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APPLICATION OF DUAL QUATERNIONS ON SELECTED PROBLEMS

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Dissertation thesis

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Plzeň, 2017

FAKULTA
APLIKOVANÝCH VĚD
ZÁPADOČESKÉ
UNIVERZITY
V PLZNI

APLIKACE DUÁLNÍCH KVATERNIONŮ NA VYBRANÉ PROBLÉMY

Jitka Prošková

Dizertační práce

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Plzeň, 2017

Acknowledgement

I would like to thank all the people who have supported me during my studies. Especially many thanks belong to my family for their moral and material support and my advisor doc. RNDr. Miroslav Lávička, Ph.D. for his guidance.

I hereby declare that this Ph.D. thesis is completely my own work and that I used only the cited sources.

Plzeň, July 20, 2017, ...

Annotation

In recent years, the study of quaternions has become an active research area of applied geometry, mainly due to an elegant and efficient possibility to represent using them rotations in three dimensional space. Thanks to their distinguished properties, quaternions are often used in computer graphics, inverse kinematics robotics or physics. Furthermore, dual quaternions are ordered pairs of quaternions. They are especially suitable for describing rigid transformations, i.e., compositions of rotations and translations. It means that this structure can be considered as a very efficient tool for solving mathematical problems originated for instance in kinematics, bioinformatics or geodesy, i.e., whenever the motion of a rigid body defined as a continuous set of displacements is investigated.

The main goal of this thesis is to provide a theoretical analysis and practical applications of the dual quaternions on the selected problems originated in geometric modelling and other sciences or various branches of technical practise. Primarily we focus on problems which are traditionally solved using quaternions and show that involving dual quaternions can simplify the designed approaches and sets them on a unifying basis.

In the first part of the thesis we recall the fundamental theory of quaternion algebra and their application for the description of the three dimensional rotations. Then we continue with dual numbers. The quaternions and dual numbers are used for the introduction of dual quaternions. Subsequently, some elementary notions dealing with dual quaternion are introduced and explained. Compared to quaternions that can represent only rotation, the dual quaternions offer a broader representation of both the rotation and translation.

In the second part of the thesis we discuss several practical applications of dual quaternions. Firstly, one of the challenging problems from geodesy is solved. The Burša-Wolf similarity transformation model is presented and a new mathematical method based on the dual quaternions is introduced and documented. Next, we deal with an interesting problem relating to structural biology, i.e., the description of the protein structure is thoroughly investigated. The well-known method for describing secondary protein structures is called SrewFit, and the dual-quaternions-improvement is designed as a new approach. The last part of the thesis is devoted to modifying existing Hermite interpolation schemes by rational spline motions with help of dual quaternions. Functionality of the designed method is illustrated on several examples.

Keywords

Quaternions, dual quaternions, datum transformation, Burša-Wolf model, secondary protein structure, ScrewFit, rational spline motion, Hermite interpolation.

Anotace

V posledních letech se studium kvaternionů stalo aktivní oblastí výzkumu aplikované geometrie díky své schopnosti jednoduše a elegantně reprezentovat rotační pohyb. Díky této vlastnosti jsou kvaterniony často využívány zejména v oblasti počítačové grafiky, inverzní kinematiky nebo také fyziky. Mimo to, je duální kvaternion také chápán jako uspořádaná dvojice kvaternionů. Duální kvaterniony jsou především vhodné pro popis přímé shodnosti, tj. složení rotace a posunutí. Tato struktura se stává tedy velmi efektivním nástrojem při řešení matematických problémů, vzniklých například v kinematice, bioinformatcie nebo geodézii, tj. vždy, když je zkoumán pohyb tuhého tělasa definovaný jako spojitá množina posunutí.

Hlavním cílem předkládané práce je poskytnout teoretické poznatky a praktické použití duálních kvaternionů na vybraných problémech, které vznikají v geometrickém modelování a dalších vědách nebo různých odvětví technické praxe. Speciálně se zaměřujeme na problémy, které jsou obvykle řešené pomocí kvaternionů a ukazují, že aplikace duálních kvaternionů dokáže zjednodušit navrhované přístupy a hlavně jim dát stejný základ.

V první části práce připomeneme fundamentální teorii kvaternionové algebry a schopnost kvaternionů popsat trojrozměrnou rotaci. Dále pokračujeme duálními čísly. Kvaterniony a duální čísla se používají při zavedení duálních kvaternionů. Následně jsou představeny některé základní pojmy vztažené k duálním kvatrnionům. Duální kvaterniony ve srovnání s kvaterniony, které dokáží reprezentovat rotaci, nám dokáží nabídnout, vzhledem k jejich schopnosti reprezentovat rotace a posunutí, širší využití.

V druhé části práce se budeme zabývat praktickým využitím duálních kvaternionů. Nejdříve se zaměříme na jeden z náročných problémů geodezie, tj. Burša-Wolf transformační model. Je zde představena a popsána nová matematická metoda založená na duálních kvaternionech. Dalším zajímavým problémem, který je zde podrobně zkoumán, je problém zaměřující se na strukturální biologii, tj. popis proteinové struktury. Použijeme metodu SrewFit, která popisuje sekundární proteinovou strukturu, a vylepšíme ji s pomocí duálních kvaternionů. Poslední část této práce je věnová na úpravě Hermitovské interpolace racionálními spline pohyby. Funkčnost navržené metody je ilustrována na několika příkladech.

Klíčová slova

Kvaterniony, duální kvaterniony, transformační metoda Burša-Wolf, sekundární proteinová struktura, metoda ScrewFit, racionální spline pohyb, hermitovská interpolace.

Glossary of notations

$\mathcal{Q}, \widehat{\mathcal{P}} \ldots$	Quaternion
1, $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$	Quaternion units
q_0	Scalar part of quaternion $\mathcal{Q}$
$\mathbf{q} = (q_1, q_2, q_3)$	Vector part of quaternion $\mathcal{Q}$
$\mathcal{Q}^*$	Conjugate quaternion to quaternion $\mathcal{Q}$
$\mathcal{Q}^{-1}$	Inverse quaternion to quaternion $\mathcal{Q}$
$\|\mathcal{Q}\|$	Norm of quaternion $\mathcal{Q}$
$\mathbb{H}$	Set of quaternions
$\mathbb{H}_p$	Set of pure quaternions
$\theta, \varphi \ldots$	Angle
z_d, $\hat{z}_d \ldots$	Dual number
ε	Dual unit
$\overline{z_d}$	Dual number conjugate to dual number z_d
$*_\varepsilon$	Dual part
i	Imaginary unit
$\mathbb{D}$	Set of dual numbers
$\mathbb{D}_p$	Set of pure dual numbers
$\mathbf{z}_d$	Dual vector
θ_d	Dual angle
$\mathcal{Q}_d$, $\widehat{\mathcal{Q}}_d \ldots$	Dual quaternion
$\mathcal{Q}_d^*$	Dual quaternion conjugate to dual quaternion $\mathcal{Q}_d$
$\overline{\mathcal{Q}_d^*}$	Dual quaternion dual conjugate to dual quaternion $\mathcal{Q}_d$
$\mathcal{Q}_d^{-1}$	Inverse dual quaternion to dual quaternion $\mathcal{Q}_d$
$\|\mathcal{Q}_d\|$	Norm of dual quaternion $\mathcal{Q}_d$
$\mathbf{v}, \mathbf{l} \ldots$	Vector
$k, s \ldots$	Scalar
$\mathbf{GL}(3, F)$	General linear group
$\mathbf{SO}(3)$	Special orthogonal group
$\mathbf{A}$,$\mathbf{R} \ldots$	Matrix
C^k	Parametric continuity of order k
G^k	Geometric continuity of order k
$\mathbf{SE}(3)$	Special Euclidean group
$\mathbb{R}$	Set of real numbers

Contents

Chapter 1

Introduction

Quaternions were invented by Sir William Rowan Hamilton (1805–1865) as an extension to complex numbers. Hamilton tried, for ten years, to create some structure similar to complex numbers and therefore he created the quaternion, an interesting mathematical notion. The unit quaternions are important, mainly for representation of three dimensional rotations, and it has been a popular tool in computer graphics for more than twenty years. This representation is better than 3×3 rotation matrices in many aspects, see Shoemake (1985). However, classical quaternions are restricted to the representation of rotations, whereas in many various areas of mathematics there is a requirement to find a more general structure, which will represent also displacement. William Kingdon Clifford (1845–1879) invented dual quaternions in the nineteenth century, see Clifford (1882), to represent rigid transformations. There is a close connection to a classical result of the spatial kinematics known as Chasles' theorem, see Murray et al. (1994) for more details. Chasles' theorem states that any rigid transformation can be described by a screw, i.e., a rotation about an axis followed by a translation in the direction of this axis. Therefore, dual quaternions are convenient to describe a composition of rotations and translations. In this thesis, we advocate that dual quaternions are in many aspects a convenient representation of the rigid transformation.

1.1 History

The geometrical interpretation of complex numbers and the method of their derivation from real numbers expanded during the nineteenth century to many

different considerations of structures of multicomponent numbers. These numbers are called *hypercomplex numbers*.

It begins with studying expressions such as $a_0\alpha_0 + a_1\alpha_1 + \cdots + a_n\alpha_n$, where n is a natural number, $a_0, a_1, \ldots, a_n$ are real numbers and $\alpha_0, \alpha_1, \ldots, \alpha_n$ are new basic units. The main requirement was to preserve common algebraic property which is that of being a field, and it is captured by nine laws governing addition and multiplication, such as $ab = ba$ and $a(bc) = (ab)c$ (commutative and associative laws for multiplication). Further, the geometric property is the existence of an absolute value $|u|$, which measures the distance of u from the origin and is multiplicative $|uv| = |u||v|$.

However, we know that the system of hypercomplex numbers can be created only for $n = 1, 2, 4, 8$, which was proven by German mathematician Adolf Hurwitz (1859–1919) in 1898, see Hurwitz (1898). If dimension n is equal to $1, 2, 4$ and 8, the algebra is known as real numbers, complex numbers or quaternions, which have all the required properties except commutative multiplication, and octonions, which have all the required properties except commutative and associative multiplication.

Many various mathematicians such as Sir William Rowan Hamilton, Arthur Cayley (1821–1895), Augustus de Morgan (1806–1871), brothers Charles Graves (1810–1860) and John Thomas Graves (1806–1870) and others started to find a new numeric field which expanded the field of complex numbers.

Hamilton wanted to extend complex numbers to a new algebraic structure with each element consisting of one real part and two distinct imaginary parts. He focused on three dimensional complex numbers known as triplets, but his effort was futile. One of Hamilton's motivations for seeking three dimensional complex numbers was to find a description of a rotation in the space corresponding to the complex numbers, where a multiplication corresponds to a rotation and a scaling in the plane. He published "Theory of Triplets", i.e., a system that would do for the analysis of three dimensional space what imaginary numbers do for two dimensional space. Hamilton had been searching for such triplets since at least 1830. It is significant to note that in this paper Hamilton makes clear that he understands the nature and importance of the associative, commutative, and distributive laws, an understanding rare at the time when no exceptions to these laws were known. Following the example of the complex numbers, he wrote the triplets of the form $a + \mathbf{i}\, b + \mathbf{j}\, c$, where $a, b, c \in \mathbb{R}$ and $\mathbf{i}^2 = \mathbf{j}^2 = -1$. Hamilton never succeeded in making this generalization, and it has later been proven that the set of three dimensional numbers is not closed under multiplication. In 1966 Kenneth O. May (1915–1977) gave an elegant proof of this, see Dam et al. (1998).

Having searched for his triplets for thirteen years, Hamilton discovered *quaternions*. In a letter he later wrote to one of his children about the discovery, he recounts that his children used to ask him each morning at breakfast: "Well,

Papa, can you multiply triplets?" To this he would reply, "No, I can only add and subtract them." His search ends with his discovery of mathematical entities he calls quaternions. The story says that on 16th October 1843 which happened to be a Monday and a council day of the Royal Irish Academy, he was walking across the Royal Canal in Dublin with his wife, when the solution to quaternions came to him in the form of an equation, which he inscribed in stone on the bridge now called the Brougham or Broom Bride. The original inscription has faded but a Quaternion plaque exists there today that reads:

> Here as walked by
> on the 16th October 1843
> Sir William Rowan Hamilton
> in a flash of genius discovered
> the fundamental formula for
> quaternion multiplication
> $\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -1$
> & cut it on a stone of this bridge.

In this formalism, Hamilton devised a four vector form of complex numbers that had the components of a four dimensional space just as two dimensional space complex numbers. Later he presented the quaternion theory of mathematics at a series of lectures at the Royal Irish Academy. The lectures gave rise to a book Hamilton (1852).

Complex numbers, quaternions and octonions have a special structure and one of the most remarkable, is their relationship with the projective geometry via the theorems of Pappus and Desargues, see Stillwell (2010).

Although Hamilton derived his work independently, it had been, discovered earlier in a nearly identical form by a mostly unknown mathematician by the name, of Olinde Rodrigues (1795–1851). In fact, Rodrigues had a much stronger grasp on the algebra of the rotations and even had the beginnings of what would later become known as Lie algebra.

Furthermore, a *biquaternions*, which were predecessors of a unit dual quaternions need to be mentioned. Biquaternions are an eight dimensional algebra consisting of quaternion numbers with complex coefficients, and were first considered by Hamilton [47]. He used this term for a quaternion $q = a + \mathbf{i}\, b + \mathbf{j}\, c + \mathbf{k}\, d$, where a, b, c, d are complex numbers. This term was later used by William Kingdon Clifford, an English mathematician and philosopher who worked extensively in many branches of pure mathematics and classical mechanics. Clifford's study of geometric algebras in both Euclidean and non-Euclidean spaces led to his invention of the biquaternion and dual algebra.

Till this time a general rigid transformation can be described by a screw. This is a combination of a rotation around the axis and a translation along a specific

straight line (the axis) in three dimensional space. Clifford's biquaternion offers one of the most elegant and efficient representations for this transformation.

Clifford adopts Hamilton's term biquaternion[1] for a different purpose, namely to denote a combination of two quaternions, algebraically combined via a new symbol ω (now ε), defined to have the property $\omega^2 = 0$.

The biquaternion can be introduced as the sum of two quaternions, when one of them is multiplied by the dual unit ω (it has eight parts):

$$\boldsymbol{q}_d = q + \omega q_\omega. \tag{1.1}$$

The symbol ω should be viewed as an operator or as an abstract algebraic entity, and not as a real number.

Clifford presented the idea of biquaternions in three papers. First mention was in *Preliminary Sketch of Biquaternions* (1873), where biquaternions are introduced. The second paper *Notes on Biquaternions* (1873) was found in Clifford's manuscripts and was probably intended as a supplement to the first paper. The third paper *Further Note on Biquaternions* (1876) is more extensive and it discusses and clarifies why the biquaternion may be interpreted in essentially two different ways, either as a generalized type of number, or as an operator, for more details see Roney (2010).

German mathematician Eduard Study (1862–1930) gathered information from Clifford's articles and in 1901 he introduced his own article *Geometrie der Dynamen*, where the term dual number is firstly used, see Perez (2003). It starts to use Study's biquaternions and Clifford's biquaternions. It is the same mathematical structure and thus the need is to introduce a new term *dual quaternions*. If you want to learn more about properties of dual numbers and dual quaternions, see for instance Roney (2010) and Clifford (1873).

1.2 State of the art

Quaternions are a very efficient tool for analyzing situations where the rotations in three dimensional space are involved. Its geometric meaning is obvious as the rotation axis and the angle can be trivially recovered. The quaternion algebra, which will be introduced, allows us to easily compose rotations. Quaternions have found their way into many different systems such as animation, inverse kinematics and physics.

Ken Shoemake popularized quaternions in the world of computer graphics, see Shoemake (1985). He introduced *spherical linear interpolation (slerp)*, which

[1] Hamilton use the term biquaternion for quaternion $q = s + \mathbf{i}\,x + \mathbf{j}\,y + \mathbf{k}\,z$, where $x, y, z \in \mathbb{C}$.

is often considered as the optimal interpolation curve between two general rotations. In animation systems quaternions are often used to interpolate between animation curves, see e.g. Dam et al. (1998). On the other hand the rotation matrices are used when many points in the space need to be transformed like the vertices of the skin of an animated model. The conversion between quaternions and matrices was introduced by Shoemake (1994) in the context of computer graphics. Another application can be found in Kavan and Žára (2005) where the dual quaternions are used.

Quaternions have played an important role in the recent development of physics. Their main use in the nineteenth century consisted in expressing physical theories. An important work where this was done was Maxwell's, see Maxwell (1873). The quaternion notation of Maxwell's equation was introduced here. However, he never really calculated with quaternions, he treated a scalar and a vector part separately. More results of application in physics were announced in Kwašniewski (2011).

Another application of quaternions can be found in mathematical models of movement. We mention a few applications, e.g. the motion of an articulated mechanical arm robot, see Heatinger et al. (2005). One of the latest articles is focused on movement in aerospace. Rigid–body attitude control is one of the canonical nonlinear control problems. A fundamental characteristic of attitude control that proves a fascinating difficulty is the topological complexity of $\mathbf{SO}(3)$. Unit quaternions are often used to parameterize $\mathbf{SO}(3)$. This parametrization is the minimal globally nonsingular representation of the rigid–body attitude. Nevertheless, unit quaternions are still used today by many authors, e.g. see Mayhew et al. (2011) or Arribas et al. (2006).

Quaternion representation is also known, in theory, of spatial curves within the Pythagorean hodographs (so called PH curves), i.e., polynomial parametric curves whose hodograph components satisfy the Pythagorean condition. These curves have many advantageous properties in computer aided geometric design, e.g. Farouki (1992), Farouki and Neff (1995) or Farouki (2008), therefore it is known as a class of special Bézier curves. The spatial PH curves were firstly introduced in Farouki and Sakkalis (1994). The advantage of the quaternion approach is that they allow us to combine PH curves and rotations in three dimensional space. In particular, Choi et al. (2002) and Farouki et al. (2002) gave an elegant quaternion description of spatial PH curves. This model has great use, see for example Jüttler and Šír (2007), Farouki et al. (2008) or Farouki and Šír (2011). In addition the PH curves are also generated through octonion algebra, see Farouki and Sakkalis (2012) for more details.

An interesting use of quaternions can be found in algorithms for Inertial Navigation System (INS). An INS may compute the attitude among other possibilities using them. This method is advantageous since it requires less computation, gives better accuracy and avoids singularity. For a deeper account of this

theory we refer the reader to Lee et al. (1998) or Ahmed and Ćuk (2005) and the references given therein.

As we have mentioned, we consider the quaternion representation as a wide area for new approaches in many branches of applied mathematics. Therefore, if you are interested in quaternions you can see some of the latest articles focused on them, e.g. Gal (2011), Longo and Vigini (2010) or Arnold et al. (2011).

The quaternions have been widely used in many branches of biology in recent years. We can find an interesting application in parts concerning proteins, e.g. the problem of predicting the tertiary structure of a protein molecules, for more details see Huliatinskyi and Rudyk (2013). This protein structure plays one of the main roles in determining the functional properties of proteins. The results can be applied in medicine, pharmaceutics or bioinformatics. Papers, Kneller and Calligari (2006) and Kneller and Calligari (2012), where the application to structural biology can be found, introduced a new method called *ScrewFit*, which is useful for the study of localizing changes in protein structure. This method is based on quaternions.

In recent years, studying dual quaternions has also been an active research area. Therefore, we mention some interesting applications. For instance, skinning is a common task in computer graphics which can be expressed by the method based on dual quaternions. It offers a very simple efficient skinning method. Due to their properties, none of the skin collapsing effects will manifest themselves. There have been several articles focusing on the generalization of established techniques for blending of the rotations to include all the rigid transformations, approaches are presented in Kavan et al. (2006) and Kavan et al. (2007). Algorithms based on dual quaternions are computationally more efficient than previous solutions and have better properties (constant speed, shortest path and coordinate invariance).

Applying dual quaternions has appeared in a kinematics equation of the robot form. The dual quaternion synthesis methodology provides a tool for the systematic design of constrained robots. Some of these results have been implemented in computer–aided design (CAD) systems. Since then, dual quaternions and their planar version have been widely used in the analysis of robotic systems, see for instance the works by Perez (2003) and Dooley and McCarthy (1991). An interesting and specific area for applying dual quaternions is hand eye calibration algorithm on an endoscopic surgery robot. Special focus is on robustness, since the error of position and orientation data provided by the robot can be large depending on the movement actually executed. The best general reference is Daniilidis (1999) or Schmidt et al. (2003). Further important research topic concerns the teleoperation of open chain serial link manipulators in laparoscopy. The paper Marinho et al. (2014) introduces a novel intuitive algorithm for robotic control of laparoscopic tools using programmable Remote Center of Motion which is based on dual quaternions.

The latest article dealing with the shortest path interpolation using dual quaternions, that are singularity–free and unambiguous, is Schilling (2011). From a different part of kinematics the paper, Wang et al. (2012) can be mentioned. This paper focuses on finding a dual quaternion solution to attitude and position control for multiple rigid body coordination. Representing rigid bodies in three dimensional space by unit dual quaternion kinematics, a distributed control strategy, together with a specified rooted-tree structure, are proposed to control the attitude and position of networked rigid bodies simultaneously with notion concision and nonsingularity. Additionally, the paper dealing with the control of an n-dof robot arm in an efficient way using dual quaternions is by Özgür and Mezouarb (2016). Of course, the task-space design problem is widely found. The paper by Marinho et al. (2015) deals with the design problem of a linear-quadratic optimal tracking controller for robotic manipulators which is modified with using the unit dual quaternion formalism. The efficiency and compactness of singularity of the representation render the unit dual quaternion a suitable framework for simultaneously describing the attitude and the position of the end-effector.

Algebra of dual quaternions has not been used in other areas of physics as frequently as it deserves. The formulation of classical electromagnetism by dual quaternions is another interesting application for them. Firstly, we found an effort to express reformulation of Maxwell's equations by using dual quaternions. It means that Maxwell's four equations could be expressed in a single equation. Further, there were derived constitutive relations and related equations which satisfy all the equations which were earlier given by using biquaternions. These dual quaternionic representations can be successfully adapted to the physical situations, see Demir and Özdas (2003) for more details. Later Maxwell's equations and the constitutive relations for electromagnetism are expressed in the terms of dual quaternionic matrices and for this purpose, new 88 matrices connected with the quaternion basis elements have been introduced, see Demir (2007) and the references given there.

Another approach based on dual quaternion is used for the space motions. The important thought was that the positions of the moving objects are represented using the dual quaternion curves without any normalization conditions, see Jütler (1994). This paper focused on rational motions described by dual quaternions. Other papers focused on a new method for tool path generation using rational Bézier cutter motions. A representing point trajectory could be used by rational Bézier dual quaternion. The Bézier dual quaternion curve corresponds to a rational Bézier motion whose point trajectories are rational Bézier curves. The influence of weights of the dual quaternion curves on the resulting rational motion can be found in Zhang et al. (2004) and Purwar and Qiaode (2005). A recent study focused on 5–axis NC machining. The rational rigid movement of a cutter is

interpolated by a B–spline curve in dual quaternion space, see Bi et al. (2010).

Current application of dual quaternion can be found in Hedgüs et al. (2012). This article is focused on the generic rational curve C in the group of Euclidean displacements. Furthermore, the linkage such that the constrained motion of one of the links of curve C is constructed. This construction is based on the factorization of polynomials over dual quaternions. Moreover, the constructive proof for the existence of a unique rational motion of minimal degree in the dual quaternion model of rigid transformation with a given rational parametric curve as trajectory, is given by Li et al. (2016).

Dual quaternions have expanded in the navigation community too. Unfortunately, researches have been aware of the benefits of them during the last decade, although quaternions were used much earlier. Thus, recent effort is to propose that dual quaternions are an elegant and efficient mathematical tool for investigating strapdown algorithms, see Wu et al. (2005) or Wu et al. (2006). Last but not least is the amazing application of dual quaternion which can be used during docking. One of the most important flying task, i.e., task for the successful implementation of autonomous rendezvous and docking, is the ability to acquire the relative position and attitude information between the chaser and the target satellites in real time, see Qiao et al. (2013) or Dong et al. (2016).

Furthermore, from the recently published papers we should mention the approach of combined position and attitude tracking controllers based on dual quaternions which can be developed with relatively low effort from existing attitude-only tracking controllers based on quaternions, see Filippe and Tsiotras (2013) and the reference given there. The next application is devoted to the H_∞ robust control problem for robot manipulators using unit dual quaternion representation, which allows a description of the end-effector transformation without decoupling rotational and translational dynamics, see Figueredo et al. (2013).

Another interesting field where the dual quaternions could be used is the area of spacecrafts. The dual quaternions are used to improve successful Quaternion Multiplicative Extended Kalman Filter for spacecraft attitude estimation. The quaternion approach has been used extensively in several NASA spacecraft. Therefore there was motivation to make improvements. This new approach can be found in Nuno et al. (2016)

The first connection between estimating of three dimensional location parameters was first introduced by Walker et al. (1991). By minimizing a single-cost function associated with the sum of the orientation and position errors, the rotation matrix and the translation vector were derived simultaneously. However, the scale parameter in the process of transformation was not considered. Therefore, the scale parameter was directly introduced into the coordinate transformation in registration of LiDAR points in work Wang et al. (2014).

Dual quaternions are applied in bioinformatics as well as quaternions. Mainly, the focus is on models of proteins and there is an effort to use dual quaternions

for its description, see Wasnik et al. (2013) and the references given there. This paper presents a method for optimal alignment of a Protein Backbone with respect to another. *Kabsch Method* is used which consists of finding the optimal translation and rotation.

1.3 Objectives and main contribution

The thesis will contribute to advancing the state of the art concerning the usage of dual quaternions in selected disciplines with promising application potential. In particular, the main objectives and challenges, which were formulated at the beginning of the dissertation task, can be summarized as follows:

- ♣ to describe the latest advances in applications of quaternions and dual quaternions on different problems originated in various (especially non-traditional) fields of technical or natural sciences;
- ♢ to identify and analyze recent methods, techniques, computations and algorithms based on quaternions which are suitable for an efficient (and simple) reformulation using dual quaternions;
- ♡ to enhance the existing framework and derive new results and algorithms for certain classes of (mainly) real-world problems that can be newly solved using the unifying approach based on dual quaternions, to focus mainly on simplifications of existing techniques;
- ♠ to implement the designed novel methods in a suitable software and to prove their functionality on particular examples and discuss advantages (or disadvantages) of traditional and newly formulated approaches.

The above formulated goals will be met in the following way. We start with giving some basic notions of quaternion algebra. Quaternions are very efficient tool for analyzing situations where the rotations in three dimensional space are involved. Further, we will present a complete algebraic structure of dual quaternions and their possibility of the representing rigid transformation. As in the above referred, dual quaternion algebra has been applied in a various fields. Therefore, we will show some examples of their applications. Advantages of the dual quaternion representation and application will be mentioned here. This thesis is an attempt to use this algebra in a special geodetic area known as datum transformation. The motivation behind the using of dual quaternion is to provide better approach and attempt to expand dual quaternions to other fields and find their advantages. The main contribution is a simplification of the original

solution of this transformation which was introduced in Prošková (2012). Furthermore, the attention is devoted to secondary protein structure, e.g. method ScrewFit which is useful for the study of localizing changes in protein structure. This method is based on quaternions. The main goal of this algorithm is to determine the relationships between sets of atoms. This part of the thesis is based on Prošková (2014). The next focus is on interpolation by rational spline motions which is an important part of the technical practice, e.g. robotics. Rational spline motions are characterized by the property that the trajectories of the points of the moving object are rational spline curves. We will focus on piecewise rational motions with the first order geometric continuity, i.e., G^1 and G^2 Hermite interpolation. We will briefly introduce a new approach to rational spline motion design, which uses dual quaternions that is mentioned in Prošková (2017).

A fundamental aspect of the proposed research aims at combining the applied mathematics and scientific computing on one side and suitably chosen topics from selected disciplines on the other side. The proposed investigation draws from results and methods which belong to various branches of not only theoretical or applied mathematics but also to other natural or technical sciences (structural biology, geodesy, kinematics etc.). The research methodology is based on the use of theoretical tools, which will be employed and adjusted to new classes of problems as well as on symbolical computations and numerical experiments. We shortly recall the contributions of the main fields.

- Principles from *algebra of quaternions and dual quaternions* will be used. The thesis needs algorithms for computing with quaternion and dual quaternion representations, and especially their applications in geometry.
- The thesis will exploit techniques of *symbolic computation*, in particular methods for solving systems of non-linear equations and elimination techniques. In addition, exact computation will be used extensively when possible.
- Principles from *computational geometry* will be used. These are needed in order to design algorithms that can be suitable for real-world applications working with mathematical objects that are assumed to be given by parameterizations.
- Advanced techniques of *geometric modelling* are used throughout the thesis. This concerns especially techniques for modelling with curves and the use of non-linear geometric representations with special properties
- Methods from *classical numerical analysis* will be used, especially when formulating and studying the modified algorithms. The thesis combines numerical and symbolic computations in order to obtain a better understanding of numerical continuation algorithms for geometric design applications.

- Fundamental principles, methods and techniques from other suitably chosen disciplines (*structural biology, geodesy, computer graphics, kinematics etc.*) will be used to enable bridge the results from applied mathematics with chosen real-life problems from these other fields.

The remainder of the thesis is organized as follows. After introduction, in Chapter 2 we recall some basic notions and facts from the quaternion geometry which are consequently used for the introduction of dual quaternions. Further, we introduce the definition of dual numbers and dual quaternions. Subsequently, dual quaternions are used for describing rigid transformation in the special Euclidean group. Since dual quaternions are composed of eight real components, 8×8 matrix representation is also introduced. The following part is devoted to practical applications of dual quaternions. The formula for computation of rotation, translation and scale parameters in the Burša–Wolf geodetic datum transformation model from two sets of co–located three dimensional coordinates is derived. Furthermore, Chapter 4 is devoted to a particular application of dual quaternions in bioinformatics where the model and the algorithm for description protein secondary structure can be found. Chapter 5 is devoted to G^1 and G^2 Hermite interpolation, which can be practically described in the form of dual quaternions where advantage is found in simplification of original approach. Finally, we conclude the thesis in Chapter 6.

Chapter 2

Preliminaries

As we have mentioned earlier, our results are based on the observations on quaternions and dual quaternions. This thesis explores the basics of the quaternion algebra, particularly its description of the three dimensional rotations. Subsequently, the notions of dual quaternion are explained. Let us therefore start our discussion with recalling some fundamental facts regarding quaternions, see e.g. Dam et al. (1998). The quaternion can represent only rotation, while the dual quaternion can do both rotation and translation. Therefore, the dual quaternion is mainly used in applications to robotics or computer graphics. Undoubted advantage of dual quaternions is that while the orientation of a rigid body is represented by nine elements in homogenous transformations, dual quaternions reduce the number of elements to four. The structure of dual algebra is very similar to complex numbers. In this thesis, we present an efficient algorithm which is based on the use of dual quaternions. Moreover, the matrix representation of these structures is explained. More details can be found e.g. in Clifford (1882) or Stachel (2004).

2.1 Quaternions

In this section, we provide a definition of quaternion algebra. The first part will be devoted to basic definition of quaternion algebra. Although this thesis is focused on dual quaternions, the basic quaternion theory is also needed for better understanding. The rest of the section will be focused on representation of rotations with quaternions.

2.1.1 Quaternion algebra

Definition 2.1. Let $\mathbf{i}^2 = \mathbf{k}^2 = \mathbf{j}^2 = \mathbf{ijk} = -1$, $\mathbf{ij} = \mathbf{k}$ a $\mathbf{ji} = -\mathbf{k}$. A *quaternion* $\mathcal{Q}$ can be written as

$$\begin{aligned} \mathcal{Q} &= (q_0, \mathbf{q}), \quad q_0 \in \mathbb{R}, \mathbf{q} \in \mathbb{R}^3 \\ &= (q_0, q_1, q_2, q_3), \quad q_0, q_1, q_2, q_3 \in \mathbb{R} \\ &= 1q_0 + \mathbf{i}\, q_1 + \mathbf{j}\, q_2 + \mathbf{k}\, q_3, \quad q_0, q_1, q_2, q_3 \in \mathbb{R}, \end{aligned}$$

where the basis elements $1, \mathbf{i}, \mathbf{j}, \mathbf{k}$ are called *quaternion units*.

Definition 2.2. The *set of quaternions* is denoted by $\mathbb{H}$.

Definition 2.3. Let $\mathcal{Q} = (0, \mathbf{q}) \in \mathbb{H}, q_0 = 0$, then $\mathcal{Q}$ is called a *pure quaternion*. The *set of all pure quaternions*[1] is denoted by $\mathbb{H}_p$.

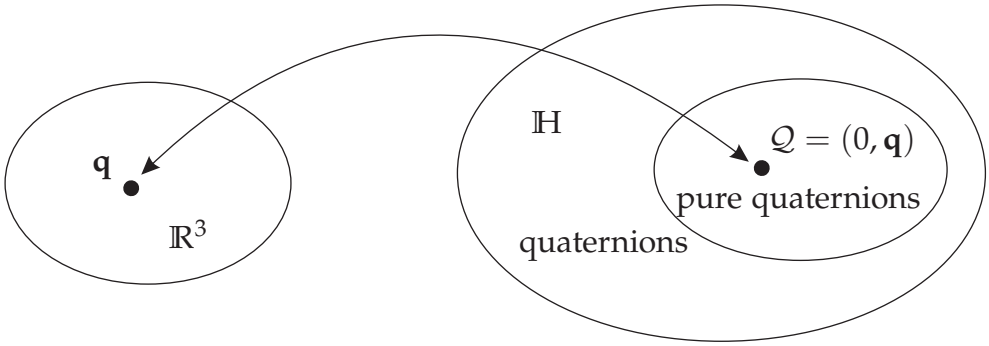

Figure 2.1: Relation between quaternions in $\mathbb{H}$ and vectors in $\mathbb{R}^3$.

Note that addition of quaternions is as simple as addition of complex numbers but the multiplication is not commutative because of the properties of quaternion units.

Definition 2.4. Let $\mathcal{Q} \in \mathbb{H}$. Then $\mathcal{Q}^* = q_0 - \mathbf{i}\, q_1 - \mathbf{j}\, q_2 - \mathbf{k}\, q_3 = q_0 - \mathbf{q}$ is called *conjugate quaternion* for a given quaternion $\mathcal{Q}$.

Definition 2.5. Let $\mathcal{Q}, \mathcal{P} \in \mathbb{H}$, where $\mathcal{Q} = (q_0, \mathbf{q})$ and $\mathcal{P} = (p_0, \mathbf{p})$. *Addition* is defined as

$$\begin{aligned} \mathcal{Q} + \mathcal{P} &= (q_0 + p_0) + (q_1 + p_1)\mathbf{i} + (q_2 + p_2)\mathbf{j} + (q_3 + p_3)\mathbf{k} \\ &= (q_0 + p_0, \mathbf{q} + \mathbf{p}). \end{aligned} \tag{2.1}$$

The multiplication rule for quaternions is the same as for polynomials, extended by the multiplicative properties of the quaternion elements $\mathbf{i}, \mathbf{j}, \mathbf{k}$.

[1] Sometimes called *imaginary quaternions*.

Definition 2.6. Let $\mathcal{Q}, \mathcal{P} \in \mathbb{H}$, where $\mathcal{Q} = (q_0, \mathbf{q})$ and $\mathcal{P} = (p_0, \mathbf{p})$. *Multiplication* is defined as

$$\mathcal{Q}\mathcal{P} = (q_0 p_0 - \mathbf{q} \cdot \mathbf{p}, \mathbf{q} \times \mathbf{p} + q_0 \mathbf{p} + p_0 \mathbf{q}), \tag{2.2}$$

where the symbols $\cdot$ and $\times$ are the standard dot product and the cross product of the vectors from $\mathbb{R}^3$.

The multiplication of quaternions is anticommutative, i.e., the equality $ab = -(ba)$ is not satisfied in general. Nevertheless, the multiplication is associative and distributive over addition.

Given two quaternions $\mathcal{Q}$ and $\mathcal{P}$, we can easily verify that it holds

$$(\mathcal{Q}\mathcal{P})^* = \mathcal{P}^* \mathcal{Q}^*. \tag{2.3}$$

Definition 2.7. Let $\mathcal{Q} \in \mathbb{H}$, $\mathcal{Q} = (q_0, \mathbf{q})$. The *norm* $\|\mathcal{Q}\|$ of the quaternion $\mathcal{Q}$ is given by

$$\|\mathcal{Q}\| = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2} = \sqrt{\mathcal{Q}\mathcal{Q}^*}, \tag{2.4}$$

thus

$$\|\mathcal{Q}\|^2 = q_0^2 + q_1^2 + q_2^2 + q_3^2 = q_0^2 + \|\mathbf{q}\|^2, \quad \|\mathcal{Q}\| \geq 0.$$

$\|\mathcal{Q}\| = 0$ if and only if $q_0 = q_1 = q_2 = q_3 = 0$, thus

$$\|\mathcal{Q}\| = 0 \Leftrightarrow \mathcal{Q} = 0.$$

Theorem 2.8. *Let $\mathcal{Q}, \mathcal{P} \in \mathbb{H}$. Then the following identities are satisfied*

$$\mathcal{Q}\mathcal{Q}^* = \|\mathcal{Q}\|^2, \tag{2.5}$$

$$\|\mathcal{Q}\mathcal{P}\| = \|\mathcal{Q}\|\|\mathcal{P}\|, \tag{2.6}$$

$$\|\mathcal{Q}\mathcal{P}\|^2 = \|\mathcal{Q}\|^2 \|\mathcal{P}\|^2 . \tag{2.7}$$

Proof. See e.g. Prošková (2009). □

Definition 2.9. Let $\mathcal{Q} \in \mathbb{H}$. If

$$\|\mathcal{Q}\| = 1, \tag{2.8}$$

then $\mathcal{Q}$ is called a *unit quaternion*. The *set of all unit quaternions* is denoted by $\mathbb{H}_1$.

Theorem 2.10. *Let $\mathcal{Q} \in \mathbb{H}$, $\mathcal{Q} \neq 0$. Then there exists a unique inverse quaternion $\mathcal{Q}^{-1}$ satisfying $\mathcal{Q}\mathcal{Q}^{-1} = \mathcal{Q}^{-1}\mathcal{Q} = 1$ which can be obtained as*

$$\mathcal{Q}^{-1} = \frac{\mathcal{Q}^*}{\|\mathcal{Q}\|^2}. \tag{2.9}$$

Proof. For more details see e.g. Prošková (2009). □

Theorem 2.11. *Let $\mathcal{Q}, \mathcal{P} \in \mathbb{H}_1$. Then the following identities are satisfied*

$$\| \mathcal{Q}\mathcal{P} \| = 1, \tag{2.10}$$
$$\mathcal{Q}^{-1} = \mathcal{Q}^{*}. \tag{2.11}$$

Proof. We can use relationship (2.6), for more details see e.g. Prošková (2009). □

Theorem 2.12. *Let $\mathcal{Q} \in \mathbb{H}_1$, then there exists a unit vector $\boldsymbol{n} \in \mathbb{R}^3$ and an angle $\frac{\theta}{2} \in \langle -\pi, \pi \rangle$ such that*

$$\mathcal{Q} = \left(\cos\frac{\theta}{2}, \boldsymbol{n} \sin\frac{\theta}{2} \right). \tag{2.12}$$

Proof. See Prošková (2009). □

Furthermore, quaternions can be also represented in the form of 2×2 complex or 4×4 real matrices in such a way that matrix multiplication corresponds to quaternion multiplication.

Definition 2.13. The 2×2 *complex matrix representation* of the quaternion $\mathcal{Q}$ has the form

$$\mathcal{Q} = q_0 + \mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3 = \begin{bmatrix} q_0 + iq_1 & q_2 + iq_3 \\ -q_2 + iq_3 & q_0 - iq_1 \end{bmatrix}, \tag{2.13}$$

where the orthogonal units $1, \mathbf{i}, \mathbf{j}, \mathbf{k}$ are represented by the matrices

$$1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{i} = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad \mathbf{j} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{k} = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} \tag{2.14}$$

and i is the ordinary imaginary unit.

As we have mentioned above, a quaternion $\mathcal{Q}$ can be also expressed by a 4×4 matrix, see Suleyman (2007) for more details.

Definition 2.14. The 4×4 *real matrix representation* of the quaternion $\mathcal{Q}$ has the form

$$\mathcal{Q} = q_0 + \mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3 = \begin{bmatrix} q_0 & q_1 & q_2 & q_3 \\ -q_1 & q_0 & -q_3 & q_2 \\ -q_2 & q_3 & q_0 & -q_1 \\ -q_3 & -q_2 & q_1 & q_0 \end{bmatrix}. \tag{2.15}$$

This expression is a useful way how to compute, e.g. the quaternion products. The quaternion product $\mathcal{S} = \mathcal{Q}\widehat{\mathcal{Q}}$, where $\mathcal{S} = s_0 + \mathbf{i}s_1 + \mathbf{j}s_2 + \mathbf{k}s_3 \in \mathbb{H}$ is described in the matrix form as

$$\mathcal{S} = \begin{bmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{bmatrix} \begin{bmatrix} \hat{q_0} \\ \hat{q_1} \\ \hat{q_2} \\ \hat{q_3} \end{bmatrix} = \begin{bmatrix} \hat{q}_0 & -\hat{q}_1 & -\hat{q}_2 & -\hat{q}_3 \\ \hat{q}_1 & \hat{q}_0 & \hat{q}_3 & -\hat{q}_2 \\ \hat{q}_2 & -\hat{q}_3 & \hat{q}_0 & \hat{q}_1 \\ \hat{q}_3 & \hat{q}_2 & -\hat{q}_1 & \hat{q}_0 \end{bmatrix} \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix}. \tag{2.16}$$

The main properties of quaternions were summarized in this chapter. These properties are required for better understanding of the following text. There exist more important issues connected with quaternions which we do not mention here for the sake of brevity (e.g. quaternion functions, quaternion analysis, differential calculus or quaternion physics). More details can be found for example in Dam et al. (1998) or Lindsay (2005).

2.1.2 Rotation using quaternions

There exist more approaches how to represent rotations in $\mathbb{R}^3$. We can mention e.g. Euler angles, the most common way to represent the attitude of a rigid body. Some sets of Euler angles are so widely used that they have trivial names such as the roll, pitch, and yaw of an airplane. Nevertheless, the main disadvantages of the Euler angles are for example that certain important functions of Euler angles have singularities or they are less accurate than unit quaternions when used to integrate incremental changes in attitude over time as it is shown in Diebel (2006). More details can be found in Pisacane (2005). Therefore, we choose quaternions because functions of unit quaternions have no singularities.

Definition 2.15. The *special orthogonal group* is defined as

$$\mathbf{SO}(3) = \{\mathbf{A} \in \mathbf{GL}(3,\mathbb{R}) \,|\, \mathbf{A}^T\mathbf{A} = \mathbf{I} \wedge \det \mathbf{A} = 1\}, \tag{2.17}$$

where $\mathbf{GL}(3,\mathbb{R})$ denotes the linear group over the set of real numbers $\mathbb{R}$.

The matrix $\mathbf{A}$ represents a rotation in $\mathbb{R}^3$ about the origin if and only if $\mathbf{A} \in \mathbf{SO}(3)$, see Park and Ravani (1997) and references therein. From the following statement we can easily see how the unit quaternions can represent rotations.

Theorem 2.16. *Each element in $\boldsymbol{SO}(3)$ can be expressed as*

$$\mathcal{P} \mapsto \mathcal{Q}\mathcal{P}\mathcal{Q}^*, \tag{2.18}$$

where $\mathcal{P}$ is a pure quaternion and $\mathcal{Q}$ is a unit quaternion.

Proof. See Gallier (2001) for instance. □

Theorem 2.17. *A unit quaternion $\mathcal{Q} = (\cos\frac{\theta}{2}, \boldsymbol{n}\sin\frac{\theta}{2})$ represents the rotation of a vector $\boldsymbol{p} \in \mathbb{R}^3$ by the angle θ along the axis given by $\boldsymbol{n}$, see Fig. 2.2. The vector $\boldsymbol{p}$ is represented by the pure quaternion $\mathcal{P} = (0, \boldsymbol{p})$. The rotated vector $\boldsymbol{p}$, represented as a pure quaternion, is*

$$\widehat{\mathcal{P}} = \mathcal{Q}\mathcal{P}\mathcal{Q}^*. \tag{2.19}$$

Proof. We can find an elegant proof of this in Dam et al. (1998). First, it is shown how a vector $\mathbf{p}$ is rotated by θ along $\mathbf{n}$, using sine, cosine and the scalar and the vector products. Then it is shown that the same result is obtained through a rotation described by quaternions. □

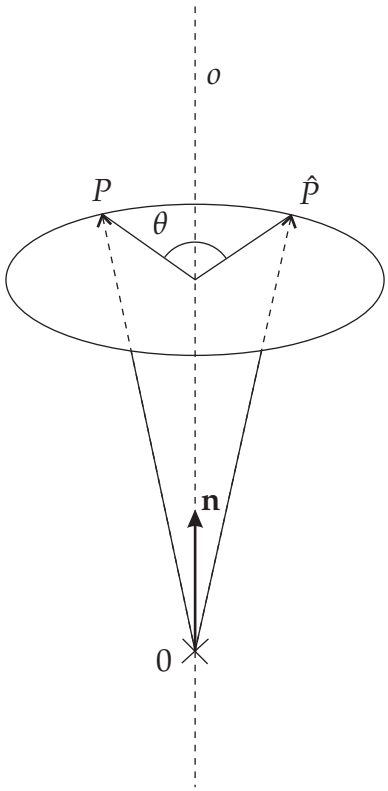

Figure 2.2: Rotation of a point P given by the position vector $\mathbf{p}$ by the angle θ along the axis o given by the vector $\mathbf{n}$.

We have a basic idea of matrix representation of the quaternions, see Definition 2.14, Equation (2.15) and Equation (2.16). Let us try to apply this formulae for the quaternion representation of rotations. Equation (2.19), i.e., $\widehat{\mathcal{P}} = \mathcal{Q}\mathcal{P}\mathcal{Q}^*$ can be expressed in matrix form as

$$\widehat{\mathcal{P}} = \begin{bmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{bmatrix} \begin{bmatrix} 0 & -p_1 & -p_2 & -p_3 \\ p_1 & 0 & -p_3 & p_2 \\ p_2 & p_3 & 0 & -p_1 \\ p_3 & -p_2 & p_1 & 0 \end{bmatrix} \begin{bmatrix} q_0 \\ -q_1 \\ -q_2 \\ -q_3 \end{bmatrix}. \tag{2.20}$$

Therefore, we get

$$\begin{aligned}
\hat{p}_1 &= p_1(q_1q_1 + q_0q_0 - q_2q_2 - q_3q_3) + p_2(2q_0q_2 - 2q_0q_3) \\
&\quad + p_3(2q_1q_3 + 2q_0q_2), \qquad (2.21)\\
\hat{p}_2 &= p_1(2q_0q_3 + 2q_1q_2) + p_2(q_0q_0 - q_1q_0 + q_2q_2 - q_3q_3) \\
&\quad + p_3(-2q_0q_1 + 2q_2q_3), \qquad (2.22)\\
\hat{p}_3 &= p_1(-2q_0q_2 + 2q_1q_3) + p_2(2q_0q_1 + 2q_2q_3) \\
&\quad + p_3(q_0q_0 - q_1q_1 - q_2q_2 + q_3q_3). \qquad (2.23)
\end{aligned}$$

The point P with the position vector $\mathbf{p} = (p_1, p_2, p_3)$ is rotated to the point $\hat{P}$ with the position vector $\hat{\mathbf{p}} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$.

2.2 Dual quaternions

A dual quaternion is considered as an ordinary quaternion whose components are dual numbers. They can represent points, lines or surfaces. Nevertheless, the most important application is a representation of the kinematics of a body, i.e., a rigid body motion. For the sake of brevity, we present at least some necessary definitions and properties dealing with dual quaternions.

2.2.1 Dual numbers

Dual numbers were invented by Clifford in 1873 but their first applications to mechanics are due to Alexandr Petrovich Kotelnikov (1865–1944), see Clifford (1873) or Kotelnikov (1895) for more details. This algebra proved to be a powerful tool for the analysis of mechanical systems as well. Dual numbers are an extension of real numbers analogous to complex numbers. The new element ε, i.e., the dual unit is added to the real numbers. This dual unit satisfies $\varepsilon^2 = 0$.

Definition 2.18. Let $a \in \mathbb{R}$, $a_\varepsilon \in \mathbb{R}$ and $\varepsilon \neq 0$, $\varepsilon^2 = 0$. A *dual number* z_d can be written as

$$z_d = a + \varepsilon a_\varepsilon, \qquad (2.24)$$

where a is the non-dual part, a_ε is the dual part and ε is the basis element.

The dual number can be written as $z_d = [a, a_\varepsilon]$. The set of all dual numbers is commutative and associative ring with a unit element.

Definition 2.19. *The set of all dual numbers* is denoted by $\mathbb{D}$.

Definition 2.20. Let $z_d = [a, a_\varepsilon] \in \mathbb{D}$, $a = 0$, then z_d is called a *pure dual number*. *The set of all pure dual numbers* is denoted by $\mathbb{D}_p$.

Definition 2.21. Let $z_d, \hat{z}_d \in \mathbb{D}$, where $z_d = [a, a_\varepsilon]$ and $\hat{z}_d = [\hat{a}, \hat{a_\varepsilon}]$, then

$$z_d = \hat{z}_d \Leftrightarrow a = \hat{a} \wedge a_\varepsilon = \hat{a_\varepsilon}. \tag{2.25}$$

The appropriate expressions for the conjugate can be obtained in a straightforward manner. The dual conjugate is analogous to the complex conjugate, see the following definition.

Definition 2.22. Let $z_d \in \mathbb{D}$. Then the dual number

$$\overline{z_d} = \overline{[a, a_\varepsilon]} = [a, -a_\varepsilon] = a - \varepsilon a_\varepsilon \tag{2.26}$$

is called *dual conjugate* to the dual number z_d.

The algebra of dual numbers satisfies the following rules for addition, multiplication and division.

Definition 2.23. Let $z_d, \hat{z}_d \in \mathbb{D}$, where $z_d = [a, a_\varepsilon]$ and $\hat{z}_d = [\hat{a}, \hat{a}_\varepsilon]$. *Addition* is defined as

$$\begin{aligned} z_d + \hat{z}_d &= [a, a_\varepsilon] + [\hat{a}, \hat{a}_\varepsilon] \\ &= (a + \varepsilon a_\varepsilon) + (\hat{a} + \varepsilon \hat{a}_\varepsilon) \\ &= (a + \hat{a}) + \varepsilon(a_\varepsilon + \hat{a}_\varepsilon). \end{aligned} \tag{2.27}$$

Definition 2.24. Let $z_d, \hat{z}_d \in \mathbb{D}$, where $z_d = [a, a_\varepsilon]$ and $\hat{z}_d = [\hat{a}, \hat{a}_\varepsilon]$. *Multiplication* is defined as

$$\begin{aligned} z_d \hat{z}_d &= [a, a_\varepsilon][\hat{a}, \hat{a}_\varepsilon] \\ &= (a + \varepsilon a_\varepsilon)(\hat{a} + \varepsilon \hat{a}_\varepsilon) \\ &= a\hat{a} + \varepsilon(a\hat{a}_\varepsilon + a_\varepsilon \hat{a}). \end{aligned} \tag{2.28}$$

Definition 2.25. Let $z_d, \hat{z}_d \in \mathbb{D}$, where $z_d = [a, a_\varepsilon]$, $\hat{z}_d = [\hat{a}, \hat{a}_\varepsilon]$ and $\hat{a} \neq 0$. *Division* is defined as

$$\begin{aligned} \frac{z_d}{\hat{z}_d} &= \frac{a + \varepsilon a_\varepsilon}{\hat{a} + \varepsilon \hat{a}_\varepsilon} \\ &= \frac{(a + \varepsilon a_\varepsilon)(\hat{a} - \varepsilon \hat{a}_\varepsilon)}{(\hat{a} + \varepsilon \hat{a}_\varepsilon)(\hat{a} - \varepsilon \hat{a}_\varepsilon)} \\ &= \frac{a\hat{a} - \varepsilon a\hat{a}_\varepsilon + \varepsilon \hat{a} a_\varepsilon - \varepsilon^2 a_\varepsilon \hat{a}_\varepsilon}{\hat{a}^2 + \varepsilon \hat{a}\hat{a}_\varepsilon - \varepsilon \hat{a}\hat{a}_\varepsilon - \varepsilon^2 \hat{a}_\varepsilon^2} \\ &= \frac{a\hat{a} + \varepsilon(\hat{a} a_\varepsilon - a\hat{a}_\varepsilon)}{\hat{a}^2} \\ &= \frac{a}{\hat{a}} - \varepsilon \left(\frac{a\hat{a}_\varepsilon - a_\varepsilon \hat{a}}{\hat{a}^2} \right). \end{aligned} \tag{2.29}$$

The division of dual numbers is very similar to division of complex numbers because the fraction is extended by the dual conjugate number. It is obvious from the previous definition that division for pure dual number is not defined. This is a fundamental difference from complex numbers because every non-zero complex number has the inverse defined.

The dual number may be used to specify the relative position between two lines in the three dimensional space. In this case, the dual number is referred to as the dual angle.

Definition 2.26. Let be given two lines m, n in three dimensional space, the angle β between these two lines and let s denote their distance. Then the *dual angle* α of these lines is defined as

$$\alpha = \beta + \varepsilon s. \tag{2.30}$$

Especially it holds

1. if the lines m, n are intersecting then $\alpha = \beta$;
2. if the lines m, n are parallel then $\alpha = \varepsilon s$;
3. it the lines m, n are coincident then $\alpha = 0$.

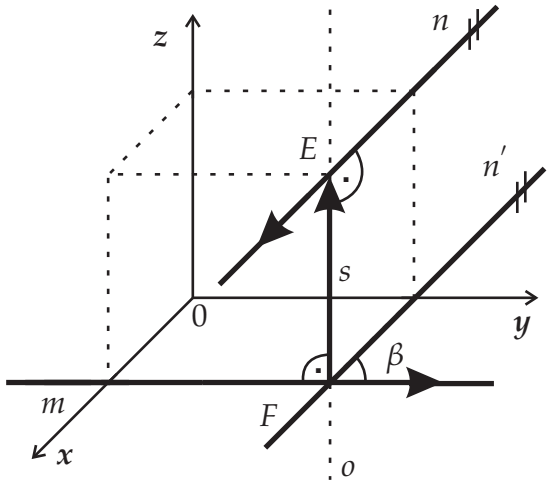

Figure 2.3: The dual angle $\alpha = \beta + \varepsilon s$ expressing the relationship between the lines m and n in space.

The dual angle enables to describe the position of an arbitrary skew line m in space according to another skew line n, see Fig. 2.3. The dual angle is a very useful tool in connection with the screw motion. For more details about the dual angle see e.g. Fischer (1998).

We emphasize that lines may be represented using dual vectors whereas transformation can be described by dual quaternions.

Definition 2.27. Let $\mathbf{a}$ and $\mathbf{a}_\varepsilon$ be the vectors and ε is the dual unit. Then the *dual vector* $\boldsymbol{z}$ is defined as

$$\mathbf{z}_d = \mathbf{a} + \varepsilon \mathbf{a}_\varepsilon. \tag{2.31}$$

Screw motions can be represented by the dual vectors at the origin, for more details see Keler (2000). The best general reference about dual vectors can be found in Stillwell (1995).

It is again also possible to introduce a matrix representation of dual numbers, i.e., the dual unit is represented by a special 2×2 matrix.

Definition 2.28. The 2×2 *matrix representation* of the dual unit ε has the form

$$\varepsilon = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \text{where} \quad \varepsilon^2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}. \tag{2.32}$$

Therefore, the dual number z_d is expressed as

$$z_d = a + \varepsilon a_\varepsilon = \begin{bmatrix} a & a_\varepsilon \\ 0 & a \end{bmatrix}. \tag{2.33}$$

2.2.2 DUAL QUATERNION ALGEBRA

Definition 2.29. A *dual quaternion* $\mathcal{Q}_d$ is defined as the sum of two standard quaternions

$$\mathcal{Q}_d = \mathcal{Q} + \varepsilon \mathcal{Q}_\varepsilon, \tag{2.34}$$

where

$$\mathcal{Q} = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k} \quad \text{and} \quad \mathcal{Q}_\varepsilon = q_{0\varepsilon} + q_{1\varepsilon}\mathbf{i} + q_{2\varepsilon}\mathbf{j} + q_{3\varepsilon}\mathbf{k} \tag{2.35}$$

are real quaternions and $1, \mathbf{i}, \mathbf{j}, \mathbf{k}$ are the usual quaternion units.

We recall that the dual unit ε commutes with the quaternion units, for example it holds $\mathbf{i}\,\varepsilon = \varepsilon\mathbf{i}$.

Definition 2.30. *The set of all dual quaternions* is denoted by $\mathbb{H}_d$.

A dual quaternion can also be considered as an 8–tuple of real numbers, i.e.,

$$\begin{aligned} \mathcal{Q}_d &= q_{0d} + q_{1d}\mathbf{i} + q_{2d}\mathbf{j} + q_{3d}\mathbf{k} \\ &= (q_0 + \varepsilon q_{0\varepsilon}) + (q_1 + \varepsilon q_{1\varepsilon})\mathbf{i} + (q_2 + \varepsilon q_{2\varepsilon})\mathbf{j} + (q_3 + \varepsilon q_{3\varepsilon})\mathbf{k}, \end{aligned} \tag{2.36}$$

where q_{0d} is the scalar part (a dual number), (q_{1d}, q_{2d}, q_{3d}) is the vector part (a dual vector), see Stachel (2004).

Definition 2.31. Let $\mathcal{Q}_d \in \mathbb{H}_d$. The *conjugation* ${\mathcal{Q}_d}^*$ of a dual quaternion $\mathcal{Q}_d$ is defined using the classical quaternion conjugation

$${\mathcal{Q}_d}^* = Q^* + \varepsilon \mathcal{Q}_\varepsilon^*. \tag{2.37}$$

Nevertheless, the dual number conjugation (2.26) can be applied to dual quaternion conjugation.

Definition 2.32. Let $\mathcal{Q}_d \in \mathbb{H}_d$. The *dual conjugate dual quaternion* $\overline{\mathcal{Q}_d^*}$ of a dual quaternion $\mathcal{Q}_d$ is defined as

$$\overline{\mathcal{Q}_d^*} = \mathcal{Q}^* - \varepsilon \mathcal{Q}_\varepsilon^*. \tag{2.38}$$

Definition 2.33. Let $\mathcal{Q}_d, \mathcal{P}_d \in \mathbb{H}_d$ where $\mathcal{Q}_d = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon$ and $\mathcal{P}_d = \mathcal{P} + \varepsilon\mathcal{P}_\varepsilon$. *Addition* is defined as

$$\mathcal{Q}_d + \mathcal{P}_d = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon + \mathcal{P} + \varepsilon\mathcal{P}_\varepsilon. \tag{2.39}$$

Definition 2.34. Let $\mathcal{Q}_d, \mathcal{P}_d \in \mathbb{H}_d$ where $\mathcal{Q}_d = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon$ and $\mathcal{P}_d = \mathcal{P} + \varepsilon\mathcal{P}_\varepsilon$. *Multiplication* is defined as

$$\mathcal{Q}_d\mathcal{P}_d = \mathcal{P} + \varepsilon(\mathcal{Q}\mathcal{P}_\varepsilon + \mathcal{Q}_\varepsilon\mathcal{P}). \tag{2.40}$$

Multiplication of dual quaternions is associative, distributive, but not commutative.

Definition 2.35. Let $\mathcal{Q}_d \in \mathbb{H}_d$, $\mathcal{Q}_d = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k} + \varepsilon q_{0\varepsilon} + \varepsilon q_{1\varepsilon}\mathbf{i} + \varepsilon q_{2\varepsilon}\mathbf{j} + \varepsilon q_{3\varepsilon}\mathbf{k}$. The *norm* $\| \mathcal{Q}_d\|$ of a dual quaternion $\mathcal{Q}_d$ is a dual scalar and it is defined as

$$\begin{aligned} \| \mathcal{Q}_d\| &= \sqrt{(q_0 + \varepsilon q_{0\varepsilon})^2 + (q_1 + \varepsilon q_{1\varepsilon})^2 + (q_2 + \varepsilon q_{2\varepsilon})^2 + (q_3 + \varepsilon q_{3\varepsilon})^2} \\ &= \sqrt{\mathcal{Q}_d^*\mathcal{Q}_d}. \end{aligned} \tag{2.41}$$

Definition 2.36. Let $\mathcal{Q}_d \in \mathbb{H}_d$. A dual quaternion is called *unit dual quaternion* if

$$\|\mathcal{Q}_d\| = 1. \tag{2.42}$$

The set of all unit dual quaternions is denoted by $\mathbb{H}_{d_1}$.

Theorem 2.37. *A dual quaternion $\mathcal{Q}_d$ is unit if and only if*

$$\| \mathcal{Q} \| = 1 \quad \wedge \quad \mathcal{Q} \cdot \mathcal{Q}_\varepsilon = 0. \tag{2.43}$$

Proof. See Prošková (2009) for more details. □

Division is defined as an inverse operation to multiplication. If the norm has a nonvanishing real part, then the dual quaternion $\mathcal{Q}_d$ has the inverse. This is an important difference from complex numbers, because every non-zero complex number has the inverse.

Theorem 2.38. *Let $\mathcal{Q}_d \in \mathbb{H}_d$, $\mathcal{Q}_d = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon$ and $\mathcal{Q} \neq 0$. Then there exists a unique inverse dual quaternion $\mathcal{Q}_d^{-1}$ satisfying $\mathcal{Q}_d\mathcal{Q}_d^{-1} = \mathcal{Q}_d^{-1}\mathcal{Q}_d = 1$ which can be obtained as*

$$\mathcal{Q}_d^{-1} = \frac{\mathcal{Q}_d^*}{\|\mathcal{Q}_d\|^2}. \tag{2.44}$$

Proof. See Prošková (2009). □

Theorem 2.39. *Let $\mathcal{Q}_d, \mathcal{P}_d \in \mathbb{H}_d$, $\mathcal{Q}_d = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon$ and $\mathcal{P}_d = \mathcal{P} + \varepsilon\mathcal{P}_\varepsilon$. Then*

$$(\mathcal{P}_d\mathcal{Q}_d)^* = \mathcal{Q}_d^*\,\mathcal{P}_d^*. \tag{2.45}$$

Proof.

$$\begin{aligned}(\mathcal{P}_d\mathcal{Q}_d)^* &= \{\mathcal{P}\mathcal{Q} + \varepsilon\,(\mathcal{P}_\varepsilon\mathcal{Q} + \mathcal{P}\mathcal{Q}_\varepsilon)\}^* \\ &= (\mathcal{P}\mathcal{Q})^* + \varepsilon\{(\mathcal{P}_\varepsilon\mathcal{Q})^* + (\mathcal{P}\mathcal{Q}_\varepsilon)^*\} \\ &= \mathcal{Q}^*\,\mathcal{P}^* + \varepsilon\,(\mathcal{Q}^*\,\mathcal{P}_\varepsilon^* + \mathcal{Q}_\varepsilon^*\,\mathcal{P}^*) \\ &= \mathcal{Q}_d^*\,\mathcal{P}_d^*.\end{aligned}$$

□

Theorem 2.40. *Let $\mathcal{Q}_d, \mathcal{P}_d \in \mathbb{H}_d$. Then $\|\mathcal{P}_d\mathcal{Q}_d\| = \|\mathcal{P}_d\|\|\mathcal{Q}_d\|$.*

Proof. Theorem 2.39 is used.

$$\|\mathcal{P}_d\mathcal{Q}_d\|^2 = (\mathcal{P}_d\mathcal{Q}_d)^*\,(\mathcal{P}_d\mathcal{Q}_d) = \mathcal{Q}_d^*\,\mathcal{P}_d^*\mathcal{P}_d\mathcal{Q}_d = \|\mathcal{P}_d\|^2\;\mathcal{Q}_d^*\mathcal{Q}_d = \|\mathcal{P}_d\|^2\|\mathcal{Q}_d\|^2 .$$

□

Analogously as in the quaternion case we can represent dual quaternions by matrices, see Suleyman (2007) for more details.

Definition 2.41. The 8×8 *matrix representation* of the dual quaternion $\mathcal{Q}_d$ has the form

$$\mathcal{Q}_d = \begin{bmatrix} \mathcal{Q} & \mathcal{Q}_\varepsilon \\ 0 & \mathcal{Q} \end{bmatrix}, \tag{2.46}$$

where $\mathcal{Q}$ and $\mathcal{Q}_\varepsilon$ are the matrix forms of the type (2.15).

The 8×8 *matrix representation* of the dual conjugate dual quaternion $\overline{\mathcal{Q}_d^*}$ has the form

$$\overline{\mathcal{Q}_d^*} = \mathcal{Q}^* - \varepsilon\mathcal{Q}_\varepsilon^* = \begin{bmatrix} \mathcal{Q}^* & -\mathcal{Q}_\varepsilon^* \\ 0 & \mathcal{Q}^* \end{bmatrix}. \tag{2.47}$$

This representation is often used in computer processing, see Bi et al. (2010). The well-known relations for the quaternion units or the dual unit are included in this matrix form.

2.2.3 Rigid motions using dual quaternions

In this section we study the operations of rotation and translation therefore the notion of rigid transformations is recalled. Rigid transformations combine the operations of rotation and translation into a single matrix multiplication. We begin by introducing the special Euclidean group which is a group of rigid transformation.

Definition 2.42. The *special Euclidean group* is defined as

$$\mathbf{SE}(3) = \left\{ \mathbf{A} | \mathbf{A} = \begin{bmatrix} \mathbf{R} & \mathbf{t} \\ 0 & 1 \end{bmatrix}, \mathbf{R} \in \mathbf{SO}(3), \mathbf{t} \in \mathbb{R}^3 \right\}, \tag{2.48}$$

i.e., $\mathbf{SE}(3)$ is the set of all rigid transformations in three dimensions.

A new method to represent the rigid transformations is based on using dual quaternions, see Prošková (2009). Dual quaternions capture in their inner structure basic information about these transformations – namely the axis of rotation along with the rotation angle about the axis and the translation along it. The composition of these transformations corresponds to the multiplication of dual quaternions.

Definition 2.43. The *associated unit dual quaternion* $\mathcal{P}_d$ to a vector $\mathbf{p} = (p_1, p_2, p_3)$ is defined as

$$\mathcal{P}_d = 1 + \varepsilon(p_1\mathbf{i} + p_2\mathbf{j} + p_3\mathbf{k}). \tag{2.49}$$

The geometric interpretation of a quaternion can be expressed in the form $\mathcal{Q} = \cos\frac{\theta}{2} + \boldsymbol{n}\sin\frac{\theta}{2}$, where $\boldsymbol{n}$ denotes the axis vector and θ the angle of rotation, see Theorem 2.12. Now, we generalize this idea for dual quaternions.

Theorem 2.44. *Let $\theta_d \in \mathbb{D}$ and $\mathcal{V}_d \in \mathbb{H}_{d_1}$, where $\theta_d = \theta + \varepsilon\theta_\varepsilon$ and $\mathcal{V}_d = b\boldsymbol{i} + c\boldsymbol{j} + d\boldsymbol{k} + \varepsilon(b_\varepsilon\boldsymbol{i} + c_\varepsilon\boldsymbol{j} + d_\varepsilon\boldsymbol{k})$. Then*

$$\mathcal{Q}_d = \cos\frac{\theta_d}{2} + \mathcal{V}_d \sin\frac{\theta_d}{2} \tag{2.50}$$

is a unit dual quaternion. Conversely, for every $\mathcal{Q}_d \in \mathbb{H}_{d_1}$ there exist $\theta_d \in \mathbb{D}$ and $\mathcal{V}_d \in \mathbb{H}_{d_1}$ with the zero scalar part which fulfills formula (2.50).

Proof. See Daniilidis (1999). □

Hence, every unit dual quaternion $\mathcal{Q}_d$, e.g. (2.50) can be described with the following parameters $\theta, \theta_\varepsilon, \mathcal{V}, \mathcal{V}_\varepsilon$, where $\mathcal{V}, \mathcal{V}_\varepsilon$ are the components of the unit dual quaternion $\mathcal{V}_d = \mathcal{V} + \varepsilon\mathcal{V}_\varepsilon$. Parameters $\theta, \theta_\varepsilon$ are the components of the dual angle, i.e., $\theta_d = \theta + \varepsilon\theta_\varepsilon$, where θ is the angle of rotation and θ_ε is the distance.

If $\theta = 2c\pi$, where $c \in \mathbb{Z}$, then $\mathcal{V}$ corresponds to a translation vector $\mathbf{v}$. The unit dual quaternion $\mathcal{Q}_d$ can be written as

$$\mathcal{Q}_d = \cos\frac{\theta_d}{2} + \mathcal{V}_d \sin\frac{\theta_d}{2} = \cos\frac{\theta + \varepsilon\theta_\varepsilon}{2} + (\mathcal{V} + \varepsilon\mathcal{V}_\varepsilon)\sin\frac{\theta + \varepsilon\theta_\varepsilon}{2}. \tag{2.51}$$

Geometric interpretation (2.51) can be considered as a screw motion and therefore every rigid transformation can be described using dual quaternions, see Murray et al. (1994).

The angle $\frac{\theta}{2}$ is the angle of revolution and the unit vector $\mathbf{v}$ which corresponds to $\mathcal{V}$ describes the axis of rotation. The distance $\frac{\theta_\varepsilon}{2}$ is the amount of translation along vector $\mathcal{V}$ and $\mathcal{V}_\varepsilon$ is the moment of the rotation axis which describes the position of the axis in three dimensional space. The moment can be described as $\mathcal{V}_\varepsilon = \mathcal{P} \times \mathcal{V}$, where $\mathcal{P}$ corresponds to the vector $\mathbf{p}$ from the origin to an arbitrary point on the axis. Therefore the dual quaternions can represent rotation with an arbitrary axis, see e.g. Kavan et al. (2006) or Kavan et al. (2007).

Theorem 2.45. *Suppose that $\boldsymbol{p} = (p_1, p_2, p_3)$ is the position vector of a point P, $\boldsymbol{t} = (t_1, t_2, t_3)$ is a translation vector and $\mathcal{Q} = (\cos\frac{\theta}{2}, \boldsymbol{n}\sin\frac{\theta}{2})$ is a unit quaternion, see Fig. 2.4. Then we can compute the image of the point P after this translation and this rotation as*

$$\widehat{\mathcal{P}}_d = \mathcal{Q}_d\, \mathcal{P}_d\, \overline{\mathcal{Q}_d^*}, \tag{2.52}$$

where $\mathcal{P}_d$, $\mathcal{Q}_d$ are the unit dual quaternions and $\mathcal{T}$ is the pure quaternion fulfilling

$$\mathcal{Q}_d = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon = \mathcal{Q} + \varepsilon\frac{\mathcal{T}\mathcal{Q}}{2} \quad \text{and} \quad \mathcal{T} = t_1\boldsymbol{i} + t_2\boldsymbol{j} + t_3\boldsymbol{k}. \tag{2.53}$$

Proof. The composition of the rotation and translation can be described as follows. Let $\mathcal{Q} \in \mathbb{H}_1$ denotes the rotation and $\mathcal{T}_d \in \mathbb{H}_{d_1}$ denotes the translation of the dual quaternion $\mathcal{P}_d \in \mathbb{H}_{d_1}$:

$$\mathcal{T}_d(\mathcal{Q}\mathcal{P}_d\overline{\mathcal{Q}^*})\overline{\mathcal{T}_d^*} = (\mathcal{T}_d\mathcal{Q})\mathcal{P}_d(\overline{\mathcal{Q}^*}\,\overline{\mathcal{T}_d^*}) = (\mathcal{T}_d\mathcal{Q})\mathcal{P}_d(\overline{\mathcal{Q}^*\mathcal{T}_d^*}) = (\mathcal{T}_d\mathcal{Q})\mathcal{P}_d\overline{(\mathcal{T}_d\mathcal{Q})^*}. \tag{2.54}$$

The multiplication $\mathcal{T}_d\mathcal{Q}$ can be expressed as

$$\mathcal{T}_d\mathcal{Q} = \left[1 + \frac{\varepsilon}{2}(t_1\mathbf{i} + t_2\mathbf{j} + t_3\mathbf{k})\right]\mathcal{Q}, \tag{2.55}$$

$$= \mathcal{Q} + \varepsilon\frac{\mathcal{T}\mathcal{Q}}{2} \quad \text{where} \quad \mathcal{T} = t_1\mathbf{i} + t_2\mathbf{j} + t_3\mathbf{k}. \tag{2.56}$$

Similarly for $\overline{(\mathcal{T}_d\mathcal{Q})^*}$ we get $\overline{(\mathcal{T}_d\mathcal{Q})^*} = Q - \varepsilon\frac{\mathcal{Q}^*\mathcal{T}^*}{2} = \mathcal{Q}^* - \varepsilon\mathcal{Q}_\varepsilon^*$. □

Moreover, the unit dual quaternions naturally represent rotation if the dual part $\mathcal{Q}_\varepsilon = 0$, see (2.19).

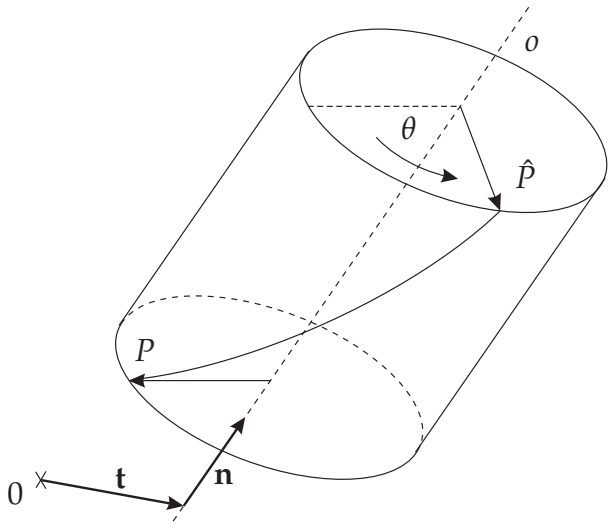

Figure 2.4: Transformation of a position vector $\mathbf{p}$ representing of the point P given by the translation vector $\mathbf{t}$ and the rotation angle θ along the axis o given by the vector $\mathbf{n}$.

Now we rewrite (2.52) to the 8×8 matrix form. The unit dual quaternions $\mathcal{Q}_d$ and $\overline{\mathcal{Q}_d^*}$ are expressed as (2.46) and (2.47). If we multiply the unit dual quaternions $\widehat{\mathcal{P}}_d = \mathcal{Q}_d \, \mathcal{P}_d \, \overline{\mathcal{Q}_d^*}$ in 8×8 matrix form, we get the 8×8 matrix

$$\widehat{\mathcal{P}}_d = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & \hat{p}_1 & \hat{p}_2 & \hat{p}_3 \\ 0 & 1 & 0 & 0 & -\hat{p}_1 & 0 & -\hat{p}_3 & \hat{p}_2 \\ 0 & 0 & 1 & 0 & -\hat{p}_2 & \hat{p}_3 & 0 & -\hat{p}_1 \\ 0 & 0 & 0 & 1 & -\hat{p}_3 & -\hat{p}_2 & \hat{p}_1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{2.57}$$

where

$$\begin{aligned} \hat{p}_1 &= q_0^2 + q_1^2 - q_2^2 - q_3^2 + 2[q_1(p_2 q_2 + p_3 q_3) - q_1 q_{0\varepsilon} + \\ &\quad q_0 q_{1\varepsilon} - q_0(p_3 q_2 - p_2 q_3) + q_3 q_{2\varepsilon} + q_2 q_{3\varepsilon}], \end{aligned} \tag{2.58}$$

$$\begin{aligned} \hat{p}_2 &= p_2(q_0^2 - q_1^2 + q_2^2 - q_3^2) + 2[q_1 q_2 + p_3(q_2 q_3 - q_0 q_1) - q_2 q_{0\varepsilon} + \\ &\quad q_3(q_0 + q_{1\varepsilon}) + q_{2\varepsilon} - q_1 q_{3\varepsilon}], \end{aligned} \tag{2.59}$$

$$\begin{aligned} \hat{p}_3 &= p_3(q_0^2 - q_1^2 - q_2^2 + q_3^2) + 2[p_2(q_0 q_1 + q_2 q_3) - q_3 q_{1\varepsilon} - \\ &\quad q_2(q_0 + q_{2\varepsilon}) + q_1(q_3 + q_{2\varepsilon}) + q_0 q_{3\varepsilon}]. \end{aligned} \tag{2.60}$$

This unit dual quaternion can be written as $\widehat{\mathcal{P}}_d = 1 + \varepsilon(\hat{p}_1\mathbf{i} + \hat{p}_2\mathbf{j} + \hat{p}_3\mathbf{k})$, i.e., the point P with the position vector $\mathbf{p} = (p_1, p_2, p_3)$ is rotated and then translated to the point $\hat{P}$ with the position vector $\hat{\mathbf{p}} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$.

Chapter 3

Burša–Wolf geodetic datum transformation model

The main aim of this chapter is to show one application of dual quaternions in one of the challenging problem of geodesy. The Burša-Wolf similarity transformation model is presented as a seven parameter model for transforming co-located 3D Cartesian coordinates between two datums. The transformation involves three translation parameters, three rotation elements and one scale factor. We will show that mathematical modelling based on dual quaternions is an elegant mathematical method which can be used to represent rotation and translation parameters. Finally, a compact formula is derived for Burša-Wolf model.

3.1 Motivation

In this section, we will present a particular application of dual quaternions in the field of geodesy. A coordinate transformation allows us to take the coordinates of a point in one coordinate system and find the new coordinates of the same point in a second coordinate system. This mathematical operation is mainly used in geodesy, but we can find its using also in photogrammetry, Geographical Information Science (GIS), computer vision and other research areas.

Spatial data are connected to the geographical location which is expressed by coordinates based on a coordinate system. The basis of the coordinate system is

called a geodetic datum which defines the size and shape of the Earth, and the origin and orientation of the coordinate systems used to map the Earth. There are many datums because different countries have used their own different datums. We can mention, for instance, that in geodesy datum transformations are used to convert coordinates related to the Czech national reference frame S-JTSK to the new reference frame WGS 84 [1] (World Geodetic System).

Similarity transformation is a type of transformation, where the scale factor is the same in all directions. The seven parameter[2] similarity transformation is widely used for the datum transformation since it, more or less, satisfies simplicity, efficiency, uniqueness and rigor. This transformation is composed of three translation parameters, one scale factor, and three rotation parameters, see Fig. 3.1. Therefore, coordinates from a three dimensional coordinate frame can be transformed into coordinates in another frame by translating the origin, applying rotation and modification of the scale. In practice, the seven transformation parameters are not always known. However, if the coordinates from two coordinate frames are known for some control points we can estimate the transformation parameters mentioned above. We can say that common coordinates at three points are sufficient for the solution of the seven parameters transformation. There are some popular seven parameter similarity transformation models such as the Burša-Wolf, which we deal with or Molodenskii model, see Molodenskii et al. (1962). The similarity transformation model is often simplified to a linear one because its parameters can be easily computed, see Leick (2003).

Existing solutions of seven parameter models solved by traditional algorithms based on rotation angles or recently quaternions are replaced by new model based on dual quaternions. We will briefly present how to represent and improve datum transformation by dual quaternions.

3.2 Burša-Wolf similarity transformation model

One of the most commonly used transformation methods in the geodetic applications is the Burša-Wolf similarity transformation model. The similarity transformation is popular due to small number of parameters involved and simplicity of the model. Our goal is to estimate all required parameters from co-located coordinates on two different datums. Burša-Wolf similarity transformation model can be written as

$$\mathbf{s}_i = \mathbf{t} + k\mathbf{R}\mathbf{p}_i, \tag{3.1}$$

[1] Dating from 1984 and last revised in 2004.

[2] This transformation is also known as 3D similarity transformation or Helmert transformation.

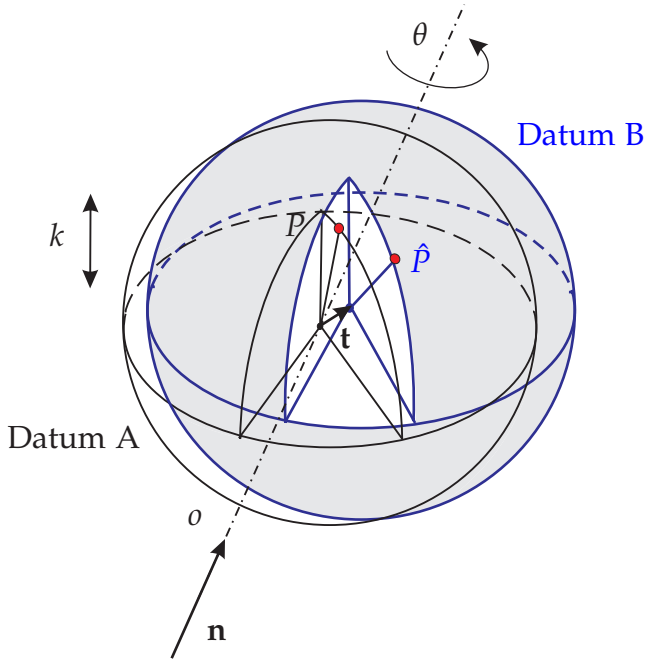

Figure 3.1: Datum shift between two geodetic datums. Apart from different ellipsoids, the centers or the rotation axes of the ellipsoids do not coincide. Transformation of a point P into $\hat{P}$, i.e., rotation by the angle θ along the axis o given by vector $\mathbf{n}$ and translation about vector $\mathbf{t}$ with scale k.

where $\mathbf{s}_i = (s_{1i}, s_{2i}, s_{3i})^T \in \mathbb{R}^3, \mathbf{p}_i = (p_{1i}, p_{2i}, p_{3i})^T \in \mathbb{R}^3$, $i = 1, \ldots, n$ are two sets of the co-located coordinates in the two different systems, $\mathbf{t} = (t_1, t_2, t_3)^T \in \mathbb{R}^3$ denotes the three translation parameters, k denotes the scale parameter and $\mathbf{R} \in \mathbf{SO}(3)$ is the rotation matrix containing three rotation parameters. In order to determine the mentioned parameters, the number of the co-located coordinates $\mathbf{s}_i, \mathbf{p}_i$ must be greater than or equal to three.

3.3 Quaternion algorithm

First, we remind one of the newest approach which is used for solving this problem. In this case, the solution of Burša-Wolf transformation model is based on quaternions. Since they are widely used to express the rotation which is included in this model. Lets us therefore start with reminding this procedure. For a deeper discussion of this method we refer the reader to Shen et al. (2008).

We define centrobaric coordinates $\triangle\mathbf{s}_i = (\triangle s_{1i}, \triangle s_{2i}, \triangle s_{3i})^T, \triangle\mathbf{p}_i =$

$(\triangle p_{1i}, \triangle p_{2i}, \triangle p_{3i})^T$, $i = 1, \ldots, n$ for the sets of the co-located coordinates as

$$\triangle \mathbf{s}_i = \mathbf{s}_i - \frac{1}{n}\sum_{i=1}^{n} \mathbf{s}_i, \quad \text{and} \quad \triangle \mathbf{p}_i = \mathbf{p}_i - \frac{1}{n}\sum_{i=1}^{n} \mathbf{p}_i, \tag{3.2}$$

Notice, that the centrobaric coordinates satisfy the equality

$$\sum_{i=1}^{n} \triangle \mathbf{s}_i = \sum_{i=1}^{n} \triangle \mathbf{p}_i = \mathbf{0}. \tag{3.3}$$

If we substitute equation (3.2) into (3.1), we obtain

$$\begin{aligned} \triangle \mathbf{s}_i &= \mathbf{t} + k\mathbf{R}\left(\triangle \mathbf{p}_i + \frac{1}{n}\sum_{i=1}^{n} \mathbf{p}_i\right) - \frac{1}{n}\sum_{i=1}^{n} \mathbf{s}_i & (3.4)\\ &= \triangle \mathbf{t} + k\mathbf{R}\triangle \mathbf{p}_i, \quad \text{where} \quad \triangle \mathbf{t} = \mathbf{t} + k\mathbf{R}\frac{1}{n}\sum_{i=1}^{n} \mathbf{p}_i - \frac{1}{n}\sum_{i=1}^{n} \mathbf{s}_i. & (3.5) \end{aligned}$$

Equation (3.4) is over-determined therefore we denote the residual vector $\mathbf{v}_i \in \mathbb{R}^3$, $i = 1, \ldots, n$ as

$$\mathbf{v}_i = \triangle \mathbf{s}_i - \triangle \mathbf{t} - k\mathbf{R}\triangle \mathbf{p}_i. \tag{3.6}$$

Now we get the following optimization problem to solve required parameters

$$\begin{aligned} \min_{k,\triangle\mathbf{t},\mathbf{R}} \sum_{i=1}^{n} \mathbf{v}_i^T \mathbf{v}_i &= \min_{k,\triangle\mathbf{t},\mathbf{R}} \sum_{i=1}^{n} (\triangle \mathbf{s}_i - \triangle \mathbf{t} - k\mathbf{R}\triangle \mathbf{p}_i)^T (\triangle \mathbf{s}_i - \triangle \mathbf{t} - k\mathbf{R}\triangle \mathbf{p}_i) & (3.7)\\ &= \min_{k,\triangle\mathbf{t},\mathbf{R}} \left[n\triangle \mathbf{t}^T \triangle \mathbf{t} + \sum_{i=1}^{n} (\triangle \mathbf{s}_i - k\mathbf{R}\triangle \mathbf{p}_i)^T (\triangle \mathbf{s}_i - k\mathbf{R}\triangle \mathbf{p}_i) \right]. & (3.8) \end{aligned}$$

Subsequently, it must be satisfied

$$\triangle \mathbf{t} = \mathbf{0}, \quad \text{i.e.,} \quad \mathbf{t} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{s}_i - k\mathbf{R}\frac{1}{n}\sum_{i=1}^{n} \mathbf{p}_i. \tag{3.9}$$

Equation (3.7) is modified and re-arranged

$$\min_{k,\mathbf{R}} \left[\sum_{i=1}^{n} \triangle \mathbf{s}_i^T \triangle \mathbf{s}_i - 2k \sum_{i=1}^{n} \triangle \mathbf{s}_i^T \mathbf{R} \triangle \mathbf{p}_i + k^2 \sum_{i=1}^{n} \triangle \mathbf{p}_i^T \triangle \mathbf{p}_i \right]. \tag{3.10}$$

It should be noted that necessary condition for an extremum of the function $F(k, x_1, \ldots, x_n) = k^2 A - kB(x_1, \ldots, x_n)$ with A constant is an extremum of the function B and $2kA - B = 0$, i.e., $k = B/2A$. Therefore, we get the new optimization problem

$$\max_{\mathbf{R}} \sum_{i=1}^{n} \triangle \mathbf{s}_i^T \mathbf{R} \triangle \mathbf{p}_i \tag{3.11}$$

and new equation which allows us to determine the scale parameter k

$$k = \sum_{i=1}^{n} \triangle \mathbf{s}_i^T \mathbf{R} \triangle \mathbf{p}_i / \sum_{i=1}^{n} \triangle \mathbf{p}_i^T \triangle \mathbf{p}_i. \tag{3.12}$$

As we have mentioned before, quaternions can represent rotation. Therefore, we substitute quaternion $\mathcal{Q} = (q_0 + \mathbf{q})$ to represent the rotation matrix $\mathbf{R}$. Then the maximization problem can be solved as

$$\max_{\mathbf{R}} \sum_{i=1}^{n} \triangle \mathbf{s}_i^T \mathbf{R} \triangle \mathbf{p}_i = \max_{\mathcal{Q}} \sum_{i=1}^{n} (q_0, \mathbf{q}^T) N \begin{pmatrix} q_0 \\ \mathbf{q} \end{pmatrix}, \tag{3.13}$$

where

$$N = \sum_{i=1}^{n} \begin{bmatrix} \triangle \mathbf{s}_i \triangle \mathbf{p}_i & -\triangle \mathbf{s}_i^T \mathbf{C}(\triangle \mathbf{p}_i) \\ -\mathbf{C}(\triangle \mathbf{s}_i) \triangle \mathbf{p}_i & \triangle \mathbf{s}_i \triangle \mathbf{p}_i^T + \mathbf{C}(\triangle \mathbf{s}_i) \mathbf{C}(\triangle \mathbf{p}_i) \end{bmatrix}, \tag{3.14}$$

and $\mathbf{C}(\mathbf{q})$ is the skew-symmetric matrix

$$\mathbf{C}(\mathbf{q}) = \begin{bmatrix} 0 & -q_3 & q_2 \\ q_3 & 0 & -q_1 \\ -q_2 & q_1 & 0 \end{bmatrix}. \tag{3.15}$$

The matrix N is real-symmetric and it contains four real-valued eigenvalues and their corresponding eigenvectors. Then the solution of the maximization problem of equation (3.13) is equal to the eigenvector corresponding to the maximal eigenvalue of N. Thus we get the solution of the unit quaternion $\mathcal{Q}$, i.e., the unit quaternion representing the best rotation is the eigenvector associated with the eigenvalue of a symmetric matrix. This quaternion is determined uniquely up to its sign. Then we compute the rotation matrix $\mathbf{R}$ as

$$\mathbf{R} = \left[q_0^2 - \mathbf{q}^T \mathbf{q} \right] \mathbf{I} + 2[\mathbf{q}\mathbf{q}^T + q_0 \mathbf{C}(\mathbf{q})], \tag{3.16}$$

where $\mathbf{I}$ denotes the 3×3 identity matrix. The rotation angles can be computed by using

$$\theta_x = \arctan \frac{r_{23}}{r_{33}}, \quad \theta_y = \arcsin(-r_{13}), \quad \theta_z = \arctan \frac{r_{12}}{r_{11}}, \tag{3.17}$$

where r_{ij} is the element of the rotation matrix $\mathbf{R}$ in the i-th row and j-th column and $\theta_x, \theta_y, \theta_z$ are the rotation angles around corresponding coordinate axes. Then the scale parametr k is computed using equation (3.12). Finally, translation parameters are obtained by equation (3.9).

3.4 Improved algorithm using dual quaternions

We use dual quaternions for description of datum transformation, where matrix representations of dual quaternions help us to simplify manipulations of equations, see Section 2.2.3 for a deeper understanding of matrix form.

Previous model based on quaternions is now adjusted with using dual quaternions. The dual quaternion transformation algorithm can be summarized in the following steps:

Algorithm 1 Dual quaternion transformation algorithm

Input: Cartesian coordinates of n stations given in a local and a global reference system.

1: Compute centrobaric coordinates $\triangle\mathbf{s}_i = (\triangle s_{1i}, \triangle s_{2i}, \triangle s_{3i})^T$, $\triangle\mathbf{p}_i = (\triangle p_{1i}, \triangle p_{2i}, \triangle p_{3i})^T$ using (3.2).

2: Express the dual unit quaternion $\mathcal{V}_{d_i}$ with the parameters $q_0, \cdots, q_3, \triangle t_1, \triangle t_2, \triangle t_3, k$ using (3.19) and determine corresponding vector $\mathbf{v}_i = (v_{1i}, v_{2i}, v_{3i})^T$.

3: Compute required parameters $q_0, \cdots, q_3, \triangle t_1, \triangle t_2, \triangle t_3, k$ by (3.24) determined by conditions (3.25).

4: Compute rotation matrix $\mathbf{R}$ using (3.16) and then rotation angles $\theta_x, \theta_y, \theta_z$ using (3.17).

5: Compute translation vector $\mathbf{t}$ using modified equation (3.5).

Output: Three rotation parameters $\theta_x, \theta_y, \theta_z$, three translation parameters t_1, t_2, t_3 and the scale parameter k.

It is possible to express residual vector $\mathbf{v}_i$ in the form of dual quaternions. First, we modify (3.6). The scale parameter $k \in \mathbb{R}$ is a constant, therefore

$$\begin{aligned} \mathbf{v}_i &= \triangle\mathbf{s}_i - \triangle\mathbf{t} - k\mathbf{R}\triangle\mathbf{p}_i \\ &= \triangle\mathbf{s}_i - \triangle\mathbf{t} - \mathbf{R}k\triangle\mathbf{p}_i \\ &= -(\triangle\mathbf{l}_i + \mathbf{R}\triangle\mathbf{r}_i), \text{ where } \triangle\mathbf{l}_i = \triangle\mathbf{t} - \triangle\mathbf{s}_i \text{ and } \triangle\mathbf{r}_i = k\triangle\mathbf{p}_i. \end{aligned} \quad (3.18)$$

Equation (3.18) expresses a rotation of the vector $\triangle\mathbf{r}_i$ and then a translation given by the translation vector $\triangle\mathbf{l}_i$. We can express this equation according to (2.52) using dual quaternions in the form

$$\mathcal{V}_{d_i} = -\mathcal{Q}_{d_i}\mathcal{R}_{d_i}\overline{\mathcal{Q}^*_{d_i}}, \quad (3.19)$$

where $\mathcal{R}_{d_i}$ is a dual unit quaternion

$$\mathcal{R}_{d_i} = 1 + \varepsilon(\triangle r_{1i}\mathbf{i} + \triangle r_{2i}\mathbf{j} + \triangle r_{3i}\mathbf{k}) = 1 + k\varepsilon(\triangle p_{1i}\mathbf{i} + \triangle p_{2i}\mathbf{j} + \triangle p_{3i}\mathbf{k}), \quad (3.20)$$

and $\mathcal{Q}_{d_i}$ is a dual unit quaternion

$$\mathcal{Q}_{d_i} = \mathcal{Q} + \varepsilon\mathcal{Q}_\varepsilon = \mathcal{Q} + \varepsilon\frac{\mathcal{L}_i\mathcal{Q}}{2}, \text{ where } \mathcal{Q} = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k} \quad (3.21)$$

$$\text{and} \quad \mathcal{L}_i = (\triangle t_1 - \triangle s_{1i})\mathbf{i} + (\triangle t_2 - \triangle s_{2i})\mathbf{j} + (\triangle t_3 - \triangle s_{3i})\mathbf{k}. \quad (3.22)$$

The quaternion $\mathcal{Q}$ is a unit quaternion and $\mathcal{L}$ is a pure quaternion. Since $\mathcal{Q}_{d_i}$ is a dual unit quaternion, we must apply the conditions (2.43), i.e.,

$$\|\mathcal{Q}\| = 1 \quad \wedge \quad \mathcal{Q}\cdot\mathcal{Q}_\varepsilon = 0. \quad (3.23)$$

From equation (3.19) we get the dual unit quaternion of the form $\mathcal{V}_{d_i} = 1 + \varepsilon(v_{1i}\mathbf{i} + v_{2i}\mathbf{j} + v_{3i}\mathbf{k})$ corresponding to the vector $\mathbf{v}_i = (v_{1i}, v_{2i}, v_{3i})^T$, where terms v_{1i}, v_{2i}, v_{3i} contains eight parameters to be solved, i.e., $q_0, \cdots, q_3, \triangle t_1, \triangle t_2, \triangle t_3, k$. Further, the transformation parameters can be determined by solving this optimization problem

$$\min_{q_0,\cdots,q_3,\triangle t_1,\triangle t_2,\triangle t_3,k} \sum_{i=1}^{n} \mathbf{v}_i^T\mathbf{v}_i = (v_{1i}, v_{2i}, v_{3i})^T(v_{1i}, v_{2i}, v_{3i}), \quad (3.24)$$

$$\|\mathcal{Q}\| = 1 \quad \wedge \quad \mathcal{Q}\cdot\mathcal{Q}_\varepsilon = 0. \quad (3.25)$$

We can use nonlinear method to solve this minimization problem, i.e., *Lagrange multipliers*. This method can also accommodate multiple constraints. Thus the problem (3.24) under the condition (2.43) can be expressed as minimizing the following Lagrange function

$$L(q_0, \cdots, q_3, \triangle t_1, \triangle t_2, \triangle t_3, k, \alpha, \beta) = \sum_{i=1}^{n} \mathbf{v}_i^T\mathbf{v}_i + \alpha(\sqrt{\mathcal{Q}\mathcal{Q}^*} - 1) + \beta(\mathcal{Q}\cdot\mathcal{Q}_\varepsilon), \quad (3.26)$$

where α and β are the Lagrange multipliers to be determined. The solution by minimizing the Lagrange function (3.26) is equivalent to solving the following non-linear system of equations

$$\begin{aligned} \frac{\partial L}{\partial q_0} &= 0, & \frac{\partial L}{\partial q_2} &= 0, & \frac{\partial L}{\partial \triangle t_1} &= 0, & \frac{\partial L}{\partial \triangle t_3} &= 0, & \frac{\partial L}{\partial k} &= 0, \\ \frac{\partial L}{\partial q_1} &= 0, & \frac{\partial L}{\partial q_3} &= 0, & \frac{\partial L}{\partial \triangle t_2} &= 0, & \frac{\partial}{\partial \alpha} &= 0, & \frac{\partial L}{\partial \beta} &= 0, \end{aligned} \quad (3.27)$$

where $q_0, \cdots, q_3, \triangle t_1, \triangle t_2, \triangle t_3, k, \alpha, \beta$ denotes unknown parameters to be solved. Because equation (3.27) is non-linear, we can find the solution numerically, e.g. by using CAS system Mathematica. Finally, the translation vector $\mathbf{t}$ can be determined by using (3.5).

3.5 Computed example and application

We consider Cartesian coordinates of seven stations given in the local and global reference systems (WGS 84) as in Table 3.1 and Table 3.2. The Fig. 3.2 shows the principle of transformation between two systems via dual quaternions. Values of this stations are taken from Garfarend and Awange (2008). The seven parameters of datum transformation are desired. Numerical example is presented to demonstrate the functionality of the designed method. The values of these stations are frequently used as in Shen et al. (2008) or Zeng and Yi (2011).

Table 3.1: Coordinates for local system (system A).

	System A		
Station name	$X(\mathrm{m})$	$Y(\mathrm{m})$	$Z(\mathrm{m})$
Solitude	4157870.237	664818.678	4775416.524
Buoch Zeil	4149691.049	688865.785	4779096.588
Hohenneuffen	4173451.354	690369.375	4758594.075
Kuehlenberg	4177796.064	643026.700	4761228.899
Ex Mergelaec	4137659.549	671837.337	4791592.531
Ex Hof Asperg	4146940.228	666982.151	4784324.099
Ex Kaisersbach	4139407.506	702700.227	4786016.645

Table 3.2: Coordinates for WGS 84 (system B).

	System B		
Station name	$X(\mathrm{m})$	$Y(\mathrm{m})$	$Z(\mathrm{m})$
Solitude	4157222.543	664789.307	4774952.099
Buoch Zeil	4149043.336	688836.443	4778632.188
Hohenneuffen	4172803.511	690340.078	4758129.701
Kuehlenberg	4177148.376	642997.635	4760764.800
Ex Mergelaec	4137012.190	671808.029	4791128.215
Ex Hof Asperg	4146292.729	666952.887	4783859.856
Ex Kaisersbach	4138759.902	702670.738	4785552.196

Now we compute the transformation parameters $\theta_x, \theta_y, \theta_z, t_1, t_2, t_3, k$ from the local geodetic system to WGS 84. We use the CAS system Mathematica where it is convenient to express dual quaternions in the 8×8 matrix form to find the transformation parameters. The optimization problem was solved using *Lagrange multipliers*. The quaternion $\mathcal{Q}$ and the translation $\triangle\mathbf{t}$ are shown in Table 3.3. The final list of results given from (3.17), (3.5), and *Lagrange multipliers* are listed in Table 3.4.

Table 3.3: Quaternion and translation parameters.

Quaternion $\mathcal{Q}$		Translation $\triangle\mathbf{t}$	
q_0	-0.9999999987474	$\triangle t_1$	-6.649×10^{-10}
q_1	-0.0000024204319	$\triangle t_2$	-3×10^{-13}
q_2	0.0000021663738	$\triangle t_3$	2.658×10^{-10}
q_3	0.0000024073178		

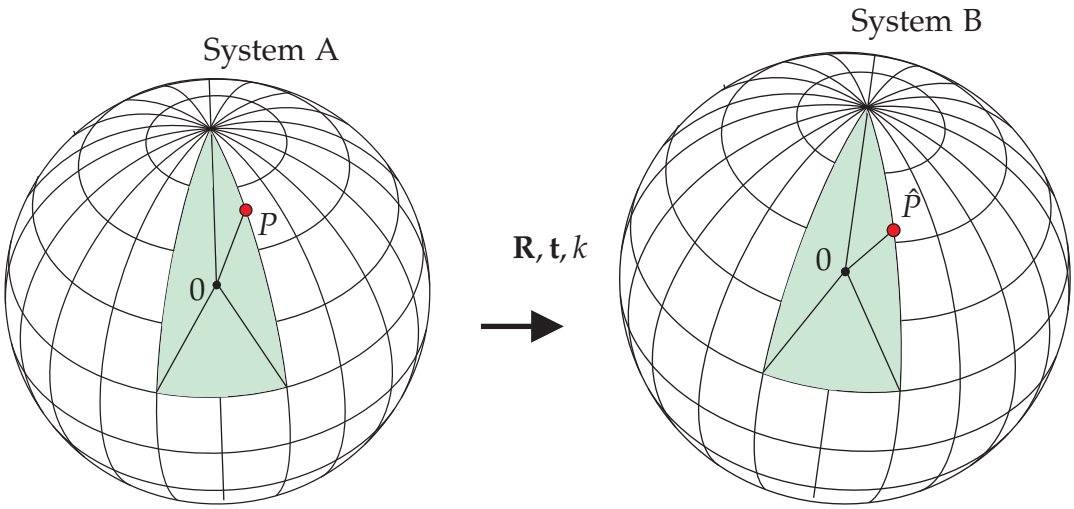

Figure 3.2: The principle of transformation from a local datum (System A) into the WGS 84 datum (System B) via the dual quaternion algorithm.

Table 3.4: Final results of dual quaternion transformation algorithm.

Rotation angles		Translation $\mathbf{t}$		Scale k	
θ_x	$-0.99850''$	t_1	$641.8908m$		
θ_y	$0.89370''$	t_2	$68.6570m$	k	1.0000055825199
θ_z	$0.99309''$	t_3	$416.4101m$		

In addition to this transformation, we compute the residual value to each point, i.e., the difference between coordinates of the system A and the new coordinates of the system A'. The coordinates of the system A' are determined using the computed transformation parameters $\mathbf{R}, \mathbf{t}, k$ and the substitution (3.1). Residuals and new values of the stations are given in Table 3.5 in the next section. Transformation parameters and transformed coordinates are equal to the parameters described by Garfarend and Awange (2008) and Shen et al. (2008).

3.6 Algorithm test

In this part, we will focus on testing two various approaches to solve datum transformation model. We found new formula for Burša-Wolf transformation model in Section 3.5 and our purpose is to compare this algorithm based on dual quaternions, with the algorithm based on quaternions.

Table 3.5: Transformed Cartesian coordinates of System A into System B (Table 3.1) using the seven datum transformation parameters of Table 3.4 computed by the dual quaternion algorithm.

Station name	$X(\mathrm{m})$	$Y(\mathrm{m})$	$Z(\mathrm{m})$
System A: Solitude	4157870.237	664818.678	4775416.524
System B	4157222.543	664789.307	4774952.099
Transformed value: A'	4157870.143	664818.543	4775416.384
Residual	0.0940	0.1351	0.1402
System A: Buoch Zeil	4149691.049	688865.785	4779096.588
System B	4149043.336	688836.443	4778632.188
Transformed value: A'	4149690.990	688865.835	4779096.574
Residual	0.0588	-0.0497	0.0137
System A: Hohenneuffen	4173451.354	690369.375	4758594.075
System B	4172803.511	690340.078	4758129.701
Transformed value: A'	4173451.394	690369.463	4758594.083
Residual	-0.0399	-0.0879	-0.0081
System A: Kuehlenberg	4177796.064	643026.700	4761228.899
System B	4177148.376	642997.635	4760764.800
Transformed value: A'	4177796.044	643026.722	4761228.986
Residual	0.0203	-0.0221	-0.0875
System A: Ex Mergelaec	4137659.549	671837.337	4791592.531
System B	4137012.190	671808.029	4791128.215
Transformed value: A'	4137659.641	671837.323	4791592.536
Residual	0.0919	0.0139	-0.0055
System A: Ex Hof Asperg	4146940.228	666982.151	4784324.099
System B	4146292.729	666952.887	4783859.856
Transformed value: A'	4146940.240	666982.145	4784324.154
Residual	-0.0118	0.0065	-0.0546
System A: Ex Kaisersbach	4139407.506	702700.227	4786016.645
System B	4138759.902	702670.738	4785552.196
Transformed value: A'	4139407.535	702700.223	4786016.643
Residual	-0.0294	0.0041	0.0017

3.6.1 Descriptive statistic

This section provides a simple view at the descriptive statistics obtained from 3070 tested points by the algorithm mentioned above, i.e., dual quaternion algorithm (*DQ algorithm*) and quaternion algorithm (*Q algorithm*). Tested points were given in local and global systems. To find the difference or distance between two set of coordinates we use *Euclidean metric.*

Comparison of algorithms can be summarized in the following steps, which are the same for both of them:

Algorithm 2 Differences between systems

Input: Cartesian coordinates of 3070 stations given in the local (system A) and the global (WGS 84–system B) reference system.

1: Compute rotations, translations and scale parameters using DQ/Q algorithm.
2: Compute new coordinates A' of the system A. The coordinates of the system A' are determined using computed transformation parameters $\mathbf{R}, \mathbf{t}, k$ and substitution (3.1).
3: Compute difference between system A and system A' using Euclidean metric.

Output: Set of values which indicates the difference between the system A and the system A' for both algorithms.

Furthermore, we get the set of values for DQ algorithm and for Q algorithm. To get some information about these data, we use descriptive statistic. Overview of these values can be found in Table 3.6. We can see from the descriptive statistic that we are not dealing with normally distributed data but rather the log-normally distributed data and this is the reason why we apply nonparametric test, a *sign test*, see Beaver et al. (2009) for more details.

3.6.2 Sign test – DQ and Q algorithm

The sign test is used to test the null hypothesis about a median $\tilde{Z}$ of a continuous distribution.

The observations in a sample of size n are $Z_1, Z_2, \ldots, Z_n$. Observations are obtained as a difference $d(A'_Q, A) - d(A'_{DQ}, A)$[3], where A'_Q and A'_{DQ} are new sets of points in WGS 84 and A is the original set of points in WGS 84. The null hypothesis is that the median $\tilde{Z}$ is equal to 0. Suppose that Z^+ is a sum of values,

[3]Euclidean distance between two points A, B is denoted as $d(A, B)$.

Table 3.6: Descriptive statistics.

	DQ algorithm	Q algorithm
minimum	0.2708	0.3333
maximum	9.2231	8.7695
average	3.4163	3.2243
sample standard deviation	1.7049	1.6847
sample variance	2.9075	2.8390
sample quantile$_{05}$	1.0087	0.9058
sample quantile$_{25}$	2.1176	1.8654
sample quantile$_{50}$	3.2470	3.0371
sample quantile$_{75}$	4.3874	4.3317
sample quantile$_{95}$	6.7545	6.3291

where $Z_i > 0$ and Z^- is a sum of values, where $Z_i < 0$. Values of Z which are exactly equal to 0 are ignored. The sum $Z^+ + Z^-$ may therefore be less than n. Null hypothesis $H_0 : \tilde{Z} = 0$ is tested that two set of values are of equal size, i.e., there is no significant difference between the methods. We choose to ignore not only values of Z that are exactly equal to zero but even values in interval $[-1, 1]$, i.e., we want to use only values that we consider as a significant difference. We get $\sum Z^+ = 580$ and $\sum Z^- = 487$. In fact these values counts the number of times where one of methods gives better results.

One-sided alternative hypotheses:

- For one-sided alternative hypothesis $H_1 : \tilde{Z} > 0$, we obtained $F_{Z^+}(x) = 0,9978$. While $0,9978 > 0,05 \Rightarrow$ we do not reject H_0 on the significance level $0,05$. It means that there is no significant difference between the methods.
- For one-sided alternative hypotheses $H_1 : \tilde{Z} < 0$, we obtained $F_{Z^-}(x) = 0,0022$. While $0,0022 < 0,05 \Rightarrow$ we reject H_0 on the significance level $0,05$ and we accept H_1 that DQ algorithm is better if we take into account only significant differences.

3.7 Light detection and ranging (LiDAR) point cloud

LiDAR (Light Detection and Ranging) is a remote sensing technology that collects three dimensional point clouds of the Earth's surface. This sys-

tem includes a Global Positioning System (GPS) and an Inertial Measurement Unit (IMU), which complement the LiDAR data with position and orientation information respectively. This technology is used for a wide range of applications including for example high-resolution topographic mapping or three dimensional surface modeling. The pairs of conjugate points from the two neighbor point clouds are given as an input. The transformation parameters need to be determined. In this solution, dual-number quaternions are used to represent the transformation between two pairs of conjugate points, see Wang et al. (2014).

The representative work on dual quaternions was first introduced by Walker et al. (1991). By minimizing a single-cost function associated with the sum of the orientation and position errors, the rotation matrix and the translation vector were derived simultaneously. However, the scale parameter in the process of transformation was not considered. Therefore, the scale parameter was directly introduced into the coordinate transformation in registration of LiDAR points in work Wang et al. (2014). We briefly show the slightly different approach which is used for solving the transformation model, more details can be found in Wang et al. (2014).

Assuming that point $\widehat{P}$ from local system is determined with quaternion $\widehat{\mathcal{P}}$. Point P from WGS 84 system is the new location of point $\widehat{P}$ and it is determined with quaternion $\mathcal{P}$. Then the dual quaternion based transformation process can be expressed as follows

$$\mathcal{P} = \mathbf{W}(\mathcal{Q})^T \mathcal{Q}_\varepsilon + k\mathbf{W}(\mathcal{Q})^T \mathbf{U}(\mathcal{Q})\widehat{\mathcal{P}}, \tag{3.28}$$

where

$$\mathbf{W}(\mathcal{Q}) = \begin{bmatrix} q_0 & -\mathbf{q}^T \\ \mathbf{q} & q_0\mathbf{I} - \mathbf{C}(\mathbf{q}) \end{bmatrix} \quad \text{and} \quad \mathbf{U}(\mathcal{Q}) = \begin{bmatrix} q_0 & -\mathbf{q}^T \\ \mathbf{q} & q_0\mathbf{I} + \mathbf{C}(\mathbf{q}) \end{bmatrix} \tag{3.29}$$

and k is scale parameter. The sum of the square distances between points P_i and P_i' is

$$f_i = (\mathcal{P}_i - \mathcal{P'}_i)^2. \tag{3.30}$$

The following equation can be derived if we substitute equation (3.28) into (3.30)

$$\begin{aligned} f_i \;=\; & (\mathcal{P}_i - \mathcal{P'}_i)^2 = [\mathbf{W}(\mathcal{Q})^T \mathcal{Q}_\varepsilon]^2 + [k\mathbf{W}(\mathcal{Q}^T)\mathbf{U}(\mathcal{Q})\widehat{\mathcal{P}}_i]^2 + \mathcal{P'}_i^T \mathcal{P'}_i \\ & + 2k[\mathbf{W}(\mathcal{Q})^T \mathcal{Q}_\varepsilon]^T [\mathbf{W}(\mathcal{Q})^T \mathbf{U}(\mathcal{Q})\widehat{\mathcal{P}}_i] - 2(\mathcal{P'}_i)^T [\mathbf{W}(\mathcal{Q})^T \mathcal{Q}_\varepsilon] \\ & - 2k(\mathcal{P'}_i)^T [\mathbf{W}(\mathcal{Q})^T \mathbf{U}(\mathcal{Q})\widehat{\mathcal{P}}_i]. \end{aligned} \tag{3.31}$$

The previous equation (3.31) can be rearranged as

$$\begin{aligned} f_i \;=\; & (\mathcal{P}_i - \mathcal{P'}_i)^2 = \mathcal{Q}_\varepsilon^T \mathcal{Q}_\varepsilon + k^2 \widehat{\mathcal{P}}_i^T \widehat{\mathcal{P}}_i + \mathcal{P'}_i^T \mathcal{P'}_i + 2k\mathcal{Q}_\varepsilon^T \mathbf{W}(\widehat{\mathcal{P}}_i)\mathcal{Q} \\ & - 2\mathcal{Q}_\varepsilon^T \mathbf{U}(\widehat{\mathcal{P}}_i)\mathcal{Q} - 2k\mathcal{Q}^T \mathbf{U}(\mathcal{P'}_i)^T \mathbf{W}(\widehat{\mathcal{P}}_i)\mathcal{Q}. \end{aligned} \tag{3.32}$$

Therefore the error norm, i.e., equation (3.7) for the similarity measurement of the proposed algorithm can be expressed as follows

$$\min_{k,\triangle\mathbf{t},\mathbf{R}} \sum_{i=1}^{n} \mathbf{v}_i^T \mathbf{v}_i = k\mathcal{Q}^T \mathbf{C}_1 \mathcal{Q} + n\mathcal{Q}_\varepsilon^T \mathcal{Q}_\varepsilon + k\mathcal{Q}_\varepsilon^T \mathbf{C}_2 \mathcal{Q} + \mathcal{Q}_\varepsilon^T \mathbf{C}_3 \mathcal{Q} + k^2 C_4 + C_5, \quad (3.33)$$

where

$$\begin{aligned} \mathbf{C}_1 &= -2\sum_{i=1}^{n} \mathbf{U}(\mathcal{P}'_i)\mathbf{W}(\widehat{\mathcal{P}}_i), \qquad \mathbf{C}_2 = 2\sum_{i=1}^{n} \mathbf{W}(\widehat{\mathcal{P}}_i), \qquad \mathbf{C}_3 = -2\sum_{i=1}^{n} \mathbf{U}(\mathcal{P}'_i), \\ C_4 &= \sum_{i=1}^{n} (\mathbf{p}_i^T \mathbf{p}_i), \qquad C_5 = \sum_{i=1}^{n} (\mathbf{p'}_i^T \mathbf{p'}_i). \end{aligned} \quad (3.34)$$

The conditions (2.43) are used, therefore we get the following equation

$$\begin{aligned} L(\mathcal{Q}, \mathcal{Q}_\varepsilon, k, \alpha, \beta) &= k\mathcal{Q}^T \mathbf{C}_1 \mathcal{Q} + n\mathcal{Q}_\varepsilon^T \mathcal{Q}_\varepsilon + k\mathcal{Q}_\varepsilon^T \mathbf{C}_2 \mathcal{Q} + \mathcal{Q}_\varepsilon^T \mathbf{C}_3 \mathcal{Q} + k^2 C_4 + C_5 \\ &\quad + \alpha(\sqrt{\mathcal{Q}\mathcal{Q}^*} - 1) + \beta(\mathcal{Q} \cdot \mathcal{Q}_\varepsilon), \end{aligned} \quad (3.35)$$

where α and β are the Lagrange multipliers. This equation (3.35) provides the optimal solution for the parameters. Considering that $\mathbf{C}_2$ and $\mathbf{C}_3$ are both skew-symmetric matrices, we obtain the following equation

$$\mathbf{A}\mathcal{Q} = \alpha\mathcal{Q}, \quad (3.36)$$

where

$$\mathbf{A} = \frac{1}{4n}(k^2 C_{22} + C_{33})\mathbf{I} + \frac{k}{2}\left[\frac{1}{n}\mathbf{C}_2^T \mathbf{C}_3 - (\mathbf{C}_1 + \mathbf{C}_1^T)\right] \quad (3.37)$$

and $\mathbf{I}$ denotes the 3×3 identity matrix. According to Walker et al. (1991), the quaternion $\mathcal{Q}$ is an eigenvector of the matrix $\mathbf{A}$ and α is the corresponding eigenvalue. Thus four solutions are derived for this equation but according to the matrix $\mathbf{A}$ which is real and symmetric, all the eigenvalues and eigenvectors are real and all the eigenvectors are orthogonal. Therefore the error will be minimized if we select the eigenvector corresponding to the largest positive eigenvalue. Detailed description of the method can be found in Wang et al. (2014).

Chapter 4

Secondary protein structure

This chapter introduces an application of dual quaternions to one interesting problem in structural biology, i.e., the description of protein structure. The secondary protein structure is a specific geometric shape and the description uses Chasles' theorem which states that any rigid body displacement can be described by a screw motion.

4.1 Motivation

The quaternions have been widely used in many branches of biology in recent years. We can find an interesting application in parts concerning proteins. Proteins are very important in almost all biological processes. Their importance can be seen in maintaining the structural integrity of the cell, transport of small molecules or the immune system. Therefore, there has been an effort to determine their structure experimentally and numerically.

A protein molecule is formed from subunits called amino acids, or to be precise, amino acid residues. An amino acid consists of a central carbon atom (C_α) and an amino group (NH_2). To the carbon are attached a hydrogen atom (H) a carboxyl group $(COOH)$ and a side chain (R) that characterizes the amino acid. The amino acids of a protein are connected in sequence with the carboxyl group of one amino acid forming a peptide bond with the amino group of the next amino acid. Proteins are made out of 20 amino acids and therefore, they can be described by a string over a 20-letter alphabet. There exist four levels of protein structure: primary, secondary, tertiary and quaternary. The primary structure of a protein is the sequence of amino acids and the secondary structure occurs when the sequence of amino acids is linked by hydrogen bonds. The tertiary

structure results from long-range contacts within the chain. The quaternary structure is the organization of protein subunits, or two or more independent polypeptide chains. The protein chains vary and thus have different chemical properties.

The peptide bond is a chemical bond formed between the carbonyl carbon (C) and the amide nitrogen (N). In protein structures, the atoms in a peptide unit are fixed in a plane with bond lengths and angles. Essentially, each peptide unit has only two degrees of freedom, given by rotations around its $N - C_\alpha$ and $C_\alpha - C$ bonds. The angle ϕ refers to the rotation around the $N - C_\alpha$ bond, and the angle ψ refers to the rotation around the $C_\alpha - C$ bond. There are many excellent sources for further details, see e.g. Branden and Tooze (1999) or Lesk (2001).

This protein structure plays one of the main role in determining the functional properties of proteins. The results can be applied in medicine, pharmaceutics, bioinformatics, etc. Another important task in biology could be determining the secondary protein structure. Many papers dealing with this problem can be found and some of them solve it by quaternion application. Complete theory dealing with the secondary protein structure may be obtained by Stryer (1988), Kabsch and Sander (1983) or Kundrot and Richards (1987). The best general reference can be found in Barlow and Thornton (1988) or Thomas (1994). Specifically, the problem of predicting the tertiary structure of a protein molecule exists, see Huliatinskyi and Rudyk (2013).

Papers, Kneller and Calligari (2006) and Kneller and Calligari (2012), where the application to structural biology can be found, are intended as the motivation for this work. In this thesis method ScrewFit, which is useful for the study of localizing changes in protein structure was introduced. This method is based on quaternions, see Kneller and Calligari (2012). The main goal of this algorithm is to determine relationships between sets of atoms.

A part of kinematics dealing with rigid transformation is known as Chasles' theorem, see Murray et al. (1994) for more details. Chasles' theorem states that any rigid transformation can be described by a screw, i.e., a rotation about an axis followed by a translation in the direction of this axis. Therefore, there is a considerable motivation to use extensions of quaternions, i.e., dual quaternions. This mathematical structure was invented by William Kingdon Clifford (1845–1879) in the nineteenth century Clifford (1882) to represent rigid transformations in space.

As in the above referred, dual quaternion algebra has been applied in various fields. We will briefly mention the transformation model of secondary protein structure. Then the method ScrewFit, which is based on quaternions will be recalled, see Kneller and Calligari (2006). The motivation behind the use of dual quaternions is to provide a better and a more stable approach and attempt to expand dual quaternions to other fields and find their advantages. The main

contribution is the simplification of the original solution of this transformation. The following part is devoted to a practical application of dual quaternions. We will see that the designed method yields surprisingly exact results.

4.2 Dual quaternion model of protein secondary structure

This section shows how dual quaternions can be efficiently used for the description of the secondary protein structure.

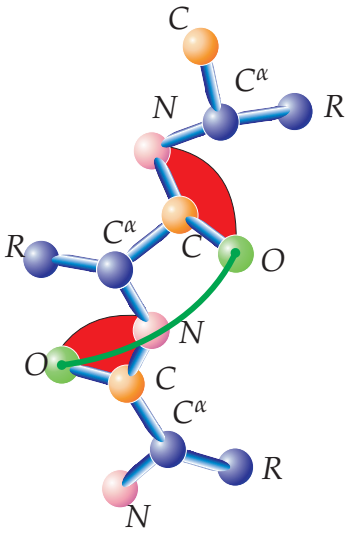

Figure 4.1: The transformation that sends one peptide plane to another one is a screw motion.

First, we remind some basic fundamentals about proteins. Secondary structure is a part of the structural biology. Proteins are biological polymers composed of amino acids, where amino acids are linked together by peptide bonds. They have complex shapes that include various folds, loops, and curves. Each shape has a particular functional property. By secondary structures of proteins we are referring to structures which describe three dimensional form of proteins.

We can mention some of the well-known secondary structure prediction methods as the *Chou-Fasman method* which uses a combination of statistical and heuristic rules, see Chou and Fasman (1974). The *GOR method* on the basis of information theory framework, see Garier et al. (1978) or the *Lim method* as a stereochemical rule-based approach for predicting secondary structure in globular proteins, see Lim (1974).

Nevertheless, these predictions were limited by the small number of proteins with solved structures and these methods were shown to be only between 56% and 60% accurate, see Kabsch and Sander (1983).

The most common protein secondary structures are α-helices. Linus Pauling (1901–1994) was American biochemist who, as the first, predicted the existence of α-helices, which was confirmed with the determination of the first three dimensional structure of a protein, myoglobin. An example of an α-helix is shown in Fig. 4.1. The protein chain can be described by local screw motions relating the $(C-O-N)$ atoms in successive peptide bonds. This method, based on screw motions, will be modified with dual quaternions. The main aim of the prediction of secondary protein structure is to find relationship between peptide bonds, i.e.,

$$(C-O-N)_j \rightarrow (C-O-N)_{j+1}. \tag{4.1}$$

The general transformation model between this peptide planes can be written as

$$\mathbf{x}_i' = \mathbf{t} + \mathbf{R}\mathbf{x}_i, \tag{4.2}$$

where $\mathbf{x}_i^T = (x_{1i}, x_{2i}, x_{3i}) \in \mathbb{R}^3, \mathbf{x'}_i^T = (x'_{1i}, x'_{2i}, x'_{3i}) \in \mathbb{R}^3$, $i = 1, 2, 3$ are two sets of coordinates corresponding $(C-O-N)$ planes, $\mathbf{R} \in \mathbf{SO}(3)$ is a rotation matrix and $\mathbf{t}^T = (t_1, t_2, t_3) \in \mathbb{R}^3$ is a translation vector.

4.3 ScrewFit - Quaternion method

The well known method for describing secondary protein structure is called *ScrewFit*. This method is based on Chasles' theorem. Therefore, quaternions are used in this method because they can represent rotation and they allow to determine precious rotation angle of secondary protein structure from

$$\mathbf{x}_i' = \mathbf{R}\mathbf{x}_i. \tag{4.3}$$

The translation vector is determined as a difference between atoms C, i.e.,

$$\mathbf{t} = \mathbf{C}_{j+1} - \mathbf{C}_j, \tag{4.4}$$

where $\mathbf{C}_{j+1}$ and $\mathbf{C}_j$ denote the positions of the C atom in peptide planes $(C-O-N)_j$ and $(C-O-N)_{j+1}$, respectively. The rotation angle φ can be computed

to solve the following equations

$$\begin{aligned} q_0 &= \cos\frac{\varphi}{2}, \\ q_1 &= n_1 \sin\frac{\varphi}{2}, \\ q_2 &= n_2 \sin\frac{\varphi}{2}, \\ q_3 &= n_3 \sin\frac{\varphi}{2}, \end{aligned} \tag{4.5}$$

where $\mathbf{n}^T = (n_1, n_2, n_3)$ is the vector of the axis of rotation.

Furthermore, some important parameters which can be used to define helical structure are mentioned.

- The number of amino acids per turn τ:

$$\tau = \frac{2\pi}{\varphi}. \tag{4.6}$$

- If the move of a set of points $\mathbf{x}$, i.e., the atoms in protein structure, is screw motion then this transformation can be expressed as

$$\hat{\mathbf{x}} \mapsto \mathbf{R}\mathbf{x} + \mathbf{t}, \tag{4.7}$$

  where $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{t} \in \mathbb{R}^3$ is translation vector and $\mathbf{R} \in \mathbf{SO}(3)$ is rotation matrix with fixed origin. Let us remind that the rotation matrix $\mathbf{R}$ has a unique axis $\mathbf{n}$ and angle φ. The axis of a rotation R is a set of all points which are invariant under this transformation, i.e., straight line which is fixed under the transformation. If we restricted to this line then the screw rotation is a translation along the line. The line has direction $\mathbf{n}$ and a point on the fixed line can be found by restricting equation (4.7) to the plane which goes through the origin perpendicular to $\mathbf{n}$ and finding the fixed point of the resulting two-dimensional rotation, see Quine (1999). The vector from the origin to a point on the axis of rigid transformation is

$$r = \frac{1}{2}\left(\mathbf{t} - (\mathbf{n}\cdot\mathbf{t})\mathbf{n} + \cot\frac{\varphi}{2}\mathbf{n}\times\mathbf{t}\right), \tag{4.8}$$

  where $\mathbf{t}_{\parallel} = (\mathbf{n}\cdot\mathbf{t})\mathbf{n}$ and $\mathbf{t}_{\perp} = \mathbf{t} - \mathbf{t}_{\parallel}$. Therefore, the helix radius ρ can be expressed as

$$\rho = \parallel r \parallel . \tag{4.9}$$

- The pitch p:

$$p = \mathbf{t}\cdot\mathbf{n}\tau. \tag{4.10}$$

- The handedness h:

$$h = \operatorname{sgn}(\mathbf{n}\cdot\mathbf{t}). \tag{4.11}$$

4.4 Improved method using dual quaternions

We denote the residual vector $\mathbf{v}_i \in \mathbb{R}^3$, as

$$\mathbf{v}_i = \mathbf{t} - \mathbf{x}'_i + \mathbf{R}\mathbf{x}_i. \tag{4.12}$$

Now, we get the following optimization problem to solve required parameters

$$\min_{\mathbf{t},\mathbf{R}} \sum_{i=1}^{n} \mathbf{v}_i^T \mathbf{v}_i. \tag{4.13}$$

It is possible to express the residual vector $\mathbf{v}_i$ in the form of dual quaternions. First, we modify (4.12) as

$$\mathbf{v}_i = \mathbf{l}_i + \mathbf{R}\mathbf{x}_i, \text{ where } \quad \mathbf{l}_i = \mathbf{t} - \mathbf{x}'_i. \tag{4.14}$$

Equation (4.14) expresses a rotation of the vector $\mathbf{x}'_i$ and then a translation given by the translation vector $\mathbf{l}_i$. We can express this equation according to (2.52) using dual quaternions in the form

$$\mathcal{V}_{d_i} = \mathcal{Q}_{d_i} \mathcal{R}_{d_i} \overline{\mathcal{Q}^*_{d_i}}, \tag{4.15}$$

where $\mathcal{R}_{d_i}$ is a unit dual quaternion

$$\mathcal{R}_{d_i} = 1 + \varepsilon(x'_{1i}\mathbf{i} + x'_{2i}\mathbf{j} + x'_{3i}\mathbf{k}), \tag{4.16}$$

and $\mathcal{Q}_{d_i}$ is a unit dual quaternion

$$\mathcal{Q}_{d_i} = \mathcal{Q} + \varepsilon\frac{\mathcal{L}_i \mathcal{Q}}{2}, \quad \text{where} \quad \mathcal{Q} = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k} \quad \text{and} \tag{4.17}$$

$$\mathcal{L}_i = (t_1 - x_{1i})\mathbf{i} + (\, t_2 - x_{2i})\mathbf{j} + (t_3 - x_{3i})\mathbf{k}. \tag{4.18}$$

Since $\mathcal{Q}_{d_i}$ is a unit dual quaternion, we must apply the conditions (2.43), i.e.,

$$\|\mathcal{Q}\| = 1 \quad \wedge \quad \mathcal{Q} \cdot \mathcal{Q}_\varepsilon = 0. \tag{4.19}$$

From equation (4.15), we get the unit dual quaternion of the form $\mathcal{V}_{d_i} = 1 + \varepsilon(v_{1i}\mathbf{i} + v_{2i}\mathbf{j} + v_{3i}\mathbf{k})$ corresponding to the vector $\mathbf{v}_i^T = (v_{1i}, v_{2i}, v_{3i})$, where terms v_{1i}, v_{2i}, v_{3i} contain seven parameters to be solved, i.e., $q_0, \ldots, q_3, t_1, t_2, t_3$. Further, the transformation parameters can be determined by solving this optimization problem

$$\min_{q_0,\ldots,q_3,t_1,t_2,t_3} \sum_{i=1}^{n} \mathbf{v}_i^T \mathbf{v}_i, \tag{4.20}$$

$$\|\mathcal{Q}\| = 1 \quad \wedge \quad \mathcal{Q} \cdot \mathcal{Q}_\varepsilon = 0. \tag{4.21}$$

We can use a nonlinear method to solve this minimization problem, i.e., *Lagrange multipliers*. Further, we compute the remaining rotation and translation parameters. Then equations (4.6), (4.8) and (4.11) are used to compute the remaining parameters. The CAS system Mathematica could be used to find the transformation parameters.

4.5 Computed examples and applications

In this part of the thesis we will focus on the algorithm based on dual quaternions designed in the previous section. This algorithm is applied to determine the local helical structure of polypeptides and proteins. We consider Cartesian coordinates of model structures of polypeptides which have been taken from the Image Library of Biological Macromolecules in Jena (Institute of Molecular Biotechnology, Jena; http://www.imb-jena.de/IMAGE.html). Numerical example is presented to demonstrate the functionality of the designed method.

Table 4.1: A comparison of results obtained from different papers. Parameters for α-helix, where τ is number of residues per turn, ρ is the radius of a helix and p is the pitch.

α-helix	τ	ρ	p
Pauling et al. (1951)	3.65	2.3	5.5
Arnott and Wonacott (1966)	3.59	2.3	5.5
Barlow and Thornton (1988)	3.54	2.3	5.4

Table 4.2: A comparison of results obtained from different papers. Parameters for 3_{10}-helix, where τ is number of residues per turn, ρ is the radius of a helix and p is the pitch.

3_{10}-helix	τ	ρ	p
Pauling et al. (1951)	3.0	1.8	6.0
Arnott & Wonacott (1966)	3.1	1.9	5.8
Barlow and Thornton (1988)	3.2	2.0	5.8

The triplet $(O - C - N)$ represents the rigid bodies so called peptide planes. The dual quaternion parameters are obtained from the fit of the $(O - C - N)$ triangle of peptide bond j onto triangle of peptide bond $j + 1$. From each set of dual quaternion parameters we can compute the direction $\mathbf{n}$ of the rotation axis, the rotation angle φ and the translation vector $\mathbf{t}$. The translation vector is computed from equation (4.20). The rotation angle φ can be computed to solve equations (4.5). Equations (4.6), (4.8) and (4.11) are used to compute the rest parameters.

Table 4.3: A comparison of quaternion and dual quaternion algorithm for different model structures. Here, τ is number of residues per turn, ρ_C is the radius of a helix with C atom on peptide plane, ρ_{C_α} is the radius of a helix with C_α atom on peptide plane, p is the pitch and h is the handedness.

α-helix					
Algorithm	τ	ρ_C	ρ_{C_α}	p	h
DQ algorithm	3.66076	1.72595	2.32996	5.30804	+
Q algorithm	3.62	1.71	2.27	5.56	+
π-helix					
DQ algorithm	4.21244	1.80627	2.59915	5.23702	+
Q algorithm	4.16	1.78	2.58	5.58	+
3_{10}-helix					
DQ algorithm	3.31652	1.47488	2.04676	5.62225	+
Q algorithm	3.28	1.46	2.03	5.89	+
β-strand					
DQ algorithm	2.03773	0.553559	0.927563	6.65063	-
Q algorithm	2.03	0.55	0.93	6.71	-
Extended helix					
DQ algorithm	2.00017	0.37281	0.546598	7.24884	-
Q algorithm	2	0.37	0.55	7.25	-

The parameters concerning this secondary structure are shown in Table 4.3. Primarily, α-helix and 3_{10}-helix were used. Naturally, the algorithm was applied to other known helices as π-helix, β-strand or extended helix. β-strand is a special type of helix, for more details see Kneller and Calligari (2006) or Aydin (2008). Helix radius depends on the reference point which lies on the helix. When the atom C is used then the radius is marked via ρ_C, when the carbon C_α atom is chosen instead then the radius is marked ρ_{C_α}. Values for pitch p or handedness h are also presented in Table 4.3. The parameters concerning this secondary structure of available helices, i.e., α-helix and 3_{10}-helix from Pauling et al. (1951), Arnott and Wonacott (1966) and Barlow and Thornton (1988) are shown in Table 4.1 and Table 4.2.

In the following part we will show results of Dual quaternion algorithm for proteins which fall into the six mentioned type of helix. The SCOP (Structural Classification of Proteins) database is one of the most relevant protein classification schemes is the structural classification of proteins. It is based on similarities of their structures and amino acid sequences. Unfortunately, the dynamic of classification of new proteins is much slower than the dynamic of discovering novel protein structures in the protein data bank (PDB). We selected representative protein for each type of helix. Every part contains graphical model of

secondary protein structure of an appropriate protein and graphical representation of main computed result, i.e., radius ρ. Graphical model of each protein is created in program *Jmol*, which is used as a molecule viewer for researchers in chemistry and biochemistry[1]. The vertical green stripes indicate α-helices found by the SrewFit method based on quaternions and the horizontal lines indicate the reference values from the dual quaternion method given in Table 4.3 with selected range 0.5.

Example 4.1. **α-helix:** Carbonmonoxy-myoglobin (PDB code 1A6G), which is included in sperm whale and belongs to the all-α class, see Vojtěchovský et al. (1999).

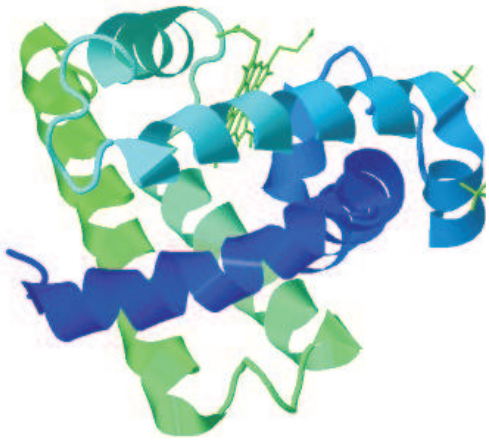

Figure 4.2: Model of secondary protein structure of the main chain of carbonmonoxy-myoglobin.

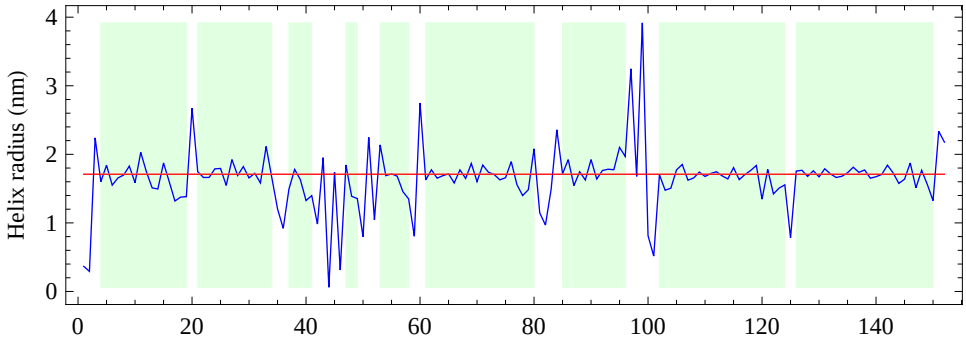

Figure 4.3: Dual quaternion description of the main chain of carbonmonoxy-myoglobin. The horizontal lines indicate the reference values from dual quaternion method given in Table 4.3 with selected range 0.5.

[1]Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/.

Example 4.2. π-helix: Monooxygenase hydroxylase is π-helix, which can be found in *Methylococcus capsulatus* (PDB code 1MTY), see Fodje and Al-Karadaghi (2002). Although once thought to be rare, short π-helices are found in 15% of known protein structures and are considered to be unstable. The dual quaternion algorithm is shown only for selected part of this protein to have a imagination about this structure.

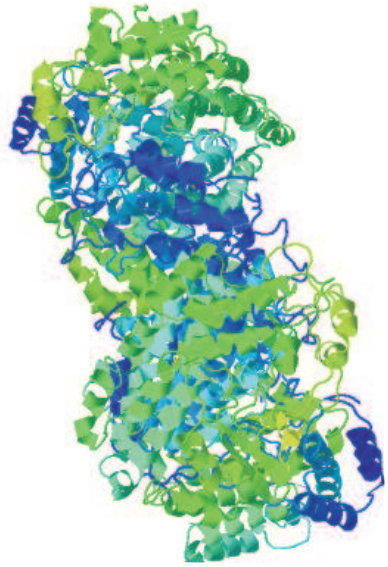

Figure 4.4: Model of secondary protein structure of the main chain of monooxygenase hydroxylase.

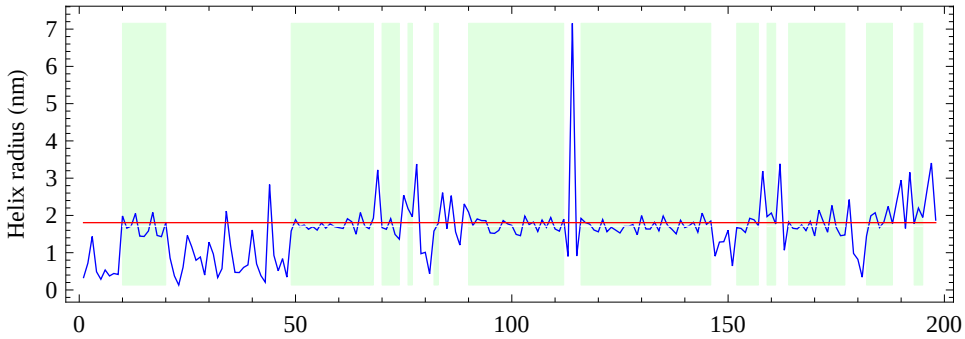

Figure 4.5: Dual quaternion description of part of the main chain of monooxygenase hydroxylase. The horizontal lines indicate the reference values from dual quaternion method given in Table 4.3 with selected range 0.5.

Example 4.3. 3_{10}-helix: The 3_{10}-helix accounts for about 4% of amino acid secondary structure states. An example of this helix is dienelactone hydrolase (PDB code 1DIN), see Vieira-Pires and Morais-Cabral (2010).

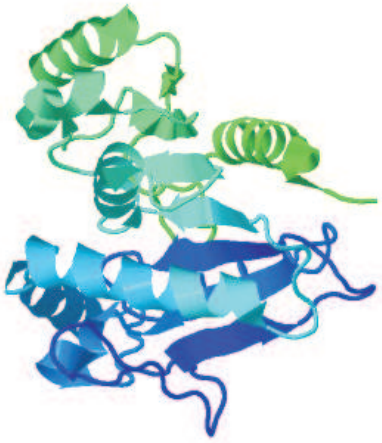

Figure 4.6: Model of secondary protein structure of the main chain of dienelactone hydrolase.

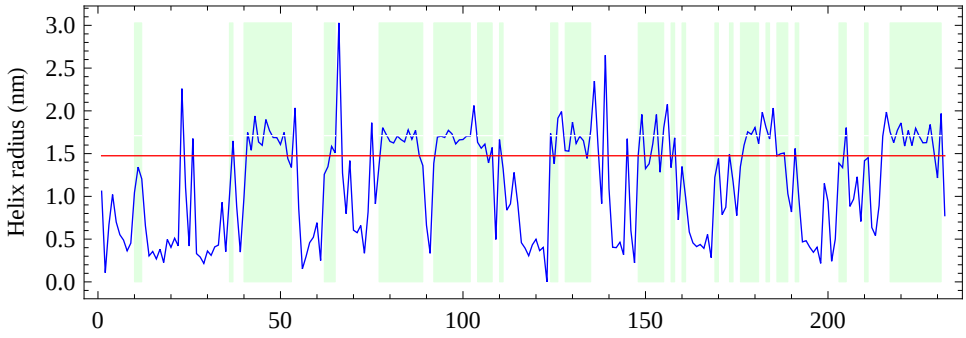

Figure 4.7: Dual quaternion description of the main chain of dienelactone hydrolase. The horizontal lines indicate the reference values from dual quaternion method given in Table 4.3 with selected range 0.5.

Example 4.4. **β-strand:** One of the known β-strand is protease inhibitor ecotin (PDB code 1ECY), see Kneller and Calligari (2006).

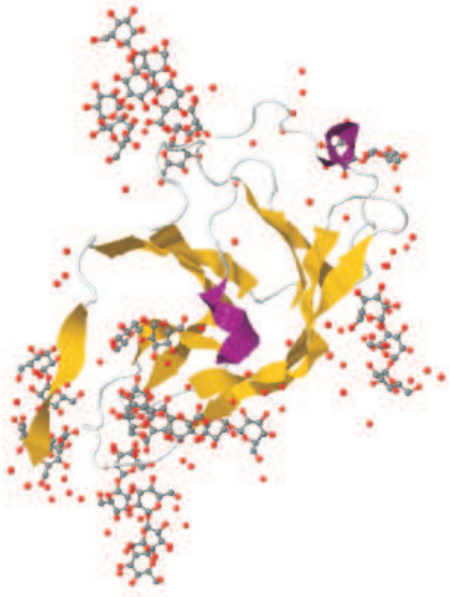

Figure 4.8: Model of secondary protein structure of the main chain of protease inhibitor ecotin.

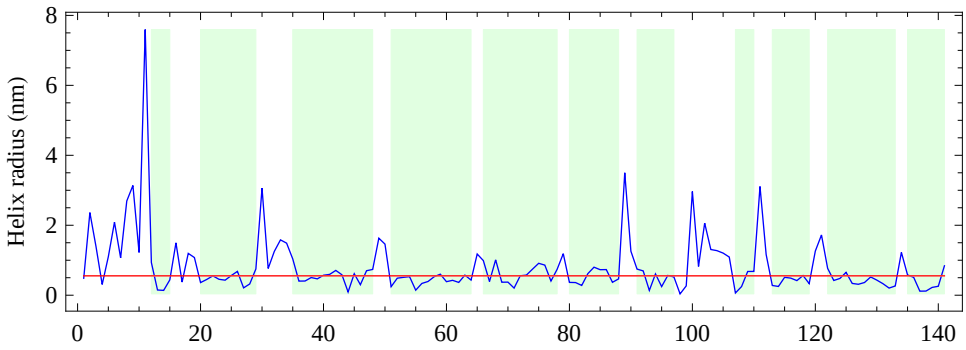

Figure 4.9: Dual quaternion description of the main chain of protease inhibitor ecotin. The horizontal lines indicate the reference values from dual quaternion method given in Table 4.3 with selected range 0.5.

Example 4.5. Extended helix: The protein crystal 5PTI of bovine pancreatic trypsin inhibitor (PDB code BPTI) was selected as an example of extended helix, see Hu and Jiang (2012).

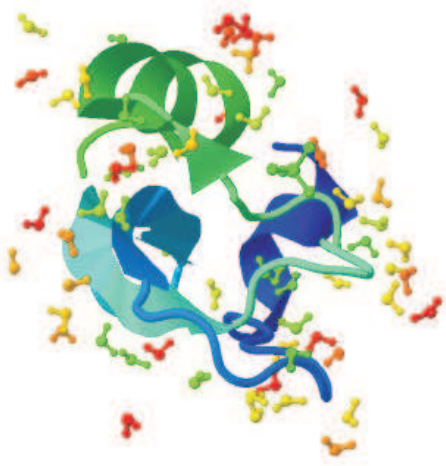

Figure 4.10: Model of secondary protein structure of the main chain of bovine pancreatic trypsin inhibitor.

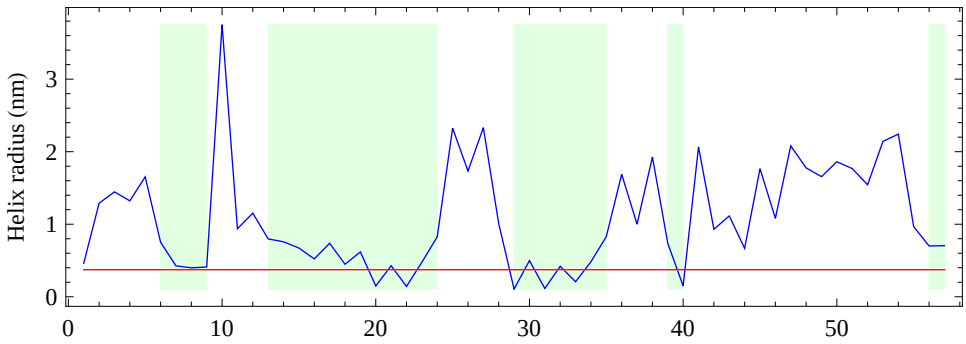

Figure 4.11: Dual quaternion description of the main chain of bovine pancreatic trypsin inhibitor. The horizontal lines indicate the reference values from dual quaternion method given in Table 4.3 with selected range 0.5.

Chapter 5

Interpolations by rational spline motions

Interpolation by rational spline motions is an important part of technical practice, e.g. robotics or computer graphics. Rational spline motions are characterized by the property that the trajectories of the points of the moving object are rational spline curves. We will focus on the most simple examples of the piecewise rational motions with the first and second order geometric continuity, in particular a parabolic G^1 Hermite interpolation and a cubic G^2 Hermite interpolation. We will briefly introduce a new approach to rational spline motion design which uses dual quaternions.

5.1 Motivation

In the computer graphics and animation, the rotational and translational motions have several important applications. In this thesis we discuss the following interpolating problem: Let be given some positions of a moving object in the three dimensional space, then a continuous motion interpolating these positions shall be found. The solution of this problem is required also in robotics, e.g. for the path planning of robot manipulators. Often, techniques for solving this problem deal separately with the positions and orientations. As an innovation, we try to combine these two parts in one step.

Recently used algorithms solving this interpolation problem were based on, e.g. Euler angles but then the trajectory of the moving object is a non-rational

curve. Another approach is to interpolate rotations using normalized quaternion curves, see Shoemake (1985) or Pletinckx (1989).

This thesis introduces dual quaternions as a tool for representing the three dimensional transformation of a rigid body. This transformation can be uniquely specified by a continuous path $q_d(t)$. Dual quaternions were invented to represent rigid transformations. Therefore, the dual quaternions prove to be very useful tool in computer graphics. Recently, the problem of the rational spline motion has been solved by Hermite interpolation based on quaternions, see Jaklič et al. (2013). This approach seems to be very interesting and efficient and therefore we modify it by dual quaternions because of their unifying properties.

5.2 Rational spline motions using quaternions

Rational spline motions are defined by the property that the trajectories of the points of the moving object are rational spline curves. A rigid body motion is described by the trajectory $\mathbf{c}(t) = (c_1(t), c_2(t), c_3(t))$ of the moving system and by the 3×3 rotation matrix $\mathbf{R}$. The trajectory of the point P given by the vector $\mathbf{p}$ is then described by the following equation

$$\widehat{\mathbf{p}}(t) = \mathbf{c}(t) + \mathbf{R}(t)\mathbf{p}. \tag{5.1}$$

It is possible to use quaternions to describe rational spline motions. Then the rotation matrix $\mathbf{R}$ in the previous equation is expressed with quaternion terms.

Theorem 5.1. *Let $\mathcal{Q} = (q_0, q_1, q_2, q_3) \in \mathbb{H}$ and $\boldsymbol{c}(t) = (c_1(t), c_2(t), c_3(t))$ be the trajectory of the rigid body motion. Then the trajectory of a point P given by the vector $\boldsymbol{p} = (p_1, p_2, p_3)$ can be described with equation (5.1), where*

$$\boldsymbol{R} = \frac{1}{\|\mathcal{Q}\|} \begin{bmatrix} q_1^2 + q_0^2 - q_2^2 - q_3^2 & 2q_0q_2 - 2q_0q_3 & 2q_1q_3 + 2q_0q_2 \\ 2q_0q_3 + 2q_1q_2 & q_0^2 - q_1^2 + q_2^2 - q_3^2 & -2q_0q_1 + 2q_2q_3 \\ -2q_0q_2 + 2q_1q_3 & 2q_0q_1 + 2q_2q_3 & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{bmatrix}. \tag{5.2}$$

Proof. The matrix $\mathbf{R}$ denotes the unitary matrix of rotation. We leave it to the reader to verify it by using equation (2.20). □

The trajectory of the point can be expressed as *a quaternion curve*, see e.g. Myung-Soo and Kee-Won (1996) for more details.

Definition 5.2. The *quaternion rational Bézier curve* is defined by $n + 1$ control points $\mathcal{R}_i \in \mathbb{H}$ as

$$q(t) = \sum_{i=0}^{n} B_i^n(t)\mathcal{R}_i, \quad t \in \langle 0, 1 \rangle, \tag{5.3}$$

where $B_i^n(t)$ are Bernstein polynomials

$$B_i^n(t) = \binom{n}{i} t^i (1-t)^{(n-i)}, \;\; i = 0, \ldots, n. \tag{5.4}$$

Rational spline motions are obtained by rational spline functions $q_i(t)$ and $c_i(t)$, where $q_i(t)$ represent the coordinates of the quaternion and $(c_1(t), c_2(t), c_3(t))$ is the trajectory of the moving frame's origin. Rational splines can be classified by the degree of their trajectories. If the quadratic polynomials $q_i(t)$ are used then the rational spherical motions are of degree four or higher, see Lenarčič and Stanišić (2010). For a purpose to get the rational spline motion (5.1) of degree four or higher the part $c_i(t)$ should be chosen as

$$c_i(t) = \frac{d_i(t)}{\| \mathcal{Q} \|}, \qquad i = 1, 2, 3, \tag{5.5}$$

where d_i are polynomials of degree four or higher.

In describing a shape using curves or surfaces, it is common to use several curve segments which are joined together with some degree of continuity. There are two types of continuity, i.e., parametric continuity and geometric continuity. The parametric continuity of order k is denoted by C^k. The geometric continuity of order k is denoted by G^k. Two curves which are parametric continuous of a certain degree are also geometric continuous of the same degree but not vice versa. We can say that parametric continuity means smoothness both of the curve and of its parametrization. Now we recall some basic facts about continuity of curves.

As we mentioned above the parametric continuity is described by the notation C^k, which is the k-th degree parametric continuity. This means that the two curves which are connected have identical the k-th degree parametric derivatives as well as all lower derivatives. If we focus on the parametric continuity C^0 of the curves then we can say that the curve segments at a joint are connected, i.e., the point at which one curve segment ends is the same point where the next segment starts. The parametric continuity C^1 means that the two curves share a common endpoint and they have the same tangent vector at their shared endpoint. We can generalize this in the following definition of the parametric continuity or order k of two trajectories.

Definition 5.3. Let us have two trajectories of the point P given by the vector $\mathbf{p}$

$$\begin{aligned} \tilde{\mathbf{p}}(t) &= \tilde{\mathbf{c}}(t) + \widetilde{\mathbf{R}}(t)\mathbf{p}, \\ \bar{\mathbf{p}}(s) &= \bar{\mathbf{c}}(s) + \bar{\mathbf{R}}(s)\mathbf{p}, \end{aligned}$$

where $\tilde{\mathbf{p}}(t)$ and $\bar{\mathbf{p}}(s)$ are the values in the intervals $[t_0, t_1]$ and $[s_0, s_1]$, respectively. Then $\tilde{\mathbf{p}}(t), \bar{\mathbf{p}}(t)$ are C^0 continuous, if

$$\tilde{\mathbf{p}}(t_1) = \bar{\mathbf{p}}(s_0). \tag{5.6}$$

If for all $i \leq k$, the i-th derivatives at $\tilde{\mathbf{p}}(t_1)$ and $\bar{\mathbf{p}}(s_0)$ are equal, then it is said that the curves are C^k continuous at the point $\tilde{\mathbf{p}}(t_1) = \tilde{\mathbf{p}}(s_0)$.

The geometric continuity conditions for quaternion curves that imply geometric continuity of motions are recalled according to Farin et al. (2002), where more details can be found.

Definition 5.4. Consider two trajectories of the point P given by the vector $\mathbf{p}$

$$\begin{aligned} \tilde{\mathbf{p}}(t) &= \tilde{\mathbf{c}}(t) + \widetilde{\mathbf{R}}(t)\mathbf{p}, \\ \bar{\mathbf{p}}(s) &= \bar{\mathbf{c}}(s) + \bar{\mathbf{R}}(s)\mathbf{p}, \end{aligned}$$

where $\tilde{\mathbf{p}}(t)$ and $\bar{\mathbf{p}}(s)$ are the values in the intervals $[t_0, t_1]$ and $[s_0, s_1]$, respectively. It is said that the curves are G^k continuous at the point $\tilde{\mathbf{p}}(t_1) = \bar{\mathbf{p}}(s_0)$ if there exists a regular reparametrization

$$\phi : [t_0, t_1] \mapsto [s_0, s_1], \text{ where } \phi' > 0, \ \phi(t_1) = s_0, \tag{5.7}$$

such that

$$\frac{d^j \tilde{\mathbf{p}}}{dt^j}(t) = \frac{d^j(\bar{\mathbf{p}} \circ \phi)}{dt^j}(t), \quad j = 1, \ldots, k \text{ for } t = t_1. \tag{5.8}$$

Subsequently, it can be written for $\bar{\mathbf{c}}$ and $\bar{\mathbf{R}}$ the following equations (5.9) and (5.10) which are equal to the condition given by equation (5.8).

$$\frac{d^j \tilde{\mathbf{c}}}{dt^j}(t) = \frac{d^j(\bar{\mathbf{c}} \circ \phi)}{dt^j}(t), \ j = 1, \ldots, k \text{ for } t = t_1, \tag{5.9}$$

$$\frac{d^j \widetilde{\mathbf{R}}}{dt^j}(t) = \frac{d^j(\bar{\mathbf{R}} \circ \phi)}{dt^j}(t), \ j = 1, \ldots, k \text{ for } t = t_1. \tag{5.10}$$

Theorem 5.5. *Let $\tilde{q}(t), \bar{q}(s)$ be two quaternion curves describing the rotations then the motions given by $\tilde{\boldsymbol{R}}$ and $\bar{\boldsymbol{R}}$ are G^0 continuous at the point $\tilde{\boldsymbol{R}}(t_1) = \bar{\boldsymbol{R}}(s_0)$ if and only if*

$$\tilde{q}(t_1) = \lambda(t_1)\bar{q}(\phi(t_1)) \text{ and } \lambda \neq 0, \tag{5.11}$$

where $\lambda : [t_0, t_1] \mapsto \mathbb{R}$ is a scalar function.

Proof. The G^k continuity conditions for a spherical , i.e, equations (5.9) and (5.10) are equivalent to equation (5.11) because of equivalence relation in the three dimensional projective space. See Ferjančič et al. (2016) for more details. □

Therefore the geometric continuity conditions are the same as the well known conditions for rational curves which are expressed in homogeneous coordinates. Equation (5.11) can be extended for derivatives as

$$\frac{d^j \tilde{q}(t)}{dt^j} = \frac{d^j(\lambda(t)\bar{q}(\phi(t))}{dt^j}, \ j = 1, \ldots, k \text{ for } t = t_1. \tag{5.12}$$

Theorem 5.6. *Let $\tilde{q}(t), \bar{q}(s)$ be two quaternion curves describing the rotations then the motions given by $\tilde{\mathbf{R}}$ and $\bar{\mathbf{R}}$ are G^1 continuous at the point $\tilde{\mathbf{R}}(t_1) = \bar{\mathbf{R}}(s_0)$ if and only if there exists a regular reparametrization*

$$\phi : [t_0, t_1] \mapsto [s_0, s_1], \text{ where } \phi' > 0, \ \phi(t_1) = s_0, \tag{5.13}$$

such that

$$\tilde{q}'(t_1) = \lambda'(t_1)\bar{q}(\phi(t_1)) + \lambda(t_1)\phi'(t_1)\bar{q}'(\phi(t_1)) \text{ and } \lambda \neq 0, \tag{5.14}$$

where $\lambda : [t_0, t_1] \mapsto \mathbb{R}$ is a scalar function.

Proof. By using Faa di Bruno's formula, the conditions, i.e., equation (5.12), can be rewritten and after its simplification the G^1 continuity is determined. □

It is possible to determine the condition for G^2 continuity as well, see the following Theorem 5.7.

Theorem 5.7. *Let $\tilde{q}(t), \bar{q}(s)$ be two quaternion curves describing the rotations then the motions given by $\tilde{\mathbf{R}}$ and $\bar{\mathbf{R}}$ are G^2 continuous at the point $\tilde{\mathbf{R}}(t_1) = \bar{\mathbf{R}}(s_0)$ if and only if there exists a regular reparametrization*

$$\phi : [t_0, t_1] \mapsto [s_0, s_1], \text{ where } \phi' > 0, \ \phi(t_1) = s_0, \tag{5.15}$$

such that

$$\begin{aligned} \tilde{q}''(t_1) &= \lambda''(t_1)\bar{q}(\phi(t_1)) + 2\lambda'(t_1)\phi'(t_1)\bar{q}'(\phi(t_1)) \\ &+ \lambda(t_1)\phi'(t_1)^2\bar{q}''(\phi(t_1)) + \lambda(t_1)\phi''(t_1)\bar{q}'(\phi(t_1)) \text{ and } \lambda \neq 0, \end{aligned} \tag{5.16}$$

where $\lambda : [t_0, t_1] \mapsto \mathbb{R}$ is a scalar function.

Proof. See Jaklič et al. (2013) for further details. □

5.3 Hermite interpolation by rational G^1 motions

This part of the thesis is focused on the G^1 Hermite interpolation. The main purpose of Hermite interpolation is to generate curves well fitted to given sample data. Firstly, we can mention the interpolation using a parabolic biarc in connection with the standard algorithm for a construction of the G^1 Hermite interpolation which can be found in Jaklič et al. (2013) and then we modify it with the help of dual quaternions.

5.3.1 G^1 HERMITE INTERPOLATION USING QUATERNIONS

This method from Jaklič et al. (2013) is based on quaternions therefore the rotation part of the spatial motion is solved via this algorithm. This leads to the separation of the rational spline motion into two independent parts, i.e., the rotation and the translation.

Let $\mathcal{Q}_0$ and $\mathcal{Q}_1$ be two unit quaternions and $\mathcal{U}_0$ and $\mathcal{U}_1$ their velocities, respectively. We would like to construct a quaternion interpolant $q : [0,1] \to \mathbb{R}^4$ interpolating these data. If the quaternions $\mathcal{U}_0, \mathcal{U}_1$ and $\mathcal{Q}_1 - \mathcal{Q}_2$ are linearly independent then it is necessary to use so-called additional quaternion $\mathcal{Q}_A$, which helps us to construct two interpolant quaternion curves $q_0 : [0,1] \to \mathbb{R}^4$ and $q_1 : [0,1] \to \mathbb{R}^4$. The quaternion curve q_0 interpolates $\mathcal{U}_0, \mathcal{Q}_0, \mathcal{Q}_A$ and q_1 interpolates $\mathcal{U}_1, \mathcal{Q}_1, \mathcal{Q}_A$ which are essentially parabolic biarcs, see Fig. 5.1. There is ensured the G^1 continuity at $\mathcal{Q}_A$. We can show that these two curves can be

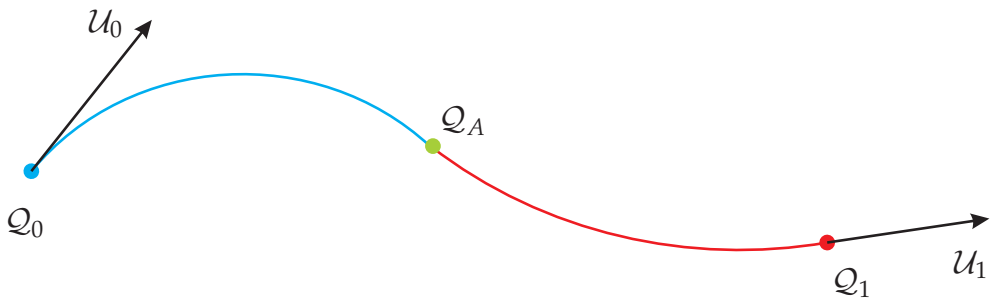

Figure 5.1: Hermite interpolation using a parabolic biarc.

written in the Berstein–Bézier form as

$$q_0(t) = \mathcal{Q}_0 B_0^2(t) + \mathcal{B}_0 B_1^2(t) + \mathcal{Q}_A B_2^2(t), \tag{5.17}$$
$$q_1(t) = \mathcal{Q}_A B_0^2(t) + \mathcal{B}_1 B_2^2(t) + \mathcal{Q}_1 B_2^2(t), \tag{5.18}$$

where B_0^2, B_1^2 and B_2^2 are the Bernstein polynomials and $\mathcal{B}_0$ and $\mathcal{B}_1$ are two unknown quaternions, see Definition 5.2.

The unknown quaternions $\mathcal{B}_0$ and $\mathcal{B}_1$ can be found by using conditions for the G^1 continuity. These conditions can be written as

$$q_0'(0) = \lambda_0^{(1)} \mathcal{Q}_0 + \phi_0^{(1)} \mathcal{U}_0, \tag{5.19}$$
$$q_1'(1) = \lambda_1^{(1)} \mathcal{Q}_1 + \phi_1^{(1)} \mathcal{U}_1, \tag{5.20}$$
$$q_0(1) = \lambda_A^{(1)} \mathcal{Q}_A + \phi_A^{(1)} q_1'(0), \tag{5.21}$$

where the parameters $\lambda_0^{(1)}, \lambda_1^{(1)}$ and $\lambda_A^{(1)}$ have to be positive. From the properties

of Bézier curves we get

$$q_0'(0) = 2(\mathcal{B}_0 - \mathcal{Q}_0), \qquad q_0'(1) = 2(\mathcal{Q}_A - \mathcal{B}_1), \tag{5.22}$$
$$q_1'(0) = 2(\mathcal{B}_1 - \mathcal{Q}_A), \qquad q_1'(1) = 2(\mathcal{Q}_1 - \mathcal{B}_1), \tag{5.23}$$

then the following equations help us to determine unknown quaternions $\mathcal{B}_0$ and $\mathcal{B}_1$ in the form

$$\mathcal{B}_0 = \mathcal{Q}_0 + \frac{1}{2}(\lambda_0^{(1)}\mathcal{Q}_0 + \phi_0^{(1)}\mathcal{U}_0), \tag{5.24}$$
$$\mathcal{B}_1 = \mathcal{Q}_1 - \frac{1}{2}(\lambda_1^{(1)}\mathcal{Q}_1 + \phi_1^{(1)}\mathcal{U}_1), \tag{5.25}$$
$$2(\mathcal{Q}_A - \mathcal{B}_0) = \lambda_A^{(1)}\mathcal{Q}_A + 2\phi_A^{(1)}(\mathcal{B}_1 - \mathcal{Q}_A). \tag{5.26}$$

Let us denote

$$\mathbf{D}_i = \frac{|\mathbf{A}^{(i)}|(\mathcal{U}_0)}{|\mathbf{A}|}, \ i = 1, \ldots, 4, \tag{5.27}$$

where $|\mathbf{A}|$ denotes the determinant of the matrix $\mathbf{A} = (\mathcal{Q}_0, \mathcal{Q}_A, \mathcal{Q}_1, \mathcal{U}_1)$. Next $\mathbf{A}^{(i)}(\mathcal{U}_0)$ denotes the matrix $\mathbf{A}$ with the i-th column replaced by the quaternion $\mathcal{U}_0$. Then Theorem 5.8 can be formulated (see Jaklič et al. (2013)).

Theorem 5.8. *Let $\mathcal{Q}_0, \mathcal{Q}_1, \mathcal{U}_0, \mathcal{U}_1$ and $\mathcal{Q}_A$ be given quaternions such that $\mathbf{A}$ is a non-singular and $\mathbf{D}_4 > 0$, see (5.27). Than a two-parametric family of G^1 continuous pairs of parabolic quaternion curves $q_0(t)$ and $q_1(t)$ defined by equations (5.24), (5.25), (5.26) and (5.27) exists.*

Proof. See Jaklič et al. (2013) for the proof. □

The quaternion algorithm above allows us to solve the rotational part of the rotational spline motion only. Nevertheless, the rational spline motion is a combination of rotations and translations, see equation (5.1). Therefore, the curve needs to be suitably translated to get the final view od the motion, see Section 5.2 for more details. The following approach using dual quaternions shows how to use rotation and translation simultaneously.

5.3.2 Improved method using dual quaternions

Dual quaternions prove to be very useful tool when used in visualization of moving objects and therefore we present here a representation formula for rational spline motions. It has been proved in Jütler (1994) that any rational motion could be represented just as a *rational dual quaternion curve*. We briefly summarized some fundamentals of using dual quaternions in Section 2.2 and now we use them to improve the original method from Jaklič et al. (2013).

Let us firstly recall the definition of dual quaternion curve.

Definition 5.9. The *dual quaternion rational Bézier curve* is defined by $n+1$ control points $\mathcal{R}_{d_i} \in \mathbb{H}_d$ as

$$q_d(t) = \sum_{i=0}^{n} B_i^n(t)\mathcal{R}_{d_i}, \;\; t \in \langle 0,1\rangle, \tag{5.28}$$

where $B_i^n(t)$ are Bernstein polynomials

$$B_i^n(t) = \binom{n}{i} t^i (1-t)^{(n-i)}, \;\; i = 0,\ldots,n. \tag{5.29}$$

Any rational spline motion (5.1) consists of two parts, one is rotational and the second one is translational. In the previous section we showed how the rotational part can be computed. Nevertheless, a construction of the translation part of the motion left. Therefore, we use dual quaternions to combine the rotation and the translation parts of the motion in one operation.

We modify equations (5.17) and (5.18) according to dual quaternion description (2.52). Hence, we get two dual quaternion curves

$$q_{d_0}(t) = \mathcal{Q}_{d_0} B_0^2(t) + \mathcal{B}_{d_0} B_1^2(t) + \mathcal{Q}_{d_A} B_2^2(t), \tag{5.30}$$

$$q_{d_1}(t) = \mathcal{Q}_{d_A} B_0^2(t) + \mathcal{B}_{d_1} B_1^2(t) + \mathcal{Q}_{d_1} B_2^2(t), \tag{5.31}$$

where $\mathcal{Q}_{d_0}, \mathcal{Q}_{d_1}, \mathcal{Q}_{d_A}, \mathcal{B}_{d_0}$ and $\mathcal{B}_{d_1}$ are unit the dual quaternions and B_0^2, B_1^2, B_2^2 are again the Bernstein polynomials, see Definition 5.9.

We solve the following interpolation problem: There are given several positions P_i, $i = 0,\ldots,m$ of a rigid body. The position P_i is composed of the position of the center c_i and by the associated rotation matrix. The rotations can be represented by the unit quaternions $\mathcal{Q}_i$. Because we usually have a non-unit quaternion describing the rotations then this quaternion has to be normalized, i.e.,

$$\mathcal{Q}_i = \mp \frac{\widehat{\mathcal{Q}_i}}{\| \widehat{\mathcal{Q}_i} \|}, \tag{5.32}$$

where $\widehat{\mathcal{Q}_i}$ is an arbitrary quaternion which is not unit, in general. The appropriate sign in equation (5.32) is chosen to satisfy

$$\mathcal{Q}_i \cdot \mathcal{Q}_{i+1} > 0, \qquad i = 0,\ldots,m, \tag{5.33}$$

which provides us that both quaternions lie on the same hemisphere. The translation can be described by a pure quaternion. We use equation (2.53)

$$\mathcal{T}_i = c_{1_i}\mathbf{i} + c_{2_i}\mathbf{j} + c_{3_i}\mathbf{k}. \tag{5.34}$$

Due to the dual quaternion description (2.52) we can combine the both quaternions and we get the unit dual quaternion

$$\mathcal{Q}_{d_i} = \mathcal{Q}_i + \varepsilon \frac{\mathcal{T}_i \mathcal{Q}_i}{2}, \tag{5.35}$$

that will be used in equations (5.30) and (5.31) and so we get two dual quaternion curves containing the translation and the rotational part. We have to mention that also Theorem 5.8 can be used to find the rotational part of the dual quaternion.

The interpolating algorithm based on dual quaternion curve can be computed in the following steps, see Algorithm 3.

Algorithm 3 Rational spline motion with continuity G^1 using dual quaternion

Input: The rotation motion defined by the quaternion curve $\hat{q}(t)$ and the trajectory $c(t)$ of the center, where $t_i = i, i = 0, \ldots, m$.

1: Normalize the rotational quaternions by equation (5.32) to get $\mathcal{Q}_i$.
2: Compute velocity $\mathcal{U}_i$ as a $\mathcal{U}_i = \mathcal{Q}_i^{(1)}$.
3: Compute translation quaternion $\mathcal{T}_i$ using (5.34).
4: Verify if $\mathcal{U}_i, \mathcal{Q}_{i+1} - \mathcal{Q}_i$ are linearly independent.
5: Determine dual quaternion curves using (5.30) and (5.31).

Output: Dual quaternion curves q_{d_i} describing the rational spline motion.

5.3.3 Computed example and application

The presented example demonstrates the functionality of the designed G^1 Hermite interpolation algorithm based on using dual quaternions. Let us consider a smooth motion defined by the quaternion curve $\hat{q}(t)$. This example is taken from Jaklič et al. (2013).

$$\hat{q}(t) = \left(t, t + \cos\left(\frac{\pi t}{4}\right), \sin\left(\frac{\pi t}{4}\right), \cos\left(\frac{\pi t}{10}\right)\right)^T \tag{5.36}$$

The trajectory of the centers is given by

$$c(t) = (3\log(t+1)\cos(t), 3\log(t+1)\sin(t), 3(t+1))^T. \tag{5.37}$$

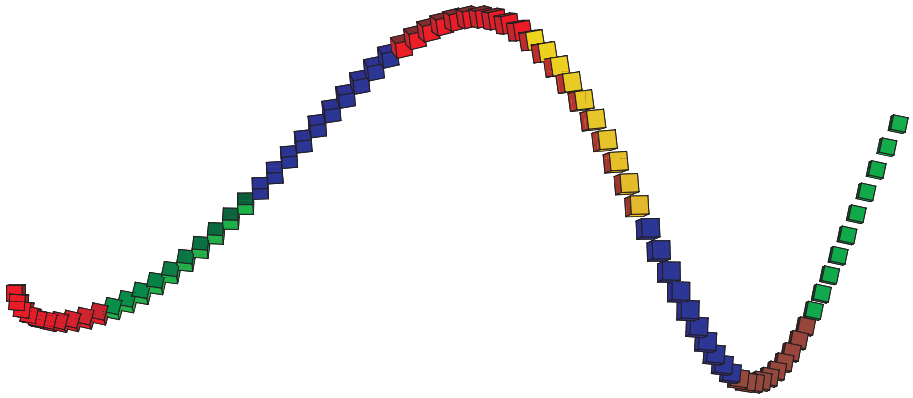

Figure 5.2: Nine positions of a cuboid point of a G^1 motion.

Table 5.1: Hausdorff distances between trajectories of an arbitrary point P of the original motion and the motion computed with Algorithm 3.

h	Hausdorff distance	Decay exponent
1	9.73262×10^{-2}	-
$\frac{1}{2}$	1.09778×10^{-1}	0.89
$\frac{1}{4}$	8.45082×10^{-2}	1.30
$\frac{1}{8}$	5.51347×10^{-2}	1.53
$\frac{1}{16}$	3.27933×10^{-2}	1.68
$\frac{1}{32}$	1.84223×10^{-2}	1.78
$\frac{1}{64}$	9.97311×10^{-3}	1.85
$\frac{1}{128}$	5.26759×10^{-3}	1.89
$\frac{1}{256}$	2.73660×10^{-3}	1.92
$\frac{1}{512}$	1.41793×10^{-3}	1.93

Firstly, we apply the individual steps as in Algorithm 3 for the values $t_i = 0, \ldots, 8$. We can see nine positions of a cuboid point of a G^1 motion in Fig. 5.2 as the result. The different colors show individual arcs of the piecewise curve, where every second quaternion $\mathcal{Q}_{2i+1}$ is the additional one. The original trajectory and the G^1 trajectory using dual quaternions can be seen in Fig. 5.3. Their distances are described in Table 5.1 which contains measured Hausdorff distances. The distances are computed for different values h. The decay exponent describes the ratio of two successive values.

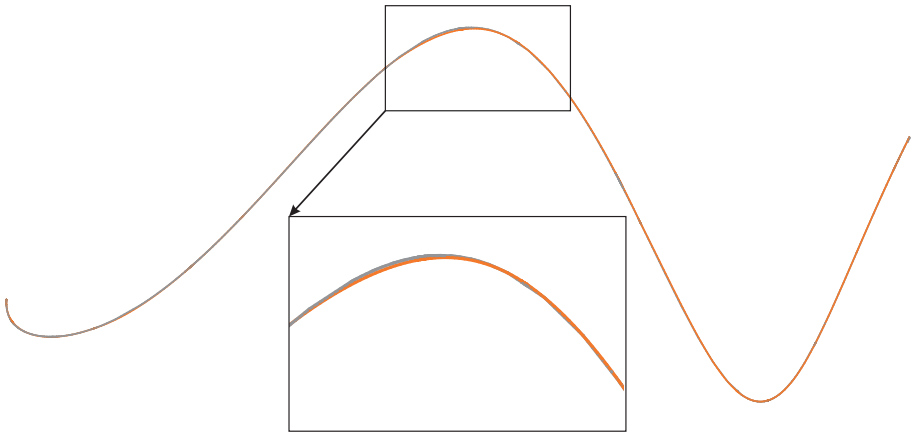

Figure 5.3: Trajectory of an arbitrary point P of the original (grey) and computed motion (orange).

5.4 Hermite interpolation by rational G^2 motions

This part of the thesis is devoted to the cubic G^2 Hermite interpolation. The cubic geometric interpolation is chosen to show the advantages of the various applications of dual quaternions considering their properties. Notice, that the main emphasis is laid on the Hermite interpolation by rational Bézier curves in space. Further, the method based on quaternions studied in see Jaklič et al. (2013) will be extended using the dual quaternions. It is easily shown that they are excellent tool to describe the G^2 rational spline motions.

5.4.1 Cubic G^2 Hermite interpolation using quaternions

Assume that a curve is determined by two points, i.e., P_0 and P_1, and two associated velocities, i.e., U_0 and U_1. The objective is to find a cubic Bézier curve $r(t)$ which interpolates given data as

$$r(0) = P_0, \qquad r'(0) = U_0, \tag{5.38}$$
$$r(1) = P_1, \qquad r'(1) = U_1. \tag{5.39}$$

The sought curve can be represented as a cubic Bézier curve, see Fig. 5.4

$$r(t) = \sum_{i=0}^{3} R_i B_i^3(t), \tag{5.40}$$

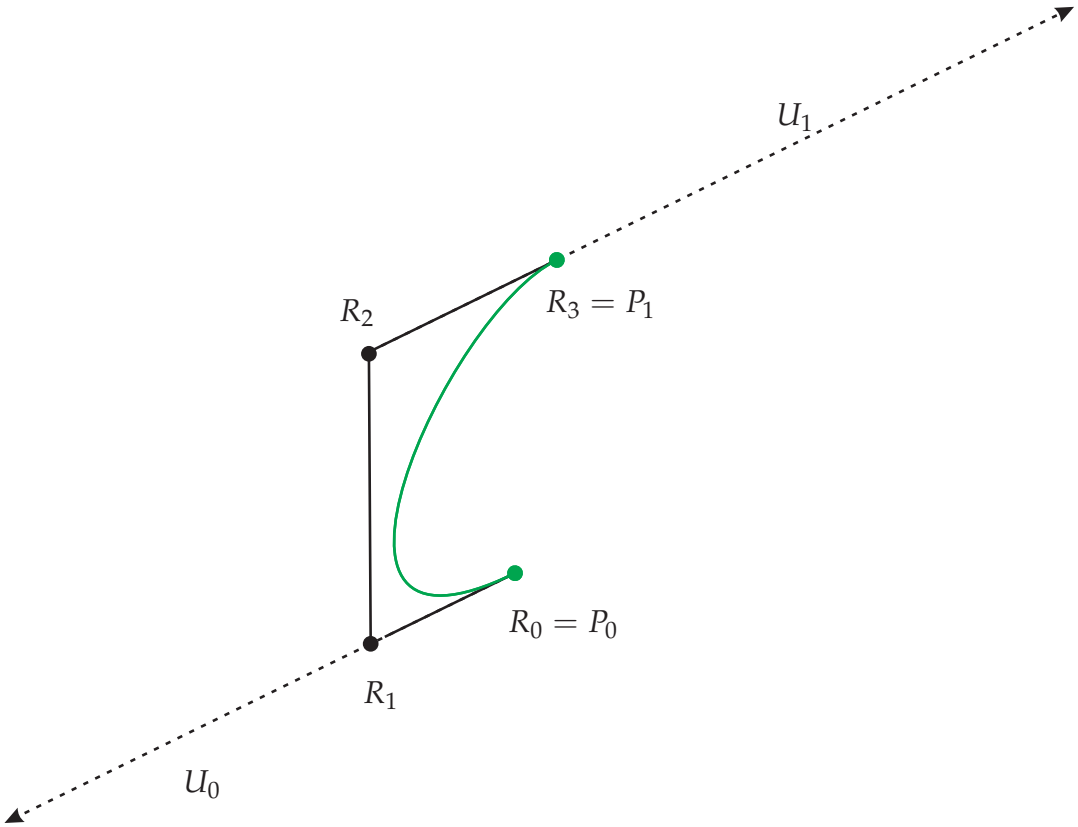

Figure 5.4: Illustrative figure – Hermite interpolation using a cubic.

where R_0, R_1, R_2, R_3 are the control points which satisfy $R_0 = P_0$, $R_1 = P_0 + \frac{U_0}{3}$, $R_2 = P_1 - \frac{U_1}{3}$ and $R_3 = P_1$. $B_i^3(t)$ are the Bernstein polynomials of degree 3, i.e.,

$$B_i^3(t) = \binom{3}{i} t^i (1-t)^{3-i}. \tag{5.41}$$

A cubic Bézier quaternion curve can be used to define a Hermite quaternion curve which interpolates two end unit quaternions. Let $\mathcal{Q}_i$ be the unit quaternion, $\mathcal{U}_i = \mathcal{Q}_i^{(1)}$ the velocity quaternion and $\mathcal{V}_i = \mathcal{Q}_i^{(2)}$ the acceleration quaternion at orientation $\mathcal{Q}_i$ for $i = 0, 1$.

Then the cubic quaternion interpolation curve $q : [0,1] \to \mathbb{H}$ can be found as

$$q(t) = \sum_{j=0}^{3} \mathcal{B}_j B_j^3(t), \tag{5.42}$$

where $\mathcal{B}_j$ are the unknown control quaternions and $B_j^3(t)$ are the Bernstein polynomials of degree 3.

The quaternion curve is G^2 continuous if the following conditions are satisfied

$$\begin{aligned} q(j) &= \lambda_j \mathcal{Q}_j, && (5.43)\\ q'(j) &= \lambda_j^{(1)} \mathcal{Q}_j + \lambda_j \phi_j^{(1)} \mathcal{U}_j, && (5.44)\\ q''(j) &= \lambda_j^{(2)} \mathcal{Q}_j + 2\lambda_j^{(1)} \phi_j^{(1)} \mathcal{U}_j + \lambda_j \phi_j^{(2)} \mathcal{U}_j + \lambda_j (\phi_j^{(1)})^2 \mathcal{U}_j^{(2)}, && (5.45)\\ \lambda_0 &= \lambda_1 = 1, && (5.46) \end{aligned}$$

where $j = 0, 1$. The parameters λ_j and ϕ_j correspond to the function λ for $j = 0, 1$ and the reparametrization ϕ for $j = 0, 1$, respectively. The remaining parameters $\lambda_j^{(n)}$ and $\phi_j^{(n)}$, where $n = 1, 2$ are the n-th derivatives for $j = 0, 1$. Moreover, the following equation has to be satisfied

$$\phi_0^{(1)} > 0, \qquad \phi_1^{(1)} > 0, \tag{5.47}$$

to guarantee the reparametrization ϕ to be regular. To obtain the following equations we have to use some basic properties of the Bézier curves mentioned at the beginning of this section

$$\begin{aligned} \mathcal{B}_0 &= \mathcal{Q}_0, \qquad \mathcal{B}_3 = \mathcal{Q}_1, && (5.48)\\ 3\Delta\mathcal{B}_0 &= \lambda_0^{(1)} \mathcal{Q}_0 + \phi_0^{(1)} \mathcal{U}_0, && (5.49)\\ 3\Delta\mathcal{B}_2 &= \lambda_2^{(1)} \mathcal{Q}_2 + \phi_2^{(1)} \mathcal{U}_2, && (5.50)\\ 6\Delta^2\mathcal{B}_0 &= \lambda_0^{(2)} \mathcal{Q}_0 + (2\lambda_0^{(1)} \phi_0^{(1)} + \phi_0^{(2)}) \mathcal{U}_0 + (\phi_0^{(2)})^2 \mathcal{V}_0, && (5.51)\\ 6\Delta^2\mathcal{B}_1 &= \lambda_1^{(2)} \mathcal{Q}_1 + (2\lambda_1^{(1)} \phi_1^{(1)} + \phi_1^{(2)}) \mathcal{U}_1 + (\phi_1^{(2)})^2 \mathcal{V}_1. && (5.52) \end{aligned}$$

The previous set of equations form a system of 24 nonlinear equations for the unknown control quaternions $\mathcal{B}_j$ for $j = 0, 1, 2, 3$ and unknown scalar parameters $\phi_i^{(1)}, \phi_i^{(2)}, \lambda_i^{(1)}, \lambda_i^{(2)}$ for $i = 0, 1$. The unknowns $\phi_0^{(1)}, \phi_0^{(2)}$ have to be positive, see equation (5.47). The set of 22 equations can be reduced to a system of 8 nonlinear equations, see Jaklič et al. (2013)

$$\begin{aligned} &\left(\frac{2}{3}\lambda_0^{(1)} + \frac{1}{6}\lambda_0^{(2)} + 1\right) \mathcal{Q}_0 + \left(\frac{1}{3}\lambda_1^{(1)} - 1\right) \mathcal{Q}_1 + \frac{1}{6}(\phi_0^{(1)})^2 \mathcal{V}_0 \\ &+ \left(\frac{2}{3}\phi_0^{(1)} + \frac{1}{3}\lambda_0^{(1)}\phi_0^{(1)} + \frac{1}{6}\phi_0^{(2)}\right) \mathcal{U}_0 + \frac{1}{3}\phi_1^{(1)} \mathcal{U}_1 = 0, && (5.53)\\ &\left(-\frac{2}{3}\lambda_1^{(1)} + \frac{1}{6}\lambda_1^{(2)} + 1\right) \mathcal{Q}_1 + \left(-\frac{1}{3}\lambda_0^{(1)} - 1\right) \mathcal{Q}_0 + \frac{1}{6}(\phi_1^{(1)})^2 \mathcal{V}_1 \\ &+ \left(-\frac{2}{3}\phi_1^{(1)} + \frac{1}{3}\lambda_1^{(1)}\phi_1^{(1)} + \frac{1}{6}\phi_1^{(2)}\right) \mathcal{U}_1 - \frac{1}{3}\phi_0^{(1)} \mathcal{U}_0 = 0. && (5.54) \end{aligned}$$

Of course Theorem 5.8 can be modified for quaternion cubic interpolation curve. Let us firstly denote

$$\mathbf{D}_{i,j} = \frac{|\mathbf{A}_i^{(j)}(\mathcal{U}_{1-i})|}{|\mathbf{A}_i|}, \quad j = 1, \ldots, 4, \text{ and } i = 0, 1, \tag{5.55}$$

where $|\mathbf{A}_i|$ denotes the determinant of matrix $\mathbf{A} = (\mathcal{Q}_i, \mathcal{Q}_{1-i}, \mathcal{U}_i, \mathcal{V}_i)$. Then Theorem 5.10 can be formulated.

Theorem 5.10. *Let $\mathcal{Q}_0, \mathcal{Q}_1, \mathcal{U}_0, \mathcal{U}_1, \mathcal{V}_0$ and $\mathcal{V}_1$ be given quaternions such that $\mathbf{A}_0$ and $\mathbf{A}_1$ are nonsingular and $\mathbf{D}_{0,4} < 0, \mathbf{D}_{1,4} > 0$. Then there exists a unique cubic interpolating quaternion curve $q(t)$ defined by equations (5.42),(5.48), (5.49), (5.50), (5.51) and (5.52) where*

$$\phi_0^{(1)} = 2\sqrt[3]{\mathbf{D}_{0,4}^2 \mathbf{D}_{1,4}}, \ \lambda_0^{(1)} = -1(3 + 2\mathbf{D}_{1,2}\sqrt[3]{\mathbf{D}_{0,4}^2 \mathbf{D}_{1,4}}), \tag{5.56}$$

$$\phi_1^{(1)} = -2\sqrt[3]{\mathbf{D}_{1,4}^2 \mathbf{D}_{0,4}}, \ \lambda_1^{(1)} = (3 + 2\mathbf{D}_{0,2}\sqrt[3]{\mathbf{D}_{1,4}^2 \mathbf{D}_{0,4}}). \tag{5.57}$$

Proof. See Jaklič et al. (2013) for the proof. □

This approach solves only the rotational part but the construction of the rational spline motion is the combination of rotations and translations as in case of G^1 Hermite interpolation, see equation (5.1). Therefore, the curve needs to be translated to get the final view od the motion, see Section 5.2 for more details.

5.4.2 Improved method using dual quaternions

Dual quaternions will be used in this section in a similar way as for G^1 Hermite interpolation due to their amazing properties. All their advantages and suitability were introduced in previous part therefore we will focus now on application part.

We can modify equations (5.42) according to dual quaternion description (2.52). Then we get the following dual quaternion curve

$$q_d(t) = \mathcal{Q}_{d_0} B_0^3(t) + \mathcal{Q}_{d_1} B_1^3(t) + \mathcal{Q}_{d_2} B_2^3(t) + \mathcal{Q}_{d_3} B_3^3(t), \tag{5.58}$$

where $\mathcal{Q}_{d_0}, \mathcal{Q}_{d_1}, \mathcal{Q}_{d_2}, \mathcal{Q}_{d_3}$ are unit dual quaternions and $B_0^3, B_1^3, B_2^3, B_3^3$ are again Bernstein polynomials, see Definition 5.9. Of course, Theorem 5.10 can be also used to find the rotational part of the dual quaternion.

The interpolating algorithm based on dual quaternion curve can be computed in the following steps, see Algorithm 4.

5.4.3 Computed example and application

The presented example demonstrates the functionality of the designed G^2 Hermite interpolation algorithm based on using dual quaternions. Let us consider smooth motion defined by the dual quaternion curve $\hat{q}(t)$ from Example 5.3.3.

Algorithm 4 Rational spline motion with continuity G^2 using dual quaternion

Input: The rotation motion defined by the quaternion curve $\hat{q}(t)$ and the trajectory $c(t)$ of the center, where $t_i = i, i = 0, \ldots, m$.

1: Normalize the rotational quaternions by equation (5.32) to get $\mathcal{Q}_i$.
2: Compute velocity $\mathcal{U}_i$ as a $\mathcal{U}_i = \mathcal{Q}_i^{(1)}$.
3: Compute quaternion $\mathcal{V}_i$ as a $\mathcal{V}_i = \mathcal{Q}_i^{(2)}$.
4: Compute translation quaternion $\mathcal{T}_i$ using (5.34).
5: Determine a dual quaternion curve using (5.58).

Output: Dual quaternion curves q_{d_i} describing rational spline motion.

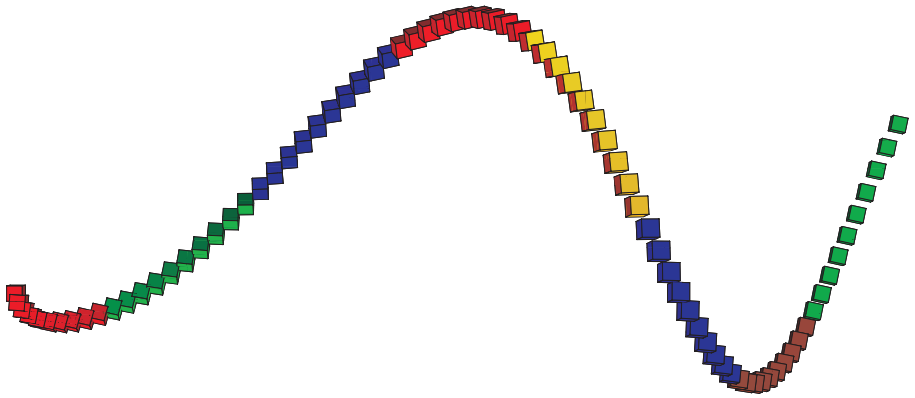

Figure 5.5: Nine positions of a cuboid point of a G^2 motion.

We apply the individual steps as in Algorithm 4 for the values $t_i = 0, \ldots, 8$. The final results are seen in Fig. 5.5 where a nine positions of a cuboid point of a G^2 motion are shown. The different colors show individual arcs of the curve. Next Fig. 5.6 shows the original trajectory and G^2 continuous trajectory using dual quaternions.

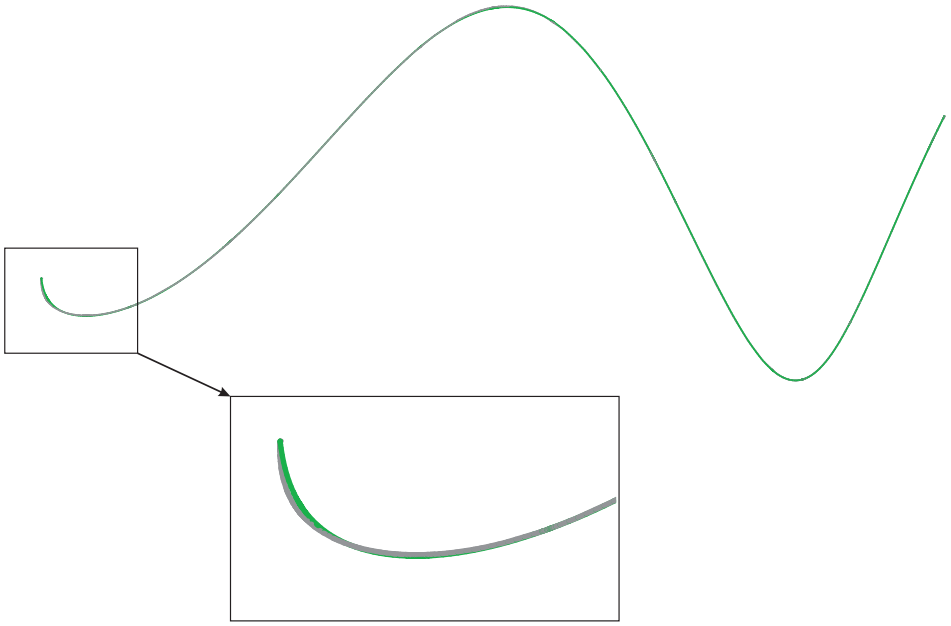

Figure 5.6: Trajectory of an arbitrary point P of the original (grey) and computed motion (green).

Table 5.2: Hausdorff distances between trajectories of an arbitrary point P of the original motion and the motion computed with Algorithm 4.

h	Hausdorff distance	Decay exponent
1	4.97979×10^{-2}	-
$\frac{1}{2}$	2.09772×10^{-2}	2.37
$\frac{1}{4}$	6.81707×10^{-3}	3.08
$\frac{1}{8}$	1.88756×10^{-3}	3.61
$\frac{1}{16}$	4.87794×10^{-4}	3.87
$\frac{1}{32}$	1.23491×10^{-4}	3.95
$\frac{1}{64}$	3.10488×10^{-5}	3.98
$\frac{1}{128}$	7.78217×10^{-6}	3.99

Their Hausdorff distances can be found in Table 5.2. The distances are computed for different values h. The decay exponent describes the ratio of two successive values.

Chapter 6

Summary

The first part of the thesis, i.e., Chapter 1 is devoted to quaternions, dual quaternions and their applications. The intriguing history of their discovery can be found at the beginning. Subsequently, the current state of the art is mentioned to show the popularity of dual quaternions, i.e., a brief description of current applications of quaternions and dual quaternions through various fields.

An important possibility of quaternions to represent rotation in $\boldsymbol{SO}(3)$ is mentioned in Chapter 2. The following part of this chapter is devoted to dual quaternions as an extension of quaternions. This structure uses two quaternions that are combined to using dual numbers. Therefore, firstly the basic definitions and properties of dual numbers were briefly mentioned. The resulting structure of dual quaternions is significant and widely used because of its ability to represent rigid transformations, i.e., spatial motions in $\boldsymbol{SE}(3)$.

Chapter 3 is devoted to a datum transformation problem of finding parameters of transformation of two coordinate systems, the local and the world one. This thesis describes one of the methods for determination of the datum transformation parameters. We use a nonlinear transformation model where we can easily use a description by dual quaternions. Main advantages of this approach are the simplification of the original solution of the datum transformation. The maximum error of the method can be estimated by the error matrix and it is similar to other methods, e.g. based on quaternions. This thesis presents one numerical example to demonstrate the introduced formula. We try to compare the models and description statistic show that both of them have probably log-normal distribution. In order to deal with comparing both algorithms, we have applied a non parametric test, a sign test. By comparing known algorithms it was found that accuracy of algorithm based on dual quaternions is better if we take into account only significant differences. Consequently, advantages of the novel approach lie in the fact that there is not needed a linearization of the non-linear transformation model and accuracy of this model is better considering given conditions.

In Chapter 4, we have presented a new algorithm based on dual quaternions for determination of the secondary structure of proteins. There is a motivation for dealing with the problem of finding parameters of transformation of peptide bonds. We used a nonlinear model to represent this transformation. In this model, we can easily use a description by dual quaternions. Expressing the rotation and translation as a dual quaternion is a convenient way to obtain the equations relating to various helix parameters. These parameters of interests in considering protein structure are residues per turn, pitch, radius or helix axis direction. The main innovation in this thesis is the use of dual quaternions to make it more efficient to keep track of the axis of rotation and translation. Advantage of this approach is again the simplification of the original solution. This thesis presents some numerical examples to demonstrate introduced formula, describing this transformation.

In the computer graphics, animation and robotics, the rotational and translational motions have several important applications. Therefore a simple algorithm for the interpolation by the rational spline motion based on dual quaternions is presented in Chapter 5. The construction of the algorithm was motivated by Jaklič et al. (2013) where a G^1 Hermite interpolation and G^2 Hermite interpolation based on quaternions were investigated. We have modified an algorithm for rational spline motion using dual quaternion approach. The rational spline motions are composed of rotational and translational parts, i.e., this motion can be easily described by dual quaternions. The main advantage of this approach is that the dual quaternions allow us to use these two transformations in only one operation, which simplifies the original method. Of course, this chapter presents some chosen examples to demonstrate the derived algorithm like the applications in previous chapters.

To sum up, let us address the objectives formulated at the beginning of the thesis. Recently, studying quaternions has become after years of using them mainly in physics and robotics again an active research area of applied geometry. New disciplines as e.g. bioinformatics, geodesy, structural biology and others based on studying a continuous set of displacements realized an important role that can be played by the quaternion algebra. However, all the proposed methods and techniques, we have found, remained only halfway. They use rotations and translations, but the algorithms exploit solely quaternions describing rotations, whereas the translations are dealt separately. And this is inefficient, especially when the dual quaternion algebra is available. Our novel approach discussed in this thesis is devoted to joining both operations (rotation and translation) in algorithms to a unique algebraic operation, for which the dual quaternion algebra is especially useful, and formulating new modified and simplified algorithms. We believe that the goals of the thesis were satisfied. We identified the latest advances in applications of quaternions and dual quaternions on selected real-world problems. Some recent methods and techniques based

on quaternions which are suitable for a reformulation using dual quaternions were analyzed and modified. New results and algorithms for certain classes of problems that can be solved using the unifying approach based on dual quaternions were designed. The functionality of the novel formulated methods on particular examples was presented and the advantages of the designed approaches were discussed. All algorithms were implemented and tested in computer algebra system Mathematica. As far as we are aware of the literature our approach to the selected problems is innovative, and it can be used also to all other problems when continuous sets of displacements are investigated.

Appendix A

Publications and citations

Publications in journals indexed on Scopus

Prošková, J. (2017). Interpolations by rational motions using dual quaternions. *Journal for Geometry and Graphics*, Accepted for publication in 2017.

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