$ is an infinitesimal rotation around $\check{\kappa}\check{b}$, ie around $\check{\mathbf{b}}$, by $\|\check{\kappa}\check{b}\| = \check{\kappa}$ radians².

Remark 4.46. This definition is the reason for the factor $\frac{1}{2}$ in the definition of the Cayley rotation on page 8.

Theorem 4.47. *A frame \check{F} is a parallel frame, if and only if $(\check{u}_l)_1 = \check{u}_l \cdot \mathbf{e}_1 = 0$.*

Proof. If \check{F} is a parallel frame, we have $(\check{u}_l)_1 = \check{u}_l \cdot \mathbf{e}_1 = (\check{F}^{\bar{1}})^{-1} \check{u} \cdot \mathbf{e}_1 = \check{\kappa}\check{b} \cdot (\check{F}^{\bar{1}}) \mathbf{e}_1 = \check{\kappa}\check{b} \cdot \check{\mathbf{t}}^{\bar{1}} \sim (\check{\mathbf{t}}^{\bar{1}} \times \check{\mathbf{t}}) \cdot \check{\mathbf{t}}^{\bar{1}} = 0$. If $(\check{u}_l)_1 = 0$, we use that $\check{u} \cdot \check{\mathbf{t}}^{\bar{1}} = \check{u} \cdot \check{\mathbf{t}}$. This follows from proposition 2.26 on page 6 and remark 4.39 on the previous page. So $0 = \check{u}_l \cdot \mathbf{e}_1 = \check{u} \cdot \check{\mathbf{t}}^{\bar{1}} = \check{u} \cdot \check{\mathbf{t}}$, that is $\check{u} \perp \check{\mathbf{t}}^{\bar{1}}$ and $\check{u} \perp \check{\mathbf{t}}$. This implies that $\check{u} \sim \check{\mathbf{t}}^{\bar{1}} \times \check{\mathbf{t}} \sim \check{\kappa}\check{b}$ and hence we have determined the rotation axis. $R_{\check{u}} = R_{\check{\kappa}\check{b}}$ follows from proposition 2.24 on page 5. \square

Proposition 4.48. *For every frame \check{F} the difference $\Delta\check{F}$ can be decomposed into $\Delta\check{F} = R_{\check{\mathbf{t}},\check{\tau}}R_{\check{\kappa}\check{b}} = R_{\check{\kappa}\check{b}}R_{\check{\mathbf{t}}^{\bar{1}},\check{\tau}}$. $\check{\tau} \in \mathcal{V}(\check{I}_1^{\bar{1}})$ is called the **discrete twist**.*

Proof. Observing $\Delta\check{F}R_{\check{\kappa}\check{b}}^{-1}\check{\mathbf{t}} = \check{F}(\check{F}^{\bar{1}})^{-1}\check{\mathbf{t}}^{\bar{1}} = \check{F}\mathbf{e}_1 = \check{\mathbf{t}}$, proposition 2.25 on page 6 shows $\Delta\check{F}R_{\check{\kappa}\check{b}}^{-1} = R_{\check{\mathbf{t}},\check{\tau}}$ for some $\check{\tau}$. Thus $\Delta\check{F} = R_{\check{\mathbf{t}},\check{\tau}}R_{\check{\kappa}\check{b}} = R_{\check{\kappa}\check{b}}R_{\check{\mathbf{t}}^{\bar{1}},\check{\tau}}$. The last equality follows from remark 4.44 on this page. \square

Remark 4.49. A parallel frame \check{P} has no discrete twist. This follows from $R_{\check{\mathbf{t}},\check{\tau}} = \Delta\check{P}R_{\check{\kappa}\check{b}}^{-1} = \text{Id}_3$.

Proposition 4.50. *Every frame \check{F} can be decomposed into $\check{F} = R_{\check{\kappa}\check{b}}\check{F}^{\bar{1}}R_{\mathbf{e}_1,\check{\tau}}$.*

Proof. $\check{F} = \Delta\check{F}\check{F}^{\bar{1}} = R_{\check{\kappa}\check{b}}R_{\check{\mathbf{t}}^{\bar{1}},\check{\tau}}\check{F}^{\bar{1}} = R_{\check{\kappa}\check{b}}\check{F}^{\bar{1}}(\check{F}^{\bar{1}})^{-1}R_{\check{\mathbf{t}}^{\bar{1}},\check{\tau}}\check{F}^{\bar{1}} = R_{\check{\kappa}\check{b}}\check{F}^{\bar{1}}R_{\underbrace{(\check{F}^{\bar{1}})^{-1}\check{\mathbf{t}}^{\bar{1}}}_{=\mathbf{e}_1},\check{\tau}}$ \square

²This is why the discrete curvature is sometimes defined as $\check{\kappa} := \check{\phi}$.

4.4.1 Discrete parallel transport

The next definition is almost an one-to-one copy of the continuous version (definition 2.71 on page 12) as we have already discretized most concepts.

Definition 4.51. The *discrete parallel transport* $\check{p}_{i_0}(v) \in \mathcal{E}(\check{I}^1)$ along the discrete curve $\check{\gamma}$ of a vector v fixed at $\check{\gamma}_{i_0}$ is

$$\check{p}_{i_0}^i(v) := \check{P}^i \left(\check{P}^{i_0} \right)^{-1} v, \quad (4.51.1)$$

where \check{P} is an arbitrary parallel frame for $\check{\gamma}$.

Remark 4.52. This is well-defined, just as in the continuous case. If \check{Q} is another parallel frame, then $(\check{Q}^0)^{-1} \check{P}^0 e_1 = (\check{Q}^0)^{-1} \check{t}^0 = e_1$, hence proposition 2.25 on page 6 implies $(\check{Q}^0)^{-1} \check{P}^0 =: R_{e_1, \alpha}$ for some fixed α . We can use induction to show $\check{P} = \Delta \check{P} \check{P}^{\bar{1}} = R_{\check{\kappa} \check{b}} \check{Q}^{\bar{1}} R_{e_1, \alpha} = \check{Q} R_{e_1, \alpha}$. Finally $\check{p}_{i_0}(v) = \check{P} \left(\check{P}^{i_0} \right)^{-1} v = \check{Q} R_{e_1, \alpha} \left(\check{Q}^{i_0} R_{e_1, \alpha} \right)^{-1} v = \check{Q} \left(\check{Q}^{i_0} \right)^{-1} v$.

Remark 4.53. $\check{p}_{i_0}(v)$ is linear in v .

Remark 4.54. A discrete parallel transport is transformed like a discrete parallel frame along the curve: $\check{p}_{i_0}(v) = \check{P} \left(\check{P}^{i_0} \right)^{-1} v = R_{\check{\kappa} \check{b}} \check{P}^{\bar{1}} \left(\check{P}^{i_0} \right)^{-1} v = R_{\check{\kappa} \check{b}} \check{p}_{i_0}^{\bar{1}}(v)$.

Remark 4.55. A **discrete parallel field** along a discrete curve $\check{\gamma}$ is the parallel transport of a point in the field along the curve $\check{\gamma}$.

4.4.2 Twisting of discrete parallel frames under deformation

Motivation This is the discrete analogue of section 2.6.2 on page 12. The following result will be used later to calculate twist forces on the rod.

Definition 4.56. A *time-varying discrete curve* $\check{\gamma}$ is a map $\check{\gamma} : \check{I} \times J \rightarrow \mathbb{R}^3$, $\check{\gamma}(i, t) := \check{\gamma}_i(t)$ with an interval J , $0 \in J \subset \mathbb{R}$; and $\check{\gamma}_i(\bullet) \in C^1$ for fixed $i \in \check{I}$.

A *discrete frame* \check{F} for a time-varying discrete curve $\check{\gamma}$ is a map $\check{F} : \check{I}^1 \times J \rightarrow SO(3)$, $\check{F}^i(t) := \check{F}(i, t)$, such that $\check{F}(\bullet, t)$ is a discrete frame for $\check{\gamma}(\bullet, t)$ for any fixed t , and $\check{F}^i(\bullet) \in C^1$ for fixed $i \in \check{I}^1$.

Remark 4.57. Vertex and edge quantities have to be reformulated, too. A **time-varying vertex quantity** α is a map $\alpha : \check{I} \times J \rightarrow G$, $\alpha_i(t) := \alpha(i, t)$ and continuous in t . A **time-varying edge quantity** is defined likewise. I continue to use \mathcal{V} and \mathcal{E} , but they denote time-varying vertex and edge quantities from now on.

Remark 4.58. A time-varying edge quantity can be parallel-transported in time, too. **Discrete parallel transport in time** is defined like the continuous variant, see remark 2.75 on page 12, only that the (time-continuous) parallel frame P stays aligned with a fixed edge that varies in time: $P(t) e_1 = \check{t}^{i_0}(t)$.

Remark 4.59. As before I use:

- $\check{\omega} \in \mathcal{E}$ for the angular velocity of \check{P} , ie $\dot{\check{P}} = [\check{\omega}] \check{P}$;
- $\check{\sigma} \in \mathcal{E}$ for the twist of \check{P} , ie $\check{\sigma} := \check{\omega} \cdot \check{t}$; and
- $\check{\psi} \in \mathcal{E}$ for the angular velocity of $R_{\check{\kappa} \check{b}}$.

Theorem 4.60. For a time-varying discrete curve $\tilde{\gamma}$ and a parallel frame \check{P} along it, the following hold:

$$\Delta\check{\sigma} = -\frac{\check{\mathbf{t}}^{\bar{1}} \times \check{\mathbf{t}}}{1 + \check{\mathbf{t}}^{\bar{1}} \cdot \check{\mathbf{t}}} \cdot (\check{\mathbf{t}}^{\bar{1}} + \check{\mathbf{t}}) \quad (4.60.1)$$

$$\check{\sigma}^b - \check{\sigma}^a = \sum_{i=a+1}^b \Delta\check{\sigma}_i \quad (4.60.2)$$

Proof. The second equation follows directly from proposition 4.11 on page 23.

We start with

$$\begin{aligned} [\check{\omega}] \check{P} &= \dot{\check{P}} = \frac{d}{dt}(\Delta\check{P} \check{P}^{\bar{1}}) = [\check{\psi}] R_{\check{\kappa}b} \check{P}^{\bar{1}} + R_{\check{\kappa}b} [\check{\omega}^{\bar{1}}] \check{P}^{\bar{1}} = [\check{\psi}] \check{P} + R_{\check{\kappa}b} [\check{\omega}^{\bar{1}}] R_{\check{\kappa}b}^{-1} R_{\check{\kappa}b} \check{P}^{\bar{1}} \\ &= [\check{\psi}] \check{P} + [R_{\check{\kappa}b} \check{\omega}^{\bar{1}}] \check{P} = [\check{\psi} + R_{\check{\kappa}b} \check{\omega}^{\bar{1}}] \check{P} \\ \iff \check{\omega} &= \check{\psi} + R_{\check{\kappa}b} \check{\omega}^{\bar{1}} \end{aligned} \quad (4.60.3)$$

We apply the dot product with $\check{\mathbf{t}}$:

$$\check{\sigma} = \check{\omega} \cdot \check{\mathbf{t}} = \check{\psi} \cdot \check{\mathbf{t}} + R_{\check{\kappa}b} \check{\omega}^{\bar{1}} \cdot \check{\mathbf{t}} = \check{\psi} \cdot \check{\mathbf{t}} + \check{\omega}^{\bar{1}} \cdot R_{\check{\kappa}b}^{-1} \check{\mathbf{t}} = \check{\psi} \cdot \check{\mathbf{t}} + \check{\omega}^{\bar{1}} \cdot \check{\mathbf{t}}^{\bar{1}} = \check{\psi} \cdot \check{\mathbf{t}} + \check{\sigma}^{\bar{1}}; \quad (4.60.4)$$

and finally see $\Delta\check{\sigma} = \check{\sigma} - \check{\sigma}^{\bar{1}} = \check{\psi} \cdot \check{\mathbf{t}}$.

$\check{\psi}$ and $\check{\mathbf{t}}$ are both independent of \check{P} . And this means that $\Delta\check{\sigma}$ is independent of the frame, too. We can choose a parallel frame that simplifies the calculations. Fix i_0 —that is I will calculate $\Delta\check{\sigma}_{i_0}$. The original parallel frame will not be used any longer. Hence without loss of generality I assume $\check{P} := (\check{\mathbf{t}} \quad \check{\mathbf{v}} \quad \check{\mathbf{p}}_{i_0}(\check{\mathbf{b}}^{i_0})) \in \mathcal{E}$ with $\check{\mathbf{v}} := \check{\mathbf{p}}_{i_0}(\check{\mathbf{b}}^{i_0} \times \check{\mathbf{t}}^{i_0})$.

The important property of this parallel frame is

$$\check{\mathbf{p}}_{i_0}(\check{\mathbf{b}}^{i_0}) = \check{\mathbf{b}}^{i_0} = R_{\check{\kappa}b}^{-1} \check{\mathbf{b}}^{i_0} = R_{\check{\kappa}b}^{-1} \check{\mathbf{p}}_{i_0}(\check{\mathbf{b}}^{i_0}) = R_{\check{\kappa}b}^{-1} R_{\check{\kappa}b} \check{\mathbf{p}}_{i_0}^{i_0-1}(\check{\mathbf{b}}^{i_0}) = \check{\mathbf{p}}_{i_0}^{i_0-1}(\check{\mathbf{b}}^{i_0}). \quad (4.60.5)$$

That is $\Delta\check{P}^{i_0}$ rotates around $\check{\mathbf{b}}^{i_0}$. In particular we have

$$\begin{aligned} \hat{\Delta}\check{P}_{i_0} &= (\check{P}^{i_0-1})^{-1} R_{\check{\kappa}b}^{i_0} \check{P}^{i_0-1} = (\check{P}^{i_0-1})^{-1} R_{\check{\mathbf{b}}^{i_0}, \check{\phi}_{i_0}} \check{P}^{i_0-1} = R_{(\check{P}^{i_0-1})^{-1} \check{\mathbf{b}}^{i_0}, \check{\phi}_{i_0}} \\ &= R_{\mathbf{e}_3, \check{\phi}_{i_0}}. \end{aligned} \quad (4.60.6)$$

From eq. (2.62.2) on page 11: $\Delta\check{\sigma}_{i_0} = \check{\omega}^{i_0} \cdot \check{\mathbf{t}}^{i_0} - \check{\omega}^{i_0-1} \cdot \check{\mathbf{t}}^{i_0-1} = \check{\mathbf{v}}^{i_0} \cdot \check{\mathbf{b}}^{i_0} - \check{\mathbf{v}}^{i_0-1} \cdot \check{\mathbf{b}}^{i_0} = (\check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1}) \cdot \check{\mathbf{b}}^{i_0}$. We can calculate $(\check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1}) \cdot \check{\mathbf{b}}^{i_0}$ using a trick. First we look at $\check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1}$:

$$\begin{aligned} \check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1} &= \check{P}^{i_0} \mathbf{e}_2 - \check{P}^{i_0-1} \mathbf{e}_2 = \check{P}^{i_0-1} \hat{\Delta}\check{P}_{i_0} \mathbf{e}_2 - \check{P}^{i_0} \hat{\Delta}\check{P}_{i_0}^{-1} \mathbf{e}_2 \\ &= \check{P}^{i_0-1} R_{\mathbf{e}_3, \check{\phi}_{i_0}} \mathbf{e}_2 - \check{P}^{i_0} R_{\mathbf{e}_3, -\check{\phi}_{i_0}} \mathbf{e}_2 \\ &= \check{P}^{i_0-1} (\cos \check{\phi}_{i_0} \mathbf{e}_2 - \sin \check{\phi}_{i_0} \mathbf{e}_1) - \check{P}^{i_0} (\cos \check{\phi}_{i_0} \mathbf{e}_2 + \sin \check{\phi}_{i_0} \mathbf{e}_1) \\ &= \cos \check{\phi}_{i_0} (\check{P}^{i_0-1} - \check{P}^{i_0}) \mathbf{e}_2 - \sin \check{\phi}_{i_0} (\check{P}^{i_0-1} + \check{P}^{i_0}) \mathbf{e}_1 \\ &= -\cos \check{\phi}_{i_0} (\check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1}) - \sin \check{\phi}_{i_0} (\check{\mathbf{t}}^{i_0-1} + \check{\mathbf{t}}^{i_0}) \end{aligned} \quad (4.60.7)$$

Hence, since $\check{\phi}_{i_0} \neq \pi$ ($\check{\gamma}$ is regular),

$$\begin{aligned} (\check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1}) (1 + \cos \check{\phi}_{i_0}) &= -\sin \check{\phi}_{i_0} (\check{\mathbf{t}}^{i_0-1} + \check{\mathbf{t}}^{i_0}) \\ \iff \check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1} &= -\frac{\sin \check{\phi}_{i_0}}{1 + \cos \check{\phi}_{i_0}} (\check{\mathbf{t}}^{i_0-1} + \check{\mathbf{t}}^{i_0}) \end{aligned} \quad (4.60.8)$$

Finally we have

$$\begin{aligned} (\dot{\check{\mathbf{v}}}^{i_0} - \dot{\check{\mathbf{v}}}^{i_0-1}) \cdot \check{\mathbf{b}}^{i_0} &= \frac{d}{dt} (\check{\mathbf{v}}^{i_0} - \check{\mathbf{v}}^{i_0-1}) \cdot \check{\mathbf{b}}^{i_0} \\ &= -\frac{\sin \check{\phi}_{i_0}}{1 + \cos \check{\phi}_{i_0}} (\dot{\check{\mathbf{t}}}^{i_0-1} + \dot{\check{\mathbf{t}}}^{i_0}) \cdot \check{\mathbf{b}}^{i_0} - \frac{d}{dt} \frac{\sin \check{\phi}_{i_0}}{1 + \cos \check{\phi}_{i_0}} (\check{\mathbf{t}}^{i_0-1} + \check{\mathbf{t}}^{i_0}) \cdot \check{\mathbf{b}}^{i_0} \\ &= -\frac{\sin \check{\phi}_{i_0}}{1 + \cos \check{\phi}_{i_0}} (\dot{\check{\mathbf{t}}}^{i_0-1} + \dot{\check{\mathbf{t}}}^{i_0}) \cdot \check{\mathbf{b}}^{i_0} - 0 \\ &= -\frac{\sin \check{\phi}_{i_0}}{1 + \check{\mathbf{t}}^{i_0-1} \cdot \check{\mathbf{t}}^{i_0}} \check{\mathbf{b}}^{i_0} \cdot (\dot{\check{\mathbf{t}}}^{i_0-1} + \dot{\check{\mathbf{t}}}^{i_0}) \\ &= -\frac{\check{\mathbf{t}}^{i_0-1} \times \check{\mathbf{t}}^{i_0}}{1 + \check{\mathbf{t}}^{i_0-1} \cdot \check{\mathbf{t}}^{i_0}} \cdot (\dot{\check{\mathbf{t}}}^{i_0-1} + \dot{\check{\mathbf{t}}}^{i_0}) \end{aligned} \quad (4.60.9)$$

For the last step I have used $\sin \check{\phi}_{i_0} \check{\mathbf{b}}^{i_0-1} = \check{\mathbf{t}}^{i_0-1} \times \sin \check{\phi}_{i_0-1} \check{\mathbf{v}}^{i_0-1} = \check{\mathbf{t}}^{i_0-1} \times (\sin \check{\phi}_{i_0} \check{\mathbf{v}}^{i_0-1} + \cos \check{\phi}_{i_0} \check{\mathbf{t}}^{i_0-1}) = \check{\mathbf{t}}^{i_0-1} \times \check{\mathbf{t}}^{i_0}$. \square

Remark 4.61. We can rewrite the first result as $\Delta \check{\sigma} = -\kappa \check{\mathbf{b}} \cdot \left(\frac{1}{2} \dot{\check{\mathbf{t}}}^{\bar{1}} + \frac{1}{2} \dot{\check{\mathbf{t}}} \right) = -\kappa \check{\mathbf{b}} \cdot \dot{\check{\mathbf{t}}}^{\check{\vee}}$. Compare this to eq. (2.77.1) on page 13.

Variational Formulation

Motivation What really interests us is the temporal twist in response to deformations of a fixed curve, ie the twist variation of parallel frames for a variation of the curve. We can use the work done so far, but we have to reformulate it using variational principles in order to obtain it as variation.

See [Bri08, chapter 1] for more details on variational principles and notation.

Theorem 4.62. *Given a (non-time-varying) discrete curve $\check{\gamma}$ and a variation $\delta \check{\gamma} \in \mathcal{V}(\check{I}; \mathbb{R}^3)$, the variational twist $\check{\sigma}[\check{\gamma}, \delta \check{\gamma}]$ of arbitrary parallel frames is*

$$\Delta \check{\sigma}[\check{\gamma}; \delta \check{\gamma}] = -\frac{\kappa \check{\mathbf{b}}}{2|\Delta \check{\gamma}|} \cdot (\delta \check{\gamma}_{\perp} - \delta \check{\gamma}_{\bar{1}}) \quad (4.62.1)$$

$$\check{\sigma}^b[\check{\gamma}; \delta \check{\gamma}] - \check{\sigma}^a[\check{\gamma}; \delta \check{\gamma}] = \sum_{i=a+1}^b \Delta \check{\sigma}_i[\check{\gamma}; \delta \check{\gamma}] \quad (4.62.2)$$

Proof. This is mainly a notational exercise.

Let \check{P} be an arbitrary parallel frame along $\check{\gamma}$, and $\check{\mathbf{v}}_{\delta \check{\gamma}}(t) := \check{\gamma} + t \delta \check{\gamma}$. Set $\mathbf{F}^i[\check{\mathbf{v}}_{\delta \check{\gamma}}(t)] := \check{Q}^i(0)$, where \check{Q} is the discrete parallel frame along the discrete time-varying curve $\check{\mathbf{v}}_{\delta \check{\gamma}}(t)$ that is constructed by parallel transporting³ \check{P}^0 along $\check{\mathbf{v}}_{\delta \check{\gamma}}^0$ in time. Hence $\check{Q} \mathbf{e}_1 \parallel \Delta \check{\mathbf{v}}_{\delta \check{\gamma}}(t)$ and \check{Q} is well-defined.

³ie parallel transporting each axis of \check{P}^0

The variation of F^i is defined as $\delta F^i [\check{v}; \delta \check{\gamma}] = \left. \frac{d}{dt} F^i [\check{\gamma} + t \delta \check{\gamma}] \right|_{t=0} = \dot{Q}^i(0) = [\check{\omega}] \check{Q}^i(0)$. From the construction of \check{Q} , we conclude that $\check{Q}(0) = \check{P}$. Let $\check{\psi}$ be defined by $\delta F^i [\check{v}; \delta \check{\gamma}] = [\check{\psi}] F^i [\check{\gamma}] = [\check{\psi}] \check{P}^i(0)$. This implies $[\check{\psi}] \check{P}^i(0) = [\check{\omega}] \check{Q}^i(0) = [\check{\omega}] \check{P}^i(0)$. Hence $\check{\psi} = \check{\omega}$ and $\check{\sigma} = \check{\omega} \cdot \check{t} = \check{\psi} \cdot \check{t}$, that is the twist of the angular velocity of the variation is exactly $\check{\sigma}$, which we have found above.

To obtain the first equation, we set $\check{\gamma}(t) := \check{\gamma} + t \delta \check{\gamma}$ and we only need to use $\frac{d}{dt} \check{\gamma} = \delta \check{\gamma}$ and $\dot{\check{t}} = \frac{d}{dt} \frac{\check{\gamma}_\perp - \check{\gamma}}{|\Delta \check{\gamma}|} = \frac{1}{|\Delta \check{\gamma}|} (\dot{\check{\gamma}}_\perp - \dot{\check{\gamma}}) = \frac{1}{|\Delta \check{\gamma}|} (\delta \check{\gamma}_\perp - \delta \check{\gamma})$. Then $\dot{\check{t}}^\perp + \dot{\check{t}} = \frac{1}{|\Delta \check{\gamma}|} (\delta \check{\gamma} - \delta \check{\gamma}_\perp + \delta \check{\gamma}_\perp - \delta \check{\gamma})$ and the equation follows. \square

Remark 4.63. $\Delta \check{\sigma} [\check{\gamma}; \delta \check{\gamma}]$ is a linear function in $\delta \check{\gamma}$, and as such immediately

$$\frac{\Delta \check{\sigma}^\perp}{\partial \check{\gamma}} = -\frac{(\check{\kappa} \check{b}_\perp)^T}{2 |\Delta \check{\gamma}|}, \quad \frac{\Delta \check{\sigma}^\perp}{\partial \check{\gamma}} = \frac{(\check{\kappa} \check{b}_\perp)^T}{2 |\Delta \check{\gamma}|}, \text{ and for all other } j: \frac{\Delta \check{\sigma}^j}{\partial \check{\gamma}} = 0. \quad (4.63.1)$$

Note that the $\check{\kappa} \check{b}$ terms are not transposed in [BWR⁺08].

Notation 4.64. Note that I have not written $\partial \Delta \check{\sigma}$ because $\Delta \check{\sigma}$ is already the (total) derivative. I don't want to derive it again: I want to refer to one specific partial derivative of which it is made up.

Discrete rod model

Summary I follow [BWR⁺08] and discretize the (dynamic) continuous curve-angle model. However, I only consider arc-length parameterized rods, that is rods whose edges have all the same length. This simplifies calculations a bit, and moreover the mathematical foundation for arc-length parameterized curvature is sound.

Definition 5.1. A *discrete rod* is a tuple $\check{\Gamma} := (\check{\gamma}, \check{\theta}, \check{r}^0)$. $\check{\gamma}$ is an arc-length parameterized time-varying discrete curve defined on $\check{I} \times T$, $\check{I} := \{0, \dots, n+1\}$, $0 \in T \subset \mathbb{R}$, and represents the **discrete centerline curve**; $\check{r}^0 : J \rightarrow \mathbb{R}^3$, $t \mapsto \check{r}^0(t)$ is the **discrete rail vector** and is parallel transported in time along $\check{\gamma}_0(\bullet)$; and $\check{\theta} \in \mathcal{E}(\check{I}^1; \mathbb{R})$ is the **discrete material frame angle** and represents the (directed) angle between the parallel transported rail vector and the material frame oriented around the edge tangents.

Remark 5.2. The rail vector \check{r} becomes an edge quantity by parallel transporting it: $\check{r} := \check{p}_0(\check{r}^0) \in \mathcal{E}(\check{I}^1)$.

Definition 5.3. The **discrete Bishop frame** $\check{B} \in \mathcal{E}(\check{I}^1)$ is a discrete parallel frame: $\check{B} := (\check{t} \quad \check{r} \quad \check{t} \times \check{r})$.

Remark 5.4. \check{B} is well-defined. It is a parallel frame:

$$\Delta \check{B} = \check{B}(\check{B}^1)^{-1} = \begin{pmatrix} R_{\check{\kappa}\check{b}} \check{t}^1 & R_{\check{\kappa}\check{b}} \check{r}^1 & R_{\check{\kappa}\check{b}}(\check{t}^1 \times \check{r}^1) \end{pmatrix} (\check{B}^1)^{-1} = R_{\check{\kappa}\check{b}} \check{B}^1 (\check{B}^1)^{-1} = R_{\check{\kappa}\check{b}}. \quad (5.4.1)$$

Remark 5.5. Because the rail vector is parallel transported in time, the twist of the angular velocity of the Bishop frame at the first edge \check{B}^0 vanishes: $\check{\sigma}^0(\bullet) = 0$.

Definition 5.6. The **discrete material frame** $\check{M} \in \mathcal{E}$ is a discrete frame: $\check{M} := \check{B}R_{\mathbf{e}_1, \check{\theta}}$.

Remark 5.7. This is also well-defined, because $\check{M}\mathbf{e}_1 = \check{B}R_{\mathbf{e}_1, \check{\theta}}\mathbf{e}_1 = \check{B}\mathbf{e}_1 = \check{t}$.

Definition 5.8. The **discrete material twist** $\check{\tau} \in \mathcal{V}$ is the discrete twist of the material frame¹ \check{M} .

Proposition 5.9. $\check{\tau} = \Delta \check{\theta}$

Proof. With remark 2.18 on page 5 we transform $\check{M} = \check{B}R_{\mathbf{e}_1, \check{\theta}} = R_{\check{\kappa}\check{b}}\check{B}^1R_{\mathbf{e}_1, \check{\theta}^1}R_{\mathbf{e}_1, \Delta \check{\theta}} = R_{\check{\kappa}\check{b}}\check{M}^1R_{\mathbf{e}_1, \Delta \check{\theta}}$. Finally proposition 4.50 on page 26 proves $\check{\tau} = \Delta \check{\theta}$. \square

¹see proposition 4.48 on page 26

5.1 Discrete rod energy

Integrated and pointwise quantities Vertex quantities like eg curvature do not make sense when seen as pointwise quantities in the discrete setting. Curvature or twist are not “concentrated” on points but distributed over the edges.

[BWR⁺08] assumes that the integrated quantities are distributed uniformly over the edges: an integrated quantity is distributed uniformly in its Voronoi cell.

In the case of discrete curves this means that an integrated vertex quantity $\alpha \in \mathcal{V}$ is distributed over half the previous edge and half the next edge. This **domain** is independent of the quantity itself. I write $\mathcal{D}_i^\mathcal{V} \in \mathcal{V}$ for the domain of the i -th vertex, and $|\mathcal{D}_i^\mathcal{V}| \in \mathcal{V}$ for its length. Since the centerline curve is arc-length parameterized, this means that the corresponding pointwise quantity $\delta\alpha \in \mathcal{V}$ is $\delta\alpha_i = \frac{\alpha_i}{|\mathcal{D}_i^\mathcal{V}|} = \frac{\alpha_i}{|\Delta\tilde{\gamma}|} \forall i \in \tilde{I}_1^1$, and $\delta\alpha_i = \frac{\alpha_i}{\frac{1}{2}|\mathcal{D}_i^\mathcal{V}|} = \frac{\alpha_i}{\frac{1}{2}|\Delta\tilde{\gamma}|} \forall i \in \{\min \tilde{I}, \max \tilde{I}\}$.

Likewise an integrated edge quantity $\beta \in \mathcal{E}$ is distributed over ‘its’ edge. Analogously I write $\mathcal{D}_i^\mathcal{E} \in \mathcal{E}$ for the domain of the i -th edge, and $|\mathcal{D}_i^\mathcal{E}| \in \mathcal{E}$ for its length. In the end this again means that the corresponding pointwise quantity is $\delta\beta^i = \frac{\beta^i}{|\mathcal{D}_i^\mathcal{E}|} = \frac{\beta^i}{|\Delta\tilde{\gamma}|} \forall i \in \tilde{I}$. No special attention has to be paid to the boundaries, because they are still ‘full’ edges.

Note that, if the curve were not arc-length parameterized, edge and vertex domains would be treated differently.

Here I have informally introduced the δ operator which transforms an integrated quantity to a pointwise one and the integration domains $\mathcal{D}^\mathcal{V}$ and $\mathcal{D}^\mathcal{E}$.

Last but not least discrete pointwise quantities $\rho \in \mathcal{V}$ and $\sigma \in \mathcal{E}$ can be interpreted as continuous quantities by setting $\rho(x) = \rho_i \forall x \in \mathcal{D}_i^\mathcal{V}$ and $\sigma(x) = \sigma^i \forall x \in \mathcal{D}_i^\mathcal{E}$.

Definition 5.10. The *integral over a discrete pointwise quantity* along a discrete curve $\tilde{\gamma}$ is defined as follows for $\alpha \in \mathcal{V}(\tilde{I})$ and $\beta \in \mathcal{E}(\tilde{J})$:

$$\int_{\tilde{\gamma}} f(\alpha) = \int_{\tilde{\gamma}} f(\alpha) dx = \sum_{i \in \tilde{I}} \int_{\mathcal{D}_i^\mathcal{V}} f(\alpha) dx = \sum_{i \in \tilde{I}} f(\alpha_i) |\mathcal{D}_i^\mathcal{V}| \quad (5.10.1)$$

$$\int_{\tilde{\gamma}} g(\beta) = \int_{\tilde{\gamma}} g(\beta) dx = \sum_{i \in \tilde{J}} \int_{\mathcal{D}_i^\mathcal{E}} g(\beta) dx = \sum_{i \in \tilde{J}} g(\beta^i) |\mathcal{D}_i^\mathcal{E}| \quad (5.10.2)$$

Remark 5.11. Then the **integral over a discrete integrated quantity** along a discrete curve $\tilde{\gamma}$ for $\alpha \in \mathcal{V}(\tilde{I})$ and $\beta \in \mathcal{E}(\tilde{J})$ is:

$$\int_{\tilde{\gamma}} f(\alpha) = \int_{\tilde{\gamma}} f(\delta\alpha) dx = \sum_{i \in \tilde{I}} \int_{\mathcal{D}_i^\mathcal{V}} f(\delta\alpha) dx = \sum_{i \in \tilde{I}} f\left(\frac{\alpha_i}{|\mathcal{D}_i^\mathcal{V}|}\right) |\mathcal{D}_i^\mathcal{V}| \quad (5.11.1)$$

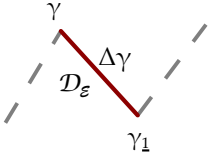
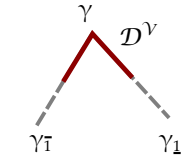
$$\int_{\tilde{\gamma}} g(\beta) = \int_{\tilde{\gamma}} g(\delta\beta) dx = \sum_{i \in \tilde{J}} \int_{\mathcal{D}_i^\mathcal{E}} g(\delta\beta) dx = \sum_{i \in \tilde{J}} g\left(\frac{\beta^i}{|\mathcal{D}_i^\mathcal{E}|}\right) |\mathcal{D}_i^\mathcal{E}| \quad (5.11.2)$$

Definition 5.12. The *potential energy of a discrete rod* $\tilde{\Gamma}$ is

$$\check{E}(\tilde{\Gamma}) := \check{E}_{bend}(\tilde{\Gamma}) + \check{E}_{twist}(\tilde{\Gamma}) \quad (5.12.1)$$

$$\check{E}_{bend}(\tilde{\Gamma}) := \frac{1}{2} \int_{\tilde{\gamma}} \alpha \check{\kappa}^2 \quad (5.12.2)$$

$$\check{E}_{twist}(\tilde{\Gamma}) := \frac{1}{2} \int_{\tilde{\gamma}} \beta \check{\tau}^2 \quad (5.12.3)$$



Remark 5.13. This is analogous to corollary 3.8 on page 16.

Remark 5.14. Applying the definition above, the energy terms become:

$$\check{E}_{bend}(\check{\Gamma}) = \frac{1}{2} \sum_{i \in \check{I}_1^{\bar{1}}} \alpha \left(\frac{\check{\kappa}_i}{|\Delta\check{\gamma}|} \right)^2 |\Delta\check{\gamma}| = \frac{1}{2} \sum_{i=1}^n \alpha \frac{\check{\kappa}_i^2}{|\Delta\check{\gamma}|} \quad (5.14.1)$$

$$\check{E}_{twist}(\check{\Gamma}) = \frac{1}{2} \sum_{i \in \check{I}_1^{\bar{1}}} \beta \left(\frac{\check{\tau}_i}{|\Delta\check{\gamma}|} \right)^2 |\Delta\check{\gamma}| = \frac{1}{2} \sum_{i=1}^n \beta \frac{\check{\tau}_i^2}{|\Delta\check{\gamma}|} \quad (5.14.2)$$

$$\check{E}(\check{\Gamma}) = \frac{1}{2} \sum_{i=1}^n \frac{\alpha \check{\kappa}_i^2 + \beta \check{\tau}_i^2}{|\Delta\check{\gamma}|} \quad (5.14.3)$$

Definition 5.15. The *discrete kinetic energy* of a discrete rod $\check{\Gamma}$ is

$$\check{E}_{kinetic} := \frac{1}{2} \int_{\check{\gamma}} \rho \pi r^2 \dot{\check{\gamma}}^2 \quad (5.15.1)$$

Remark 5.16. If we apply definition 5.10 on the facing page, we see

$$\begin{aligned} \check{E}_{kinetic} &= \frac{1}{2} \rho \pi r^2 \frac{|\Delta\check{\gamma}|}{2} \dot{\check{\gamma}}_0^2 + \sum_{i \in \check{I}_1^{\bar{1}}} \frac{1}{2} \rho \pi r^2 |\Delta\check{\gamma}| \dot{\check{\gamma}}_i^2 + \frac{1}{2} \rho \pi r^2 \frac{|\Delta\check{\gamma}|}{2} \dot{\check{\gamma}}_{n+1}^2 \\ &= \frac{1}{2} \frac{\check{m}}{2} \dot{\check{\gamma}}_0^2 + \sum_{i \in \check{I}_1^{\bar{1}}} \frac{1}{2} \check{m} \dot{\check{\gamma}}_i^2 + \frac{1}{2} \frac{\check{m}}{2} \dot{\check{\gamma}}_{n+1}^2 \end{aligned} \quad (5.16.1)$$

with the mass quantity $\check{m} := \rho \pi r^2 |\Delta\check{\gamma}| \in \mathcal{V}(\check{I})$.

Thus we can interpret the vertices as mass particles, whereas the first and last one only have half the mass of the other vertices. This makes sense.

5.2 Discrete quasistatic material frames

Quasistatic material frame condition We can carry over the quasistatic material frame condition from section 3.7 on page 19 easily:

$$\frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\theta}} = 0 \text{ for any edge that is not subject to boundary conditions.} \quad (5.16.2)$$

Proposition 5.17. In the isotropic case, twist is distributed uniformly over the rod:

$$\frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\theta}} = 0 \implies \Delta \check{\theta} = \check{\tau} = \text{const.} \quad (5.17.1)$$

Proof. The following only holds for edge indices $\in \check{I}_1^{\bar{1}}$. Using $\check{\tau} = \Delta \check{\theta} = \check{\theta} - \check{\theta}^{\bar{1}}$ and applying the chain rule leads to

$$0 = \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\theta}} = \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}} \frac{\partial \check{\tau}}{\partial \check{\theta}} + \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}_1} \frac{\partial \check{\tau}_1}{\partial \check{\theta}} = \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}} - \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}_1} \iff \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}} = \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}_1}. \quad (5.17.2)$$

Lastly we determine the partial derivative $\frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}} = \frac{\beta}{|\Delta \check{\gamma}|} \check{\tau}$ and substitute to obtain

$$\frac{\beta}{|\Delta \check{\gamma}|} \check{\tau} = \frac{\beta}{|\Delta \check{\gamma}|} \check{\tau}_1 \iff \check{\tau} = \check{\tau}_1 \iff \check{\tau} = \text{const.} \quad (5.17.3)$$

□

Corollary 5.18. *If the material frame of one end of the rod is free, that is there are no material frame boundary conditions for it, there is no twist: $\check{\tau} = 0$.*

Proof. I assume the first material is free. The other case is similar. We can apply (5.16.2) to the first edge, too: $0 = \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\theta}^0} = \frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}_1} \frac{\partial \check{\tau}_1}{\partial \check{\theta}^0} = -\frac{\partial \check{E}(\check{\Gamma})}{\partial \check{\tau}_1} = -\frac{\beta}{|\Delta \check{\gamma}|} \check{\tau}_1 \iff \check{\tau}_1 = 0$. As $\check{\tau}$ is constant, the statement follows. □

Corollary 5.19. $\check{E}_{twist}(\check{\Gamma}) = \frac{1}{2} \beta \frac{(\check{\theta}^n - \check{\theta}^0)^2}{n |\Delta \check{\gamma}|}$

Proof. With proposition 4.11 on page 23:

$$\check{\theta}^n - \check{\theta}^0 = \sum_{i \in \check{I}_1^{\check{\Gamma}}} \Delta \check{\theta} = \sum_{i \in \check{I}_1^{\check{\Gamma}}} \check{\tau} = \sum_{i=1}^n \check{\tau} = n \check{\tau}. \quad (5.19.1)$$

So $\check{\tau} = \frac{\check{\theta}^n - \check{\theta}^0}{n}$. Substituting into (5.14.2) yields:

$$\check{E}_{twist}(\check{\Gamma}) = \frac{1}{2} \sum_{i=1}^n \beta \frac{\check{\tau}_i^2}{|\Delta \check{\gamma}|} = \frac{1}{2} \sum_{i=1}^n \beta \frac{(\check{\theta}^n - \check{\theta}^0)^2}{n^2 |\Delta \check{\gamma}|} = \frac{1}{2} \beta \frac{(\check{\theta}^n - \check{\theta}^0)^2}{n |\Delta \check{\gamma}|}. \quad (5.19.2)$$

□

Summary I have shown that the discrete rod behaves just like the continuous rod in the isotropic case. Both exhibit constant twist rates along the rod, and zero twist if one or both ends is not fixed against untwisting.

Simulation using constrained Lagrangian mechanics

Motivation We have a simplified potential energy term for the discrete rod. The next steps usually are setting up the Lagrangian equations and constraints, and solving for the forces.

[BWR⁺08] uses the **Fast Manifold Projection** algorithm to solve the constrained system. It is described in [GHF⁺07] and [Gol10] with helpful insights from [BFA02].

It works by solving the forces of the unconstrained system first, integrating them, and then “correcting” this unconstrained integration step by projecting it back onto the constraint manifold¹.

Thus we need to calculate the forces of the unconstrained system first.

6.1 Force calculation in the unconstrained system

6.1.1 Unconstrained Lagrangian system

The **Lagrangian function** of the discrete rod is

$$L(\check{\Gamma}) := \check{E}_{kinetic}(\check{\Gamma}) - \check{E}(\check{\Gamma}). \quad (6.0.1)$$

The discrete curve $\check{\gamma}$ satisfies the **Euler-Lagrange equation**:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\check{\gamma}}} = \frac{\partial L}{\partial \check{\gamma}}. \quad (6.0.2)$$

Then the force $\check{\mathbf{f}} \in \mathcal{V}(\check{I})$ is, according to [Arn89],

$$\check{\mathbf{f}} := \frac{d}{dt} \frac{\partial L}{\partial \dot{\check{\gamma}}} = \frac{\partial L}{\partial \check{\gamma}} = -\frac{\partial \check{E}}{\partial \check{\gamma}} = -\frac{\partial \check{E}_{bend}}{\partial \check{\gamma}} - \frac{\partial \check{E}_{twist}}{\partial \check{\gamma}}. \quad (6.0.3)$$

6.1.2 Bending force calculation

We calculate $\frac{\partial \check{E}_{bend}}{\partial \check{\gamma}_i}$:

$$\frac{\partial \check{E}_{bend}}{\partial \check{\gamma}_i} = \frac{\alpha}{|\Delta \check{\gamma}|} \left(\check{\kappa} \check{\mathbf{b}}_{i+1} \cdot \frac{\partial \check{\kappa} \check{\mathbf{b}}_{i+1}}{\partial \check{\gamma}_i} + \check{\kappa} \check{\mathbf{b}}_i \cdot \frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \check{\gamma}_i} + \check{\kappa} \check{\mathbf{b}}_{i-1} \cdot \frac{\partial \check{\kappa} \check{\mathbf{b}}_{i-1}}{\partial \check{\gamma}_i} \right). \quad (6.0.4)$$

¹see [Arn89, chapter 4]

The equation above is only valid for $i \in \tilde{I}_1^1$. For $i \in \{\min \tilde{I}, \max \tilde{I}\}$, the first or last dot product does not appear. I only calculate one of the partial derivatives. The others are special cases and follow immediately from this one, see [BWR⁺08].

I start with

$$\begin{aligned} \frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \check{\gamma}_i} &= \frac{\partial}{\partial \check{\gamma}_i} \left(2 \frac{\check{\mathbf{t}}^{i-1} \times \check{\mathbf{t}}^i}{1 + \check{\mathbf{t}}^{i-1} \cdot \check{\mathbf{t}}^i} \right) = \frac{\partial}{\partial \check{\gamma}_i} \left(2 \frac{\Delta \check{\gamma}^{i-1} \times \Delta \check{\gamma}^i}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} \right) \\ &= \frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^{i-1}} \frac{\partial \Delta \check{\gamma}^{i-1}}{\partial \check{\gamma}_i} + \frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^i} \frac{\partial \Delta \check{\gamma}^i}{\partial \check{\gamma}_i} = \frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^{i-1}} - \frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^i}. \end{aligned} \quad (6.0.5)$$

Because of the antisymmetry of $\check{\kappa} \check{\mathbf{b}}$, $\frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^{i-1}} = -\frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^i}$ up to swapping of variables. We only need to calculate $\frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^i}$:

$$\begin{aligned} \frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^i} &= \frac{\partial}{\partial \Delta \check{\gamma}^i} \left(2 \frac{\Delta \check{\gamma}^{i-1} \times \Delta \check{\gamma}^i}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} \right) \\ &= \frac{2 \frac{\partial}{\partial \Delta \check{\gamma}^i} \left([\Delta \check{\gamma}^{i-1}] \Delta \check{\gamma}^i \right)}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} - \frac{2 \Delta \check{\gamma}^{i-1} \times \Delta \check{\gamma}^i}{(|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i)^2} \frac{\partial}{\partial \Delta \check{\gamma}^i} (|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i) \\ &= \frac{2 [\Delta \check{\gamma}^{i-1}]}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} - \frac{2 \Delta \check{\gamma}^{i-1} \times \Delta \check{\gamma}^i}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} \frac{(\Delta \check{\gamma}^{i-1})^T}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} \\ &= \frac{2 [\Delta \check{\gamma}^{i-1}] - \check{\kappa} \check{\mathbf{b}}_i (\Delta \check{\gamma}^{i-1})^T}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} = \frac{1}{|\Delta \check{\gamma}|} \frac{2 [\check{\mathbf{t}}^{i-1}] - \check{\kappa} \check{\mathbf{b}}_i (\check{\mathbf{t}}^{i-1})^T}{1 + \check{\mathbf{t}}^{i-1} \cdot \check{\mathbf{t}}^i}. \end{aligned} \quad (6.0.6)$$

Knowing this, we can immediately deduce² $\frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^{i-1}}$:

$$\frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \Delta \check{\gamma}^{i-1}} = -\frac{2 [\Delta \check{\gamma}^i] + \check{\kappa} \check{\mathbf{b}}_i (\Delta \check{\gamma}^i)^T}{|\Delta \check{\gamma}|^2 + \Delta \check{\gamma}^{i-1} \cdot \Delta \check{\gamma}^i} = -\frac{1}{|\Delta \check{\gamma}|} \frac{2 [\check{\mathbf{t}}^i] + \check{\kappa} \check{\mathbf{b}}_i (\check{\mathbf{t}}^i)^T}{1 + \check{\mathbf{t}}^{i-1} \cdot \check{\mathbf{t}}^i} \quad (6.0.7)$$

Finally

$$\frac{\partial \check{\kappa} \check{\mathbf{b}}_i}{\partial \check{\gamma}_i} = -\frac{1}{|\Delta \check{\gamma}|} \frac{2 [\check{\mathbf{t}}^i] + \check{\kappa} \check{\mathbf{b}}_i (\check{\mathbf{t}}^i)^T}{1 + \check{\mathbf{t}}^{i-1} \cdot \check{\mathbf{t}}^i} - \frac{1}{|\Delta \check{\gamma}|} \frac{2 [\check{\mathbf{t}}^{i-1}] - \check{\kappa} \check{\mathbf{b}}_i (\check{\mathbf{t}}^{i-1})^T}{1 + \check{\mathbf{t}}^{i-1} \cdot \check{\mathbf{t}}^i}. \quad (6.0.8)$$

6.1.3 Twisting force calculation

Calculating $\frac{\partial \check{E}_{twist}}{\partial \check{\gamma}}$ is a bit more challenging. $\check{\gamma}$ does not occur in our formulation of \check{E}_{twist} . However, we can use the chain rule to obtain

$$\frac{\partial \check{E}_{twist}}{\partial \check{\gamma}_i} = \sum_{j=0}^n \frac{\partial \check{E}_{twist}}{\partial \check{\theta}^j} \frac{\partial \check{\theta}^j}{\partial \check{\gamma}_i}. \quad (6.0.9)$$

I assume that there are material frame boundary conditions for both ends. Otherwise $\frac{\partial \check{E}_{twist}}{\partial \check{\theta}^j} = 0$ and we are done.

²the swap of variables flips the sign in front of $\check{\kappa} \check{\mathbf{b}}_i$

Because of section 5.2 on page 33 $\frac{\partial \check{E}_{twist}}{\partial \check{\theta}^i} = 0$ for $i \in \bar{I}_1^1$ and we only have to consider the partial derivatives for³ $i \in \{\min \check{I}, \max \check{I}\}$:

$$\frac{\partial \check{E}_{twist}}{\partial \check{\theta}^n} = \frac{\partial}{\partial \check{\theta}^n} \left(\frac{1}{2} \beta \frac{(\check{\theta}^n - \check{\theta}^0)^2}{n |\Delta \check{\gamma}|} \right) \stackrel{(5.19)}{=} \beta \frac{\check{\theta}^n - \check{\theta}^0}{n |\Delta \check{\gamma}|} \quad (6.0.10)$$

$$\frac{\partial \check{E}_{twist}}{\partial \check{\theta}^0} = \frac{\partial}{\partial \check{\theta}^0} \left(\frac{1}{2} \beta \frac{(\check{\theta}^n - \check{\theta}^0)^2}{n |\Delta \check{\gamma}|} \right) \stackrel{(5.19)}{=} -\beta \frac{\check{\theta}^n - \check{\theta}^0}{n |\Delta \check{\gamma}|} \quad (6.0.11)$$

Calculating $\frac{\partial \check{\theta}^j}{\partial \check{\gamma}_i}$ is a bit tricky. How does the material angle change if the curve is deformed? The answer is: it does not.

However, as we have seen in section 4.4.2 on page 27, parallel frames do change and twist under variation. And with them the parallel rail field, too, which determines the material frame together with the material frame angle $\check{\theta}$. The material frame does not change because it is quasistatic (which is obvious if we assume for a moment that the end tangents are fixed, too). Thus the material frame angle $\check{\theta}$ has to change to counteract the additional twisting of the parallel rail field. We have

$$\frac{\partial \check{\theta}^j}{\partial \check{\gamma}_i} = -\frac{\check{\sigma}^j}{\partial \check{\gamma}_i} \quad (6.0.12)$$

$\frac{\check{\sigma}^j}{\partial \check{\gamma}_i}$ is nothing else but the variational twist around $\check{\gamma}_i$. For $\delta \check{\gamma}_i \in \mathbb{R}^3$:

$$\frac{\check{\sigma}^j}{\partial \check{\gamma}_i} \delta \check{\gamma}_i = \check{\sigma}^j(0) \text{ with } \dot{\check{\gamma}}_i(0) = \delta \check{\gamma}_i. \quad (6.0.13)$$

In remark 5.5 on page 31 I have established that $\check{\sigma}_0 = 0$ due to the time-parallel transport of the rail vector. Thus $\frac{\partial \check{\theta}^0}{\partial \check{\gamma}_i} = 0$ and we only have to examine $\frac{\partial \check{\sigma}^n}{\partial \check{\gamma}_i}$.

We use theorem 4.62 on page 29 to obtain:

$$\frac{\partial \check{\theta}^n}{\partial \check{\gamma}_i} = -\frac{\check{\sigma}^n}{\partial \check{\gamma}_i} = -\sum_{j=1}^n \frac{\Delta \check{\sigma}^j}{\partial \check{\gamma}_i} \stackrel{(4.63)}{=} -\frac{\Delta \check{\sigma}^{i+1}}{\partial \check{\gamma}_i} - \frac{\Delta \check{\sigma}^{i-1}}{\partial \check{\gamma}_i} = -\frac{(\check{\kappa} \check{\mathbf{b}}_{i+1})^T - (\check{\kappa} \check{\mathbf{b}}_{i-1})^T}{2 |\Delta \check{\gamma}|} \quad (6.0.14)$$

With this we can finally write out the expression for the twist force

$$\frac{\partial \check{E}_{twist}}{\partial \check{\gamma}_i} = -\frac{\beta}{2n |\Delta \check{\gamma}|^2} (\check{\theta}^n - \check{\theta}^0) \left((\check{\kappa} \check{\mathbf{b}}_{i+1})^T - (\check{\kappa} \check{\mathbf{b}}_{i-1})^T \right) \quad (6.0.15)$$

6.2 Integration

The rod is integrated by applying the forces using the symplectic **semi-implicit Euler method** as described in [HLW06, chapter 1]:

$$\dot{\check{\gamma}}^{unconstrained}(t+1) := \dot{\check{\gamma}}(t) + \frac{\check{\mathbf{f}}}{\check{m}} h \quad (6.0.16)$$

$$\check{\gamma}^{unconstrained}(t+1) := \check{\gamma}(t) + \dot{\check{\gamma}}(t+1)h, \quad (6.0.17)$$

with timestep h .

³Note that [BWR⁺08] states that the partial derivative for $\check{\theta}^0$ is 0. This is not true.

Remark 6.1. If you compare the force terms, you see that both have the material parameters α or β as linear attenuators. Thus scaling both α and β by the same factor λ has the same effect as scaling the timestep h by λ when it comes to calculating the forces.

This lets us infer that (a) this discrete rod model most certainly has redundant parameters; (b) huge values in α or β are equivalent to using huge timesteps, which usually is a bad idea; and (c) only the ratio $\alpha : \beta$ is important for the dynamic behavior of the system .

6.3 Constraints and boundary conditions

Motivation The avid reader has probably noticed that the main problem with the unconstrained integration step is not the probable violation of the boundary conditions but the certain violation of the rod inextensibility.

Thus the main task of the Fast Manifold Projection algorithm is to enforce the inextensibility constraints.

Before I present the Fast Manifold Projection algorithm, I want to mention the different constraints that are possible.

Inextensibility constraints Different sources suggest different constraints for enforcing the constant length of the edges of the discrete rod:

- [BWR⁺08] suggests using $\Delta\tilde{\gamma} \cdot \Delta\tilde{\gamma} - |\Delta\tilde{\gamma}|^2 = 0 \iff \Delta\tilde{\gamma}^2 - |\Delta\tilde{\gamma}|^2 = 0$ with gradient $2\Delta\tilde{\gamma}^T$.
- [GHF⁺07] suggests using $\frac{\Delta\tilde{\gamma}^2}{|\Delta\tilde{\gamma}|} - |\Delta\tilde{\gamma}| = 0$ with gradient $\frac{2\Delta\tilde{\gamma}^T}{|\Delta\tilde{\gamma}|}$.
- [Gol10] suggests using $\frac{\Delta\tilde{\gamma}^2}{2|\Delta\tilde{\gamma}|} - \frac{|\Delta\tilde{\gamma}|}{2} = 0$ with gradient $\frac{\Delta\tilde{\gamma}^T}{|\Delta\tilde{\gamma}|}$.

[Gol10] states that his last constraint is most robust, because the gradient is weighted depending on the length of the edge and almost normalized. I share his view on this.

So the inextensibility constraints are:

$$0 = C^i(\tilde{\gamma}_{i+1}, \tilde{\gamma}_i) := \frac{(\Delta\tilde{\gamma}^i)^2}{2|\Delta\tilde{\gamma}|} - \frac{|\Delta\tilde{\gamma}|}{2} \quad (6.1.1)$$

with gradients

$$\frac{\partial C^i}{\partial \tilde{\gamma}_{i+1}} = \frac{(\Delta\tilde{\gamma}^i)^T}{|\Delta\tilde{\gamma}|} \quad (6.1.2)$$

$$\frac{\partial C^i}{\partial \tilde{\gamma}_i} = -\frac{(\Delta\tilde{\gamma}^i)^T}{|\Delta\tilde{\gamma}|} \quad (6.1.3)$$

Rigid body constraints One of the most important use cases in the simulation of a discrete rod is attaching it to rigid bodies. The question is how to attach it. I am only going to cover the case when a rigid body is attached to the first vertex, respectively the first edge.

The first vertex has to be “fixed” relative to the rigid body. The second vertex has to be “fixed”, too, because otherwise it is impossible to impose material frame boundary conditions that are consistent over time. If the first and second vertex are “fixed” relative to the rigid body, the first tangent is “fixed” as well and $\tilde{\theta}^0$ can be determined using the orientation of the rigid body and the initial boundary conditions.

I assume that the state of the rigid body is described by 4 quantities: (a) its position $\mathbf{r} \in \mathbb{R}^3$; (b) its velocity $\dot{\mathbf{r}} \in \mathbb{R}^3$; (c) its orientation $\mathbf{q} \in \mathbb{H}$, a unit quaternion; and (d) its angular velocity⁴ $2\dot{\mathbf{q}}^*$. I denote the initial state quantities by \mathbf{r}_0 and \mathbf{q}_0 .

⁴see [Ebe10] for a deduction of this

Then the rigid body constraints are:

$$0 = C_r^{unit}(\mathbf{q}) := \mathbf{q} \cdot \mathbf{q} - 1 \quad (6.1.4)$$

$$0 = C_r^0(\mathbf{q}, \check{\gamma}_0, \mathbf{r}) := \mathbf{q}\mathbf{q}_0^*(\check{\gamma}_0(0) - \mathbf{r}_0)\mathbf{q}_0\mathbf{q}^* - (\check{\gamma}_0 - \mathbf{r}) = 0 \quad (6.1.5)$$

$$0 = C_r^1(\mathbf{q}, \check{\gamma}_1, \mathbf{r}) := \mathbf{q}\mathbf{q}_0^*(\check{\gamma}_1(0) - \mathbf{r}_0)\mathbf{q}_0\mathbf{q}^* - (\check{\gamma}_1 - \mathbf{r}) = 0 \quad (6.1.6)$$

The gradient of C_{unit} is: $\frac{\partial C_r^{unit}}{\partial \mathbf{q}} = \frac{\partial(\mathbf{q} \cdot \mathbf{q} - 1)}{\partial \mathbf{q}} = \frac{\partial(\mathbf{q} \cdot \mathbf{q} - 1)}{\partial \mathbf{q}} = 2\mathbf{q}^T$. See appendix B on page 51 for calculation of the gradients of C_r^0 and C_r^1 .

6.4 Fast Manifold Projection algorithm

Motivation I have already described the general idea of the Fast Manifold Projection algorithm in the introduction. This section is going to look at the algorithm in detail.

6.4.1 Constrained Lagrangian system

Definition 6.2. A constrained Lagrangian system consists of:

1. the motion $\mathbf{x} : \mathbb{R} \rightarrow \mathbb{R}^n, t \mapsto \mathbf{x}(t), \mathbf{x} \in C^2$;
2. the potential function $U : \mathbb{R}^n \rightarrow \mathbb{R}$;
3. the mass matrix $M \in \mathbb{R}^{n \times n}$, M positive definite and symmetric;
4. the constraint function $C : \mathbb{R}^n \rightarrow \mathbb{R}^m, C \in C^2$;
5. the constraint manifold $S = \{\mathbf{x} \mid C(\mathbf{x}) = 0\}$;
6. the Lagrange multiplier $\lambda : \mathbb{R} \rightarrow \mathbb{R}^m$; and
7. the Lagrangian function $\hat{L}(\mathbf{x}, \dot{\mathbf{x}}, \lambda) := \frac{1}{2}\dot{\mathbf{x}}^T M \dot{\mathbf{x}} - U(\mathbf{x}) + C(\mathbf{x})^T \cdot \lambda$; whereas n is called the **dimension of the system**, and m specifies the number of constraints on the system.

Remark 6.3. This definition is paraphrased from [GHF⁺07]. See also [Arn89, chapter 4] and [MR99].

Proposition 6.4. A motion \mathbf{x} that satisfies the Euler-Lagrange equation for some Lagrange multiplier λ always stays in S : $\mathbf{x}(t) \in S$.

Proof. The Lagrangian system \hat{L} has the combined coordinates (\mathbf{x}, λ) . Thus the Euler-Lagrange equations for it are:

$$\frac{d}{dt} \frac{\partial \hat{L}}{\partial \dot{\mathbf{x}}} = \frac{\partial \hat{L}}{\partial \mathbf{x}} \iff M\ddot{\mathbf{x}} = \frac{\partial C^T}{\partial \mathbf{x}}(\mathbf{x})\lambda - \frac{\partial U}{\partial \mathbf{x}}(\mathbf{x}) \quad (6.4.1)$$

$$\frac{d}{dt} \frac{\partial \hat{L}}{\partial \dot{\lambda}} = \frac{\partial \hat{L}}{\partial \lambda} \iff 0 = C(\mathbf{x}) \quad (6.4.2)$$

$\mathbf{x}(t) \in S$ immediately follows from the second equation. □

Definition 6.5. $\mathbf{R}(x) := \partial_x C^T(x)\lambda$ is called the **constraint force**.

Remark 6.6. The constraint force \mathbf{R} is always perpendicular to the manifold S , and performs no work. See [Arn89].

6.4.2 Projection step

General idea We are given a discretized constrained Lagrangian system. During the simulation unconstrained steps and projection steps alternate.

Let the result of an unconstrained step be denoted by \mathbf{x}_0 . It is obtained by integrating the unconstrained Lagrangian system L :

$$L(\mathbf{x}, \dot{\mathbf{x}}) := \frac{1}{2} \dot{\mathbf{x}}^T M \dot{\mathbf{x}} - U(\mathbf{x}). \quad (6.6.1)$$

The corresponding Euler-Lagrange equation is:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{x}}} = \frac{\partial L}{\partial \mathbf{x}} \iff M \ddot{\mathbf{x}} = -\frac{\partial U}{\partial \mathbf{x}}(\mathbf{x}). \quad (6.6.2)$$

If you compare the constrained with the unconstrained system, you notice that the equation of motion of the unconstrained system (obviously) lacks the constraint force. This means that the unconstrained step integrates the motion without applying the constraint force.

The idea behind the Fast Manifold Projection algorithm is to apply this constraint force in retrospect while minimizing the required displacement and energy change due to the additional movement.

Proposition 6.7. *The appropriate metric tensor for the Lagrangian system is the mass matrix M . M is called the **Lagrangian metric**.*

Proof. See [Fra12, p 54–55] □

Definition 6.8. *The inner product \cdot_M is defined as: $\mathbf{a} \cdot_M \mathbf{b} := \mathbf{a} M \mathbf{b}$.*

Definition 6.9. $S_c = \{\mathbf{x} \mid C(\mathbf{x}) = c\}$

Remark 6.10. $S = S_0$

Algorithm Starting with \mathbf{x}_0 the algorithm iteratively moves towards the constraint manifold using Newton iterations that are constrained to be orthogonal to level set of the constraint function at the starting point.

The algorithm assumes $C(\mathbf{x}_i + \delta \mathbf{x}) \approx C(\mathbf{x}_i) + \partial_{\mathbf{x}} C(\mathbf{x}_i) \delta \mathbf{x}$. It uses this to determine $\mathbf{x}_{i+1} := \mathbf{x}_i + \Delta \mathbf{x}^i$ with $C(\mathbf{x}_{i+1}) \approx 0$ by searching for $\Delta \mathbf{x}^i \perp_M TS_{C(\mathbf{x}_i)}^{\mathbf{x}_i}$ with $\partial_{\mathbf{x}} C(\mathbf{x}_i) \Delta \mathbf{x}^i = -C(\mathbf{x}_i)$.

In fact, if the iteration starts with \mathbf{x}_i :

1. determine $\boldsymbol{\lambda}^i \in \mathbb{R}^m$ by solving

$$\left(\partial_{\mathbf{x}} C(\mathbf{x}_i) M^{-1} \partial_{\mathbf{x}} C^T(\mathbf{x}_i) \right) \boldsymbol{\lambda}^i = -C(\mathbf{x}_i); \quad (6.10.1)$$

2. then set

$$\Delta \mathbf{x}^i := M^{-1} \partial_{\mathbf{x}} C^T(\mathbf{x}_i) \boldsymbol{\lambda}^i; \quad (6.10.2)$$

3. finally obtain $\mathbf{x}_{i+1} := \mathbf{x}_i + \Delta \mathbf{x}^i$;
4. check whether $C(\mathbf{x}_{i+1}) \approx 0$ and break, if the approximation is sufficiently good; otherwise
5. iterate

Remark 6.11. The linear equation that has to be solved in 6.4.2 is only of dimension $\approx 2n \times 2n$ compared to $\approx 5n \times 5n$ for other approaches. See [GHF⁺07].

Proposition 6.12. $\Delta \mathbf{x}^i \perp_M TS_{C(\mathbf{x}_i)}^{\mathbf{x}_i}$

Proof. With $TS_{C(\mathbf{x}_i)}^{\mathbf{x}_i} = \ker \partial_{\mathbf{x}} C(\mathbf{x}_i)$, for $\boldsymbol{\xi} \in TS_{C(\mathbf{x}_i)}$:

$$\boldsymbol{\xi} \cdot_M \Delta \mathbf{x}^i = \boldsymbol{\xi}^T M M^{-1} \partial_{\mathbf{x}} C^T(\mathbf{x}_i) \boldsymbol{\lambda}^i = \boldsymbol{\lambda}^i \cdot \partial_{\mathbf{x}} C(\mathbf{x}_i) \boldsymbol{\xi} = 0 \quad (6.12.1)$$

□

Remark 6.13. The algorithm would perform an orthogonal projection, if $\partial_{\mathbf{x}} C(\mathbf{x}_i) = \text{const}$ along \mathbf{x}_i .

6.4.3 Generalized mass matrix

Simple case In the simplest case the mass matrix M is a diagonal matrix that contains particle masses and the corresponding \mathbf{x} vector contains particle positions. This is the case for the inextensibility constraints of a discrete rod.

$M \leftrightarrow \dot{\mathbf{x}}$ correspondence $\dot{\mathbf{x}}$ and M are connected through the Lagrangian. Even though the Fast Manifold Projection algorithm does not use $\dot{\mathbf{x}}$ directly, M and $\dot{\mathbf{x}}$ need to be compatible in the following way:

$\frac{1}{2} \dot{\mathbf{x}}^T M \dot{\mathbf{x}}$ must be equal the kinetic energy of the Lagrangian system. M need not contain mass values anymore. Hence, it is called **generalized mass matrix**. Likewise \mathbf{x} and $\dot{\mathbf{x}}$ are then called **generalized position** and **generalized velocity**.

I stress this, because [BWR⁺08] states an incorrect generalized velocity for the rigid body coupling that is caused by such an incompatibility.

Rigid body case If rigid body constraints are included, everything gets more complicated. In particular the orientation of the rigid body \mathbf{q} , a quaternion, is part of the generalized position vector \mathbf{x} .

[BWR⁺08] uses the 3×3 inertia tensor I of the rigid body in the generalized mass matrix and states that the generalized velocity is the angular velocity of the body expressed using quaternions: $2\mathbf{q}^{-1}\dot{\mathbf{q}}$, which can be interpreted as \mathbb{R}^3 vector. However, it is not possible to give a generalized position that fits.

Instead you have to use the quaternion as generalized position and its derivative as generalized velocity. The generalized mass matrix is not just the tensor of inertia. The following paragraph deduces the correct generalized mass matrix.

Rotational energy from quaternion derivative The angular velocity $\boldsymbol{\omega} \in \mathbb{R}^3$ is equal to $2\mathbf{q}^{-1}\dot{\mathbf{q}}$ (without proof). The kinetic energy of rotation T is $T := \frac{1}{2}\boldsymbol{\omega}^T I \boldsymbol{\omega}$, whereas I is the inertia tensor of the rigid body.

The quaternion multiplication by \mathbf{q}^{-1} in $2\mathbf{q}^{-1}\dot{\mathbf{q}}$ can be replaced by a 3×4 matrix \hat{Q} , ie $\boldsymbol{\omega} = \hat{Q}\dot{\mathbf{q}}$. Then $T = \frac{1}{2}\dot{\mathbf{q}}^T \hat{Q}^T I \hat{Q} \dot{\mathbf{q}}$.

If we set $M := 2\hat{Q}^T I \hat{Q}$, we can set $\mathbf{x} := \mathbf{q}$ and $\dot{\mathbf{x}} := \dot{\mathbf{q}}$ and everything fits together. Note that in this case the generalized mass matrix has to be updated after every iteration in the projection algorithm because \hat{Q} depends on \mathbf{q} , which changes in every iteration. See also [Bet06].

6.4.4 Velocity update

Position filter [GHF⁺07] formulates the algorithm as velocity filter in spirit of [BFA02]. A **velocity filter** is an algorithm that changes the velocity of a particle before its final position in the integration step is calculated. [BWR⁺08] use it like a **position filter**, ie it only filters the position of a particle to fulfill a property.

Motivation Because changing the position of a particle without changing its velocity during integration would result in incorrect motions, a **velocity update** has to be performed after the Fast Manifold Projection algorithm has run. It calculates the change of velocity needed to directly move the particle to its final position and applies it to its velocity. This is carried over for the generalized case, too.

Examples Let $\tilde{\gamma}^{unconstrained}(t)$ denote the position of the vertices of a discrete rod after unconstrained integration, $\tilde{\gamma}(t+1)$ after projection, and $\tilde{\gamma}(t)$ at the beginning. Likewise denote $\dot{\tilde{\gamma}}^{unconstrained}(t)$, $\dot{\tilde{\gamma}}(t+1)$, and $\dot{\tilde{\gamma}}(t)$. Then

$$\dot{\tilde{\gamma}}(t+1) := \dot{\tilde{\gamma}}^{unconstrained}(t) + \frac{\tilde{\gamma}(t+1) - \tilde{\gamma}^{unconstrained}(t)}{h}. \quad (6.13.1)$$

Likewise the angular velocity of a rigid body is updated by:

1. determining the rotation from the old orientation of the rigid body to the orientation after the projection;
2. determining its axis and angle;
3. dividing the angle by h ; and
4. using the axis and scaled angle as new angular velocity.

6.4.5 Critique

The Fast Manifold Projection does not preserve energy well, and it has none of the sound properties discussed in [HLW06]: it is a simple projection method that is neither symmetric nor symplectic.

6.5 Torque transfer

Torque is not transferred by the Fast Manifold projection. It has to be transferred manually between discrete rods and attached rigid bodies.

An attached rigid body simply applies its torque to the discrete rod by updating the material angle $\check{\theta}$ in the corresponding material frame boundary condition when it is turning.

The discrete rod has to transfer its torque explicitly. [BWR⁺08] calculate the discrete rod's torque by applying the principles of virtual displacement and immediately obtain $|\beta \frac{\check{\theta}^n - \check{\theta}^0}{n |\Delta \tilde{\gamma}|} | \check{t}^0$ for the torque.

Implementation

Motivation I have implemented the discrete rod model of [BWR⁺08] in C++ and I want to share my experience.

Framework The following external frameworks were used:

AntTweakBar for the user interface,

GoogleTest for unit testing,

OpenGL for graphics, and

SFML for the window management.

Scenarios I have created the following scenarios:

Free rod A rod can move around freely, or one or both of its ends can be fixed. The same can be done to the material frame at the ends. Twist can be induced to observe it buckle.

Mitchell's instability A rod is closed into a ring. The ends are twisted before they are closed. Depending on the twist of the closed ends and the material parameters α and β , the rod remains stable or it suddenly buckles. The critical twist has been calculated analytically and I was able to observe the predicted behavior near the critical twist.

Wilberforce pendulum A rigid body is attached to a rod that is fixed above. The rigid body turns along the vertical axis and twists the rod. When the rod starts buckling, the spin of the rigid body slows down until it stops. Then, because of gravity, the rod starts unbuckling and the rigid body resumes spinning, etc.

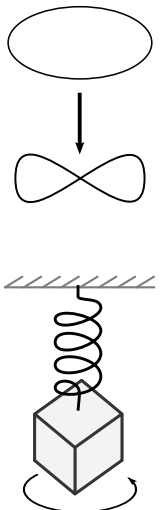
My code has issues with numerical stability in this scenario.

Numerical Stability and Fast Manifold Projection My experience with the Fast Manifold Projection algorithm is not a positive one. It quickly loses energy and I had to fine-tune my constraints to make it converge quickly.

I had issues with a non-moving rod degenerating after several thousand frames in the scenario for Mitchell's instability. Error forces start oscillating between the vertices and it starts moving at some point.

Boundary Conditions [BWR⁺08] is not clear on how to update the material frames between frames. Specifically the treatment of the boundary conditions is not explained.

The material frame boundary conditions specify a start and end material frame and the material angles are chosen accordingly. I have talked about the ambiguity of the static curve-



angle model before and the discrete curve-angle model with these boundary conditions has the same problem.

The solution for the quasistatic frame in the isotropic case has no 'memory'¹. So instead I compute the new Bishop frame, and then, based on it, temporary material frames for the first and last edge using the old material angles. I compare them to the target material frames specified by the boundary conditions and compute an angle difference that is used to update the material angles. This approach fails if the material frame turns more than π in one frame.

¹The anisotropic solution in [BWR⁺08] uses an iterative solver that starts with the old material angles.

Conclusion

We have gone a long way: from skew-symmetric matrices to quaternions, from continuous differential geometry to discrete differential geometry, and from the twisting of parallel frames under deformation to forces on rods.

Moreover I have touched the physical modeling of rods and Lagrangian mechanics as well as the actual implementation of a discrete rod simulator.

In all this it has become clear that the treatment of rods can go much deeper than I was able to sketch here, and that rods and especially discrete rods can serve as starting point to studies in many different areas of mathematics and physics.

Nonetheless I have only discussed the smaller half of the ‘Discrete Elastic Rods’ paper: anisotropic bending response, collision detection and an in-depth treatment of the rigid body coupling would have gone way beyond the time frame of this thesis.

Further Reading The follow-up paper [BAV⁺10] is a good starting point for other interesting points of view. The book [AP10] offers an in-depth treatment of the physics in rod and shell modeling. Finally the journal article [BS99] provides a more abstract and mathematically satisfying view on rods and the Lagrange top.

Additional proofs

A.1 Cayley transform (2.38)

Theorem A.1 (Cayley transform). For $\mathbf{u} \in S^2$, $\alpha \in (-\pi, \pi)$:

$$\tilde{\mathbf{u}} := \tan \frac{\alpha}{2} \mathbf{u} \tag{A.1.1}$$

$$(\text{Id}_3 - [\tilde{\mathbf{u}}])^{-1} (\text{Id}_3 + [\tilde{\mathbf{u}}]) = R_{\mathbf{u}, \alpha} \tag{A.1.2}$$

Proof. I set $\phi := \tan \frac{\alpha}{2}$, $U := [\tilde{\mathbf{u}}]$ and $Q := (\text{Id}_3 - U)^{-1} (\text{Id}_3 + U)$. I have split the proof into multiple parts:

1. $\text{Id}_3 - A$ is invertible for all $A \in so(3)$:

$$(\text{Id}_3 - A) \mathbf{v} = 0 \iff \mathbf{v} = A\mathbf{v} = \underbrace{\mathbf{a}}_{A=[\mathbf{a}]} \times \mathbf{v} \implies \mathbf{v}^2 = (\mathbf{a} \times \mathbf{v}) \cdot \mathbf{v} = 0 \iff \mathbf{v} = 0 \tag{A.1.3}$$

2. $Q \in O(3)$:

$$\begin{aligned} QQ^T &= (\text{Id}_3 - U)^{-1} (\text{Id}_3 + U) (\text{Id}_3 + U)^T (\text{Id}_3 - U)^{-T} \\ &= (\text{Id}_3 - U)^{-1} \underbrace{(\text{Id}_3 + U) (\text{Id}_3 - U)}_{=\text{Id}_3 - U^2, \text{Id}_3 \text{ and } U \text{ commute}} (\text{Id}_3 + U)^{-1} \\ &= (\text{Id}_3 - U)^{-1} (\text{Id}_3 - U) (\text{Id}_3 + U) (\text{Id}_3 + U)^{-1} = \text{Id}_3 \end{aligned} \tag{A.1.4}$$

3. $Q \in SO(3)$ —only $\det Q = 1$ needs to be proved:

$$\det Q = \det (\text{Id}_3 - U)^{-1} \det (\text{Id}_3 + U) = \frac{\det (\text{Id}_3 + U)}{\det (\text{Id}_3 - U)} = \frac{\det (\text{Id}_3 + U)}{\det (\text{Id}_3 - U)^T} = \frac{\det (\text{Id}_3 + U)}{\det (\text{Id}_3 + U)} = 1 \tag{A.1.5}$$

4. Thus theorem 2.21 on page 5 yields $Q = R_{\mathbf{v}, \beta}$ with $\mathbf{v} \in S^2$, $\beta \in (-\pi, \pi]$.

5. $\mathbf{v} = \mathbf{u}$:

$$(\text{Id}_3 \pm U) \mathbf{u} = \mathbf{u} \pm \phi \mathbf{u} \times \mathbf{u} = \mathbf{u} \tag{A.1.6}$$

$$Q\mathbf{u} = (\text{Id}_3 - U)^{-1} (\text{Id}_3 + U) \mathbf{u} = (\text{Id}_3 - U)^{-1} \mathbf{u} = \mathbf{u} \tag{A.1.7}$$

With proposition 2.25 on page 6 $\mathbf{v} = \mathbf{u}$ follows.

6. $Q = R_{\mathbf{u}, \alpha} \iff P = R_{\mathbf{e}_1, \alpha}$ with $P := F^{-1}QF$:

If we choose $\mathbf{w} \perp \mathbf{u}$, we can perform a change of coordinates using $F := (\mathbf{u} \quad \mathbf{w} \quad \mathbf{u} \times \mathbf{w})$:

$$\begin{aligned} P &= F^{-1}QF = F^{-1}(\text{Id}_3 - U)^{-1}FF^{-1}(\text{Id}_3 + U)F = (\text{Id}_3 - F^{-1}UF)^{-1}(\text{Id}_3 + F^{-1}UF) \\ &\stackrel{(2.13)}{=} (\text{Id}_3 - [\phi F^{-1}\mathbf{u}])^{-1}(\text{Id}_3 + [\phi F^{-1}\mathbf{u}]) = (\text{Id}_3 - [\phi \mathbf{e}_1])^{-1}(\text{Id}_3 + [\phi \mathbf{e}_1]) \end{aligned} \quad (\text{A.1.8})$$

$$R_{\mathbf{e}_1, \alpha} = R_{F^{-1}\mathbf{u}, \alpha} = F^{-1}R_{\mathbf{u}, \alpha}F \quad (\text{A.1.9})$$

7. $P = R_{\mathbf{e}_1, \alpha}$:

We verify $Pe_2 = \cos \alpha e_2 + \sin \alpha e_3$.

$$Pe_2 = \cos \alpha e_2 + \sin \alpha e_3 \iff (\text{Id}_3 + [\phi \mathbf{e}_1])e_2 = (\text{Id}_3 - [\phi \mathbf{e}_1])(\cos \alpha e_2 + \sin \alpha e_3) \quad (\text{A.1.10})$$

Expanding the left and right hand side separately we obtain

$$(\text{Id}_3 + [\phi \mathbf{e}_1])e_2 = e_2 + \phi \mathbf{e}_1 \times e_2 = e_2 + \phi e_3 \quad (\text{A.1.11})$$

$$\begin{aligned} (\text{Id}_3 - [\phi \mathbf{e}_1])(\cos \alpha e_2 + \sin \alpha e_3) &= \cos \alpha e_2 + \sin \alpha e_3 - \phi \cos \alpha \underbrace{\mathbf{e}_1 \times e_2}_{e_3} - \phi \sin \alpha \underbrace{\mathbf{e}_1 \times e_3}_{-e_2} \\ &= (\cos \alpha + \phi \sin \alpha)e_2 + (\sin \alpha - \phi \cos \alpha)e_3 \end{aligned} \quad (\text{A.1.12})$$

With basic trigonometric identities we get the desired results

$$\cos \alpha + \phi \sin \alpha = \cos \alpha + \sin \alpha \frac{\sin \frac{\alpha}{2}}{\cos \frac{\alpha}{2}} = \frac{\cos \alpha \cos(-\frac{\alpha}{2}) - \sin \alpha \sin(-\frac{\alpha}{2})}{\cos \frac{\alpha}{2}} = \frac{\cos \frac{\alpha}{2}}{\cos \frac{\alpha}{2}} = 1 \quad (\text{A.1.13})$$

$$\sin \alpha - \phi \cos \alpha = \sin \alpha - \cos \alpha \frac{\sin \frac{\alpha}{2}}{\cos \frac{\alpha}{2}} = \frac{\sin \alpha \cos(-\frac{\alpha}{2}) + \cos \alpha \sin(-\frac{\alpha}{2})}{\cos \frac{\alpha}{2}} = \frac{\sin \frac{\alpha}{2}}{\cos \frac{\alpha}{2}} = \phi \quad (\text{A.1.14})$$

□

A.2 Twisting of parallel frames under deformation ([BWR⁺08]'s ansatz)

Sources For an overview, see [War09]. For the definition of writhe, see [Ful71]. See [Ful78], [Can04], and [vdHPR07] for more details. The following proof sketch makes use of the results in [Vri05].

Proof sketch. [Vri05] only deals with closed rods. So we close our rod using, eg the principles described in [vdHPR07]. The closed rod is closed in a way that leaves the total twist and linking number of the open rod unchanged. Let $\bar{L} > L$ denote the length of the closed rod. We start with equation (7) from [Vri05]:

$$\frac{\partial W_r[R(t, \lambda)]}{\partial \lambda} = -\frac{1}{2\pi} \int_0^1 \left(\frac{\partial T(t, \lambda)}{\partial \lambda} \times T(t, \lambda) \right) \cdot \frac{\partial T(t, \lambda)}{\partial t} dt. \quad (\text{A.1.15})$$

Written in my notation:

$$\begin{aligned} \frac{\partial W_r[\gamma(s, t)]}{\partial t} &= -\frac{1}{2\pi} \int_0^{\bar{L}} \left(\frac{\partial \mathbf{t}(s, t)}{\partial t} \times \mathbf{t}(s, t) \right) \cdot \frac{\partial \mathbf{t}(s, t)}{\partial s} ds = -\frac{1}{2\pi} \int_{\gamma} (\dot{\mathbf{t}} \times \mathbf{t}) \cdot \mathbf{t}' ds \\ &= -\frac{1}{2\pi} \int_{\gamma} (\mathbf{t} \times \mathbf{t}') \cdot \dot{\mathbf{t}} ds = -\frac{1}{2\pi} \int_{\gamma} \kappa \mathbf{b} \cdot \dot{\mathbf{t}} ds. \end{aligned} \quad (\text{A.1.16})$$

A.2. TWISTING OF PARALLEL FRAMES UNDER DEFORMATION ([BWR⁺08]'S ANSATZ)

With this, we use equation (2) from [Vri05]:

$$\Delta \dot{L}k [\gamma(s, t)] = \Delta \dot{T}w [\gamma(s, t)] + \dot{W}r [\gamma(s, t)]. \quad (\text{A.1.17})$$

The linking number $\Delta Lk [\gamma(s, t)]$ is always an integer, thus $\Delta \dot{L}k [\gamma(s, t)] = 0$.

The total twist is defined as $\Delta Tw [\gamma(s, t)] := \frac{1}{2\pi} \int_{\gamma} \tau ds = \frac{1}{2\pi} \int_{\gamma} \theta' ds = \frac{\theta(L) - \theta(0)}{2\pi}$, so

$$\begin{aligned} 0 &= \Delta \dot{T}w [\gamma(s, t)] + \dot{W}r [\gamma(s, t)] = \frac{\dot{\theta}(L) - \dot{\theta}(0)}{2\pi} - \frac{1}{2\pi} \int_{\gamma} \kappa \mathbf{b} \cdot \dot{\mathbf{t}} ds \\ \Leftrightarrow \dot{\theta}(\bar{L}) - \dot{\theta}(0) &= \int_{\gamma} \kappa \mathbf{b} \cdot \dot{\mathbf{t}} ds \end{aligned} \quad (\text{A.1.18})$$

As the rod is closed, the material frame cannot change. With an argument similar to section 6.1.3 on page 36, you can argue that $\dot{\theta}(\bar{L}) - \dot{\theta}(0)$ denotes the negative twist variation of an arbitrary parallel frame, ie $\sigma(\bar{L}) - \sigma(0) = -(\dot{\theta}(\bar{L}) - \dot{\theta}(0)) = -\int_{\gamma} \kappa \mathbf{b} \cdot \dot{\mathbf{t}} ds$. \square

Differentiation of the rigid body constraint

Motivation The constraint $0 = C(\mathbf{q}, \mathbf{r}, \mathbf{x}) := \mathbf{q}\bar{\mathbf{x}}\mathbf{q}^* + \mathbf{r} - \mathbf{x}$ is given for coupling the rigid body to the rod. $\frac{\partial}{\partial \mathbf{r}} C$ and $\frac{\partial}{\partial \mathbf{x}} C$ are straightforward to calculate:

$$\frac{\partial}{\partial \mathbf{r}} C = \text{id}_3, \quad \frac{\partial}{\partial \mathbf{x}} C = -\text{id}_3 \quad (\text{B.0.1})$$

However $\frac{\partial}{\partial \mathbf{q}} C = \frac{\partial}{\partial \mathbf{q}} (\mathbf{q}\bar{\mathbf{x}}\mathbf{q}^*)$ requires more consideration. We need a linearized derivative that can be used in the constraint Jacobi matrix. For this linearized form we need to look at how to write a quaternion multiplication in matrix form, after we identify quaternions with vectors in \mathbb{R}^4 .

Derivative in quaternion form I use the usual variational ansatz as is common for total derivatives:

If we can find a linear function A , such that $(\mathbf{q} + \mathbf{h})\mathbf{v}(\mathbf{q} + \mathbf{h})^* = \mathbf{q}\mathbf{v}\mathbf{q}^* + A\mathbf{h} + O(\|\mathbf{h}\|^2)$, then $A = \frac{\partial}{\partial \mathbf{q}} (\mathbf{q}\mathbf{v}\mathbf{q}^*)$. Consequently:

$$(\mathbf{q} + \mathbf{h})\mathbf{v}(\mathbf{q} + \mathbf{h})^* = (\mathbf{q} + \mathbf{h})\mathbf{v}(\mathbf{q}^* + \mathbf{h}^*) \quad (\text{B.0.2})$$

$$= \mathbf{q}\mathbf{v}\mathbf{q}^* + \mathbf{q}\mathbf{v}\mathbf{h}^* + \mathbf{h}\mathbf{v}\mathbf{q}^* + \mathbf{h}\mathbf{v}\mathbf{h}^* \quad (\text{B.0.3})$$

$$= \mathbf{q}\mathbf{v}\mathbf{q}^* + \mathbf{q}\mathbf{v}\mathbf{h}^* + \mathbf{h}\mathbf{v}\mathbf{q}^* + O(\|\mathbf{h}\|^2) \quad (\text{B.0.4})$$

The last step is correct because $\|\mathbf{h}\mathbf{v}\mathbf{h}^*\| = \|\mathbf{v}\| \|\mathbf{h}\| \|\mathbf{h}^*\| = \|\mathbf{v}\| \|\mathbf{h}\|^2$. You can quickly verify that $A\mathbf{h} := \mathbf{q}\mathbf{v}\mathbf{h}^* + \mathbf{h}\mathbf{v}\mathbf{q}^*$ is linear, so we have found the derivative:

Theorem B.1. *The derivative of $\mathbf{q}\mathbf{v}\mathbf{q}^*$ in quaternion form is:*

$$\frac{\partial}{\partial \mathbf{q}} (\mathbf{q}\mathbf{v}\mathbf{q}^*) (\mathbf{h}) = \mathbf{q}\mathbf{v}\mathbf{h}^* + \mathbf{h}\mathbf{v}\mathbf{q}^* \quad (\text{B.1.1})$$

Quaternion multiplication in matrix form

Lemma B.2. *The left quaternion application function $q_l : \mathbb{H} \rightarrow \mathbb{H}, q(\mathbf{p}) = \mathbf{q}\mathbf{p}$ for $\mathbf{q} = s + \mathbf{v}$ can be written as*

$$q_l : \mathbb{R}^4 \mapsto \mathbb{R}^4, q(\mathbf{p}) = Q_l \mathbf{p} \quad (\text{B.2.1})$$

with

$$Q_l := \begin{pmatrix} s & -\mathbf{v}^T \\ \mathbf{v} & s \text{Id}_3 + [\mathbf{v}] \end{pmatrix} \in \mathbb{R}^{4 \times 4} \quad (\text{B.2.2})$$

Lemma B.3. *The right quaternion application function $q_r : \mathbb{H} \rightarrow \mathbb{H}$, $q(\mathbf{p}) = \mathbf{p}q$ for $q = s + \mathbf{v}$ can be written as*

$$q_r : \mathbb{R}^4 \mapsto \mathbb{R}^4, q(\mathbf{p}) = Q_r \mathbf{p} \quad (\text{B.3.1})$$

with

$$Q_r := \begin{pmatrix} s & -\mathbf{v}^T \\ \mathbf{v} & s \text{Id}_3 - [\mathbf{v}] \end{pmatrix} \in \mathbb{R}^{4 \times 4} \quad (\text{B.3.2})$$

Proof. I only prove the second lemma here: the first is proved similarly.

With $\mathbf{p} = t + \mathbf{w}$ the product $\mathbf{p}q$ can be written as

$$(t + \mathbf{w})(s + \mathbf{v}) = \begin{pmatrix} t \\ \mathbf{w} \end{pmatrix} \begin{pmatrix} s \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} st - \mathbf{w} \cdot \mathbf{v} \\ t\mathbf{v} + s\mathbf{w} + \mathbf{w} \times \mathbf{v} \end{pmatrix} \quad (\text{B.3.3})$$

$$= \begin{pmatrix} s & -\mathbf{v}^T \\ \mathbf{v} & s \text{Id}_3 - [\mathbf{v}] \end{pmatrix} \begin{pmatrix} t \\ \mathbf{w} \end{pmatrix} \quad (\text{B.3.4})$$

□

Similarly you can immediately verify:

Lemma B.4. *The quaternion conjugation mapping $\mathbb{H} \rightarrow \mathbb{H}$, $q \mapsto q^*$ can likewise be written as $\mathbb{R}^4 \mapsto \mathbb{R}^4$, $q \mapsto Cq$ with*

$$C = \begin{pmatrix} 1 & \\ & -\text{Id}_3 \end{pmatrix} \quad (\text{B.4.1})$$

Remark B.5. Similarly to writing $[\mathbf{v}]$ for the skew-symmetric matrix that corresponds to the left cross-multiplication with a vector \mathbf{v} , I will use the following notation for matrices that correspond to a left or right multiplication with a quaternion:

$$[\mathbf{q}]_l \mathbf{p} = \mathbf{q}\mathbf{p} = [\mathbf{p}]_r \mathbf{q} \quad (\text{B.5.1})$$

Derivative in matrix form With the help of these lemmas, we can write the quaternion derivative in matrix form:

Theorem B.6. *The derivative of $q\mathbf{v}q^*$ written in matrix form is:*

$$\frac{\partial}{\partial \mathbf{q}} (q\mathbf{v}q^*) = 2 \begin{pmatrix} 0 & \\ \mathbf{w} & -t \text{Id}_3 - [\mathbf{w}] \end{pmatrix} \text{ with } \begin{pmatrix} t \\ \mathbf{w} \end{pmatrix} = q\mathbf{v} \quad (\text{B.6.1})$$

Proof. Set $\mathbf{p} := \mathbf{q}\mathbf{v} = t + \mathbf{w}$, and note that $\mathbf{v} = \begin{pmatrix} 0 \\ \mathbf{v} \end{pmatrix}$. Thus $\mathbf{q}\mathbf{v}^* = -\mathbf{q}\mathbf{v} = -\mathbf{p}$. We obtain:

$$\frac{\partial}{\partial \mathbf{q}} (\mathbf{q}\mathbf{v}\mathbf{q}^*) (\mathbf{h}) = \mathbf{q}\mathbf{v}\mathbf{h}^* + \mathbf{h}\mathbf{v}\mathbf{q}^* = (\mathbf{q}\mathbf{v})\mathbf{h}^* + \mathbf{h}(\mathbf{q}\mathbf{v}^*)^* = \mathbf{p}\mathbf{h}^* + \mathbf{h}(-\mathbf{p})^* \quad (\text{B.6.2})$$

$$= [\mathbf{p}]_l \mathbf{h}^* + [-\mathbf{p}^*]_r \mathbf{h} = [t + \mathbf{w}]_l \begin{pmatrix} 1 & \\ & -\text{Id}_3 \end{pmatrix} \mathbf{h} + [-t + \mathbf{w}]_r \mathbf{h} \quad (\text{B.6.3})$$

$$= \begin{pmatrix} t & -\mathbf{w}^T \\ \mathbf{w} & t \text{Id}_3 + [\mathbf{w}] \end{pmatrix} \begin{pmatrix} 1 & \\ & -\text{Id}_3 \end{pmatrix} \mathbf{h} + \begin{pmatrix} -t & -\mathbf{w}^T \\ \mathbf{w} & -t \text{Id}_3 - [\mathbf{w}] \end{pmatrix} \mathbf{h} \quad (\text{B.6.4})$$

$$= \begin{pmatrix} t & \mathbf{w}^T \\ \mathbf{w} & -t \text{Id}_3 - [\mathbf{w}] \end{pmatrix} \mathbf{h} + \begin{pmatrix} -t & -\mathbf{w}^T \\ \mathbf{w} & -t \text{Id}_3 - [\mathbf{w}] \end{pmatrix} \mathbf{h} \quad (\text{B.6.5})$$

$$= 2 \begin{pmatrix} 0 & \\ \mathbf{w} & -t \text{Id}_3 - [\mathbf{w}] \end{pmatrix} \mathbf{h} \quad (\text{B.6.6})$$

□

Corollary B.7. *The derivative of $\mathbf{q}\mathbf{v}\mathbf{q}^*$ written in matrix form transformed back into \mathbb{R}^3 is:*

$$\frac{\partial}{\partial \mathbf{q}} (\mathbf{q}\mathbf{v}\mathbf{q}^*) = 2 \begin{pmatrix} \mathbf{w} & -t \text{Id}_3 - [\mathbf{w}] \end{pmatrix} \text{ with } \begin{pmatrix} t \\ \mathbf{w} \end{pmatrix} = \mathbf{q}\mathbf{v} \quad (\text{B.7.1})$$

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