Computations of form and stability of rotating drops with finite elements

*Berechnungen von Form und Stabilität rotierender Tropfen
mit finiten Elementen*

Von der Fakultät für Mathematik, Informatik und Naturwissenschaften
der Rheinisch-Westfälischen Technischen Hochschule Aachen
zur Erlangung des akademischen Grades eines
Doktors der Naturwissenschaften genehmigte Dissertation

vorgelegt von

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Tag der mündlichen Prüfung: 15. Dezember 2003

Diese Dissertation ist auf den Internetseiten der Hochschulbibliothek online verfügbar.

At this point I would like to thank Prof. Josef Bemelmans for proposing this problem to me and for his excellent supervision. I would like to thank Prof. Gerhard Dziuk for introducing the finite element theory to me, for providing suitable literature and his help concerning the discretisation of curvature related problems. Further, I would like to thank Alfred Schmidt and Kunibert Siebert for their finite element toolbox **ALBERT** and for answering a bunch of beginner's questions concerning finite elements.

Abstract

We consider the problem of a drop rotating rigidly at a fixed angular velocity. The centrifugal forces are balanced by surface tension alone. Such a drop is described by the Young-Laplace equation:

$$2H = 4r^2\omega^2 + C, \quad \int_{\Omega} dx = \text{const.}$$

Here H denotes the mean curvature, r the orthogonal distance to the axis of rotation, C the Lagrange multiplier for the volume constraint, $\Omega \subset \mathbb{R}^3$ the region enclosed by the drop surface and ω the angular velocity.

Subject of this work is the numerical computation of the bifurcation of shape families from explicitly known axisymmetric drops. The bifurcation parameter is ω .

This problem has been treated numerically by R.A. Brown and L.E. Scriven in 1980 [[BROWN and SCRIVEN 1980a](#)]. We present an algorithm which avoids an explicit global parametrisation of the drop surface and does not impose a meridional reflective symmetry on the drop shapes, using ideas introduced by G. Dziuk for computing evolutionary surfaces [[DZIUK 1991](#)].

The results of the numerical experiments extend the results formerly found by Brown and Scriven and reveal several new branches of spheroidal drop shapes. Furthermore drop shapes of annular type have been computed branching from an axisymmetric family of tori which was found by R. Gulliver [[GULLIVER 1984](#)].

Zusammenfassung

Wir betrachten einen Tropfen, der als starrer Körper mit konstanter Winkelgeschwindigkeit rotiert. Dabei steht die Zentrifugalkraft im Gleichgewicht mit der Oberflächenspannung; andere Kräfte werden nicht berücksichtigt. Solch ein Tropfen wird von der Young-Laplace Gleichung beschrieben:

$$2 H = 4 r^2 \omega^2 + C, \quad \int_{\Omega} dx = \text{const.}$$

Dabei bezeichnet H die mittlere Krümmung, r den Abstand von der Rotationsachse, C den Lagrangeschen Multiplikator für die Volumenbedingung, $\Omega \subset \mathbb{R}^3$ das Gebiet, das der Tropfen einnimmt und ω die Winkelgeschwindigkeit.

Der Gegenstand der Untersuchung ist die numerische Berechnung von Familien von Tropfen, die von explizit bekannten zylindersymmetrischen Familien abzweigen. Der Verzweigungsparameter ist ω .

Dieses Problem wurde bereits 1980 von R.A. Brown und L.A. Scriven numerisch behandelt [[BROWN and SCRIVEN 1980a](#)]. Wir stellen einen Algorithmus vor, der eine explizite globale Parametrisierung der Oberfläche des Tropfens vermeidet und ohne die Annahme einer meridialen Spiegelsymmetrie auskommt. Benutzt werden dazu Ideen von G. Dziuk zur Berechnung von Flächen, die sich unter dem Krümmungsfluß entwickeln [[DZIUK 1991](#)].

Die Ergebnisse der numerischen Experimente erweitern die Resultate von Brown und Scriven und zeigen etliche neue Verzweigungen. Außerdem wurden Tropfen vom Typ eines Torus berechnet, welche von einer zylindersymmetrischen Familie abzweigen, die von R. Gulliver gefunden wurde [[GULLIVER 1984](#)].

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Chapter 1

Introduction

This work is concerned with the numerical computation of the equilibrium figures of rotating drops subject to surface tension and centrifugal forces alone.

Such drops were already studied by J.A.F. Plateau in the first half of the nineteenth century. He made experiments with drops immersed in a tank of liquid of almost the same density as the drop and used a wooden shaft to turn the drops at constant angular velocity. Newer experiments were performed in the context of the low gravity fluid dynamics experiments of the Spacelab in the eightieth and ninetieth of the 20th century. This time, an acoustic multi-pole field was used to initiate the rotation of the drops.

The physical experiments and analytical and numerical works performed in the (roughly) 160 years following Plateau's experiments suggest that the equations governing this problem show an interesting bifurcation behaviour with a rich variety of solution families. However, no strict analytical proof exists yet for the existence of any of the bifurcation phenomena observed by either physical or numerical experiments. The attempt to give a short history of related works is made below in [Section 1.2](#).

In this work we describe a numerical method which uses parametric finite elements on the surface of the drop and, in addition, uses a local adaptive refinement strategy and methods to counter-balance the degeneration of the surface mesh.

This enables us to compute geometrically complicated surfaces without running into coordinate singularities and to handle multiply-connected surfaces like annuli.

Furthermore, for the first time in the numerical treatment of this problem no artificial symmetries are imposed on the drop shapes. Thus our path-tracking algorithm is able to compute a much larger part of the solution-set than it was possible to compute with previous numerical method. Particularly we found several solution-branches not known before.

The remainder of this work is structured as follows:

First we present the physical problem with the corresponding mathematical model and give a short historical overview. After introducing the necessary definitions and notations we present the exact solutions known presently.

In the second part of this work we explain the discretisation of the differential equation describing the drops and the path-tracking algorithm. The numerical methods for the surface mesh are described in detail in the third chapter. Finally, the last chapter presents the results of the numerical experiments.

The implementation of our algorithm for the computation of the drop-shapes (see Algorithm 2.6.1 on page 58) was based on version 0.2 of the finite element toolbox ALBERT [SCHMIDT and SIEBERT 1998]. The toolbox ARPACK [LEHOUCQ et al. 1998] was used as back-end for the eigenvalue computations needed for solving the bifurcation equations.

1.1 The physical model

We consider a rotating drop held together by its surface tension alone. Gravitational forces are neglected.

The drop rotates as a rigid body with constant angular velocity ω around the z -axis. The surface tension is proportional to the mean curvature with a constant factor σ . Moreover, the mass-density ρ of the drop is constant.

The aim is to compute the shape of the drop in dependence on ω under the constraint of a prescribed volume V . So we are searching for compact embedded surfaces $\Gamma \subset \mathbb{R}^3$ which satisfy the differential equation derived from the physical model described above.

Let $\Omega \subset \mathbb{R}^3$ be the region enclosed by Γ . Then the drop's energy E in its rest-system is given by

$$E = E_{surf} + E_{rot} - C(|\Omega| - V),$$

with the surface energy $E_{surf} := \sigma|\Gamma|$, the rotational energy $\omega^2 \frac{\rho}{2} \int_{\Omega} r^2 dx$ and the Lagrange-parameter C accounting for the volume-constraint. r denotes the distance from the axis of rotation. The drop rotates around the z - or x_3 -axis where a point $P \in \mathbb{R}^3$ has the components $(x, y, z) \equiv (x_1, x_2, x_3)$.

Without loss of generality (see the remark at the end of this section on page 4) we can assume that $V = \frac{4}{3}\pi$. Division of E by σ then yields the normalised energy

$$\hat{E} := \frac{1}{\sigma} E = |\Gamma| - \frac{1}{2} \hat{\omega}^2 \frac{\rho}{\sigma} \int_{\Omega} r^2 dx - \bar{C}(|\Omega| - \frac{4}{3}\pi), \text{ with } \bar{C} := \frac{\hat{C}}{\sigma},$$

Substituting $\bar{\omega}^2 := \frac{\rho}{8\sigma} \hat{\omega}^2$ one gets rid of the constants ρ and σ . So the only parameter left is the normalised angular velocity $\bar{\omega}$:

$$(1.1) \quad \bar{E} = |\Gamma| - 4\bar{\omega}^2 \bar{M} - \bar{C}(|\Omega| - \frac{4}{3}\pi)$$

where $\bar{M} := \int_{\Omega} r^2 dx$ is the normalised moment of inertia.

In the following we are only concerned with the normalised energy of equation (1.1) and so we omit the bars. For the remainder E , ω , M and C each denote the quantities $\bar{E}$, $\bar{\omega}$, $\bar{M}$ and $\bar{C}$ of equation (1.1).

The energy functional E describes a drop rotating at constant angular velocity ω . However, the natural parameter for a freely rotating drop would be its angular momentum. Such a drop is described by another functional R (the so called ‘‘Routhian’’) which is related to E by a Legendre-transformation (see any standard text-book for theoretical mechanics, for example [LANDAU and LIFSCHITZ 1990, Chapter VII]).

$$(1.2) \quad R := E - \omega \frac{\partial E}{\partial \omega} = |\Gamma| + 8 \frac{L^2}{2M} - C(|\Omega| - \frac{4}{3}\pi).$$

The formal first and second variation of E and R are given by:

Preserved angular velocity ω	Preserved angular momentum L
$E = \Gamma - 4\omega^2 M - C(\Omega - \frac{4}{3}\pi)$	$R = \Gamma + 4 \frac{L^2}{M} - C(\Omega - \frac{4}{3}\pi)$
$\delta E = \delta \Gamma - 4\omega^2 \delta M - C \delta \Omega $	$\delta R = \delta \Gamma - 4 \frac{L^2}{M^2} \delta M - C \delta \Omega $
$\delta^2 E = \delta^2 \Gamma - 4\omega^2 \delta^2 M - C \delta^2 \Omega $	$\delta^2 R = \delta^2 \Gamma - 4 \frac{L^2}{M^2} \delta^2 M - C \delta^2 \Omega $ $+ 8 \frac{L^2}{M^3} (\delta M)^2$

Because of $\omega^2 = L^2/M^2$ it is clear that E and R have the same stationary points. Obviously, a rigid body rotating at constant angular velocity has a constant angular momentum and vice versa.

However, in the second variation of R there is the additional term $8 \frac{L^2}{M^3} (\delta M)^2 \geq 0$. So there may be stationary points which are minima of R but not of E . The reason is that the conservation of angular momentum is an additional constraint on the admissible perturbations.

Another important difference is that the Euler-Lagrange-equations derived from the variation of R are integro-differential equations. In contrast, the variation of E yields ‘‘only’’ partial differential equations. The reason is that the first variation of R contains the term $M = \int_{\Omega} r^2 dx$ explicitly while the first variation of E only contains the first variation of M .

The Euler-Lagrange equations for the first variation of E are

$$(1.3) \quad 2 H_{\Gamma} \nu_{\Gamma} \equiv -\Delta_{\Gamma} \text{id}_{\Gamma} = (4\omega^2 r^2 + C) \nu_{\Gamma}, \quad \int_{\Gamma} \text{id}_{\Gamma} \nu_{\Gamma} d\Gamma = 4\pi.$$

Here Δ_{Γ} denotes the Laplace-Beltrami operator, ν the outer normal-field and $\text{id}_{\Gamma} : \Gamma \rightarrow \Gamma : x \mapsto x$ the identity mapping on Γ . Furthermore the volume constraint has been transformed into an integral over the surface Γ by virtue of Gauß’ formula, using $\text{div id}_{\mathbb{R}^3} = 3$.

The unknowns in equation (1.3) above are the surface Γ itself and the Lagrange-multiplier C for the volume constraint. ω enters as a parameter. A brief derivation of the Euler-Lagrange equations is in Section 2.1 on page 22.

We note that by applying a scaling transformation $x \mapsto \lambda \cdot x$ ($\lambda > 0$) a solution Γ of the Euler-Lagrange equations (1.3) is transformed into a solution Γ^λ of the Equation

$$2 H_{\Gamma^\lambda} \nu_{\Gamma^\lambda} \equiv -\Delta_{\Gamma^\lambda} \text{id}_{\Gamma^\lambda} = \left(4 \frac{\omega^2}{\lambda^3} r^2 + \frac{C}{\lambda}\right) \nu_{\Gamma^\lambda} x, \quad \int_{\Gamma^\lambda} \text{id}_{\Gamma^\lambda} \nu_{\Gamma^\lambda} d\Gamma^\lambda = 4 \pi \lambda^3.$$

This follows easily from the facts that $H_{\Gamma^\lambda} = \frac{1}{\lambda} H_\Gamma$ and $\nu_{\Gamma^\lambda} = \nu_\Gamma$.

The goal is now to find bifurcations from the two explicitly known families of solutions to (1.3), which are described in Section 1.4. The angular velocity ω is used as bifurcation parameter. The path-tracking algorithm and the discretisation of equation (1.3) will be described in Chapter 2 below.

1.2 Historical Overview

The following is a brief summary of some analytical and numerical results concerning the computation of shape and stability of equilibrium configurations of rotating drops. The list is – of course – incomplete.

1843 J.A.F. Plateau Plateau made physical experiments with a drop immersed in a tank of liquid of almost the same density as the drop. The apparatus is shown in

Figure 1.1 From the translation of Plateau’s essay in [PLATEAU 1863].

Figure 1.1(a). By turning the vertically mounted shaft the drop could be brought into rotation. Some of the figures observed by Plateau are shown in Figure 1.1(b) on the preceding page. The experiments were published in [PLATEAU 1843] and later in English translation in [PLATEAU 1863].

1869 A. Beer He found a family of exact solutions to (1.3). The derivation can be found in his book [BEER 1869], a short outline is given in Section 1.4 below.

1914 Lord Rayleigh By a Taylor-series expansion [RAYLEIGH 1914] found that certain annular equilibrium shapes are stable in the cylinder-symmetric setting.

1965 S. Chandrasekhar He found, by considering oscillations around a linearisation of (1.3), estimates for the value of the angular velocity at which the drop-shapes found by Beer become unstable, see [CHANDRASEKHAR 1965].

1968 L.A. Slobozhanin The annular axisymmetric solutions are actually unstable; [MYSHKIS et al. 1987] gives a short outline of Slobozhanin's work, see also [SLOBOZHANIN 1968].

1980 R.A. Brown, L.E. Scriven They performed numerical experiments with a finite element method, investigating bifurcations from the axisymmetric family found by Beer. They found three families of bifurcations – a two-lobed, a three-lobed and a four-lobed family – which are no longer cylinder-symmetric, but allow only discrete rotation-groups of order 2, 3 and 4. The results were published in [BROWN and SCRIVEN 1980a]. We will comment further on their numerical method below, as our work extends their results.

1982 H.C. Wente He considered stationary rotating drops held together by self-gravitation *and* surface tension in [WENTE 1982] and showed that every such a drop possesses a reflective symmetry about its equatorial plane.

1984 R. Gulliver He found a (more or less) explicit expression for axisymmetric annular solutions of (1.3), very similar to the representation of the simply connected

Figure 1.2 T.G. Wang's repetition of Plateau's experiments. The pictures are taken from [WANG 1988].

axisymmetric shapes found by [BEER 1869]. We comment further on those two families in Section 1.4 below.

1985 T.G. Wang Wang repeated and extended Plateau's experiments, using drops of water immersed into a tank of glycerin.

Figure 1.2 on the preceding page shows some of the drop shapes he observed, together with a sketch of the apparatus he has used.

Wang had also a major part in the drop-dynamics experiments of the *Spacelab 3* mission in 1985. There, an acoustic multi-pole field was used to initiate the rotation of the centimetre-sized water-drops, see [WANG 1988]. The experiments were continued on subsequent Spacelab flights. Figure 1.3 originates from the *USML2* flight in 1995 and shows the development of a freely rotating two-lobed drop.

Figure 1.3 Development of a freely rotating two-lobed drop, *USML2* space-lab flight in 1995

1987 F. Brulois Brulois developed a method to estimate up to arbitrary accuracy the maximum value of the angular velocity ω up to which the drops of Beer's axisymmetric family of drops are still stable, see [BRULOIS 1987].

1.3 Notation and Fundamental Definitions

1.3.1 Analysis in $\mathbb{R}^n$

1.3.1 DEFINITION (NATURAL NUMBERS, REAL NUMBERS)

$\mathbb{N} := \{1, 2, \dots\}$ denotes the set of natural numbers, $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ denotes the set of natural numbers including zero. The set of real numbers is denoted by $\mathbb{R}$.

Further $\mathbb{R}^+ := \{x \in \mathbb{R} \mid x > 0\}$ and $\mathbb{R}^{\geq 0}, \mathbb{R}^{\leq 0}, \mathbb{R}^{> 0} \equiv \mathbb{R}^+, \mathbb{R}^{< 0}$ denote as usual the sets of non-negative, non-positive, positive and negative real numbers.

1.3.2 DEFINITION (SCALAR PRODUCTS)

Let $n, m \in \mathbb{N}$ For $x, y \in \mathbb{R}^n$. we denote by $x \cdot y := \langle x, y \rangle := x^T y$ the Euclidean scalar product. For $A = (a_{ij}), B = (b_{ij}) \in \mathbb{R}^{m \times n}$ we denote by $A : B := \sum_{i=1}^m \sum_{j=1}^n a_{ij} b_{ij}$, the standard scalar product of A with B in the vector space $\mathbb{R}^{m \times n}$.

The summation convention is used whenever it is unambiguous: for $a = (a_i)$, $b = (b_i) \in \mathbb{R}^n$ we write

$$a_i b_i := a \cdot b = \sum_{i=1}^n a_i b_i,$$

and similarly for other indexed quantities.

1.3.3 DEFINITION (POLYNOMIAL SPACES P_k)

For $k \in \mathbb{N}_0$ and $\Omega \subset \mathbb{R}^n$ we denote by $P_k(\Omega)$ the vector space of polynomials $p : \Omega \rightarrow \mathbb{R}$ of degree less or equal to k .

1.3.4 DEFINITION (PARTIAL DERIVATIVES, GRADIENTS)

For $\Omega \subset \mathbb{R}^n$ open and $f : \Omega \rightarrow \mathbb{R}$ differentiable we denote the partial derivatives of f by

$$\nabla_i f = D_i f := \frac{\partial f}{\partial x_i}$$

and the gradient of f by

$$\nabla f = Df := (\nabla_1 f, \dots, \nabla_n f).$$

For $v \in \mathbb{R}^n$ we denote by

$$f_v = \frac{\partial f}{\partial v} := v \cdot \nabla f$$

the directional derivative of f in direction v .

For a multi-index $s = (s_1, \dots, s_n) \in \mathbb{N}_0^n$ the mixed partial derivatives are denoted by

$$\nabla^s f := \nabla_1^{s_1} \dots \nabla_n^{s_n} f.$$

1.3.5 DEFINITION (CONTINUOUS FUNCTION SPACES C^k , C_0^k)

For $\Omega \subset \mathbb{R}^n$ open and bounded we define

$$C^0(\bar{\Omega}) := \{f : \bar{\Omega} \rightarrow \mathbb{R} \mid f \text{ continuous}\}$$

and for $k \in \mathbb{N}$

$$C^k(\bar{\Omega}) := \{f : \bar{\Omega} \rightarrow \mathbb{R} \mid f \text{ is } k\text{-times continuously differentiable on } \Omega, \\ \nabla^s f \text{ can be continuously extended to } \bar{\Omega} \text{ for all } s \in \mathbb{N}_0^n, |s| \leq k\}.$$

$C^0(\bar{\Omega})$ and $C^k(\bar{\Omega})$ are Banach spaces with the norms

$$\|f\|_{\sup(\Omega)} := \sup_{x \in \Omega} |f(x)|, \text{ respectively } \|f\|_{C^k(\bar{\Omega})} := \sum_{|s| \leq k} \|\nabla^s f\|_{\sup(\Omega)}.$$

Spaces of continuous functions with compact support are denoted by

$$C_0^k(\bar{\Omega}) := \{f \in C^k(\bar{\Omega}) \mid \text{supp } f \Subset \Omega\}.$$

Finally

$$C^\infty(\bar{\Omega}) := \bigcap_{k \in \mathbb{N}} C^k(\bar{\Omega}) \quad \text{and} \quad C_0^\infty(\bar{\Omega}) := \bigcap_{k \in \mathbb{N}} C_0^k(\bar{\Omega}).$$

1.3.6 DEFINITION (HÖLDER-SPACES $C^{k,\alpha}(\bar{\Omega})$, LIPSCHITZ SPACES $C^{0,1}(\bar{\Omega})$)

Let $\Omega \subset \mathbb{R}^n$ open and bounded and $\alpha \in [0, 1]$, $f : \bar{\Omega} \rightarrow \mathbb{R}$. We define

$$\text{höl}_\alpha(f) := \sup_{\substack{x, y \in \bar{\Omega} \\ x \neq y}} \frac{|f(x) - f(y)|}{|x - y|^\alpha}.$$

Then for $k \in \mathbb{N}_0$ we define Banach-spaces

$$C^{k,\alpha}(\bar{\Omega}) := \{f \in C^k(\bar{\Omega}) \mid \text{höl}_\alpha(\nabla^s f) < \infty \text{ for all } s \in \mathbb{N}_0^n, |s| = k\}$$

with

$$\|f\|_{C^{k,\alpha}(\bar{\Omega})} := \|f\|_{C^k(\bar{\Omega})} + \sum_{|s|=k} \text{höl}_\alpha(\nabla^s f).$$

Functions in $C^{0,\alpha}(\bar{\Omega})$ are called Hölder-continuous on $\bar{\Omega}$.

Functions in $C^{0,1}(\bar{\Omega})$ are called Lipschitz-continuous on $\bar{\Omega}$.

1.3.7 DEFINITION (LEBESGUE-SPACES $L_p(\Omega)$)

Let $\Omega \subset \mathbb{R}^n$ open, $f : \Omega \rightarrow \mathbb{R}$ measurable and $p \in [1, \infty)$. We define

$$\|f\|_{L_p(\Omega)} := \sqrt[p]{\int_{\Omega} |f|^p dx} \quad \text{and} \quad \|f\|_{L_\infty(\Omega)} := \text{ess sup}_{x \in \Omega} |f(x)|.$$

Then the Lebesgue-space $L_p(\Omega)$ is defined as

$$L_p(\Omega) := \{f : \Omega \rightarrow \mathbb{R} \mid f \text{ measurable and } \|f\|_{L_p(\Omega)} < \infty\}.$$

REMARK 1.3.1 $L_2(\Omega)$ with the scalar product $(f, g)_{L_2(\Omega)} := \int_{\Omega} fg$ is a Hilbert-space.

1.3.8 DEFINITION (SOBOLEV-SPACES H_p^k AND $\mathring{H}_p^k$)

Let $\Omega \subset \mathbb{R}^n$ open. Let $k \in \mathbb{N}_0$ and $p \in [1, \infty)$. We define

$$\|f\|_{H_p^k(\Omega)} := \left(\sum_{|s| \leq k} \|\nabla^s f\|_{L_p(\Omega)}^p \right)^{1/p}$$

and the Sobolev-spaces $H_p^k(\Omega)$ and $\mathring{H}_p^k(\Omega)$ as the closures

$$H_p^k(\Omega) := \overline{\{f \in C^\infty(\Omega) \mid \|f\|_{H_p^k(\Omega)} < \infty\}}$$

and

$$\mathring{H}_p^k(\Omega) := \overline{\{f \in C_0^\infty(\Omega) \mid \|f\|_{H_p^k(\Omega)} < \infty\}}$$

with respect to the $H_p^k(\Omega)$ norm.

In the case of $p = 2$ we set $H^k(\Omega) := H_2^k(\Omega)$ and $\mathring{H}^k(\Omega) := \mathring{H}_2^k(\Omega)$.

REMARK 1.3.2 $H_p^k(\Omega)$ and $\mathring{H}_p^k(\Omega)$ are Banach spaces, $H_2^k(\Omega)$ and $\mathring{H}_2^k(\Omega)$ with the scalar product $(f, g)_{H_2^k(\Omega)} := \sum_{|s| \leq k} \int_{\Omega} \nabla^s f \cdot \nabla^s g$ are Hilbert-spaces.

1.3.9 DEFINITION (WEAK DERIVATIVE)

Let $\Omega \subset \mathbb{R}^n$ open, $f : \Omega \rightarrow \mathbb{R}$ measurable and s any multi-index. Then a locally integrable function $v : \Omega \rightarrow \mathbb{R}$ is called the s^{th} weak derivative of f if it satisfies

$$(1.4) \quad \int_{\Omega} v \varphi = (-1)^{|s|} \int_{\Omega} f \nabla^s \varphi \quad \text{for all } \varphi \in C_0^{|s|}(\Omega).$$

For $k \in \mathbb{N}_0$ the set of all k -times weakly differentiable functions is denoted by $W^k(\Omega)$.

REMARK 1.3.3 We use the same notation for weak and for “ordinary” derivatives if it is unambiguous. So the s^{th} weak derivative of a function f is denoted by $\nabla^s f$ and the like for the weak gradient, divergence and the directional derivatives.

Using Definition 1.3.9 it is possible to get an alternative characterisation of the Sobolev space H_p^k :

1.3.10 DEFINITION (THE SPACE W_p^k)

Let $\Omega \subset \mathbb{R}^n$ open. Let $k \in \mathbb{N}_0$ and $p \in [1, \infty)$. We define

$$W_p^k(\Omega) := \{f \in W^k(\Omega) \mid \nabla^s f \in L_p(\Omega) \text{ for all } |s| \leq k\}.$$

1.3.11 THEOREM

Let $\Omega \subset \mathbb{R}^n$ open. Let $k \in \mathbb{N}_0$ and $p \in [1, \infty)$. Then it holds:

$$(W_p^k(\Omega), \|\cdot\|_{H_p^k(\Omega)}) = H_p^k(\Omega).$$

Proof: For example [GILBARG and TRUDINGER 2001, Section 7.9] or [EVANS 1998, Section 5.3] □

1.3.2 Differential geometry

Analysis on manifolds is treated in detail – for example – in [AUBIN 1982], [CARMO 1992], [CARMO 1993] and relevant aspects can also be found in [WLOKA 1982] and [GILBARG and TRUDINGER 2001]. However we do not need the notion of differentiability and curvature for the most general case, but only for the case of 2 dimensional isometric immersions into $\mathbb{R}^3$. Therefore we give the most basic definitions for the general case, but the covariant derivative and the curvature will only be defined for the case of n -dimensional isometric immersions into $\mathbb{R}^{n+1}$.

Differential manifolds For the most part the following definitions are cited from [AUBIN 1982] and also in some cases from [GALLOT et al. 1993].

1.3.12 DEFINITION (MANIFOLD, CHART, PARAMETRISATION, ATLAS)

1. A Hausdorff topological space Γ is called a topological manifold of dimension n if each point of Γ has a neighbourhood homeomorphic to $\mathbb{R}^n$.
2. A local chart on Γ is a pair (Ω, ϕ) with $\Omega \subset \Gamma$ open and ϕ a homeomorphism of Ω onto an open set of $\mathbb{R}^n$.
3. The mapping $\phi^{-1} : \phi(\Omega) \rightarrow \Omega$ is called a parametrisation or coordinate system of Ω .
4. A set $(\Omega_i, \phi_i)_{i \in I}$ of local charts of Γ such that $\Gamma = \bigcup_{i \in I} \Omega_i$ is called an atlas of Γ .

1.3.13 DEFINITION (C^k -MANIFOLD, ORIENTABLE MANIFOLD)

An atlas $(\Omega_i, \phi_i)_{i \in I}$ of Γ is called of class C^k if all changes of coordinate

$$\phi_i \circ \phi_j^{-1} : \phi_j(\Omega_i \cap \Omega_j) \rightarrow \mathbb{R}^n$$

are of class C^k . Two atlases of class C^k are called equivalent if their union is an atlas of class C^k . A differentiable manifold of class C^k is a manifold together with an equivalence class of C^k atlases. A differentiable manifold is called orientable if there exists an atlas so that the Jacobi-determinants for all changes of coordinate are positive.

Analogous definitions are valid for the differentiability classes C^∞ and $C^{k,\alpha}$.

1.3.14 DEFINITION (DIFFERENTIABLE MAPPING, IMMERSION, EMBEDDING)

A mapping $f : \Gamma \rightarrow \Xi$ between two differentiable manifolds Γ of dimension n and Ξ of dimension m , both of class C^k , is called differentiable of class C^r in $P \in \Gamma$, $r \leq k$, if the mapping $\phi_Q \circ f \circ \phi_P^{-1}$ is differentiable of class C^r at $\phi_P(P)$ for local charts (Ω_P, ϕ_P) around $P \in \Gamma$ and (Ω_Q, ϕ_Q) around $Q := f(P) \in \Xi$. The rank of f in P is defined as the rank of $\phi_Q \circ f \circ \phi_P^{-1}$ in $\phi_P(P)$.

A differentiable mapping f is called immersion if its rank in each point of Γ is equal to n . An immersion f is called embedding if it is a homeomorphism of Γ onto $f(\Gamma)$ where $f(\Gamma)$ has the topology induced by Ξ .

1.3.15 DEFINITION (TANGENT VECTOR)

A tangent vector at $P \in \Gamma$ is a map $X : f \rightarrow X(f) \in \mathbb{R}$, defined on the set of real-valued functions differentiable in a neighbourhood of P , which satisfies

1. $X(\lambda f + \mu g) = \lambda X(f) + \mu X(g) \quad \forall \lambda, \mu \in \mathbb{R}$,
2. $X(fg) = f(P)X(g) + g(P)X(f)$.

The tangent space $T_P\Gamma$ of Γ at P is the set of all tangent vectors at $P \in \Gamma$.

REMARK 1.3.4 It follows from 1. and 2. that $X(f) = 0$ for all tangent vectors X at $P \in \Gamma$ and all differentiable functions f with $\nabla(f \circ \phi^{-1})(\phi(P)) = 0$ for a local chart (Ω, ϕ) around P .

REMARK 1.3.5 The tangent space $T_P\Gamma$ of Γ at p has a natural vector space structure (as has any set of real-valued functions).

If $\Phi : \Omega \subset \mathbb{R}^n \rightarrow \Gamma$ is a coordinate system of a neighbourhood of P then the tangent vectors

$$\left(\frac{\partial}{\partial x_i} \right)_P \quad \text{defined by} \quad \left(\frac{\partial}{\partial x_i} \right)_P (f) := \left(\frac{\partial(f \circ \Phi^{-1})}{\partial x_i} \right)_{\Phi^{-1}(P)}$$

form a basis of $T_P\Gamma$.

1.3.16 DEFINITION (TANGENT SPACE, COTANGENT SPACE, TENSOR BUNDLE)

1. The tangent space $T\Gamma$ of Γ is defined as the fiber bundle $T\Gamma := \bigcup_{P \in \Gamma} T_P\Gamma$.
2. The cotangent space $T^*\Gamma$ of Γ is defined as the fiber bundle $T^*\Gamma := \bigcup_{P \in \Gamma} T_P^*\Gamma$, where $T_P^*\Gamma$ denotes the dual of $T_P\Gamma$.
3. The tensor bundle $T_s^r\Gamma$ of type (r, s) of Γ is defined as the bundle of tensor products $\bigcup_{P \in \Gamma} \overset{r}{\otimes} T_P\Gamma \otimes \overset{s}{T_P^*\Gamma}$.

1.3.17 DEFINITION (DIFFERENTIAL SECTION, VECTOR FIELD, TENSOR FIELD)

1. A section of the fiber bundle (E, π, Γ) is a differentiable map $\xi : \Gamma \rightarrow E$, such that $\pi \circ \xi(P) = P$ for all $P \in \Gamma$.
2. A differentiable vector field on Γ is a section of $T\Gamma$, carrying its natural fiber bundle structure: In this case π is the mapping $\pi : T\Gamma \rightarrow \Gamma : X \in T_P\Gamma \mapsto P$.
3. A differentiable tensor field of type (r, s) on Γ is a section of $T_s^r\Gamma$.

1.3.18 DEFINITION (METRIC, FIRST FUNDAMENTAL FORM)

A Riemannian metric on Γ is a differentiable tensor field g of type $(0, 2)$ on Γ such that $g(P)$ is a scalar-product on $T_P\Gamma \times T_P\Gamma$.

g is also called first fundamental form of the Riemannian manifold Γ .

Analysis on Hyper-Surfaces In the following $\Gamma \subset \mathbb{R}^{n+1}$ is an n -dimensional C^2 -immersion into $\mathbb{R}^{n+1}$. We identify the tangent space $T_P\Gamma$ at a point $P \in \Gamma$ with the affine hyper-plane of $\mathbb{R}^{n+1}$ which is tangential to Γ at P .

Γ has the Riemannian metric induced by the Euclidean metric of $\mathbb{R}^{n+1}$ so that $\Gamma \hookrightarrow \mathbb{R}^{n+1}$ by construction is an *isometric* immersion.

1.3.19 DEFINITION (TANGENTIAL DERIVATIVES, LAPLACE-BELTRAMI OPERATOR)

Let $\Gamma \subset \mathbb{R}^{n+1}$ be an isometric C^2 -immersion of dimension n . We denote its (local) outer unit normal field by $\nu_\Gamma = (\nu_1, \dots, \nu_{n+1}) : \Gamma \rightarrow \mathbb{R}^{n+1}$.

1. For a function $f \in C^1(\Gamma)$ the tangential gradient $\nabla_\Gamma f$ is defined as

$$\nabla_\Gamma f := \nabla f - (\nabla f \cdot \nu_\Gamma) \nu_\Gamma.$$

The tangential derivative $\delta_i^\Gamma f$ of f in direction i is defined as the i -th component of $\nabla_\Gamma f$ ($1 \leq i \leq n+1$):

$$\nabla_\Gamma f = (\delta_1^\Gamma f, \dots, \delta_{n+1}^\Gamma f).$$

2. For a vector field $w = (w_1, \dots, w_{n+1}) \in (C^1(\Gamma))^{n+1}$ the tangential divergence $\nabla_\Gamma \cdot w$ is defined as

$$\nabla_\Gamma \cdot w := \nabla \cdot w - (\nabla w_i \cdot \nu_\Gamma) \nu_i.$$

3. For a function $g \in C^2(\Gamma)$ the Laplace-Beltrami operator $\Delta_\Gamma g$ is defined as

$$\Delta_\Gamma g := \nabla_\Gamma \cdot \nabla_\Gamma g.$$

REMARK 1.3.6 This definition makes sense only if f and w are extended to a neighbourhood of Γ , for example constant in normal direction. However, $\nabla_\Gamma f$ and $\nabla_\Gamma \cdot w$ do not depend on the extension, but only on the values of f and w on Γ .

Let $(e_i | 1 \leq i \leq n+1)$, denote the standard basis of $\mathbb{R}^{n+1}$. If e_i , $1 \leq i \leq n+1$, is not orthogonal to $T_P \Gamma$ in $P \in \Gamma$, then a neighbourhood of P can be parametrised as a graph over the hyperplane $E_i := \langle e_j | 1 \leq j \leq n+1, j \neq i \rangle_{\mathbb{R}}$. The components of $\nabla_\Gamma f$ are the covariant derivatives of f in direction e_j , $j \neq i$. If $e_i \in (T_P \Gamma)^\perp$ then the corresponding component of $\nabla_\Gamma f$ is zero.

REMARK 1.3.7 In the following we will omit the upper index from the directional tangential derivatives whenever it is unambiguous, so $\delta_i f \equiv \delta_i^\Gamma f$, ($1 \leq i \leq n+1$, f as in Definition 1.3.19 on the page before).

With w and g as in Definition 1.3.19 on the preceding page we get the following expressions for the tangential divergence and the Laplace-Beltrami operator:

$$\nabla_\Gamma \cdot w = \delta_i w_i, \quad \Delta_\Gamma g = \delta_i \delta_i g.$$

1.3.20 DEFINITION (WEINGARTEN-MAP)

Let $\Gamma \subset \mathbb{R}^{n+1}$ be an isometric C^2 -immersion of dimension n with a (local) outer unit normal field $\nu_\Gamma = (\nu_1, \dots, \nu_{n+1}) : \Gamma \rightarrow \mathbb{R}^{n+1}$.

The Weingarten-map $II = (II_1, \dots, II_{n+1}) : \Gamma \rightarrow \mathbb{R}^{(n+1) \times (n+1)}$ is defined as

$$(1.5) \quad II_i := \nabla_\Gamma \nu_i, \quad 1 \leq i \leq n+1.$$

REMARK 1.3.8 Defined this way the Weingarten-map II is the usual second fundamental form (see for example [CARMO 1992]), but written in the coordinate frame of the embedding space $\mathbb{R}^{n+1}$, where the tangent space $T_P \Gamma$ at a point $P \in \Gamma$ is identified with the geometrical tangent hyper-plane (as sub-space of $\mathbb{R}^{n+1}$) of Γ at P .

$T_P \Gamma \subset \mathbb{R}^{n+1}$ is an invariant sub-space of $II(P) \in \text{Hom}(\mathbb{R}^{n+1}, \mathbb{R}^{n+1})$ and $II(P)((T_P \Gamma)^\perp) = \{0\}$, which implies that $\nu_\Gamma(P)$ is always an eigenvector of $II(P)$ with eigenvalue 0.

1.3.21 DEFINITION (PRINCIPAL-, MEAN- AND GAUSSIAN-CURVATURE)

For $P \in \Gamma$ the eigenvalues κ_i , $1 \leq i \leq n$ of the second fundamental form $II(P)|_{T_P \Gamma \times T_P \Gamma}$ are called principal curvatures of Γ at P . The mean curvature H_Γ , the curvature vector Y_Γ and the Gauss curvature K_Γ at P are defined as

$$(1.6) \quad H_\Gamma := \frac{1}{n} \sum_{i=1}^n \kappa_i, \quad Y_\Gamma := n H_\Gamma \nu_\Gamma, \quad K_\Gamma := \prod_{i=1}^n \kappa_i.$$

REMARK 1.3.9 In the special case $n = 2$ the mean *and* Gaussian curvature can be computed from II (instead of the restriction $II|_{T\Gamma \times T\Gamma}$) as follows:

$$(1.7) \quad H_\Gamma = \frac{1}{2} \text{trace} II, \quad K_\Gamma = \det(II + I_3) - 2H_\Gamma - 1.$$

1.3.22 LEMMA (A FORMULA FOR THE MEAN CURVATURE VECTOR)

Let $\Gamma \subset \mathbb{R}^{n+1}$ be an isometric C^2 -immersion of dimension n . Let $\text{id}_\Gamma : \Gamma \rightarrow \Gamma : P \mapsto P$ be the identity mapping on Γ . Then the following holds

$$(1.8) \quad -\Delta_\Gamma \text{id}_\Gamma = Y_\Gamma.$$

Proof: Under the premises of Lemma 1.3.22 let $\nu_\Gamma = (\nu_1, \dots, \nu_{n+1})$ be the outer unit normal field of Γ . We then have for a point $X = (X_1, \dots, X_{n+1}) \in \Gamma$ and $1 \leq i \leq n+1$:

$$\begin{aligned} \Delta_\Gamma X_i &= \delta_j \delta_j X_i &= \delta_j (\nabla_j X_i - \langle \nabla X_i, \nu_\Gamma \rangle \nu_j) \\ &= \delta_j (\delta_{ij} - \nu_i \nu_j) &= -\delta_j (\nu_i \nu_j) \\ &= -\underbrace{\nu_j \delta_j \nu_i}_{=0} - \nu_i \delta_j \nu_j \\ &= -\nu_i \delta_j \nu_j \\ &\stackrel{(1.5)}{=} -\text{trace}(II(X)) \nu_i = -n H_\Gamma \nu_i. \end{aligned}$$

□

1.3.23 LEMMA (INTEGRATION BY PARTS)

For an isometric C^2 -immersion $\Gamma \subset \mathbb{R}^{n+1}$ without boundary and $f \in C^1(\Gamma)$ the formula for integration by parts is

$$(1.9) \quad \int_\Gamma \nabla_\Gamma f \, do = - \int_\Gamma f Y_\Gamma \, do.$$

Proof: A detailed proof is given in [GILBARG and TRUDINGER 2001], chapter 16. □

1.3.24 COROLLARY

From Lemma 1.3.23 it follows immediately for $f, g \in C^1(\Gamma)$:

$$(1.10) \quad \int_\Gamma f \Delta_\Gamma g \, do = \int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma g \, do.$$

Proof: Under the assumptions of Corollary 1.3.24 we have by product-rule:

$$\int_\Gamma \nabla_\Gamma \cdot (f \nabla_\Gamma g) \, do = \int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma g \, do + \int_\Gamma f \nabla_\Gamma \cdot \nabla_\Gamma g \, do.$$

On the other hand it follows from Lemma 1.3.23

$$\int_\Gamma \nabla_\Gamma \cdot (f \nabla_\Gamma g) \, do = - \int_\Gamma f \underbrace{\langle \nabla_\Gamma g, Y_\Gamma \rangle}_{=0} \, do.$$

□

Wloka defines in [WLOKA 1982, pp. 92] Sobolev-spaces H^s , $s \in \mathbb{R}$, on Hölder-manifolds:

1.3.25 DEFINITION (SOBOLEV-SPACES $H^s(\Gamma)$, $H^{-s}(\Gamma)$)

Let Γ be a compact Riemannian $C^{k,\alpha}$ -manifold of dimension n , $k \in \mathbb{N}_0$, $\alpha \in [0, 1]$ with $\alpha = 1$ in case $k = 0$. Let $(\Omega_l, \Phi_l)_{l \in L}$ be a finite $C^{k,\alpha}$ -atlas of Γ and ϕ_l a subordinate partition of unity (i.e. $\text{supp}(\phi_l) \subset \Omega_l$). Let $s \leq k + \alpha$, if $\alpha \in \{0, 1\}$ and $s < k + \alpha$ otherwise.

By definition $v : \Gamma \rightarrow \mathbb{R}$ belongs to $H^s(\Gamma)$ if all functions

$$(v \cdot \phi_l) \circ \Phi_l^{-1} : \Phi_l(\Omega_l) \rightarrow \mathbb{R}, \quad l \in L,$$

belong to $\mathring{H}^s(\Phi_l(\Omega_l))$. Together with the scalar-product

$$\langle v, w \rangle_s := \sum_l \langle (v \cdot \phi_l) \circ \Phi_l^{-1}, (w \cdot \phi_l) \circ \Phi_l^{-1} \rangle_{H^s(\mathbb{R}^n)}$$

$H^s(\Gamma)$ is a Hilbert-space.

For $s > 0$ we denote by $H^{-s}(\Gamma)$ the dual space of $H^s(\Gamma)$.

REMARK 1.3.10 The above definition implicitly defines the notion of weak derivatives for a $C^{k,\alpha}$ -manifold, using the same construction as in the definition of differential mappings on manifolds, Definition 1.3.14 on page 10.

[WLOKA 1982, pp. 92] shows that the Sobolev-spaces $H^s(\Gamma)$ – given the prerequisites of Definition 1.3.25 – are well-defined and in particular that $\langle \cdot, \cdot \rangle_s$ only depends up to norm-equivalence on the special choice of the atlas and the local chart.

Definition 1.3.25 covers especially the case of the discrete surfaces of class $C^{0,1}$ constructed by the finite element approach of Section 2.4.1 on page 42 below.

1.3.3 Some aspects from bifurcation theory

The following section gives in brief some notations needed to motivate the approach sketched in Chapter 2. We cite from [CHOW and HALE 1996].

For the remainder of this section we assume that X and Z are Banach-spaces and Λ is an open set in a Banach space. $M : \Lambda \times X \rightarrow Z$ is continuously Frechet differentiable. $D_x M(\lambda, x)$ denotes the Frechet-derivative of M with respect to its second argument evaluated at (λ, x) . Λ is called the *parameter set*. We are interested in solutions of the equation

$$(1.11) \quad M(\lambda, x) \stackrel{!}{=} 0$$

for $\lambda \in \Lambda$, $x \in X$. Let $\mathcal{S} \subset \Lambda \times X$ denote the set of solutions of (1.11) and for any $\lambda \in \Lambda$ define

$$\mathcal{S}_\lambda := \{x \in \mathcal{S} \mid (\lambda, x) \in \mathcal{S}\}.$$

1.3.26 DEFINITION (BIFURCATION POINT)

For any open set $U \subset X$ we define the equivalence relation $\sim_U$ on the set $\{\mathcal{S}_\lambda \mid \lambda \in \Lambda\}$ by setting $\mathcal{S}_\lambda \sim_U \mathcal{S}_\mu : \iff \mathcal{S}_\lambda \cap U$ is homeomorphic to $\mathcal{S}_\mu \cap U$. A point $\lambda_c \in \Lambda$ is called a bifurcation point for $\mathcal{S}$ if, for any neighbourhood $V \subset \Lambda$ of λ_c , there is an $x_c \in \mathcal{S}_{\lambda_c}$ and a neighbourhood $U \subset X$ of x_c such that there are $\lambda_1, \lambda_2 \in V$ with $\mathcal{S}_{\lambda_1} \not\sim_U \mathcal{S}_{\lambda_2}$.

REMARK 1.3.11 Particularly, $\lambda_c \in \Lambda$ is called a bifurcation point if there is an $x_c \in \mathcal{S}_{\lambda_c}$ and a neighbourhood $V_c \times U_c \subset \Lambda \times X$ of (λ_c, x_c) such that for any $\lambda \in V_c \setminus \{\lambda_c\}$ there is more than one solution, that is, $|\mathcal{S}_\lambda| > 1$. We note that Definition 1.3.26 covers more general types of bifurcations.

We state now a version of the implicit function theorem on Banach spaces.

1.3.27 THEOREM (IMPLICIT FUNCTION THEOREM)

Suppose X, Y, Z are Banach spaces, $U \subset X, V \subset Y$ are open sets, $F : U \times V \rightarrow Z$ is continuously (Frechet-)differentiable, $(x_0, y_0) \in U \times V$, $F(x_0, y_0) = 0$ and its Frechet-derivative $D_x F(x_0, y_0)$ with respect to x has a bounded inverse.

Then there is a neighbourhood $U_1 \times V_1 \subset U \times V$ of (x_0, y_0) and a function $f : V_1 \rightarrow U_1$, $f(y_0) = x_0$ such that $F(x, y) = 0$ for $(x, y) \in U_1 \times V_1$ if and only if $x = f(y)$.

If $F \in C^k(U \times V, Z)$, $k \geq 1$ or analytic in a neighbourhood of (x_0, y_0) , then $f \in C^k(V_1, X)$ or f is analytic in a neighbourhood of y_0 .

Proof: [CHOW and HALE 1996, Section 2.2] □

This means that $D_x F(x_0, y_0)$ has no bounded inverse at a bifurcation point.

The Liapunov-Schmidt method reduces the bifurcation problem for a certain class of problems to solving a finite set of equations in a finite number of unknowns. We will omit a description of this method here and only cite [CHOW and HALE 1996] with the following result which is based on the method of Liapunov-Schmidt:

1.3.28 THEOREM (BIFURCATION FROM A SIMPLE EIGENVALUE)

Let X and Z be real Banach-spaces, $\Lambda \subset \mathbb{R}$ open and $M : \Lambda \times X \rightarrow Z$ defined by

$$\begin{aligned} M(\lambda, x) &= Bx - \lambda Ax + N(\lambda, x), \\ N(\lambda, 0) &= 0, \quad D_x N(\lambda, 0) = 0, \end{aligned}$$

with $B, A \in L(X, Z)$ and $N \in C^1(\Lambda \times X, Z)$ with continuous mixed second Frechet-derivative $D_{\lambda x} N$.

If λ_0 is a simple eigenvalue of the pair (B, A) with eigenvector y_0 , then there is a $\delta > 0$ and C^1 -functions

$$(1.12) \quad \begin{aligned} \lambda^*(u) &= \lambda_0 + O(\|u\|), \\ x^*(u) &= u y_0 + O(\|u\|^2) \end{aligned}$$

for $|u| < \delta$, $u \in \mathbb{R}$, such that $M(\lambda^*(u), x^*(u)) = 0$. All zeroes of M near $(\lambda_0, 0)$ are either $(\lambda, 0)$ or given by $(\lambda^*(u), x^*(u))$.

Proof: [CHOW and HALE 1996, remarks at the beginning of Section 5.5 and Theorem 5.3] $\square$

REMARK 1.3.12 If λ_0 is an eigenvalue of the pair (B, A) with eigenvector y_0 , then $(B - \lambda_0 A) y_0 = 0$. As $D_x M(\lambda, x) = B - \lambda_0 A$, Theorem 1.3.28 on the preceding page states that under the given assumptions it is sufficient to look at the eigenvalues of $D_x M(\lambda, x)$ to determine a bifurcation point.

Moreover, the eigenvector y_0 approximates the solution-family branching off at $(\lambda_0, 0)$ in the sense stated more precisely in equation (1.12) above.

1.4 Exact solutions

Up to now two families of exact solutions to the Euler-Lagrange equations (1.3) are known. One was already discovered by A. Beer [BEER 1869] in the 19th century. It is a one-parameter family of drops having the topological type of a sphere. The other one was detected by R. Gulliver [GULLIVER 1984] in 1984 and has the topology of a torus.

Both families consist of surfaces of revolution where the generating curve is given in the following integral form:

$$(1.13) \quad \boxed{\begin{aligned} u(r) &= \int_{r_-}^r \frac{v(\rho)}{\sqrt{1 - v^2(\rho)}} d\rho, \quad r_- \leq r \leq r_+ \\ v(\rho) &:= \omega^2 \rho^3 + a \rho + b/\rho. \end{aligned}}$$

b and c are constants which depend on the angular velocity ω . For drops of the topological type of the sphere one has $r_- = 0$, r_+ is the equatorial radius, $b = 0$ and a is the mean curvature of the drop at the axis of rotation.

For annular drops r_- and r_+ denote the inner and outer radii of the torus.

Both families meet at a point where the inner radius of the annular shapes and the thickness at the axis of rotation of the simply connected drops both approach 0 (Figure 1.4).

Figure 1.4 Limit surfaces of annular and simply connected family

Figure 1.5 ω - L phase diagram for exact annular and simply connected solutions.

The value of ω at the “meeting point” in the chosen normalisation is exactly $\omega^2 = 1/2$ (see equation (1.15) below and Figure 1.5).

Obviously, between the meeting point and the turning point (maximal value of ω) of each of the families there are two solutions for each value of ω .

1.4.1 Solutions of spheroidal type

A derivation of the formulas for the coefficient a in (1.13) on the preceding page can be found in [BEER 1869, pp. 158]. A short summary is also in the appendix of [CHANDRASEKHAR 1965], for example. We will just present the resulting expressions.

To get an explicit expression for a in (1.13) one has to use the parameter k defined as

$$(1.14) \quad k := \frac{8\sigma}{\rho \hat{\omega}^2 r_1^3} = \frac{1}{r_1^3 \bar{\omega}^2} \equiv \frac{1}{r_1^3 \omega^2}$$

instead of the angular velocity ω (normalisation as chosen in Section 1.1). Here r_1 denotes the radius of the drop at its equator.

Figure 1.6 Computation of the spheroidal drop shapes.

Using the elliptic integrals $F(c, \varphi)$ and $E(c, \varphi)$ of first and second kind in Legendre normal form,

$$F(c, \varphi_1) := \int_0^{\varphi_1} \frac{d\varphi}{\sqrt{1 - c^2 \sin^2 \varphi}} \quad \text{and} \quad E(c, \varphi_1) := \int_0^{\varphi_1} \sqrt{1 - c^2 \sin^2 \varphi} d\varphi,$$

one first expresses the ratio u_1/r_1 of half of the drop's thickness at the axis of rotation to the equatorial radius r_1 (see Figure 1.6):

$$\frac{u_1}{r_1} = \frac{u(r_1)}{r_1} = \left(\frac{k}{2m} - \frac{m}{2} \right) F(c, \varphi_1) + m E(c, \varphi_1) - \sqrt{1 - c^2 \sin^2 \varphi_1},$$

with

$$\begin{aligned} m &= \sqrt[4]{2k + k^2} \\ c &= \frac{1}{m} \sqrt{\frac{m^2}{2} + \frac{1+2k}{4}} = \sqrt{\frac{1}{2} + \frac{1+2k}{4m^2}} = \sqrt{\frac{1}{2} + \frac{1+2k}{4\sqrt{2k+k^2}}} \\ \varphi_1 &= 2 \arctan \frac{1}{m} = 2 \arctan \frac{1}{\sqrt[4]{2k+k^2}}. \end{aligned}$$

Then one uses the volume constraint to compute the constants ω^2 , r_1 and a as functions of k :

$$(1.15) \quad \omega^2 = \frac{1}{2} \left(1 - \frac{u_1}{r_1} \frac{k-1}{k} \right), \quad r_1 = \sqrt[3]{\frac{1}{\omega^2 k}}, \quad a = \frac{1}{r_1} \frac{k-1}{k}.$$

The generating curve $u(r)$ of the surface of revolution can then be computed from its integral representation (1.13) with $b = 0$, $r_- = 0$ and $r_+ = r_1$. Clearly, for a drop of thickness 0 at $r = 0$ one has $u_1 = 0$ and therefore $\omega^2 = 1/2$. Figure 1.7 on the next page gives an overview over the possible drop shapes for some values of ω .

Figure 1.7 Meridional sections through some spheroidal shapes at different values of ω . Only the “right” half of the section is shown. The abscisse shows the distance to the axis of rotation. The thickness of the shapes at $r = 0$ is a monotonically increasing function of the parameter k defined in (1.14).

Figure 1.8 Meridional section through some annular shapes at different values of ω^2 . Only the “right” half of the section is shown. The abscisse shows the distance to the axis of rotation. One observes that the equatorial radius of the torus becomes very large for small ω .

1.4.2 Solutions of annular type

Gulliver [GULLIVER 1984] proves the existence of a family of tori as well as the existence of the meeting point with the spheroidal family (Figure 1.5 on page 17). However, the constants a , b , r_- and r_+ are not given in closed form but have to be computed

numerically from the following equations (ω^2 given):

$$(1.16a) \quad 1 \stackrel{!}{=} \omega^2 r_-^3 + a r_- + b \frac{1}{r_-} \stackrel{!}{=} \omega^2 r_+^3 + a r_+ + b \frac{1}{r_+} \quad (\text{smoothness at equator}),$$

$$(1.16b) \quad 0 \stackrel{!}{=} F(a, b) := \int_{r_-}^{r_+} \frac{\omega^2 \rho^3 + a \rho + b \frac{1}{\rho}}{\sqrt{1 - (\omega^2 \rho^3 + a \rho + b \frac{1}{\rho})^2}} d\rho \quad (\text{surface must be closed}),$$

$$(1.16c) \quad \frac{2\pi}{3} \stackrel{!}{=} V(a, b) := \pi \int_{r_-}^{r_+} \rho^2 \frac{\omega^2 \rho^3 + a \rho + b \frac{1}{\rho}}{\sqrt{1 - (\omega^2 \rho^3 + a \rho + b \frac{1}{\rho})^2}} d\rho \quad (\text{volume constraint}).$$

Chapter 2

The path tracking problem

In this chapter we will first derive expressions for the first and second variation of the (normalised) energy E of a drop which rotates rigidly at constant angular velocity ω , held together by surface tension alone:

$$E(\Gamma, C) = |\Gamma| - 4\omega^2 \int_{\Omega} r^2 - C(3|\Omega| - 4\pi).$$

We use the notation of Section 1.1 which means that $\Omega \subset \mathbb{R}^3$ is the interior of the drop, bounded by the surface $\Gamma := \partial\Omega$. The distance from the axis of rotation is denoted by $r = \sqrt{x_1^2 + x_2^2}$, where $\mathbb{R}^3 = \{(x_1, x_2, x_3) \mid x_1, x_2, x_3 \in \mathbb{R}\}$. $C \in \mathbb{R}$ is the Lagrange-parameter for the volume constraint.

“Solutions” are pairs (Γ, C) which are critical points of E , where $\Gamma \subset \mathbb{R}^3$ is a compact closed immersion of dimension 2 and $C \in \mathbb{R}$.

Under the assumption that the prerequisites of Theorem 1.3.28 on page 15 hold we know that the solution set of E is locally – and in the absence of bifurcation points – a one-parameter family, parametrised by the angular velocity ω . Branch-points in the sense of Definition 1.3.26 on page 15 are just points where two or more one-parameter families come together.

Before arriving at a *fully*-discrete scheme for the computation of drop shapes we will first use the second variation of E to construct a Newton iteration for a *semi*-discrete regime where each step of the Newton iteration is established by solving certain partial differential equations exactly. This is described in Section 2.3 below.

The fully-discrete scheme is introduced by means of a finite element method in Section 2.4.

In this setup “path-tracking” means that we start with an exactly known solution (Γ_0, C_0) at an angular velocity ω_0 and use this solution as initial value for the Newton scheme to construct a new solution (Γ_1, C_1) at a different angular velocity ω_1 . This is iterated to compute a discrete subset $\{(\Gamma_i, C_i) \mid i \in \mathbb{N}\}$ of the solution set of E , always using the previous solution (Γ_{i-1}, C_{i-1}) as initial value for the Newton iteration which constructs (Γ_i, C_i) .

To get a more thorough picture of the solution set the path-tracking algorithm checks for bifurcation points between (Γ_{i-1}, C_{i-1}) and (Γ_i, C_i) . If there is a bifurcation point a new instance of the path-tracking algorithm is started to track down the new branches originating from there.

We start by deriving the full and linearised Euler-Lagrange equations for the critical points of E .

2.1 First and second variation of the energy functional

In the following $\Gamma \subset \mathbb{R}^3$ is assumed to be an immersed compact surface of class $C^{k,\alpha}$ with $k \in \mathbb{N}$, $k \geq 3$, $\alpha \in (0, 1)$. We will be more specific on the value of k and α when we are discussing the linearised Euler-Lagrange equation below.

We will give expressions for the first and second variation of

$$\begin{aligned}
 E(\Gamma, C) &= |\Gamma| - 4\omega^2 \int_{\Omega} r^2 dx - C(3|\Omega| - 4\pi) \\
 (2.1) \quad &= \underbrace{\int_{\Gamma} do}_{=:E_{\text{surf}}(\Gamma)} - 4\omega^2 \underbrace{\int_{\Omega} r^2 dx}_{=:E_{\text{rot}}(\Gamma)} - C \underbrace{\left(\int_{\Gamma} \text{id}_{\Gamma} \cdot \nu_{\Gamma} do - 4\pi \right)}_{=:E_{\text{vol}}(\Gamma, C)}.
 \end{aligned}$$

and the corresponding Euler-Lagrange equations. The second variation $\delta^2 E$ will be derived for perpendicular perturbations only. $\delta^2 E$ will be given in scalar terms of the signed length of the perturbations as well as in terms of the perturbations themselves.

The following is of course well known; the variation of the surface energy is treated in great detail in [NITSCHKE 1975], for example.

2.1.1 The first variation of $E(\Gamma, C)$

Let $\varphi \in (C^{k,\alpha}(\Gamma))^3$. For $\varepsilon > 0$ define the variation $\Gamma_{\varphi}(\varepsilon)$ of Γ with respect to φ as

$$\Gamma_{\varphi}(\varepsilon) := \{x + \varepsilon\varphi(x) \mid x \in \Gamma\}.$$

We note that $\Gamma_{\varphi}(\varepsilon)$ is again of class $C^{k,\alpha}$ and defines again an immersed compact surface provided ε is small enough. This follows from the boundedness of the curvature of Γ .

Then, for $K \in \mathbb{R}$ the first variation $\delta E(\Gamma, C)[\varphi, K]$ of E at (Γ, C) in direction of (φ, K) is

$$\delta E(\Gamma, C)[\varphi, K] = \frac{d}{d\varepsilon} E(\Gamma_{\varphi}(\varepsilon), C + \varepsilon K) \Big|_{\varepsilon=0}.$$

First variation δE_{surf} of the surface energy

$$\begin{aligned}
(2.2) \quad \delta E_{\text{surf}}(\Gamma)\varphi &= \frac{d}{d\varepsilon} E_{\text{surf}}(\Gamma_\varphi(\varepsilon)) \Big|_{\varepsilon=0} = \frac{d}{d\varepsilon} \int_{\Gamma_\varphi(\varepsilon)} do_\varepsilon \Big|_{\varepsilon=0} \\
&= \int_{\Gamma} \nabla_{\Gamma} \text{id}_{\Gamma} : \nabla_{\Gamma} \varphi \, do \stackrel{(1.10)}{=} - \int_{\Gamma} \Delta_{\Gamma} \text{id}_{\Gamma} \cdot \varphi \, do.
\end{aligned}$$

First variation δE_{rot} of the rotational energy Obviously, the first variation is just the surface integral over Γ of the centrifugal energy-density $-4\omega^2 r^2$ multiplied by the distance of the perturbed surface $\Gamma_\varphi(\varepsilon)$ from the original surface Γ :

$$(2.3) \quad \delta E_{\text{rot}}(\Gamma_\varphi(\varepsilon))\varphi = \frac{d}{d\varepsilon} E_{\text{rot}}(\Gamma_\varphi(\varepsilon)) \Big|_{\varepsilon=0} = -4\omega^2 \int_{\Gamma} r^2 \varphi \cdot \nu_{\Gamma} \, do.$$

This is clear from the additivity of the Riemann-integral (this is the classical setup, Γ is of class $C^{k,\alpha}$).

First variation δE_{vol} of the volume constraint From the same reasoning as is used in the case of $\delta E_{\text{rot}}(\Gamma_\varphi(\varepsilon))\varphi$ above follows:

$$\begin{aligned}
(2.4) \quad \delta E_{\text{vol}}(\Gamma, C)[\varphi, K] &= \frac{d}{d\varepsilon} E_{\text{vol}}(\Gamma_\varphi(\varepsilon), C + \varepsilon K) \Big|_{\varepsilon=0} \\
&= -C \int_{\Gamma} \varphi \cdot \nu_{\Gamma} \, do - K \left(\int_{\Gamma} \text{id}_{\Gamma} \cdot \nu_{\Gamma} \, do - 4\pi \right).
\end{aligned}$$

Summarising the above formulas (2.2)-(2.4) we get the following expression for the first variation $\delta E(\Gamma, C)[\varphi, K]$ of the energy $E(\Gamma, C)$ in direction of (φ, K) :

$$\begin{aligned}
(2.5) \quad \delta E(\Gamma, C)[\varphi, K] &= \frac{d}{d\varepsilon} E(\Gamma_\varphi(\varepsilon), C + \varepsilon K) \Big|_{\varepsilon=0} \\
&= - \int_{\Gamma} \Delta_{\Gamma} \text{id}_{\Gamma} \cdot \varphi \, do - 4\omega^2 \int_{\Gamma} r^2 \varphi \cdot \nu_{\Gamma} \, do - C \int_{\Gamma} \varphi \cdot \nu_{\Gamma} \, do \\
&\quad - K \left(\int_{\Gamma} \text{id}_{\Gamma} \cdot \nu_{\Gamma} \, do - 4\pi \right).
\end{aligned}$$

By definition it holds for a stationary point $\delta E(\Gamma, C)[\varphi, K] = 0$ for all $(\varphi, K) \in C^{\alpha,k}(\Gamma) \times \mathbb{R}$. So it follows from the fundamental Lemma of the calculus of variations that a stationary point of E satisfies the Euler-Lagrange equations:

$$(2.6) \quad \boxed{-\Delta_{\Gamma} \text{id}_{\Gamma} = (4\omega^2 r^2 + C)\nu_{\Gamma}, \quad \int_{\Gamma} \text{id}_{\Gamma} \cdot \nu_{\Gamma} \, do = 4\pi.}$$

This is exactly equation (1.3) on page 3 from the introductory section Section 1.1.

REMARK 2.1.1 (2.6) is a partial differential equation defined on a surface which is itself the major unknown in (2.6). This seems to be a “chicken and egg” problem. But, this, however is not so. (2.6) has to be understood in terms of either local charts, or by interpreting id_{Γ} as a function on another, explicitly known manifold close (in some sense) to a solution Γ of (2.6).

In either case the above Euler-Lagrange equations are a system of coupled, highly non-linear partial differential equations.

2.1.2 The second variation of $E(\Gamma, C)$

The expressions for the second variation $\delta^2 E$ of E are far more complicated than equation (2.4). Particularly, it makes a major difference whether one allows arbitrary perturbations or only perturbations perpendicular to the surface Γ , and the interconnection between different kinds of perturbations is quite involved.

In the following we only consider orthogonal perturbations $\varphi \in (C^{k-1,\alpha}(\Gamma))^3$, where “orthogonal” means $\langle \varphi, \nu \rangle \varphi = \varphi$. For any $\varphi \in (C^{k-1,\alpha}(\Gamma))^3$ we define $\bar{\varphi} := \langle \varphi, \nu \rangle$.

First we state some well-known identities which are needed in the derivation of the second variation.

2.1.1 LEMMA (CALCULUS ON SURFACES)

Let $\Gamma \subset \mathbb{R}^3$ be an immersed surface of class $C^{k,\alpha}$ and $\psi \in (C^{k-1,\alpha}(\Gamma))^3$ an orthogonal variation with $k \geq 3$, $\alpha \in (0, 1)$. Then the following holds:

Variation of the unit normal field

$$(2.7) \quad \frac{d}{d\varepsilon} (\nu_{\Gamma_\psi(\varepsilon)}) \big|_{\varepsilon=0} = -(\nabla_\Gamma \psi)^{tr} \nu_\Gamma.$$

Variation of the curvature vector

$$(2.8) \quad -\frac{d}{d\varepsilon} (Y_{\Gamma_\psi(\varepsilon)}) \big|_{\varepsilon=0} = \frac{d}{d\varepsilon} (\Delta_{\Gamma_\psi(\varepsilon)} \text{id}_{\Gamma_\psi(\varepsilon)}) \big|_{\varepsilon=0} \\ = \nu_\Gamma \nu_\Gamma \cdot \Delta_\Gamma \psi + 2 \nu_\Gamma \nabla_\Gamma \psi : \nabla_\Gamma \nu_\Gamma + (\nabla_\Gamma \psi)^{tr} \cdot Y_\Gamma.$$

Divergence of an orthogonal perturbation

$$(2.9) \quad \nabla_\Gamma \cdot \psi = \psi \cdot Y_\Gamma.$$

Square of the Weingarten map

$$(2.10) \quad \nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma = \kappa_1^2 + \kappa_2^2 = -\nu_\Gamma \cdot \Delta_\Gamma \nu_\Gamma,$$

where κ_1 and κ_2 denote the principal curvatures of Γ .

Laplace-Beltrami operator of an orthogonal perturbation

$$(2.11) \quad \nu_\Gamma \cdot \Delta_\Gamma \psi = \Delta_\Gamma \bar{\psi} + \bar{\psi} (\nu_\Gamma \cdot \Delta_\Gamma \nu_\Gamma) \stackrel{(2.10)}{=} \Delta_\Gamma \bar{\psi} - \bar{\psi} (\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma).$$

Proof: We omit the proof of the equations (2.7) and (2.8). The derivation is elementary but in parts lengthy. The variation of the surface area and unit normal field have been dealt with elsewhere quite intensively, see for example [NITSCHKE 1975].

Equation (2.9) is clear because ψ has no tangential components:

$$\begin{aligned} \nabla_\Gamma \cdot \psi &= \nabla_\Gamma \cdot (\langle \psi, \nu_\Gamma \rangle \nu_\Gamma) \\ &= \langle \psi, \nu_\Gamma \rangle \nabla_\Gamma \cdot \nu_\Gamma + \underbrace{\langle (\nabla_\Gamma \psi) \cdot \nu_\Gamma, \nu_\Gamma \rangle}_{=0} + \underbrace{\langle (\nabla_\Gamma \nu_\Gamma) \cdot \psi, \nu_\Gamma \rangle}_{=0} \\ &= \langle \psi, \nu_\Gamma \rangle 2 H_\Gamma = \langle \psi, Y_\Gamma \rangle. \end{aligned}$$

Equation (2.10) is a simple application of the product rule:

$$0 = \nu_\Gamma \cdot \nabla_\Gamma \nu_\Gamma = \nabla_\Gamma \cdot (\nu_\Gamma \cdot \nabla_\Gamma \nu_\Gamma) = \nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma + \nu_\Gamma \Delta_\Gamma \nu_\Gamma.$$

It is clear that $\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma = \kappa_1^2 + \kappa_2^2$ because $\nabla_\Gamma \nu_\Gamma$ can be diagonalised in each point of Γ .

Equation (2.11) follows from the chain-rule and by exploiting orthogonality relations:

$$\begin{aligned} \nu_\Gamma \cdot \Delta_\Gamma \psi &= \nu_\Gamma \cdot (\Delta_\Gamma (\bar{\psi} \nu_\Gamma)) = \nu_\Gamma \cdot (\nu_\Gamma \Delta_\Gamma \bar{\psi} + \bar{\psi} \Delta_\Gamma \nu_\Gamma + 2 \nabla_\Gamma \nu_\Gamma \cdot \nabla_\Gamma \bar{\psi}) \\ &= \Delta_\Gamma \bar{\psi} + \bar{\psi} \nu_\Gamma \cdot \Delta_\Gamma \nu_\Gamma + 2 \underbrace{\nu_\Gamma \cdot \nabla_\Gamma \nu_\Gamma}_{=0} \cdot \nabla_\Gamma \bar{\psi} \stackrel{(2.10)}{=} \Delta_\Gamma \bar{\psi} - \bar{\psi} (\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma). \end{aligned}$$

□

We will now employ Lemma 2.1.1 on the facing page to derive an expression for the second variation of the drop energy. For $\varphi, \psi \in (C^{k,\alpha}(\Gamma))^3$ and $K, J \in \mathbb{R}$ the second variation $\delta^2 E(\Gamma, C)$ of E at (Γ, C) in direction of (φ, K) and (ψ, J) is

$$\delta^2 E(\Gamma, C)[\varphi, K][\psi, J] = \delta(\delta E(\Gamma, C)[\varphi, K])[\psi, J] = \frac{d}{d\varepsilon} (\delta E(\Gamma_\psi(\varepsilon), C + \varepsilon J)[\varphi, K]) \Big|_{\varepsilon=0}.$$

Second variation $\delta^2 E_{\text{surf}}$ of the surface energy: As a consequence of (2.8) on the preceding page we have:

$$\begin{aligned} \delta^2 E_{\text{surf}}(\Gamma)[\varphi][\psi] &= \frac{d}{d\varepsilon} \left(- \int_{\Gamma_\psi(\varepsilon)} \Delta_{\Gamma_\psi(\varepsilon)} \text{id}_{\Gamma_\psi(\varepsilon)} \cdot \varphi \, do \right) \Big|_{\varepsilon=0} \\ &= - \int_\Gamma \frac{d}{d\varepsilon} (\Delta_{\Gamma_\psi(\varepsilon)} \text{id}_{\Gamma_\psi(\varepsilon)}) \Big|_{\varepsilon=0} \cdot \varphi \, do - \int_\Gamma \Delta_\Gamma \text{id}_\Gamma \cdot \varphi \nabla_\Gamma \cdot \psi \, do \\ &\stackrel{(2.8)}{=} - \int_\Gamma (\nu_\Gamma \nu_\Gamma \cdot \Delta_\Gamma \psi + 2 \nu_\Gamma \nabla_\Gamma \psi : \nabla_\Gamma \nu_\Gamma + (\nabla_\Gamma \psi)^{\text{tr}} \cdot Y_\Gamma) \cdot \varphi \, do \\ &\quad - \int_\Gamma \Delta_\Gamma \text{id}_\Gamma \cdot \varphi \psi \cdot Y_\Gamma \, do \\ (2.12) \quad &= - \int_\Gamma \varphi \cdot \Delta_\Gamma \psi + 2 \varphi \cdot \nu_\Gamma \nabla_\Gamma \psi : \nabla_\Gamma \nu_\Gamma + \underbrace{\varphi_i \delta_i \psi_j (Y_\Gamma)_j}_{=0} \, do \\ &\quad - \int_\Gamma \Delta_\Gamma \text{id}_\Gamma \cdot \varphi \psi \cdot Y_\Gamma \, do \\ &= - \int_\Gamma \psi \cdot \Delta_\Gamma \varphi \, do - 2 \underbrace{\int_\Gamma \varphi \cdot \nu_\Gamma \nabla_\Gamma \psi : \nabla_\Gamma \nu_\Gamma \, do}_{=: I_1} \\ &\quad - \int_\Gamma \psi \cdot Y_\Gamma \Delta_\Gamma \text{id}_\Gamma \cdot \varphi \, do. \end{aligned}$$

I_1 can be transformed using integration by parts:

$$\begin{aligned} I_1 &= \int_\Gamma \varphi \cdot \nu_\Gamma \nabla_\Gamma \psi : \nabla_\Gamma \nu_\Gamma \, do \\ (2.13) \quad &= - \int_\Gamma \underbrace{\psi \cdot \nabla_\Gamma \nu_\Gamma}_{=0} \nabla_\Gamma (\varphi \cdot \nu_\Gamma) \, do - \int_\Gamma \varphi \cdot \nu_\Gamma \psi \cdot \Delta_\Gamma \nu_\Gamma \, do. \end{aligned}$$

Substituting (2.13) in (2.12) and using equation (2.10) from Lemma 2.1.1 on page 24 we arrive at the following expression of the second variation of the surface energy:

$$(2.14) \quad \begin{aligned} \delta^2 E_{\text{surf}}(\Gamma)[\varphi][\psi] = & - \int_{\Gamma} \psi \cdot \Delta_{\Gamma} \varphi \, do - 2 \int_{\Gamma} \psi \cdot \nu_{\Gamma} \varphi \cdot \nu_{\Gamma} (\nabla_{\Gamma} \nu_{\Gamma} : \nabla_{\Gamma} \nu_{\Gamma}) \, do \\ & + \int_{\Gamma} \psi \cdot Y_{\Gamma} Y_{\Gamma} \cdot \varphi \, do. \end{aligned}$$

It follows from (2.11) on page 24 that (2.14) depends only on the scalar functions $\bar{\varphi} = \varphi \cdot \nu_{\Gamma}$ and $\bar{\psi} = \psi \cdot \nu_{\Gamma}$:

$$(2.15) \quad \begin{aligned} \delta^2 E_{\text{surf}}(\Gamma)[\varphi][\psi] = & - \int_{\Gamma} \bar{\psi} \nu_{\Gamma} \cdot \Delta_{\Gamma} (\bar{\varphi} \nu_{\Gamma}) \, do - 2 \int_{\Gamma} \bar{\psi} \bar{\varphi} (\nabla_{\Gamma} \nu_{\Gamma} : \nabla_{\Gamma} \nu_{\Gamma}) \, do \\ & - \int_{\Gamma} \bar{\psi} 2 H_{\Gamma} \bar{\varphi} 2 H_{\Gamma} \, do \\ = & - \int_{\Gamma} \bar{\psi} \Delta_{\Gamma} \bar{\varphi} \, do - \int_{\Gamma} \bar{\psi} \bar{\varphi} (\nabla_{\Gamma} \nu_{\Gamma} : \nabla_{\Gamma} \nu_{\Gamma}) \, do \\ & - \int_{\Gamma} 2 H_{\Gamma} (\bar{\psi} \bar{\varphi} 2 H_{\Gamma}) \, do. \end{aligned}$$

□

Second variation $\delta^2 E_{\text{rot}}$ of the rotational energy:

$$(2.16) \quad \begin{aligned} \delta^2 E_{\text{rot}}(\Gamma)[\varphi][\psi] &= \frac{d}{d\varepsilon} \delta E_{\text{rot}}(\Gamma_{\psi(\varepsilon)})(\varphi) \Big|_{\varepsilon=0} \\ &= -4 \omega^2 \frac{d}{d\varepsilon} \left(\int_{\Gamma_{\psi(\varepsilon)}} r_{\varepsilon}^2 \nu_{\Gamma_{\psi(\varepsilon)}} \cdot \varphi \, do \right) \Big|_{\varepsilon=0} \\ &= -4 \omega^2 \left(\int_{\Gamma} \varphi \cdot \frac{d}{d\varepsilon} (r_{\varepsilon}^2 \nu_{\Gamma_{\psi(\varepsilon)}}) \Big|_{\varepsilon=0} \, do + \int_{\Gamma} r^2 \nu_{\Gamma} \cdot \varphi \nabla_{\Gamma} \cdot \psi \, do \right), \end{aligned}$$

with

$$r_{\varepsilon}^2 := (x_1 + \varepsilon \psi_1)^2 + (x_2 + \varepsilon \psi_2)^2 = r^2 + 2\varepsilon (x_1 \psi_1 + x_2 \psi_2) + o(\varepsilon^2).$$

and $\text{id}_{\Gamma} = (x_1, x_2, x_3)$, $\psi = (\psi_1, \psi_2, \psi_3)$.

Inserting the above relation and (2.7) (variation of the normal field) from Lemma 2.1.1 on page 24 into (2.16) above we get

$$\begin{aligned} \delta^2 E_{\text{rot}}(\Gamma)[\varphi][\psi] = & -4 \omega^2 \left(\int_{\Gamma} 2 \varphi \cdot \nu_{\Gamma} (x_1 \psi_1 + x_2 \psi_2) \, do - \int_{\Gamma} r^2 \underbrace{\varphi \cdot (\nabla_{\Gamma} \psi)^{\text{tr}} \cdot \nu_{\Gamma}}_{=0} \, do \right) \\ & - 4 \omega^2 \int_{\Gamma} r^2 \nu_{\Gamma} \cdot \varphi \nabla_{\Gamma} \cdot \psi \, do. \end{aligned}$$

Using $\psi = (\psi \cdot \nu_\Gamma) \nu_\Gamma$ we finally arrive at the following expressions:

$$(2.17) \quad \begin{aligned} \delta^2 E_{\text{rot}}(\Gamma)[\varphi][\psi] &= -8\omega^2 \int_{\Gamma} \varphi \cdot \nu_\Gamma \psi \cdot \nu_\Gamma (x_1 \nu_1 + x_2 \nu_2) do \\ &\quad - 4\omega^2 \int_{\Gamma} \psi \cdot Y_\Gamma r^2 \nu_\Gamma \cdot \varphi do \end{aligned}$$

$$(2.18) \quad \Longleftrightarrow \quad \delta^2 E_{\text{rot}}(\Gamma)[\varphi][\psi] = -8\omega^2 \int_{\Gamma} \bar{\varphi} \bar{\psi} (x_1 \nu_1 + x_2 \nu_2) do - 4\omega^2 \int_{\Gamma} 2 H_\Gamma \bar{\psi} \bar{\varphi} r^2 do.$$

□

Second variation $\delta^2 E_{\text{vol}}$ of the volume constraint:

$$\begin{aligned} \delta^2 E_{\text{vol}}(\Gamma, C)[\varphi, K][\psi, J] &= \frac{d}{d\varepsilon} (\delta E_{\text{vol}}(\Gamma_{\psi(\varepsilon)}, C + \varepsilon J)[\varphi, K]) \Big|_{\varepsilon=0} \\ &= -\frac{d}{d\varepsilon} \left((C + \varepsilon J) \int_{\Gamma_{\psi(\varepsilon)}} \varphi \cdot \nu_{\Gamma_{\psi(\varepsilon)}} do + K \left(\int_{\Gamma_{\psi(\varepsilon)}} \text{id}_{\Gamma_{\psi(\varepsilon)}} \cdot \nu_{\Gamma_{\psi(\varepsilon)}} do - 4\pi \right) \right) \Big|_{\varepsilon=0}. \end{aligned}$$

Taking into account that the variation of the normal field is tangential to Γ whereas ψ and φ are orthogonal variations the expressions for the second variation of the volume constraint are

$$(2.19) \quad \delta^2 E_{\text{vol}}(\Gamma, C)[\varphi, K][\psi, J] = -J \int_{\Gamma} \varphi \cdot \nu_\Gamma do - K \int_{\Gamma} \psi \cdot \nu_\Gamma do - C \int_{\Gamma} Y_\Gamma \cdot \psi \nu_\Gamma \cdot \varphi do$$

$$(2.20) \quad \Longleftrightarrow \quad \delta^2 E_{\text{vol}}(\Gamma, C)[\varphi, K][\psi, J] = -J \int_{\Gamma} \bar{\varphi} do - K \int_{\Gamma} \bar{\psi} do - C \int_{\Gamma} 2 H_\Gamma \bar{\psi} \bar{\varphi} do.$$

□

By summing up the different expressions for the second variation of E_{surf} , E_{rot} and E_{vol} given in the equations (2.14), (2.17) and (2.19) (respectively (2.15), (2.18) and (2.20) for the scalar case) we finally arrive at an expression for the second variation $\delta^2 E(\Gamma, C)[\varphi, K][\psi, J]$ of $E(\Gamma, C)$ at (φ, K) and (ψ, J) :

$$(2.21) \quad \begin{aligned} \delta^2 E[\varphi, K][\psi, J] &= - \int_{\Gamma} \psi \cdot \Delta_\Gamma \varphi do - 2 \int_{\Gamma} \psi \cdot \nu_\Gamma \varphi \cdot \nu_\Gamma (\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma) do \\ &\quad - 8\omega^2 \int_{\Gamma} \varphi \cdot \nu_\Gamma \psi \cdot \nu_\Gamma (x_1 \nu_1 + x_2 \nu_2) do \\ &\quad - J \int_{\Gamma} \varphi \cdot \nu_\Gamma do - K \int_{\Gamma} \psi \cdot \nu_\Gamma do \\ &\quad + \int_{\Gamma} Y_\Gamma \cdot \psi \varphi \cdot \underbrace{(Y_\Gamma - (4\omega^2 r^2 + C) \nu_\Gamma)}_{\equiv 0 \text{ if } (\Gamma, C) \text{ is a solution of (2.6)}} do. \end{aligned}$$

Using $\bar{\varphi} = \varphi \cdot \nu_\Gamma$ and $\bar{\psi} = \psi \cdot \nu_\Gamma$ this can be written in scalar terms:

$$\begin{aligned}
 \delta^2 E[\varphi, K][\psi, J] = & - \int_\Gamma \bar{\psi} \Delta_\Gamma \bar{\varphi} \, do - \int_\Gamma \bar{\psi} \bar{\varphi} (\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma) \, do \\
 & - 8\omega^2 \int_\Gamma \bar{\varphi} \bar{\psi} (x_1 \nu_1 + x_2 \nu_2) \, do \\
 & - J \int_\Gamma \bar{\varphi} \, do - K \int_\Gamma \bar{\psi} \, do \\
 & + \int_\Gamma 2 H_\Gamma \bar{\psi} \bar{\varphi} \underbrace{(2 H_\Gamma - 4\omega^2 r^2 - C)}_{\equiv 0 \text{ if } (\Gamma, C) \text{ is a solution of (2.6)}} \, do.
 \end{aligned}
 \tag{2.22}$$

We remark that the residual $R_{(\Gamma, C, \omega)} := 2 H_\Gamma - (4\omega^2 r^2 + C)$ vanishes if the second variation is evaluated at a solution (Γ, C) of the non-linear Euler-Lagrange equation (2.6). So the last integral in (2.21) and (2.22) is zero in this case.

The linearisations of the non-linear Euler-Lagrange equation (2.6) are the Euler-Lagrange equations implied by the expressions (2.21) and (2.22) for the second variation $\delta^2 E$, evaluated at a solution (Γ, C) . The non-linear Euler-Lagrange equation (2.6) is repeated here for clarity.

$$(2.6) \quad -\Delta_\Gamma \text{id}_\Gamma = (4\omega^2 r^2 + C)\nu_\Gamma, \quad \int_\Gamma \text{id}_\Gamma \cdot \nu_\Gamma \, do = 4\pi.$$

$$(2.23) \quad \begin{cases} -\Delta_\Gamma \varphi - 2\nu_\Gamma (\kappa_1^2 + \kappa_2^2) \nu_\Gamma \cdot \varphi - 8\omega^2 \nu_\Gamma (x_1 \nu_1 + x_2 \nu_2) \nu_\Gamma \cdot \varphi - K \nu_\Gamma = 0, \\ \int_\Gamma \varphi \cdot \nu_\Gamma \, do = 0. \end{cases}$$

$$(2.24) \quad -\Delta_\Gamma \bar{\varphi} - \nu_\Gamma (\kappa_1^2 + \kappa_2^2) \bar{\varphi} - 8\omega^2 (x_1 \nu_1 + x_2 \nu_2) \bar{\varphi} - K = 0, \quad \int_\Gamma \bar{\varphi} \, do = 0.$$

We note that (2.23) is a coupled system of partial differential equations for the components of the orthogonal perturbation φ while (2.24) is a single partial differential equation for the signed length $\bar{\varphi}$ of φ .

2.2 The linear Euler-Lagrange equations

As a preparation for the continuous (in the sense of non-discrete) Newton method described in Section 2.3 below we continue by examining the linear Euler-Lagrange equations (2.23) and (2.24) for the non-homogeneous case. For brevity we define

$$\begin{aligned}
 a_\Gamma &:= 8\omega^2 (x_1 \nu_1 + x_2 \nu_2) + 2(\kappa_1^2 + \kappa_2^2) \\
 \bar{a}_\Gamma &:= 8\omega^2 (x_1 \nu_1 + x_2 \nu_2) + (\kappa_1^2 + \kappa_2^2).
 \end{aligned}
 \tag{2.25}$$

Note that $\bar{a}_\Gamma$ is *not* equal to a_Γ and – violating the conventions introduced above – a_Γ and $\bar{a}_\Gamma$ are *both* scalar quantities.

Γ is still assumed to be of class $C^{k,\alpha}$, $k \geq 3$, so a_Γ and $\bar{a}_\Gamma$ are of class $C^{k-2,\alpha}$. We are interested in solutions (φ, K) with $\varphi \in C^{k,\alpha}(\Gamma)$, $K \in \mathbb{R}$.

$$(2.26) \quad -\Delta_{\Gamma} \varphi - a_{\Gamma} \nu_{\Gamma} \cdot \varphi \nu_{\Gamma} - K \nu_{\Gamma} = f, \quad \int_{\Gamma} \varphi \cdot \nu_{\Gamma} do = b.$$

$$(2.27) \quad -\Delta_{\Gamma} \bar{\varphi} - \bar{a}_{\Gamma} \bar{\varphi} - K = \bar{f}, \quad \int_{\Gamma} \bar{\varphi} do = b.$$

For the right hand side (f, b) we assume that $f \in C^{k-2, \alpha}(\Gamma)$ and $b \in \mathbb{R}$ is just a real number. When used in the continuous Newton method below (f, b) will be the residual of the non-linear Euler-Lagrange equations (2.6). So later we will have $f = R_{(\Gamma, C, \omega)} \nu_{\Gamma}$, $b = \int_{\Gamma} \text{id}_{\Gamma} \cdot \nu_{\Gamma} do - 4\pi$.

REMARK 2.2.1 (2.26) and (2.27) have the structure of a Neumann-problem. The *Fredholm alternative* – which is not quoted in this work – defines compatibility conditions for the right-hand side in order that (2.26) and (2.27) have a solution, see for example [EVANS 1998, Appendix D.5].

Specifically, it is necessary for the scalar equation (2.27) that $\bar{f} + K \in N((-\Delta_{\Gamma} - \bar{a}_{\Gamma})^*)^{\perp}$, where $N(\cdot)$ denotes the kernel of a linear operator and $V^{\perp}$ the orthogonal complement of a Hilbert (sub-)space. A^* is the adjoint of a bounded linear operator A on a Hilbert space.

This determines the value of K . However, the Fredholm alternative does not provide an explicit expression for K in this general setup.

The problems (2.26) and (2.27) are ill-posed in the sense that we do not have uniqueness of a solution. Therefore we continue by examining the Lie-symmetries of the non-linear Euler-Lagrange equation (2.6) and their consequences for its linearisation.

2.2.1 Lie-symmetries

When omitting the volume constraint the non-linear Euler-Lagrange equation (2.6) is invariant with respect to the one-parameter groups of scalings, rotations about the axis of rotation and translations in direction of the axis of rotation. The three symmetries span a 3-dimensional Lie-group which maps any solution of (2.6) to another solution of (2.6).

Thus any solution of (2.6) which is not invariant with respect to this Lie-group generates a differential manifold of solutions. As a consequence, the homogeneous linearised equations have non-trivial solutions in this case.

Scalings: The invariance with respect to scalings is broken by imposing the volume constraint, so we need not discuss it further. We refer here to the remark on page 4 at the end of Section 1.1.

Translations in x_3 -direction: The invariance with respect to translations in direction of the axis of rotation could be dealt with in a like-wise manner: we just could impose the constraint that the centre of mass remains at the origin and deduce from this a linearised centre-of-mass constraint in the same way we deduced the linearised volume constraint. It is – maybe – remarkable that the homogeneous linearisation just ends up in $\int_{\Gamma} \bar{\varphi} x_3 d\sigma = 0$.

We will omit the proof because we do not need this result. Instead, we use the following theorem to break the translational invariance in x_3 -direction:

2.2.1 THEOREM (EQUATORIAL REFLECTIVE SYMMETRY, [WENTE 1982])

A solution Γ of class C^2 of (2.6) owns a reflective symmetry with respect to the (x_1, x_2) -plane, where the x_3 -axis is the axis of rotation.

Proof: The reference to Wente’s publication which contains the proof is in the heading of the theorem above. We just like to remark that in his work Wente also takes self-gravitation into account, proving the result stated in the theorem in a far more general regime. $\square$

Wente’s theorem means that we can eliminate the translational invariance in the x_3 -direction by cutting the drop at its equatorial plane and imposing Dirichlet boundary conditions on the x_3 -component of the solutions of (2.6) and Neumann boundary conditions on the x_1 and x_2 components. We remark that by Theorem 2.2.1 the attribute “equatorial” is well-defined.

REMARK 2.2.2 *Cutting the drop at its equatorial plane is just a matter of a clever treatment of (2.6) and its linearisations (2.26) and (2.27). It has no effect on existence and regularity of solutions for the equations above (although – by construction – it has a **serious** effect on the uniqueness).*

In the discussion of the regularity of the solutions of the linearisations of (2.6) we will not dissect the drop at its equatorial plane but instead use reflectively symmetric Ansatz-functions, see Definition 2.2.2 on page 32.

In the treatment of the discretisation of the Newton scheme the boundary conditions will be used explicitly, because the Theorem 2.2.1 saves half of the computation time. We will, nevertheless, not consistently use definitions like Γ^+ for the “upper” half of the drop-surface and so on. We will rather comment on the regime in use at the start of each section for the remainder of our analysis.

Axial symmetry about the x_3 -axis The invariance of the non-linear Euler-Lagrange equations (2.6) under the action of a one-parameter Lie-group G implies that the image of a solution (Γ, C) under the infinitesimal generator $\mathcal{G}$ of G is a solution of the linearised equations. $\mathcal{G} \cdot (\Gamma, C)$ will be a non-trivial solution if (Γ, C) is *not* invariant under the action of G .

While this is clear we want to establish the fact explicitly for the case of the one-parameter group R of rotations around the x_3 -axis, the axis of rotation. As subgroup of

$GL(3, \mathbb{R})$ we have the following presentation for R and its infinitesimal generator $\mathcal{R}$:

$$(2.28) \quad G = \left\{ g(\varepsilon) := \begin{pmatrix} \cos \varepsilon & -\sin \varepsilon & 0 \\ \sin \varepsilon & \cos \varepsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} \mid \varepsilon \in \mathbb{R} \right\}, \quad \mathcal{R} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The canonical action of the Group G on a solution (Γ, C) of the non-linear Euler-Lagrange equation generates a differentiable family of solutions $G \cdot (\Gamma, C) := \{(g(\varepsilon) \cdot \Gamma, C) \mid \varepsilon \in \mathbb{R}\}$. We can expand the mapping $\varepsilon \mapsto g(\varepsilon) \cdot \Gamma$ into a Taylor-series around $\varepsilon = 0$ because G is a Lie-group. Up to first order in ε we thus arrive at $g(\varepsilon) \cdot \Gamma = \Gamma + \varepsilon \mathcal{R} \cdot \Gamma + o(\varepsilon^2)$.

This induces an orthogonal perturbation $\Theta := \langle \mathcal{R} \cdot \text{id}_\Gamma, \nu_\Gamma \rangle \nu_\Gamma \in C^{k-1, \alpha}(\Gamma)$ which is – by construction – a solution of the linearised Euler-Lagrange equation (2.23). We have at a point $X = (x_1, x_2, x_3) \in \Gamma$ that

$$\Theta(X) = (\mathcal{R} \cdot X) \nu_\Gamma = (-x_2 \nu_1 + x_1 \nu_2) \nu_\Gamma.$$

So clearly $\Theta \equiv 0$ if and only if Γ is invariant under the action of G . We note that the same holds for $\bar{\Theta}(X) = (-x_2 \nu_1 + x_1 \nu_2)$ with respect to the scalar version (2.24) of the linearisation.

This means that in the presence of symmetry breaking – if Γ is not axially symmetric – we can eliminate the singularity of the second variation $\delta^2 E(\Gamma, C)$ by allowing only perturbations which are transversal to Θ respectively to $\bar{\Theta}$ in the scalar case.

The notion of “transversal” will be made explicit in the next section when we define weak solutions for the linearised Euler-Lagrange equations (2.23) and (2.24).

We remark at this point that earlier numerical methods for the computation of equilibrium shapes of rotating drops employed by others – the work of [BROWN and SCRIVEN 1980a] being the one of greatest importance – were imposing an artificial reflective symmetry about a meridional plane of the drop surface. The boundary conditions implied by dissecting the drop at this plane also eliminate the singularity of the second variation $\delta^2 E(\Gamma, C)$. We do not use this technique because we do not want to impose artificial symmetry constraints.

Figure 2.1 The action of an infinitesimal rotation

Figure 2.2 Rotations violate the Neumann boundary conditions implied by an artificial dissection at a meridional plane

2.2.2 Weak solutions of the linearisation

We are going to define the notion of a weak solution for both the vector-valued and the scalar-valued non-homogeneous linearised Euler-Lagrange equations defined in (2.26) and (2.27) on page 29. The most important step is choosing an appropriate function space which will contain the weak solutions.

In the following we lower the differentiability-class for the surface Γ to $C^{k,\alpha}$ with $k \geq 2$ (we previously required $k \geq 3$). More specifically in the following we assume that $\Gamma \subset \mathbb{R}^3$ is an isometrically immersed compact surface of class $C^{k,\alpha}$ with $k \geq 2$ and $0 < \alpha < 1$. And we assume that Γ possesses a reflective symmetry about the (x_1, x_2) -plane.

Therefore we can decompose Γ as follows:

$$\Gamma^+ := \Gamma \cap (\mathbb{R}^2 \times \mathbb{R}^+), \quad \Gamma^- := \Gamma \cap (\mathbb{R}^2 \times \mathbb{R}^-), \quad \Sigma := \partial\Gamma^+ \equiv \partial\Gamma^-.$$

Let $\mathcal{I} : \mathbb{R}^3 \rightarrow \mathbb{R}^3 : (x_1, x_2, x_3) \mapsto (x_1, x_2, -x_3)$ denote the reflection about the (x_1, x_2) -plane. We obviously have

$$\Gamma = \Gamma^+ \cup \Sigma \cup \Gamma^- \quad \text{and} \quad \Gamma^- = \mathcal{I} \cdot \Gamma^+.$$

In preparation for the definition of weak solutions we introduce the following notations:

2.2.2 DEFINITION (FUNCTION SPACES FOR THE WEAK SOLUTIONS)

Under the assumption listed above we define the following function spaces on Γ :

reflectively symmetric scalar functions

$$W_{\pm}(\Gamma) := \{v \in H^1(\Gamma) \mid v(X) = v(\mathcal{I} \cdot X) \quad \forall X \in \Gamma\}.$$

reflectively symmetric vector-valued functions

$$W_{\pm}(\Gamma) := \{(v_1, v_2, v_3) \in (H^1(\Gamma))^3 \mid v_3(X) = -v_3(\mathcal{I} \cdot X) \quad \forall X \in \Gamma\}.$$

axially *asymmetric* scalar functions

$$W_{\odot}(\Gamma) := \{v \in H^1(\Gamma) \mid \int_{\Gamma} \bar{\Theta} v \, d\sigma = 0\},$$

where $\bar{\Theta}$ is the action of the infinitesimal generator of the group of rotations about the x_3 -axis, as defined in the previous section, that is $\bar{\Theta} = -x_2 \nu_1 + x_1 \nu_2$ for $X = (x_1, x_2, x_3) \in \Gamma$.

axially *asymmetric* vector-valued functions

$$W_{\odot}(\Gamma) := \{v \in (H^1(\Gamma))^3 \mid \int_{\Gamma} \Theta \cdot v \, d\sigma = 0\},$$

where Θ is the action of the infinitesimal generator of the group of rotations about the x_3 -axis, as defined in the previous section, that is $\Theta = (-x_2 \nu_1 + x_1 \nu_2) \nu_{\Gamma}$ for $X = (x_1, x_2, x_3) \in \Gamma$.

scalar mean-value constraint

$$\mathbb{W}(\Gamma) := \{v \in H^1(\Gamma) \mid \int_{\Gamma} v \, do = 0\}.$$

We note that any function $\tilde{v}$ in the affine linear space $\mathbb{W}^b(\Gamma) := \mathbb{W}(\Gamma) + \frac{b}{|\Gamma|}$ satisfies the non-homogeneous volume constraint $\int_{\Gamma} \tilde{v} \, do = b$, $b \in \mathbb{R}$.

vector-valued mean-value constraint

$$\mathbb{W}(\Gamma) := \{v \in (H^1(\Gamma))^3 \mid \int_{\Gamma} v \cdot \nu_{\Gamma} \, do = 0\}.$$

We note that any function $\tilde{v}$ in the affine linear space $\mathbb{W}^b(\Gamma) := \mathbb{W}(\Gamma) + \frac{b}{|\Gamma|} \nu_{\Gamma}$ satisfies the non-homogeneous volume constraint $\int_{\Gamma} \tilde{v} \, do = b$, $b \in \mathbb{R}$.

orthogonal weak vector-fields

$$W^{\perp}(\Gamma) := \{v \in (H^1(\Gamma))^3 \mid \langle v, \nu_{\Gamma} \rangle \nu_{\Gamma} = v\}.$$

We note that $W^{\perp}(\Gamma)$ is well defined because Γ is of class $C^{k,\alpha}$ and so $\nu_{\Gamma} \in C^{k-1,\alpha}(\Gamma)$ holds ($k \geq 2$).

2.2.3 LEMMA

Under the assumptions on Γ used in Definition 2.2.2 on the facing page it holds:

1. $W_{\pm}(\Gamma)$, $W_{\circ}(\Gamma)$ and $\mathbb{W}(\Gamma)$ are closed subspaces of $H^1(\Gamma)$.

$$W(\Gamma) := W_{\pm}(\Gamma) \cap W_{\circ}(\Gamma) \cap \mathbb{W}(\Gamma)$$

is a Hilbert-space. Moreover, for any number $b \in \mathbb{R}$,

$$W(\Gamma) + \frac{b}{|\Gamma|} = W_{\pm}(\Gamma) \cap W_{\circ}(\Gamma) \cap \mathbb{W}^b(\Gamma).$$

2. $W_{\pm}(\Gamma)$, $W_{\circ}(\Gamma)$, $\mathbb{W}(\Gamma)$ and $W^{\perp}(\Gamma)$ are closed subspaces of $(H^1(\Gamma))^3$.

$$W(\Gamma) := W_{\pm}(\Gamma) \cap W_{\circ}(\Gamma) \cap W^{\perp}(\Gamma) \cap \mathbb{W}(\Gamma)$$

is a Hilbert-space. Moreover, for any number $b \in \mathbb{R}$,

$$W(\Gamma) + \frac{b}{|\Gamma|} \nu_{\Gamma} = W_{\pm}(\Gamma) \cap W_{\circ}(\Gamma) \cap W^{\perp}(\Gamma) \cap \mathbb{W}^b(\Gamma).$$

3. The “orthogonal lift”

$$^{\perp} : H^1(\Gamma) \rightarrow W^{\perp}(\Gamma) : v \mapsto v \nu_{\Gamma}$$

is an isomorphism between Hilbert-spaces.

4. If Γ is axially symmetric with respect to the x_3 -axis, then it holds that $W_{\circ}(\Gamma) = H^1(\Gamma)$ and $W_{\circ}(\Gamma) = (H^1(\Gamma))^3$.

Proof:

ad 1. $\underline{W}_\pm(\Gamma)$ is the kernel of the operation of the involution $\mathcal{I}$ on $H^1(\Gamma)$ and hence $\underline{W}_\pm(\Gamma)$ is closed. $\underline{W}_\odot(\Gamma)$ and $\underline{W}(\Gamma)$ are kernels of continuous functionals. In the case of $\underline{W}_\odot(\Gamma)$ the continuity follows from the fact that $\nu_\Gamma \in C^{k-1,\alpha}(\Gamma)$, $k \geq 2$, which especially means that $\underline{W}_\odot(\Gamma)$ is well-defined. It follows $W(\Gamma) := \underline{W}_\pm(\Gamma) \cap \underline{W}_\odot(\Gamma) \cap \underline{W}(\Gamma) \leq H^1(\Gamma)$ is a Hilbert-space.

Now, for any constant function $\tilde{b} \in H^1(\Gamma)$ with $\tilde{b} \equiv b$, $b \in \mathbb{R}$, it is clear that $\tilde{b} \in \underline{W}_\pm(\Gamma) \cap \underline{W}_\odot(\Gamma)$ because the constant functions on Γ share all symmetries with Γ .

This establishes the relation $W(\Gamma) + \frac{b}{|\Gamma|} = \underline{W}_\pm(\Gamma) \cap \underline{W}_\odot(\Gamma) \cap \underline{W}^b(\Gamma)$.

ad 2. For $\underline{W}_\pm(\Gamma)$, $\underline{W}_\odot(\Gamma)$ and $\underline{W}(\Gamma)$ we can conclude as in the scalar case above. $W^\perp(\Gamma)$ is a Hilbert-space because of 3.

It is clear that $\underline{W}_\pm(\Gamma) \cap \underline{W}_\odot(\Gamma) \cap W^\perp(\Gamma)$ contains the unit normal field ν_Γ and hence all functions which are constant in normal direction. It therefore holds $W(\Gamma) + \frac{b}{|\Gamma|} \nu_\Gamma = \underline{W}_\pm(\Gamma) \cap \underline{W}_\odot(\Gamma) \cap W^\perp(\Gamma) \cap \underline{W}^b(\Gamma)$.

ad 3. We note that $\nu_\Gamma \in C^{k-1,\alpha}(\Gamma)$ and hence $^\perp$ clearly is well defined because Γ is compact. $^\perp$ is one-to-one because we have an explicit expression for its inverse; it holds for $v \in H^1(\Gamma)$, $w \in W^\perp(\Gamma)$:

$$(\bar{v}^\perp) \stackrel{\text{def}}{=} \langle v \nu_\Gamma, \nu_\Gamma \rangle = v \quad \text{and} \quad \bar{w}^\perp \stackrel{\text{def}}{=} \langle w, \nu_\Gamma \rangle \nu_\Gamma = w.$$

$^\perp$ is continuous because $\nabla_\Gamma \nu_\Gamma \in C^{k-2,\alpha}(\Gamma)$, $k \geq 2$, is bounded because $\Gamma \subset \mathbb{R}^3$ is compact. Therefore we have for $u, v \in H^1(\Gamma)$:

$$\begin{aligned} \|(u - v)^\perp\|_{(H^1(\Gamma))^3}^2 &= \int_\Gamma |u - v|^2 \|\nu_\Gamma\|^2 do \\ &\quad + \int_\Gamma \|\nu_\Gamma\|^2 \|\nabla_\Gamma(v - u)\|^2 do + \int_\Gamma |v - u|^2 \|\nabla_\Gamma \nu_\Gamma\|^2 do \\ &\leq \|u - v\|_{H^1(\Gamma)}^2 + \|(\nabla_\Gamma \nu_\Gamma)^2\|_{L^\infty(\Gamma)} \|u - v\|_{L_2(\Gamma)}^2 \\ &\leq (1 + \|\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma\|_{L^\infty(\Gamma)}) \|u - v\|_{H^1(\Gamma)}^2. \end{aligned}$$

Similarly, $^\perp$ (the inverse of $\cdot^\perp$) is bounded. By the same argument we have for $w, p \in W^\perp(\Gamma)$

$$\|\bar{w} - \bar{p}\|_{H^1(\Gamma)}^2 \leq (1 + \|\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma\|_{L^\infty(\Gamma)}) \|(w - p)^\perp\|_{(H^1(\Gamma))^3}^2.$$

ad 4. If Γ is axially symmetric, then it holds that Θ and $\bar{\Theta}$ are identically zero.

□

REMARK 2.2.3 To summarise the above constructions: $\underline{W}(\Gamma) \leq H^1(\Gamma)$ and $W(\Gamma) \leq (H^1(\Gamma))^3$ are well-defined Hilbert-spaces. They relate to the Lie-symmetries of the linearised Euler-Lagrange equations (2.27) and (2.26) on page 29 in that they

incorporate already the linearised volume constraint, the orthogonality constraint with respect to the infinitesimal generator of the group of rotations about the x_3 -axis and they break the translational invariance in the direction of the x_3 -axis.

This means that $\underline{W}(\Gamma)$ and $W(\Gamma)$ are transversal to the three-dimensional space spanned by the infinitesimal generators of the Lie-symmetry group of the Euler-Lagrange equation. Therefore the non-trivial solutions of the linearised Euler-Lagrange equations induced by the Lie-symmetry group are not contained in the Ansatz-spaces $\underline{W}(\Gamma)$ and $W(\Gamma)$.

2.2.4 DEFINITION (WEAK SOLUTIONS OF THE LINEARISATION)

Let $\Gamma \subset \mathbb{R}^3$ be an isometrically immersed compact surface of class $C^{k,\alpha}$ with $k \geq 2$ and $0 < \alpha < 1$ which possesses a reflective symmetry about the (x_1, x_2) -plane. Let $f \in (C^{k-2,\alpha}(\Gamma))^3$, $b \in \mathbb{R}$.

1. For $u \in \underline{W}(\Gamma)$, $K \in \mathbb{R}$ we say that $(u + \frac{b}{|\Gamma|}, K)$ is a weak solution of the linearised Euler-Lagrange equation (2.27) if

$$(2.29) \quad \int_{\Gamma} \nabla_{\Gamma} u \cdot \nabla_{\Gamma} \eta \, do - \int_{\Gamma} \bar{a}_{\Gamma} u \eta \, do = \int_{\Gamma} \left(\bar{f} + \bar{a}_{\Gamma} \frac{b}{|\Gamma|} + K \right) \eta \, do$$

for all $\eta \in \underline{W}(\Gamma)$, where $\bar{a}_{\Gamma} = 8\omega^2(x_1\nu_1 + x_2\nu_2) + \nabla_{\Gamma}\nu_{\Gamma} : \nabla_{\Gamma}\nu_{\Gamma}$ as defined in (2.25) on page 28.

2. For $w \in W(\Gamma)$, $K \in \mathbb{R}$ we say that $(w + \frac{b}{|\Gamma|}\nu_{\Gamma}, K)$ is a weak solution of the linearised Euler-Lagrange equation (2.26) if

$$(2.30) \quad \int_{\Gamma} \nabla_{\Gamma} w : \nabla_{\Gamma} \chi \, do - \int_{\Gamma} a_{\Gamma} \nu_{\Gamma} \cdot w \nu_{\Gamma} \cdot \chi \, do = \int_{\Gamma} \left(f + a_{\Gamma} \frac{b}{|\Gamma|} \nu_{\Gamma} + K \nu_{\Gamma} \right) \cdot \chi \, do$$

for all $\chi \in W(\Gamma)$, where $a_{\Gamma} = 8\omega^2(x_1\nu_1 + x_2\nu_2) + 2\nabla_{\Gamma}\nu_{\Gamma} : \nabla_{\Gamma}\nu_{\Gamma}$ as defined in equation (2.25).

REMARK 2.2.4 We will *not* analyse existence and uniqueness of solutions of (2.29) and (2.30) above.

2.2.5 THEOREM (REGULARITY OF WEAK SOLUTIONS)

Assume that the prerequisites of Definition 2.2.4 hold.

1. Let $(u, K) \in \underline{W}(\Gamma) \times \mathbb{R}$ be a weak solution of the scalar equation (2.29) in Definition 2.2.4 above. Then it holds that $u \in C^{k,\alpha}(\Gamma)$.
2. Let $(w, K) \in W(\Gamma) \times \mathbb{R}$ be a weak solution of the vector-valued equation (2.30) in Definition 2.2.4 above. Then it holds that $w \in (C^{k,\alpha}(\Gamma))^3$.

Proof: First, let $(u, K) \in \underline{W}(\Gamma) \times \mathbb{R}$ be a weak solution of the scalar equation (2.29). Then $u \in H^1(\Gamma)$ and u is a weak solution of the elliptic equation

$$-\Delta_{\Gamma} u + c u = g \quad \text{with} \quad c := -\bar{a}_{\Gamma}, \quad g := \bar{f} + K.$$

Since Γ is of class $C^{k,\alpha}$ with $k \geq 2$, $\alpha \in (0, 1)$, we have that

$$c = -\bar{a}_\Gamma = 8\omega^2(x_1\nu_1 + x_2\nu_2) + \nabla_\Gamma\nu_\Gamma : \nabla_\Gamma\nu_\Gamma \in C^{k-2,\alpha}(\Gamma), \quad \bar{f} = f \cdot \nu_\Gamma \in C^{k-2,\alpha}(\Gamma).$$

Furthermore, in a local chart there holds

$$-\Delta_\Gamma u = -|g|^{1/2} D_i \left(g^{ij} \sqrt{|g|} D_j u \right),$$

where $(g_{ij}) \in \mathbb{R}^{2 \times 2}$ are the components of the Riemannian metric of Γ in the chosen coordinate system, $g^{ik}g_{kj} = \delta_{ij}$ and $|g|$ the determinant of (g_{ij}) . For a $C^{k,\alpha}$ -manifold we have $g_{ij} \in C^{k-1,\alpha}(\Gamma)$.

It follows then by [AUBIN 1982, Theorem 4.18] that $u \in C^{k,\alpha}(\Gamma)$. We would like to mention at this point that Aubin's theorem requires that $c > 0$ on Γ but this is only needed to prove existence and uniqueness of a solution. The regularity of a solution is only affected by the regularity of the coefficients of the equation.

The important result is that a solution of the scalar linearised Euler-Lagrange equations is of the same differentiability class as Γ itself.

For any weak solution $(w, K) \in W(\Gamma) \times \mathbb{R}$ of the vector-valued linearised Euler-Lagrange equations (2.30) we note that the term $a_\Gamma \nu_\Gamma \nu_\Gamma \cdot w$ – which couples the equations – is of class $C^{k-2,\alpha}$ and can be added to the right-hand side. What remains is a Poisson-equation on a manifold which is covered by Aubin's theorem. $\square$

2.2.6 THEOREM (EQUIVALENCE OF SCALAR AND VECTOR-VALUED SOLUTIONS)

Let $\Gamma \subset \mathbb{R}^3$ be an isometrically immersed compact surface of class $C^{k,\alpha}$ ($k \geq 2$ and $0 < \alpha < 1$) which possesses a reflective symmetry about the (x_1, x_2) -plane.

For $f \in (C^{k-2,\alpha}(\Gamma))^3$ and $b \in \mathbb{R}$ the following holds:

If each of the equations (2.29) and (2.30) of Definition 2.2.4 on the preceding page has a unique solution $(u, \tilde{K}) \in W(\Gamma) \times \mathbb{R}$ respectively $(w, K) \in W(\Gamma) \times \mathbb{R}$ then

$$(2.31) \quad u \nu_\Gamma \equiv w \quad \text{and} \quad \tilde{K} = K.$$

Particularly, it holds that $v \nu_\Gamma \in C^{k,\alpha}(\Gamma)$.

Proof: Assume that $(u, \tilde{K}) \in W(\Gamma) \times \mathbb{R}$ and $(w, K) \in W(\Gamma) \times \mathbb{R}$ are the unique weak solutions of the scalar respectively vector-valued linearised Euler-Lagrange equations.

Then we first have $u^\perp = u \nu_\Gamma \in W(\Gamma)$ because $\nu_\Gamma \in C^{k-1,\alpha}(\Gamma)$ and $k \geq 2$ and so $u^\perp \in H^1(\Gamma)$.

By substituting $(u^\perp, \tilde{K})$ and an arbitrary test-function $\chi \equiv \langle \chi, \nu_\Gamma \rangle \nu_\Gamma \equiv \bar{\chi} \nu_\Gamma \in W(\Gamma)$

into the right hand side of equation (2.30) it follows:

$$\begin{aligned}
& \int_{\Gamma} \nabla_{\Gamma}(u \nu_{\Gamma}) : \nabla_{\Gamma}(\bar{\chi} \nu_{\Gamma}) \, do - \int_{\Gamma} a_{\Gamma} \nu_{\Gamma} \cdot (u \nu_{\Gamma}) \nu_{\Gamma} \cdot (\bar{\chi} \nu_{\Gamma}) \, do - K \int_{\Gamma} \nu_{\Gamma} \cdot (\bar{\chi} \nu_{\Gamma}) \, do \\
&= \int_{\Gamma} \nu_{\Gamma} \cdot \nu_{\Gamma} \nabla_{\Gamma} u \cdot \nabla_{\Gamma} \bar{\chi} \, do + \int_{\Gamma} (\nabla_{\Gamma} \nu_{\Gamma} : \nabla_{\Gamma} \nu_{\Gamma}) u \bar{\chi} \, do - \int_{\Gamma} a_{\Gamma} u \bar{\chi} \, do - \tilde{K} \int_{\Gamma} \bar{\chi} \, do \\
&= \underbrace{\int_{\Gamma} \nabla_{\Gamma} u \cdot \nabla_{\Gamma} \bar{\chi} \, do + \int_{\Gamma} \underbrace{(\nabla_{\Gamma} \nu_{\Gamma} : \nabla_{\Gamma} \nu_{\Gamma} - a_{\Gamma})}_{=-\bar{a}_{\Gamma}} u \bar{\chi} \, do - \tilde{K} \int_{\Gamma} \bar{\chi} \, do}_{\text{left-hand side of the scalar linearisation (2.29)}} \\
&= \int_{\Gamma} \bar{f} \bar{\chi} \, do, \quad \text{because } \bar{\chi} \text{ is an admissible scalar test-function} \\
&= \int_{\Gamma} f \cdot \nu_{\Gamma} \bar{\chi} \cdot \nu_{\Gamma} \, do.
\end{aligned}$$

The term in the last line is the right hand side of the vector-valued linearisation (2.30). This already establishes that $(u \nu_{\Gamma}, \tilde{K})$ is a weak solution of the vector-valued linearisation and hence – by the regularity result established in Theorem 2.2.5 on page 35 – we have $u \nu_{\Gamma} \in C^{k,\alpha}(\Gamma)$, despite the fact that ν_{Γ} is only of class $C^{k-1,\alpha}$.

From the assumption of uniqueness we then get $(u \nu_{\Gamma}, \tilde{K}) = (w, K)$. $\square$

2.3 The continuous Newton iteration

We will now describe a Newton-type iteration to construct a new solution (Γ_{m+1}, C_{m+1}) at an altered angular velocity $\omega_{m+1} := \omega_m + \varepsilon_{\omega}$ from a known C^{∞} solution (Γ_m, C_m) at angular velocity ω_m (with $m \in \mathbb{N}$).

To avoid confusion we like to comment on the kind of indices used throughout this section. The index “ m ” in the statement above is used to indicate that Γ_m and Γ_{m+1} arise as two distinct surfaces during the path-tracking algorithm. Because Γ_{m+1} is constructed by a Newton iteration we will need an additional index which denotes the sequence of surfaces constructed during that Newton iteration. For this we will use *upper* indices in brackets. An equivalent notation is used for the Lagrange-multipliers

For example, $(\Gamma_m^{(l)}, C_m^{(l)})$ denotes the l^{th} approximation constructed by the Newton-algorithm from the m^{th} exact solution (Γ_m, C_m) in the course of the path-tracking algorithm. In particular we have

$$(\Gamma_m, C_m) = (\Gamma_m^{(0)}, C_m^{(0)}) \quad \text{and} \quad (\Gamma_{m+1}, C_{m+1}) := \lim_{l \rightarrow \infty} (\Gamma_m^{(l)}, C_m^{(l)})$$

provided that the Newton method converges.

We are here in the semi-discrete regime, “discrete” because of the Newton iteration and because we track down solution paths in discrete steps with respect to the angular velocity ω , but only *semi*-discrete because the Newton iteration described here will be established in terms of $C^{k,\alpha}$ solutions of the linearised Euler-Lagrange equations (2.29) and (2.30) above, with $k \geq 2$ and $\alpha \in (0, 1)$.

This means that at this point of our analysis we discretise with respect to ω . The discretisation “in space” – putting it in analogy to time-dependent problems – will be defined later by a finite element method.

Algorithm 2.3.1 A modified Newton iteration. In the algorithm below X and Y are Banach spaces. We assume that the operator $A : X \rightarrow Y$ is Frechet-differentiable with $L := DA$ and that L has a bounded inverse.

Parameters: tolerances $\varepsilon_x, \varepsilon_y$, line-search limit j_{max} , iteration limit l_{max}

- 1: choose a start value $\Xi_0 \in X$
 - 2: $l := 0$
 - 3: **repeat**
 - 4: $d_l := (L(\Xi_l))^{-1} [A \Xi_l]$
 - 5: choose $\lambda_l \in \mathbb{R}$ with $h_l(\lambda_l) = \min_{0 \leq i \leq j_{max}} h_l(2^{-i})$ where $h_l(\tau) := \|A(\Xi_l - \tau d_l)\|_Y$
 - 6: $\Xi_{l+1} := \Xi_l - \lambda_l d_l$
 - 7: $l := l + 1$
 - 8: **until** $l > l_{max}$ **or** ($\|\Xi_{l+1}\|_X \leq \varepsilon_x$ **and** $\|A(\Xi_{l+1})\|_Y \leq \varepsilon_y$)
-

Algorithm 2.3.1 shows the general layout of the Newton iteration we are using.

We like to stress here that the entire discretisation is purely experimental. We do not even know whether the Newton-directions computed in each iteration step of the Newton-scheme exist, nor whether the operators defined in the following section are (Frechet-) differentiable.

A proof of convergence of the discretisation is entirely beyond the scope of this work.

In the following we assume that in the course of the path-tracking algorithm we have arrived at a “point” (Γ_m, C_m) . The goal is to develop a consistent notation which would define a Newton iteration if we knew that all quantities existed.

Because we are not concerned with convergence and hence will not perform the limiting process $(\Gamma_{m+1}, C_{m+1}) = \lim_{l \rightarrow \infty} (\Gamma_m^{(l)}, C_m^{(l)})$ we drop the lower index and set $(\Gamma, C) := (\Gamma_m, C_m)$ in the following. For the same reason we set $\omega := \omega_{m+1}$.

2.3.1 The differential operators

Let $\Xi_0 \equiv (\Gamma^{(0)}, C^{(0)}) := (\Gamma, C)$ where $\Gamma \subset \mathbb{R}^3$ is a compact immersed surface of class C^∞ .

Because the curvature of Γ is bounded there is an open set $U_0^{k,\alpha} \subset (C^{k,\alpha}(\Gamma))^3$ so that each $\varphi \in U_0^\infty := U_0^{k,\alpha} \cap (C^\infty(\Gamma))^3$ defines a diffeomorphism $\text{id}_\Gamma + \varphi : \Gamma \rightarrow \Gamma_\varphi$ with

$$\Gamma_\varphi := \{\text{id}_\Gamma(X) + \varphi(X) \mid X \in \Gamma\}$$

where Γ_φ is again of class C^∞ .

We remark that the Banach spaces $C^{j,\beta}(\Gamma_\varphi)$ and $C^{j,\beta}(\Gamma)$ are norm-equivalent for $j \leq k$ and $\beta \leq \alpha$ and that the norm-equivalence between them is controlled by the $C^{j,\beta}(\Gamma)$ -norm of $\text{id}_\Gamma + \varphi$. Similarly, the Sobolev spaces $H_p^s(\Gamma_\varphi)$ and $H_p^s(\Gamma)$, $s < j + \beta$, are

equivalent where the equivalence is controlled by the $H_p^s(\Gamma)$ norm of $\text{id}_\Gamma + \varphi$ (chain rule) and the $H_\infty^1(\Gamma)$ norm of $\text{id}_\Gamma + \varphi$ (transformation formula for integrals).

By actually identifying the spaces $C^{j,\beta}(\Gamma_\varphi)$ and $C^{j,\beta}(\Gamma)$ we can define an operator

$$(2.32) \quad A^\infty : U_0^\infty \times \mathbb{R} \rightarrow C^{k-2,\alpha}(\Gamma) \times \mathbb{R} : (\varphi, K) \mapsto (R_{(\Gamma_\varphi, K, \omega)}, \int_{\Gamma_\varphi} \text{id}_{\Gamma_\varphi} \cdot \nu_{\Gamma_\varphi} do - 4\pi),$$

where

$$R_{(\Gamma_\varphi, K, \omega)} := 2H_{\Gamma_\varphi} - (4\omega^2 r^2 + K) = -\nu_{\Gamma_\varphi} \cdot \Delta_{\Gamma_\varphi} \text{id}_{\Gamma_\varphi} - (4\omega^2 r^2 + K)$$

is the residual of the non-linear Euler-Lagrange equations (2.6) on page 23. This notation was already introduced when discussing the second variations (2.21) and (2.22) of the normalised energy E on page 28.

The operator A is continuous on $U_0^\infty \times \mathbb{R}$ and U_0^∞ is dense in $U_0^{k,\alpha}$ so that we can extend A to a continuous operator on $U_0^{k,\alpha} \times \mathbb{R}$. We note that A is Gateaux-differentiable on $U_0^\infty \times \mathbb{R}$ and we *assume* in the following that A is indeed Frechet-differentiable on $U_0^{k,\alpha} \times \mathbb{R}$.

To formulate the iteration step of the Newton iteration we need an expression for $DA(\varphi, K)$ only at points $(\varphi, K) \in U_0^\infty \times \mathbb{R}$ where DA denotes the Frechet-derivative of the operator A . The expression for $DA(\varphi, K)$ is implied by the vector-valued linearised Euler-Lagrange equations (2.23) on page 28:

$$(2.33) \quad \begin{aligned} DA(\varphi, K) : (C^{k,\alpha}(\Gamma_\varphi))^3 \times \mathbb{R} &\rightarrow C^{k-2,\alpha}(\Gamma_\varphi) \times \mathbb{R}, \\ (\psi, J) &\mapsto \left(-\nu_{\Gamma_\varphi} \cdot \Delta_{\Gamma_\varphi} \psi - a_{\Gamma_\varphi} \nu_{\Gamma_\varphi} \nu_{\Gamma_\varphi} \cdot \psi - L + R_{(\Gamma_\varphi, K, \omega)} Y_{\Gamma_\varphi} \cdot \psi, \int_{\Gamma_\varphi} \psi \cdot \nu_{\Gamma_\varphi} do \right). \end{aligned}$$

The 0th-order term a_{Γ_φ} was defined by equation (2.25) on page 28 and is governed by the square of the second fundamental form of Γ_φ .

The expression $(R_{(\Gamma_\varphi, K, \omega)} Y_{\Gamma_\varphi} \cdot \psi)$ is the correction introduced by the fact that we necessarily linearise at a *non*-stationary point (Γ_φ, K) of the drop-energy, compare with equation (2.21) on page 27.

We can make $R_{\Gamma_\varphi, K, \omega}$ arbitrarily small by choosing the start value Γ closer to a solution of the Euler-Lagrange equation (2.6). In the Newton iteration Algorithm 2.3.1 on the facing page we will therefore use the following approximation

$$L(\varphi, K)[\psi, J] := \left(-\nu_{\Gamma_\varphi} \cdot \Delta_{\Gamma_\varphi} \psi - a_{\Gamma_\varphi} \psi \cdot \nu_{\Gamma_\varphi} - L, \int_{\Gamma_\varphi} \psi \cdot \nu_{\Gamma_\varphi} do \right).$$

instead of $DA(\varphi, K) \approx L(\varphi, K)$.

As we have seen in the discussion of the linearised Euler-Lagrange equations the operator A and its approximate linearisation L are *not* invertible in general. The reason is that A – in the way A is defined above – has a non-trivial Lie-symmetry group.

We will resolve this problem by constructing the Newton-correction in special Ansatz-spaces, see Remark 2.2.3 on page 34.

2.3.2 The iteration step

Using the notation of the preceding section we are now able to constitute the iteration step of the Newton algorithm Algorithm 2.3.1 on page 38 in our special case.

Let $\Xi_l = (\text{id}_{\Gamma^{(l)}}, C^{(l)}) \in (C^{k,\alpha}(\Gamma^{(0)}))^3 \times \mathbb{R}$ be the point generated in the previous iteration step, where $\Gamma^{(l)}$ is the associated surface. We then generate $\Gamma^{(l+1)}$ and thereby $\Xi_{l+1} = (\text{id}_{\Gamma^{(l+1)}}, C^{(l+1)})$ by the following (sub-) steps:

Algorithm 2.3.2 The iteration step of the continuous Newton iteration

- 1: On $\Gamma^{(l)}$ solve the *scalar* Euler-Lagrange equations *weakly* for $(\tilde{\psi}_l, K_l) \in W(\Gamma^{(l)}) \times \mathbb{R}$, as defined in Definition 2.2.4 on page 35:

$$(2.34) \quad \int_{\Gamma^{(l)}} \nabla_{\Gamma^{(l)}} \tilde{\psi}_l \cdot \nabla_{\Gamma^{(l)}} \eta \, do - \int_{\Gamma^{(l)}} \bar{a}_{\Gamma^{(l)}} \tilde{\psi}_l \eta \, do = \int_{\Gamma^{(l)}} \left(\bar{f} + \bar{a}_{\Gamma^{(l)}} \frac{b}{|\Gamma^{(l)}|} + K_l \right) \eta \, do$$

for all $\eta \in W(\Gamma^{(l)})$ with “right-hand side”

$$(f, b) := A(\Xi_l) = (R_{(\Gamma^{(l)}, C^{(l)}, \omega)}, \int_{\Gamma^{(l)}} \text{id}_{\Gamma^{(l)}} \cdot \nu_{\Gamma^{(l)}} \, do)$$

and let $\bar{\psi}_l := \tilde{\psi}_l + \frac{b}{|\Gamma^{(l)}|}$. The special choice of the Ansatz space $W(\Gamma^{(l)}) \subset H^1(\Gamma^{(l)})$ eliminates the non-uniqueness caused by the Lie-symmetries as explained in Section 2.2 above.

- 2: Set $\psi_l := \bar{\psi}_l \nu_{\Gamma^{(l)}}$. By the regularity Theorem 2.2.5 on page 35 and the equivalence Theorem 2.2.6 on page 36 we have $\psi_l \in C^{k,\alpha}(\Gamma^{(l)})$ and (ψ_l, K_l) is the solution of the vector-valued linearised Euler-Lagrange equation (2.26). This implies

$$d_l := (\psi_l, K_l) = (L(\text{id}_{\Gamma^{(l)}}, C^{(l)}))^{-1} A(\text{id}_{\Gamma^{(l)}}, C^{(l)}).$$

- 3: Choose $\lambda_l \in \mathbb{R}^+$ as explained in Algorithm 2.3.1 on page 38 and generate

$$\Xi_{l+1} = (\text{id}_{\Gamma^{(l+1)}}, C^{(l+1)}) := (\text{id}_{\Gamma^{(l)}}, C^{(l)}) - \lambda_l (\psi_l, K_l) = \Xi_l - \lambda_l d_l,$$

where $\Gamma^{(l+1)} := \{\text{id}_{\Gamma^{(l)}}(X) - \lambda_l \psi_l(X) \mid X \in \Gamma^{(l)}\} = \Gamma^{(l)} - \lambda_l \psi_l$, see Figure 2.3.

REMARK 2.3.1 1. The Newton iteration produces a sequence of surfaces and associated function spaces, which are generated by the diffeomorphisms

$$\Psi_l := \text{id}_{\Gamma^{(l)}} - \lambda_l \psi_l \in C^{k,\alpha}(\Gamma^{(l)}), \quad l \in \mathbb{N}_0.$$

In the definition of the operator A and its approximate linearisation L we have identified all those function spaces with the corresponding spaces over $\Gamma^{(0)}$. The identification is arranged by chaining up all diffeomorphisms $\Psi_0, \dots, \Psi_{j-1}$ which lead to a surface $\Gamma^{(j)}$. The relation between the function spaces is demonstrated by the following diagram for the case of $C^{k,\alpha}$:

$$(2.35) \quad \begin{array}{ccccccc} \Gamma^{(0)} & \xrightarrow{\Psi_0} & \Gamma^{(1)} & \xrightarrow{\Psi_1} \dots \xrightarrow{\Psi_{l-1}} & \Gamma^{(l)} & \xrightarrow{\Psi_l} & \dots \\ C^{k,\alpha}(\Gamma^{(0)}) & \xleftarrow{\Psi_0^*} & C^{k,\alpha}(\Gamma^{(1)}) & \xleftarrow{\Psi_1^*} \dots \xleftarrow{\Psi_{l-1}^*} & C^{k,\alpha}(\Gamma^{(l)}) & \xleftarrow{\Psi_l^*} & \dots \end{array}$$

Figure 2.3 Displacement in normal direction during the Newton iteration

Here $\Phi * f(x) = f(\Phi(x))$ denotes the pull-back which maps a space $C^{k,\alpha}(\Gamma^{(l)})$ back to $C^{k,\alpha}(\Gamma^{(l-1)})$. The equivalence between $C^{k,\alpha}(\Gamma^{(l)})$, $l \in \mathbb{N}$, and the “base”-space $C^{k,\alpha}(\Gamma^{(0)})$ is controlled by the $C^{k,\alpha}$ -norm of the chain of diffeomorphisms $\Psi_{l-1} \circ \dots \circ \Psi_0$.

2. We have formulated the iteration step of the Newton algorithm in terms of $C^{k,\alpha}$ -spaces to indicate in which norm convergence possibly could take place. This should probably be weakened. However, choosing for example a H_p^k -norm one would still need to have H_∞^1 -estimates for the diffeomorphisms Ψ_j , $j \in \mathbb{N}$, to control the equivalence of the function spaces over the sequence of surfaces generated by the Newton iteration.
3. Requiring the initial surface to be of differentiability class C^∞ is not a restriction. The initial surfaces for the path-tracking algorithm are chosen from the exactly known families of surfaces which are indeed C^∞ -manifolds.
4. To actually establish convergence of the Newton iteration in any appropriate norm one would need to have a priori estimates for the solutions of the linearised Euler-Lagrange equations. To establish such estimates one needs control over the 0th-order term $-a_\Gamma$ respectively $-\bar{a}_\Gamma$. However, a_Γ is governed by $\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma$, the square of the second fundamental form. Already in the course of the annular family established by [GULLIVER 1984] the term $\nabla_\Gamma \nu_\Gamma : \nabla_\Gamma \nu_\Gamma$ diverges when the annular shapes approach the spheroidal family at $\omega^2 = 1/2$, see Section 1.4.
5. It is important that control over the regularity of the surface is not destroyed during the Newton-algorithm. While the smoothness of the initial manifold guarantees that each surface $\Gamma^{(l)}$ is again smooth, it is the equivalence Theorem 2.2.6 on page 36 which guarantees that we do not lose regularity by computing only the normal component of the Newton-directions ψ_l . Here, “loss of regularity” means *loss of information* about the norm of the derivatives of ψ_l in the given function space.

2.4 The discretised Newton iteration

The Euler-Lagrange equations derived in Section 2.1 which constitute the Newton iteration described in the previous section are defined on the surface of the drop. We do not want to use a global parametrisation to avoid coordinate singularities. Using, for example, a polar coordinate system one even could not represent the exactly known solution families in that coordinate system (see Figure 2.4).

Figure 2.4 A parametrisation by a polar coordinate system fails even along the family of exact spheroidal solutions found by [BEER 1869]. The red spots mark the points where the radius vector intersects the surface.

Therefore we follow the method developed in [DZIUK 1991] for parametric mean-curvature flow and adapt it to our problem. In this approach one defines finite element spaces on discretised surfaces and solves the differential equations on the surfaces without using an explicit parametrisation in the sense that the local parametrisations are defined by the triangulation itself. The construction of these *parametric finite elements* is described below in Section 2.4.1.

In the following sections we use these parametric finite elements to discretise the continuous Newton iteration defined in the preceding Section 2.3 and to discretise the eigenvalue problem originating from the bifurcation equations in the sense of Theorem 1.3.28 on page 15.

Finally we will give an overview of the complete discrete path-tracking algorithm used in this work.

2.4.1 Iso-parametric triangulations

First we need to construct a discretisation Γ_h of a smooth surface Γ to have an initial value for the discretisation of the path-tracking algorithm. The notion “iso-parametric triangulation” will be justified in the following Section 2.4.2.

We start by giving the necessary notations:

2.4.1 DEFINITION (REGULAR SIMPLEX)

Let $P_1, \dots, P_{n+1} \in \mathbb{R}^q$, with $n, q \in \mathbb{N}$, $n \leq q$, such that $P_1 - P_{n+1}, \dots, P_n - P_{n+1}$ are linearly independent. The regular n -simplex T with vertices $P_1, \dots, P_{n+1}$ is the convex hull of the points $P_1, \dots, P_{n+1}$.

$$(2.36) \quad T := \text{conv}(P_1, \dots, P_{n+1}) = \{X \in \mathbb{R}^q \mid X = \sum_{i=1}^{n+1} \lambda_i P_i, \lambda_i \in \mathbb{R}^{\geq 0}, \sum_{i=1}^{n+1} \lambda_i = 1\}.$$

For $X \in T$ the components of the $(n+1)$ -tuple $(\lambda_1, \dots, \lambda_{n+1})$ are called the barycentric coordinates of X with respect to T .

For $k \leq n$ a regular k -simplex with vertices $Q_1, \dots, Q_{k+1} \in \{P_1, \dots, P_{n+1}\}$ is called a k -sub-simplex of T . Any $(n-1)$ -sub-simplex of T is called a face of T . Any 1-sub-simplex of T is called an edge of T .

REMARK 2.4.1 We introduce the following notation:

The diameter of T and the radius of the largest n -dimensional ball contained in T are denoted by

$$h(T) := \text{diam}(T) \quad \text{and} \quad \rho(T) := \max\{r \in \mathbb{R}^+ \mid B_r^T(X) \subset T, X \in T\},$$

where $B_r^T(X)$ denotes the n -dimensional section of the q -dimensional ball with radius r around $X \in \mathbb{R}^q$ with the affine sub-space of dimension n containing T .

2.4.2 DEFINITION (REGULAR TRIANGULATION, CONFORMING TRIANGULATION)

Let $q, n \in \mathbb{R}$, $n \leq q$ and $N \in \mathbb{N}$. Let $T_j \subset \mathbb{R}^q$, $1 \leq j \leq N$, be regular n -simplices and let

$$h := \max_{1 \leq j \leq N} h(T_j), \quad \overline{\Gamma}_h := \bigcup_{j=1}^N T_j \quad \text{and} \quad \mathcal{T}_h := \bigcup_{j=1}^N \{T_j\}.$$

1. $\mathcal{T}_h$ is called a conforming triangulation if for any $T_j, T_l \in \mathcal{T}_h$ with $T_j \neq T_l$ the intersection $T_j \cap T_l$ is either empty or a proper k -sub-simplex of T_j ($k < n$).
2. A vertex P of a regular n -simplex $T_j \in \mathcal{T}_h$ is called a non-conforming vertex of $\mathcal{T}_h$ if there is a regular n -simplex $T_l \in \mathcal{T}_h$ such that P is not a vertex of T_l , but $P \in T_l$.
3. A sequence $(\mathcal{T}_{h_j})_{j \in \mathbb{N}}$ of triangulations is called shape-regular if

$$\sup_{j \in \mathbb{N}} \max_{T \in \mathcal{T}_{h_j}} \frac{h(T)}{\rho(T)} < \infty.$$

REMARK 2.4.2 We note that for any regular triangulation $\mathcal{T}_h$ of regular n -simplices its associated simplicial domain $\Gamma_h \subset \mathbb{R}^q$ is an n -dimensional $C^{0,1}$ -immersion into $\mathbb{R}^q$. For a smooth n -dimensional immersion Γ we say that Γ_h and $\mathcal{T}_h$ interpolate Γ if for any vertex $P \in \mathcal{T}_h$ we have $P \in \Gamma$.

In our case the above definitions are only needed for the case of conforming triangulations consisting of regular 2-simplices in $\mathbb{R}^3$.

To get a discretisation of an initial surface for the path-tracking algorithm the goal is now to construct a $C^{0,1}$ -immersion Γ_h^d which is locally parametrised by polynomials of a given degree d and which approximates a smooth surface Γ . To this aim we start with a conforming triangulation $\mathcal{T}_h$ which interpolates Γ .

It is possible to construct such a triangulation from local charts (see [KALIK and WENDLAND 1992]), but this is not necessary in our case. Our initial surface will either be a spheroid close to the unit-sphere or an annular surface close to a circular torus. In both cases we have a global parametrisation and can choose an initial “macro”-triangulation which interpolates the smooth surface. Later, this macro-triangulation is refined sufficiently often to yield a good approximation of Γ . The details of the refinement process and how to maintain regularity of the triangulation is described in the following chapter in the sections 3.3 and 3.4.

Therefore, at this point we just assume that we already have a conforming triangulation $\mathcal{T}_h^1 := \mathcal{T}_h$ which interpolates a smooth surface Γ .

If the desired order of the polynomial parametrisation is 1 then we are done. Otherwise we use Lagrange-polynomials of order d over a reference-simplex to define higher-order approximations of Γ by the procedure described below. We define the following notations:

2.4.3 DEFINITION (REFERENCE SIMPLEX, LAGRANGE POLYNOMIALS)

The regular n -simplex $\hat{T} \subset \mathbb{R}^{n+1}$ defined by

$$\hat{T} := \{(\lambda_1, \dots, \lambda_{n+1}) \mid \lambda_i \in \mathbb{R}^{\geq 0}, \sum_{i=1}^{n+1} \lambda_i = 1\}$$

is called the n -dimensional reference simplex.

For given $d \in \mathbb{N}$ we denote by $m(n, d)$ the dimension of the vector space $P_d(\hat{T})$ of polynomials of degree d over $\hat{T} \subset \mathbb{R}^{n+1}$. The canonical Lagrange-interpolation nodes on $\hat{T}$ are denoted by $\hat{Q}_j$ and the nodal basis functions by $\hat{p}_j$, $j = 1, \dots, m(n, d)$.

REMARK 2.4.3 Per definition we have $\hat{p}_j(\hat{Q}_i) = \delta_{ij}$. Examples for $n = 2$ and $d = 1, 2$ are shown in Figure 2.5(b) on the facing page.

We give now the construction of a $C^{0,1}$ surface Γ_h^d which is locally parametrised over the reference simplex $\hat{T}$ by polynomials of degree d and interpolates the smooth surface Γ . An example is illustrated in Figure 2.5(a) on the next page.

We still assume that we have a given regular triangulation $\mathcal{T}_h^1$ which interpolates the smooth surface Γ and also a well defined projection $\Pi_\Gamma : \Gamma_h^1 \rightarrow \Gamma : P \mapsto \Pi_\Gamma(P) \in \Gamma$. In general Π_Γ exists only if the triangulation $\mathcal{T}_h^1$ is fine enough.

For any regular n -simplex $\bar{T} \in \mathcal{T}_h^1$ with vertices $Q_1, \dots, Q_{n+1} \in \mathbb{R}^q$ we denote by $\Phi_T^1 : \hat{T} \rightarrow T$ the affine linear parametrisation which maps each vertex $\hat{Q}_i$ of $\hat{T}$ to the vertex Q_i of $\bar{T}$, so we have

$$\Phi_T^1(\hat{Q}_i) = Q_i, \quad 1 \leq i \leq (n+1).$$

Figure 2.5 Parametrisation with Lagrange finite elements

- (a) The figure shows an octahedron as “macro”-triangulation and the resulting interpolation of the unit-sphere with quadratic Lagrange elements. The images Q_i of the Lagrange nodes $\hat{Q}_i$ of the reference element $\hat{T}$ are obtained by first mapping $\hat{T}$ with an affine-linear transformation to each face of the octahedron. Then the non-vertex Lagrange nodes of the affine-linear image are projected to the sphere. Φ_T^2 is the resulting local parametrisation which interpolates the sphere at the points Q_i .

- (b) Lagrange nodes and basis-functions for linear and quadratic finite elements. n denotes the dimension of the reference element $\hat{T} \subset \mathbb{R}^{n+1}$. d is the polynomial degree of the Ansatz-functions and $m(n, d)$ is the number of Lagrange nodes, which is also the number of the Lagrange Ansatz-functions for given n and d .

$n = 2, d = 1$

$$\begin{aligned} m(n, d) &= 3, \\ \hat{Q}_1 &= (1, 0, 0), \quad \hat{Q}_2 = (0, 1, 0), \quad \hat{Q}_3 = (0, 0, 1), \\ \hat{p}_j(\lambda_1, \lambda_2, \lambda_3) &= \lambda_j \end{aligned}$$

$n = 2, d = 2$

$$\begin{aligned} m(n, d) &= 6, \\ \hat{Q}_1 &= (1, 0, 0), \quad \hat{Q}_2 = (0, 1, 0), \quad \hat{Q}_3 = (0, 0, 1), \\ \hat{Q}_4 &= (0, \tfrac{1}{2}, \tfrac{1}{2}), \quad \hat{Q}_5 = (\tfrac{1}{2}, 0, \tfrac{1}{2}), \quad \hat{Q}_6 = (\tfrac{1}{2}, \tfrac{1}{2}, 0), \end{aligned}$$

$$\hat{p}_j(\lambda_1, \lambda_2, \lambda_3) = \begin{cases} 2\lambda_j(\lambda_j - 1) & j = 1, 2, 3, \\ 4\lambda_2\lambda_3 & j = 4, \\ 4\lambda_3\lambda_1 & j = 5, \\ 4\lambda_1\lambda_2 & j = 6. \end{cases}$$

By $\bar{Q}_i := \Phi_T^1(\hat{Q}_i)$, $(n+1) < i \leq m(n, d)$, we denote the images of the non-vertex Lagrange-nodes of $\hat{T}$ on the simplex $\bar{T}$ and set

$$Q_i := \Pi_\Gamma(\bar{Q}_i) = \Pi_\Gamma \circ \Phi_T^1(\hat{Q}_i), \quad (n+1) < i \leq m(n, d).$$

This defines a polynomial mapping Φ_T^d by interpolating the points $Q_i \in \Gamma$ with the Lagrange-polynomials $\hat{p}_i$, $1 \leq i \leq m(n, d)$,

$$(2.37) \quad \Phi_T^d : \hat{T} \rightarrow T := \Phi_T^d(\hat{T}) : \lambda = (\lambda_1, \dots, \lambda_{n+1}) \mapsto \sum_{i=1}^{m(n, d)} \hat{p}_i(\lambda) Q_i.$$

REMARK 2.4.4 By construction T interpolates the surface Γ in its Lagrange-nodes $Q_i = \Phi_T^d(\hat{Q}_i)$. If the base-triangulation $\mathcal{T}_h^1$ is fine enough, then $\Phi_T^d : \hat{T} \rightarrow T$ is a diffeomorphism. If Φ_T^d is a diffeomorphism for all $\bar{T} \in \mathcal{T}_h^1$ then

$$\Gamma_h^d := \bigcup_{\bar{T} \in \mathcal{T}_h^1} \sum_{i=1}^{m(n, d)} \hat{p}_i(\hat{T}) (\Pi_\Gamma \circ \Phi_{\bar{T}}^1(\hat{Q}_i))$$

is a $C^{0,1}$ -surface which is piecewise polynomial of degree d over the reference element $\hat{T}$. The continuity of Γ_h^d is clear, because the parametrisation with Lagrange-polynomials over the reference elements respects the simplicial hierarchy of $\mathcal{T}_h^1$. Therefore neighbouring elements have compatible Lagrange-nodes in their intersection (see the example in Figure 2.5(a) on the preceding page).

In the following we will also need $C^{0,1}$ -surfaces which do not originate from the interpolation of an underlying smooth surface Γ . For these surfaces we can generalise our definitions in the following sense:

2.4.4 DEFINITION (ISO-PARAMETRIC n -SIMPLEX)

Let $Q_i \in \mathbb{R}^q$, $1 \leq i \leq m(n, d)$, such that the mapping

$$\Phi_T^d : \hat{T} \rightarrow T := \Phi_T^d(\hat{T}) : \lambda = (\lambda_1, \dots, \lambda_{n+1}) \mapsto \sum_{i=1}^{m(n, d)} \hat{p}_i(\lambda) Q_i$$

is a diffeomorphism. Then T is called an iso-parametric n -simplex with vertices $Q_1, \dots, Q_{n+1}$ and non-vertex nodes $Q_{n+2}, \dots, Q_{m(n, d)}$.

REMARK 2.4.5 Likewise it is possible to define conforming iso-parametric “triangulations” $\mathcal{T}_h^d$ as sets of compatible iso-parametric n -simplices in the sense that intersecting iso-parametric n -simplices have compatible Lagrange-nodes in their intersection.

In this sense $\mathcal{T}_h^d$ is in the following such a conforming iso-parametric triangulation which does not necessarily arise from the interpolation of a smooth surface. Its associated $C^{0,1}$ -immersion will be denoted by $\Gamma_h^d := \bigcup_{T \in \mathcal{T}_h^d} T$. Because for any degree d the first $(n+1)$ Lagrange-nodes of the reference-element $\hat{T}$ are its vertices, we have always a canonical *linear* triangulation $\mathcal{T}_h^1$ and an associated immersion Γ_h^1 which interpolate the discrete surface Γ_h^d .

We will omit the upper index which indicates the polynomial degree of the local parametrisation over the reference element $\hat{T}$ when it is either clear from the context or does not matter.

2.4.2 Iso-parametric finite elements

We define parametric finite elements on a discrete surface Γ_h^d which are piece-wise polynomial of degree d or 1 over the reference simplex $\hat{T}$.

We define for $s \in \{1, d\}$

$$(2.38) \quad W_h^s(\Gamma_h^d) := \{v_h \in C^{0,1}(\Gamma_h^d) \mid \Phi_h^d * v_h := (v_h \circ \Phi_T^d) \in P_s(\hat{T}) \quad \forall T \in \mathcal{T}_h^d\}.$$

The finite element space $W_h^d(\Gamma_h^d)$ is virtually *iso*-parametric as the local parametrisation of Γ_h^d over the reference simplex is polynomial of degree d . In particular we have

$$\text{id}_{\Gamma_h^d} \in (W_h^d(\Gamma_h^d))^q.$$

This justifies our notion of an “iso-parametric triangulation” introduced in the preceding section.

For given $s \in \{1, d\}$ the canonical nodal basis $\{v_h^i \mid i = 1, \dots, \dim(W_h^s(\Gamma_h^d))\}$ of the finite element space $W_h^s(\Gamma_h^d)$ is defined by the images of the Lagrange-nodes of the reference element:

$$\{Q_i \mid i = 1, \dots, \dim(W_h^s(\Gamma_h^d))\} = \bigcup_{T \in \mathcal{T}_h^d} \{\Phi_T^d(\hat{Q}_j) \mid 1 \leq j \leq m(n, s)\}.$$

The basis functions v_h^i are then uniquely determined by requiring $v_h^i(Q_j) = \delta_{ij}$. We note that the first $(n+1)$ Lagrange-nodes $\hat{Q}_1, \dots, \hat{Q}_{n+1}$ for any polynomial degree d are the vertices of the reference element $\hat{T}$. This implies that it is possible to define the finite element space $W_h^1(\Gamma_h^d)$ of piecewise linear functions for any polynomial order $d \in \mathbb{N}$ of the parametrisation.

By Definition 1.3.25 on page 14 and the following remark 1.3.10 we know that the Hilbert-space $H^1(\Gamma_h^d)$ is well defined. It follows easily that $W_h^s < H^1(\Gamma_h^d)$, $s \in \{1, d\}$.

From [CIARLET and RAVIART 1972] we quote the following interpolation estimates:

2.4.5 THEOREM

Let $\Gamma \subset \mathbb{R}^q$ be a smooth compact immersed surface. Let $H^{d+1}(\Gamma)$ be continuously embedded into $C^0(\Gamma)$. By $I_h^d : H^{d+1}(\Gamma) \rightarrow W_h^d(\Gamma_h^d)$ we denote the interpolation operator which interpolates a function $\varphi \in H^{d+1}(\Gamma)$ in the Lagrange-nodes $\{Q_i\} \in \Gamma_h^d$. We note that I_h^d is hereby uniquely determined. Further we denote by $\pi : \Gamma_h^d \rightarrow \Gamma$ the lift in normal direction with respect to Γ .

It then holds for any function $\varphi \in W_h^d(\Gamma_h^d)$:

$$(2.39) \quad \|\varphi - \pi(I_h^d \varphi)\|_{H^m(\Gamma)} \leq c h^{d+1-m} \|\varphi\|_{H^{d+1}(\Gamma)}, \quad \text{with } m = 0, 1,$$

$$(2.40) \quad \|\pi^{-1} \varphi - I_h^d \varphi\|_{H^m(T)} \leq c h^{d+1-m} \|\pi^{-1} \varphi\|_{H^{d+1}(T)}, \quad \text{with } 0 \leq m \leq d+1.$$

Proof: [CIARLET and RAVIART 1972, Theorem 5] □

REMARK 2.4.6

The regular iso-parametric n -simplex $T = \Phi_T^d(\hat{T}) \in \mathcal{T}_h^d$ is a C^∞ -manifold. Thus the spaces $H^m(T)$ are well defined and make sense for $0 \leq m \leq d+1$, where the upper bound $d+1$ is maximal in the sense that derivatives of order higher than d of the local parametrisation Φ_T^d are constant.

2.4.3 A finite element formulation of the Newton iteration

Based on the weak formulation (Definition 2.2.4 on page 35) of the scalar linearised Euler-Lagrange equations (2.24) we will now formulate a finite element discretisation of the continuous Newton iteration Algorithm 2.3.2 on page 40.

The goal is to approximate the solutions of the non-linear Euler-Lagrange equations (2.6) on page 23 in the context of iso-parametric discrete surfaces $\Gamma_h^d \subset \mathbb{R}^3$ of dimension 2 and their corresponding iso-parametric finite element spaces $W_h^d(\Gamma_h^d)$ as defined in the previous section. We will drop the upper index because we do not mix discretisations of different polynomial degree here, so for $d \in \mathbb{N}$ fixed we set $\Gamma_h := \Gamma_h^d$ and $W_h(\Gamma_h) := W_h^d(\Gamma_h^d)$.

Moreover, the surfaces generated during the Newton iteration will be indexed by upper indices *in brackets*. So $\Gamma_h^{(l)}$ is the l^{th} surface in the Newton iteration. In particular (l) does *not* denote the polynomial degree of the parametrisation.

We begin by writing down the discrete analogon of the continuous iteration step Algorithm 2.3.2 on page 40 of the modified Newton iteration Algorithm 2.3.1 on page 38. The details will be discussed afterwards, see the Remarks 2.4.7 to 2.4.11 on pages 49–51.

Let $\Xi_h^{(l)} = (\text{id}_{\Gamma_h^{(l)}}, C_h^{(l)}) \in (W_h(\Gamma_h^{(l)}))^3 \times \mathbb{R}$ be the point generated by the previous iteration step of a discretisation of the modified Newton algorithm. We use the following notations:

- $\Gamma_h^{(l)} \subset \mathbb{R}^2 \times \mathbb{R}^+$ is an iso-parametric surface *with* boundary $\Sigma_h^{(l)} \subset \mathbb{R}^2 \times \{0\}$.
- We *define* the discrete residual $R_h^{(l)}$ of the non-linear Euler-Lagrange equations by the following expression:

$$(2.41) \quad R_h^{(l)} := 2 H_h(\Gamma_h^{(l)}) - 2\omega^2 r^2 - C_h^{(l)}.$$

The discrete mean curvature $H_h(\Gamma_h^{(l)})$ is *defined* in Section 3.2, Definition 3.2.4 on page 62. We note that $R_h^{(l)} \in W_h(\Gamma_h^{(l)})$ and refer to Remark 2.4.10 and Remark 2.4.11 on page 51.

- We *define* a discrete version $\bar{a}_h^{(l)}$ of the 0th-order term $\bar{a}_\Gamma$ of the scalar linearised Euler-Lagrange equations:

$$\bar{a}_h^{(l)} := (II_h(\Gamma_h^{(l)}) : II_h(\Gamma_h^{(l)})) + 8\omega^2 (x_1 \nu_1 + x_2 \nu_2),$$

where the discrete Weingarten-map $II_h(\Gamma_h^{(l)})$ is *defined* in Section 3.2, Definition 3.2.4 on page 62.

- We remind of the notation $\bar{\Theta} := (-x_2, \nu_1 + x_1 \nu_2)$. $\bar{\Theta}$ is generated by the action of the infinitesimal generator $\mathcal{R}$ of the symmetry group of rotations around the x_3 -axis and is a solution of the scalar linearised Euler-Lagrange equations. $\bar{\Theta}$ is non-trivial when the cylinder-symmetry of the surface is broken, see equation (2.28) on page 31.

Next we generate $\Gamma_h^{(l+1)}$ and thereby $\Xi_h^{(l+1)} = (\text{id}_{\Gamma_h^{(l+1)}}, C_h^{(l+1)}) \in (W_h(\Gamma_h^{(l+1)})) \times \mathbb{R}$ using the following (sub-) steps as explained in Algorithm 2.4.1:

Algorithm 2.4.1 The iteration step of the discrete Newton iteration

- 1: On $\Gamma_h^{(l)}$ solve the following system of equations for $(\bar{\psi}_h^{(l)}, K_h^{(l)}) \in W_h(\Gamma_h^{(l)}) \times \mathbb{R}$ and $\theta^{(l)} \in \mathbb{R}$:

$$(2.42a) \quad \int_{\Gamma_h^{(l)}} \nabla_{\Gamma_h^{(l)}} \bar{\psi}_h^{(l)} \cdot \nabla_{\Gamma_h^{(l)}} \bar{\eta}_h \, do - \int_{\Gamma_h^{(l)}} \bar{a}_h^{(l)} \bar{\psi}_h^{(l)} \bar{\eta}_h \, do - K_h^{(l)} \int_{\Gamma_h^{(l)}} \bar{\eta}_h \, do - \theta^{(l)} \int_{\Gamma_h^{(l)}} \bar{\Theta} \bar{\eta}_h \, do = \int_{\Gamma_h^{(l)}} R_h^{(l)} \bar{\eta}_h \, do,$$

$$(2.42b) \quad \int_{\Gamma_h^{(l)}} \bar{\psi}_h^{(l)} \, do = C_h^{(l)},$$

$$(2.42c) \quad \int_{\Gamma_h^{(l)}} \bar{\psi}_h^{(l)} \bar{\Theta} \, do = 0,$$

for all $\bar{\eta} \in W_h(\Gamma_h^{(l)})$. See Remark 2.4.9 on the next page below.

- 2: Generate an orthogonal perturbation $\psi_h^{(l)} \in (W_h(\Gamma_h^{(l)}))^3$ using an L_2 -projection with the appropriate boundary conditions. See also Remark 2.4.7 below.

$$(2.43) \quad \begin{cases} \int_{\Gamma_h^{(l)}} \psi_h^{(l)} \cdot \eta_h \, do = \int_{\Gamma_h^{(l)}} \bar{\psi}_h^{(l)} \nu_{\Gamma_h^{(l)}} \cdot \eta_h \, do, \\ \text{for all } \eta_h = (\eta_h^1, \eta_h^2, \eta_h^3) \in (W_h(\Gamma_h^{(l)}))^3 \text{ with } \eta_h^3|_{\Sigma_h^{(l)}} \equiv 0, \\ \text{where } \psi_h^{(l)} = (\psi_{h,1}^{(l)}, \psi_{h,2}^{(l)}, \psi_{h,3}^{(l)}) \in (W_h(\Gamma_h^{(l)}))^3 \text{ with } \psi_{h,3}^{(l)}|_{\Sigma_h^{(l)}} \equiv 0. \end{cases}$$

- 3: Choose $\lambda_l \in \mathbb{R}^+$ as explained in Algorithm 2.3.1 on page 38 (but see Remark 2.4.11 below) and set

$$(2.44) \quad \Xi_h^{(l)} = (\text{id}_{\Gamma_h^{(l+1)}}, C_h^{(l+1)}) := (\text{id}_{\Gamma_h^{(l)}}, C_h^{(l)}) - \lambda_l (\psi_h^{(l)}, K_h^{(l+1)}),$$

where

$$\Gamma_h^{(l+1)} := \{\text{id}_{\Gamma_h^{(l)}}(X) - \lambda_l \psi_h^{(l)}(X) \mid X \in \Gamma_h^{(l)}\} = (\Gamma_h^{(l)})_{-\lambda_l \psi_h^{(l)}}.$$

REMARK 2.4.7 (PERTURBATIONS IN NORMAL DIRECTION)

In step 2 of the discretised iteration step Algorithm 2.4.1 we have to use an L_2 -projection to construct a vector-valued perturbation because the normal-field $\nu_{\Gamma_h^{(l)}}$ is *discontinuous* across element boundaries. This means that $\nu_{\Gamma_h^{(l)}} \bar{\psi}_h^{(l)} \notin (W_h(\Gamma_h^{(l)}))^3$.

Another possibility than using an L_2 -projection to construct a vector-valued perturbation in normal direction is to define a continuous approximate normal field $\nu_h \in (W_h(\Gamma_h^{(l)}))^3$ and set $\psi_h^{(l)} := \bar{\psi}_h^{(l)} \nu_h$. The construction of such an approximate normal field is discussed in Section 3.1 in the next chapter.

REMARK 2.4.8 (POLYNOMIAL DEGREE OF THE FINITE ELEMENT SPACE)

The discretised Newton iteration does *not* work for linearly discretised parametric surfaces. The reason is the 0th-order term $\bar{a}_h(\Gamma_h^{(l)})$ which contains the square of the discrete Weingarten-map $II_h(\Gamma_h^{(l)})$. We present experimental convergence tests with respect to the L_2 - and L_∞ -norm for II_h in the Tables 3.1 to 3.4 on pages 65–68 in the next chapter. The numerical experiments suggest that II_h converges with respect to the L_2 - and L_∞ -norm to the continuous Weingarten-map of the underlying smooth surface if the polynomial degree of the interpolating iso-parametric surface is at least 2, but that we have no convergence in the linear case.

REMARK 2.4.9 (BREAKING OF LIE-SYMMETRIES)

1. For the continuous Newton iteration (Algorithm 2.3.2 on page 40) we were using an Ansatz-space of reflectively symmetric functions with respect to the (x_1, x_2) -plane to break the translational invariance of the linearised equations in x_3 -direction.

To do so in the context of finite elements would imply to choose an iso-parametric triangulation which shares the reflective symmetry. But then an Ansatz-space consisting of reflectively symmetric functions would just result in a linear system with block-matrices composed of identical blocks, overlapping only for the nodes located in the equatorial plane. Exploiting the block-matrix structure to reduce the number of unknowns by roughly one half is equivalent to dissecting the drop at its equatorial plane and imposing the natural boundary conditions implied by the dissection.

For the system of scalar equations (2.42) which determine the signed length of the (discrete) orthogonal perturbation this implies homogenous Neumann boundary conditions.

2. Likewise, in the continuous setup the volume constraint as well as the transversality condition with respect to the infinitesimal rotations around the x_3 -axis were resolved by using appropriate Ansatz-functions. This is not possible in the finite-element regime because the goal is to use basis-functions with small simply connected support in order to generate sparse matrices. But it is in general not possible for such functions to satisfy integral constraints which prescribe *global* properties.

Therefore we have to use the transversality constraints (2.42b) and (2.42c) when solving of the discretised linear Euler-Lagrange equation (2.42). This is the reason why (2.42) is a saddle-point problem while the corresponding differential equation (2.34) in the first (sub-) step in the continuous scheme – Algorithm 2.3.2 on page 40 – is not.

REMARK 2.4.10 (EQUIVALENCE OF THE FINITE ELEMENT SPACES)

As introduced in Section 2.3.1 we use the notation

$$(\Gamma_h)_{\psi_h} := \{\text{id}_{\Gamma_h}(X) + \psi_h(X) \mid X \in \Gamma_h\}$$

with $\psi_h \in (W_h(\Gamma_h))^3$. If $(\Gamma_h)_{\psi_h}$ is again a $C^{0,1}$ -immersion then it is also naturally an iso-parametric triangulated surface because $\text{id}_{\Gamma_h} + \psi_h$ is piecewise a polynomial of degree d over the reference element. This implies that the finite element spaces $W_h((\Gamma_h)_{\psi_h})$ and

$W_h(\Gamma_h)$ are isomorphic and norm-equivalent with respect to the H^1 -norm. This is clear because by construction it holds for any $\varphi_h \in W_h(\Gamma_h) < C^{0,1}(\Gamma_h)$ that $\varphi_h \in H_\infty^1(\Gamma_h)$ and *additionally* φ_h and Γ_h are piecewise of class C^∞ (see [ADAMS 1975, Theorem 3.35]).

Therefore we can apply the chain-rule to the pull-back $\psi_h * f_h = f_h \circ \psi_h$ of any function $f_h \in W_h((\Gamma_h)_{\psi_h})$ and so we have $\psi_h * f_h \in W_h(\Gamma_h)$. In particular the notion of a weak-solution is equivalent for $W_h((\Gamma_h)_{\psi_h})$ and $W_h(\Gamma_h)$.

In the discrete regime there is – analogous to Remark 2.3.1 on page 40 – a chain of (weak) diffeomorphisms

$$\Psi_h^{(l)} := \text{id}_{\Gamma_h^{(l)}} - \lambda_l \psi_h^{(l)} \in (W_h(\Gamma_h^{(l)}))^3, l \in \mathbb{N}_0.$$

We can sketch the situation by the following diagram:

$$(2.45) \quad \begin{array}{ccccccc} \Gamma_h^{(0)} & \xrightarrow{\Psi_h^{(0)}} & \Gamma_h^{(1)} & \xrightarrow{\Psi_h^{(1)}} & \dots & \xrightarrow{\Psi_h^{(l-1)}} & \Gamma_h^{(l)} & \xrightarrow{\Psi_h^{(l)}} & \dots \\ W_h(\Gamma_h^{(0)}) & \xleftarrow{\Psi_h^{(0)*}} & W_h(\Gamma_h^{(1)}) & \xleftarrow{\Psi_h^{(1)*}} & \dots & \xleftarrow{\Psi_h^{(l-1)*}} & W_h(\Gamma_h^{(l)}) & \xleftarrow{\Psi_h^{(l)*}} & \dots \end{array}$$

Analogous to the continuous case the equivalence between $W_h(\Gamma_h^{(0)})$ and $W_h(\Gamma_h^{(l)})$ is controlled by the $H_\infty^1(\Gamma_h^{(0)})$ -norm of the chain of (weak) diffeomorphisms $\Psi_h^{(l-1)} \circ \dots \circ \Psi_h^{(0)}$.

REMARK 2.4.11 (STOPPING CRITERION)

As stopping criterion for the discretised Newton method we use a norm of the discrete residual $R_h^{(l)}$ of the non-linear Euler-Lagrange equations as defined in equation (2.41).

The proper norm, of course, would be the operator norm of the right-hand side of the weak formulation (2.42) used in the iteration step (Algorithm 2.4.1 on page 49) above *with respect to the finite element space* $W_h(\Gamma_h^{(0)})$.

From Remark 2.4.10 on the preceding page we see that the computation of this norm would be quite involved. Instead, we use a norm – which one is explained at the end of this remark – of $R_h^{(l)}$ with respect to $W_h(\Gamma_h^{(l)})$. For the continuous case this practice is justified by the fact that we actually have a solution if the continuous Newton iteration converges and the residual of the non-linear Euler-Lagrange equations with respect to the limit surface is zero. So we can hope that a small discrete residual $R_h^{(l)}$ with respect to $W_h(\Gamma_h^{(l)})$ indicates that we have arrived at a good approximation of a smooth drop-shape.

However, it is not clear that the norm of $R_h^{(l)}$ with respect to $W_h(\Gamma_h^{(l)})$ can be used for the step-size control in Algorithm 2.3.1 on page 38 which determines the value of λ_l in each iteration step. The step-size control is intended to enforce convergence when the initial value is *not* close to a solution.

Because the operator norm of the right-hand side of (2.42) with respect to the finite dimensional space $W_h(\Gamma_h^{(l)})$ is just an Euclidean scalar-product we chose the Euclidean standard scalar-product with respect to the nodal basis of $W_h(\Gamma_h^{(l)})$.

REMARK 2.4.12 (SOLVERS FOR THE DISCRETE SYSTEM)

In the nodal basis of $W_h(\Gamma_h^{(l)})$ implied by the Lagrange-nodes of the iso-parametric discrete surface $\Gamma_h^{(l)}$ the linear system (2.42) takes the form

$$(2.46) \quad \left(\begin{array}{c|c} A & B \\ \hline B^{\text{tr}} & 0 \end{array} \right) \cdot \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix},$$

where $A \in \mathbb{R}^{N \times N}$, $B \in \mathbb{R}^{N \times 2}$, $x, b \in \mathbb{R}^N$ and $y, c \in \mathbb{R}^2$, given N is the dimension of $W_h(\Gamma_h^{(l)})$.

We note that A itself is not invertible in general and not positive (semi-) definite. This means that a Schur-complement reformulation of (2.46) is in general not possible. In addition the non-definiteness of A makes it necessary to use a solver for quadratic indefinite systems. We chose to use the `symmlq`-solver which is an iterative *CG*-like solver based on the Lanczos-algorithm, see [PAIGE and SAUNDERS 1975].

It is also not straight-forward to arrive at a good preconditioner, again because A is indefinite. During our experiments we were using a level 1 $\text{ILU}(k)$ -preconditioner for the system matrix as described in [BARRETT et al. 1994, pp. 74]. The important feature of an $\text{ILU}(k)$ -preconditioner S for A is that the profile of S depends only on the profile of A but not on the values of the non-zero entries of A . Therefore a large part of the costly computations to generate the preconditioner can be shared between the iteration-steps of the Newton iteration. In addition we were using the *Gibs-King* algorithm which computes a permutation of the basis of $W_h(\Gamma_h^{(l)})$ to minimise the fill-in of an LU -factorisation. Without such a permutation an $\text{ILU}(k)$ -preconditioner is computationally too costly and only reduces the number of iterations of the solver but does not reduce the computation time.

To be precise, if S is an $\text{ILU}(1)$ -preconditioner for A , then we were using the matrix

$$\left(\begin{array}{c|c} S & 0 \\ \hline 0 & 1 \end{array} \right)$$

as a left-preconditioner for the entire system. Using the $\text{ILU}(1)$ -preconditioner S for A is of course purely experimental. It appears that S often is positive definite and can therefore be used as the matrix of a scalar product; otherwise it would not be straightforward to use it in the left-preconditioner above. The reason why S is in many cases a good preconditioner for A is probably that A has only a few negative eigenvalues.

The general technique of preconditioning is for example explained in [BRAESS 1997] or again in [BARRETT et al. 1994].

2.4.4 An error indicator

In the course of the path-tracking algorithm the surface mesh is heavily deformed. We resolve the degeneration of the surface-elements implied by this deformation by the mesh-smoothing techniques described in the Section 3.4 of Chapter 3 below.

To counterbalance the change in the local node-density which is even amplified by mesh-smoothing (see Figure 3.11 on page 85) we use a local mesh-refinement strategy. The decision which elements should be refined or coarsened is governed by an ad-hoc error indicator which assigns a local error to each element of the iso-parametric triangulation. The indicator function we are using is modelled after an a posteriori error estimator derived by [VERFÜRTH 1994] for quasi-linear elliptic problems.

For an element $T \in \mathcal{T}_h$ with diameter h_T the quantity $\eta_{T,1}$ defined by

$$(2.47) \quad \eta_{T,1}^2 := C_0^2 h_T^2 \| -\Delta_{\Gamma_h} \text{id}_{\Gamma_h} - (4\omega^2 r^2)\nu_{\Gamma_h} \|_{L_2(T)}^2 + C_1^2 h_T \| [[\nu_{\Gamma_h}]] \|_{L_2(\partial T)}^2$$

is used as an indicator for the local H^1 -error. C_0 and C_1 are constants which can be chosen to adapt the error indicator to the real error for exactly known surfaces. $[[\cdot]]$ denotes the jump across element boundaries.

Modelled after an L_2 -estimator derived by [BÄNSCH and SIEBERT 1995] for semi-linear problems we can use $\eta_{T,2}$ defined by

$$(2.48) \quad \eta_{T,2}^2 := C_0^2 h_T^4 \| -\Delta_{\Gamma_h} \text{id}_{\Gamma_h} - (4\omega^2 r^2)\nu_{\Gamma_h} \|_{L_2(T)}^2 + C_2^2 h_T^3 \| [[\nu_{\Gamma_h}]] \|_{L_2(\partial T)}^2$$

as an ad-hoc L_2 -error-indicator.

Below in Chapter 4 we will compare the global error indicators

$$\eta_1 := \sqrt{\sum_{T \in \mathcal{T}_h} \eta_{T,1}^2} \quad \text{and} \quad \eta_2 := \sqrt{\sum_{T \in \mathcal{T}_h} \eta_{T,2}^2}$$

with the real H^1 - and L_2 -errors of some approximate solutions generated by the Newton scheme.

For the adaption of the mesh with the error indicator $\eta_{T,1}$ or $\eta_{T,2}$ we were using the *equal distribution strategy* which aims at equally distributing the error over all mesh elements in the sense of squared mean values. This is explained in detail in [ERIKSON and JOHNSON 1991].

We remark that we leave the topology of the mesh unchanged during the discrete Newton iteration which generates the drop-shapes. It was our experience that mesh-adaption in between the iteration steps caused the Newton method to fail completely. We therefore adapt the mesh after the Newton iteration has terminated using the error indicators described above.

2.5 The solving of the bifurcation equation

2.5.1 Finding of bifurcation points

As a necessary condition for the existence of a bifurcation point in the sense of Definition 1.3.26 on page 15 the linearised Euler-Lagrange equation (2.23) on page 28 must have non-trivial solutions. Using the notations of the Newton iteration described in the

previous sections this means that 0 is an eigenvalue of the Fréchet-derivative $L_\omega(\Xi)$ of the non-linear operator $A_\omega(\Xi)$ (assuming that A is Fréchet-differentiable with respect to ω and Ξ). If A_ω is continuously Fréchet-differentiable then the spectrum of the linearisation depends continuously on ω and Theorem 1.3.28 on page 15 guarantees that at a simple eigenvalue 0 of L_ω there is indeed a bifurcation point. Additionally, the same theorem establishes that the corresponding eigenfunction of L_ω approximates the drop-shapes of the new branch.

The remarks above motivate the Algorithm 2.5.1 for the finding of branch points and constructing an initial value for the path-tracking algorithm such that we can track down the new branch. The method arises naturally from the approximation property of the eigenfunctions corresponding to a 0 eigenvalue and was used before by others, see for example [BROWN and SCRIVEN 1980a].

Algorithm 2.5.1 Flow-chart for the finding of new branches during the path-tracking algorithm. The adaptive computation of the drop shapes is illustrated in Algorithm 2.6.1 on page 58. n^- denotes the number of negative eigenvalues of the linearised operator (see (2.50) on the next page).

A central point of Algorithm 2.5.1 is the computation of all negative eigenvalues of the linearised operator. In the compact notation used above this means to find the smallest few eigenvalues of L_ω where the eigenvalues of L_ω are determined by solving the equation

$$(2.49) \quad L_\omega \Xi = \lambda \Xi$$

for Ξ and λ . We remark that there are only finitely many negative eigenvalues because the spectrum of the Laplace-Beltrami operator Δ_Γ (Γ compact Riemannian) is bounded from below, see [AUBIN 1982, Theorem 4.2].

Further, all (discrete) bifurcations we have found during our numerical experiments were bifurcations from “effectively” simple eigenvalues in the sense that occasionally a multiplicity of 2 was caused by the invariance of the linearised differential equation with respect to (infinitesimal) rotations around the x_3 -axis.

Our final remark in this section is that Algorithm 2.5.1 on the preceding page is a “shooting”-method. If it doesn’t find a new branch at a value of ω^{br} where an eigenvalue changes its sign then this does *not* imply that there is no branch-point. This is clear because the convergence of the Newton iteration depends on its initial value.

2.5.2 The discretisation of the bifurcation equation

For completeness we give here the discretisation of the eigenvalue equation (2.49) where we use the notations introduced in the construction of the discrete Newton iteration in the previous section. The discretisation of the eigenvalue equation follows from the first (sub-) step of the discrete Newton iteration-step Algorithm 2.4.1 on page 49. We assume that $(\Gamma_h, C_h) \equiv (\Gamma_{h,k}, C_{h,k}) \equiv \Xi_{h,k}$ is the k^{th} -surface constructed during the discrete path-tracking algorithm ($k \in \mathbb{N}$). So (Γ_h, C_h) is an approximate limit of the discrete Newton method. We then arrive at the following discrete eigenvalue-problem which has to be solved for $(\bar{\psi}_h, K_h) \in W_h(\Gamma_h) \times \mathbb{R}$, $\theta \in \mathbb{R}$:

$$(2.50) \quad \left\{ \begin{array}{l} \int_{\Gamma_h} \nabla_{\Gamma_h} \bar{\psi}_h \cdot \nabla_{\Gamma_h} \bar{\eta}_h \, do - \int_{\Gamma_h} \bar{a}_h \bar{\psi}_h \bar{\eta}_h \, do \\ \quad - K_h^{(l)} \int_{\Gamma_h} \bar{\eta}_h \, do - \theta^{(l)} \int_{\Gamma_h} \bar{\Theta} \bar{\eta}_h \, do = \lambda \int_{\Gamma_h} \bar{\psi}_h \bar{\eta}_h \, do, \\ \int_{\Gamma_h} \bar{\psi}_h \, do = 0, \\ \int_{\Gamma_h} \bar{\psi}_h \bar{\Theta} \, do = 0, \\ \text{for all } \bar{\eta} \in W_h(\Gamma_h). \end{array} \right.$$

See Remark 2.4.9 on page 50 for a discussion of the imposed constraints and the Neumann boundary conditions.

2.5.3 Solvers for the constraint eigen-problem

The matrices of the linear system (2.50) in the nodal basis of $W_h(\Gamma_h)$ implied by the Lagrange-nodes of the iso-parametric discrete surface Γ_h are just the same as for the solution of the linear system in the discrete Newton method with the exceptions that the mass-matrix $M \in \mathbb{R}^{N \times N}$ appears on the right-hand side of the matrix equation. Using

the same notation as for the matrix equation (2.46) on page 52 for the linear-system of the discrete Newton iteration-step we get the following generalised eigenvalue-problem:

$$(2.51) \quad \left(\begin{array}{c|c} A & B \\ \hline B^{\text{tr}} & 0 \end{array} \right) \cdot \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \left(\begin{array}{c|c} M & 0 \\ \hline 0 & 0 \end{array} \right) \begin{bmatrix} x \\ y \end{bmatrix},$$

where the unknowns are the eigenvalues λ and the eigenvectors $(x, y)^{\text{tr}}$.

[BROWN and SCRIVEN 1980a] use a Cholesky decomposition of A to transform (2.51) into a standard eigenvalue problem which then is solved using the Lanczos-algorithm. For large linear systems this leads to problems even when using a permutation to reduce the bandwidth of the Cholesky factorisation. The reason is that the matrices generated by a LU-factorisation from a sparse matrix are no longer sparse.

Apart from this the Cholesky decomposition seems to lead to problems for large systems in the sense that the solver for the standard eigenvalue problem failed to converge.

Another – possibility sometimes called “shift and invert” – is to choose an $s \in \mathbb{C}$ such that

$$\left(\begin{array}{c|c} A & B \\ \hline B^{\text{tr}} & 0 \end{array} \right) - s \left(\begin{array}{c|c} M & 0 \\ \hline 0 & 0 \end{array} \right)$$

is invertible and use the inverse of this matrix to transform (2.51) into a standard eigenvalue problem. This method is described in detail in [LEHOUCQ et al. 1998].

For both methods it is essential to first compute a permutation of the nodal basis of $W_h(\Gamma_h)$ basis which minimises the fill-in of LU-factorisations. The permutation dramatically reduces the amount of memory needed for the Cholesky-factorisation and in the case of the “shift and invert” method it is needed for the ILU(k)-preconditioner in the inversion of the matrix, see our Remark 2.4.12 on page 52.

After converting the generalised eigenvalue problem (2.51) to standard form the Lanczos algorithm can be used to compute approximations to all negative eigenvalues and the corresponding eigenfunctions. For this purpose we have employed the *ARPACK* package, see [LEHOUCQ et al. 1998].

2.6 The discrete path-tracking algorithm

This last section of Chapter 2 gives finally an overview over the complete discrete path-tracking algorithm which is sketched in the flow-chart Algorithm 2.6.1 on page 58.

The goal is to compute a discrete set $\mathcal{S}_h = \{(\Gamma_h^k, C_h^k)\}$ of iso-parametric surfaces each approximating a smooth solution (Γ^k, C^k) of the non-linear Euler-Lagrange equations (2.6) on page 23. $\mathcal{S}_h$ should have the property that, whenever (Γ^k, C^k) and (Γ^{k+1}, C^{k+1}) enclose a bifurcation point $(\Gamma^{\text{br}}, C^{\text{br}})$, then $(\Gamma^{\text{br}}, C^{\text{br}})$ as well as a discrete set of approximate solutions belonging to the new branch should also be part of $\mathcal{S}_h = \{(\Gamma_h^k, C_h^k)\}$. It is, of course, impossible to achieve this goal with our method (see our remark at the end of Section 2.5.1).

The flow-chart Algorithm 2.6.1 on the following page illustrates the discrete path-tracking algorithm. A central part is the computation of the discrete drop-shapes. To generate a single new surface Γ_h^{k+1} at a new angular velocity $\omega_{k+1} := \omega_k + \Delta_\omega$ from its predecessor Γ_h^k the following steps are needed:

- improve the regularity of the surface mesh by mesh-smoothing techniques, see Section 3.4 below,
- compute an intermediate new surface with the discrete Newton iteration, see Section 2.4,
- adapt the iso-parametric triangulation to the non-linear Euler-Lagrange equations (2.6) using the error indicators described in Section 2.4.4 – do this at least once even if the accumulated error indicator is below the given bound. The latter is used to counterbalance the redistribution of the nodes caused by the deformation of the mesh and by the mesh-smoothing.

This procedure is iterated until a given bound for the accumulated error indicator (see Section 2.4.4 above) is fulfilled.

Another point is that we have to adapt the step size Δ_ω with respect to the angular velocity. If Δ_ω is too large then the initial value for the Newton iteration is too far away from the new solution at $\omega_k + \Delta_\omega$ and the Newton iteration does not converge. We use a simple “divide by 2 and multiply by $\sqrt{2}$ ” scheme as shown in the flow-chart Algorithm 2.6.1 on the next page.

The finding of bifurcation points was already described in Algorithm 2.5.1 on page 54 (Section 2.5). It searches for branch points and if it finds one, it tries to generate a new discrete surface Γ_h^{new} which already belongs to the new branch. If it finds such a Γ_h^{new} then a new instance of the path-tracking Algorithm 2.6.1 on the next page is started, this time with Γ_h^{new} as initial surface.

The following Chapter 3 deals with numerical methods of iso-parametric triangulations in general and the last Chapter 4 deals with the results of our numerical experiments.

Algorithm 2.6.1 Flow-chart for the adaptive computation of drop-shapes as part of the path-tracking algorithm. The finding of bifurcation points is illustrated in Algorithm 2.5.1 on page 54.

Chapter 3

Numerical methods for iso-parametric meshes

The implementation of the discretisation of the path-tracking algorithm described in the previous chapter was based on version 0.2 of the finite element toolbox ALBERT [SCHMIDT and SIEBERT 1998]. ALBERT provides abstract data-structures and library functions for the management of locally adaptive finite element algorithms on simplicial meshes in space-dimension 2 and 3. It supplies the user with predefined Lagrange finite element spaces up to polynomial degree 4, including the management of degrees of freedom, numerical quadrature and the abstract implementation of adaptive algorithms.

The treatment of parametric meshes was already well prepared to a certain extent, in particular the geometric dimension of the mesh-coordinates was separated from the dimension of the reference simplex. Based on the frame-work provided by the provisional version 0.2 of ALBERT we have implemented support for iso-parametric surfaces meshes up to arbitrary polynomial degree ALBERT supports.

This chapter is concerned with four important aspects which arise in the handling of iso-parametric meshes *without* discussing the actual coding of the algorithms in the context of ALBERT.

In the first two sections we define discrete versions of geometric quantities, namely the outer unit normal field and – far more important – the notion of a discrete curvature for $C^{0,1}$ -surfaces.

The third Section 3.3 discusses in brief local mesh refinement and coarsening. In Section 3.4 we explain in greater detail mesh-smoothing techniques. Mesh-smoothing is a crucial point when using “moving-mesh” methods like our discretisation of the path-tracking algorithm in the previous chapter.

3.1 Approximate normals

For the implementation of the discrete Newton iteration as well as for the mesh-smoothing algorithm we need a continuous approximate normal field for a discrete

n -dimensional (hyper-) surface $\Gamma_h^d \subset \mathbb{R}^{n+1}$ and for its linear interpolation Γ_h^1 . In the following we can drop the upper index and set $\Gamma_h := \Gamma_h^d$ and $W_h(\Gamma_h) := W_h^d(\Gamma_h^d)$.

[SCHMIDT 1993] defines a continuous approximate normal field by an averaging process effectively lumping the mass-matrix of the finite element space W_h as is explained below.

At a Lagrange-node $P \in \Gamma_h$ we define an average normal $\nu_h^{av}(P)$ as a weighted mean-value of the element normals of its adjacent triangles,

$$(3.1) \quad \tilde{\nu}_h^{av} := \frac{\sum_{T \in S(P)} |T| \nu_T}{\sum_{T \in S(P)} |T|}, \quad \nu_h^{av}(P) := \frac{1}{\|\tilde{\nu}_h^{av}(P)\|} \tilde{\nu}_h^{av}(P),$$

where $S(P)$ denotes the “star” around P (meaning the set of elements adjacent to P) and ν_T the exact unit normal field of the iso-parametric n -simplex T . The approximate normal-field $\nu_h^{av} \in W_h$ is then the Lagrange-interpolation between the values $\nu_h^{av}(P)$ at the nodes of the iso-parametric triangulation $\mathcal{T}_h$.

[SCHMIDT 1993] remarks that we get the same value for ν_h^{av} when defining it by the L_2 -projection of ν_T to $(W_h(\Gamma_h))^{n+1}$

$$(3.2) \quad (\tilde{\nu}_h^{L_2}, \psi_h)_{L_2(\Gamma_h)} := \sum_{T \in \mathcal{T}_h} (\nu_T, \psi_h)_{L_2(T)} \quad \forall \psi_h \in W_h(\Gamma_h), \quad \nu_h^{L_2} := \frac{1}{\|\tilde{\nu}_h^{L_2}\|} \tilde{\nu}_h^{L_2},$$

if we use lumping for the mass-matrix on the left-hand side or a simple formula for the numerical quadrature on the left-hand side. So $\nu_h^{L_2} = \nu_h^{av}$ in this case. The topic of lumping and the associated error-estimates are described in [THOMÉE 1980].

In the presence of ill-shaped elements it might be better to use the angles $\angle(P, T)$ adjacent to the point P as weight factor instead of the area $|T|$ of its adjacent elements (see the figure below for the notation):

$$(3.3) \quad \tilde{\nu}_h^{\angle}(P) := \sum_{T \in S(P)} \angle(P, T) \nu_T, \quad \nu_h^{\angle}(P) := \frac{1}{\|\tilde{\nu}_h^{\angle}(P)\|} \tilde{\nu}_h^{\angle}(P).$$

The difference between ν_h^{av} , $\nu_h^{L_2}$ and $\nu_h^{\angle}$ should be neglectable for regular-shaped iso-parametric triangulations. $\nu_h^{\angle}$ probably gives better results at the vertices P , because it stresses the fact that the direction of the normal at P is a *local* property of the surface Γ_h at P .

We note that the computational costs for the path-tracking algorithm described in the previous chapter are governed by the computation of the eigenvalues of the linearised Euler-Lagrange equations. This means that the computational costs of the three different averaging processes (3.1)-(3.3) are not an issue here.

We have implemented all three methods in the context of the finite element-toolbox ALBERT. Generally, we were using the exact L_2 -projection $\nu_h^{L_2}$ as defined in equation

(3.2) for the discretised Newton iteration described in the previous chapter and the angle-weighted averaged normals $\nu_h^\angle$ of equation (3.3) in the projection step of the mesh-smoothing algorithm, which is described in detail in Section 3.4.4.

We will not comment further on our particular choice and use the notation ν_h for either of the three possibilities.

3.2 Curvature for Discrete Surfaces

The linearisations (2.23) and (2.24) on page 28 of the Euler-Lagrange Equations (2.6) on page 23 contains the square sum $\kappa_1^2 + \kappa_2^2 = \det II^2 = 2(2H^2 - K)$ of the principal curvatures of the surface Γ of the drop. The present formulation of the Newton iteration needs a point-wise definition of this quantity as well as a point-wise definition of the mean-curvature for the computation of the residual in each Newton-step.

This would not be a problem for surfaces of class at least C^2 . However, the surfaces Γ_h^n of the discretised Newton iteration are only of class $C^{0,1}$. So it is not obvious how to define a good point-wise approximation for the curvature needed for the discretisation of the Newton-scheme.

In this section we define a discrete curvature for surfaces of class $C^{0,1}$. At the end we will present some experimental convergence tests for $C^{0,1}$ -surfaces obtained by finite element approximations.

3.2.1 Definition of the Discrete Curvature

3.2.1 DEFINITION (PROJECTION)

Let $W < X$, X a vector space. $\Pi \in L(X, W)$ is called a projection from X onto W , if Π is surjective and idempotent.

3.2.2 LEMMA (H^{-1} -PROJECTION)

Let Γ be a compact $C^{0,1}$ manifold without boundary, $W < H^1(\Gamma_h)$. Further, we denote by $\langle\langle \cdot, \cdot \rangle\rangle : H^{-1}(\Gamma) \times H^1(\Gamma) \rightarrow \mathbb{R}$ the dual pairing. Then the map

$$\Pi : H^{-1}(\Gamma) \rightarrow W$$

defined by

$$(\Pi v, \psi)_{L_2(\Gamma)} = \langle\langle v, \psi \rangle\rangle \quad \forall \psi \in W$$

is a projection from $H^{-1}(\Gamma)$ onto $(W, \|\cdot\|_{L_2(\Gamma)})$.

Proof: This is clear because the L_2 -norm is weaker than the H_2^1 -norm. □

REMARK 3.2.1 In general $(W, \|\cdot\|_{L_2(\Gamma)})$ is not a Hilbert-space even if $W < H^1(\Gamma_h)$ is closed.

For smooth C^2 -surfaces $\Gamma \subset \mathbb{R}^{n+1}$ we have the identity

$$Y_\Gamma = -\Delta_\Gamma \text{id}_\Gamma, \quad \text{with } Y_\Gamma := n H \nu.$$

as was shown in Lemma 1.3.22 on page 13. So it follows for all $\psi \in (H^1(\Gamma))^{n+1}$

$$\int_\Gamma Y_\Gamma \cdot \psi \, d\Gamma = - \int_\Gamma \Delta_\Gamma \text{id}_\Gamma \cdot \psi \, d\Gamma = \int_\Gamma \nabla_\Gamma \text{id}_\Gamma \cdot \nabla_\Gamma \psi \, d\Gamma.$$

3.2.3 DEFINITION (DISCRETE CURVATURE VECTOR)

Let Γ_h be a $C^{0,1}$ approximation of a C^2 manifold $\Gamma \subset \mathbb{R}^{n+1}$ with $W_h \leq H^1(\Gamma_h)$ such that $\text{id}_{\Gamma_h} \in (W_h)^{n+1}$. Then the discrete curvature vector $Y_h \in (W_h)^{n+1}$ is defined as the solution of

$$(3.4) \quad (Y_h, \psi_h)_{L_2(\Gamma_h)} = (\nabla_{\Gamma_h} \text{id}_{\Gamma_h}, \nabla_{\Gamma_h} \psi_h)_{L_2(\Gamma_h)} \quad \forall \psi_h \in (W_h)^{n+1}.$$

This definition follows [SCHMIDT 1993]. There it is shown that Y_h is the H^{-1} projection of the functional $-\Delta_{\Gamma_h} \text{id}_{\Gamma_h} \in H^{-1}(\Gamma_h)$ defined by

$$\langle \langle -\Delta_{\Gamma_h} \text{id}_{\Gamma_h}, \psi \rangle \rangle := -(\nabla_{\Gamma_h} \text{id}_{\Gamma_h}, \nabla_{\Gamma_h} \psi)_{L_2(\Gamma_h)} \quad \text{for } \psi \in H^1(\Gamma_h).$$

The experimental convergence tests for the case of a sphere presented in [SCHMIDT 1993] show approximate linear convergence in the L^2 and L^∞ norms for quadratic Lagrange elements and no convergence for linear elements.

For the definition of the scalar mean and Gaussian curvature we have a look at the Weingarten map. Again, let Γ be a smooth surface. Then the principal curvatures are the non-zero eigenvalues of the Weingarten map

$$II : \Gamma \rightarrow \mathbb{R}_{\text{sym}}^{3 \times 3} : x \mapsto \nabla_\Gamma \nu_\Gamma(x),$$

which is just the differential of the Gauß-map trivially extended to $T_p \Gamma^\perp$ and written in Cartesian coordinates, see Remark 1.3.8 on page 12.

To derive a weak formulation for II we multiply the equation $II_j = \nabla_\Gamma(\nu_\Gamma)_j$ by a test-function $\psi \in H^1(\Gamma)$ and integrate over Γ . Then using the integration by parts formula (1.9) from on page 13 we arrive at

$$\int_\Gamma II_j \cdot \psi \, do = \int_\Gamma \nabla_\Gamma(\nu_\Gamma)_j \cdot \psi \, do = - \int_\Gamma (\nu)_j \nabla_\Gamma \cdot \psi \, do - 2 \int_\Gamma H(\nu_\Gamma)_j \psi \cdot \nu \, do.$$

We employ this relation to define a discrete Weingarten map II_h on a discrete surface Γ_h :

3.2.4 DEFINITION (DISCRETE WEINGARTEN MAP)

Let Γ_h be an $C^{0,1}$ approximation of a C^2 manifold $\Gamma \subset \mathbb{R}^{n+1}$ with $W_h \subset H^1(\Gamma_h)$ such that $\text{id}_{\Gamma_h} \in (W_h)^{n+1}$. Then the discrete Weingarten map $II_h \in (W_h)^{(n+1) \times (n+1)}$ is defined as the solution of

$$(3.5) \quad ((II_h)_j, \psi_h)_{L_2(\Gamma_h)} = -((\nu_h)_j, \nabla_{\Gamma_h} \cdot \psi_h)_{L_2(\Gamma_h)} - ((\nu_h)_j, Y_h \cdot \psi_h)_{L_2(\Gamma_h)} \\ \text{for all } \psi_h \in (W_h)^{n+1},$$

where Y_h is the discrete curvature vector defined in (3.4) and ν_h is the (discontinuous) normal field of Γ_h .

The discrete mean curvature H_h and discrete Gaussian curvature K_h (the latter only in the case of $n = 2$) are defined by

$$(3.6) \quad H_h := \frac{1}{2} \text{trace} II_h, \quad K_h := \det(II_h + I_3) - 2H_h - 1.$$

REMARK 3.2.2 $II_h \in (W_h)^{(n+1) \times (n+1)}$ is the H^{-1} projection of the functional

$$\nabla_{\Gamma_h} \nu_h \in (H^{-1}(\Gamma_h))^{(n+1) \times (n+1)}$$

defined by

$$\langle \langle \nabla_{\Gamma_h} \nu_h, \psi \rangle \rangle := -((\nu_h)_j, \nabla_{\Gamma_h} \cdot \psi)_{L_2(\Gamma_h)} - ((\nu_h)_j, Y_h \cdot \psi)_{L_2(\Gamma_h)} \quad \forall \psi \in (H^1(\Gamma_h))^{n+1}.$$

3.2.2 Convergence tests

Figure 3.1 Surface meshes for testing our definition of the discrete curvature. The defining equations for the surfaces are 3.7b to 3.7d on this page. A picture for 3.7a has been omitted as it is of the same type as the surface shown in (a), but with smaller Gaussian curvature.

Table 3.1 to 3.4 on pages 65–68 show the results of our experimental convergence tests with piecewise polynomial discretisations of degree 1, 2, 3 and 4 for the following model problems (see Figure 3.1):

$$(3.7a) \quad (x - z^2)^2 + y^2 + z^2 - 1 = 0$$

$$(3.7b) \quad (x - z^2)^2 + (y - z^2)^2 + z^2 - 1 = 0$$

$$(3.7c) \quad x^2 + (2y)^2 + \left(\frac{2}{3}z\right)^2 - 1 = 0$$

$$(3.7d) \quad x^2 + y^2 + z^2 - 1 = 0$$

The underlying macro triangulation for the discretisation of all model-problems is an icosahedron. The discrete surface Γ_h is just the interpolation of the exact shape Γ with Lagrange-polynomials. Γ is viewed as a graph in approximate normal direction over the discrete surface Γ_h .

At first the mesh was refined adaptively until the L_2 error with respect to the exact surface was below 0.005. Afterwards the meshes were refined globally by doubly bisecting the elements in each refinement step.

The tables 3.1 to 3.4 on pages 65–68 show the number of unknowns, the maximal mesh width, the relative L_2 and L_∞ errors and the experimental order of convergence (*EOC*) of the discrete mean and Gaussian curvatures H_h and K_h as defined in (3.6).

For the normalisation of the relative errors we use the curvature of the exact surfaces defined by 3.7a to 3.7d on the page before:

$$\mathcal{E}_{C,r} := \frac{\|C - C_h\|_{L_r(\Gamma_h)}}{\|C\|_{L_r(\Gamma_h)}}, \quad \text{where } C \in \{K, H\}, \quad r \in \{2, \infty\}.$$

As usual, the experimental order of convergence is defined as

$$EOC := \frac{\log \frac{\mathcal{E}_j}{\mathcal{E}_{j+1}}}{\log \frac{h_j}{h_{j+1}}}.$$

While it is not surprising that the discrete curvatures originating from Definition 3.2.4 on page 62 do not converge for linearly interpolated surfaces, the experimental order of convergence for higher order parametrisations is surprising.

The tables 3.1 to 3.4 on pages 65–68 suggest that for Lagrange-interpolates of polynomial degree k the experimental order of convergence for the discrete curvature is greater than $k - 1$, provided that $k > 1$.

It should be stressed that we did *not* interpolate the curvatures of the C^∞ surfaces defined by 3.1 to 3.4 on pages 65–68 with finite elements, but just the surfaces themselves. This means that the errors shown in Table 3.1 to 3.4 on pages 65–68 are not mere interpolation errors. We would have expected values for the *EOC* of at most $k - 1$, but not greater.

It should also be stressed that the results for the less complicated surfaces (3.7c) (an ellipsoid) and (3.7d) (a sphere) (see Table 3.3 on page 67 and 3.4 on page 68) are not as suggestive as the results for the more complicated surfaces. Table 3.3 on page 67 and 3.4 on page 68 show a *decreasing EOC* as the number of unknowns increases.

This might indicate that the values for the *EOC* as shown in the tables 3.1 on the next page and 3.2 on page 66 just did not stabilise yet.

We presume that it is sufficient to use Lagrange finite elements of order 2 for the parametrisation of the discretised surfaces; even with respect to the L_∞ -norm the discretised curvature of the interpolating surface seems to converge to the exact curvature of the C^∞ surface.

To our knowledge no analytical results are known with respect to this problem.

Table 3.1 Discrete curvature, problem 1, relative errors

Polynomial degree: 1									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
2593	0.135	0.79	.	1.4	.	0.19	.	0.36	.
10366	0.0689	0.87	-0.16	2.2	-0.61	0.19	0.055	0.36	-0.028
41458	0.0361	0.9	-0.041	2.1	0.015	0.19	-0.0011	0.4	-0.15
165826	0.0199	0.91	-0.022	2.3	-0.12	0.19	-0.0065	0.42	-0.081
663298	0.0114	0.91	-0.0072	2.3	-0.02	0.19	-0.0042	0.43	-0.024
2653186	0.00654	0.91	-0.0023	2.3	-0.0059	0.19	-0.0021	0.43	-0.0092

Polynomial degree: 2									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
522	0.372	1.7	.	2.5	.	0.15	.	0.48	.
2082	0.206	1.	0.85	2.7	-0.14	0.085	0.92	0.31	0.75
8322	0.118	0.54	1.2	1.5	1.	0.044	1.2	0.15	1.3
33282	0.0681	0.2	1.8	0.69	1.4	0.02	1.4	0.067	1.5
133122	0.0382	0.082	1.6	0.44	0.78	0.0099	1.3	0.044	0.74
532482	0.0219	0.032	1.7	0.13	2.2	0.0047	1.3	0.018	1.6
2129922	0.0123	0.015	1.4	0.044	1.9	0.0023	1.2	0.0088	1.2

Polynomial degree: 3									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
848	0.488	1.5	.	3.6	.	0.13	.	0.49	.
3386	0.32	2.1	-0.83	5.4	-1.	0.15	-0.26	0.58	-0.4
13538	0.191	1.1	1.1	6.3	-0.3	0.087	1.	0.62	-0.12
54146	0.11	0.17	3.5	1.3	2.9	0.022	2.5	0.17	2.3
216578	0.064	0.054	2.1	0.46	1.9	0.0068	2.1	0.083	1.4
866306	0.0359	0.014	2.3	0.13	2.2	0.0018	2.3	0.026	2.
3465218	0.0202	0.0036	2.4	0.034	2.3	0.00046	2.4	0.0069	2.3

Polynomial degree: 4									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
754	0.549	4.5	.	13.	.	0.3	.	1.4	.
3010	0.324	1.6	2.	8.6	0.77	0.12	1.8	0.75	1.2
12034	0.196	0.34	3.1	1.5	3.5	0.035	2.4	0.24	2.3
48130	0.121	0.04	4.4	0.5	2.2	0.0048	4.1	0.055	3.
192514	0.0697	0.0047	3.9	0.046	4.3	0.00074	3.4	0.0092	3.2
770050	0.0402	0.00061	3.7	0.0062	3.6	9.1e-05	3.8	0.0012	3.7
3080194	0.0232	7.4e-05	3.8	0.00068	4.	1.1e-05	3.8	0.00015	3.8

Table 3.2 Discrete curvature, problem 2, relative errors

Polynomial degree: 1									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
2673	0.205	1.7	.	1.9	.	0.39	.	0.69	.
10686	0.0957	1.4	0.22	1.7	0.14	0.24	0.64	0.59	0.21
42738	0.0508	1.5	-0.11	2.3	-0.44	0.2	0.29	0.37	0.75
170946	0.0263	1.7	-0.19	3.3	-0.56	0.19	0.057	0.37	-0.025
683778	0.0151	1.8	-0.091	3.7	-0.21	0.19	-0.0025	0.41	-0.17
2735106	0.00864	1.8	-0.033	3.7	-0.037	0.2	-0.0041	0.43	-0.085

Polynomial degree: 2									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
970	0.368	2.7	.	5.2	.	0.25	.	0.58	.
3874	0.204	4.4	-0.83	11.	-1.3	0.15	0.9	0.42	0.52
15490	0.116	2.4	1.1	6.4	1.	0.073	1.2	0.31	0.53
61954	0.0673	0.96	1.7	3.8	0.95	0.039	1.2	0.21	0.71
247810	0.0379	0.34	1.8	1.6	1.5	0.018	1.3	0.087	1.6
991234	0.0214	0.11	2.	0.47	2.2	0.0085	1.4	0.039	1.4

Polynomial degree: 3									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
1559	0.468	12.	.	19.	.	0.45	.	0.84	.
6230	0.322	13.	-0.15	29.	-1.1	0.34	0.73	1.1	-0.78
24914	0.19	10.	0.39	50.	-1.1	0.19	1.2	1.4	-0.4
99650	0.113	1.3	4.	8.	3.5	0.055	2.3	0.43	2.3
398594	0.0653	0.36	2.3	3.6	1.4	0.022	1.7	0.27	0.82
1594370	0.0373	0.086	2.6	0.88	2.5	0.0062	2.2	0.1	1.8

Polynomial degree: 4									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
1874	0.477	15.	.	39.	.	0.45	.	1.2	.
7490	0.304	8.	1.4	58.	-0.87	0.22	1.6	1.3	-0.16
29954	0.196	1.2	4.3	9.2	4.2	0.055	3.2	0.45	2.5
119810	0.115	0.22	3.3	3.1	2.	0.013	2.7	0.14	2.2
479234	0.0655	0.022	4.1	0.34	3.9	0.0019	3.5	0.026	3.
1916930	0.0374	0.0024	3.9	0.025	4.7	0.00023	3.8	0.0032	3.7

Table 3.3 Discrete curvature, problem 3, relative errors

Polynomial degree: 1									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
1799	0.2	0.76	.	1.4	.	0.19	.	0.45	.
7190	0.117	0.83	-0.14	1.7	-0.39	0.18	0.056	0.39	0.25
28754	0.0674	0.83	-0.0022	1.7	0.028	0.18	0.019	0.43	-0.2
115010	0.0384	0.83	-0.0086	1.7	-0.098	0.18	-0.0021	0.48	-0.17
460034	0.0218	0.83	-0.0067	1.7	0.0033	0.18	-0.0034	0.54	-0.2
1840130	0.0127	0.84	-0.0037	1.8	-0.012	0.18	-0.0019	0.59	-0.19

Polynomial degree: 2									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
514	0.295	0.69	.	1.6	.	0.086	.	0.27	.
2050	0.19	0.49	0.77	1.7	-0.23	0.06	0.81	0.23	0.41
8194	0.107	0.21	1.5	1.1	0.85	0.026	1.4	0.12	1.1
32770	0.0588	0.069	1.8	0.47	1.4	0.011	1.5	0.063	1.1
131074	0.0309	0.025	1.6	0.17	1.6	0.0049	1.2	0.031	1.1
524290	0.0159	0.011	1.3	0.056	1.7	0.0024	1.1	0.013	1.3
2097154	0.00833	0.0051	1.2	0.026	1.2	0.0012	1.1	0.0064	1.1

Polynomial degree: 3									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
1082	0.309	2.2	.	8.3	.	0.23	.	1.	.
4322	0.198	0.76	2.3	3.4	2.	0.09	2.1	0.59	1.2
17282	0.131	0.16	3.8	1.2	2.6	0.025	3.1	0.19	2.8
69122	0.0788	0.041	2.7	0.31	2.6	0.0067	2.6	0.063	2.1
276482	0.0457	0.011	2.5	0.086	2.4	0.0017	2.5	0.019	2.2
1105922	0.0259	0.0027	2.4	0.024	2.2	0.00044	2.4	0.0052	2.3
4423682	0.0145	0.00067	2.4	0.0063	2.3	0.00011	2.4	0.0014	2.3

Polynomial degree: 4									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
978	0.443	7.5	.	72.	.	0.39	.	4.1	.
3906	0.265	0.23	6.8	2.5	6.5	0.04	4.4	0.36	4.7
15618	0.153	0.024	4.1	0.24	4.3	0.0056	3.6	0.065	3.1
62466	0.0908	0.0027	4.2	0.027	4.2	0.00063	4.2	0.0059	4.6
249858	0.0527	0.00034	3.8	0.004	3.5	8e-05.	3.8	0.0012	2.9
999426	0.0297	4.3e-05	3.6	0.00057	3.4	1e-05.	3.6	0.00018	3.4
3997698	0.0168	5.5e-06	3.6	9.9e-05	3.1	1.3e-06	3.6	2.8e-05	3.2

Table 3.4 Discrete curvature, problem 4, relative errors

Polynomial degree: 1									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
2346	0.126	0.41	.	1.1	.	0.17	.	0.43	.
9378	0.0717	0.41	-0.015	1.2	-0.19	0.18	-0.014	0.47	-0.13
37506	0.0407	0.42	-0.0048	1.2	0.088	0.18	-0.0062	0.45	0.085
150018	0.0231	0.42	-0.0038	1.2	0.012	0.18	-0.0041	0.44	0.012
600066	0.0131	0.42	-0.0022	1.2	0.0027	0.18	-0.0023	0.44	0.0022
2400258	0.00743	0.42	-0.0012	1.2	0.0011	0.18	-0.0012	0.48	-0.13

Polynomial degree: 2									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
202	0.395	0.052	.	0.18	.	0.021	.	0.082	.
802	0.242	0.025	1.5	0.13	0.74	0.0055	2.7	0.031	2.
3202	0.138	0.0073	2.2	0.048	1.7	0.0014	2.5	0.01	2.
12802	0.0784	0.0019	2.4	0.016	1.9	0.00034	2.4	0.0033	2.
51202	0.0441	0.00049	2.4	0.0053	2.	8.6e-05	2.4	0.001	2.
204802	0.0249	0.00012	2.4	0.0017	2.	2.2e-05	2.4	0.00033	2.
819202	0.014	3.1e-05	2.4	0.00053	2.	5.4e-06	2.4	0.00011	2.
3276802	0.00787	7.7e-06	2.4	0.00017	2.	1.4e-06	2.4	3.3e-05	2.

Polynomial degree: 3									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
272	0.515	0.27	.	2.5	.	0.11	.	0.54	.
1082	0.284	0.096	1.7	0.52	2.6	0.048	1.5	0.23	1.4
4322	0.154	0.021	2.5	0.12	2.4	0.011	2.4	0.06	2.2
17282	0.0863	0.0048	2.5	0.037	2.	0.0028	2.4	0.02	1.9
69122	0.0486	0.0012	2.4	0.01	2.2	0.0007	2.4	0.0061	2.1
276482	0.0273	0.00031	2.4	0.0032	2.	0.00018	2.4	0.0019	2.
1105922	0.0154	7.8e-05	2.4	0.001	2.	4.5e-05	2.4	0.00061	2.
4423682	0.00856	2e-05.	2.4	0.00034	1.9	1.1e-05	2.4	0.0002	1.9

Polynomial degree: 4									
#unkn.	h_{max}	$\mathcal{E}_{K,2}$	EOC	$\mathcal{E}_{K,\infty}$	EOC	$\mathcal{E}_{H,2}$	EOC	$\mathcal{E}_{H,\infty}$	EOC
162	0.793	0.14	.	0.86	.	0.058	.	0.26	.
642	0.448	0.025	2.9	0.14	3.2	0.012	2.7	0.056	2.7
2562	0.244	0.0015	4.7	0.0081	4.7	0.0008	4.5	0.0039	4.4
10242	0.144	0.00028	3.2	0.003	1.9	0.00014	3.4	0.0015	1.8
40962	0.0817	1.9e-05	4.7	0.00026	4.3	9.7e-06	4.6	0.00014	4.2
163842	0.0464	2.8e-06	3.4	7.5e-05	2.2	1.4e-06	3.4	3.8e-05	2.3
655362	0.0261	2.4e-07	4.2	1.5e-05	2.8	1.2e-07	4.2	7.5e-06	2.8
2621442	0.0146	3.4e-08	3.4	5.4e-06	1.8	1.7e-08	3.4	2.7e-06	1.8

3.3 Local refinement and coarsening

ALBERT implements local mesh-refinement and coarsening by the *newest-vertex* bisection method as described in detail in [SCHMIDT and SIEBERT 2000]. At the beginning each element T of a shape-regular conforming triangulation is assigned a dedicated refinement edge. When an element is bisected, the refinement edges of its children are the edges opposite the newest vertex, see Figure 3.2. Algorithm 3.3.1 sketches the algorithm which removes non-conforming nodes in the sense of Definition 2.4.2 on page 43 above. [BÄNSCH 1991] shows that in the case of a fixed triangulated domain the newest-vertex bisection method guarantees the shape-regularity and conformance of the refined meshes.

Algorithm 3.3.1 Local refinement of a triangular mesh. We start with a triangulation $\mathcal{T}$ and a set $F \subset \mathcal{T}$ of elements which are marked for refinement.

- 1: $k := 0, \mathcal{T}_0 := \mathcal{T}$
 - 2: **repeat**
 - 3: $k := k + 1$
 - 4: generate $\mathcal{T}_k$ from $\mathcal{T}_{k-1}$ by bisecting all elements $T \in F$
 - 5: set $F := \{T \in \mathcal{T}_{k+1} \mid T \text{ has a non-conforming vertex}\}$
 - 6: **until** $F = \emptyset$
-

The case of an iso-parametric triangulation $\mathcal{T}_h^d$ can be handled similar to the case of planar triangulations described above. In the following we will use the notation introduced in Section 2.4.1. In the linearly parametrised case $d = 1$ there is actually *no* difference.

If $d \geq 2$ then the only difference to the planar case is the following: the assignment of coordinates to the newly introduced nodes is more difficult. The coordinates are chosen such that the coordinates of the new nodes interpolate the old surface Γ_h^d . A natural choice is to map the Lagrange-nodes of the two child-elements of the appropriately bisected reference element $\hat{T}$ to the bisected iso-parametric element T by means of the local parametrisation Φ_T^d . Figure 3.3 on the following page shows an example for the case of $d = n = 2$.

Figure 3.2 Refinement and coarsening of a conforming patch. The refinement edges are indicated by the dashed red lines. The blue dotted lines in the patch on the right mark the edges which would be inserted in the next refinement step.

Figure 3.3 Refinement of an iso-parametric element of degree 2. The coordinates of the new nodes are the images under Φ_T^2 of the children of the refined reference element. The new edge which bisects the reference element $\hat{T}$ and the iso-parametric element is shown in red, as well as the new nodes.

Because the identity mapping $\text{id}_{\Gamma_h^d}$ of the iso-parametric discrete surface Γ_h^d is itself contained in the iso-parametric finite element space $W_h^d(\Gamma_h^d)$ this choice for the new coordinates during the refinement of an iso-parametric element is just the usual interpolation step which maps a finite element function from the coarse mesh to the refined mesh.

Finally we remark that during the construction of an interpolation Γ_h^d of a given smooth immersed (hyper-)surface Γ we have to project the new nodes to the smooth surface Γ . We do this by first performing the interpolation step described above and afterwards use the lift in approximate normal direction with respect to the *discrete* surface to project the new coordinates to Γ .

3.4 Mesh smoothing

During the path-tracking algorithm for the drop shapes the surface mesh used in the discretisation of the problem may degenerate and develop very acute and very obtuse angles (see Figure 3.4(b) on the next page). Therefore it is a crucial point of the algorithm to counterbalance this degeneration by mesh-smoothing techniques, which eliminates this problem as shown in Figure 3.4(c) on the facing page.

3.4.1 Subdivision of obtuse angles

ALBERT uses the “newest vertex” algorithm (see Section 3.3) for mesh-adaption. This guarantees a stable triangulation in the planar case ([BÄNSCH 1991]).

Figure 3.4 Two-lobed drop with obtuse angles

(a) Two-lobed drop, $\omega \simeq 0.208$, result of path-tracking without mesh-smoothing
 (b) Magnification of central region of (a)
 (c) Same value of ω , created by path-tracking with mesh-smoothing

However, as the surface mesh is subject to large deformations during the path-tracking algorithm, the stability of the triangulation is no longer guaranteed by this scheme. Therefore in [SCHMIDT 1993] – prior to the mesh-adaption step – the longest edge of each element is chosen as the refinement-edge, so that the largest angle will be divided when an element is refined. Subsequent bisections to resolve hanging nodes follow the newest-vertex scheme (in contrast to [MITCHELL 1989]), because this reduces the number of bisection steps needed to get a conformal triangulation again.

Figure 3.5 Examples for subdivision of large angles

(a) 3 choices for the refinement edge (in blue). Angles of children need not be less obtuse than angles of the parent element.
 (b) Subsequent refinement steps (coloured). Topmost triangle: acute angles less sharp.
 (c) Refine by red edges: acute angles cannot improve.
 (d) Flip-flop effect: which each step alternately either obtuse or right angles occur.

We note that there is no guarantee that the children of a bisected element have significantly less obtuse angles. Nevertheless, choosing the largest edge as refinement edge might make things less worse. This is shown in Figure 3.5(b).

In addition to just reassigning the refinement edges [SCHMIDT 1993] also actively refines

obtuse angles greater than a certain limit, $\frac{2\pi}{3}$ being the limit of choice.

We adopt his techniques. However, we want to avoid the flip-flop effect illustrated in Figure 3.5(d) on the preceding page: there, when bisecting an element only once in each step of our path-tracking algorithm (or in a time-step for time dependent problems), obtuse and right angles alternate from each refinement step to the next.

Also, we do not always reassign the refinement edges to be opposite the largest angle in each element, but only when one of the interior angles indeed is obtuse, that is, larger than $\frac{\pi}{2}$. This way, our algorithm benefits from the robustness of the newest-vertex scheme locally, in regions where the triangulation is highly regular. It doesn't make sense to reassign the refinement edges in nearly equilateral triangles.

So, with regard to the division of obtuse angles, we arrive at Algorithm 3.4.1.

Algorithm 3.4.1 Mesh adaption and subdivision of obtuse angles

```

1: for all  $T \in \Gamma_h$  do
2:   if largest angle of  $T > \frac{\pi}{2}$  then
3:     reassign refinement edge to longest edge
4:   end if
5: end for
6: Adapt mesh, using newest vertex scheme. Number of bisections for refinement and
   coarsening in each element is  $n$  (dimension of surface). Remove hanging nodes with
   newest vertex scheme.
7: for all  $T \in \Gamma_h$  do
8:   if largest angle of  $T > \frac{2\pi}{3}$  then
9:     bisect  $T$ , using largest edge as refinement edge
10:    remove hanging nodes with newest vertex scheme
11:   end if
12: end for

```

3.4.2 Vertex displacement

The mesh-smoothing method described in the previous section tries to improve the mesh quality by refinement techniques. This changes the topology of the triangulation but leaves already present vertices in place. It is not possible with this method to counterbalance the development of a distinct anisotropy in the node-density during the path-tracking algorithm, as indicated in Figure 3.5(d) on the preceding page.

Another possibility to improve the mesh quality is to leave the topological structure of the mesh unchanged and instead change the coordinates of the vertices to improve the triangulation, which is the subject of the subsequent sections.

While there are also “direct” methods available, which compute optimised coordinates for all vertices simultaneously – see e.g. [BALENDRA 1999] for a very brief outline – we have chosen a single-step method.

In the single-step setup, we loop over all vertices of the mesh and displace the vertices, sequentially, based on the shape of the “star” $S(P)$ around each vertex P , the union of

Algorithm 3.4.2 Outline of combined averaging and optimisation based smoothing (see [CANANN et al. 1998] for details)

```

1:  $k := 0$ 
2: repeat
3:   for all  $P \in \Gamma_h$  do
4:     if  $k < 2$  then
5:       use some averaging method (e.g. Laplacian smoothing (3.9)) to move  $P$ 
6:     else if  $P$  never moved by opt. based method and local mesh quality good enough then
7:       use some averaging method (e.g. Laplacian smoothing (3.9)) to move  $P$ .
8:     else
9:       use optimisation based smoothing (e.g. using the Distortion Metric (3.15))
10:    end if
11:  end for
12:   $k := k + 1$ 
13: until no more nodes found to move

```

all triangles adjacent to P . This “main-loop” is then repeated until the mesh reaches a satisfactory state.

We expect – without further investigation – that a single-step method is more stable in the case of parametric meshes, because the displacement of each vertex will be small even for highly distorted meshes, and so it is easier to project the displaced nodes back to the surface.

Some existing single-step approaches In the literature there is the notion of “averaging methods”, where the new position $A(P)$ of a node P is computed directly from the data of its element neighbourhood $S(P)$, using an explicit mapping $A : S(P) \rightarrow \mathbb{R}^m$ where m is the dimension of the embedding space. Two examples are “Laplacian smoothing” (3.9) – the new position of P is the average of the end points of the edges adjacent to P – and averaging about certain interior angles, as in (3.12) on page 79.

In contrast to this, one finds the notion of “optimisation based” methods, which compute the new location by minimising a functional F defined on the element-neighbourhood $S(P)$ of P . Actually, the most commonly used averaging methods are just special cases of optimisation based methods where the minimiser P_{min} of F can be computed by a closed, comparatively simple formula, see (3.8) and (3.10) on page 78.

Algorithm 3.4.2 gives a very short outline of a combined method, as described in [CANANN et al. 1998]. It uses computational cheap averaging methods in regions where the local mesh quality is good enough, and invokes optimisation based smoothing only for sufficiently ill-shaped elements. This technique aims at reducing the computational cost of an optimisation-based smoothing method considerably by still retaining a highly regular mesh.

For optimisation based methods, the simplest way to decrease the value of the smoothing-functional F locally is a steepest descent method in the direction opposite to the gradient of F .

In contrast to this method [DJIDJEV 2000] proposes to use the search direction of the previous iteration-step of the main-loop of his single-step algorithm for the update of a new search direction in a conjugate-gradient manner (see Algorithm 3.4.3 on the facing page). Unluckily in the examples we have tried this leads to a non-stable smoothing-algorithm, in the sense that the conjugate-gradient method (CG-method) Algorithm 3.4.3 on the next page converges more slowly than the more simpler steepest decent method.

The problem might be that the gradient of the smoothing-functional F at P can be altered a lot when a neighbouring node is moved. Therefore, the gradients and CG-directions of the previous iteration might not contain enough information about the current state.

It has to be noted, though, that in the single-step approach a lot of parameters come into play which influence the smoothing-algorithm: for example the maximum distance to move a node inside its patch $S(P)$, the accuracy of the computation of the local minimiser (good local accuracy does *not* imply good global quality!), the order in which the nodes are displaced. Those parameters do not only influence the efficiency of the mesh-smoothing, but also the final state. Thus the reason that we could not use the CG-style method presented in [DJIDJEV 2000] simply might be that our parameters were not suitable for doing so.

Single-step method for parametric meshes For the moment we are only concerned with piecewise linearly parametrised surface meshes. A simple extension to local parametrisations of higher polynomial degree is given at the end of this paragraph.

We do not use the combined Algorithm 3.4.2 on the page before: as illustrated below in Figure 3.10 on page 85, the global redistribution of the vertices caused by the averaging methods (3.9) and (3.12) is significantly different from the redistribution caused by the most powerful smoothing-functionals (3.15) and (3.16). (3.15) and (3.16) tend to increase the node-density in regions of high curvature (where a highly refined mesh is needed), but (3.9) and (3.12) do not.

Therefore we use a pure optimisation-based approach, but avoid unnecessary work by only moving nodes where the smoothing-functional has a large gradient and so the expected improvement of the local mesh quality is high enough.

Regardless of whether using a direct or a single-step method, it is an important constraint for the displacement of the nodes that they must remain *on* the surface. As a global parametrisation of the discrete surface is not available, it would be hard to incorporate this constraint directly into the computation of the vertex displacements. Instead, one first computes the optimised node positions ignoring the on-surface constraint. Afterwards, the displaced nodes are projected back to the original surface. The projection is a crucial and non-trivial step of the smoothing algorithm and is therefore explained in detail in Section 3.4.4 on page 88 below.

This way the computation of the new coordinates is simplified, but the smoothed mesh still interpolates the discrete surface Γ_h , and the additional error introduced by mesh-smoothing is a mere interpolation error. The problem of projecting a point to the discrete surface Γ_h is addressed in Section 3.4.4. The general approach for a single-step

Algorithm 3.4.3

CG method for a smoothing-functional, see [FLETCHER and REEVES 1964]

Parameters: Gradient tolerance: t_{grad} Iteration limit for CG iterations: j_{CG} Iteration limit for line-search: l_{line} **Start:**

```

1:  $P_0 := P$ 
2:  $g_0 := \nabla F(P_0)$ 
3:  $d_0 := -g_0$ 
4:  $j := 0$ ;
5: while  $\|g_j\| > t_{grad}$  and  $j < j_{CG}$  do
6:   compute projection  $\hat{S}(P_k)$  of  $S(P_j)$  w.r.t. approximate tangential plane  $T_{P_j}(\Gamma_{h,0})$ 
   at  $P_j$ 
7:    $s_j := \frac{1}{2} \frac{1}{\|g_j\|} \text{dist}(P_j, \partial \hat{S}(P_j))$ 
8:   line-search: find a local minimum  $\hat{F}(P_{j,l^*}) < \hat{F}(P_j)$  on the discrete set
    $L_j := \{P_{j,l} := P_j - 2^{-l} s_j g_j \mid 0 \leq l \leq l_{line}\}$ .
9:   if  $P_{j,l^*}$  does not exist then
10:     break out of the loop
11:   end if
12:    $P_{j+1} := \Pi_{\Gamma_{h,0}}(P_{j,l^*})$ 
13:    $g_{j+1} := \nabla F(P_{j+1})$ 
14:    $\beta_j := \frac{\|g_{j+1}\|^2}{\|g_j\|^2}$ 
15:    $d_{j+1} := -g_{j+1} + \beta_j d_j$ 
16:    $j := j + 1$ 
17: end while
18: if  $j > 0$  then
19:   replace  $P$  by  $P_j$ 
20: end if

```

algorithm for parametric meshes is to remember the original surface $\Gamma_{h,0} := \Gamma_h$ at the start of the single-step algorithm. This involves only storage of the coordinates of the nodes of the original mesh as the topological structure of the mesh does not change during the smoothing process. Then we are able to iterate the single-step smoothing method and produce a sequence $\Gamma_{h,k}$, $k = 1, 2, \dots$ of triangulations, where in each step the stored coordinates of the original surface are used to compute the projection back to $\Gamma_{h,0} \equiv \Gamma_h$. In the following we denote this projection by $\Pi_{\Gamma_{h,0}}$ ([SCHMIDT 1993]).

In our implementation, we first project the element-neighbourhood $S(P)$ of a vertex $P \in \Gamma_{h,k}$ to an approximate tangential (with respect to $\Gamma_{h,0}$) plane at P . Then we compute the new position $\hat{P}$ of P with respect to the projected star $\hat{S}(P)$. Compared to allowing arbitrary displacements in $\mathbb{R}^3$ this stabilises the node-displacement with respect to the projection $\Pi_{\Gamma_{h,0}}$ in regions of high curvature, because the displaced node $\hat{P}$ remains closer to the original surface. Especially this approach inhibits displacements which only lead off the surface and would be annihilated by the subsequent projection step.

Algorithm 3.4.4 Optimisation-Based Mesh-Smoothing Algorithm. In order to apply this algorithm to different smoothing-functionals with comparable stop-conditions, the smoothing-functional F and its gradient are scaled by the extremal values of F on the current triangulation.

Parameters: Iteration limit: k_{max}

Minimal number of iterations: k_{min}

Tolerances for extremal angles: $t_{\alpha_{min}}, t_{\alpha_{max}}$

Minimal number of moved nodes: n_{min}

Optimisation tolerance: t_{opt}

Gradient tolerance: t_{grad}

Start:

```

1:  $\Gamma_{h,0} := \Gamma_h$ 
2:  $F_0 := \sum_{P \in \Gamma_{h,0}} F(P)$ 
3:  $k := 0$ 
4: repeat
5:    $\Gamma_{h,k+1} := \Gamma_{h,k}$ 
6:    $n_{moved} := 0$ 
7:    $F_{min} := \min_{P \in \Gamma_{h,k+1}} F(P), F_{max} := \max_{P \in \Gamma_{h,k+1}} F(P), F_{scale} := F_{max} - F_{min}.$ 
8:   for all  $P \in \Gamma_{h,k+1}$ , sorted in descending order w.r.t.  $\|\nabla F(P)\|$  do
9:     if  $\|\nabla F(P)\| < t_{grad} \cdot F_{scale}$  then
10:       continue with next node
11:     end if
12:     if  $1/2 \cdot dist(P, \partial \hat{S}(P)) \cdot \|\nabla F(P)\| > t_{opt} \cdot F_{scale}$  then
13:       try to displace  $P$  by CG-method, see Algorithm 3.4.3 on the preceding page
14:       if  $P$  was moved by CG-method then
15:          $n_{moved} := n_{moved} + 1$ 
16:       end if
17:     end if
18:   end for
19:   compute extremal angles  $\alpha_{min}$  and  $\alpha_{max}$ 
20:    $F_{k+1} := \sum_{P \in \Gamma_{h,k+1}} F(P)$ 
21:    $k := k + 1$ 
22: until  $k > k_{max}$  {iteration limit exceeded} or
       $F_k > F_{k-1}$  {total mesh quality did not improve} or
       $n_{moved} < n_{min}$  {only a few nodes were moved} or
       $(k > k_{min}$  {minimal number of iterations completed}
      and
       $(\alpha_{min} > t_{\alpha_{min}}$  and  $\alpha_{max} < t_{\alpha_{max}}$  {angles good enough}))
```

In order to find good new position $\hat{P}$ for P inside the projected element neighbourhood $\hat{S}(P)$ – such that $F(\hat{P})$ is close to minimal – a few steps (typically 2 or 3) of a non-linear conjugate gradient method are applied (see Algorithm 3.4.3 on page 75). This was inspired by [DJIDJEV 2000], though we were not able to copy his method, see the remarks on page 74.

The main part of our optimisation-based smoothing algorithm is described in Algorithm 3.4.4 on the facing page. Suitable choices for the optimisation functional F are investigated in Section 3.4.3 below.

Parametrisations of higher polynomial degree So far our approach only covers piecewise linearly-parametrised surfaces. As described in [SCHMIDT 1993] for a surface Γ_h which's elements are parametrised with Lagrange-polynomials of degree 2 or greater the smoothing algorithm acts only on the vertex-nodes of the discretised surface Γ_h : the vertex nodes constitute a triangulated surface Γ_h^{lin} which is then smoothed as described above, with the difference that the projection $\Pi_{\Gamma_{h,0}}$, of course, uses the non-linear parametrisation of Γ_h .

After the smoothing-algorithm has terminated, producing a smoothed triangular surface mesh $\Gamma_{h,k}^{lin}$, the none-vertex Lagrange-nodes of each element with respect to the chosen polynomial parametrisation are projected by $\Pi_{\Gamma_{h,0}}$ to Γ_h , hereby generating the non-linearly parametrised smoothed mesh.

For the parametrisation with quadratic Lagrange-polynomials this means that the mid-points of the edges of $\Gamma_{h,k}^{lin}$ are projected to $\Gamma_{h,0}$ and constitute the non-vertex nodes of the final mesh.

3.4.3 Smoothing functionals

For evaluating the local mesh-quality we use a functional $F(P)$ defined on the star $S(P)$ around a vertex P of the triangulation.

To fix the notation (see the figure on the right) let N denote the number of the triangles T_i around P , $1 \leq i \leq N$, so $S(P) = \bigcup_{i=1}^N T_i$.

For $1 \leq i \leq N$ let Q_i , $1 \leq i \leq N$, $Q_{N+1} := Q_1$, be the vertices of S such that Q_i , Q_{i+1} and P are the vertices of T_i . Further let $v_i := Q_i - P$, with $v_{N+1} := v_1$, denote the edges adjacent to P and $w_i := Q_{i+1} - Q_i = v_{i+1} - v_i$, $w_{N+1} := w_1$, the edges opposite to P .

The non-unit element normals are denoted by $\nu_i := v_i \wedge v_{i+1}$ ($1 \leq i \leq N$). The normals nu_i have been omitted from the figure on the right.

Finally $\alpha_i := \angle(w_i, -v_i)$, $\beta_i := \angle(v_{i+1}, w_i)$ and $\gamma_i := \angle(v_i, v_{i+1})$ denote the interior angles of T_i , $1 \leq i \leq N$ as shown in the drawing above.

In the case of a parametric surface Γ_h , we actually do not use $S(P)$, but its projection $\hat{S}(P)$ to an approximate tangential plane at P . However, to simplify notation we will not distinguish between $S(P)$ and $\hat{S}(P)$ in the following, and assume that $S(P)$ is planar, but embedded into $\mathbb{R}^3$.

For the derivation of the formulas for the gradients of the smoothing-functionals it has to be noted that P is the independent variable and

$$\nabla \|\nu_i(P)\| = \frac{\nu_i(P)}{\|\nu_i(P)\|} \wedge w_i.$$

This is clear because $\|\nu_i\|$ is the volume of the parallelogram spanned by w_i and v_i . So the steepest-ascent direction clearly is orthogonal to w_i , moving P away from w_i , and the amount of increase is proportional to $\|w_i\|$ (which is independent from P).

There are several possible choices for F . In his survey about unstructured mesh generation [OWEN 1998] gives a brief summary and large list of references. In our work we have considered and implemented the following smoothing-functionals:

Discrete Laplacian The length of the edges adjacent to P is minimised:

$$(3.8) \quad \begin{aligned} F_{\Delta}(P) &:= \sum_{i=1}^N \|v_i\|^2, \\ \nabla F_{\Delta}(P) &= -2 \sum_{i=1}^N v_i. \end{aligned}$$

The exact position of the minimum of F_{Δ} can be computed easily, it is just the mean value of the vertices Q_i , $1 \leq i \leq N$. This method is the probably most often used averaging smooth-method. The new position of P is given by

$$(3.9) \quad A_{\Delta}(P) := \frac{1}{N} \sum_{i=1}^N Q_i.$$

F_{Δ} can be viewed as the energy of a mechanical system where the edges adjacent to P are replaced by linear springs. This was probably the motivation for the following averaging method.

Torsion Springs In [ZHOU and SHIMADA 2000] the energy of a torsion-spring system is used:

$$(3.10) \quad F_{tors}(P) := \sum_{i=1}^N (\alpha_i^2 + \beta_i^2).$$

The authors define an iterative process, which decreases F_{tors} : rotate the interior edges v_i of $S(P)$ around their starting points Q_i until the edges half the angles

at Q_i . The new position for P is the average of the coordinates of the end-points of the rotated edges. This can be used to define an iteration which finally yields a minimiser for F_{tors} by a limiting process. For convenience let $\bar{\nu}$, $\|\bar{\nu}\| = 1$, be an approximate normal at P (just $(0, 0, 1)$ in the 2-dimensional case). Then let $P_{tors,0} := P$ and for $k \in \mathbb{N}_0$ define

$$(3.11) \quad P_{tors,k+1} := \frac{1}{N} \sum_{i=1}^N \left(\|v_{i+1}(P_{tors,k})\| \left(\bar{\nu} \wedge \frac{\frac{w_{i+1}}{\|w_{i+1}\|} + \frac{w_i}{\|w_i\|}}{\left\| \frac{w_{i+1}}{\|w_{i+1}\|} + \frac{w_i}{\|w_i\|} \right\|} \right) + Q_{i+1} \right).$$

Compared with the computations described by [ZHOU and SHIMADA 2000] this formula avoids trigonometric functions at the cost of additional square-roots.

The exact position of the minimiser can be obtained by the limit

$$(3.12) \quad A_{tors}(P) := \lim_{k \rightarrow \infty} P_{tors,k}.$$

We did not investigate whether there exists an explicit formula for the minimiser, though this would be an interesting point for the application of (3.10) as smoothing-functional.

The authors do not use (3.12), but apply in each step of the smoothing algorithm only one iteration step of (3.11).

Conformal Energy

[SCHMIDT 1993] uses the “conformal energy” E_C of [HUTCHINSON 1991],

$$E_C(x) := \int_{D_N} \|\nabla x\|^2 - 2 \int_{D_N} \|x_u \wedge x_v\|,$$

where D_N is the regular N -polygon inscribed into the unit-circle and $x : D_N \rightarrow S(P) : (u, v) \mapsto x(u, v)$ denotes a parametrisation of $S(P)$ over D_N . It holds that $E_C(x) \geq 0$ and $E_C(x) = 0$ if and only if x is a conformal parametrisation.

In the discrete case one restricts oneself to (continuous!) parametrisations which map the facets of D_N linearly to the facets of $S(P)$ (so vertices are mapped to vertices and the central of D_N is mapped to P). This yields the following formula for the “conformal energy” $E_C(P)$ of $S(P)$, where $\alpha := \frac{2\pi}{N}$:

$$(3.13) \quad \begin{aligned} F_{con}(P) &:= E_C(P) = \sum_{i=1}^N \left(\frac{\|v_i\|^2 + \|v_{i+1}\|^2 - 2 \cos(\alpha) \langle v_i, v_{i+1} \rangle}{2 \sin(\alpha)} - \|\nu_i\| \right), \\ \nabla F_{con}(P) &= - \sum_{i=1}^N \left(\frac{1 - \cos(\alpha)}{\sin \alpha} (v_i + v_{i+1}) + \frac{\nu_i}{\|\nu_i\|} \wedge w_i \right), \end{aligned}$$

with $\nu_i = v_i \wedge v_{i+1}$ (see the figure on page 77 for the notation). A detailed derivation of (3.13) can be found in [SCHMIDT 1993].

It has to be noted, however, that in the planar case F_{con} is identical to F_{edge} , up to a factor and an additive constant, as long as the triangles are not inverted (see

Figure 3.6 Contour plots of some smoothing-functionals. The position of the minimum is indicated by the central node. For the smoothing-functionals see equations (3.8)–(3.16).

Figure 3.6(a) and Figure 3.6(b)). This follows from:

$$\begin{aligned} & \|v_{i+1}\|^2 - 2 \langle v_{i+1}, v_i \rangle + \|v_i\|^2 = \|v_{i+1} - v_i\|^2 = \|Q_{i+1} - Q_i\|^2 = \|w_i\|^2 \\ \iff & -2 \cos(\alpha) \langle v_i, v_{i+1} \rangle = \cos(\alpha) (\|w_i\|^2 - \|v_i\|^2 - \|v_{i+1}\|^2) \quad (1 \leq i \leq N). \end{aligned}$$

So we get

$$\begin{aligned} (3.14) \quad F_{con}(P) &= \sum_{i=1}^N \left(\frac{\|v_i\|^2 + \|v_{i+1}\|^2 - 2 \cos(\alpha) \langle v_i, v_{i+1} \rangle}{2 \sin(\alpha)} - \|v_i\| \right) \\ &= \sum_{i=1}^N \left(\frac{1 - \cos(\alpha)}{2 \sin(\alpha)} (\|v_i\|^2 + \|v_{i+1}\|^2) + \frac{1}{2} \cot(\alpha) \|w_i\|^2 \right) - 2 |S(P)| \\ &= \frac{1 - \cos(\alpha)}{\sin(\alpha)} F_{\Delta}(P) + \frac{1}{2} \cot(\alpha) \sum_{i=1}^N \|w_i\|^2 - 2 |S(P)|. \end{aligned}$$

Neither the boundary edges w_i nor the area $|S(P)|$ of $S(P)$ depend on the position of the central node P . In the parametric case, when P is constrained to move on the

Figure 3.7 Contour plots of some smoothing-functionals for a highly distorted patch. Edges leading to inverted triangles are shown in red.

surface Γ_h , F_{con} penalises loss of area, which might explain why [SCHMIDT 1993] observed that in the parametric case this method is slightly better than mere Laplacian smoothing.

However, as we project $S(P)$ to an approximate tangent plane at P , our algorithm doesn't see this difference. The only remaining difference to Laplacian smoothing is the weight-factor $\frac{1-\cos(\alpha)}{\sin(\alpha)}$, which changes the order in which our optimisation based single-step mesh-smoothing Algorithm 3.4.4 on page 76 displaces the nodes.

Distortion Metric In [CANANN et al. 1998] a so called “distortion metric” is used. For any triangle $T_i \subset S(P)$ the quantity $\mathcal{D}(T_i)$ defined as

$$\mathcal{D}(T_i) := \frac{\|v_i\|^2 + \|v_{i+1}\|^2 + \|w_i\|^2}{2\|\nu_i\|}$$

is used as a measure the distortion of T_i from the equilateral form. Up to a factor $\mathcal{D}(T_i)$ is the ratio of the sum of the squared edge lengths of T_i to its area. It is

minimal for equilateral triangles. The smoothing-functional for this case is

$$\begin{aligned}
 F_{dist}(P) &:= \sum_{i=1}^N \mathcal{D}(T_i) = \sum_{i=1}^N \frac{\|v_i\|^2 + \|v_{i+1}\|^2 + \|w_i\|^2}{2 \|\nu_i\|} \\
 &= \sum_{i=1}^N (|\cot \alpha_i| + |\cot \beta_i| + |\cot \gamma_i|) \\
 &= \sum_{i=1}^N \frac{|\langle v_i, v_{i+1} \rangle| + |\langle v_{i+1}, w_i \rangle| + |\langle v_i, w_i \rangle|}{\|\nu_i\|}, \\
 \nabla F_{dist}(P) &:= - \sum_{i=1}^N \left(\frac{v_i + v_{i+1}}{\|\nu_i\|} + \frac{F_{dist}(P)}{2 \|\nu_i\|^2} \nu_i \wedge w_i \right).
 \end{aligned}
 \tag{3.15}$$

Squared Cotangens The following is a modification of (3.15); the sum is taken over the square of the cotangens of the interior angles:

$$\begin{aligned}
 F_{cot^2}(P) &:= \sum_{i=1}^N (\cot^2(\alpha_i) + \cot^2(\beta_i) + \cot^2(\gamma_i)) \\
 &= \sum_{i=1}^N \frac{\langle v_i, v_{i+1} \rangle^2 + \langle v_{i+1}, w_i \rangle^2 + \langle v_i, w_i \rangle^2}{\|\nu_i\|^2}, \\
 \nabla F_{cot^2}(P) &= -2 \sum_{i=1}^N \frac{\langle v_i, v_{i+1} \rangle (v_i + v_{i+1}) + \langle v_i + v_{i+1}, w_i \rangle w_i + F_{cot^2}(P) \nu_i \wedge w_i}{\|\nu_i\|^2}.
 \end{aligned}
 \tag{3.16}$$

Contour-plots of the smoothing-functionals (3.8)–(3.16) are shown in Figure 3.6 on page 80. In compliance with (3.14), F_Δ and F_{con} have the same level-sets inside the region where the triangles of the patch are not inverted. Figure 3.6(d) and 3.6(e) on page 80 illustrate that F_{dist} and F_{cot^2} diverge when the central nodes approaches a position which leads to degenerated triangles. This has a stabilising effect for our single step Algorithm 3.4.4 on page 76, because triangles become less easily inverted.

In contrast to this, F_Δ , F_{tors} and F_{con} are continuous across “degeneration”-lines, so that Algorithm 3.4.4 on page 76 additionally has to check for inverted triangles. As illustrated in Figure 3.7 on the page before, there are even cases where the minimiser for F_Δ (and also for F_{con}) is located outside the patch $S(P)$ around P .

Mesh-smoothing for a planar test-domain As a first test for the behaviour of the smoothing-functionals listed above, we apply the two averaging methods (3.9) and (3.11) and the optimisation-based Algorithm 3.4.4 on page 76 with the smoothing-functionals listed above to the planar triangulation shown in Figure 3.8 on the next page.

This figure was created by deforming a globally refined rectangular domain. The colouring measures the quality of the elements in terms of the minimum and maximum angles (blue is better). The overall minimum and maximum angles were 6.86 and 155.39 degrees.

The mesh-smoothing was carried out until Algorithm 3.4.4 on page 76 terminated because it couldn't find any better node-position up to machine-precision.

The final angles – see Table 3.5 – show only very little difference between explicit Laplacian smoothing, optimisation based Laplacian smoothing and optimisation based smoothing with the conformal energy F_{con} (Figures 3.9(a) to 3.9(d) on the following page).

This was, of course, to be expected, as this only difference between F_{Δ} and F_{con} is the weight factor $\frac{1 - \cos(\alpha)}{\sin(\alpha)}$, which compensates for the number of edges adjacent to each node (see equation (3.14) on page 80).

Figure 3.8 Planar test triangulation

Table 3.5 Extremal angles for the triangulated domain from Figure 3.9 on the following page, after mesh-smoothing

	minimum angle	maximum angle
Laplacian, explicit	12.96	100.21
Torsion Springs	12.19	97.50
Laplacian, opt. based	13.81	100.86
Conformal Energy	12.93	99.79
Distortion Metric	21.08	97.20
Squared Cotangents	21.33	96.32

The domain of the first test-case has also been chosen as an example to illustrate another effect of mesh smoothing. As shown in Figure 3.10 on page 85, the smoothing-functionals differ in the way they redistribute the nodes globally. F_{Δ} (and so F_{con} and F_{tors}) produce high-quality triangles in the top-region, at the cost of the triangles in the quenched bottom region of the example domain, while F_{dist} and F_{cot^2} achieve a more fair distribution of acute angles.

Mesh-smoothing for parametric test-cases We will now apply the smoothing-algorithm to a parametric example. The torsion-spring energy will be used no longer.

Figure 3.11 on page 85 shows the development of triangulations of the surface shown in figure Figure 3.12(a) on page 86. The surface originates from a globally refined icosahedron inscribed into the unit-sphere. The resulting mesh was heavily deformed and afterwards refined, either globally (Figure 3.11(a) on page 85) or locally (Figure 3.11(b) on page 85).

The initial triangulation has some quite obtuse angles, resulting from the deformation of the underlying sphere.

Figure 3.9 Distribution of angles with different smoothing-functionals. The colours indicate the element quality in terms of the size of the interior angles (blue is better).

Figure 3.11 on the next page shows a big difference in the behaviour of the various smoothing-functionals with respect to the topology of the surface mesh. In the globally refined case the results of the more complicated smoothing-functionals F_{dist} and F_{cot^2} are much better than the results achieved by smoothing with the conformal energy F_{con} . Again, the diagrams demonstrate that there is only little difference between Laplacian smoothing and smoothing with the conformal energy.

Excessive mesh-smoothing – in this examples we were using 200 iterations – can severely change the node-distribution over the surface-mesh; the tips of the lobes in Figure 3.11 are only covered by a very coarse mesh after the smoothing-algorithm has finished. However, one notes that the smoothing-functionals tend to move nodes to regions of high curvature, where a high resolution is needed. A local mesh-adaption strategy can afterwards compensate the coarse-mesh structure in regions of low curvature.

As a final example, we present how the smoothing-functionals behave when applied to our path-tracking problem. This will also explain why we were using F_{cot^2} , defined in (3.16), rather than Laplacian smoothing (or the essentially equivalent conformal energy F_{con}). For the test we chose the two-lobed family of solutions which branches off from the exact solutions found by Beer (see Section 1.4 on page 16). This is the simplest non-cylinder-symmetric branch but it already develops a distinct constriction around the origin when the angular velocity ω approaches 0, as shown in Figure 3.14 on page 87.

Figure 3.10 Top and bottom parts of Figure 3.9 on the preceding page, bottom part magnified. Mesh-smoothing changes the local node-density

Figure 3.11 Mesh-smoothing for the parametric example mesh shown in Figure 3.12 on the next page. The two diagrams show the development of the maximal angle for the indicated smoothing-functionals for the surface meshes shown in Figure 3.12(a) on the following page.

Figure 3.12 Geometry and smoothed-meshes for a parametric example. Only the locally refined case is shown. The colours reflect the local mesh-quality (dark blue is better).

(a) Initial mesh

(b) Conformal Energy

(c) Distortion Metric

(d) Squared Cotangents

Figure 3.13 Different smoothing-functionals acting on the two-lobed family. The goal was to keep the minimal angle above 30° , starting from very regular triangulation at $\omega \approx 0.55$. (a) shows that smoothing with F_{dist} and F_{cot^2} achieve this goal very well.

Figure 3.14 Result of path-tracking using optimisation based mesh-smoothing with either F_{con} or F_{cot^2}

(a) Drop shape at $\omega \approx 0.12$ (b) Magnified central region of (a), smoothed using F_{cot^2} (c) Magnified central region of (a), smoothed using F_{con}

The test-runs started at $\omega \approx 0.55$ and stopped at $\omega \approx 0.12$. Figure 3.13 shows that neither optimisation based smoothing with the Conformal Energy F_{con} nor explicit Laplacian smoothing are able to keep the mesh in good shape, and the corresponding test-runs broke down at $\omega \approx 0.12$, the last value shown in Figure 3.13.

While the same diagram also shows that there is little difference between F_{dist} and F_{cot^2} , we nevertheless chose F_{cot^2} as it yielded better results for annular drop shapes. We will not discuss this here further, but the example for the planar Figure 3.10 on page 85 and the first parametric test-case Figure 3.11 on page 85 already indicate that F_{cot^2} yields slightly better results than F_{dist} , though at a higher computational cost.

3.4.4 Projection to discretised surfaces

As a part of the mesh-smoothing Algorithm 3.4.4 on page 76 we need to project the displaced nodes back to $\Gamma_{h,0}$. So we need a projection

$$\Pi_{\Gamma_{h,0}} : U(\Gamma_{h,0}) \rightarrow \Gamma_{h,0}$$

which maps points from a neighbourhood $U(\Gamma_{h,0})$ of $\Gamma_{h,0}$ onto the surface.

A crucial part of our mesh-smoothing algorithm is the method described in [SCHMIDT 1993]. We give a detailed description as it has to be analysed carefully to be able to implement it in a stable way.

In order to implement the projection $\Pi_{\Gamma_{h,0}}$ efficiently, one first searches for the triangle onto which a point P will be projected. To this aim for points $P \in \Gamma_{h,k}$ one maintains mappings $P \mapsto T_P^k$, where $T_P^k \subset \Gamma_{h,0}$ is the element that P was projected to in the previous iteration of the smoothing algorithm – that is, when $\Gamma_{h,k}$ was generated ($k \in \mathbb{N}$). For T_P^0 one just selects one of the elements adjacent to P .

T_P^k will be close to the element to which $P \in \Gamma_{h,k}$ will be projected in the k -th run of the smoothing-algorithm, because the amount of displacement caused by the single-step method in each iteration step is not very large.

Algorithm 3.4.5 Projection of a node P to $\Gamma_{h,0}$

- 1: start with a triangle $T_P \in \Gamma_{h,0}$
 - 2: **repeat**
 - 3: let $T := T_P$
 - 4: compute barycentric coordinates $(\lambda_1, \lambda_2, \lambda_3)$ of P w.r.t. T
 - 5: **if** $\lambda_k < 0$ for one $k \in \{1, 2, 3\}$ **then**
 - 6: replace T by the corresponding neighbour in $\Gamma_{h,0}$
 - 7: **end if**
 - 8: **until** $\lambda_i > 0$, $i = 1, 2, 3$
 - 9: let $T_P := T$
 - 10: project P along an approximate normal onto T_P .
-

Starting with T_P^k , one uses Algorithm 3.4.5 to find T_P^{k+1} and to compute $\Pi_{\Gamma_{h,0}}(P)$. Line 4 of Algorithm 3.4.5 – the computation of the barycentric coordinates – is the crucial point and will be more detailed now.

Linear case First, we will present the computation of the barycentric coordinates for the linear case, where $\Gamma_{h,0}$ is parametrised locally by linear Lagrange finite elements; the method will later be extended to parametrisations of higher polynomial degree.

Let P be a point off the surface and $T \subset \Gamma_{h,0}$ an element of the triangulation of $\Gamma_{h,0}$ with vertices P_i , $i = 1, 2, 3$. Let ν_i , $i = 1, 2, 3$ be the approximate normals (refapproxnormals) at the vertices of T .

The idea is to compute the barycentric coordinates $\lambda = (\lambda_0, \lambda_1, \lambda_2)$ of P with respect to the triangle $\hat{T}$ parallel to T , which is inscribed into the skew-prism defined by the approximate normals ν_i , $1 \leq i \leq 3$, of T (see Figure 3.15).

Let ν_T (not shown in the figure) be the (non-approximate) unit-normal of T and

$$Q_i := P_i + \frac{\langle P - P_3, \nu_T \rangle}{\langle \nu_i, \nu_T \rangle} \nu_i$$

be the vertices of $\hat{T}$.

Of course, instead of P_3 any of the other two vertices of T could also be used as origin.

λ can then be computed by solving the linear system

$$(3.17) \quad \begin{cases} \lambda_1(Q_1 - Q_3) + \lambda_2(Q_2 - Q_3) = (P - Q_3) \\ \lambda_3 = 1 - \lambda_1 - \lambda_2 \end{cases}$$

Figure 3.15 Projection to triangulations

(3.17) has a unique solution, provided that the skew-prism is not degenerated. If the barycentric coordinates are all positive, then P is located inside $\hat{T}$.

In the linearly parametrised case, the projection $\Pi_{\Gamma_{h,0}}^{lin}$ of P to $\Gamma_{h,0}$ is then simply defined as

$$(3.18) \quad \Pi_{\Gamma_{h,0}}^{lin} := \sum_{i=1}^3 \lambda_i P_i.$$

[SCHMIDT 1993] observed that in some cases the Projection-Algorithm 3.4.5 on the preceding page will run into loops. As we found out the reason for this are not mere rounding errors. The skew-prisms defined by the approximate normals at the vertices of each element do *not* constitute a unique subdivision of a neighbourhood of $\Gamma_{h,0}$, as was intended.

This is illustrated in Figure 3.16 on the following page. The walls of the skew-prisms are pieces of ruled surfaces, in general being parts of hyperboloids. The skew-prisms intersect each other and leave holes between them.

The errors are still small as long as the mesh is fine enough and the jump of the element normals between neighbouring elements are not too large. However, the errors are several orders of magnitude larger than rounding errors, and they can become large in regions where the mesh is not fine enough to resolve the curvature of the surface (in the sense that the jump of the element normals between neighbouring triangles is large).

The algorithm has to take this into account; when it runs into a loop, it just picks one of the elements of the loop-path as target element and projects to an edge which corresponds to a negative barycentric coordinate λ_{k^*} and “repairs” the remaining two barycentric coordinates by adding $-\frac{1}{2}\lambda_{k^*}$.

Figure 3.16 Projection to discrete surfaces. In general the skew-prisms overlap and leave holes between them, they are ruled surfaces.

It would have been possible to avoid the problems shown in figure Figure 3.16 by not defining the skew-prism by parallel translation of the elements T of $\Gamma_{h,0}$. Instead, one could have defined the vertices Q_i of the top triangle $\hat{T}$ in Figure 3.15 on the preceding page by moving the points P_i the same distance along the average normals ν_i until $\hat{T}$ contained the point P . But this would lead to a quadratic equation for the barycentric coordinates, which would have been computationally more costly to solve than solving the linear equation (3.17).

Higher order parametrisations Still following [SCHMIDT 1993], we first proceed as in the linear case and determine T_P and the barycentric coordinates $(\lambda_1, \lambda_2, \lambda_3)$ of P with respect to the triangulation defined by the vertex nodes of $\Gamma_{h,0}$. The goal is then to project P along the direction of g defined as the weighted mean value

$$g := \sum_{i=1}^3 \lambda_i \nu_i$$

to the non-linearly parametrised surface.

The point where $G := \{P + s g \mid s \in \mathbb{R}\}$ meets the element T (if it meets it at all) is a zero of the function $d_{P,g,T}(\lambda_1, \lambda_2)$ defined by

$$(3.19) \quad d_{P,g,T}(\lambda_1, \lambda_2) := \Psi_T(\lambda_1, \lambda_2) - P - \frac{\langle \Psi_T(\lambda_1, \lambda_2) - P, g \rangle}{\|g\|^2} g.$$

Here $\Psi_T(\lambda_1, \lambda_2)$ denotes the parametrisation of T over the reference simplex, choosing λ_1 and λ_2 as coordinates as in (3.17). $d_{P,g,T}(\lambda_1, \lambda_2)$ is the perpendicular line from G to $\Psi_T(\lambda_1, \lambda_2)$, so it is a mapping from the reference triangle to $G^\perp$.

We can try to solve the non-linear equation (3.19) by a Newton iteration. For the case that one of the components of the solution $\lambda = (1 - \lambda_1 - \lambda_2, \lambda_1, \lambda_2)$ is negative, [SCHMIDT 1993] suggests to proceed to the corresponding neighbour as described in Algorithm 3.4.5 on page 88.

Figure 3.17 Projection to parametric surfaces, polynomial degree is 2

Unluckily, there are some complications. Two of the possible cases are illustrated in Figure 3.17, which shows quadratic parametrisations of two neighbouring elements. The straight lines in blue and red in the interior of the top-triangles indicate possible search-directions g .

The blue line in Figure 3.17(a) shows the “good” case where the projection along g hits the same element as found by the linear projection $\Pi_{\Gamma_{h,0}}^{lin}$. The red line originated from the pale-red coloured top-triangle on the right, but the non-linear projection should end up in left the element with the blue boundary.

However, it is not that easy to for a computer to efficiently find out that the “blue” element is indeed the right one for the red line in Figure 3.17(a). This is demonstrated in Figure 3.17(b), which shows – slightly rotated to give a better view – the left element, where the quadratic parametrisation is extended beyond the boundaries of the element.

The left, dark blue line in Figure 3.17(b) does not hit the quadratic parametrised surface at all. In this case equation (3.19) does not provide information about a neighbour which might contain the projection.

So it is not possible to apply the Projection-Algorithm 3.4.5 on page 88 blindly. To cope with this case, our implementation falls back to a brute-force search. If a solution of (3.19) cannot be found, traversing neighbouring elements until it succeeds.

This alone still does not suffice. The orange line on the right in Figure 3.17(b) on the preceding page hits the surface obtained by extending the quadratic parametrisation beyond the boundary of the element twice. This shows that a negative component of the barycentric coordinates obtained as a solution of (3.19) does not necessarily mean that the point should be projected to a neighbouring element.

So if the brute-force search still fails, the start-values for the Newton iteration are altered in the hope to eventually catch the correct solution.

This works in most cases. Otherwise, when a vertex-node cannot be projected, the node simply remains in place during the corresponding iteration of the smoothing-algorithm.

When non-vertex nodes cannot be projected, our implementation just skips the projection step. This means that the corresponding node remains in the place which is defined by the barycentric coordinates of its associated Lagrange node. In the case of 2-dimensional Lagrange elements this is just the mid-point of the edge which connects the neighbouring vertices.

Chapter 4

Numerical results

In this chapter we present the results of our numerical experiments.

We will begin with experimental convergence tests with respect to the discretised Newton iteration described in Section 2.4. In particular, we present *EOC*-tests with respect to the real L_2 - and H^1 -errors for approximations of some explicitly known solutions. Furthermore, we will compare the ad-hoc error indicators introduced in Section 2.4.4 with the real L_2 - and H^1 -errors. We use some members of the axially symmetric families of spheroidal and annular drop shapes discussed in Section 1.4.

In the last sections of this final chapter we will present the results of our experimental numerical computations. Our computations – although completely experimental – illustrate nevertheless the capabilities of our approach:

1. our algorithm does *not* rely on artificial symmetry constraints
2. it *cannot* suffer from coordinate singularities
3. it is able to treat drop shapes of arbitrary topology

The third point is a consequence of using a local parametrisation over the reference element. We stress that 3. does *not* mean that we are able to compute “through changes of topology”. Our numerical method preserves the topological class of the (discrete) surface because it preserves by construction the number of “holes” of the surface.

4.1 Experimental convergence tests

4.1.1 Convergence of the discrete Newton iteration

For a sequence of iso-parametric triangulations $\mathcal{T}_{h_j}$ we define the *experimental order of convergence* (*EOC*) – as usual – by

$$EOC_j := \frac{\log \frac{\mathcal{E}_j}{\mathcal{E}_{j+1}}}{\log \frac{h_j}{h_{j+1}}},$$

where $\mathcal{E}_j := \|u - u_{h_j}\|$ denotes the error between the discrete solution u_{h_j} and the exact solution u in any appropriate norm.

Table 4.1 Errors and *EOC*s for a spheroidal drop shape at $\omega \approx 0.7138$

h_{max}	$\ \Gamma - \Gamma_h\ _{L_2}$	<i>EOC</i>	$\ \Gamma - \Gamma_h\ _{H^1}$	<i>EOC</i>	$\ \Gamma - \Gamma_h\ _{L_\infty}$	<i>EOC</i>	$\ \Gamma - \Gamma_h\ _{H_\infty^1}$	<i>EOC</i>
0.159	0.000323	.	0.013	.	0.000342	.	0.0115	.
0.08	$2.78e - 05$	3.58	0.00309	2.1	$4.39e - 05$	3.	0.00366	1.67
0.0401	$3.37e - 06$	3.04	0.000798	1.96	$6.47e - 06$	2.76	0.00137	1.42
0.02	$4.26e - 07$	2.99	0.000202	1.98	$1.05e - 06$	2.63	0.000457	1.59
0.01	$5.38e - 08$	2.99	$5.07e - 05$	1.99	$1.59e - 07$	2.71	0.00013	1.82

Table 4.2 Errors and *EOC*s for an annular drop shape at $\omega \approx 0.7069$

h_{max}	$\ \Gamma - \Gamma_h\ _{L_2}$	<i>EOC</i>	$\ \Gamma - \Gamma_h\ _{H^1}$	<i>EOC</i>	$\ \Gamma - \Gamma_h\ _{L_\infty}$	<i>EOC</i>	$\ \Gamma - \Gamma_h\ _{H_\infty^1}$	<i>EOC</i>
0.17	0.00035	.	0.0148	.	0.000455	.	0.0115	.
0.0849	0.000128	1.46	0.00763	0.954	0.000204	1.16	0.0124	-0.115
0.0425	$1.58e - 05$	3.02	0.00183	2.07	$3.52e - 05$	2.54	0.00409	1.61
0.0213	$2.06e - 06$	2.94	0.000449	2.03	$5.82e - 06$	2.6	0.00116	1.81

Table 4.1 and Table 4.2 show the L_2 -, L_∞ -, H^1 - and H_∞^1 -errors for the approximation of a spheroidal and an annular shape (see Figure 4.1 on the next page), both members of the exactly known axially symmetric families of solutions to equation (2.6). The discrete surfaces were generated by the discrete Newton iteration described in the previous chapter using iso-parametric Lagrange-elements of polynomial degree 2. In each iteration of the convergence test the surface mesh was globally refined by doubly bisecting each element (see Section 3.3).

The *EOC* of the L_2 - and H^1 -errors shown in the tables 4.1 and 4.2 is nearly optimal in the sense that it is close to the approximation order of the Lagrange interpolation operator, see Theorem 2.4.5 on page 47.

We note that the first *EOC*-value is not always of the magnitude of the interpolation order which is explained by the fact that the initial triangulation used in the convergence tests was very coarse; in general *EOC*-tests are only meaningful for sufficiently refined meshes.

This is also illustrated by the diagrams shown in the Figures 4.2 to 4.5 on pages 96–99. The figures show the results of a test-run which started with a very coarse approximation of a sphere as initial surface for the path-tracking algorithm. Then the discrete path-tracking algorithm described in the previous chapter (see the flow-chart shown in Algorithm 2.6.1 on page 58) generated an initial family of coarse iso-parametric surfaces approximating the exact axially symmetric solutions described in Section 1.4.

Each of the coarse initial iso-parametric triangulations was then globally refined effectively halving the mesh-constant in each refinement step. The labels “level i ” to the right of the keys at the bottom of the figures denote the i^{th} refinement-step, so the maximal

Figure 4.1 Drop shapes used during the *EOC*-tests shown in Table 4.1 and 4.2

mesh-width of a triangulation at “level 5” is approximately 16-times smaller than the mesh-width of the corresponding “level 1” triangulation.

The final value of ω in the figures on the following pages is close to the value which marks the turning point where the spheroidal family bends back to meet the annular drop shapes (see Figure 1.5 on page 17).

Figure 4.2 shows the *EOC* for the L_2 - and H^1 -errors while tracking the axially-symmetric family of spheroidal drop-shapes. For the finer meshes the *EOC* seems again to approach the approximation order of the Lagrange interpolation operator, in accordance with the behaviour shown in Table 4.1 and Table 4.2.

4.1.2 Accuracy of the error indicators

In Section 2.4.4 we have introduced two residual ad-hoc error indicators for controlling the local adaption of the surface grids. We repeat them here for the sake of clarity:

$$(2.48) \quad \eta_{T,2}^2 := C_0^2 h_T^4 \| -\Delta_{\Gamma_h} \text{id}_{\Gamma_h} - (4\omega^2 r^2)\nu_{\Gamma_h} \|_{L_2(T)}^2 + C_2^2 h_T^3 \| [[\nu_{\Gamma_h}]] \|_{L_2(\partial T)}^2$$

$$(2.47) \quad \eta_{T,1}^2 := \tilde{C}_0^2 h_T^2 \| -\Delta_{\Gamma_h} \text{id}_{\Gamma_h} - (4\omega^2 r^2)\nu_{\Gamma_h} \|_{L_2(T)}^2 + \tilde{C}_1^2 h_T \| [[\nu_{\Gamma_h}]] \|_{L_2(\partial T)}^2$$

By summing up the local contributions of each element of the iso-parametric triangulations $\mathcal{T}_h$ we arrive at the global quantities

$$\eta_1 := \sqrt{\sum_{T \in \mathcal{T}_h} \eta_{T,1}^2} \quad \text{and} \quad \eta_2 := \sqrt{\sum_{T \in \mathcal{T}_h} \eta_{T,2}^2},$$

which we use to measure the error of the discretisation in the path-tracking algorithm. More specifically, either the value η_1 or η_2 is used as the stopping criterion for the mesh-adaption in Algorithm 2.6.1 on page 58.

Figure 4.2 *EOC* for L_2 - and H^1 -errors while tracking the spheroidal family

It is important to understand that it is not possible to determine constants C_0 and C_1 such that either η_1 or η_2 approximate the real error uniformly in ω because we compute the errors and the error indicators with respect to the L_2 - and H^1 -spaces on each surface. Those spaces are isomorphic for smooth surfaces of the same topological type but they are not *isometric*. Moreover, the iso-parametric finite element spaces W_h are not even isomorphic for the different discrete surfaces generated during the path-tracking if the mesh is refined or coarsened in between.

Finally, Figure 4.4 on the following page and Figure 4.5 on page 99 show the values of the real errors and the error indicator η_2 and η_1 using a logarithmic scale on the ordinate.

We note that the “noise” at $\omega \approx 0.71$ in some of the diagrams is caused by the bifurcation point which leads to the 3-lobed family.

4.1.3 Eigenvalue computation

Although the accuracy of eigenvalue computation is an important issue for the path-tracking algorithm – because it determines the position of the bifurcation points – we will be rather brief here. Figure 4.3 shows the first 5 eigenvalues of the linearised Euler-Lagrange equation for some of the drop-shapes computed during the convergence tests discussed in the previous two sections. We note that the figure actually shows the smallest 5 eigenvalues for 4 levels of global refinement – though this is hardly recognisable in the diagram on the left. The right diagram is just a magnified part of the left diagram and shows the 5th eigenvalue. Still only the coarsest discretisation – the red line – can be clearly distinguished from all the others which are just plotted one over another.

Figure 4.3 The first five eigenvalues, computed for some of the shapes used for the experimental convergence tests shown on the pages before

Figure 4.4 L_2 -errors and error-indicators while tracking the spheroidal family

Figure 4.5 H^1 -errors and error-indicators during path-tracking

4.2 Bifurcation diagrams and drop-shapes

We start this section by comparing the bifurcation diagram Figure 4.6 – computed by [BROWN and SCRIVEN 1980a] – with the results of our own computations. Brown and Scriven were investigating numerically the bifurcations from the axially symmetric family of spheroidal shapes (see Section 1.4). We remark that Figure 4.7 on the next page – showing the results of our own numerical experiments – has its axis interchanged with respect to Figure 4.6. Generally, we illustrate the bifurcations by plotting the angular momentum L against the angular velocity ω . Using either (ω, L) - or (L, ω) -diagrams is a natural choice because L is the proper parameter to describe freely rotating drops while the equations for the equilibrium shapes take as simpler when choosing ω as parameter.

Figure 4.6 Bifurcation diagram as computed by [BROWN and SCRIVEN 1980a]

FIGURE 4. Shape families, their stability and bifurcations, for drops isolated and so rotating at constant angular momentum. Shapes are stable along solid branches, unstable along broken ones.

We have chosen ω for the abscissa because it is the bifurcation parameter for our path-tracking algorithm.

We remind in this respect of the introductory Section 1.1 for the relation between the two variants of the energy functional which use either the angular velocity or the angular momentum as the bifurcation parameter.

The notion of an n -lobed drop shape used in Figure 4.6 on the facing page and Figure 4.7 will be made clear by the pictures on the following pages. The first difference between the two bifurcation diagrams is that Figure 4.7 shows many bifurcations not present in Figure 4.6. Besides the two-, three and four-lobed families already found by [BROWN and SCRIVEN 1980a] there are a five- and a six-lobed branch which bifurcate directly from the axially symmetric family. All families bifurcating from the axially symmetric family also have sub-branches (though Figure 4.7 doesn't show it for the five-lobed branch).

The major reason why we were able to find discrete solutions not found by Brown and Scriven is that they used a global parametrisation to represent the drop shapes. Another reason is that they were imposing an artificial meridional reflective symmetry.

Another difference between Figure 4.6 and 4.7 is that the scales of the axes do not match. The reason is that Brown and Scriven did not compensate for dissecting the drop at its equatorial and the assumed meridional symmetry-plane. This means that their angular momentum differs from ours by a factor of 4.

Figure 4.7 Bifurcation diagram resulting from Algorithm 2.6.1 on page 58

Figure 4.7 on the preceding page does not contain all the bifurcations we have found. We will present more detailed diagrams below which concentrate on certain parts of the solution family rather than presenting an overview over the entire set of discrete solutions computed by our path-tracking algorithm.

We have the conjecture that beyond the six-lobed family there are no further bifurcations from the main branch. We believe so because the eigenvalues of the linearised Euler-Lagrange equation seem to approach zero when tracking down the main branch beyond the bifurcation point of the six-lobed family towards smaller values of ω . Figure 4.8 shows the smallest few eigenvalues of the linearised Euler-Lagrange equations for the axially symmetric family of spheroidal solutions.

Figure 4.8 Spectrum of the linearised Euler-Lagrange equations for the axially symmetric spheroidal family after the turning point

4.2.1 Two-lobed spheroidal shapes

The first bifurcation from the axially symmetric family of spheroidal drop shapes occurs at a value of $\omega \approx 0.5599$ which is in accordance with the value reported in [BROWN and SCRIVEN 1980a]. We note that [WENTE 1982] has developed a method to estimate the actual value of ω to arbitrary accuracy. We note, however, that the value determined by the path-tracking method is inherently inexact because the linearization of the Euler-Lagrange equations becomes singular at a branch point which leads to numerical difficulties in the discretisation.

Figure 4.9 shows a sequence of members of the two-lobed family of drop shapes. The two-lobed drops seem to approach a limiting surface consisting of two spheres touching each other in one point as ω approaches 0.

Figure 4.9 Two-lobed drop shapes

The value of ω which marks the bifurcation point for the two-lobed family is important because it marks the onset of instability for the axially symmetric spheroidal family. Beyond this point the linearization has negative eigenvalues – regardless whether one imposes the additional constraint of conservation of angular momentum. This means

that all spheroidal shapes for larger values of ω are (presumably) only saddle-points of the underlying energy functional.

It is remarkable in this respect that the first part of the *two-lobed* family might be stable if one imposes the constraint of conservation of angular momentum. Figure 4.10 shows that at the beginning of the two-lobed branch the (discretised) linearization has only positive eigenvalues when the angular momentum is conserved by the admissible perturbations. This was already found out by Brown and Scriven.

Figure 4.10 Spectrum of the linearised Euler-Lagrange equations for the two-lobed branch under the constraint of conserve angular momentum. The strange transversal lines at the right of the spectrum are just an artifact of the numerical construction of the initial value for the Newton iteration: the eigenvalue leading off to a new branch changes it multiplicity at the bifurcation point.

The two-lobed family has an interesting sub-branch which starts at $\omega \approx 0.262$. The form of the drops is illustrated in Figure 4.11 on the facing page. Brown and Scriven also found a sub-branch of similar shape at $\omega \approx 0.255$. However, they reported that the so called “peanut-shaped” branch reconnects to the two-lobed branch at a smaller value of the angular velocity. We could not reproduce their result. In fact, the branch of “peanut-shaped” discrete surfaces found by us branches off to *larger* values of ω .

It is interesting that this new family of surfaces passes through several turning points and – up to the point where we terminated our path-tracking algorithm – develops an additional constriction after each turnaround in the ω - L diagram. Figure 4.12 and 4.13

on page 106 and 107 illustrate the “development” of the constrictions in greater detail (this is *not* a development in time; all surfaces are equilibrium figures).

We have the conjecture that this sub-branch of the two-lobed family develops arbitrary many constrictions while “winding up” itself in the (ω, L) -plane.

We will see below that a similar behaviour seems to be typical for all sub-branches of the three- and four-lobed families and for the five- and six-lobed family bifurcating from the main branch.

Figure 4.11 Sub-branch of the two-lobed family branching at $\omega \approx 0.262$. The notion “Branch 1-2-3-4-5-6-7” indicates which eigenvalue was approaching 0 at each turning point, leading to the next turnaround.

Figure 4.12 Two-lobed sub-branch, view from the top. The black cross marks the axis of rotation.

branch 1-2, $\omega=0.2624$

branch 1-2, $\omega=0.3721$

branch 1-2, $\omega=0.4551$

branch 1-2-3, $\omega=0.3255$

Figure 4.13 Two-lobed sub-branch, continued from Figure 4.12 on the preceding page

branch 1-2-3-4, $\omega=0.4332$

branch 1-2-3-4-5, $\omega=0.3413$

branch 1-2-3-4-5-6, $\omega=0.4226$

branch 1-2-3-4-5-6-7, $\omega=0.3515$

4.2.2 Three- and four-lobed shapes

Like the two-lobed branch the three- and four-lobed branches seem to approach a limit surface consisting of spheres of equal size when ω tends to zero. Figure 4.14 illustrates this for the case of the three-lobed branch.

Figure 4.14 Three-lobed branch at $\omega = 0.1056$. This figure also illustrates the effectiveness of the mesh-smoothing algorithm and the concept of using a local parametrisation over the reference simplex which allows for surfaces with self-intersection.

More interesting is the behaviour of the sub-branch which bifurcates from the three-lobed family at $\omega \approx 0.42$, see Figure 4.15 on the next page. First we note that the sub-branch leads to both, smaller and larger values of ω . It seems to be tangential to the three-lobed branch in the (ω, L) -plane. The sub-branch shows again the “winding-up” behaviour

Figure 4.15 Three-lobed sub-branch breaking the meridional reflective symmetry

similar to the sub-branch of the two-lobed family, and it is highly probable that it continues beyond the point where we stopped our computations. However, the important point is that it develops a sub-sub-branch which breaks the meridional reflective symmetry.

The way this happens seems to be typical for the sub-branches in the respect that not all lobes develop constrictions simultaneously but only some of them.

Concerning the four-lobed shapes we just remark that they exhibit a similar behaviour as the three-lobed families. They seem to approach a four-sphere limit when ω tends to zero. The bifurcation diagram Figure 4.7 on page 101 shows sub- and sub-sub-branches which are related to the geometrically simpler “parent” branches by shrunk or grown lobes and additional constrictions, just as it was the case for the three-lobed family.

4.2.3 Five- and six-lobed spheroidal shapes

The five- and six-lobed bifurcations differ from the two-, three- and four-lobed variants. They do not approach a limit surface consisting of spheres of equal size, but instead wind-up in the (ω, L) -phase-space, see Figure 4.16. We are rather brief here and just present some pictures on the following pages.

Figure 4.16 “Winding-up” of the two-, five- and six-lobed families

Figure 4.17 Five-lobed drop shapes

$\omega = 0.7239$ $\omega = 0.7138$ $\omega = 0.5731$ $\omega = 0.4491$

Figure 4.18 Five-lobed shapes after and before “winding-up” in the (ω, L) -plane

Figure 4.19 Members of the six-lobed branch shown in the bifurcation diagram Figure 4.7 on page 101. The bottom-right shape belongs to the sub-branch.

4.2.4 Annular drop shapes

The results of our computations with respects to bifurcations from the axially symmetric annular shapes are summarised in the bifurcation diagram shown in Figure 4.20.

Figure 4.20 Bifurcations from the axially symmetric family of annular shapes

We remark that the “pearl-necklet”-like shape does not seem to be the final bifurcation of this kind. We have the conjecture that for decreasing ω there is a countable number of bifurcations, each one incrementing the number of constriction by 1 with respect to its predecessor.

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Index of Notations

$C^\infty(\bar{\Omega})$	smooth functions, p. 7
$C^k(\bar{\Omega})$	continuously differentiable functions, p. 7
$C^{0,\alpha}(\bar{\Omega})$	Hölder-continuous functions, p. 8
$C^{k,\alpha}(\bar{\Omega})$	differentiable functions with Hölder-continuous derivatives, p. 8
$C_0^\infty(\bar{\Omega})$	smooth functions with compact support, p. 7
$C_0^k(\bar{\Omega})$	continuously differentiable functions with compact support, p. 7
$C^{0,1}(\bar{\Omega})$	Lipschitz-continuous functions, p. 8
$\text{conv}(\cdot)$	convex hull, p. 43
DA	Frechet-derivative of the operator A , p. 14
Δ_Γ	Laplace-Beltrami operator of Γ , p. 11
$\nabla_\Gamma \cdot w$	tangential divergence of w , p. 11
$\nabla_\Gamma f$	tangential gradient of f , p. 11
δE	first variation of E , p. 22
$\delta^2 E$	second variation of E , p. 25
$\delta_i^\Gamma f$	directional tangential derivative of f , p. 11
$\nabla^s f$	mixed partial derivatives, $s = (s_1, \dots, s_n) \in \mathbb{N}_0^n$, p. 7
∇_i, D_i, ∇, D	partial derivatives and gradient, p. 7
$\frac{\partial f}{\partial v}$	directional derivative in direction v , p. 7
EOC	experimental order of convergence, p. 64, 93
Γ_h	triangulated or discrete surface, p. 43
Γ_h^d	iso-parametric surface of degree d , p. 46
H_Γ	mean curvature of Γ , p. 12
H_h	discrete scalar mean curvature, p. 63
$\mathring{H}_p^k(\Omega)$	Sobolev-space with trace zero on $\partial\Omega$, p. 8
$H_p^k(\Omega)$	Sobolev-space, p. 8
Π	Weingarten-map, p. 12
Π_h	discrete Weingarten map, p. 62
K_Γ	Gaussian curvature of Γ , p. 12
K_h	discrete Gaussian curvature, p. 63
$(\lambda_1, \dots, \lambda_{n+1})$	barycentric coordinates, p. 44
$L_p(\Omega)$	Lebesgue-space, p. 8
$m(n, d)$	$\dim(P_d(\mathbb{R}^n))$, p. 44
$\mathbb{N}$	natural numbers, p. 6
ν_T	unit normal of the iso-parametric n -simplex T , p. 60

ν_h	approximate discrete unit normal field, p. 60
Φ_T^d	polynomial parametrisation of degree d over $\hat{T}$, p. 46
P_k	polynomials over $\mathbb{R}^n$ of degree at most k , p. 7
$\Phi * \cdot$	pull back w.r.t. to Φ , p. 41
$\hat{p}_j$	j^{th} -Lagrange polynomial, p. 44
$\mathbb{R}$	real numbers, p. 6
$\mathbb{R}^+$	positive real numbers, p. 6
$S(P)$	the “star” of P , the elements adjacent to the vertex, p. 60, 72
$\hat{S}(P)$	projected element neighbourhood, p. 75
$A : B$	Euclidean scalar product between matrices, p. 6
$x \cdot y, \langle x, y \rangle$	Euclidean scalar product, p. 6
$T\Gamma$	tangent bundle, p. 11
$T_P\Gamma$	tangent space of Γ at P , p. 10
$\mathcal{T}_h$	triangulation, p. 43
$\mathcal{T}_h^d$	iso-parametric triangulation of degree d , p. 46
$\hat{T}$	reference simplex, p. 44
$W_h^d(\Gamma_h^d)$	finite element space over Γ_h^d , p. 47
Y_Γ	curvature vector, p. 12
Y_h	discrete curvature vector, p. 62

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