

An Eulerian Discontinuous Galerkin Method for the Numerical Simulation of Interfacial Transport

Christina Kallendorf



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An Eulerian Discontinuous Galerkin Method for the Numerical Simulation of Interfacial Transport

Vom Fachbereich Maschinenbau an der Technischen Universität Darmstadt zur Erlangung des akademischen Grades eines Doktor-Ingenieurs (Dr.-Ing.) genehmigte

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Nomenclature

Abbreviations

Arbitrary Lagrangian Eulerian
Discontinuous Galerkin
Discontinuous Galerkin method
Evolving Surface Finite Element method
Finite Area method
Finite Difference method
Finite Element method
Finite Volume method
Interior Penalty
Local Discontinuous Galerkin
Marker and Cell
Particle in Cell
Piecewise Linear Interface Calculation
Surface Finite Element method
Simple Line Interface Calculation
Volume of Fluid

Dimensionless numbers

Hatta number
Peclet number
Reynolds number
Weber number
Characteristic length scale
Characteristic velocity scale

Operators

Trace of an operator matrix
Laplace operator
Multiplier
Divergence
Curl operator
Gradient
Surface divergence

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$\nabla^{(\mathfrak{s})}$	Surface gradient
$P^{\mathfrak{s}}$	Surface projection tensor
\mathcal{E}_{u^j}	Euler operator
D_i	Total derivative

Symbols

$\eta^{(i)}$	Dynamic viscosity of phase <i>i</i>
$p^{(i)}$	Pressure of phase <i>i</i>
(φ, θ, r)	Spherical coordinate system
$\{\{\cdot\}\}$	Average operator
<i>u</i>	Dependent variables
z	Independent variables, including time where applicable
$F^*(\Phi_h^+,\Phi_h^-)$	Numerical flux function
$\frac{d}{dt}$	Total time derivative
$\mathfrak{B}^{(1)}$	Part of the domain occupied by the inner phase
$\mathfrak{B}^{(2)}$	Part of the domain occupied by the outer phase
G	Phase Interface
$\gamma^{(\mathfrak{s})}$	Excess surface physical quantity
HeunC	Heun's confleunt function given by
	HeunC $(a_1, a_2, a_3, a_4, a_5, s) = \sum_{n=0}^{\infty} v_n(a_1, a_2, a_3, a_4, a_5) s^n$
[[·]]	Jump operator
(\cdot, \cdot)	Inner product
\mathcal{F}	Arbitrary smooth function
<i>G</i>	Arbitrary smooth function
¢	Intersection of the interface with the boundary of the domain
<i>A</i>	Coefficient matrix
<i>I</i>	Identity matrix
M	Mass matrix
$oldsymbol{M}^E$	Cell-face mass matrix
Ω	Problem domain
Ω_h	Computational domain
$\partial \Omega$	Boundary of the domain
$\Phi \ \ldots \ldots \ldots$	Level Set function
Σ_h^{γ}	Narrow band tube around the interface
$n^{(\mathfrak{s})}$	Unit normal vector
$w^{(\mathfrak{s})}$	Speed of the interface S
τ	Penalty parameter
Θ	Conservation law density
$u^{(i)} (i = 1, 2) \ldots$	Material velocity of the subdomain $\mathfrak{B}^{(i)}$ (<i>i</i> = 1, 2)
Ψ	Conservation law spatial fluxes
n	Outward unit normal vector of $\partial \Omega$
$oldsymbol{n}^{j}$	Normal vector to the <i>j</i> th grid cell
<i>s</i>	Unit normal to the curve \mathfrak{C} , tangent to the interface
<i>D</i>	Dimension of the domain

<i>h</i>	Characteristic grid size
I^{γ}	Set of cells included in the Narrow Band
K_j	jth grid cell
$L^2(\Omega)$	Equivalent classes of measurable, squarely integrable functions on
	Ω up to null sets
l_i^j	Langrange polynomials
$P^k(K)$	Polynomials on cell K whose order is at most k
$S(c, \boldsymbol{x}, t) \ldots \ldots$	Source term
S^d	Differentiation matrix in <i>d</i> -th spatial component

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We	Weber number
<i>L</i>	Characteristic length scale
u_{∞}	Characteristic velocity scale

Operators

tr	Trace of an operator matrix
Δ	Laplace operator
Λ^i	Multiplier
$\nabla \cdot$	Divergence
$\nabla \times$	Curl operator
∇	Gradient
$\nabla^{(\mathfrak{s})}$	Surface divergence

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$\nabla^{(\mathfrak{s})}$	Surface gradient
$P^{\mathfrak{s}}$	Surface projection tensor
\mathcal{E}_{u^j}	Euler operator
D_i	Total derivative

Symbols

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$\Omega \ \ldots \ldots \ldots \ldots$	Problem domain
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$\Theta \ \ldots \ldots \ \ldots$	Conservation law density
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S^d	Differentiation matrix in <i>d</i> -th spatial component

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1 Introduction

1.1 Motivation

In various applications, it is important to model, simulate and compute processes on surfaces, curves or on more general submanifolds. Most of these processes are governed by partial differential equations (PDEs) on surfaces, or on submanifolds, respectively. Depending on the application, the problem domain is either steady, or deforming, or moving and deforming at the same time. These distinct cases imply an increasing complexity of the problem. Areas of interest range from fluid mechanics, bio-chemistry and medical imaging to image processing. Q

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For example, in image processing, surface differential equations on steady surfaces are involved when smoothing and regularizing images (Diewald, Preußer, Rumpf, and Strzodka, 2001). Denoising (Bertalmío, Cheng, Osher, and Sapiro, 2001) as well as deblurring (Cheng, 2000) of images is achieved by solving surface diffusion equations, for instance, in brain imaging (Mémoli, Sapiro, and Thompson, 2004).

In biochemistry, the interaction of pairs of chemicals, called morphogenes, in the epithelial, i.e. outer, layer of growing organisms is modelled by reaction-diffusion equations on the organisms' surface (Leung and Berzins, 2003a). Morphogenes have been used in modelling spatial pattern formation and the regeneration of body cells such as receptor cells in the eye of a Drosophila (Koch and Meinhardt, 1994). Coat markings of mammals as well as the formation of skeletal pattern are assigned to morphogenes (Maini, Painter, and Nguyen Phong Chau, 1997). These morphogenesis processes are goverended by differential equations on *deforming* surfaces.

In fluid mechanics, the transport of mass, energy or momentum on phase interfaces is a topic of increasing importance. Here, interfacial transport is modelled by PDEs on the phase interface and therefore, on *moving* and *deforming* interfaces. In particular, it is often inevitable to examine the transport of surface active substances on the moving interface, such as emulsifiers or detergents. For their surface active behavior, these compounds are known as surface active agents, or shortly *surfactants* (Schramm, 2000). The transport of these substances on two-phase interfaces is governed by convectiondiffusion equation defined on evolving surfaces. These surfaces may change rapidly with respect to geometry or topology.

Introduction

Because their structure includes both a part which has affinity to nonpolar media and one part that has an affinity to polar media, surfactants absorb at interfaces that separate media of different polarity. During adsorption, the surfactant molecules form a monolayer on the interface between the immiscible phases, destroying the cohesive forces between the polar and non-polar molecules and replacing them. While the hydrophilic head of the adsorbed surfactant molecule orients itself towards the polar phase, the hydrophobic tail lies either flat on the interface, or aligns itself to the less polar liquid (Gecol, 2007), if the interface is sufficiently occupied. As a consequence of the adsorption process, most types of surfactants reduce the interfacial free energy, i.e. the surface tension (Tricot, 1997a). This implies that the surface tension of a surfactant covered interface is lower than the one of a clean interface. Furthermore, the interfacial tension is comparatively lower in interfacial regions of high surfactant concentration. When the surfactant is not uniformly distributed, a Marangoni force is introduced by the gradient that exists in surfactant concentration. This Marangoni force is directed from regions of high surfactant concentration to regions of low surfactant concentration along the interface (Kas-Danouche, Papageorgiou, and Siegel, 2004).

Numerous industrial processes that involve two-phase or free surface flows require controlling mechanisms of the surface tension. Fur this purpose, surfactants are usually added to either of the phases.

Silicone surfactants are used as stabilizing agents for polyetherane foam by reducing interfacial tension and, consequently, promoting the formation of a coherent interfacial film (Snow, Pernisz, and Braun, 2006). They function as stabilizer of foams, for instance, in enhanced oil recovery or drilling operations.

Surfactants are used to control the formation of small droplets in industrial emulsification processes by lowering the surface tension, and hence facilitating the droplet breakup and preventing coalescence (Janssen, Boon, and Agterof, 1994; Eggleton, Tsai, and Stebe, 2001). Surfactants are commonly added to stabilize emulsions, i.e. mixtures of two or more immiscible fluids, such as oil and water. Emulsions are present not only in food, cosmetic and pharmaceutical products, but they are also frequently applied in technical processes. For instance, emulsions are used as cooling lubricants in order to minimize both frictional effects and temperature during machining processes, for instance, in metal fabrication (Doll and Sharma, 2011). Emulsified fuels, where water droplets are dispersed in the fuel and stabilized by a surfactant additive, are used in automotive technology in order to minimize emissions. For example, water in diesel dispersions have been investigated as direct fuel substitutes that can be utilized with little or no modifications in existing diesel engines by Nadeem, Rangkuti, Anuar, Haq, Tan, and Shah (2006). They were reported to significantly reduce the emissions of NO_x , CO, SO_x as well as particle matter.

Coating forms an important aspect of numerous industrial manufacturing processes in order to protect, functionalize and lubricate surfaces. Surfactants are often employed as additives to facilitate coating processes by reducing the surface tension (Tricot, 1997b). At the same time, several processes involve coating liquids that are surfactant

solutions, and surface and bulk rheology of these solutions naturally impacts the coating properties.

From the numerical perspective, evolving interfacial physical quantities along a moving deformable surface is a highly challenging task. The surface differential operators involved require a thoughtful approximation that is distinct from the available discretizations of standard differential operators. Depending on the method applied, tracking or capturing an interface also requires great expertise. In most research works a Lagrangian grid is used to track the phase interface and employed to discretize interfacial equations, implying that these equations are only solved on the interface, see e.g. Ceniceros (2003), James and Lowengrub (2004), Kruijt-Stegeman, van de Vosse, and Meijer (2004), Lai, Tseng, and Huang (2008), Lee and Pozrikidis (2006), Muradoglu and Tryggvason (2008) or Zhang, Eckmann, and Ayyaswamy (2006).

In the present work, a numerical framework for solving interfacial convection-diffusion problems is established. In contrast to these traditional approaches, the method presented here does **not** treat interfacial transport problems by establishing a Lagrangian, i.e. interfacial grid, but instead, it is founded on maintaining the Eulerian grid. Up to now, considerably fewer works on numerical simulations of interfacial equations are based on such an Eulerian approach. Several limited examples are given by Bertalmío, Cheng, Osher, and Sapiro (2001), Greer (2006), Greer, Bertozzi, and Sapiro (2006), Burger (2009) as well as Dziuk and Elliott (2009) for various interfacial differential equations. Especially when the a surface moves and deforms quickly, as in the case of a fluidic interface, an Eulerian representation of the surface differentials has favorable properties. Beyond, the method can be easily combined with an interface capturing technique that presumes an implicit representation of the interface.

For this purpose, the Discontinuous Galerkin (DG) method is employed, which incorporates favorable features of both Finite Element (FE) and Finite Volume (FV) methods. The DG method has become increasingly popular in the past decades, as it combines polynomial approximations of arbitrary order with the use of numerical fluxes to approximate integrals over the cell boundaries. Consequently, the DG approach is highly convenient for hyperbolic problems. At the same time, it is flexible with respect to the domain's geometry and achieves $O(h^p)$ order of convergence. Importantly, the use of numerical fluxes establishes a local block structure of the discretization, which supports parallel computing, and allows to incorporate boundary conditions easily. The treatment of surface convection-diffusion equations by the DG method highly benefits from these features, and to the author's knowledge, it is the first published work that pursues an Eulerian approach for resolving surface differential operators in the context of a DG method.

A parallelized and modular package for the numerical simulation of interfacial transport problems is designed. The library, developed in C#, discretizes both interfacial convection and convection-diffusion equations by a DG method, and is integrated in the existing software framework *BoSSS* initiated by Kummer (2012). Here, the surface convection-diffusion equation is extended into the underlying three-dimensional space by identifying the surface gradient with the projection of the standard gradient to

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its tangential part. In this way, the interfacial transport problem can be discretized based on the existent Eulerian grid, at the same time admitting an implicit interface representation as the zero-isocontour of a Level Set function. In contrast to the Langrangian approach, this Eulerian approach is highly suitable for moving and deforming interfaces and allows for an accurate resolution of the interface.

1.2 Thesis Outline

The present work is structured as follows.

The surface differential equations under consideration focus on the general case of interfacial transport in fluid mechanical applications. For this reason, in chapter 2, starting from the standard postulates of continuum mechanics, the derivation of local mass balance laws for the bulk phases and for the phase interface for some arbitrary physical quantity are provided, following Wang and Oberlack, 2011. The resulting equations are then employed to derive the equations of the physical model under consideration, i.e. the Navier–Stokes equations for two phases, including interfacial jump conditions, and the interfacial convection–diffusion equation describing material transport at a two–phase interface.

Chapter 3 gives a comprehensive overview of existing numerical research on surface and interfacial transport. Available methods are classified as traditional *Lagrangian approaches*, where the submanifold itself is resolved by a Lagrangian grid, or as *Eulerian approaches*, where the interfacial problem is extended into the underlying threedimensional domain and discretized on basis of the given Eulerian grid. Special attention is paid to existing works dealing with interfacial transport in fluid mechanical applications. In this context, the method selected for the treating the interfacial equations highly depends on the approach employed for tracking or capturing the interface. Therefore, numerical methods that are available for representing the phase interphase are additionally outlined in chapter 3.

The solver developed within the context of this work is based on a Discontinuous Galerkin (DG) discretization of the transport problem. For this reason, the fundamentals of the DG method are explained in chapter 4 with a particular focus on the PDEs relevant to the subsequent work. Its characteristic features are underlined, pointing out to the motivation for founding the subsequent approximations on a DG scheme. Against this background, chapter 4 further motivates the design of the method presented, incorporating an interface capturing approach by a Level Set function and an Eulerian approach for resolving the surface differentials.

In the Eulerian formulation, however, the conserved form of the interfacial balance law is destroyed by the extension of the interfacial differential equation to the threedimensional domain. This fact has been identified as an obstacle at the initial project phase. From the viewpoint of numerical accuracy, the conserved form of a differential equation is always favorable to reduce numerical errors and preserve the quantity numerically. In chapter 5, infinite sets of conservation laws have been discovered by using the direct construction method, i.e. by applying local conservation law multipliers (Kallendorf, Cheviakov, Oberlack, and Wang, 2012). These conserved forms constitute a well-suited basis for discretizing the interfacial transport equation by a DG scheme, while maintaining an implicit representation of the interface. The obtained results are also applicable to the construction of more general balance laws for other excess surface physical quantities. The system of governing equations is subsequently rewritten in a fully conserved form in the three-dimensional domain.

In chapter 6, general exact solutions to the interfacial transport of a solute on the spherical surface with both convective and diffusive terms are developed (Kallendorf, Fath, Oberlack, and Wang, 2015). The transport of insoluble surfactant in a Stokes flow setting is investigated, where a spherical shaped inner phase is dispersed in an outer phase. The model is simplified by assuming that the impact of the surfactant on surface tension is negligible. Its investigation has been motivated by the lack of exact solutions to the interfacial transport problem. The general solutions derived involve Heun's confluent functions, and for the steady case, it is shown that these solutions collapse to a simple exponential form. Furthermore, for the purely diffusive problem, exact solutions are constructed using Legendre polynomials.

The embedded interfacial transport problem is discretized on a small subdomain of the original domain only, which is given by a Narrow Band tube of few cells thickness around the interface. As this narrow band changes position and structure in accordance with the interface, it is not created as an independent physical grid, but rather induced from the full grid through selective storage allocation and extraction of the relevant entries, or coordinates, respectively. Chapter 7 describes how such a coordinate based Narrow Band is implemented within the software framework BoSSS (Kummer, 2012). Furthermore, a method for extending values to newly acquired cells of this subdomain is developed and analysed in chapter 8. This tool, which is based on employing a pseudo-timestepping scheme, is essential when discretizing problems on a dynamically moving Narrow Band.

Chapter 8 describes the Eulerian DG scheme that is established in the present work for discretizing interfacial transport equations. This implementation is based on simplest forms of the conservation laws that have been developed in chapter 5. The convection-diffusion equation is discretized by a simple operator splitting scheme, which motivates to solve the purely convective and the purely diffusive parts of the conserved form independently. Computational examples of all of the three forms of surface transport equation are developed and solved for both two-and three-dimensional underlying domains. Based on exact solutions to the two-dimensional examples, a study of convergence is presented, where the purely convective equation, both on a steady and on a moving surface, as well as the purely diffusive equation on a steady surface are considered. Illustrations of sample problems are provided for problems of all mentioned complexities, i.e. for steady, but complex, moving as well as moving and deforming surfaces. Q

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To conclude, chapter 9 summarizes the results achieved within the context of the present thesis. This chapter concludes with an outlook of further improvements and ideas for continued research.

2 Equations of the Physical Model

2.1 Transport Equations in Two-Phase Flow

In this section, starting from the standard postulates of continuum mechanics, local mass balance laws for the bulk phases and for the phase interface are derived for some arbitrary physical quantity. The derivation presented here is adopted from Wang and Oberlack (2011), who established, in addition to the classical mass balance laws for the bulks in a three-phase setting, local mass balance laws for phase interfaces and contact lines. The resulting equations are then employed to derive the equations of the physical model under consideration, i.e. the Navier – Stokes equations for two phases, including interfacial jump conditions, and the material transport equations at a two-phase interface and in the bulks.

2.1.1 Mass Balance Laws in a Two-Phase Setting

Let Γ denote a physical variable charaterizing a partial aspect of a state of a body at time *t*. A material domain $\Omega(t)$ of the body under consideration is chosen with respect to which the physical variable is evaluated. For this purpose, a setting with two immiscible phases is assumed, considering a material domain Ω which is decomposed into two disjoint subdomains $\mathfrak{B}^{(1)}$ and $\mathfrak{B}^{(2)}$ occupied by the distinct phases. The two phases are separated by a curved surface \mathfrak{S} , the phase interface, which can be identified with a two-dimensional, moving, orientable and mathematically singular surface in the three-dimensional Euclidian space. This surface is singular in the sense that a vanishing interface thickness is considered, across which the physical quantities may be discontinuous.

In fact, in multiphase systems, an interface is rather given by a thin transition layer of only few molecular layers thickness, across which physical quantities, such as mass or momentum, change smoothly but rapidly. But as the thickness of this interfacial transition zone ranges at the nanometer scale, the interface is infinitely thin as compared to the dimensions of the adjacent bulks and can be considered as a two-dimensional continuum, with its own material properties, for instance, surface tension.

The material domain Ω is bounded by an outer boundary $\partial \Omega = \partial \mathfrak{B}^{(1)} \cup \partial \mathfrak{B}^{(2)} \cup \mathfrak{C}$ in Lagrangian representation, where the curve \mathfrak{C} denotes the intersection of the interface \mathfrak{S} with the domain's boundary $\partial \Omega$. As depicted in figure 2.1, *n* denotes the outward

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unit normal vector of $\partial\Omega$ and $n^{(s)}$ the unit normal of the interface \mathfrak{S} , pointing from $\mathfrak{B}^{(1)}$ into $\mathfrak{B}^{(2)}$. In addition, the unit normal *s* to the curve \mathfrak{C} , which is tangent to the interface and oriented outward from the system, is needed in the following derivations.

Denoting the total time derivative by $\frac{d}{dt}$, the time rate of change of the physical variable Γ of the body per unit time can be decomposed into

$$\frac{d\Gamma}{dt} = F + P + S,\tag{2.1}$$

destinguishing the flux *F* of the variable from outside into the body through the surface $\partial\Omega$, its production *P* within the domain as well as its supply *S*, or source by action, at a distance from outside of the body. The physical variable can be specified by means of densities $\gamma^{(i)}$, in each subdomain $\mathfrak{B}^{(i)}$, i = 1, 2, and density $\gamma^{(s)}$, on the interface \mathfrak{S} , repectively, in Eulerian representation, i.e.

$$\Gamma = \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \gamma^{(i)} \, dv + \int_{\mathfrak{S}} \gamma^{(\mathfrak{s})} \, da.$$
(2.2)

On the interface, densities of the respective surface excess amounts are employed. The surface excess $N_l^{(s)}$ of a component l corresponds to the difference between its actual amount present in the real system, and its amount in a reference system if its concentration within the adjacent bulks is extended to a chosen geometrical dividing surface (Mitropoulos, 2008). The dividing surface, i.e. singular interface, is usually located where the surface excess of the solvent is zero, as depicted in figure 2.2. Likewise, the terms on the right hand side can be expressed in integral form employing

- the non-convective bulk flux densities of Γ (per unit surface area), $\phi^{(i)}$ (*i* = 1, 2), through the material outer surfaces $\partial \mathfrak{B}^{(i)}$ of the bulk phases $\mathfrak{B}^{(i)}$,
- the non-convective surface flux density of Γ (per unit line length), φ^(s), through the outer boundary curve C of the phase interface G,



Figure 2.2: Surface excess concentration in a two-component system according to Mitropoulos (2008). The concentration profile is given as a function of distance normal to the phase boundary. The surface excess is the sum of shaded areas above and below of the dividing surface. Usually, the dividing surface is chosen as the zero surface excess of the solvent.

- the bulk and surface production densities, $\pi^{(i)}$ (in the bulk phases $\mathfrak{B}^{(i)}$, i = 1, 2) and $\pi^{(s)}$ on the phase interface, respectively,
- as well as the bulk and surface supply rate densities $\zeta^{(i)}$ (in the bulk phases $\mathfrak{B}^{(i)}$, i = 1, 2) and $\zeta^{(s)}$, on the interface, respectively.

Using these densities, one immediately obtains

$$P = \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \pi^{(i)} \, dv + \int_{\mathfrak{S}} \pi^{(\mathfrak{s})} \, da$$
(2.3)

$$S = \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \zeta^{(i)} \, dv + \int_{\mathfrak{S}} \zeta^{(\mathfrak{s})} \, da.$$
(2.4)

With respect to the non-convective fluxes, one assumes that the surface flux vector $\phi_C^{(s)}$ per unit length at the curve \mathfrak{C} depends on the coordinate $x^{\mathfrak{C}}$ of \mathfrak{C} , the time t and the line normal s and has the form

$$\phi_C^{(\mathfrak{s})} = \phi_C^{(\mathfrak{s})} \left(\boldsymbol{x}^{\mathfrak{C}}, t, \boldsymbol{s} \right) = -\phi^{(\mathfrak{s})} \cdot \boldsymbol{s}.$$
(2.5)

The equality on the right hand side results from the Cauchy lemma for the line flux density, which implies a linear dependence if the line flux density $\phi_C^{(s)}$ depends on the normal at the line *s*. In sum,

$$F = -\sum_{i=1}^{2} \int_{\partial \mathfrak{B}^{(i)}} \phi^{(i)} \cdot \boldsymbol{n} \, da - \int_{\mathfrak{C}} \phi^{(\mathfrak{s})} \cdot \boldsymbol{s} \, dl.$$
(2.6)

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As the partial volume $\mathfrak{B}^{(i)}$ is enclosed by the set $\partial \mathfrak{B}^{(i)} \cup \mathfrak{S}$, Gauss' divergence theorem can be applied to the surface density integrals in identity (2.6), i.e.

$$\int_{\partial \mathfrak{B}^{(i)}} \boldsymbol{\phi}^{(i)} \cdot \boldsymbol{n} \, da = \int_{\mathfrak{B}^{(i)}} \nabla \cdot \boldsymbol{\phi}^{(i)} \, dv - \int_{\mathfrak{S}} \boldsymbol{\phi}^{(i)} \cdot \boldsymbol{n}^{(\mathfrak{s})} \, da \, , \, i = 1, 2.$$

Inserting density integrals (2.3), (2.4) and (2.6) into equation (2.1) yields a mass balance statement in a setting with two phases in integral form:

$$\sum_{i=1}^{2} \frac{d}{dt} \int_{\mathfrak{B}^{(i)}(t)} \gamma^{(i)} dv + \frac{d}{dt} \int_{\mathfrak{S}} \gamma^{(\mathfrak{s})} da$$

$$= \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} (\pi^{(i)} + \zeta^{(i)} - \nabla \cdot \phi^{(i)}) dv$$

$$+ \int_{\mathfrak{S}} (\pi^{(\mathfrak{s})} + \zeta^{(\mathfrak{s})}) da + \sum_{i=1}^{2} \int_{\mathfrak{S}} \phi^{(i)} \cdot \mathbf{n}^{(\mathfrak{s})} da - \int_{\mathfrak{C}} \phi^{(\mathfrak{s})} \cdot \mathbf{s} dl.$$
(2.7)

2.1.2 The Geometric Surface

With respect to the subsequent considerations, the notions of a parametric surface representation and of surface differentials will be needed. An evolving surface that is oriented by the normal field $n^{(s)}$ can be represented by a local mapping $x_i^{(s)} = \hat{x}_i^{(s)}(\boldsymbol{\xi}^{(s)},t), i = 1, ..., D$, introducing a set of parameters $\boldsymbol{\xi}^{(s)} = (\xi_1^{(s)}, \xi_2^{(s)})$ in a threedimensional setting, or a single parameter $\boldsymbol{\xi}^{(s)} = \boldsymbol{\xi}^{(s)}$, in the two-dimensional case, which is denoted as a one-dimensional vector here. As one important property, the local velocity field of the interface is given by the local time derivative of this mapping,

$$\boldsymbol{w}^{(\mathfrak{s})}(\boldsymbol{x},t) = \left. \frac{\partial \hat{\boldsymbol{x}}^{(\mathfrak{s})}}{\partial t} \right|_{\boldsymbol{\xi}^{(\mathfrak{s})}}.$$
(2.8)

Furthermore, a curvilinear coordinate system can be introduced on the surface based on the parametric form. The partial derivatives of the local mapping define its tangential vectors f_i , i.e.

$$\boldsymbol{f}_{i}(\boldsymbol{\xi}^{(\mathfrak{s})},t) = \frac{\partial \hat{\boldsymbol{x}}^{(\mathfrak{s})}}{\partial \xi_{i}^{(\mathfrak{s})}}(\boldsymbol{\xi}^{(\mathfrak{s})},t) , \ i = 1, \dots, D-1,$$

which correspond to the tangent base vectors of a curvilinear coordinate system on the surface, provided that the mapping is sufficiently smooth. The normalization

$$e_i(\boldsymbol{\xi}^{(s)}, t) = \frac{1}{\|\boldsymbol{f}_i\|} \boldsymbol{f}_i(\boldsymbol{\xi}^{(s)}, t), \ i = 1, \dots, D-1$$

yields a set of orthonormal basis vectors with scale factors

$$h_i = \left\| \frac{\partial \hat{\boldsymbol{x}}^{(\mathfrak{s})}}{\partial \xi_i^{(\mathfrak{s})}} \right\| , \ i = 1, \dots, D - 1.$$



Figure 2.3: The surface projection of a given vector w is indicated in blue.

These vectors span an orthogonal curvilinear coordinate system which allows to introduce surface differentials defined on the surface only. The interfacial normal vector is obtained through

$$\boldsymbol{n}^{(\mathfrak{s})}$$
 = \boldsymbol{e}_3 = $rac{\boldsymbol{e}_1 \times \boldsymbol{e}_2}{|\boldsymbol{e}_1 \times \boldsymbol{e}_2|},$

in case D = 3, or by a vector orthonormal to e_1 , in case D = 2, respectively. Within this context, the surface gradient of a scalar function c is given by

$$\nabla^{(\mathfrak{s})}c = \boldsymbol{e}_1 \frac{1}{h_1} \frac{\partial c}{\partial \xi_1^{(\mathfrak{s})}} + \boldsymbol{e}_2 \frac{1}{h_2} \frac{\partial c}{\partial \xi_2^{(\mathfrak{s})}},$$

for D = 3, or

$$\nabla^{(\mathfrak{s})}c = \boldsymbol{e}_1 \frac{1}{h_1} \frac{\partial c}{\partial \xi_1^{(\mathfrak{s})}},$$

when D = 2, respectively. The surface divergence of a vector field $v^{(s)} = v^{(s)}(\xi_1^{(s)}, \xi_2^{(s)})$ in parametric coordinates is a divergence given in curvilinear coordinates in a lowerdimensional domain, i.e. for the case D = 3,

$$\nabla^{(\mathfrak{s})} \cdot \boldsymbol{v}^{(\mathfrak{s})} = \frac{1}{h_1 h_2} \frac{\partial \left(h_2 \boldsymbol{v}_1^{(\mathfrak{s})}\right)}{\partial \xi_1^{(\mathfrak{s})}} + \frac{1}{h_1 h_2} \frac{\partial \left(h_1 \boldsymbol{v}_2^{(\mathfrak{s})}\right)}{\partial \xi_2^{(\mathfrak{s})}}.$$

For a bulk field that is well defined and smooth up to the surface from at least one side, the surface differentials may be identified with the tangential parts of the standard differential operators in Cartesian form. Parts tangential to the interface of a vector or vector field are obtained by the surface projection tensor

$$P^{(\mathfrak{s})} \equiv I - n^{(\mathfrak{s})} \otimes n^{(\mathfrak{s})}, \tag{2.9}$$

which involves only the surface (or interfacial) normal vector $n^{(s)}$. In this manner, the surface gradient of a scalar field c is given by

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$$\nabla^{(\mathfrak{s})}c = \boldsymbol{P}^{\mathfrak{s}}\nabla c = \nabla c - \left(\nabla c \cdot \boldsymbol{n}^{(\mathfrak{s})}\right)\boldsymbol{n}^{(\mathfrak{s})},\tag{2.10}$$

and the surface divergence of a vector field u by

$$\nabla^{(\mathfrak{s})} \cdot \boldsymbol{u} = \operatorname{tr} \left(\boldsymbol{P}^{\mathfrak{s}} \nabla \boldsymbol{u} \right) = \nabla \cdot \boldsymbol{u} - \boldsymbol{n}^{(\mathfrak{s})} \cdot \left(\nabla \boldsymbol{u} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right), \tag{2.11}$$

where tr(A) denotes the trace of a matrix A. In fact, the resulting expressions as well as the solution of the extended equations on the surface, or interface, respectively, are independent of the chosen extension, see also Delfour and Zolésio (2011).

2.1.3 Transport Theorems for the Bulks

In order to achieve local forms of the balance laws on the bulks and on the interface, an extended form of Reynold's transport theorem can be applied to exchange time derivatives and integration over the bulks on the left hand side of equation (2.7). For this purpose, it is assumed that all quantities are continuous in each of the subdomains.

Introducing the material velocities in the subdomains, $u^{(i)}$ (i = 1, 2) in addition to the speed $w^{(s)}$ of the interface \mathfrak{S} , the transport theorem then yields, for the bulks,

$$\frac{d}{dt} \int_{\mathfrak{B}^{(i)}} \gamma^{(i)} dv = \int_{\mathfrak{B}^{(i)}} \frac{\partial \gamma^{(i)}}{\partial t} dv + \int_{\partial \mathfrak{B}^{(i)}} \gamma^{(i)} \left(\boldsymbol{u}^{(i)} \cdot \boldsymbol{n} \right) da + (-1)^{i-1} \int_{\mathfrak{S}} \gamma^{(i)} \left(\boldsymbol{w}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) da , \quad i = 1, 2.$$
(2.12)

Here, Gauss divergence theorem may be applied. Taking into account that each volume $\mathfrak{B}^{(i)}$ is enclosed by the surface $\partial \mathfrak{B}^{(i)} \cup \mathfrak{S}$, equation (2.12) may be rewritten as

$$\frac{d}{dt} \int_{\mathfrak{B}^{(i)}} \gamma^{(i)} dv = \int_{\mathfrak{B}^{(i)}} \frac{\partial \gamma^{(i)}}{\partial t} dv + \int_{\mathfrak{B}^{(i)}} \nabla \cdot \left(\gamma^{(i)} \boldsymbol{u}^{(i)}\right) dv + (-1)^{i-1} \int_{\mathfrak{S}} \gamma^{(i)} \left(\left(\boldsymbol{w}^{(\mathfrak{s})} - \boldsymbol{u}^{(i)} \right) \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) da , \ i = 1, 2.$$
(2.13)

The sum of identities (2.13) for both of the bulk phases then results in

$$\sum_{i=1}^{2} \frac{d}{dt} \int_{\mathfrak{B}^{(i)}} \gamma^{(i)} dv = \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \frac{\partial \gamma^{(i)}}{\partial t} dv + \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \nabla \cdot \left(\gamma^{(i)} \boldsymbol{u}^{(i)}\right) dv + \int_{\mathfrak{S}} \left[\gamma \left(\boldsymbol{w}^{(\mathfrak{s})} - \boldsymbol{u} \right) \cdot \boldsymbol{n}^{(\mathfrak{s})} \right] da, \qquad (2.14)$$

where the integrals over \mathfrak{S} can be restated by the interfacial jump operator

$$\llbracket \gamma \rrbracket = \gamma^{(2)} - \gamma^{(1)}.$$

2.1.4 Transport and Divergence Theorems for the Interface

The contour and surface integrals in equation (2.7) can be rewritten and summarized in a similar fashion as the integrals over the bulks by employing specific transport and divergence theorems. Petryk and Mróz (1986) established a transport theorem for surface integrals, which can be applied to treat the integral over the interface \mathfrak{S} with normal vector $n^{(\mathfrak{s})}$ that moves with velocity $w^{(\mathfrak{s})}$ and is enclosed by the curve \mathfrak{C} :

$$\frac{d}{dt} \int_{\mathfrak{S}} \gamma^{(\mathfrak{s})} \, da = \int_{\mathfrak{S}} \left(\frac{\delta^{\mathfrak{s}} \gamma^{(\mathfrak{s})}}{\delta^{\mathfrak{s}} t} + \gamma^{(\mathfrak{s})} \left(\boldsymbol{w}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) H^{\mathfrak{s}} \right) \, da + \int_{\mathfrak{C}} \gamma^{(\mathfrak{s})} \left(\boldsymbol{w}^{(\mathfrak{s})} \cdot \boldsymbol{s} \right) \, dl, \qquad (2.15)$$

where $H^{\mathfrak{s}} = \nabla^{\mathfrak{s}} \cdot \mathbf{n}^{(\mathfrak{s})}$ is twice the mean curvature. Here, $\frac{\delta^{\mathfrak{s}}}{\delta^{\mathfrak{s}}t}$ denotes the normal time derivative which is the time derivative for a given point on the surface following the normal trajectory of the surface.

Equation (2.15) is then applied to the last term of the left hand side of equation (2.7). In order to eliminate the contour integrals from equation, the surface divergence theorem (see, for instance, Ecker (2004)) can be used. Employing the material velocity component tangent to the surface as the tangential surface velocity, i.e. $w_t^{(s)} = (w^{(s)} \cdot s) \cdot s$, one has

$$\int_{\mathfrak{C}} \gamma^{(\mathfrak{s})} \left(\boldsymbol{w}^{(\mathfrak{s})} \cdot \boldsymbol{s} \right) dl = \int_{\mathfrak{C}} \gamma^{(\mathfrak{s})} \left(\boldsymbol{w}_{t}^{(\mathfrak{s})} \cdot \boldsymbol{s} \right) dl = \int_{\mathfrak{C}} \gamma^{(\mathfrak{s})} \left(\boldsymbol{u}^{(\mathfrak{s})} \cdot \boldsymbol{s} \right) dl$$
$$= \int_{\mathfrak{S}} \left(\nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})} \boldsymbol{u}_{t}^{(\mathfrak{s})} \right) - \gamma^{(\mathfrak{s})} H^{(\mathfrak{s})} \left(\boldsymbol{u}_{t}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) \right) da$$
$$= \int_{\mathfrak{S}} \nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})} \boldsymbol{u}_{t}^{(\mathfrak{s})} \right) da. \tag{2.16}$$

Altogether, inserting identities (2.16) into (2.15) and replacing the resulting identity in (2.14), the left hand side of equation can be decomposed into volume integrals over the bulks and surface integrals over the interface as follows

$$\frac{d\Gamma}{dt} = \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \frac{\partial \gamma^{(i)}}{\partial t} \, dv + \sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \nabla \cdot \left(\gamma^{(i)} \boldsymbol{u}^{(i)}\right) \, dv + \int_{\mathfrak{S}} \left[\gamma \left(\boldsymbol{w}^{(\mathfrak{s})} - \boldsymbol{u} \right) \cdot \boldsymbol{n}^{(\mathfrak{s})} \right] \, da \\
+ \int_{\mathfrak{S}} \left(\frac{\delta^{\mathfrak{s}} \gamma^{(\mathfrak{s})}}{\delta^{\mathfrak{s}} t} + \gamma^{(\mathfrak{s})} \left(\boldsymbol{w}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) H^{\mathfrak{s}} \right) \, da + \int_{\mathfrak{S}} \nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})} \boldsymbol{u}_{t}^{(\mathfrak{s})}\right) \, da. \tag{2.17}$$

Furthermore, on the right hand side of equation (2.7), the surface divergence theorem can be employed to replace the contour integral by surface integrals, yielding

$$\int_{\mathfrak{C}} \phi^{(\mathfrak{s})} \cdot \boldsymbol{s} \, dl = \int_{\mathfrak{S}} \left(\nabla^{(\mathfrak{s})} \cdot \phi^{(\mathfrak{s})} - H^{(\mathfrak{s})} \left(\phi^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) \right) \, da. \tag{2.18}$$

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2.1.5 Mass Balance Laws of the Bulks and of the interface

Employing the transport and divergence theorems as indicated in subsections 2.1.3 and 2.1.4, the integral form of the mass balance law (2.7) can be stated by surface and volume integrals only:

$$\sum_{i=1}^{2} \int_{\mathfrak{B}^{(i)}} \left(\frac{\partial \gamma^{(i)}}{\partial t} + \nabla \cdot \left(\gamma^{(i)} \boldsymbol{u}^{(i)} + \boldsymbol{\phi}^{(i)} \right) - \pi^{(i)} - \zeta^{(i)} \right) dv + \int_{\mathfrak{S}} \left(\frac{\delta^{\mathfrak{s}} \gamma^{(\mathfrak{s})}}{\delta t} + \nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})} \boldsymbol{u}_{t}^{(\mathfrak{s})} \right) - \left(\pi^{(\mathfrak{s})} + \zeta^{(\mathfrak{s})} \right) - \left[\gamma \left(\boldsymbol{w}^{(\mathfrak{s})} - \boldsymbol{u} \right) \cdot \boldsymbol{n}^{(\mathfrak{s})} - \boldsymbol{\phi} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right] \right) da = \int_{\mathfrak{S}} \left(\nabla^{(\mathfrak{s})} \cdot \boldsymbol{\phi}^{(\mathfrak{s})} + H^{(\mathfrak{s})} \left(\boldsymbol{\phi}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) - \gamma^{(\mathfrak{s})} H^{(\mathfrak{s})} \left(\boldsymbol{w}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) \right) da.$$
(2.19)

Due to the arbitrary choice of the integration domains, both in the volume and in the surface integrals appearing in the above equation, the integrands must vanish identically. For each phase i = 1, 2, one obtains the local balance equations

$$\frac{\partial \gamma^{(i)}}{\partial t} + \nabla \cdot \left(\gamma^{(i)} \boldsymbol{u}^{(i)}\right) + \nabla \cdot \Phi^{(i)} - \pi^{(i)} - \zeta^{(i)} = 0 \quad \text{in} \quad \mathfrak{B}^{(i)}, \ i = 1, 2.$$
(2.20)

For a material surface, the local form of the general balance law on the interface \mathfrak{S} , in turn, is given by

$$\frac{\delta^{(\mathfrak{s})}\gamma^{(\mathfrak{s})}}{\delta t} + \nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})}\boldsymbol{u}_{t}^{(\mathfrak{s})}\right) + \gamma^{(\mathfrak{s})}H^{(\mathfrak{s})}\left(\boldsymbol{u}^{(\mathfrak{s})}\cdot\boldsymbol{n}^{(\mathfrak{s})}\right) + \nabla^{(\mathfrak{s})}\cdot\boldsymbol{\phi}^{(\mathfrak{s})} - H^{(\mathfrak{s})}\left(\boldsymbol{\phi}^{(\mathfrak{s})}\cdot\boldsymbol{n}^{(\mathfrak{s})}\right) - \pi^{(\mathfrak{s})} - \zeta^{(\mathfrak{s})} + \left[\!\left[\boldsymbol{\phi}\cdot\boldsymbol{n}^{(\mathfrak{s})}\right]\!\right] = 0 \text{ on } \mathfrak{S}.$$
(2.21)

Surface integrals in equation (2.19) are often rearranged by using the additional identity

$$\int_{\mathfrak{S}} \left(\nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})} \boldsymbol{u}^{(\mathfrak{s})} \right) - \gamma^{(\mathfrak{s})} H^{(\mathfrak{s})} \left(\boldsymbol{u}^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) \right) \, da = \int_{\mathfrak{S}} \nabla^{(\mathfrak{s})} \cdot \left(\gamma^{(\mathfrak{s})} \boldsymbol{u}^{(\mathfrak{s})}_t \right) \, da. \tag{2.22}$$

When the surface is material, the normal time derivative is related to the total and partial time derivatives by the equation

$$\frac{d\gamma^{(\mathfrak{s})}}{dt} = \frac{\delta^{\mathfrak{s}}\gamma^{(\mathfrak{s})}}{\delta^{\mathfrak{s}}t} + \boldsymbol{u}_{t}^{(\mathfrak{s})} \cdot \nabla^{\mathfrak{s}}\gamma^{(\mathfrak{s})} = \frac{\partial\gamma^{(\mathfrak{s})}}{\partial t} + \boldsymbol{u}^{(\mathfrak{s})} \cdot \nabla^{\mathfrak{s}}\gamma^{(\mathfrak{s})},$$
(2.23)

where $u_t^{(s)}$ is the tangential part of the surface velocity field and the surface differential operators are defined as in subsection 2.1.2.

2.2 Conservation of Mass and Linear Momentum

The Navier – Stokes equations for a setting with two phases can be derived from equations (2.19) and (2.21). In the two - phase system, the identities

$$\gamma^{(i)} = \rho^{(i)} , \ \gamma^{(\mathfrak{s})} = \rho^{(\mathfrak{s})} , \ \phi^{(i)} = \phi^{(\mathfrak{s})} = 0 , \ \zeta^{(i)} = \zeta^{(\mathfrak{s})} = 0 , \ \pi^{(i)} = \pi^{(\mathfrak{s})} = 0$$
(2.24)

are employed for the balance of mass, where $\rho^{(i)}$, i = 1, 2 denote the bulk densities and $\rho^{(s)}$ the surface density, respectively. As a result, one obtains the continuity equation

$$\frac{\partial \rho^{(i)}}{\partial t} + \nabla \cdot \left(\rho^{(i)} \boldsymbol{u}^{(i)}\right) = 0 \text{ in } \mathfrak{B}^{(i)}$$
(2.25)

and the interfacial mass balance yields the classical jump balance equation:

$$\llbracket \rho \left(\boldsymbol{w}^{(\mathfrak{s})} - \boldsymbol{u} \right) \cdot \boldsymbol{n}^{(\mathfrak{s})} \rrbracket^{(i)} = 0 \text{ on } \mathfrak{S}, \tag{2.26}$$

when the surface density is neglected. It should be remarked that this condition always holds for material interfaces, which is assumed in the present work.

The balance of linear momentum is implied by using the identities

$$\begin{split} \gamma^{(i)} &= \rho^{(i)} \boldsymbol{u}^{(i)} , \ \gamma^{(\mathfrak{s})} = \rho^{(\mathfrak{s})} \boldsymbol{u}^{(\mathfrak{s})} , \ \phi^{(i)} = -\boldsymbol{T}^{(i)} , \ \phi^{(\mathfrak{s})} = -\boldsymbol{T}^{(\mathfrak{s})} , \\ \zeta^{(i)} &= \rho^{(i)} \boldsymbol{g} , \ \zeta^{(\mathfrak{s})} = \rho^{(\mathfrak{s})} \boldsymbol{g} , \ \pi^{(i)} = 0 , \ \pi^{(\mathfrak{s})} = 0 , \end{split}$$

where *g* denotes the gravitational force per unit mass and $T^{(i)}$ and $T^{(s)}$ the stress tensors. The stress tensors are commonly decomposed into istropic and dynamic parts, which yields $T^{(i)} = -p^{(i)}I + (T^{(i)})^D$, i = 1, 2 for the Cauchy stress, where $p^{(i)}$ is the hydrostatic pressure in the respective phase i = 1, 2. The surface dynamic stress is neglected within this context, i.e. only the surface tension $\sigma^{(s)}$ remains and $T^{(s)} = \sigma^{(s)}I^{(s)}$. Inserting the above identities in the bulk and interfacial balance laws yields the balance of linear momentum in the bulks

$$\frac{\partial \left(\rho^{(i)} \boldsymbol{u}^{(i)}\right)}{\partial t} + \nabla \cdot \left(\rho^{(i)} \boldsymbol{u}^{(i)} \otimes \boldsymbol{u}^{(i)}\right) = -\nabla p^{(i)} + \nabla \cdot \left(\boldsymbol{T}^{(i)}\right)^{D} + \rho^{(i)} \boldsymbol{g} \text{ in } \mathfrak{B}^{(i)}$$

and on the interface

$$\frac{\delta^{\mathfrak{s}}\left(\rho^{(\mathfrak{s})}\boldsymbol{u}^{(\mathfrak{s})}\right)}{\delta t} + \nabla^{(\mathfrak{s})}\cdot\left(\rho^{(\mathfrak{s})}\boldsymbol{u}^{(\mathfrak{s})}\otimes\boldsymbol{u}^{(\mathfrak{s})}_{t}\right) + \rho^{(\mathfrak{s})}\boldsymbol{u}^{(\mathfrak{s})}H^{(\mathfrak{s})}\left(\boldsymbol{w}^{(\mathfrak{s})}\cdot\boldsymbol{n}^{(\mathfrak{s})}\right)$$
$$= \left[\!\left[\rho\boldsymbol{u}\left(\boldsymbol{w}^{(\mathfrak{s})}-\boldsymbol{u}\right)\cdot\boldsymbol{n}^{(\mathfrak{s})}+\boldsymbol{T}\cdot\boldsymbol{n}^{(\mathfrak{s})}\right]\!\right]^{(i)} + \rho^{(\mathfrak{s})}\boldsymbol{g} + \nabla^{(\mathfrak{s})}\boldsymbol{\sigma}^{(\mathfrak{s})}-H^{(\mathfrak{s})}\boldsymbol{\sigma}^{(\mathfrak{s})}\boldsymbol{n}^{(\mathfrak{s})} \text{ on }\mathfrak{S}.$$

Taking into account the continuity equation (8.3), the usual form of the bulk equations is obtained

$$\rho^{(i)}\frac{\partial \boldsymbol{u}^{(i)}}{\partial t} + \rho^{(i)}\boldsymbol{u}^{(i)} \cdot \nabla \boldsymbol{u}^{(i)} = -\nabla p^{(i)} + \nabla \cdot \left(\boldsymbol{T}^{(i)}\right)^{D} + \rho^{(i)}\boldsymbol{g} \text{ in } \mathfrak{B}^{(i)}$$
(2.27)

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Likewise, by applying equation (2.26), the interfacial balance collapses to the classic jump conditions on the interface

$$\llbracket \rho \left(\boldsymbol{u} - \boldsymbol{u}^{(s)} \right) \left(\boldsymbol{w}^{(s)} - \boldsymbol{u} \right) - p \boldsymbol{I} + (\boldsymbol{T})^{D} \rrbracket^{(i)} \cdot \boldsymbol{n}^{(s)} + \nabla^{(s)} \cdot \sigma^{(s)} - H^{(s)} \left(\sigma^{(s)} \cdot \boldsymbol{n}^{(s)} \right) = 0 \text{ on } \mathfrak{S},$$

when the interfacial density and the surface dynamic stress is neglected. For material interfaces, the first term in the jump condition vanishes, as the material velocity and the local velocity of the surface coincide. This leads to the simplified condition

$$\llbracket -p\boldsymbol{I} + (\boldsymbol{T})^{D} \rrbracket^{(i)} \cdot \boldsymbol{n}^{(\mathfrak{s})} = -\nabla^{(\mathfrak{s})} \cdot \sigma^{(\mathfrak{s})} + H^{(\mathfrak{s})} \left(\sigma^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) \text{ on } \mathfrak{S}.$$
(2.28)

Additionally, the balance laws of angular momentum in the bulks and on the interface can be derived from the balance laws (2.20) and (2.21), see, for instance, Wang and Oberlack (2011). One important implication is the fact that the Cauchy stress tensor must be symmetric for non-polar continua. The present work assumes a setting with an incompressible two-phase flow with constant densities $\rho^{(i)}$, i = 1, 2. In the incompressible flow system, the deformation tensor is given by the identity

$$(\boldsymbol{T}^{(i)})^{D} = \eta^{(i)} \left(\nabla \boldsymbol{u}^{(i)} + \nabla \left(\boldsymbol{u}^{(i)} \right)^{T} \right)$$
(2.29)

where M^T denotes the transpose of the matrix M. Identity (2.29) is inserted into equations (2.28) and (2.27). In addition to the jump condition (2.28), the interface requires further coupling conditions. Condition (2.26) requires continuity of the velocity field in normal direction across the interface,

$$\llbracket \boldsymbol{u} \cdot \boldsymbol{n}^{(\mathfrak{s})} \rrbracket = 0 \text{ on } \mathfrak{S}, \tag{2.30}$$

which, combined with a no slip condition, yields continuity of the velocity field across the interface

$$\llbracket \boldsymbol{u} \rrbracket = 0 \text{ on } \mathfrak{S}, \tag{2.31}$$

as the phases are viscuous, immiscible and no phase transition takes place. The characteristic velocity scale u_{∞} , the characteristic length scale L and the Reynolds number $\operatorname{Re}^{(i)} = \tilde{\rho} L u_{\infty} / \eta^{(i)}$ are employed to introduce the non-dimensional variables,

$$\overline{x}_i = \frac{x_i}{L}, \ \overline{t} = \frac{t}{L/u_{\infty}}, \ \overline{u}^{(i)} = \frac{u^{(i)}}{u_{\infty}}, \ \overline{p}^{(i)} = \frac{p^{(i)}}{\tilde{\rho}u_{\infty}^2}, \ \overline{g} = \frac{Lg}{u_{\infty}^2}$$
(2.32)

with a parameter $\tilde{\rho}$ yet to be specified. The introduction of non-dimensional variables yields the non-dimensional Navier - Stokes equations for an incompressible two - phase flow setting:

$$\overline{\nabla} \cdot \overline{\boldsymbol{u}}^{(i)} = 0 \text{ in } \mathfrak{B}^{(i)}, \tag{2.33}$$

$$\frac{\rho^{(i)}}{\tilde{\rho}} \left(\frac{\partial \overline{\boldsymbol{u}}^{(i)}}{\partial \overline{t}} + \left(\overline{\boldsymbol{u}}^{(i)} \cdot \overline{\nabla} \right) \overline{\boldsymbol{u}}^{(i)} \right) = -\overline{\nabla} \overline{p}^{(i)} + \frac{1}{\operatorname{Re}^{(i)}} \overline{\nabla} \cdot \left(\overline{\nabla} \overline{\boldsymbol{u}}^{(i)} + \overline{\nabla} \left(\overline{\boldsymbol{u}}^{(i)} \right)^T \right) \text{ in } \mathfrak{B}^{(i)}, \quad (2.34)$$

where $\overline{\nabla}$ denotes the nabla operator with respect to the non-dimensional coordinate system. The non-dimensional interfacial continuity conditions are given by

$$\llbracket \overline{\boldsymbol{u}} \rrbracket = 0 \text{ on } \mathfrak{S}, \tag{2.35}$$

and in normal direction off the interface,

$$[\overline{\boldsymbol{u}} \cdot \overline{\boldsymbol{n}}^{(\mathfrak{s})}] = 0 \text{ on } \mathfrak{S}, \tag{2.36}$$

as $n^{(s)} = \overline{n}^{(s)}$. Furthermore, employing the surface tension σ_0 of a clean interface to establish $\overline{\sigma}^{(s)} = \sigma^{(s)}/\sigma_0$ and the Weber number

We =
$$\frac{\tilde{\rho} L u_{\infty}^2}{\sigma_0}$$
,

condition (2.28) transforms to

$$\left[\!\left[-\overline{p}\boldsymbol{I}+\overline{\nabla}\overline{\boldsymbol{u}}+\overline{\nabla}\overline{\boldsymbol{u}}^{T}\right]\!\right]^{(i)}\cdot\overline{\boldsymbol{n}}^{(\mathfrak{s})}=-\overline{\nabla}^{(\mathfrak{s})}\cdot\overline{\sigma}^{(\mathfrak{s})}+\overline{H}^{(\mathfrak{s})}\left(\overline{\sigma}^{(\mathfrak{s})}\cdot\overline{\boldsymbol{n}}^{(\mathfrak{s})}\right) \text{ on }\mathfrak{S},$$

with the assumption that the temperature remains constant. At this point, it is important to note that a common parameter $\tilde{\rho}$ has been introduced for both of the densities, which may be, for instance, identical to $\tilde{\rho} = (\rho^{(1)} + \rho^{(2)})/2$.

2.3 Surfactant Transport Equations

In many applications, one is interested in the transport process of a solute whose concentration is small and whose influence on the flow field is negligible. Such a solute is considered as a passive constituent which is convected by the fluid flow and whose relative motion to the fluid flow is modeled by a diffusive flux. More specifically, in the present work interest focusses on the transport of surface active agents, or shortly, surfactants. Denote by $c^{(i)}$, i = 1, 2, the concentration of surfactant in each of the bulks and by c^{s} the surface excess density of surfactant. In the bulks and on the interface, the densities of the physical variable are provided by the surfactant concentration, i.e.

$$\gamma^{(i)} = c^{(i)} \quad \text{and} \quad \gamma^{(\mathfrak{s})} = c^{\mathfrak{s}}. \tag{2.37}$$

It is assumed that no chemical reactions take place within or outside of the domain or the interface, i.e. no further solute is created within Ω , implying

$$\pi^{(i)} = 0, \quad \pi^{(\mathfrak{s})} = 0, \quad \zeta^{(i)} = 0, \quad \zeta^{(\mathfrak{s})} = 0.$$
 (2.38)

Furthermore, let $D^{(s)}$ denote the diffusion coefficient on the interface, and $D^{(i)}$, i = 1, 2 the diffusion coefficients in the bulks, respectively. For each bulk phase, Fick's first law

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can be applied for the diffusive flux, i.e. $j^{(i)} = -D^{(i)} \nabla c^{(i)}$, establishing the convectiondiffusion equation of surfactant concentration in each bulk

$$\frac{\partial c^{(i)}}{\partial t} + \nabla \cdot \left(c^{(i)} \ \boldsymbol{u}^{(i)}\right) - D^{(i)} \nabla \cdot \nabla c^{(i)} = 0 \text{ in } \mathfrak{B}^{(i)}, \ i = 1, 2.$$
(2.39)

Similarly, the mass balance equation of the solute on the interface \mathfrak{S} can be established by the general local balance equation (2.21) by means of the identifications (2.38) and Fick's first law for the diffusive flux,

$$\phi^{(\mathfrak{s})} = -D^{(\mathfrak{s})} \nabla^{(\mathfrak{s})} c^{\mathfrak{s}} \text{ on } \mathfrak{S}, \tag{2.40}$$

resulting in the interfacial transport equation of surfactant

$$\frac{\delta^{(\mathfrak{s})}c^{\mathfrak{s}}}{\delta t} + \nabla^{(\mathfrak{s})} \cdot \left(c^{\mathfrak{s}}\boldsymbol{u}_{t}^{(\mathfrak{s})}\right) + H^{(\mathfrak{s})}c^{\mathfrak{s}}(\boldsymbol{n}^{(\mathfrak{s})} \cdot \boldsymbol{u}^{(\mathfrak{s})}) - D^{(\mathfrak{s})}\nabla^{(\mathfrak{s})} \cdot \nabla^{(\mathfrak{s})}c^{\mathfrak{s}} = S \text{ on }\mathfrak{S},$$
(2.41)

where the flow of mass from and to the bulks is summarized by the source term *S*,

$$S = D^{(1)} \nabla c^{(1)}|_{\mathfrak{S}} \cdot \boldsymbol{n}^{(\mathfrak{s})} - D^{(2)} \nabla c^{(2)}|_{\mathfrak{S}} \cdot \boldsymbol{n}^{(\mathfrak{s})}.$$
(2.42)

In equation (2.41), identities (2.22) and may be (2.23) employed, yielding

$$\frac{\mathrm{d}c^{\mathfrak{s}}}{\mathrm{d}t} + c^{\mathfrak{s}} \nabla^{(\mathfrak{s})} \cdot \boldsymbol{u}^{(\mathfrak{s})} - D^{(\mathfrak{s})} \nabla^{(\mathfrak{s})} \cdot \nabla^{(\mathfrak{s})} c^{\mathfrak{s}} = S \text{ on } \mathfrak{S}.$$
(2.43)

At the same time, the bulk equations (2.39) are coupled to the surface equations by

$$(-1)^{(i)} D^{(i)} \nabla c^{(i)}|_{\mathfrak{S}} \cdot \boldsymbol{n}^{(\mathfrak{s})} = k_{ad}^{(i)} c_{\mathfrak{s}}^{(i)} \left(c_{\infty}^{\mathfrak{s}} - c^{\mathfrak{s}}\right) - k_{de}^{(i)} c^{\mathfrak{s}} \qquad \text{on } \mathfrak{S}.$$
(2.44)

Here, c_{∞}^{s} is the upper bound of the surfactant concentration that can be accommodated at the interface, $c_{s}^{(i)}$ is the bulk concentration of surfactant immediately adjacent to the interface and $k_{ad}^{(i)}$ and $k_{de}^{(i)}$ denote adsorption and desorption coefficients of each phase, respectively. In addition to the non-dimensional variables introduced in equations (2.32), the maximal packing number c_{∞} of the interface and total surfactant concentration in the bulks C_{∞} as well as the Péclet numbers for the bulks and for the interface

$$\operatorname{Pe}^{(i)} = \frac{u_{\infty}L}{D^{(i)}}$$
 and $\operatorname{Pe}^{(\mathfrak{s})} = \frac{u_{\infty}L}{D^{(\mathfrak{s})}}$

are used for establishing a non-dimensional form of the surfactant transport equations. By employing the non-dimensional concentrations

$$\overline{c}^{(\mathfrak{s})} = \frac{c^{(\mathfrak{s})}}{c_{\infty}}, \ \overline{c}^{(i)} = \frac{c^{(i)}}{C_{\infty}},$$

one obtains the non-dimensional form of equations

$$\frac{\partial \overline{c}^{(i)}}{\partial \overline{t}} + \overline{\nabla} \cdot \left(\overline{c}^{(i)} \ \overline{u}^{(i)}\right) - \frac{1}{\operatorname{Pe}^{(i)}} \overline{\nabla} \cdot \overline{\nabla} \overline{c}^{(i)} = 0 \text{ in } \mathfrak{B}^{(i)}, i = 1, 2 \text{ and} \qquad (2.45)$$

$$\frac{\partial \overline{c}^{(\mathfrak{s})}}{\partial \overline{t}} + (\overline{\boldsymbol{u}} \cdot \overline{\nabla}) \,\overline{c}^{(\mathfrak{s})} + \overline{c}^{(\mathfrak{s})} \overline{\nabla}^{(\mathfrak{s})} \cdot \overline{\boldsymbol{u}} - \frac{1}{\operatorname{Pe}^{(\mathfrak{s})}} \overline{\nabla}^{(\mathfrak{s})} \cdot \overline{\nabla}^{(\mathfrak{s})} \overline{c}^{(\mathfrak{s})} = \overline{S} \text{ on } \mathfrak{S}, \tag{2.46}$$

where the source term S in non-dimensional form is given by

$$\overline{S} = \frac{1}{\operatorname{Pe}^{(1)}} \overline{\nabla} \overline{c}^{(1)}|_{\mathfrak{S}} \cdot \overline{\boldsymbol{n}}^{(\mathfrak{s})} - \frac{1}{\operatorname{Pe}^{(2)}} \overline{\nabla} \overline{c}^{(2)}|_{\mathfrak{S}} \cdot \overline{\boldsymbol{n}}^{(\mathfrak{s})}.$$
(2.47)

A number of non-dimensional parameters is commonly employed for the adsorption and desorption terms in boundary condition (2.44),

$$La^{(i)} = \frac{C_{\infty}k_{ad}^{(i)}}{k_{de}^{(i)}}, Ha^{(i)} = \frac{Lk_{ad}^{(i)}C_{\infty}}{u_{\infty}}, k = \frac{c_{\infty}}{C_{\infty}L},$$

where La is the Langmuir number, that characterizes the ratio between adsorption and desorption kinetics, Ha is the Hatta number, that indicates the ratio between the mass flux and the advective flux on the interface, and k is the non-dimensional adsorption length. By means of these parameters, one obtains

$$(-1)^{(i)}\overline{\nabla}\overline{c}^{(i)}|_{\mathfrak{S}} \cdot \overline{\boldsymbol{n}}^{(\mathfrak{s})} = -\operatorname{k}\operatorname{Ha}^{(i)}\operatorname{Pe}^{(i)}\left(\overline{c}_{\mathfrak{s}}^{(i)}\left(1-\overline{c}^{(\mathfrak{s})}\right) - \frac{1}{\operatorname{La}^{(i)}}\overline{c}^{(\mathfrak{s})}\right)$$
(2.48)

Due to the hydrophobic effect, the presence of surfactants may have a significant impact on the surface tension, i.e. on the surface free energy per unit area. When an interface of a surfactant solution is freshly formed, its surface tension σ is close to the surface tension of a clean surface, σ_0 , and decays to its equilibrium value during the adsorption of surfactants. Therefore, it is usually termed dynamic surface tension in presence of surfactants. Gibb's derived a thermodynamic relationship between the surface excess concentration, the bulk concentrations and a change in surface tension, and a variety of adsorption isotherms may be employed to relate the surface excess conentration adsorbed at the interface and bulk concentrations, see e.g. Eastoe and Dalton (2000). Langmuir's isotherm is probably the most commonly used non-linear isotherm, based on the assumptions that the change of surfactant concentration that is due to adsorption is proportional to both the bulk concentration and the number of vacant sites on the surface while the change caused by desorption is proportional to the number of adsorption greecies. The resulting surface equation of state is often employed when considering the impact of surfactant adsorption

$$\sigma_0 - \sigma = -RTc^{\mathfrak{s}}_{\infty} \ln\left(1 - \frac{c^{\mathfrak{s}}}{c^{\mathfrak{s}}_{\infty}}\right),\tag{2.49}$$

where R is the ideal gas constant and T the absolute temperature. As pointed out previously, in the present work, the influence of surfactant on the surface tension as

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well as an exchange with the bulks are not considered. Therefore, equations (2.49), (2.48), (2.45) and (2.47) are not taken into account in the discretization presented. Throughout the subsequent work, equations will be presented in non-dimensional form and overlines are omitted, unless stated otherwise.

3 State of the Art of Numerical Methods

The numerical simulation of the transport of mass at fluidic interfaces constitutes a major challenge, as such processes are modelled by equations defined on moving and deforming submanifolds of the original domain. Commonly, one has to deal with interfacial convection-diffusion equations which involve differential operators defined on the submanifolds. These differential operators are usually represented in curvilinear coordinates. Alternatively, they may be identified with those parts of the standard differential operators that are tangential to the interface. The choice of an adequate numerical method for treating these equations highly depends on the representation of the surface or interface. This chapter provides a brief overview of numerical methods which have been employed until today for representing fluidic interfaces and of numerical approaches for dealing with surface and interfacial equations. Additionally, existing works which include interfacial surfactant transport are outlined.

3.1 Treatment of Fluidic Interfaces

Over the past 50 years, several distinct approaches for the numerical treatment of fluidic interfaces have been developed. Those methods that are most important in order to understand the numerical treatment of interfacial equations are recapitulated in this section.

3.1.1 Particle Methods

In early approaches, sets of massless markers have been introduced which are employed to locate and track the position of the interface. An Eulerian grid is maintained, requiring additional storage of the coordinates of these virtual particles which are evolved with the (interpolated) velocity field. However, in cases of topology changes such as droplet breakup or coalescence, markers may accumulate in one region or get lost in others, requiring a redistribution. These methods originate in the Marker and Cell method (MAC) first introduced 1965 by Harlow and coworkers at the Los Alamos Laboratories for the treatment of free surfaces in viscous incompressible flows by Finite Difference schemes (Welch, Harlow, Shannon, and Daly, 1965; Harlow and

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Welch, 1965). This method was developed from their earlier Particle in Cell method (PIC). While the original MAC method used the massless markers only to determine if grid cells contained fluid or not, de Sousa, Mangiavacchi, Nonato, Castelo, Tomé, Ferreira, Cuminato, and McKee (2004) incorporate the computation of surface normals and curvature and on this basis, the resolution of the interface. The MAC method uses markers in the whole liquid domain, so-called volume markers. As a simplification, a restriction of markers located on the surface only, so-called surface markers, has been suggested by Aulisa, Manservisi, and Scardovelli, 2004; Chen, Johnson, Raad, and Fadda, 1997 in later works.

3.1.2 Volume of Fluid Methods

In Volume of Fluid methods (VOF), commonly attributed to Noh and Woodward (1976), marker particles were then replaced by a marker function which is constant in each fluid, i.e. the characteristic function χ_i of each fluid *i*. Here, the advection equation of the marker function is approximated in an integral sense as a conservation law

$$\frac{\partial}{\partial t} \int_{V_i} \chi_i \, dx + \int_{\partial V_i} \chi_i \left(\boldsymbol{u} \cdot \boldsymbol{n}^i \right) \, d\sigma,$$

where V_i denotes the volume occupied by fluid *i* and n^i denotes its outer normal. In this way, mass conservation can be achieved while discontinuities at the interface are taken into account at the same time. A so-called color function is established through a normalization by cell volume, providing volume fractions, or area fractions, respectively, in each computational cell. The advection of the color function requires a location of the interface in order to be able to approximate the volume boundary integral. For this purpose, volume or area fraction data is used locally to reconstruct a discontinuous interface. Here, fractions in a defined neighbourhood of cells intersected by the interface are employed. Although is is robust and vastly mass conserving, the VOF method struggles with numerical diffusion, which causes the interface to become spread throughout more than one cell width. Furthermore, interface reconstruction is rather tedious and constitutes the focus of research. One of the earliest algorithms introduced by Noh and Woodward (1976) is the well known SLIC (Simple Line Interface Calculation) algorithm, later improved by Chorin (1980), which assumes the interface to be parallel to either of the coordinate axes, always perpendicular to the direction of the advection.

In an algorithm proposed by Hirt and Nichols Hirt and Nichols (1981), the interface is also aligned with the coordinate axes but in depends on the interfacial normal which is reconstructed from volume fractions of neighbouring cells. A method proposed by Youngs (1984) takes up this idea, and the interface is reconstructed as straight lines in each computational cell whose orientation is determined through its normal vector. This method is known today as the PLIC (Piecewise Linear Interface Calculation) method. As one remarkable feature, by this linear reconstruction scheme second order accuracy could be achieved.



Figure 3.1: The three-dimensional Level Set function that embeds a circle.

3.1.3 Level Set Methods

In Level Set methods, devised by Osher and Sethian (1988), an auxiliary smooth (or at least Lipschitz continuous) function $\Phi : \mathbb{R}_+ \times \mathbb{R}^D \to \mathbb{R}$ is introduced, which embeds the fluid interface at each point of time into the higher, *D*-dimensional domain. The interface is represented implicitly as the zero-isocontour of this so-called Level Set function, i.e.

$$\mathfrak{S} = \left\{ \boldsymbol{x} \in \mathbb{R}^{D} : \Phi\left(t, \boldsymbol{x}\right) = 0 \right\},$$
(3.1)

which is advected by the flow field according to the Level Set advection equation (see Osher and Fedkiw (2003), Osher and Sethian (1988), or Peng, Merriman, Osher, Zhao, and Kang (1999))

$$\frac{\partial \Phi}{\partial t} + (\boldsymbol{u} \cdot \nabla \Phi) = 0 \text{ in } \Omega.$$
(3.2)

In fact, the Level Set function can be considered as a special marker function which is advected with the flow. With evolving time, however, the function Φ may become undesirably flat or steep near the interface, in this way imposing shocks and severe inaccuracies. Commonly, it is then replaced by a signed distance function d(x), i.e. a function that maps each point to its signed distance onto the zero-isocontour and thus, assures a normalized gradient. A signed distance function whose zero Level Set is identical to the original zero isocontour can be constructed by the Fast Marching Method that goes back to Chopp (1993). In a first step, called *initialization* phase, a signed distance function is reconstructed on all vertices that are cut by the interface. This can be achieved either by means of a geometric approach or scaling of the original Level Set function on the vertices. In a second step, known as extension phase, the approximated signed distance function is successively extended to neighbouring cells (Gross and Reusken, 2011).

Alternatively, the re-initialization of the Level Set function can be achieved through a PDE based pseudo-timestepping procedure. In a pseudo-timestepping approach proposed, for instance, by Peng, Merriman, Osher, Zhao, and Kang (1999) as well as

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Sussman, Smereka, and Osher (1994) a virtual time variable is introduced and the initial value problem

$$\frac{\partial \widetilde{\Phi}}{\partial \tau} + \operatorname{sign}(\widetilde{\Phi}_0) \left(\|\widetilde{\Phi}\| - 1 \right) = 0$$
$$\widetilde{\Phi}_0(\boldsymbol{x}) = \widetilde{\Phi}(0, \boldsymbol{x}) = \Phi(\boldsymbol{x})$$

is solved until a steady state solution Φ is attained. This stationary solution yields the desired signed distance function and replaces the original Level Set function.

3.1.4 ALE Methods

In arbitrary Lagrangian-Eulerian (ALE) methods, accredited to Franck and Lazarus (1964), Noh (1964) and Hirt, Amsden, and Cook (1974), the most favorable features of Eulerian and Lagrangian approaches are coupled by allowing arbitrarily moving grids. The nodes of the computational mesh may be associated with material points, being moved with the continuum in a Lagragian fashion, or may be held fixed in an Eulerian manner, or advanced with an arbitrary grid velocity. Usually, both approaches are combined, employing a Lagrangian description in the neighbourhood of moving boundaries or interfaces, while maintaining an Eulerian description in more distant regions. In this way, one strives to achieve a higher resolution than in an Eulerian approach, still being able to handle more severe distortions as in a purely Lagrangian approach. As one essential aspect, ALE approaches employ suitable remeshing techniques, using mesh regularization or mesh adaptation such as mesh refinement at high distortions. The equations are treated in a fixed reference domain, consisting of reference coordinates. Both mesh and material are moved with respect to this reference domain. Correspondingly, the reference domain requires an adaptation both of the differential quantities and of integral expressions. Here, the convective velocity which is the relative velocity between the mesh and the material, plays an important role and indicates the Eulerian or Lagrangian character of the method. Although ALE methods have been mainly employed to treat problems in structural mechanics and fluid-structure interactions, they have been applied to compressible and incompressible flow problems, and have been used to treat free surface flows by Hughes, Liu, and Zimmermann (1981) as well as Ramaswamy and Kawahara (1987).

3.2 Treatment of Surface Problems

Traditionally, the discretization of surface or interface problems is based on a Lagrangian approach, employing curvilinear coordinates. In this case, the interface has to be approximated numerically, implying that for unsteady surfaces, a resolution has to be available in each time step. The computational domain is reconstructed and is used to discretize the problem on the surface, or interface, respectively. More recently, few authors have attempted to treat surface (or interface) transport problems



Figure 3.2: Examples of surface meshes employed in Lagrangian approaches.

by constructing an adequate extension into the underlying domain, and employ an Eulerian approach for discretizing the problem.

3.2.1Lagrangian Approaches

Finite Element Methods have already been applied to surface problems in the late 80s by Dziuk (1988) with surfaces specified by splines. Their application to arbitrary, possibly moving surfaces, however, is a fairly new area of research. Most commonly, the surface \mathfrak{S} is approximated by a triangulated mesh \mathfrak{S}_h with vertices residing on the original surface. An example of a surface mesh is given by figure 3.2. On these grids suitable finite element spaces of sufficiently smooth functions are constructed, usually consisting of continuous polynomials that are affine linear on the simplices, for instance by Dziuk and Elliott (2007b). In this way, weak forms of the surface differential equations are generated easily. In case of dynamic, i.e. moving or deforming interfaces, Dziuk and Elliott (2007a) developed a method where the nodes of the interfacial triangulation are advected by the motion velocity, requiring space-time finite element spaces of basis polynomials. This method is commonly referred to as the Surface Finite Element Method (SFEM) in applications with stationary surfaces (Dziuk and Elliott, 2007b) or Evolving Surface Finite Element Method (ESFEM) (Dziuk and Elliott, 2007a), on instationary geometries, respectively.

Calhoun, Helzel, and LeVeque (2008) as well as Wu, Deng, and Chen (2008) adopted similar approaches in Finite Volume schemes, using surface triangulations as grid cells for the Finite Volume schemes. Using Finite Volume schemes on interfacial grids, however, requires a fairly high effort with respect to the regularity of the grid cells. In particular, the ratio of the sizes of the cells influences the CFL condition (Calhoun, Helzel, and LeVeque, 2008). Lenz, Nemadjieu, and Rumpf (2008) have used evolving simplicial meshes, similar to Dziuk and Elliott (2007a), when treating the interfacial

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equations by Finite Volume methods. The grid discretization suggested by Nemadjieu (2010) is founded on a polygonial mesh where the cell vertices lie on motion trajectories with respect to the initial polygonal surface. In research presented by J. Li (2006), the interface is tracked by a series of marker points based on which the grid cells are generated. Tukovic and Jasak (10-12 June 2008), in turn, use a computational mesh that moves and deforms with the motion of the interface, i.e. an ALE method where the grid boundaries yield the interface in two-phase flow problems. Here, all cell faces of the polyhedral control volumes that coincide with the interface constitute the mesh which their face centered Finite Area method (FAM) is based on.

3.2.2 Eulerian Approaches

In case of moving or deforming interfaces, however, the above approaches are less adequate, since they require an adaptation in every time step and re-meshing after certain periods of time (Dziuk and Elliott, 2007a; Elliott and Eilks, 2008; Lenz, Nemadjieu, and Rumpf, 2008). A better representation of the interfacial differential operators may then be given extrinsically, based on the Eulerian grid. This is achieved by an orthogonal projection of the standard operators onto parts tangential to the interface. Here, an implicit representation of the interface, for instance, by means of a Level Set function, yields the orthogonal projection without any difficulties (Dziuk and Elliott, 2008). A weak formulation of a corresponding Eulerian convection-diffusion equation is provided by Dziuk and Elliott (2009). In this manner, the interfacial equations are embedded into a subset of the higher dimensional domain. Now all computations can be performed on the fixed Eulerian grid of the three-dimensional domain. Here, to restrict computational costs and guarantee regularity of the Level Set function up to a certain extent, a small neighborhood of the interface - a narrow band around the interface – is used as the new computational domain, typically consisting of few grid cells in the normal direction to the interface only (Bertalmío, Cheng, Osher, and Sapiro, 2001; Greer, 2006; Greer, Bertozzi, and Sapiro, 2006; Burger, 2009). Within this context, Deckelnick, Dziuk, Elliott, and Heine (2010) propose an unfitted FE discretization to mimic curved boundaries. This method, however, is restricted to first order basis polynomials, as the unfitted finite elements lead to ill-conditioned mass matrices. As another approach, each point can be mapped to one of its closest points on the surface. Following this approach developed by Ruuth and Merriman (2008) and Macdonald and Ruuth (2008), all standard differential operators only consist of tangential components and replace the surface differential operators. As an alternative to embedding the problem into a formulation in the higher dimensional domain, Olshanskii, Reusken, and Grande (2009) introduce a method that builds on the restriction of a Finite Element space defined on a triangulation of the outer domain. Here, the PDE on the surface is discretized by time-independent Finite Element spaces that are induced by triangulations of the higher-dimensional domain.



Figure 3.3: An extension of the surface concentration $c^{\mathfrak{s}} = \cos^2(\varphi)$ to isocontours of the Level Set function.

3.3 Interfacial Transport in Two-Phase Flows

The coupling of interfacial transport of substances, for instance surfactants, to flow problems is a very recent area of research and only few related works exist. Its challenge does not only lie in the numerical treatment of the interfacial equations on moving and deforming submanifolds, but also in the fact that three interdependent problems have to be solved simultaneously. First of all, the Navier Stokes equations need to be solved for the flow field, respecting the surface tension force (and possibly, the Marangoni force,) determined by the position and geometry of the interface, on the one hand, and by the distribution of interfacial substances, on the other hand. Second, the interface that is advected by the flow field has to be tracked or captured. Third, the interfacial transport equation, depending both on the flow field and the interfacial properties, has to be evolved.

In this section, a brief overview of existing works is provided. The transport of surfactants has been included in various low Reynolds number settings, for instance by Stone and Leal (1990a), Milliken, Stone, and Leal (1993), Li and Pozrikidis (1997), Pozrikidis (2004), Yon and Pozrikidis (1998), Blyth and Pozrikidis (2004a), Pawar and Stebe (1996), Eggleton, Pawar, and Stebe (1999) and Eggleton, Tsai, and Stebe (2001). Here, the flow field is obtained by a boundary integral method which is generally limited to Stokes and inviscid flow settings. As one of the first works published in this context, Stone and Leal (1990a) numerically studied moderate and large deformations of drops in axisymmetric extensional flows that are due to the presence of insoluble surfactants. Using a linear surface tension model, they investigated the effect of variations in interfacial tension on the deformation and breakup of drops. These numerical investigations have been extended by Milliken, Stone, and Leal (1993) who replaced the equations of state by a nonlinear model and additionally addressed the effect of the viscosity ratio between the drop and the surrounding fluid. The method

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of Stone and Leal (1990a) has been adopted by Pawar and Stebe (1996), and Eggleton, Pawar, and Stebe (1999) and Eggleton, Tsai, and Stebe (2001) to study effects of surface saturation and surfactant interaction for a drop in axisymmetric extensional flow when insoluble surfactants are present. Linear equations of state have been used by Pawar and Stebe (1996) and non-linear equations of state by Eggleton, Pawar, and Stebe (1999) and Eggleton, Tsai, and Stebe (2001). Special attention is paid to stagnant cap effects (Eggleton, Pawar, and Stebe, 1999) that may eventually cause the breakup of droplets (Eggleton, Tsai, and Stebe, 2001). The setting introduced by Stone and Leal (1990a) was further generalized by Li and Pozrikidis (1997) who considered three-dimensional non-axisymmetric flows.

The interfacial equation describing the transport of surfactants has been treated in these boundary integral frameworks by Finite Difference methods (FDM) in orthogonal (Stone and Leal, 1990a; Milliken, Stone, and Leal, 1993) or non-orthogonal (Li and Pozrikidis, 1997) curvilinear coordinates, based on unstructured interfacial grids.

In subsequent works, the FDM has been replaced by FVM or FEM. Yon and Pozrikidis (1998) have used interfacial marker points to create an unstructed grid on the interface and to establish a Finite Volume scheme. Within this context, the authors investigated the deformation of a droplet in the presence of surfactants on shear flow. Furthermore, simulations of a perdiodic two-layer channel flow are employed by Blyth and Pozrikidis (2004a) to examine the influence of surfactants on Marangoni instabilities. Pozrikidis (2004) creates a surface grid of curved triangular elements based on which a FEM approximation is established. The grid is constructed from a set of marker points that are transported with the normal component of the flow field, i.e. in an ALE fashion. On this basis, the transport of surfactants on the deformation of a drop in shear flow are computed numerically. Additionally, Pozrikidis (2004) compares the FEM approximation with their previously used FVM scheme.

A combined application of a Cartesian mesh for solving the Navier Stokes equations by FDM and of Lagrangian marker particles to treat the interfacial transport is presented by Lai, Tseng, and Huang (2008). Here, the interface, represented by a parametric form, is treated as an immersed boundary that moves with the flow field and exerts an interfacial force to the fluids (Lai, Tseng, and Huang, 2008). This method does not require an interpolation of interfacial values to couple the equations. Specific to this approach is the reformulation of the interfacial convection-diffusion that takes interfacial stretching into account (Huan, Lai, and Tseng, 2008). However, a redistribution of the Lagrangian markers becomes necessary by interfacial deformation.

Drumright-Clarke and Y.Y.Renardy (2004) as well as Renardy, Renardy, and Cristini (2002) present a VOF approach to treat the effect of insoluble surfactants on drop deformation and breakup, approximating the Navier Stokes equations by FDM on a Cartesian rectangular grid. The position of the interface is reconstructed using a PLIC method. Here, the volume of surfactant is computed in each grid cell and divided by the respective interfacial area to reconstruct the interfacial concentration. A coupling of the flow field and surfactant transport is achieved by a continuous surface

stress formulation, however, with a restriction to a linear equation of state. Another approach that combines the treatment of insoluble surfactants with a VOF method is presented by James and Lowengrub (2004). In contrast to other works, the surfactant concentration is not tracked directly, but expressed by surfactant mass and surface area. These quantities are evolved independently by means of a FV scheme. The surfactant concentration is then recovered by the ratio of surfactant mass per surface area. This approach is unique in the sense that an exact conservation of surfactant mass can be easily achieved, as it is tracked directly. The surfactant concentration can be related to the surface tension by arbitrary, possibly non-linear equations of state. Simulations of drops in extensional flow are used as test cases, focussing particularly on drop retraction and breakup. The idea of tracking surfactant mass and surface area separately has been taken up by Yang (2007) and applied to an ALE appraoch, i.e. the equations are discretized on basis of moving, unstructured, triangular grids. In a very distinct approach that was first introduced by Xu and Zhao (2003), the interfacial surfactant transport equation is treated globally by Eulerian differential operators where the interfacial differential operators are identified with the tangential parts of standard differential operators. This idea has been motivated by using an implicit representation of the interface by means of a Level Set function. In a subsequent paper Xu, Li, Lowengrub, and Zhao (2006) coupled this method to an immersed interface approach for solving Stokes problems is presented.

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4 An Introduction to DG Methods

The next chapter provides a brief introduction to Discontinuous Galerkin (DG) methods. Especially, it focusses on the DG discretization of first and second order PDEs that are involved in the subsequent work. Its most characteristic features are outlined, motivating the use of the DG method. This chapter concludes with an account for the design of the numerical method presented in this thesis.

4.1 Discontinuous Galerkin methods – A Selected Overview

4.1.1 The Discontinuous Galerkin Discretization

The Discontinuous Galerkin (DG) method was originally introduced by Reed and Hill (1973). Motivated by the neutron transport equation, the authors suggested to use discontinuous basis functions in the Galerkin discretization of hyperbolic equations. Instead of linking the element variables through a continuity requirement as in Finite Element methods (FEM), a coupling between neighbouring elements is achieved through numerical fluxes that are employed in the boundary integrals. These numerical fluxes, or slope limiters, are adopted from Finite Volume methods (FVM). At the same time, DG schemes allow for an approximation of convection dominated problems by polynomials of arbitrary order. Thus, in principle, the DG approach can be seen as a hybrid method that strives to combine elements of FEM and FVM, although it is often assigned to either of them. Source terms and time derivatives, in contrast, remain fully decoupled between elements.

Starting from a simple hyperbolic equation in a scalar variable Φ ,

$$\frac{\partial \Phi}{\partial t} + \nabla \cdot (\Phi \ \boldsymbol{u}) = 0 \text{ in } \Omega \times (0, T) , \qquad (4.1)$$
$$\Phi|_{t=0} = \Phi_0 \text{ in } \Omega$$

for some given constant velocity vector u, the DG discretization is briefly reviewed in this section. In fact, the above equation (4.1) corresponds to the Level Set advection equation in an incompressible flow setting. More detailed information on DG and its numerical aspects are given in Hesthaven and Warburton (2008), Cockburn (2004), Cockburn, Karniadakis, and Shu (2000) and B. Q. Li (2006). For a thorrow review of

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numerical analysis on the DG method, the interested reader may refer to Di Pietro and Ern (2012).

As a starting point, the problem domain Ω is approximated by a computational domain $\Omega_h \approx \Omega$ that is discretized by a structured or unstructered grid. The grid consists of a set of a set of *J* cells $\mathfrak{T}_h = \{K_j : j = 1, ..., J\}$, i.e.

$$\Omega_h = \bigcup_{j=1,\dots,J} K_j \ ,$$

with characteristic cell size h. In the present work, the vectors that are normal to the cells' edges, pointing away from cell K_j , are denoted by n^j , where the edge indices are omitted.

In the DG approach, the solution of equation (4.1) is approximated by a function Φ_h in the finite element space

$$V_h^k = \left\{ v \in L^2(\Omega_h) : v|_K \in P^k(K), \ K \in \mathfrak{T}_h \right\}.$$

Within this context, $P^k(K)$ denotes the set of all polynomials on K whose order is at most k. The space $L^2(\Omega_h)$ is the space of measurable, squarely integrable functions (up to null sets) on Ω_h , equipped with the inner product

$$(f,g) = \int_{\Omega_h} f(\boldsymbol{x}) g(\boldsymbol{x}) d\boldsymbol{x}.$$

For this purpose, for each *j*-th cell, a set of basis polynomials, $\{\varphi_i^j : i = 1, ..., N_p\}$, of arbitrary polynomial order *N*, is defined locally. All field variables are then approximated by piecewise *N*-th order polynomials, i.e. by a linear combination of basis polynomials. For instance, the Level Set variable Φ is approximated by

$$\Phi_{h}(t,\boldsymbol{x}) = \sum_{j=1}^{J} \sum_{i=1}^{N_{p}} \Phi^{j,i}(t) \varphi_{i}^{j}(\boldsymbol{x}),$$

where the coefficients $\{\Phi^{j,i}(t) : j = 1, ..., J; i = 1, ..., N_p\}$ form the set of discrete DG coordinates. The basis polynomials are chosen such that their support contains only one element, yielding local approximations

$$\Phi_{h}^{j}(t,\boldsymbol{x}) = \sum_{i=1}^{N_{p}} \Phi^{j,i}(t) \varphi_{i}^{j}(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in K_{j}.$$
(4.2)

Hence, the global approximation of each field is given by the direct sum of these J local approximations

$$\Phi_{h}(t, \boldsymbol{x}) = \bigoplus_{j=1}^{J} \Phi_{h}^{j}(t, \boldsymbol{x}).$$

Likewise, u_h denotes the DG approximation of the velocity field. The dimension of the computational domain determines the relation between the number N_p of local

basis functions and the polynomial order of the scheme. In fact, if D = 1, it holds that $N_p = N + 1$, if D = 2, $N_p = (N + 1)(N + 2)/2$ and in three dimensions,

$$N_p = \frac{(N+1)(N+2)(N+3)}{6}.$$

A Galerkin formulation is given by discretizing equation (4.1) in this manner, multiplying by a test function and integrating over each cell. The equation is then required to be satisfied in a Galerkin sense, i.e.

$$\int_{K_j} \frac{\partial \Phi_h}{\partial t} v \, d\boldsymbol{x} + \int_{K_j} \nabla \cdot (\Phi_h \, \boldsymbol{u}_h) \, v \, d\boldsymbol{x} = 0$$

for all test functions $v \in V_h^k$. As the space V_h^k is spanned by the set of basis polynomials, it is sufficient to demand

$$\int_{K_j} \frac{\partial \Phi_h}{\partial t} \varphi_i^j \, d\boldsymbol{x} + \int_{K_j} \nabla \cdot (\Phi_h \, \boldsymbol{u}_h) \, \varphi_i^j \, d\boldsymbol{x} = 0$$

for all basis polynomials $i = 1, ..., N_p$, in each cell $K_j \in \mathfrak{T}_h$. Finally, Gauss' integral theorem yields the weak form:

$$\int_{K_j} \frac{\partial \Phi_h}{\partial t} \varphi_i^j \, d\boldsymbol{x} - \int_{K_j} (\Phi_h \, \boldsymbol{u}_h) \cdot \nabla \varphi_i^j \, d\boldsymbol{x} + \int_{\partial K_j} \Phi_h \, \boldsymbol{u}_h \cdot \boldsymbol{n}^j \, \varphi_i^j \, d\boldsymbol{s} = 0, \quad i = 1, \dots, N_p. \quad (4.3)$$

Assuming discontinuity, the limits

$$\lim_{\boldsymbol{y} \to \boldsymbol{x}; \boldsymbol{y} \in K_j} \Phi_h(\boldsymbol{y}) = \Phi_h^+, \ \lim_{\boldsymbol{y} \to \boldsymbol{x}; \boldsymbol{y} \notin K_j} \Phi_h(\boldsymbol{y}) = \Phi_h^-$$

at the cell boundaries generally differ. Therefore, the flux at the boundary integrals is modelled by numerical flux functions $F^*(\Phi_h^+, \Phi_h^-)$ that are borrowed from FV schemes. As a result, in each cell K_j , equation (4.3) is discretized by

$$\int_{K_j} \frac{\partial \Phi_h}{\partial t} \varphi_i^j d\boldsymbol{x} - \int_{K_j} (\Phi_h \, \boldsymbol{u}_h) \cdot \nabla \varphi_i^j d\boldsymbol{x} + \int_{\partial K_j} \boldsymbol{F}^* (\Phi_h^+, \Phi_h^-) \cdot \boldsymbol{n}^j \varphi_i^j d\boldsymbol{s} = 0, \quad i = 1, \dots, N_p. \quad (4.4)$$

For stability and well – posedness of the method, the numerical fluxes are required to be *conservative*, i.e. single-valued on each edge, *consistent* with the orginal flux, i.e. in this example,

$$F^*(\Phi, \Phi) \cdot n^j = \Phi \ u \cdot n^j$$

and *monotone*, meaning nondecreasing in its first argument and nonincreasing in the second (Hesthaven and Warburton, 2008). The definition of numerical fluxes most commonly involves the jump operator

$$\llbracket c \rrbracket = c^+ n^j - c^- n^j$$
 and $\llbracket u \rrbracket = u^+ \cdot n^j - u^- \cdot n^j$

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and the average operator

$$\{\{c\}\} = \frac{c^+ + c^-}{2} \text{ and } \{\{u\}\} = \frac{1}{2}(u^+ + u^-)$$

for some scalar c and some vector u. A variety of numerical fluxes is readily available from FVM. As examples, consider the central Lax Friedfrichs flux which is often employed when the flux has no specified direction. In contrast, an upwinding flux scheme

$$F^{*}\left(\Phi_{h}^{+},\Phi_{h}^{-}
ight)\cdot n^{j}=\lim_{s\downarrow0}\Phi_{h}\left(x-su
ight)\;u\cdot n^{j}$$

selects the upstream values at the elements' edges. In this way, it accounts for the fact that information is transported along the characteristics of a simple advection equation, such as (4.1), or in other words,

$$\boldsymbol{F}^{*}\left(\Phi_{h}^{+},\Phi_{h}^{-}\right)\cdot\boldsymbol{n}^{j} = \begin{cases} \Phi_{h}^{+}\boldsymbol{u}\cdot\boldsymbol{n}^{j} & \text{if} \quad \boldsymbol{n}^{j}\cdot\boldsymbol{u} \geq 0\\ \Phi_{h}^{-}\boldsymbol{u}\cdot\boldsymbol{n}^{j} & \text{if} \quad \boldsymbol{n}^{j}\cdot\boldsymbol{u} < 0 \end{cases}$$

Only the DG modes of the discretization are dependent on time, resulting in

$$\frac{\partial \Phi_h^j}{\partial t}(t, \boldsymbol{x}) = \sum_{i=1}^{N_p} \frac{d\Phi^{j,i}}{dt}(t) \varphi_i^j(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in K_j.$$
(4.5)

Therefore, the global approximation is the solution to the discrete problem

$$\sum_{j=1}^{J}\sum_{i=1}^{N_{p}}\frac{d\Phi^{j,i}}{dt}\int_{K_{j}}\varphi_{i}^{j}\varphi_{i}^{j}d\boldsymbol{x}-\sum_{j=1}^{J}\sum_{i=1}^{N_{p}}\Phi^{j,i}\int_{K_{j}}\varphi_{i}^{j}\boldsymbol{u}_{h}\cdot\nabla\varphi_{i}^{j}d\boldsymbol{x}$$
(4.6)

$$+\sum_{j=1}^{J}\int_{\partial K_{j}}\boldsymbol{F}^{*}\left(\Phi_{h}^{+},\Phi_{h}^{-}\right)\cdot\boldsymbol{n}^{j}\varphi_{i}^{j}\,d\boldsymbol{s}=0,\quad i=1,\ldots,N_{p}$$
(4.7)

with suitable boundary fluxes, where an adequate time stepping scheme is employed.

4.1.2 Discrete Quantities

To develope a matrix based representation of the discretization of a simple advection equation, for instance equation (4.1), the mass matrix M with entries

$$M_{i,k}^{j} = \int_{K_{j}} \varphi_{i}^{j}(x) \varphi_{k}^{j}(x) dx \quad i, k = 1, \dots, N_{p}; \ j = 1, \dots, J$$

and the differentiation matrix S^d in each dimensional component d = 1, ..., D,

$$S_{i,k}^{d,j} = \int_{K_j} \varphi_i^j \frac{\partial \varphi_k^j}{\partial x_d} \, dx \quad i,k = 1,\dots,N_p \; ; \; j = 1,\dots,J,$$





(a) Approximation by zero order polynomials

(b) Approximation by higher order polynomials

Figure 4.1: The discontinuous Galerkin discretization of a one-dimensional function. Higher order approximation with discontinuities, as compared to a zero-order approximation.

are introduced. Furthermore, the insertion of numerical fluxes in discretization (4.6) requires an approximation of traces on the element's edges, i.e. a cell - face mass matrix M^E for each edge $e_j \subset \partial K_j$, j = 1, ..., J

$$M_{i,k}^{j,E} = \int_{e_j} \varphi_i^j(\sigma) \varphi_k^j(\sigma) \mathbf{n}_e^j d\sigma \quad i,k = 1, \dots, N_p \; ; \; j = 1, \dots, J.$$

In case of a constant flow field u, the DG discretization of equation can expressed in matrix form by

$$\boldsymbol{M} \cdot \frac{d\boldsymbol{\Phi}}{dt} + \boldsymbol{M}^E \cdot \boldsymbol{\Phi} - \sum_{d=1}^D u_d \, \boldsymbol{S}^d \cdot \boldsymbol{\Phi} = 0,$$

where $\Phi = {\Phi^{j,i}(t) : j = 1, ..., J; i = 1, ..., N_p}$. In principal, a simple monomial basis may be employed for the above approximation. However, a monomial basis usually yields ill conditioned matrices. For this reason, it is commonly orthogonalized, for instance, by a Gram-Schmidt procedure, with respect to the inner product space $L^2(\Omega_h)$.

In this way, the mass matrix attains a diagonal form. Identity (4.2) represents the modal approximation of the variables which is also employed in the present work. It should be pointed out that alternatively, based on a set of N_p local quadrature points

$$\left\{ \boldsymbol{x}_{i}^{j}:\ i=1,\ldots,N_{p}
ight\}$$

one can also define a nodal approximation

$$\Phi_{h}(t,\boldsymbol{x}) = \sum_{i=1}^{N_{p}} \widehat{\Phi}^{j,i}(\boldsymbol{x}_{i}^{j},t) l_{i}^{j}(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in K_{j},$$



Figure 4.2: The rotation of Enzensberger's Stern surface around its *z*-axis, represented by a Level Set function. The DG method supports an easy discretization of the advection equation, a high resolution by fifth order polynomials and its numerical solution on multiple cores.

where interpolating Lagrange polynomials $\{l_i^j : l_i^j(\boldsymbol{x}_n^j) = \delta_{in}, i, n = 1, ..., J\}$ are used to express the polynomials in each *j*-th element. The modes of the modal approximation can be transformed to nodal values by means of a generalized Vandermonde matrix.

In the discrete forms of the equation considered, any suitable time stepping procedure, implicit or explicit, may be employed for treating the time derivative. Regarding linear hyperbolic equations, the use of explicit time stepping schemes is uncritical, as the DG discretization follows the characteristics of the equation. It should be mentioned that in case of nonlinear hyperbolic equations, however, special attention needs to be paid to both stability and accuracy of the method. Within this context, Runge-Kutta DG methods that were devised by Cockburn and Shu (1989), Cockburn, Hou, and Shu (1990) and Cockburn and Shu (1998b) have become well-established. Combining total variation diminishing (TVD) Runge-Kutta solvers with local projection limiters, the authors achieve convergence in regions where shocks occur while maintaining accuracy in smooth regions. Finally, the discretization in time defines the system of discrete equations which needs to be solved for the DG coefficients.

4.1.3 DG Methods for Second Order PDEs

Within a DG scheme, higher order PDEs are generally not as straightforward to implement as in FEM. For further illustration, a diffusion problem, equipped with mixed boundary conditions, is employed. The boundary of the domain $\partial\Omega$ is assumed to partitioned into a region $\partial\Omega_D$, where a Dirichlet boundary condition is imposed, and a region $\partial\Omega_N$, where a Neumann boundary condition holds, such that $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$. The problem under consideration is given by

$$\frac{\partial c}{\partial t} - \nabla \cdot (\boldsymbol{A}(\boldsymbol{x}, t) \cdot \nabla c) = 0 \text{ in } \Omega \times (0, T)$$

$$c|_{\partial\Omega_D} = c_D \text{ and } (\boldsymbol{A}(\boldsymbol{x}, t) \cdot \nabla c)|_{\partial\Omega_N} = g_N,$$

$$c|_{t=0} = c_0 \text{ in } \Omega,$$
(4.8)

where the coefficient matrix A is always assumed to be symmetric and positive semidefinite and the functions g_N, c_D are sufficiently smooth. The coefficients may be constant, or variable in space and time.

In the simplest case of the Laplacian operator, i.e. where A = I, the diffusion equation (4.8) was initially treated as a first order equation with central fluxes, where the variable's gradient was replaced by the differentiation matrix. Although being numerically stable, this intuitive approach prove to be inconsistent, generating incorrect solutions, as shown by Zhang and Shu (2003). A new strategy is pursued by Bassi and Rebay (1997a) who treat equation (4.8) by breaking it down to a system of two first order equations. To each of these equations, a weak Galerkin formulation with suitable numerical fluxes is applied.

In other words, for each partial derivative, an auxiliary variable q_h^i , i = 1, ..., D is introduced, corresponding to a weak derivative in variational form. An approximate solution $(c_h, q_h) \in V_h^k \times W_h^k$ is then sought, where q_h belongs to the vector valued finite element space

$$\boldsymbol{W}_{h}^{k} = \left\{ \boldsymbol{w} \in \left(L^{2}\left(\Omega_{h}\right) \right)^{D} : v|_{K} \in P^{k}(K)^{D}, K \in \mathfrak{T}_{h} \right\},\$$

and solves the system of equations

$$\int_{K_j} \frac{\partial c_h}{\partial t} \varphi_i^j d\boldsymbol{x} + \int_{K_j} \boldsymbol{q_h} \cdot \nabla \varphi_i^j d\boldsymbol{x} - \int_{\partial K_j} \boldsymbol{F}_q^* \left(c_h^+, c_h^-, \boldsymbol{q_h}^+, \boldsymbol{q_h}^- \right) \boldsymbol{n}^j \varphi_i^j d\boldsymbol{s} = 0$$
(4.9)

$$\int_{K_j} \boldsymbol{q}_h \, \varphi_i^j \, d\boldsymbol{x} + \int_{K_j} c_h \cdot \nabla \varphi_i^j \, d\boldsymbol{x} - \int_{\partial K_j} \boldsymbol{F}_c^* \left(c_h^+, c_h^-, \boldsymbol{q_h}^+, \boldsymbol{q_h}^- \right) \boldsymbol{n}^j \, \varphi_i^j \, d\boldsymbol{s} = 0 \qquad (4.10)$$
$$\forall \ i = 1, \dots, N_p, \ j = 1, \dots, J$$

in a Galerkin sense.

The respective boundary conditions are included within the flux functions in an adequate manner, implying they are imposed in a weak sense. The choice of the most convenient fluxes constitutes the challenge of this formulation, as stability and accuracy of the scheme highly depend on the fluxes. But also the structure of the stiffness matrices is determined to a great extent by the fluxes, for instance, with respect to symmetry or the number of non-zero entries. By now, a wide range of methods has emerged for treating equation system (4.9) optimally, which is reviewed by Castillo (2006) and Arnold, Brezzi, Cockburn, and Marini (2000).

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DG method	$oldsymbol{F}_{c}^{*}$	$\boldsymbol{F}_{\boldsymbol{q}}^{*}$
Bassi and Rebay (1997a)	$\{\{c_h\}\}$	$\{\{q_h\}\}$
LDG by Cockburn and Shu (1998a)	$\{\{c_h\}\} - \boldsymbol{\beta}\llbracket c_h\rrbracket$	$\{\{\boldsymbol{q}_h\}\} - \tau \llbracket c_h \rrbracket + \boldsymbol{\beta} \llbracket \boldsymbol{q}_h \rrbracket$
Brezzi et al.(1999)	$\{\{c_h\}\}$	$\{\{\boldsymbol{q}_h\}\} - \tau \llbracket c_h \rrbracket$
IP by Douglas and Dupont (1976)	$\{\{c_h\}\}$	$\{\{\nabla c_h\}\} - \tau \llbracket c_h \rrbracket$

Table 4.1: Selected DG methods for second order PDEs and their numerical fluxes

DG methods developed for second order PDEs are not only characterized by the formulation of fluxes. Another important aspect is given by the fact that the auxiliary variables are not necessarily maintained. Instead, they can be successively eliminated from the system. As indicated, the numerical fluxes may depend on the traces of both of the approximations c_h and q_h in the considered cell and its neighbouring cell. Additionally, a dependency on ∇c_h , i.e. on the derivatives of c_h as specified through the differentiation matrix, may be given. In fact, the fluxes exclusively depend either on q_h or on ∇c_h . The latter case is not of interest in the present work, and is generally combined with a definition of the fluxes that allow for an elimination of the auxiliary variables. Examples of these methods are the Interior Penalty method given by Douglas and Dupont (1976) or the approach proposed by Baumann and Oden (1999a).

In the Local DG (LDG) scheme, originally presented by Cockburn and Shu (1998a), as well as the method introduced by Brezzi, Manzini, Marini, Pietra, and Russo (1999), numerical fluxes depend on q_h only. As one characteristic feature, these schemes are local in the sense that the approximation q_h allows for a local resolution in terms of c_h (Cockburn and Shu, 1998a). This claim may be achieved by choosing the fluxes in the second equation to depend only on the interior and exterior values of c_h . The aforementioned numerical fluxes are indicated in table 4.1 above. An extension of LDG methods to diffusion problems with space-and time-dependent, symmetric and positive definite tensors A is suggested by Cockburn and Dawson (2000), based on an approach that has been presented by Arbogast, Wheeler, and Yotov (1997).

Cockburn and Dawson (2000) introduce an additional set of auxiliary variables, $\theta_h = (\theta_h^k, k = 1, ..., D)$ representing the coefficient matrix applied to the computational variable. Equations (4.9) are then replaced by the Galerkin formulation

$$\int_{K_j} \frac{\partial c_h}{\partial t} \varphi_i^j d\mathbf{x} + \int_{K_j} \boldsymbol{\theta}_h \cdot \nabla \varphi_i^j d\mathbf{x} - \int_{\partial K_j} \boldsymbol{F}_{\theta}^* \left(c_h^+, c_h^-, \boldsymbol{\theta}_h^+, \boldsymbol{\theta}_h^- \right) \boldsymbol{n}^j \varphi_i^j d\mathbf{s} = 0$$

$$- \int_{K_j} \boldsymbol{q}_h \varphi_i^j d\mathbf{x} - \int_{K_j} c_h \cdot \nabla \varphi_i^j d\mathbf{x} + \int_{\partial K_j} \boldsymbol{F}_c^* \left(c_h^+, c_h^-, \boldsymbol{q}_h^+, \boldsymbol{q}_h^- \right) \boldsymbol{n}^j \varphi_i^j d\mathbf{s} = 0$$

$$\int_{K_j} \boldsymbol{\theta}_h \varphi_i^j d\mathbf{x} = \int_{K_j} \boldsymbol{A}(\mathbf{x}, t) \cdot \boldsymbol{q}_h \varphi_i^j d\mathbf{x} \quad \forall \ i = 1, \dots, N_p, \ j = 1, \dots, J.$$

4.2 Hamilton-Jacobi Equations

LDG methods have proved to be valuable for treating a wider range of PDEs that are not in conserved form. One class of first order PDEs which are no conservation laws is given by Hamilton-Jacobi equations. Hamilton-Jacobi equations involve a Hamiltonian function *H*, which may be nonlinear and variable in space, and their general form is

$$\frac{\partial \Phi}{\partial t} + H\left(\frac{\partial \Phi}{\partial x_1}, \dots, \frac{\partial \Phi}{\partial x_D}, x_1, \dots, x_D\right) = 0 \text{ in } \Omega \times (0, T) , \qquad (4.11)$$
$$\Phi|_{t=0} = \Phi_0 \text{ in } \Omega.$$

Typical examples of Hamilton-Jacobi equations are the Burgers equation without viscosity, or the Eikonal equation that can be employed in a pseudo-timestepping procedure to re-initialize the Level Set function. As DG methods rely on a conserved form of the equations in order to apply the discretization scheme, initial value problems of type (4.11) require a suitable workaround.

Beyond, problems of type (4.11) often do not admit classical, i.e. sufficiently smooth solutions, but rather general solutions which fulfill the Hamilton-Jacobi equation almost everywhere. This class of solutions is Lipschitz continuous, but may include discontinuous derivatives, independent of the smoothness of the initial value or boundary conditions. In fact, generalized solutions of problem (4.11) are not necessarily unique, requiring the numerical scheme to select the solutions that are relevant to the underlying problem. Fur this purpose, Crandall and Lions (1983) introduced the notion of viscosity solutions. By now, two approaches for treating the above problem can be destinguished.

First, Hu and Shu (1998) introduced a Runge Kutta DG discretization of the nonlinear problem if the Hamiltonian depends only on the partial derivatives. Differentiation of the equation yields a system of *D* conservation laws in the derivatives.

$$\frac{\partial \boldsymbol{v}}{\partial t} + \nabla H\left(\boldsymbol{v}_1, \dots, \boldsymbol{v}_D\right) = 0 \text{ in } \Omega \times (0, T)$$
(4.12)

$$\nabla u = \boldsymbol{v} \quad \text{in} \quad \Omega \times (0, T) \tag{4.13}$$

Here, the original variable is determined by a least squares procedure where the integration constant remains to be specified. Later, this method was reinterpreted by Li and Shu (2005) who suggested to refine the space of test and Ansatz functions such that they are curl free in each element. Nevertheless, determining the practically relevant solution is an intricate issue when following this approach.

The second idea, which goes back to Yan and Osher (2011), relies on a smart application of the LDG approach. A pair of variables (p_l, q_l) is introduced for each of the derivatives $\partial \Phi / \partial x_l$, l = 1, ..., D, while the Hamiltonian is replaced by a monotone, consistent numerical flux function H^* . A system of 2D additional first order equations needs to be solved to determine derivatives in the Galerkin sense, using an upwinding and a downwinding scheme each.

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In summary, this leads to the following DG formulation of the above equation:

$$\int_{K_j} \frac{\partial \Phi_h}{\partial t} \varphi_i^j d\boldsymbol{x} + \int_{K_j} H^* \left(p_1, \dots, p_D, q_1, \dots, q_D \right) \varphi_i^j d\boldsymbol{x} = 0$$

$$\int_{K_j} p_l \varphi_i^j d\boldsymbol{x} - \int_{K_j} \Phi_h \frac{\partial \varphi_i^j}{\partial x_l} d\boldsymbol{x} + \int_{\partial K_j} \Phi_h^+ n_l^j \varphi_i^j d\boldsymbol{s} = 0$$

$$\int_{K_j} q_l \varphi_i^j d\boldsymbol{x} - \int_{K_j} \Phi_h \frac{\partial \varphi_i^j}{\partial x_l} d\boldsymbol{x} + \int_{\partial K_j} \Phi_h^- n_l^j \varphi_i^j d\boldsymbol{s} = 0$$
for $i = 1, \dots, N_p$, $l = 1, \dots, D$, $j = 1, \dots, J$

$$(4.14)$$

which is further discretized by a suitable time-stepping scheme. Within this context, the DG approach does not only offer far more flexibility with respect to the Hamiltonian *H*, which may be variable in space, non-convex, nonlinear. More importantly, as Yan and Osher (2011) point out, this LDG approximation grasps complete information of the partial derivatives, making it possible to catch their characteristics. In this manner, the scheme accounts for points of discontinuity of the derivatives where values of the up - and downwinding fluxes are usually distinct. As the authors claim, for piecewise constant approximations, series of approximate solutions converge to a viscosity solution of the problem.

4.3 Choice of Method

4.3.1 The DG Method for Fluid Applications

The numerical method designed in the present thesis for treating interfacial transport is based on the DG Method. The newly developed software library is integrated in an existing DG code, which is currently extended to two – phase flow problems. But for which reasons has this method been chosen over others, such as the FVM?

This chapter has underlined that the DG approach has some remarkable advantages over other numerical methods for solving purely convective, or convection dominated problems. Being able to use an arbitrary polynomial degree for the approximation of the problem, an arbitrarily high order of accuracy can be achieved. Thus, as Cockburn (2004) points out, high order approximations of smooth solutions can be generated, while high resolutions of non – smooth solutions can be obtained. Simultaneously, complex geometries can be handled, as the discontinuous approximation allows for elements of arbitrary shapes (Cockburn, 2004). Boundary values are easily incorporated in boundary fluxes of the DG formulation. Due to the local block structure of operator matrices and block diagonal structure of the mass matrices, DG methods are particularly suitable for parallelization. In times of emerging supercomputers and multiple processor architectures, this is a very important issue. Benefitting from these features, the DG method enjoys increasing popularity in various areas and recently, in fluid mechanics.

An existing number of other established numerical solvers that implement the DG method has also been used for applications in fluid mechanics. The most well – known is probably the nudg code by Hesthaven and Warburton (2008), based on the nodal DG method and available both in Matlab and C++. The Fluid Dynamics group of TU Darmstadt started to develop its own DG solver *Bo*unded Support Spectral Solver (*BoSSS*) in 2009, pursuing an object oriented design in a five-layered library (Kummer, 2012). In contrast to other solvers, *BoSSS* was coded in C# for the *.NET* and *mono* framework and hence, can be easily run on Linux/UNIX and supercomputers/clusters (x86, x86_64, IA-64 architectures), requiring only a single compilation. The code implementation is fully MPI parallel and a parallel database for storing application data is provided. In addition, core routines for large linear systems have been written for GPUs.

In the past decade, DG methods have been increasingly applied to single phase flows. Following the development of methods for treating higher order PDEs, simulations of the steady Stokes problem were presented, for instance, by Schötzau, Schwab, and Toselli (2003) as well as Cockburn, Kanschat, Schötzau, and Schwab (2002). The treatment of incompressible Navier – Stokes equations is provided, for example, by Cockburn, Kanschat, and Schötzau (2005), Shahbazi (2007), Girault, Rivière, and Wheeler (2010) as well as Baumann and Oden (1999b). Compressible Navier – Stokes equations are considered in Bassi and Rebay, 1997a, Baumann and Oden (1999b), Cockburn and Shu (1997) and Bassi and Rebay (1997b). Applications range from simulations of the Taylor vortex problem (Shahbazi, 2007), of laminar viscous flow around the NACA0012 airfoil (Bassi and Rebay, 1997a), to mechanical heart valves simulations (Shahbazi, 2007). An incorporation of free surfaces is attempted by Grooss and Hesthaven (2006) as well as Grooss (2005).

4.3.2 The Level Set Method for Representing Fluidic Interfaces

The method that is developed in the context of this work assumes an implicit representation of the interface by a zero-level isocontour of a Level Set function. The critical reader may wonder why this may be a suitable choice when attempting to discretize an equation on the interface itself.

It is a well-known fact that several numerical approaches for computing the fluid interface are available. Fundamentally, a choice between an interface tracking approach, where the interface is tracked through the trajectories of fluid particles, or an interface capturing approach, where the interface is captured implicitly through a marker function, has to be made.

Interface tracking approaches, most prominently, MAC and ALE methods, are generally more intricate in multi-flow applications where interface moves and deforms. In particular, large interface deformations require tedious remeshing or re-distribution of markers. Relevant geometric quantities, such as the surface normal or curvature, need to be reconstructed with high effort. Additionally, topology changes, for instance, disconnecting interfaces, impose severe limitations to these methods.

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In contrast, interface capturing methods, such as the VOF and Level Set method, provide more flexibility with respect to interfacial dynamics and are very well able to handle changing topologies, making them particularly attractive for fluid mechanical problems. At the same time, their implementation is based on the underlying Eulerian grid and they are claimed to be robust. VOF methods enjoy high popularity for their excellent conservation properties. Nevertheless, they are usually only first or second order accurate. For this reason, VOF methods appear to be less adequate in a DG context where high order accuracy should be exploited. The Level Set approach, in turn, supports high order interface resolution and the DG method is well-suited for solving the hyperbolic differential equation, by which the smooth marker function is advected. In fact, the method has been adopted by a number of other authors using DG schemes, such as Owkes and Desjardins (2013), or Chen, Zhao, Yang, and Sai (2011), or Marchandise, Geuzaine, Chevaugeon, and Remacle (2007), or Marchandise and Remacle (2006).

The discretization of the Level Set equation, however, may lead to numerical dissipation, that can be usually observed by a loss of mass in areas of high curvature or areas which are underresolved. Re-initialization and mass loss are frequently mentioned as the major shortcomings of the Level Set approach. However, only little mass loss was reported when employing the Level Set approach within the context of DG discretizations.

The Level Set approach offers another imminent advantage. Although the interface is represented only implicitly, several geometric quantities can be directly obtained. As the gradient of the Level Set function is always perpendicular to its isocontours, the surface normal is given by the normalized gradient,

$$\boldsymbol{n}^{(s)} = \frac{\nabla \Phi}{\|\nabla \Phi\|}.$$
(4.15)

4.3.3 An DG based Extension Approach for the Interfacial Transport Equation

The objective of the present work is the development of a numerical solver for interfacial transport that is based on a DG scheme. At the same time, an implicit representation of the interface by means of a Level Set function should be supported and maintained. Two distinct strategies for resolving all interfacial quantities and approximating surface differential operators can now be pursued: either a Lagrangian or an Eulerian approach.

In a Lagrangian approach, the interface itself yields the domain that is to be discretized. In order to enable an explicit discretization of variables and operators on the iterface itself, however, an explicit representation of the interface is necessary. When capturing the interface implicitly, for instance, by means of a Level Set function, however, a Lagrangian method requires to locate points on the interface in every single time step. Then, a grid structure needs to be established based on these points, requiring a tedious sorting procedure. Especially in three-dimensional problems, a number of degenerate cases has to be considered. Additionally, the number of interfacial nodes degree needs to be sufficiently high such that the accuracy of the interfacial representation, achieved by the implicit method, can be maintained. For these reasons, a Lagrangian approach was not considered to be the most adequate choice for disretizing in the present context.

The second option is given by an Eulerian approach, where all computational quantities are extended to the underlying computational domain and all differential operators are embedded into the higher dimensional space. The interfacial transport problem can be discretized based on the existent Eulerian grid, at the same time admitting an implicit interface representation. In addition, the underlying numerical scheme can be easily applied, making results for numerical analysis and order of convergence available. An Eulerian approach has been applied in few other works, and is still not fully developed, motivation its use also from a research perspective. Against this background, an Eulerian approach is the focus of this thesis.

In summary, the algorithm consists of three steps. First, all quantities such as initial or boundary values, need to be extended in a reasonable manner. In this way, the interfacial surfactant concentration $c^{(s)} : \mathfrak{S} \to \mathbb{R}$, and the initial surfactant concentration, respectively, are replaced by a variable $c : \Sigma \to \mathbb{R}$ such that $c|_{\mathfrak{S}} = c^{(s)}$. Both for reasons of efficiency and regularity, the extension is limited to a subset Σ of Ω only, where $\mathfrak{S} \subset \Sigma$.

Second, the embedding of the interfacial differential operators can be achieved by identifying them with the tangential parts of standard differential operators, employing the projection tensor (2.9). The surface gradient is then replaced by tangential part of the standard gradient (2.10) and the surface divergence, respectively, by the trace of the tangential gradient (2.11). Using a Level Set function for the capturing the interface, the interfacial normal is obtained by the normalized Level Set gradient, i.e. by identity (4.15). Alternatively, it is possible to apply standard differential operators, if all quantities are extended by mapping each node to its closest point on the interface. As a mapping to closest points is always orthogonal, the differential operators attain only tangential parts in this case and an application of the tangential projection becomes redundant. Closest points could be easily determined if the Level Set function attains signed distance property. In the present context, however, this is not guaranteed and a mapping to closest points is not considered. Finally, in a third step, the reformulated equation is solved on $\Sigma \subset \Omega$. Using the above identities, extended formulation of the surfactant transport equation (2.46) is given by

$$\frac{\partial c}{\partial t} + (\boldsymbol{u} \cdot \nabla) c + c \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla \boldsymbol{u}) - \alpha \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla (\boldsymbol{P}^{\mathfrak{s}} \nabla c)) = S \text{ in } \Sigma, \qquad (4.16)$$

where the coefficient is either given by $\alpha = 1/\text{Pe}^{(s)}$, or in the particular case of no diffusion, $\alpha = 0$.

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5 New Conservation Laws of Surface Transport Equations

Until recently, surface, or interfacial differential equations have most commonly been treated numerically by Lagrangian approaches. However, as pointed out in chapter 3, Lagrangian methods reach their limits when the interface moves or deforms. The present work, in contrast, focusses on the development of a new Eulerian approach for treating interfacial transport equations based on a DG method. An Eulerian approach requires to re-write all equations in an extended form that embeds the interfacial quantities in the underlying three-dimensional domain. In order to employ a DG scheme properly, conserved forms of these extended surface transport equations are necessary. Such conservation laws are constructed in the following chapter and have been developed by Kallendorf, Cheviakov, Oberlack, and Wang (2012). Equations of the interfacial convection and convection-diffusion describing the transport of surfactants, and more general interfacial balance laws, in the context of a three-dimensional incompressible two-phase flow are considered. In both convection and convection-diffusion settings, infinite families of conservation laws that essentially involve surfactant concentration are derived, using the direct construction method. The obtained results are also applicable to the construction of the general balance laws for other excess surface physical quantities. The system of governing equations is subsequently rewritten in a fully conserved form in the three-dimensional domain.

5.1 Motivation for Constructing Conservation Laws

The present work assumes an implicit representation of the interface by a Level Set function. When the interface is implicitly defined, interfacial differential operators may be given extrinsically based on the Eulerian grid. Here, an orthogonal projection, as defined by (2.9), of the standard operators onto parts tangential to the interface is used. An implicit representation of the interface, for instance, by means of a Level Set function, yields the orthogonal projection without any difficulties, see also Dziuk and Elliott (2008). In contrast to the local parametric form, this representation of interfacial operators is always available.

The following analysis assumes a setting where numerically, the closed interface \mathfrak{S} is represented by an implicit approach using a Level Set function $\Phi : \mathbb{R}^3 \to \mathbb{R}$, i.e.

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 $\mathfrak{S} = \{ x \in \Omega : \Phi(x) = 0 \}$. The Level Set function Φ is transported by the flow field u according to

$$\Phi_t + \boldsymbol{u} \cdot \nabla \Phi = 0 \text{ in } \Omega, \tag{5.1}$$

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where the index *t* indicates the local time derivative $\partial/\partial t$. Incompressibility of the flow yields the continuity equation

$$\nabla \cdot \boldsymbol{u} = 0 \text{ in } \Omega, \tag{5.2}$$

implying that the above equation can simply be given in the conserved form by

$$\Phi_t + \nabla \cdot (\boldsymbol{u} \, \Phi) = 0 \text{ in } \Omega \tag{5.3}$$

when multiplying (5.2) by Φ and adding equation (5.1). Identifying the interfacial differential operators with interfacial projection of the differential operators to their tangential parts, one obtains the extended convection-diffusion surfactant transport equation

$$c_t + \boldsymbol{u} \cdot \nabla c + c \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla \boldsymbol{u}) - \alpha \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla (\boldsymbol{P}^{\mathfrak{s}} \nabla c)) = 0 \operatorname{in} \Omega, \qquad (5.4)$$

or more generally, the extended general interfacial balance law without the source term (S = 0),

$$\gamma_t^{(\mathfrak{s})} + \boldsymbol{u} \cdot \nabla \gamma^{(\mathfrak{s})} + \gamma^{(\mathfrak{s})} \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla \boldsymbol{u}) - \alpha \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla (\boldsymbol{P}^{\mathfrak{s}} \boldsymbol{\theta})) = 0 \operatorname{in} \Omega$$
(5.5)

in the form to be investigated below.

A weak formulation of a corresponding Eulerian convection-diffusion equation is provided by Dziuk and Elliott (2009). Still, this formulation is a major obstacle for numerical methods that split up any differential terms by Gaussian product rule and thus, require equations in divergence form. Discontinuous Galerkin methods are just one example. Here, a projection of differential operators onto their tangential parts can only be implemented by incorporating aggravating source terms.

Nevertheless, conservation laws can be constructed algorithmically using the direct construction method described by Anco and Bluman (2002a), Anco and Bluman (2002b), Bluman, Cheviakov, and Anco (2009) and Bluman, Cheviakov, and Anco (2010). The direct construction method does not require the use of Noether's theorem, and, in fact, supersedes it for equations that do not admit a variational formulation (Bluman, Cheviakov, and Anco, 2009; Bluman, Cheviakov, and Anco, 2010). The method has been implemented in the symbolic software package GeM for Maple (Cheviakov, 2007) and successfully used to compute conservation laws of many nonlinear models, such as the equations of magnetohydrodynamics equilibria (Cheviakov, 2010). Many other examples can be found in Bluman, Cheviakov, and Anco (2010).

Here, a conserved form of both the interfacial convection and the convection-diffusion equations is provided, describing the transport of surfactants in incompressible twophase flow based on a Level Set formulation of the interface. The transport of surfactants is taken only as an illustrative example of a much wider class of interfacial balance laws. The direct construction method of conservation laws is briefly outlined in Section 5.2. In Section 5.3, the direct construction method is used to derive infinite families of conservation laws for the considered interfacial surfactant transport equations, both in the convection and the convection-diffusion settings, as well as for more general interfacial balance equations. The derived families of conservation laws involve arbitrary functions. Using the obtained conservation laws for the surfactant transport equation, the corresponding systems of partial differential equations are written in fully conserved forms, which form the basis for the following numerical implementation within a DG scheme. Here, the remaining equations of the system are provided in a conserved form as they stand.

5.2 Construction of Conservation Laws using the Direct Method

For a given system of partial differential equations, it is often important to find its divergence-type conservation laws, i.e., expressions of the form

$$\frac{\partial \Theta}{\partial t} + \nabla \cdot \Psi = 0 \tag{5.6}$$

that hold on the solutions of the given system. In (5.6), the conservation law density Θ and the spatial fluxes Ψ^i , i = 1, 2, 3, can depend on independent and dependent variables of the given equations, as well as their partial derivatives, and possibly on nonlocal (integral) quantities.

Conservation laws of the form (5.6) provide the mathematical expression of basic conservation principles holding for a given model, such as conservation of mass, energy, momentum, charge, etc.. They are also used for multiple other purposes, such as existence, uniqueness, and global solution behavior analysis or linearisation mappings. An important application, which is in the focus of the current contribution, is the formulation of a given system of equations in a *fully conserved form*, which makes the application of many modern numerical methods straightforward, as discussed above.

An algorithmic way to seek local conservation laws (5.6) of a given system of PDEs is provided by the direct construction method (Anco and Bluman, 2002a; Anco and Bluman, 2002b; Bluman, Cheviakov, and Anco, 2009; Bluman, Cheviakov, and Anco, 2010). Existence of conservation laws is often associated with symmetries through the famous Noether's theorem. However, this only holds for equations that follow from a variational principle, which is often not the case for equations arising in applications. Even when equations are variational, it turns out that Noether's theorem is not the optimal way for conservation law computations. On the other hand, the direct construction method is practically efficient whether or not the given equations are variational.

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The direct construction method is now briefly overviewed in application to a general PDE system

$$R^{\sigma} = 0, \quad \sigma = 1, \dots, N \tag{5.7}$$

of *N* partial differential equations, with independent variables $z = (z^1, ..., z^n)$, one of which can be time, and *m* dependent variables $u = (u^1, ..., u^m)$. The intention is to find conservation laws

$$\sum_{i=1,\dots,n} \frac{\partial \Psi^i}{\partial z^i} = 0 \tag{5.8}$$

of the PDE system (5.7). Expressions (5.8) coincide with (5.6) when one of the independent variables is time and others are spatial variables x^i , i = 1, ..., D.

Consider an Euler operator with respect to each dependent variable u^j , written as

$$\mathcal{E}_{u^{j}} = \frac{\partial}{\partial u^{j}} - \mathrm{D}_{i} \frac{\partial}{\partial u^{j}_{i}} + \dots + (-1)^{s} \mathrm{D}_{i_{1}} \dots \mathrm{D}_{i_{s}} \frac{\partial}{\partial u^{j}_{i_{1} \dots i_{s}}} + \dots$$
(5.9)

in terms of the total derivative operators

$$D_{i} = \frac{\partial}{\partial z^{i}} + u_{i}^{j} \frac{\partial}{\partial u^{j}} + u_{ii_{1}}^{j} \frac{\partial}{\partial u_{i_{1}}^{j}} + u_{ii_{1}i_{2}}^{j} \frac{\partial}{\partial u_{i_{1}i_{2}}^{j}} + \dots,$$
(5.10)

where $u_{i_1...i_s}^j \equiv \partial^s u^j / \partial z^{i_1} \dots \partial z^{i_s}$ and $u_{ii_1...i_s}^j \equiv \partial^{s+1} u^j / \partial z^i \partial z^{i_1} \dots \partial z^{i_s}$ are partial derivatives of order *s* and *s* + 1, respectively.

The idea of the direct construction method is based on the fact that any divergence expression is annihilated by an Euler operator with respect to each u^j :

$$\mathcal{E}_{u^{j}}\left(\sum_{i=1,\dots,n}\frac{\partial\Psi^{i}}{\partial z^{i}}\right) \equiv 0, \quad j=1,\dots,m.$$
(5.11)

Vice versa, if an expression is annihilated by all Euler operators, then it is a divergence expression (5.8).

One seeks conservation laws as linear combinations of given equations R^{σ} with unknown multipliers Λ^{σ} :

$$\Lambda^{\sigma} R^{\sigma} \equiv \sum_{i=1,\dots,n} \frac{\partial \Psi^{i}}{\partial z^{i}} = 0.$$
(5.12)

The unknown multipliers may be chosen by a user to depend on independent and dependent variables and perhaps partial derivatives of dependent variables up to some prescribed order. Due to (5.11), the multipliers Λ^{σ} are found from the *determining equations*

$$\mathcal{E}_{u^{j}}(\Lambda^{\sigma}R^{\sigma}) = 0, \quad j = 1, ..., m.$$
 (5.13)

After the linear determining equations (5.13) are solved and multipliers Λ^{σ} are found, one proceeds to finding conservation law density and fluxes by means of (5.12). Methods of flux computation are reviewed in Cheviakov, 2010. In particular, one of these

methods requires the knowledge of point symmetries (Bluman, Cheviakov, and Anco, 2010) of a given system of equations. For completeness, point symmetries of the equations (5.1), (5.2), (5.4) considered in the current chapter are given in Appendix A.1.

The direct construction method is implemented in the symbolic software package GeM for Maple (Cheviakov, 2007) which has been used for the computations in the present work.

In Section 5.3 below, the direct construction method is used to discover infinite families of conservation laws of the system of equations (5.2), (5.3), and (5.4) and in particular, to write all those equations in the conserved form. This is done for the cases of both zero and nonzero diffusion coefficient α .

It is important to note that the majority of PDE systems arising in applications can be written in a *solved form* with respect to some leading derivatives. It has been proven that for such systems, *all of their local conservation laws* follow from some multipliers through linear combinations (5.12) see, e.g. Bluman, Cheviakov, and Anco (2010). The equations considered below, in both convection and convection-diffusion settings, can be written in a solved form.

In seeking conservation laws, one naturally avoids *trivial* conservation laws like $\nabla \times (\cdot) \equiv 0$, or those whose fluxes and density vanish on solutions of the given system. For details, see Bluman, Cheviakov, and Anco (2010).

5.3 Conserved Form of the Equations

In this section, it is assumed that sets of initial values and boundary conditions are provided where necessary; they will not be stated explicitly. These conditions will neither influence nor be influenced by the construction of the conserved form of the considered differential equations.

5.3.1 Conservation Laws of Surfactant Transport without Diffusion

In the case of no surface diffusion (α = 0), the governing equations (5.2), (5.3), (5.4) in the index notation can be written as

$$R^1 = \nabla \cdot \boldsymbol{u} = 0 \quad \text{in } \Omega, \tag{5.14a}$$

$$R^{2} = \Phi_{t} + \nabla \left(\boldsymbol{u} \cdot \Phi \right) = 0 \text{ in } \Omega, \qquad (5.14b)$$

$$R^{3} = c_{t} + \boldsymbol{u} \cdot \nabla c - c \,\boldsymbol{n}^{(s)} \cdot \left(\nabla \boldsymbol{u} \cdot \boldsymbol{n}^{(s)}\right) = 0 \text{ in } \Omega.$$
(5.14c)

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Equations (5.14a) and (5.14b) are in the conserved form as they stand. Now the objective is to seek multipliers Λ^1 , Λ^2 , Λ^3 of conservation laws for the equations (5.14) such that the linear combination

$$\mathbf{\Lambda} \cdot \mathbf{R} = \frac{\partial \Theta}{\partial t} + \nabla \cdot \mathbf{\Psi} = 0.$$
 (5.15)

yields a conservation law and the conserved density Θ involves the surfactant concentration *c*. Consequently, one must take $\Lambda^3 \neq 0$.

The first step is to choose the dependence of the multipliers Λ^i for the direct construction method.

It can be shown that choosing multipliers independent of second-order derivatives does not yield any solution of the equations determining the multipliers (5.13). Hence to construct any conservation form (5.15) with $\Lambda^3 \neq 0$, a dependence of the multipliers on the second-order spatial derivatives of physical quantities is necessary (Bluman, Cheviakov, and Anco, 2010).

One is successful when using the multiplier ansatz

$$\Lambda^{i} = \Lambda^{i}(t, \boldsymbol{x}, \Phi, c, \boldsymbol{u}, \partial\Phi, \partial c, \partial\boldsymbol{u}, \partial^{2}\Phi, \partial^{2}c, \partial^{2}\boldsymbol{u}),$$
(5.16)

where

$$\partial \Phi \equiv \left\{ \frac{\partial \Phi}{\partial x^k}, \, k = 1, 2, 3 \right\}, \quad \partial^2 \Phi \equiv \left\{ \frac{\partial^2 \Phi}{\partial x^j \partial x^k}, \, j, k = 1, 2, 3 \right\}$$

are sets of first-order and second-order derivatives of Φ , or *c* and components of *u*, respectively. In (5.16), one may additionally include time derivatives of components of *u* but does not need to include time derivatives of Φ and *c*, since the latter are defined by spatial derivatives through the equations (5.14b), (5.14c).

Requiring that the conservation law (5.15) holds and solving the multiplier determining equations (5.11), one obtains an infinite set of admitted conservation law multipliers Λ^1 , Λ^2 , Λ^3 . Importantly, the multiplier Λ^3 can be nonzero. It has a general form

$$\Lambda^{3} = \|\nabla\Phi\| \ \mathcal{K}(\Phi, \, c \, \|\nabla\Phi\|), \tag{5.17}$$

where \mathcal{K} is an arbitrary sufficiently smooth function of its arguments. The form of the multipliers Λ^1 , Λ^2 is highly complicated; however, a rather simple explicit form of an equivalent conservation law can be found. The following statement holds.

Principal Result 1. (a) The system of surfactant transport equations in the absence of surface diffusion (5.14a),(5.14b) and (5.14c) admits an infinite family of conservation laws given by

$$\frac{\partial}{\partial t}\mathcal{G}(\Phi, c \|\nabla\Phi\|) + \nabla \cdot (\boldsymbol{u} \,\mathcal{G}(\Phi, c \|\nabla\Phi\|)) = 0 \quad in \ \Omega,$$
(5.18)

where G is an arbitrary sufficiently smooth function of its arguments.

- (b) Each of the conservation laws (5.18) with $\mathcal{G} \neq 0$ is a conserved form of the dynamic equation (5.14c) for the surfactant concentration.
- (c) The conservation laws (5.18) can be written in the material form as

$$\frac{d}{dt}\mathcal{G}(\Phi, c \,\|\nabla\Phi\|) = 0, \tag{5.19}$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \nabla$$

denotes the material derivative. This means that the quantity G is invariant to a fixed particle.

(*d*) The arbitrary functions \mathcal{K} and \mathcal{G} are related by

$$\mathcal{K}(\Phi, c \|\nabla\Phi\|) = \frac{\partial \mathcal{G}}{\partial \xi}(\Phi, \xi)|_{\xi=c\|\nabla\Phi\|}.$$
(5.20)

Remark 1. To preserve the number of independent equations in the rewritten system, as compared to the equation system (5.14), \mathcal{G} has to be chosen as an invertible function in its second argument. With this restriction, the surfactant transport equation without diffusion, (5.14c), can be replaced by the conserved form (5.18).

Statement (b) follows from the observation that, since Λ^3 given by (5.17) is generally nonzero, the linear combination (5.15) essentially involves the surfactant transport equation (5.14c). Statement (c) is a direct consequence of the incompressibility condition (5.2). This indicates that in the pure convection case, $\mathcal{G}(\Phi, c \| \nabla \Phi \|)$ is a material conservation quantity.

The statement (a) follows from the direct construction method. A straightforward way to verify that (5.18) holds on solutions of (5.14) is as follows. Denote the differential consequences of equation $R^2 = 0$ (5.14b) with respect to spatial coordinates x^j by

$$R_j^2 = \frac{\partial}{\partial x^j} \Phi_t + \frac{\partial}{\partial x^j} \left(\boldsymbol{u} \cdot \nabla \Phi \right) = 0, \quad j = 1, 2, 3,$$
(5.21)

and denote $\mathcal{G}(\Phi, c \| \nabla \Phi \|) = \widetilde{\mathcal{G}}(\Phi, c^2 \| \nabla \Phi \|^2) = \widetilde{\mathcal{G}}$ for simplicity of notation. Then a direct computation yields

$$\frac{\partial}{\partial t} \left(\mathcal{G}(\Phi, c \| \nabla \Phi \|) \right) + \nabla \cdot \left(u \mathcal{G}(\Phi, c \| \nabla \Phi \|) \right)$$

$$\equiv \frac{\partial}{\partial t} \widetilde{\mathcal{G}} + \nabla \cdot \left(u \widetilde{\mathcal{G}} \right)$$

$$= \left\{ \widetilde{\mathcal{G}} - \Phi D_1 \widetilde{\mathcal{G}} - 2c^2 \| \nabla \Phi \|^2 D_2 \widetilde{\mathcal{G}} \right\} R^1 + \left\{ D_1 \widetilde{\mathcal{G}} \right\} R^2$$

$$+ \left\{ 2c \| \nabla \Phi \|^2 D_2 \widetilde{\mathcal{G}} \right\} R^3 + \sum_{j=0}^3 \left\{ 2c^2 D_2 \widetilde{\mathcal{G}} \frac{\partial \Phi}{\partial x^j} \right\} R_j^2$$

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where $D_1 \tilde{\mathcal{G}}$, $D_2 \tilde{\mathcal{G}}$ denote the partial derivatives of $\tilde{\mathcal{G}}$ by its first and second argument respectively. Consequently, the divergence expression (5.18) is indeed a linear combination of the equations $R^1 = 0$, $R^2 = 0$, $R^3 = 0$ (5.14) and the differential consequences $R_j^2 = 0$ (5.21) with multipliers given in the curly brackets, and the Principal Result 1 is fully established.

Remark 2. In the case where $\mathcal{G}(\Phi, c \| \nabla \Phi \|) = 1$, formula (5.18) reduces to the incompressibility condition (5.14a). Simplest concentration-dependent conservation laws in the family (5.18) can be obtained, for example, by setting $\mathcal{G}(\Phi, c \| \nabla \Phi \|) = (c \| \nabla \Phi \|)^p$, $p \in \mathbb{N}$, and are given by

$$\frac{\partial}{\partial t} \left[(c \| \nabla \Phi \|)^p \right] + \nabla \cdot \left[\boldsymbol{u} \ (c \| \nabla \Phi \|)^p \right] = 0.$$
(5.22)

In particular, when *p* is an even number, the density and the fluxes in (5.22) do not involve square roots which are due to $|\nabla \Phi|$.

Another possible case of interest for applications is the separated form $\mathcal{G}(\Phi, c | \nabla \Phi |) = F_1(\Phi)F_2(c \| \nabla \Phi \|)$, where F_1 and F_2 are suitable arbitrary functions.

5.3.2 Conservation Laws of Surfactant Transport including Diffusion

In the presence of diffusion, i.e. $\alpha = 1/Pe$, the extended surfactant dynamic equations take the form

$$\tilde{R}^1 = \nabla \cdot \boldsymbol{u} = 0 \text{ in } \Omega, \qquad (5.23a)$$

$$\tilde{R}^2 = \Phi_t + \nabla \cdot (\boldsymbol{u} \cdot \Phi) = 0 \text{ in } \Omega, \qquad (5.23b)$$

$$\tilde{R}^{3} = c_{t} + \boldsymbol{u} \cdot \nabla c - c\boldsymbol{n}^{(s)} \cdot \left(\nabla \boldsymbol{u} \cdot \boldsymbol{n}^{(s)}\right) - \frac{1}{\operatorname{Pe}} \operatorname{tr}\left(\boldsymbol{P}^{s} \nabla \left(\boldsymbol{P}^{s} \nabla c\right)\right) = 0 \text{ in } \Omega.$$
(5.23c)

Similar to the purely convective case, for the system (5.23), there exist no conservation laws where the multipliers depend only on independent and dependent variables as well as first order derivatives of the dependent variables. Hence, no *c*-dependent conservation law can be constructed (Cheviakov, 2007).

If the multiplier dependence is further generalized to include second order derivatives of Φ , then one finds an infinite family of sets of local conservation law multipliers corresponding to *c*-dependent conservation laws. Such multipliers are given by

$$\Lambda^{1} = \Phi \mathcal{F}(\Phi) \|\nabla\Phi\|^{-1} \sum_{i=1,...,n} \sum_{j=1,...,n} \left(\frac{\partial}{\partial x^{j}} \left(c \frac{\partial \Phi}{\partial x^{j}} \right) - cn_{i}n_{j} \frac{\partial^{2} \Phi}{\partial x^{i} \partial x^{j}} \right),$$

$$\Lambda^{2} = -\mathcal{F}(\Phi) \|\nabla\Phi\|^{-1} \sum_{i=1,...,n} \sum_{j=1,...,n} \left(\frac{\partial}{\partial x^{j}} \left(c \frac{\partial \Phi}{\partial x^{j}} \right) - cn_{i}n_{j} \frac{\partial^{2} \Phi}{\partial x^{i} \partial x^{j}} \right),$$

$$\Lambda^{3} = \mathcal{F}(\Phi) \|\nabla\Phi\|, \qquad (5.24)$$

where \mathcal{F} is an arbitrary sufficiently smooth function. The conservation law density Θ and the fluxes Ψ^i are again found directly using the flux determining equation (5.15). The following result holds.

Principal Result 2. (a) The system of surfactant transport equations (5.23a), (5.23b) and (5.23c) in the case of a nonzero surface diffusion ($\alpha \neq 0$) admits an infinite family of conservation laws given by

$$\frac{\partial}{\partial t} \left(c \mathcal{F}(\Phi) \| \nabla \Phi \| \right) + \nabla \cdot \left(\boldsymbol{A} \, \mathcal{F}(\Phi) \| \nabla \Phi \| \right) = 0 \quad in \ \Omega, \tag{5.25}$$

where

$$\boldsymbol{A} = c \, \boldsymbol{u} - \frac{1}{Pe} \, \boldsymbol{P}^{(s)} \nabla c \tag{5.26}$$

and \mathcal{F} is an arbitrary sufficiently smooth function of its argument, cf. (5.24).

(b) Each of the conservation laws (5.25) with $\mathcal{F} \neq 0$ is a conserved form of the dynamic equation (5.23c) for the surfactant concentration. In this case (5.23c) can be replaced by (5.25).

The simplest concentration-dependent conservation law of the family (5.25) is obtained by setting $\mathcal{F}(\Phi) = 1$, and has the form

$$\frac{\partial}{\partial t} \left(c \| \nabla \Phi \| \right) + \nabla \cdot \left(\boldsymbol{u} \, c \| \nabla \Phi \| \right) = \frac{1}{\operatorname{Pe}} \nabla \cdot \left(\| \nabla \Phi \| \boldsymbol{P}^{(\mathfrak{s})} \nabla c \right) \text{ in } \Omega.$$
(5.27)

Remark 3. As it is expected, one can observe that when $\alpha = 0$, formulas (5.25) collapse to a subfamily of conservation laws (5.18) for the no-diffusion case, with

$$\mathcal{G}(\Phi, c \|\nabla \Phi\|) = \mathcal{F}(\Phi) c \|\nabla \Phi\|.$$

Remark 4. Conservation laws (5.25), as well as conservation laws (5.18) for the nodiffusion case, are dimensionally consistent for any choice of dimension units for the arbitrary functions \mathcal{F} and \mathcal{G} .

Remark 5. The extended surface excess concentration scaled by the surface area element is a conserved quantity of the interfacial transport equation, i. e. the extended concentration variable is conserved on each level set isocontour. This fact also implies that the speed of interfacial diffusion depends on the streching of the interface.

The surface area element of a parametrisable (and sufficiently smooth) interface is given by the norm of its normal vector. When the interface is embedded by the level set function, its surface normal is given by the gradient of the level set variable, i.e. its surface area element is $\|\nabla \Phi\|$. Therefore, the extended surface excess concentration scaled by the surface area element is given by the expression $c \|\Phi\|$, which is the conserved quantity of the respective equations.

5.3.3 Conservation Laws of General Interfacial Balance Laws

Conserved forms of the surfactant transport equation (5.4) in the convection-diffusion setting were constructed in Section 5.3.2 above. The equation (5.4) follows from a surface extension of the Fick's law, i.e., identity (2.40). However, it is easy to see that neither the obtained multipliers (5.24), nor the conservation laws (5.25) themselves

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depend on the choice of the surface diffusion law. This allows for the following generalization.

Let $\gamma^{(s)}$ be some excess surface physical quantity on the surface \mathfrak{S} whose non-convective flux can be expressed as the surface projection of an arbitrary vector in the form $\phi^{(s)} = P^s \cdot \theta$. The balance law for $\gamma^{(s)}$ in the absence of the source term is given by (5.5), which is almost identical to the surfactant transport equation (5.4), (5.23c). It follows that the analysis of Section 5.3.2 can be carried over to a system of equations (5.23a), (5.23b), (5.5), to obtain an infinite family of conservation laws

$$\frac{\partial}{\partial t} \left(\gamma^{(\mathfrak{s})} \mathcal{F}^{\gamma}(\Phi) \| \nabla \Phi \| \right) + \nabla \cdot \left(\boldsymbol{A}^{\gamma} \mathcal{F}^{\gamma}(\Phi) \| \nabla \Phi \| \right) = 0, \tag{5.28}$$

where

$$\boldsymbol{A}^{\gamma} = \gamma^{(\mathfrak{s})}\boldsymbol{u} + \boldsymbol{\phi}^{(\mathfrak{s})} = \gamma^{(\mathfrak{s})}\boldsymbol{u} + \boldsymbol{P}^{\mathfrak{s}}\boldsymbol{\theta}, \quad i = 1, 2, 3,$$
(5.29)

for any excess surface physical quantity $\gamma^{(s)}$. In (5.28), \mathcal{F}^{γ} is an arbitrary sufficiently smooth function.

5.3.4 Conservation Laws in the Presence of Source Terms

So far, only surfactant transport equations and balance laws that do not involve source terms have been considered. In many cases the source terms may occur, e.g. for the surfactant transport equation when adsorption or desorption from both the adjoining bulk phases to the interface or chemical production on the interface take place.

Generally, when a transport equation contains a source term, it may not be written in a fully conserved form, except for some special cases. However, using the previously derived conserved forms for the no-source case, one can rewrite a transport equation with sources in a more compact form. As an example, consider a surfactant transport equation with sources. It can be written in the form

$$R^{3*} = \tilde{R}^3 - S(c, \boldsymbol{x}, t)$$

= $c_t + c \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla \boldsymbol{u}) - \alpha \operatorname{tr} (\boldsymbol{P}^{\mathfrak{s}} \nabla c) - S(c, \boldsymbol{x}, t)$
= 0 in Ω . (5.30)

A linear combination of (5.23a), (5.23b) and the above equation (5.30) by the multipliers (5.24) yields

$$\begin{split} \Lambda^{1}\tilde{R}^{1} + \Lambda^{2}\tilde{R}^{2} + \Lambda^{3}R^{3*} \\ &= \Lambda^{1}\tilde{R}^{1} + \Lambda^{2}\tilde{R}^{2} + \Lambda^{3}\tilde{R}^{3} - \Lambda^{3}S(c, \boldsymbol{x}, t) \\ &= \frac{\partial}{\partial t}\left(c\mathcal{F}(\Phi) \|\nabla\Phi\|\right) + \nabla \cdot \left(\boldsymbol{A}\mathcal{F}(\Phi) \|\nabla\Phi\|\right) - \Lambda^{3}S(c, \boldsymbol{x}, t) = 0. \end{split}$$

Consequently, the interfacial convection-diffusion equation with sources can be rewritten as

$$\frac{\partial}{\partial t} \left(c \mathcal{F}(\Phi) \| \nabla \Phi \| \right) + \nabla \left(\mathbf{A} \mathcal{F}(\Phi) \| \nabla \Phi \| \right) = \mathcal{F}(\Phi) \| \nabla \Phi \| S(c, \mathbf{x}, t) \text{ in } \Omega.$$

Similarly, the purely convective surfactant dynamics equation can be rewritten as

$$\frac{\partial}{\partial t} \mathcal{G}(\Phi, c \| \nabla \Phi \|) + \nabla \cdot (\boldsymbol{u} \, \mathcal{G}(\Phi, c \| \nabla \Phi \|))$$

= $\| \nabla \Phi \| \frac{\partial \mathcal{G}}{\partial \xi}(\Phi, \xi) |_{\xi = c \| \nabla \Phi \|} (\Phi, c \| \nabla \Phi \|) S(c, \boldsymbol{x}, t) \text{ in } \Omega.$

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6 Exact Solutions to the Interfacial Surfactant Transport Equation

Sets of exact solutions to interfacial convection-diffusion equations, which describe the interfacial transport of insoluble surfactants in a two-phase flow, are derived in the following chapter. The results presented have been achieved by Kallendorf, Fath, Oberlack, and Wang (2015) in collaboration. The investigated model is based on a Stokes flow setting where a spherical shaped inner phase is dispersed in an outer phase. Neglecting the influence of surface tension, general exact solutions to the surfactant conservation law on the spherical surface with both convective and diffusive terms are provided by means of Heun's confluent function. For the steady case, it is shown that these solutions collapse to a simple exponential form. Furthermore, for the purely diffusive problem, exact solutions are constructed using Legendre polynomials. The present analytical study can be considered as a first step towards a more general investigation in which the Marangoni number is small but the Marangoni effect may be not negligible. For such cases, perturbative solutions in small Marangoni number or small inverse Biot number (rapid exchange of surfactants to the bulk phases) up to a certain order may be obtained, in which the analytical solutions obtained in the present study is employed as the base state.

6.1 Motivation

Existing research on exact solutions to interfacial transport problems is still sparse and mainly focussed on the transport without the diffusive part. The numerical treatment of interfacial surfactant transport, however, motivates the development of exact solutions to the convection-diffusion problem, primarily as a mean to validate the numerical method.

A setting of a Stokes flow past a bubble or drop is commonly assumed as the basis when investigating interfacial transport analytically, for admitting exact solutions to the flow problem. In case the Peclet number is high, interfacial diffusion may be neglected and the interfacial equation reduces to a purely convective problem. For this case, stationary solutions of the surfactant transport for a Stokes flow past bubbles or drops have been analytically derived by Sadhal and Johnson (1983), Johnson and Sadhal (1983) and Harper (1982). This setting is commonly referred to as the stagnant

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cap model. Here, the adsorbed surfactants are swept to the rear end of the drop or bubble. A diffusion boundary-layer theory for the distribution of surfactant within the bulks around the stagnant cap bubble is presented by Harper (2004) and Harper (1974), where the surface excess is assumed to be related linearly to the bulk concentration and provides the boundary condition to the transport problem in the bulks. Wang, Papageorgiu, and Maldarelli (1999) investigate convection-diffusion in the bulk phases along with the convective transport at the interface as well as the Marangoni force created by the surfactants present. Furthermore, the effect of insoluble surfactants on small drop deformations in linear flows is theoretically derived by Vlahovska, Bławzdziewicz, and Loewenberg (2009). All these analytical solutions are obtained with various simplifications and are available only for steady cases. There exists no exact analytical solution of the unsteady surfactant transport equation including the effects of both convection and diffusion.

In the present chapter, steady and special unsteady analytical solutions of interfacial surfactant transport on a spherical droplet in a Stokes flow are provided, where the deformation of the droplet surface and the dependence of the surface tension on the surfactant concentration are neglected, corresponding to the assumptions of both the small capillary number and the small Marangoni number, respectively. This chapter is structered as follows. The governing equations that describe the Stokes flow around a spherical droplet, and the interfacial transport of insoluble surfactants on a spherical surface, are presented in section 6.2. In section 6.3, solutions to the general interfacial transport problem are derived in subsection 6.3.1, and in particular, its steady state solution, is discussed in subsection 6.3.2. In addition, in subsection 6.3.3, unsteady solutions to the initial value problem, which is dominated by diffusion, are constructed. In section 6.4, the results are summarized and discussed.

The present analytical study can be considered as a first step towards a more general investigation in which the Marangoni number is small but the Marangoni effect may be not negligible. For such cases, perturbative solutions in small Marangoni number or small inverse Biot number (rapid exchange of surfactants to the bulk phases) up to a certain order may be obtained, in which the analytical solutions obtained in the present study is employed as the base state.

6.2 Governing Equations

The present chapter is focussed on an axisymmetric fluid flow problem with a uniform inflow velocity U along the *z*-axis. A setting with two immiscible incompressible phases is considered, where a droplet shaped inner phase $\mathfrak{B}^{(i)}$ is dispersed in an outer phase $\mathfrak{B}^{(o)}$ with different dynamic viscosities η^i , and η^o , respectively. The droplet is assumed to maintain a rigid spherical shape of radius r_0 . It corresponds to the assumption of the small capillary number. The flow is dominated by the viscous forces such that inertia can be neglected and additionally, it is assumed to be stationary. Consequently, the flow field is governed by the Stokes equations

$$\eta^{(k)} \Delta \boldsymbol{u}^{(k)} = \nabla p^{(k)} \text{ and } \nabla \cdot \boldsymbol{u}^{(k)} = 0$$
(6.1)

in each of the phases $\mathfrak{B}^{(k)}$ with k = i, o, where $u^{(k)}$ and $p^{(k)}$ are the velocity and the pressure of phase k. In a spherical coordinate system (φ, θ, r) , the problem is independent of φ due to the symmetry with respect to the *z*-axis, $\theta = 0, \Pi$. A stream function $\Psi^{(k)}$ is introduced that is valid in both of the phases k = i, o. It yields the divergence - free velocity field by the identities

$$u_{\varphi}^{(k)} = \frac{1}{r^2 \sin(\theta)} \frac{\partial \Psi^{(k)}}{\partial \theta} \text{ and } u_r^{(k)} = -\frac{1}{r \sin(\theta)} \frac{\partial \Psi^{(k)}}{\partial r} \text{ for } k = i, o.$$

Applying the curl operator to the moment equation in (6.1) reduces the problem to requiring

$$0 = \nabla \times \left(\nabla \times \left(\nabla \times \boldsymbol{u}^{(k)} \right) \right) = \frac{1}{r \, \sin(\theta)} \mathfrak{L}^2 \left(\mathfrak{L}^2 \Psi^{(k)} \right) \boldsymbol{e}_{\varphi},$$

where the operator $\mathfrak{L}^2 \Psi^{(k)}$ is defined by

$$\mathfrak{L}^{2}\Psi \coloneqq \frac{\partial^{2}\Psi^{(k)}}{\partial r^{2}} + \frac{\sin(\theta)}{r^{2}}\frac{\partial}{\partial\theta}\left(\frac{1}{\sin(\theta)}\frac{\partial\Psi^{(k)}}{\partial\theta}\right)$$

Thus, the moment equation reduces to the equation $\mathfrak{L}^4 \Psi^{(k)} = 0$ which is solved by choosing $\Psi^{(k)} = r^n \sin^2(\theta)$, $n \in \mathbb{N}$. The remaining constants are determined by requiring regularity, the uniform inflow condition far distant from the sphere and further conditions on the spherical interface \mathfrak{S} that separates the phases, including the continuity of the tangential velocity field as well as vanishing radial components

$$u_r^{(o)}(r_0) = u_r^{(i)}(r_0) = 0$$
 and $[\![u_\theta(r_0)]\!] = 0$

and the continuity of the stress,

$$\eta^{o} \frac{\partial u_{r}^{o}}{\partial r} \Big|_{r=r_{0}} = \eta^{i} \frac{\partial u_{r}^{i}}{\partial r} \Big|_{r=r_{0}} \text{ and }$$
$$\eta^{o} \left(r \frac{\partial}{\partial r} \left(\frac{u_{\theta}^{o}}{r} \right) + \frac{1}{r} \frac{\partial u_{r}^{o}}{\partial \theta} \right) \Big|_{r=r_{0}} = \eta^{i} \left(r \frac{\partial}{\partial r} \left(\frac{u_{\theta}^{i}}{r} \right) + \frac{1}{r} \frac{\partial u_{r}^{i}}{\partial \theta} \right) \Big|_{r=r_{0}}$$

where the Marangoni effect is neglected, corresponding to the assumption of the small Marangoni number. In this manner, the well-known solution for the velocity field, also



Figure 6.1: Stokes flow around a spherical droplet.

known as the Hadamard-Rybczynski solution (Hadamard, 1911; Rybczynski, 1911), is obtained, in the outer phase

$$u_{r}^{o} = \cos\left(\theta\right) U \left(-\frac{r_{0}}{2} \frac{2+3\frac{\eta^{i}}{\eta^{o}}}{1+\frac{\eta^{i}}{\eta^{o}}} \frac{1}{r} + 1 + \frac{r_{0}^{3}}{2} \frac{\frac{\eta^{i}}{\eta^{o}}}{1+\frac{\eta^{i}}{\eta^{o}}} \frac{1}{r^{3}}\right)$$
$$u_{\theta}^{o} = -\sin\left(\theta\right) U \left(-\frac{r_{0}}{4} \frac{2+3\frac{\eta^{i}}{\eta^{o}}}{1+\frac{\eta^{i}}{\eta^{o}}} \frac{1}{r} + 1 - \frac{r_{0}^{3}}{4} \frac{\frac{\eta^{i}}{\eta^{o}}}{1+\frac{\eta^{i}}{\eta^{o}}} \frac{1}{r^{3}}\right),$$
(6.2)

and the inner phase

$$u_{r}^{i} = \cos\left(\theta\right) U \left(-\frac{1}{2} \frac{1}{1 + \frac{\eta^{i}}{\eta^{o}}} + \frac{1}{2r_{0}^{2}} \frac{1}{1 + \frac{\eta^{i}}{\eta^{o}}}r^{2}\right)$$
$$u_{\theta}^{i} = -\sin\left(\theta\right) U \left(-\frac{1}{2} \frac{1}{1 + \frac{\eta^{i}}{\eta^{o}}} + \frac{1}{r_{0}^{2}} \frac{1}{1 + \frac{\eta^{i}}{\eta^{o}}}r^{2}\right).$$
(6.3)

For illustration, the streamlines of the solution are depicted in figure 6.1.

In addition, the interfacial convection-diffusion equation of surfactant excess concentration $c^{(\mathfrak{s})}$ will be investigated in the form

$$\frac{\partial c^{(\mathfrak{s})}}{\partial t} + \boldsymbol{u} \cdot \nabla c^{(\mathfrak{s})} + c^{(\mathfrak{s})} \nabla^{(\mathfrak{s})} \cdot \boldsymbol{u}_t + c^{(\mathfrak{s})} V^{(\mathfrak{s})} \nabla^{(\mathfrak{s})} \cdot \boldsymbol{n}^{(\mathfrak{s})} - D^{(\mathfrak{s})} \nabla^{(\mathfrak{s})} \cdot \nabla^{(\mathfrak{s})} c^{(\mathfrak{s})} = 0, \qquad (6.4)$$

with constant diffusion coefficient $D^{(s)}$ and normal velocity of the interface $V^{(s)} = u \cdot n^{(s)}$ and tangential velocity u_t .

Here, the investigation of the interfacial transport of surfactant is restricted to applications in the absence of adsorption and desorption from both of the adjoining bulks to the interface. The differential operator $\nabla^{(s)}$ denotes the surface gradient. In a curvilinear coordinate system, spanned by the vectors

$$\boldsymbol{e}_{\varphi} = \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \\ 0 \end{pmatrix} \text{ and } \boldsymbol{e}_{\theta} = \begin{pmatrix} \cos(\theta)\cos(\varphi) \\ \cos(\theta)\sin(\varphi) \\ -\sin(\theta) \end{pmatrix}$$

with respect to spherical surface parameters (φ , θ), the surface gradient of a scalar function *c* is given by

$$\nabla^{(\mathfrak{s})}c = \frac{1}{r\,\sin(\theta)}\frac{\partial c}{\partial \varphi}\boldsymbol{e}_{\varphi} + \frac{1}{r}\frac{\partial c}{\partial \theta}\boldsymbol{e}_{\theta},$$

while the surface divergence of a tangential vector field u_t may be expressed by

$$\nabla^{(\mathfrak{s})} \cdot \boldsymbol{u}_t = \frac{1}{r^2 \, \sin(\theta)} \frac{\partial(u_{\varphi} \, r)}{\partial \varphi} + \frac{1}{r^2 \, \sin(\theta)} \frac{\partial(u_{\theta} \, r \, \sin(\theta))}{\partial \theta}.$$

Applying these identities and inserting the specification of the flow field on the interface for $r = r_0$ from (6.2) and (6.3), i.e.

$$u_{\theta}^{\mathfrak{s}} = u_{\theta}^{i}(r_{0}) = u_{\theta}^{o}(r_{0}) = -\frac{U}{2\left(1 + \frac{\eta^{i}}{\eta^{o}}\right)} \sin\left(\theta\right) \text{ and } u_{\varphi}^{\mathfrak{s}} = 0,$$
(6.5)

equation (6.4) can be rewritten as

$$\frac{\partial c^{\mathfrak{s}}}{\partial t} - \frac{\sin\left(\theta\right)}{2\left(1 + \frac{\eta^{i}}{\eta^{o}}\right)} U \frac{\partial c^{\mathfrak{s}}}{\partial \theta} - \frac{U\cos\left(\theta\right)}{\left(1 + \frac{\eta^{i}}{\eta^{o}}\right)} \frac{c^{\mathfrak{s}}}{r_{0}} \\
= D^{(\mathfrak{s})} \left(\frac{1}{r_{0}\tan\left(\theta\right)} \frac{\partial c^{\mathfrak{s}}}{\partial \theta} + \frac{\partial^{2}c^{\mathfrak{s}}}{\partial \theta^{2}} + \frac{1}{r_{0}\sin^{2}\left(\theta\right)} \frac{\partial^{2}c^{\mathfrak{s}}}{\partial \varphi^{2}}\right).$$
(6.6)

The velocity U, radius r_0 , and a surface reference concentration $c_{\infty}^{\mathfrak{s}}$ are employed to non-dimensionalize equation (6.6) by introducing $\tilde{c}^{\mathfrak{s}} = c^{\mathfrak{s}}/c_{\infty}^{\mathfrak{s}}$ as well as $\tilde{t} = t U/r_0$. In this manner, one obtains

$$\operatorname{Pe}^{(\mathfrak{s})}\left(\left(1+\frac{\eta^{i}}{\eta^{o}}\right)\frac{\partial\tilde{c}^{\mathfrak{s}}}{\partial\tilde{t}}-\frac{\sin(\theta)}{2}\frac{\partial\tilde{c}^{\mathfrak{s}}}{\partial\theta}-\cos(\theta)\tilde{c}^{\mathfrak{s}}\right)=\frac{1}{\tan(\theta)}\frac{\partial\tilde{c}^{\mathfrak{s}}}{\partial\theta}+\frac{\partial^{2}\tilde{c}^{\mathfrak{s}}}{\partial\theta^{2}}+\frac{1}{\sin^{2}(\theta)}\frac{\partial^{2}\tilde{c}^{\mathfrak{s}}}{\partial\varphi^{2}},\quad(6.7)$$

where the Péclet number is defined by

$$\operatorname{Pe}^{(\mathfrak{s})} = \frac{Ur_0}{D^{(\mathfrak{s})} \left(1 + \frac{\eta^i}{\eta^o}\right)}.$$

In the following, all tildes denoting the non-dimensional quantities are omitted and the surfactant transport equation in non-dimensional form is used.

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6.3 Exact Solutions

In this section, three cases are investigated to obtain the corresponding exact solutions of the differential equation (6.7).

6.3.1 Unsteady Solution

Separation of variables yields a solution of the unsteady transport equation (6.7). Assuming that the solution takes the form

$$c^{\mathfrak{s}}(\theta,\varphi,t) = \Sigma_{k,l} S_{k,l}(\theta) T_k(t) W_l(\varphi), \tag{6.8}$$

one obtains a system of ordinary differential equations for an enumerable set of predefined λ_k and $\mu_k \in \mathbb{R}, k \in \mathbb{N}$:

$$\frac{dT_k(t)}{dt} = -\frac{\lambda_k^2}{\operatorname{Pe}^{(\mathfrak{s})}\left(1 + \frac{\eta^i}{\eta^o}\right)} T_k(t), \tag{6.9}$$

$$\frac{d^2 W_l(\varphi)}{d\varphi^2} = -\mu_l^2 W_l(\varphi), \tag{6.10}$$

$$\frac{d^2 S_{k,l}(\theta)}{d\theta^2} = \left(\frac{\mu_k^2}{\sin^2(\theta)} - \left(\lambda_k^2 + \operatorname{Pe}^{(\mathfrak{s})}\cos(\theta)\right)\right) S_{k,l}(\theta)$$
(6.11)

$$-\left(\operatorname{Pe}^{(\mathfrak{s})}\frac{\sin(\theta)}{2} + \frac{1}{\tan(\theta)}\right)\frac{dS_{k,l}(\theta)}{d\theta}.$$
(6.12)

Obviously, the solution of $T_k(t)$ of equation (6.9) is given by

$$T_k(t) = \exp\left(-\frac{\lambda_k^2}{\operatorname{Pe}^{(\mathfrak{s})}\left(1 + \frac{\eta^i}{\eta^o}\right)}t\right),\tag{6.13}$$

and

$$W_l(\varphi) = B_l^1 \sin(\mu_l \varphi) + B_l^2 \cos(\mu_l \varphi)$$
(6.14)

is the solution of equation (6.10) with suitable constants B_l^1 and B_l^2 . More specifically, the set of functions W_l forms a basis of the continuous, periodic functions in $[0, 2\pi]$ for integers $\mu_l = l \in \mathbb{N}$.

In order to transform the trigonometrical coefficients into polynomial coefficients, we apply the transformations $S_{k,l}(\theta) = \hat{S}_{k,l}(s) \cdot \exp(\operatorname{Pe}^{(\mathfrak{s})}/2\cos(\theta))$ and $s = 1/2\cos(\theta) + 1/2$. Hence, (6.12) reduces to the following equation:

$$\frac{d^2 \hat{S}_{k,l}}{ds^2} + \frac{\operatorname{Pe}^{(\mathfrak{s})} s^2 + s(2 - \operatorname{Pe}^{(\mathfrak{s})}) - 1}{s(s-1)} \frac{d \hat{S}_{k,l}}{ds} - \left(\frac{\lambda_k^2}{s(s-1)} + \frac{l^2}{4s^2(s-1)^2}\right) \hat{S}_{k,l} = 0.$$
(6.15)

The computer algebra system Maple17 (Waterloo Maple Inc. 2013) yields the solution

$$\hat{S}_{k,l}(s) = C_{k,l}^{1} (s(s-1))^{\frac{l}{2}} \exp(\operatorname{Pe}^{(\mathfrak{s})} s) \operatorname{HeunC}\left(\operatorname{Pe}^{(\mathfrak{s})}, l, l, -\operatorname{Pe}^{(\mathfrak{s})}, -\lambda_{k}^{2} + \frac{l^{2}}{2} + \frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}, s\right) + C_{k,l}^{2} s^{-\frac{l}{2}} (s-1)^{\frac{l}{2}} \exp(\operatorname{Pe}^{(\mathfrak{s})} s) \operatorname{HeunC}\left(\operatorname{Pe}^{(\mathfrak{s})}, -l, l, -\operatorname{Pe}^{(\mathfrak{s})}, -\lambda_{k}^{2} + \frac{l^{2}}{2} + \frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}, s\right)$$

$$(6.16)$$

to equation (6.15), where HeunC denotes Heun's confluent function, see also Olver, Lozier, Boisvert, and Clark (2010).

Within this context, the general Heun's confluent function (Olver, Lozier, Boisvert, and Clark, 2010) HeunC($a_1, a_2, a_3, a_4, a_5, s$) can be given by a series

HeunC
$$(a_1, a_2, a_3, a_4, a_5, s) = \sum_{n=0}^{\infty} v_n(a_1, a_2, a_3, a_4, a_5) s^n$$
,

where the coefficients are defined recursively by the equations

$$A_n v_n = B_n v_{n-1} + C_n v_{n-2}, \ n = 1, 2, \dots$$
(6.17)

with

$$\begin{split} A_n &= 1 + \frac{a_2}{n}, \\ B_n &= 1 + \frac{a_2 + a_3 - 1 - a_1}{n} + \frac{a_5 - (-a_1 + a_2 + a_3)/2 + a_1 a_2/2 + a_2 a_3/2}{n^2}, \\ C_n &= \frac{a_1}{n^2} \left(\frac{a_4}{a_1} + \frac{a_2 + a_3}{2} + n - 1 \right), \end{split}$$

and $v_{-1} = 0$, $v_0 = 1$, and its radius of convergence for *s* equals one.

With respect to the solution under consideration, the short denotation

$$\operatorname{HeunC}_{k,l}(\theta) \equiv \operatorname{HeunC}\left(\operatorname{Pe}^{(\mathfrak{s})}, l, l, -\operatorname{Pe}^{(\mathfrak{s})}, -\lambda_k^2 + l^2/2 + \operatorname{Pe}^{(\mathfrak{s})}/2, s\right)$$

is introduced for Heun's confluent function with the coefficients

$$A_{n} = 1 + \frac{l}{n},$$

$$B_{n} = 1 + \frac{2l - \operatorname{Pe}^{(\mathfrak{s})} - 1}{n} + \frac{-\operatorname{Pe}^{(\mathfrak{s})} \lambda_{k}^{2} + l^{2} + \operatorname{Pe}^{(\mathfrak{s})} - l + 1/2l \operatorname{Pe}^{(\mathfrak{s})}}{n^{2}},$$

$$C_{n} = \frac{\operatorname{Pe}^{(\mathfrak{s})} (-2 + l + n)}{n^{2}}.$$
(6.18)

The remaining constants of solution (6.16) need to be specified from the following available conditions. First, one infers $C_{k,l}^2 = 0$, $k, l \in \mathbb{N}$, from the smoothness condition

$$\left. \frac{\mathrm{d}S(s)}{\mathrm{d}s} \right|_{\theta=0,\theta=\pi} = 0. \tag{6.19}$$

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Second, the remaining constants for each λ_k and μ_l , $k, l \in \mathbb{N}$, are provided either by the initial distribution or by the conservation of mass

$$\int_{\partial A} c_0^{\mathfrak{s}}(\theta, \varphi) \, dA = \int_{\partial A} c^{\mathfrak{s}}(t, \theta, \varphi) \, dA, \tag{6.20}$$

where $c_0^{\mathfrak{s}}(\theta, \varphi)$ is the initial mass distribution.

It is noted that for an axisymmetric initial distribution, i.e. in the case of l = 0, the solution (6.16) is no longer valid, as both parts are linearly dependent. In this case, the solution of (6.15) takes the form

$$\hat{S}_{k}(\theta) = C_{k}^{1} \operatorname{HeunC}_{k,0}(\theta) + C_{k}^{2} \operatorname{HeunC}_{k,0}(\theta) \int^{\theta} \frac{\exp(-\frac{\operatorname{Pe}^{(s)}}{2}\cos(\sigma))}{\operatorname{HeunC}_{k,0}(\sigma)^{2}(\sin(\sigma))} d\sigma.$$

Nevertheless, due to the smoothness condition (6.19), the second constant C_k^2 must be zero and this solution collapses to an identical set of functions as (6.16) for the case of l = 0.

It is important to note that the given set of Heun functions, however, does not yield sets of finite polynomial series allowing for a partitioning of arbitrary initial values. Nevertheless, initial value problems can be designed when restricting initial distributions to the form $c_0^{\mathfrak{s}}(\theta) = \sum_{k,l} c_{k,l} S_k(\theta) W_l(\varphi)$ where the functions S_k and W_l are defined as above, yielding

$$c^{\mathfrak{s}}(\theta,t) = \sum_{k,l} c_{k,l} \left(\frac{-\sin^2(\theta)}{4}\right)^{\frac{l}{2}} W_l(\varphi) \operatorname{HeunC}_{k,l}(\theta) \exp\left(\operatorname{Pe}^{(\mathfrak{s})} \frac{\cos(\theta)+1}{2}\right) \exp\left(\frac{-\lambda_k^2 t}{\operatorname{Pe}^{(\mathfrak{s})}\left(1+\frac{\eta i}{\eta^o}\right)}\right). \quad (6.21)$$

Consider, for instance, an axisymmetric problem with initial distribution

$$c_0^{\mathfrak{s}}(\theta) = \exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos(\theta)\right) - \frac{1}{2}\exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos(\theta)\right) \operatorname{HeunC}\left(\operatorname{Pe}^{(\mathfrak{s})}, 0, 0, -\operatorname{Pe}^{(\mathfrak{s})}, -4 + \frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}, \frac{1}{2}\cos(\theta) + \frac{1}{2}\right).$$

Then the solution is given by the function

$$c^{\mathfrak{s}}(\theta, t) = \exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos(\theta)\right) - \frac{1}{2}\exp\left(\frac{-4t}{\operatorname{Pe}^{(\mathfrak{s})}\left(1 + \frac{\eta^{i}}{\eta^{o}}\right)} + \frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos(\theta)\right)\operatorname{HeunC}\left(\operatorname{Pe}^{(\mathfrak{s})}, 0, 0, -\operatorname{Pe}^{(\mathfrak{s})}, -4 + \frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}, \frac{1}{2}\cos(\theta) + \frac{1}{2}\right),$$

which is illustrated in figure 6.2.



Figure 6.2: An unsteady problem and the steady state solution for $Pe^{(s)} = 0.5$. In the unsteady case, the surfactant accumulates at the rear end of the droplet. In the steady state, which is depicted on the right, the maximum of surfactant accumulates at the rear end of the droplet, while a minimum is attained at the inlet.

6.3.2 Steady solution

Due to the axi-symmetry of the flow field, the steady solution of equation (6.7) is also axisymmetric. For this case, its solution can be expressed as a more simplistic function. For this purpose, we consider the steady and axisymmetric case of equation (6.7),

$$\frac{d^2c^{\mathfrak{s}}}{d\theta^2} + \frac{1}{\tan\left(\theta\right)}\frac{dc^{\mathfrak{s}}}{d\theta} + \operatorname{Pe}^{(\mathfrak{s})}\frac{\sin\left(\theta\right)}{2}\frac{dc^{\mathfrak{s}}}{d\theta} + \operatorname{Pe}^{(\mathfrak{s})}\cos\left(\theta\right)c^{\mathfrak{s}} = 0,$$

which reduces, after integration, to the first order ODE:

$$\sin\left(\theta\right)\frac{dc^{\mathfrak{s}}}{ds} + \frac{\mathrm{Pe}^{(\mathfrak{s})}}{2}\sin^{2}\left(\theta\right)c^{\mathfrak{s}} = C,\tag{6.22}$$

with an unknown constant *C*. The general solution of the above equation (6.22), composed of the general solution of the homogeneous equation and a particular solution of the inhomogeneous equation, is given by

$$c^{\mathfrak{s}}(\theta) = C_1 \exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos\left(\theta\right)\right) + C \, \exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos\left(\theta\right)\right) \int_0^{\theta} \frac{\exp\left(-\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos\left(\sigma\right)\right)}{\sin\left(\sigma\right)} \, d\sigma \, .$$

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Again, due to the smoothness condition (6.19), the constant C must be zero. The remaining coefficient C_1 can be obtained, e.g. from the total dimensionless initial concentration c_0^5 due to mass conservation on the surface:

$$m^{\mathfrak{s}} = 2\pi r_0^2 \int_0^{\pi} c_0^{\mathfrak{s}}(\theta) \sin(\theta) \, d\theta = \int_0^{2\pi} \int_0^{\pi} C_1 \exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos\left(s\right)\right) r_0^2 \sin(\theta) d\theta d\varphi$$
$$= C_1 2\pi r_0^2 \int_0^{\pi} \exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\cos\left(\theta\right)\right) \sin(\theta) d\theta d\varphi$$
$$= C_1 r_0^2 \frac{\pi}{\operatorname{Pe}^{(\mathfrak{s})}} \left(\exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\right) - \exp\left(-\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2}\right)\right),$$

which yields

$$C_1 = \frac{m^{\mathfrak{s}} \operatorname{Pe}^{(\mathfrak{s})}}{2\pi r_0^2 \sinh(\operatorname{Pe}^{(\mathfrak{s})}/2)}.$$
(6.23)

Thus, with a given initial mass m^{s} , the stationary solution to the interfacial surfactant transport equation is

$$c^{\mathfrak{s}}(\theta) = \frac{m^{\mathfrak{s}} \operatorname{Pe}^{(\mathfrak{s})}}{2\pi r_0^2 \sinh(\operatorname{Pe}^{(\mathfrak{s})}/2)} \exp\left(\frac{\operatorname{Pe}^{(\mathfrak{s})}}{2} \cos\left(\theta\right)\right).$$
(6.24)

This distribution has been mentioned by Blyth and Pozrikidis, 2004b without any theoretical derivation. An exemplary surfactant distribution in the steady state is depicted in figure 6.2b.

Remark 6. Solution (6.24) coincides with the general unsteady solution (6.21) of the evolution equation (6.7) for the axisymmetric case l = 0 and for the mode $k = 0, \lambda_0 = 0$, as for this mode, HeunC₀ (θ) \equiv 1. This can be easily proven using the expansion formula. Following identities (6.18), for $\lambda_0 = 0$ one has $A_n = 1, B_n = 1 - (1 + \text{Pe}^{(\mathfrak{s})})/n + \text{Pe}^{(\mathfrak{s})}/n^2, C_n = \text{Pe}^{(\mathfrak{s})}(n-2)/n^2$. By means of (6.17) and $v_{-1} = 0$ and $v_0 = 1$, these equations yield

$$v_1 = (1 - (1 + Pe^{(s)}) + Pe^{(s)}) 1 + 0 = 0$$

$$v_2 = 0 + \frac{Pe^{(s)}(2 - 2)}{n^2} 1 = 0,$$

...

$$v_i = 0, \ i > 0.$$

Thus, if the general unsteady solution (6.21) includes the mode $\lambda_0 = 0$, it converges to the steady solution for $t \to \infty$.

6.3.3 Solution of unsteady surfactant transportation without convection

In this section, a setting with an extremely slow inflow or high diffusivity of the surfactant is investigated, such that the diffusion is dominant and the convective term

is negligible. Without convection, the unsteady problem can be completely solved by a combination of polynomials. In particular, any initial distribution can be decomposed by polynomials and an unsteady concentration may be deduced. Within this context, equation (6.7) reduces to

$$\operatorname{Pe}^{(\mathfrak{s})}\left(1+\frac{\eta^{i}}{\eta^{o}}\right)\frac{\partial c}{\partial t} = \frac{\partial^{2}c}{\partial\theta^{2}} + \frac{1}{\tan\left(\theta\right)}\frac{dc}{d\theta} + \frac{1}{\sin^{2}\left(\theta\right)}\frac{\partial^{2}c}{\partial\varphi^{2}}.$$
(6.25)

Applying again a separation Ansatz (6.8), requires the three sets of functions to satisfy a system of ODEs which consists of equations (6.9), (6.10) and in addition

$$\frac{d^2 S_{k,l}\left(\theta\right)}{d\theta^2} + \lambda_k^2 S_{k,l}\left(\theta\right) + \frac{\cos\left(\theta\right)}{\sin\left(\theta\right)} \frac{dS_{k,l}\left(\theta\right)}{d\theta} - \frac{\mu_l^2}{\left(\sin\left(\theta\right)\right)^2} S_{k,l}\left(\theta\right) = 0, \tag{6.26}$$

where the sets of constants λ_k and μ_l are determined by the initial value of the problem. The solutions for $T_k(t)$ and $W_k(\varphi)$, i.e. (6.13) and (6.14), remain unchanged for the present case of pure diffusion. Employing a transformation variables $s = \cos(\theta)$, the solution to equation (6.26) can be obtained, for instance, by Maple17 (Waterloo Maple Inc. 2013) and is given by a linear combination of Legendre functions of the first ($P_n^m(s)$) and second kind ($Q_n^m(s)$),

$$S_{k,l}(\theta) = C_{k,l}^1 P_n^m(\cos(\theta)) + C_{k,l}^2 Q_n^m(\cos(\theta))$$
(6.27)

with $m = \mu_l$ and

$$n = \frac{1}{2}\sqrt{1+4\lambda_k^2} - \frac{1}{2}.$$
 (6.28)

As the Legendre functions of the second kind are singular in $s = \pm 1$, i.e. $\theta = 0, \pi$, the smoothness condition across the poles again implies that $C_{k,l}^2 = 0$. If *n* as defined by equation (6.28) and $m = \mu_l = l$ are non - negative integers, the corresponding Legendre functions of first the kind are orthogonal. Due to the identity

$$P_n^m(s) = \frac{(1-s^2)^{m/2}}{n! \ 2^n} \frac{d^{m+n}}{ds^{m+n}} \left(s^2 - 1\right)^n$$

arbitrary polynomials in $\cos(\theta)$ and $\sin(\theta)$ can be obtained from these Legendre functions. In this way, solutions of the diffusion problem can be generated for arbitrary initial distributions.

Remark 7. For $\text{Pe}^{(s)} \ll 1$, equation (6.12) simplifies to equation (6.26). Then, for nonnegative integers $m = \mu_l = l$ and n such that λ_k satisfies equation (6.28), and the solution simplifies to Legendre functions of the first kind, $P_n^m(s)$. Consequently, the solution of the purely diffusive problem coincides with the solution of equation (6.7) when assuming that $\text{Pe}^{(s)} \ll 1$. Q



Figure 6.3: A diffusion dominated problem for the initial distribution of $c_0^{\mathfrak{s}}(\theta) = \cos^2(\theta)$.

For axisymmetric initial distributions, $\mu_l = 0$, and by the restriction of *n* as defined by (6.28) to positive integers, Legendre functions of the first kind simply coincide with regular Legendre polynomials

$$P_n(s) = \frac{1}{n! \, 2^n} \frac{d^n}{ds^n} \left(s^2 - 1\right)^n.$$

and form a complete orthonormal basis of $L^2([0,\pi])$. Using eigenvalues that satisfy $k = \frac{1}{2}\sqrt{1+4\lambda_k^2} - \frac{1}{2}$ for all $k \in \mathbb{N}_0$, a solution corresponding to any axisymmetric initial distribution can be constructed and the limit is a continuous as well as continuously differentiable function. For instance, the initial distribution $c_0^{\mathfrak{s}}(\theta) = \cos^2(\theta)$ implies that only the two modes $\lambda_0 = 0$ as well as $\lambda_2 = \sqrt{6}$ are not equal zero, and the unsteady surfactant concentration is given by

$$c^{\mathfrak{s}}(\theta,t) = \frac{1}{3} + \left(\cos^2\left(\theta\right) - \frac{1}{3}\right) \exp\left(\frac{-6t}{\operatorname{Pe}^{(\mathfrak{s})}\left(1 + \frac{\eta^i}{\eta^o}\right)}\right).$$

This allows for the determination the surface excess concentration throughout the full time scale, as depicted in figure 6.3. Here, the surfactant equally distributes on the spherical surface, reaching the well-known equal distribution $c^{\mathfrak{s}}(\theta) = 1/3$.

6.4 Discussion and Conclusions

In the present chapter, general solutions to interfacial convection-diffusion equations on a spherical surface have been constructed. The obtained solutions represent the surface excess concentration of a solute, such as surfactants, on a spherical droplet in a two-phase immiscible incompressible Stokes flow. In the present investigation, the

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deformation of the droplet, the Marangoni effect as well as surfactant exchange with the bulks have been neglected. In contrast to known previous results, unsteady surfactant transport on the interface that includes diffusion, or is even dominated by diffusion, is covered. With respect to the most general form of the equation, the surface excess concentration derived here combines exponential functions with Heun's confluent functions. Consequently, general properties can be concluded, as, in particular, the steady state solution to the problem. Furthermore, solutions to the purely diffusive equation can be constructed using Legendre polynomials. Such analytical solutions are of great importance for numerical simulations of interfacial transport problems as benchmark solutions.

In a potential further investigation, when the Marangoni effect, i.e. the influence of surfactant on surface tension and thereby on the flow field, is taken into account, the set of solutions to the unsteady interfacial transport obtained in the present study can be employed as the base state. In a setting with large Biot numbers, i.e. when the ratio of surfactant exchange with the bulk phases is high, or when the Marangoni number is small, approximative analytic solutions can be achieved by a perturbation analysis. In this context, the base order concentration distribution is obtained from the interfacial transport equation governed by the given Hadamard-Rybczynski flow, as indicated. The first order correction of the Hadamard-Rybczynski terminal velocity can then be performed based on the present base-order surfactant concentration, which has been applied to non-diffusive surfactants, for instance by Stone and Leal (1990b). Provided that the deformation of the drop is small, it is possible to regard the surfactant transport by projecting the surfactant concentration back onto a sphere, which has been presented by Vlahovska, Bławzdziewicz, and Loewenberg (2009).

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7 A Narrow Band Method for the Eulerian Approach

The embedded interfacial transport equation is discretized on a small subdomain of the original domain only, which is called the Narrow Band. In this way, the number of degrees of freedom and consequently, the computational effort, are reduced. At the same time, well-posedness of the embedded equation can be assured because regions of singularities in the gradient of the Level Set function are excluded. This Narrow Band is a dynamic computational domain that changes position and structure in accordance with the Level Set function. For this reason, it is not created as an independent physical grid. Instead it is induced from the full computational domain through selective storage allocation and extraction of all relevant entries, or coordinates, respectively. In particular, this approach takes advantage of the local band structure of the matrices in a DG approximation. This chapter describes how such a coordinate based Narrow Band is developed which extrapolates quantities to new Narrow Band cells and at the same time, accurately preserves them on the interface. This method is necessary for treating problems on a dynamically moving Narrow Band.

7.1 A Coordinate Based Narrow Band Approach

The subgrid The embedding of the interfacial transport problem into higher – dimensional space is solved only on a small extract of the original Eulerian grid. This subgrid consists of cells close to the interface. In this way, computational effort is optimized, while guaranteeing well – posedness of the Eulerian formulation. This subgrid is formed by all cells that include isocontours of the Level Set function up to a constant, depending on the grid resolution *h* and a constant $\gamma > 0$:

$$\Sigma_h^{\gamma} = \bigcup_{j \in I^{\gamma}} K_j , I^{\gamma} = \{j = 1, \dots, J : \exists \boldsymbol{x} \in K_j : |\Phi(\boldsymbol{x})| \le \gamma h\}.$$

It can be considered as a narrow band tube around the interface and for this reason, it is called the Narrow Band. Figure 7.1 illustrates Narrow Band structures in a two -dimensional Cartesian domain with respect to a circle, an eccentric circle, an ellipse and Zalesak's notched disk, which will be used within the subsequent test cases. In the software framework Bosss, the implementation of the Narrow Band is based

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Figure 7.1: Examples of a Narrow Band

on the class SubGrid¹ by Kummer (2012). It provides both a quadrature execution mask for the Narrow Band and a bit array which verifies whether a cell belongs to the subgrid or not. The Narrow Band is a subgrid delivered from the LevelSetTracker of the Level Set variable. It comprises all cells that include the subdomain located between the zero isocontours of two level sets which are parallel to the original one. The cell mask of the subgrid is used to determine which quadrature nodes form part of the Narrow Band. These nodes are then utilised for numerical integration when computing operator matrices. Otherwise, only a bit entry is stored, i.e. the matrix entry remains sparse. The cells of the subgrid receive their own local cell indices, in descending order for odd, and in ascending order for even rows, in the same fashion as the full grid. An example is given by figure 7.2 which illustrates both global subgrid indices and local subgrid indices on two processors for the simple case of a circle. Mappings between the local subgrid cells and the local cells of the

 $^{^1} BoSSS. Foundation. SubGrid\\$

full grid are established by the methods LocalCellIndex2SubgridIndex² and SubgridIndex2LocalCellIndex³. On this basis, local matrix and coordinate blocks can be extracted from the full grid quantities, and can be sorted back to the respective quantities in the full spatial domain.



(a) Global indices on Ω_h





(b) Local indices on processor 1





(c) Local indices of Σ_h^γ on processor 1



(d) Global subgrid indices on Σ_{h}^{γ}

(e) Local indices on processor 2

(f) Local indices of Σ_h^{γ} on processor 2

Figure 7.2: Mapping of local coordinates of the full grid and of the Narrow Band with respect to two processors.

Coordinate mappings in the subgrid Variables on the subgrid are provided by the class SubgridCoordinateMapping ⁴ developed by the author, which extends the standard class CoordinateMapping ⁵. It manages all entries of the mapping that fall within the range of the subgrid, SubGridValues ⁶, by their indices, SubGridIndices ⁷. In the method Compress, the corresponding entries of the local coordinates are extracted to the local array of subgrid values. The counterpart of this method,

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²BoSSS.Foundation.SubGrid.LocalCellIndex2SubgridIndex

³BoSSS.Foundation.SubGrid.SubgridIndex2LocalCellIndex

⁴BoSSS.Foundation.SubgridCoordinateMapping

⁵BoSSS.Foundation.CoordinateMapping

⁶BoSSS.Foundation.SubgridCoordinateMapping.SubGridValues

⁷BoSSS.Foundation.SubgridCoordinateMapping.SubGridIndices

Decompress, copies all entries of the subgrid values to their respective positions in the coordinate mapping. All other entries are then filled with zeros.

Operator matrices in the subgrid As all entries of the operator matrix outside of the Narrow Band are allocated as sparse entries, the part of the operator matrix that is relevant to the Narrow Band needs to be determined and extracted. Taking advantage of the local block structures of the DG scheme, this operation can be performed blockwise. Each cell block that is associated with a grid cell of the Narrow Band is extracted. Likewise, cell blocks are selected which are linked to any neighbouring cell included in the Narrow Band. In multiprocessing, this procedure requires both local coordinate indices, for accessing matrix rows, and global coordinate indices, for accessing matrix columns. Local coordinate indices are provided by the subgrid indices of the associated subgrid coordinate mapping. In order to construct global coordinate indices, a global index array of the subgrid cells and a global array of their subgrid neighbours need to be computed by looping over all processors. Then, the initial row

		6	7	8	9	10	11	
		•••		•••	•••			
4		0	0	0	0	$N_{4,10}$	$N_{4,11}$	
5		$N_{5,6}$	0	0	$N_{5,9}$	$N_{5,10}$	$N_{5,11}$	
6		D_6	$N_{6,7}$	$N_{6,8}$	$N_{6,9}$	$N_{6,10}$	0	
7		$N_{7,6}$	D_7	$N_{7,8}$	$N_{7,9}$	0	0	
4 5 6 7	····	0 $N_{5,6}$ D_6 $N_{7,6}$	0 0 $N_{6,7}$ D_7	0 0 $N_{6,8}$ $N_{7,8}$	0 $N_{5,9}$ $N_{6,9}$ $N_{7,9}$	$N_{4,10}$ $N_{5,10}$ $N_{6,10}$ 0	$N_{4,11}$ $N_{5,11}$ 0 0	··· ··· ···

(a) Full grid matrix, processor 1

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	0	1	2	3
0	D_6	$N_{6,5}$	$N_{6,10}$	$N_{6,9}$
1	$N_{5,6}$	D_5	$N_{5,10}$	$N_{5,9}$
(b)	Subgrie	d matri	ix, proce	essor 1

Figure 7.3: Matrices associated with the full grid and with the Narrow Band with respect to the example illustrated by figures 7.2. On top, selected matrix blocks for the local grid cells with indices 4 - 7 are shown. Diagonal blocks D_i are indexed by the local cell index *i*, neighbour blocks with the global cell neighbour *k* are equipped with both indices, $N_{i,k}$. At the bottom, the compressed matrix with the excerpted matrix blocks of the original matrix is shown for the local subgrid cells 0, 1.

position of the diagonal matrix block which should be extracted is determined by the local cell index multiplied by the DOFs per cell. These diagonal blocks are transferred to the next free diagonal block of the compressed matrix in ascending order. Next, the blocks corresponding to the neighbouring cells in the full grid matrix are accessed through the global cell indices per cell. If the respective cell forms part of the Narrow



Figure 7.4: Illustration of an extrapolated concentration on level set isocontours

Band, the block is copied to the compressed matrix and positioned by means of the global subgrid indices that have been gathered initially.

7.2 The Pseudo-timestepping Method for Extending Data

When employing an Eulerian approach to treat interfacial problems, it is first necessary to construct a representation of all relevant surface quantities on the underlying Eulerian grid. In each time step, a meaningful extension of the density variable to the updated Narrow Band has to be performed which, at the same time, conserves this quantity on the interface at a high level of accuracy. This method is particularly important when the subgrid changes position and structure in accordance with the Level Set function. Greer, Bertozzi, and Sapiro (2006) have recommended to start off with variables that are constant in normal direction with respect to the interface. This means, an extension \tilde{c} of a given variable c that solves the boundary value problem

$$\nabla \tilde{c} \cdot \boldsymbol{n}^{(s)} = 0 \text{ in } \Sigma_h^{\gamma}$$

$$\tilde{c} = c \text{ on } \mathfrak{S}.$$
(7.1)

as illustrated by figure 7.4 is employed. In this way, numerical errors that are caused by the degeneration of the diffusion operator in normal direction off the interface can be reduced.

The extension \tilde{c} may be constructed explicitly by mapping each quadrature node in the Narrow Band Σ_h^{γ} to its closest point on the interface \mathfrak{S} . In the following, this method is referred to as the Closest Point method (CPM). Although this approach is fast with respect to performance, its parallelization is an intricate issue, since the closest interfacial point may be located on a different processor than the original quadrature node.

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For this reason, in the present work, a distinct method is adopted, called the pseudotimestepping method (PTM). Here, an extension \tilde{c} of given data c is achieved by solving the pseudo-timestepping equation

$$\frac{\partial \tilde{c}}{\partial \tau} + \operatorname{sign}(\Phi) \nabla \tilde{c} \cdot \nabla \Phi = 0 \text{ in } \Sigma_h^{\gamma}, \ \tau > 0$$

$$\tilde{c}(0, \boldsymbol{x}) = c(\boldsymbol{x})$$
(7.2)

with respect to the artificial parameter τ until reaching a steady state. The steady state solution \tilde{c} then provides the extended quantity. As the zero-isocontour of the Level Set function Φ is also a zero-isocontour of its signum function, \tilde{c} identical with c on the interface.

This method has been suggested by Greer, Bertozzi, and Sapiro (2006) and mimics a pseudo-timestepping scheme developed by Zhao, Chan, Merriman, and Osher (1996) for re-initializing Level Set functions in multiphase problems. This approach is furthermore employed to regularize data by performing a limited small number of pseudo-timesteps after solving the interfacial advection-diffusion for some time steps.

Equation (7.2) is a linear Hamilton-Jacobi equation. It can be approximated by a special type of an LDG scheme that has been previously outlined in section 4.2, resulting in:

$$\int_{K_j} \frac{\partial \tilde{c}_h}{\partial t} \varphi_i^j d\boldsymbol{x} + \int_{K_j} \Phi_h \nabla \Phi_h \cdot \boldsymbol{p} \varphi_i^j d\boldsymbol{x} = 0$$
(7.3)
$$\int_{K_j} \boldsymbol{p} \varphi_i^j d\boldsymbol{x} - \int_{K^j} \tilde{c}_h \nabla \varphi_i^j d\boldsymbol{x} + \int_{\partial K^j} \boldsymbol{F}^* (c_h^+, c_h^-) \cdot \boldsymbol{n} \varphi_i^j d\boldsymbol{s} = 0$$
for $i = 1, \dots, N_p$, $j = 1, \dots, J \in \Sigma_h^{\gamma}$.

The novel idea of the scheme proposed here lies in the modification of numerical fluxes. Originally, when LDG schemes are applied to Hamilton-Jacobi equations, weak formulations of partial derivatives are introduced in pairs, employing a standard upwinding and downwinding flux each. However, in problem (7.2), information is transported along with the interfacial normal $n^{(s)}$ instead of the cell normal. Beyond, information is always directed away from the interface. Thus, only a form that utilizes an upwinding scheme is necessary.

For this reason, the author of this thesis employs the following numerical flux, when approximating the partial derivatives of \tilde{c} :

$$\boldsymbol{F}^{*}(c_{h}^{+},c_{h}^{-})\cdot\boldsymbol{n} = \begin{cases} c_{h}^{+}\boldsymbol{e}^{l}\cdot\boldsymbol{n} & \text{if } \boldsymbol{n}^{(\mathfrak{s})}\cdot\boldsymbol{n} \geq 0\\ c_{h}^{-}\boldsymbol{e}^{l}\cdot\boldsymbol{n} & \text{if } \boldsymbol{n}^{(\mathfrak{s})}\cdot\boldsymbol{n} < 0 \end{cases}$$

For stability, in the discrete equation (7.3), the sign function is replaced by the Level Set function itself.

Within the BoSSS framework, extension methods are provided within the namespace Extension⁸. A single instance of the class LDGExtension⁹, for the PTM, performs the extension and replaces the coordinates of the respective mapping. Alternatively, the static method AnsatzConstruction provided by the class ClosestPoint¹⁰ determines and assigns the closest points to the mapping's coordinates. By standard, it is recommended to use the PTM, as the CPM is restricted to usage on a single processing unit only.

7.3 Numerical performance

The pseudo-timestepping approach requires the user to fix a meaningful end time T which is somehow minimal with respect to performance. In fact, a limited number of timesteps is usually sufficient in order to achieve a meaningful extension of a given variable to new grid cells, even if this extension is not precisely constant in normal direction off the interface.

Most importantly, the original concentration function needs to be conserved on the interface. This aspect is investigated in the following. Three of the two-dimensional examples presented at the beginning of this chapter in figure 7.1, i.e. a circle, an ellipse and a deformed circle are employed for an analysis of the surface error. As a benchmark, results of the CPM are employed for comparing the quality of the attained solution. It must be remarked that the CPM cannot be applied to constant basis polynomials and that the respective results for the PTM are only enlisted for completeness.

In all of the three cases, the pseudo-timestepping scheme is performed up to an end time 0.2 for at least 200 timesteps. Numerical tests indicate that for these examples, the resulting solutions of both methods are similarly close to a function that is constant in normal direction off the interface when chosing this end time. The relative L^2 -error is computed on the Level Set isocontour with respect to the original, unaltered variable

$$e_{\Gamma_h} = \frac{\|\tilde{c} - c\|_{L^2(\Gamma_h)}}{\|c\|_{L^2(\Gamma_h)}}$$

and is constructed using hierarchical moment fitting quadrature rules of order eight which have been provided by Müller, Kummer, and Oberlack (2013).

The surface errors on a circle, a deformed circle and an ellipse when performing the pseudo-timestepping method on the set of cells intersected by the surface are illustrated by figure 7.5. The resulting slopes of regression lines in comparison with the CPM are given by table 7.1 and are nearly identical for both methods. With respect to an accurate conservation of the surface variable, the PTM is as suitable as the CPM.

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⁸BoSSS.Application.Extension

⁹BoSSS.Application.Extension.LDGExtension

¹⁰BoSSS.Application.Extension.ClosestPoint

A Narrow Band Method for the Eulerian Approach

	Circle		Ellipse		Deformed circle	
p	CPM	PTM	CPM	PTM	CPM	PTM
0	-	0.88	-	0.97	-	1.01
1	2.01	2.03	1.92	1.95	1.98	2.00
2	2.88	2.87	2.87	3.06	2.96	2.96

Table 7.1: Surface mass loss of the CPM and PTM for different test problems in comparison.

The selected test cases show nearly identical slopes of regression lines for both methods. The resulting slopes of the regression lines are enlisted in table 7.1. In the test cases shown, optimal convergence rates of nearly p + 1 that may be expected from a DG scheme are achieved.

From the viewpoint of numerical accuracy, none of the methods needs to be preferred. However, the only PTM can be applied when the discretization is based on a polynomial basis of order 0 or when the numerical computation is performed on multiple processors. Beyond, in contrast to the CPM, the PTM is easily implemented for grids formed by more cells than simply the cut cells. To conclude, figures 7.6 and 7.7 illustrate the effect of the PTM. Figure 7.6 shows the extended subgrid variable on the Narrow Band in a two-dimensional domain and its extrapolation to newly acquired grid cells when the interface is moved. Here, a deformed circle rotates around the origin. When the induced subgrid loses or gains cells, the PTM is performed until T = 0.3, i.e. for few time steps only. Figure 7.7 underlines that the PTM may as well be used for applications where the surface undergoes topological changes, such as the collision or break up of drops. Here, an initial surface concentration has been prescribed on a Narrow Band that includes all cut cells and their next neighbouring cells. With the evolving surface, the Narrow Band changes structure and position, and the surface concentration is moved accordingly, by applying the PTM.



Figure 7.5: Error of mass loss on the interface when applying the pseudo-timestepping method up to an pseudo-end time of T = 0.2. At this end time, the obtained solution is close to the extrapolation generated by the closest point method.

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Figure 7.6: Repeated extrapolation of an initial concentration of $c(x) = x^2$ onto a moving Narrow Band around a deformed circle. The PTM is used to extend data to new subgrid cells when the surface is rotated around the origin.



Figure 7.7: Extension by the pseudo - timestepping based method on a surface that represents the breakup of a droplet.

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8 The Eulerian DG Algorithm and Numerical Results

The objective of the present work is the numerical approximation and solution of the interfacial transport problem by a DG scheme. As it provides excellent mass conservation properties when combined with DG methods and as it is flexible for capturing interfaces with distortions and topological changes, the Level Set method was required for representing the interface. Against this background, an Eulerian approach has been chosen for the interfacial transport problem. Here, the interfacial equation is approximated based on the existing Eulerian grid, instead of traditional Lagrangian approaches, similar to the Level Set approach for capturing the interface. The use of Eulerian methods for the discretization of interfacial equations is not very common, but still promising. In particular, tedious interface reconstruction and remeshing can be avoided.

The resulting numerical scheme for discretizing and solving the interfacial transport problem is described in this chapter. It is based on an Eulerian DG method and employs conserved forms of the underlying transport equations that have been developed in chapter 5. As the convection-diffusion equation can be treated by a first order differential operator splitting scheme, diffusive and convective parts of the equation are discretized separately. Various test scenarios are developed in a two-dimensional setting which are used to verify the respective discretizations and analyse the order of convergence. Examples in three-dimensional domains illustrate how surface problems can be successfully solved numerically by the method presented.

8.1 Discretization of surface transport equations

The interfacial transport equation is numerically discretized by a DG scheme in **Eulerian form**, based on the given Cartesian mesh. All surface differential operators are extended to the underlying higher dimensional domain and identified with tangential parts of the standard differential operators. This is achieved by employing the surface projection tensor P^{s} according to equations (2.10) and (2.11).

The resulting form of the interfacial transport equation is then given by equation (5.4). Furthermore, the phase interface is represented implicitly as the zero-isocontour of a Level Set function Φ which is advected by the flow field in an incompressible setting

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according to equation (3.2). In the Eulerian formulation, all transport equations are extended to a Narrow Band Σ_h^{γ} of level set isocontours up to a defined width around the interface, as devised in chapter 7.

Sets of conservation laws (5.27) derived in chapter 5 (see also Kallendorf, Cheviakov, Oberlack, and Wang (2012)) enhance a DG discretization of the interfacial transport equation in the Eulerian formulation. Simple forms of these conservation laws are employed in the method presented. In summary, the aim of this chapter is the numerical discretization and solution of the following system of equations

$$\frac{\partial}{\partial t} \Phi + \nabla \cdot (\boldsymbol{u} \, \Phi) = 0 \text{ in } \Omega \times]0, T]$$

$$\Phi(\boldsymbol{x}, 0) = \Phi_0(\boldsymbol{x}) \text{ in } \Omega$$
(8.1)

$$\frac{\partial}{\partial t} \left(c \| \nabla \Phi \| \right) + \nabla \cdot \left(\boldsymbol{u} \, c \| \nabla \Phi \| \right) = \frac{1}{\operatorname{Pe}^{(\mathfrak{s})}} \nabla \cdot \left(\| \nabla \Phi \| \boldsymbol{P}^{(\mathfrak{s})} \nabla c \right) \text{ in } \Sigma_{h}^{\gamma} \times]0, T] \qquad (8.2)$$

$$c(\boldsymbol{x}, 0) = c_{0} \left(\boldsymbol{x} \right) \text{ in } \Sigma_{h}^{\gamma}$$

$$\text{where } \boldsymbol{P}^{(\mathfrak{s})} \nabla c = \nabla c - \left(\nabla c \cdot \boldsymbol{n}^{(\mathfrak{s})} \right) \boldsymbol{n}^{(\mathfrak{s})} \text{ in } \Sigma_{h}^{\gamma}$$

$$\text{and } \boldsymbol{n}^{(\mathfrak{s})} = \frac{\nabla \Phi}{\| \nabla \Phi \|} \text{ in } \Sigma_{h}^{\gamma}$$

$$\text{and } \nabla \cdot \boldsymbol{u} = 0 \text{ in } \Omega \times [0, T]. \qquad (8.3)$$

Equation (8.2) is treated by a first order operator splitting scheme. For this purpose, assume a discretization by N timesteps of the temporal horizon,

 $\{0 = t^0 < \ldots t^k < t^{k+1} < \ldots < t^N = T\}$, and denote the solution at time t^k by c^k . Roughly speaking, in each timestep the convective part of equation (8.2) given by

$$\frac{\partial}{\partial t} \left(c \left\| \nabla \Phi \right\| \right) + \nabla \cdot \left(\boldsymbol{u} \, c \left\| \nabla \Phi \right\| \right) = 0 \text{ in } \Sigma_h^{\gamma} \times \left] t^k, t^{k+1/2} \right]$$
(8.4)

is solved for $c^{k+1/2}$ at an intermediate time $t^{k+1/2}$, using c^k as an initial value. Next, the solution $c^{k+1/2}$ is employed as the initial value when computing the solution c^{k+1} of the purely diffusive equation, i.e.

$$\frac{\partial}{\partial t} \left(c \| \nabla \Phi \| \right) = \frac{1}{\operatorname{Pe}^{(\mathfrak{s})}} \nabla \cdot \left(\| \nabla \Phi \| \boldsymbol{P}^{\mathfrak{s}} \nabla c \right) \text{ in } \Sigma_{h}^{\gamma} \times \left[t^{k+1/2}, t^{k+1} \right], \tag{8.5}$$

which is then the solution of equation (8.2) at time t^{k+1} for the initial value c^k . It is important to note that the conservation laws of the convective and the diffusive part of the extended equation (5.4), i.e. equations (8.4) and (8.5), correspond to the convective and the diffusive parts, respectively, of conservation law (8.2) which has been derived in chapter 5.

All of these conservation laws are treated by a common algorithmic structure. The equations are discretized in the density variable $\Psi \equiv c \|\nabla \Phi\|$ and require a coupling to the Level Set advection equation. The concentration c^k can be obtained from the density variable Ψ^k at time t^k by division through the surface area element $\|\nabla \Phi_k\|$, which is computed from the updated Level Set variable Φ^k .

When initiating the solution process, the initial surface excess concentration c_0^5 is extended to an initial variable c^0 that is defined in the Narrow Band around the initial Level Set function Φ^0 . By a pointwise multiplication by the surface area element, the initial value Ψ^0 of the density variable is obtained. At the beginning of each time step, the evolution of the Level Set function is performed first. Within this context, the Level Set equation is discretized by using an upwinding scheme for the numerical fluxes and a third order Runge-Kutta TVD time-stepping scheme. In case the evolved level set isocontours up to the specified bandwidth intersect additional Cartesian grid cells, the Narrow Band is amplified. All quantities are then extrapolated using the pseudo-timestepping method introduced in chapter 7. Next, the transport equation as an equation in Ψ , is solved. Finally, the extended surface concentration c^k at time step t^k is generated from Ψ^k by a pointwise division through the surface area element. The structure of this algorithm is outlined in algorithm 1.

```
Algorithm 1 Solve Interfacial Transport Problem
Input: Level Set function \Phi^0, surface excess concentration c^{\mathfrak{s}}, grid \Omega_h,
temporal discretization {t_0 = t^0 < \dots t^n < t^{n+1} < \dots < t^N = T}
Output: Extended concentration c^N
   for t^n < t^N do
      if t^0 = t_0 then
         Compute subgrid \Sigma^0
         Extend c_0^{\mathfrak{s}} to c^0 on \Sigma^0
         Compute \|\nabla \Phi^0\| from \Phi^0
         \Psi^0 \leftarrow c^0 \|\nabla \Phi^0\|
      else
         Solve Level set advection for \Phi^n
         Compute subgrid \Sigma^n
         if \Sigma^n \notin \Sigma^{n-1} then
            Extend \Psi^{n-1} onto \Sigma^n
         end if
      end if
      Solve extended surface transport problem for \Psi^n
      t^{n+1} \leftarrow t^n
   end for
   c^N \leftarrow \Psi^N / \| \nabla \Phi^N \|
   return c^N
```

The computational structure for discretizing and solving the surface transport problems is integrated in the existent code framework BoSSS in various projects. The software code developed is fully MPI parallel. Numerical results presented in the following sections are computed utilizing two to four nodes of an Intel[®] Xeon[®] Processor E5-4650 on Lichtenberg cluster (TU Darmstadt) with a node memory expansion 128 GByte per node.

Numerical errors are provided for the concentration variable c and are measured on the surface Γ_h with respect to exact solutions c_{ex} of the surface concentration on the surface.

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As the solution of the extended equation on the surface, or interface, respectively, is analytically independent of the chosen extension (see also Delfour and Zolésio (2011)), accuracy of the numerical solution needs to be investigated on the surface. Here, L^2 error estimates on the Level Set isocontour are constructed using hierarchical moment fitting quadrature rules of order eight, which have been provided by Müller, Kummer, and Oberlack (2013). In order to account for the influence of errors in quadrature, relative errors i.e.

$$e_{\Gamma_h} = \frac{\|c_{ex} - c\|_{L^2(\Gamma_h)}}{\|c_{ex}\|_{L^2(\Gamma_h)}}$$
(8.6)

are computed.

8.2 Surface Transport Equations without Diffusion

This section treats the interfacial problem without diffusion, i.e. the system of equations (8.1),(8.2) and (8.3) is considered where the second equation replaced by equation (8.4). Solving the convective part of equation (8.2) only is necessary for a simple operator splitting scheme, and represents the case where the surface diffusion is negligible. The purpose of the following test problems is *not* the simulation of a physical problem, but exclusively the numerical analysis of the method presented.

8.2.1 Numerical Results

In the following, for convenience, the jump and average operators on all outer edges of the Narrow Band Σ_h^{γ} are simply given by

$$\{\{c_h\}\} = c_h^+, \ \llbracket c_h \rrbracket = c_h^+ \boldsymbol{n}^j,$$

where n^j denotes the normal vector oriented outward of the border edge of the Narrow Band and c_h^+ is the value of the boundary cell located inside of the Narrow Band. The density variable Ψ is approximated by a linear combination of DG polynomials

$$\Psi_{h}(t,x) = \sum_{j=1}^{J} \sum_{i=1}^{N_{p}} \Psi^{j,i}(t) \varphi_{i}^{j}(x)$$
(8.7)

such that for each point t^k in the temporal discretization

$$\Psi_h(t^k) \in V_h^p = \left\{ v \in L^2\left(\Sigma_h^\gamma\right) \colon v|_K \in P^p(K), \forall K \in \mathfrak{I}_{h,\gamma} \right\}.$$
(8.8)

Here, $\mathfrak{I}_{h,\gamma} \subset \mathfrak{T}_h$ denotes the set of all cells contained in the Narrow Band Σ_h^{γ} that is associated with the Level Set function Φ_h at time t^k .



Figure 8.1: Code structure of the Bosss application by which the surface transport problem without diffusion is discretized and solved.

The numerical objective is determining a function (8.7), which satisfies requirement (8.8) and solves the DG formulation

$$\int_{K_j} \frac{\partial \Psi_h}{\partial t} \varphi_i^j d\boldsymbol{x} - \int_{K_j} (\Psi_h \boldsymbol{u}_h) \cdot \nabla \varphi_i^j d\boldsymbol{x} + \sum_{e \in E^j} \int_e \left(\{ \{ \boldsymbol{u}_h \, c_h \} \} + \left| \boldsymbol{n}^j \cdot \boldsymbol{u}_h \right| \frac{\llbracket c_h \rrbracket}{2} \right) \cdot \boldsymbol{n}^j \varphi_i^j \, ds = 0$$
(8.9)

for all cells $K_j \in \mathfrak{I}_{h,\gamma}$ and all basis polynomials $\varphi_i^j \in V_h^p$ for the given initial value (in Ψ). Here, E^j denotes the set of all edges of cell j. The numerical flux employed in the respective edge integrals is an upwinding flux. Equation (8.9) is discretized by a Runge-Kutta TVD3 scheme in time. The degree of basis polynomials is always one lower than the basis degree used for the Level Set function. A rough overview of the code structure that implements the approximation and solution of the respective initial value problem is provided by figure 8.1, which outlines the functionality of the new classes.

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Figure 8.2: Relative error and order of convergence of the interfacial convection problem with respect to a circular surface. The extended equation is discretized by polynomial degrees 0, 1 and 2, starting with an initial concentration of $x^2/(x^2 + y^2)$. The Narrow Band embraces all cells that include Level Set isocontours up to the absolute value 2h.

Investigation of steady 2D problems Numerical errors of the Eulerian discretization of the interfacial transport problem without diffusion are considered by means of two simple test settings. In both cases, the underlying flow field is tangential with respect to the initial surface, implying a configuration with a steady geometry. It should be remarked that the results presented solely focus on the performance of the numerical solver, without assuming any physical background, i.e. the flow field is **not** subject to an incompressible two-phase flow with interfacial jumps.

As a first example, a unit circle exposed to a rotational field u(x, y) = (-y, x) is considered. In polar coordinates the surface transport equation without diffusion is given by

$$\frac{\partial c^{\mathfrak{s}}}{\partial t} + \frac{r}{r_0} \frac{\partial c^{\mathfrak{s}}}{\partial \varphi} = 0 \text{ on } \mathfrak{S}, \tag{8.10}$$

i.e. for $r = r_0$. For a given initial concentration the solution of equation (8.10) is obtained from the method of characteristics. When transformed to Cartesian coordinates, for an initial concentration $c_0^{s}(x, y)$ the solution is given by

$$c^{\mathfrak{s}}(x, y, t) = c_0^{\mathfrak{s}}(x\cos(t) + y\sin(t), x\sin(t) - y\cos(t)).$$

Figure 8.2 illustrates the relative error after 200 time steps, evaluated at time $\overline{T} = 0.2$, for polynomial degrees 0, 1 and 2, when starting with an initial concentration of $x^2/(x^2+y^2)$. The Narrow Band is defined by the level set isocontours of absolute value 2h. On the left, results for the case of a Level Set function with signed distance property are shown. The slopes of the resulting linear regression lines are 0.92 for a zero order discretization, 1.88 for a first order discretization, and 2.88 for second order polynomials. On the right, in contrast, a polynomial Level Set function is applied, yielding linear fits with idential slopes.

In a similar fashion, solutions to the convection problem on an ellipse can be derived, employing elliptic coordinates to the convection problem on an ellipse in parametric form,

$$\hat{\boldsymbol{x}}^{(s)}(\varphi, r, \mu_0) = \left(\begin{array}{c} r \cosh(\mu_0) \cos(\varphi) \\ r \sinh(\mu_0) \sin(\varphi) \end{array} \right),$$

where $r \cosh(\mu_0) = a$ and $r \sinh(\mu_0) = b$ are the semi-minor and semi-major axes of the fixed elliptic surface.

Again assuming a tangential velocity field $u(x, y) = (-\frac{a}{b}y, \frac{b}{a}x)$, one obtains the surfactant transport equation without diffusion in elliptic coordinates:

$$\frac{\partial c^{\mathfrak{s}}}{\partial t} + \frac{r}{r_0} \frac{\sin\left(\varphi\right)\cos\left(\varphi\right)}{\left(\cosh\left(\mu_0\right)\right)^2 - \cos^2\left(\varphi\right)} c^{\mathfrak{s}} + \frac{r}{r_0} \frac{\partial c^{\mathfrak{s}}}{\partial \varphi} = 0.$$
(8.11)

For a prescribed initial distribution $c_0^{\mathfrak{s}}(\varphi)$ the solution of the surface transport equation on an ellipse in elliptic coordinates is given by

$$c^{\mathfrak{s}}(\varphi,t) = c_0^{\mathfrak{s}}(t-\varphi) \left(\frac{b^2 \left(\cos(\varphi)\cos(t) + \sin(\varphi)\sin(t)\right)^2 + a^2 \left(\cos(\varphi)\sin(t) - \sin(\varphi)\cos(t)\right)^2}{b^2 \cos^2(\varphi) + a^2 \sin^2(\varphi)} \right)^{1/2}.$$

Hence, after a transformation to Cartesian coordinates, the initial distribution $c_0^s(x, y)$ yields the solution

$$c^{\mathfrak{s}}(x,y,t) = \frac{\left(c_0^{\mathfrak{s}} \|\nabla\Phi\|\right) \left(x\cos(t) + \frac{a}{b}y\sin(t), y\cos(t) - \frac{b}{a}x\sin(t)\right)}{\|\nabla\Phi(x,y)\|}.$$

Figure 8.3 illustrates the relative surface error and order of convergence for a setting with an initially constant surface excess concentration at value 1.0, which is extended by the constant value to the Narrow Band. Parameters of the ellipse are given by a = 0.8 and b = 1.2. The error is computed at $\overline{T} = 0.25$, which is discretized by 500 equidistant timesteps. The Narrow Band is defined by the level set isocontours of absolute value 1*h* and 3*h* in order to investigate the influence of the width of the Narrow Band. In fact, computations on Narrow Band structures have been performed by other authors, but the configuration of the Narrow Band has not been addressed.

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Figure 8.3: Relative error and order of convergence of the interfacial convection problem with respect to an ellipse. The extended equation is discretized by polynomial degrees 0, 1 and 2, starting with an initially constant concentration $c(x) \equiv 1.0$. The Narrow Band embraces all cells that include Level Set isocontours up to the absolute value 1h and 3h.

Nearly optimal results are achieved on a Narrow Band of width 3*h*, depicted on the left, where the computed slopes of the regression lines are 0.73 for a zero order discretization, 1.83 for a first order discretization, and 3.15 for second order polynomials. Computing the same test case on a thinner band tube of (critical) width 1*h* around the surface only, results in slopes of the regression lines of 0.41 for a zero order discretization, 1.28 for a first order discretization, and 2.37 for second order polynomials. In addition, the computation has been performed on a Narrow Band is defined by the level set isocontours of absolute value 2*h*. In this case the slopes of the resulting linear regression lines are 0.59 for a zero order discretization, 1.57 for a first order discretization, and 2.98 for second order polynomials.

These numerical results allow for the following interpretations. The discretization by a DG scheme enables the numerical approximation and discretization of purely convective interfacial transport problems by polynomials of arbitrary order. The order of convergence has been investigated for discretizations using up to second order polynomials for the computational variable, and up to third oder polynomials for the Level Set variable, respectively. Results are summarized in table 8.1.

In both of the test cases that include steady surfaces, for different configurations, convergence rates are close to p + 1, when the width of Narrow Band is chosen with at least 2h. In summary, the expectation of a DG scheme are met. Convergence for zero

	Circle, signed distance	Circle, poly- nomial	Ellipse, polynomial		
width p	2h	2h	1h	2h	3h
0	0.92	0.92	0.41	0.59	0.73
1	1.88	1.88	1.28	1.56	1.83
2	2.88	2.88	2.37	2.98	3.15

Table 8.1: Summary of computed slopes of regression lines for different twodimensional scenarios and distinct polynomial degrees p. Different widths of the Narrow Band and different structures of the Level Set function are considered.

order basis polynomials, however, is slightly suboptimal. This may be explained by the strong dependence on boundary values in this case.

When using the Eulerian approach presented for the numerical computation of the interfacial transport problem, the width of the narrow band tube around the interface needs to be parametrized, identifying those cells of the underlying computational domain which are used for the discretization of the equation. Test cases on an ellipse have been run for three different configurations, i.e. band widths 1h, 2h and 3h. Numerical results indicate that an increase of the width of the Narrow Band may improve the order of convergence. This behaviour can be viewed to be natural because the degrees of freedom with respect to the discretization of the interface remain fixed, while the degrees of freedom employed for the approximation of the extended problem increase.

Furthermore, numerical errors have been investigated for different underlying Level Set functions because the Level Set function is coupled to the transport equation through the surface area element. For this purpose, both polynomial and irrational functions have been used, such that signed distance property has been attained only in some of the test settings. In the studies performed, no negative impact of different structures of the Level Set function could be observed. In contrast to diffusion problems, this behaviour has actually been anticipated, as the surface area element affects the solution only by a pointwise multiplication or division, and not the numerical scheme itself.

Investigation of unsteady problems Next, an example of the purely convective problem on an unsteady surface is investigated, which is given by a counter-clockwise rotation of an ellipsoid around the *z*-axis. Figure 8.4 illustrates the three-dimensional problem for a quarter rotation, when combining the solution of the Level Set equation, followed by an extension of the density variable onto the new subgrid and the solution of the interfacial transport equation without diffusion in conserved form given by the method presend.



Figure 8.4: Quarter rotation of an ellipsoid around the *z*-axis, starting with an initial concentration function $c_0(x) = y^2$. The computed solution is obtained by solving the surface transport equation without diffusion and the Level Set equation. Values are extrapolated to new Narrow Band cells by utilizing the pseudo-timestepping method.

The problem in two dimensions, i.e. the rotation of an ellipse by a field u(x, y) = (-y, x), is employed for analysing the error when the solution of the Level Set equation and an extrapolation to new Narro Band cells by a pseudo-timestepping scheme are combined with the solution of the convection equation. As a remark, interfacial jumps and the impact of exchange with the bulk phases are not considered in this investigation.

Within this context, a conserved form of the interfacial convection problem proves to be a powerful tool for determining exact solutions as follows. The initial Level Set function that describes an ellipse in Cartesian coordinates (x, y) is given by

$$\Phi_0(x,y) = \frac{x^2}{a^2} + \frac{y^2}{b^2} - 1.0$$

Its advection by the rotational field results in the Level Set function

$$\Phi(x, y, t) = \frac{\tilde{x}^2}{a^2} + \frac{\tilde{y}^2}{b^2} - 1.0$$

with $\tilde{x} = x \cos(t) + y \sin(t), \ \tilde{y} = y \cos(t) - x \sin(t),$

which embeds the rotated elliptic surface. For each time step the resulting surface line element is given by

$$\|\nabla\Phi(x,y,t)\| = 2\left(\left(\frac{\tilde{x}}{a^2} + \frac{\tilde{y}}{b^2}\right)^2\right)^{1/2}.$$

Inserting the Ansatz

$$c(x, y, t) = \mathcal{F}(x, y, t) \|\nabla \Phi(x, y, t)\|^{-1}$$
(8.12)

into equation 8.4, the remaining equation in \mathcal{F} is solved by functions

$$\mathcal{F}(x,y,t) = \left\| \nabla \Phi(x,y,t) \right\|^{-1} c_0(\tilde{x},\tilde{y}).$$

Equation (8.12) then yields the concentration function for the initial value problem. The resulting L^2 -surface error after 760 timesteps with timestep size 0.001, after performing a rotation by 90°, is given in table (8.2).

With an exception of the first data point, all computed erros decrease notably with increasing polynomial degree. Computed slopes of the resulting regression lines are 0.7 for zero order polynomials, 2.03 for first order polynomials and 2.58 for the case of a second order discretization. These convergence rates nearly meet the expectations of the DG scheme, but are still slightly suboptimal. In this respect, the result convenes with the numerical performance of the convection problem on a steady surface. Furthermore, for this problem the decrease of numerical errors with decreasing edge length is not as steep as expected, which is probably originated in the lack of optimization with respect to the number of pseudo-timesteps and the width of the Narrow Band.

8.3 Surface Transport Equations dominated by Diffusion

In this section, the diffusive part (8.5) of the surface transport equation (5.27) is investigated. Physically, the purely diffusive form of the equation is relevant to two-phase

h	<i>p</i> = 0	<i>p</i> = 1	<i>p</i> = 2
0.425	6.692482E-001	1.590755E+000	4.172316E+000
0.2125	3.907067E-001	3.046398E-002	1.221666E-002
0.10625	2.365996E-001	1.061694E-002	5.143001E-003
0.053125	1.365673E-001	6.457332E-003	2.833721E-003
0.0265625	1.010066E-001	3.095253E-003	1.144462E-003

Table 8.2: Surface error terms for the purely convective problem when imposing a quarter rotation on an ellipse.

flow settings with an extremely slow inflow or high diffusivity of the surfactant, where the diffusion is dominant and the convective term is negligible. Further applications are settings with steady surfaces, such as heat conduction on a rigid surface. The purpose of the test problems presented here is *not* the simulation of the physical problem, but exclusively the introduction and numerical investigation of the method presented for the diffusive form of the equation.

The discretization of the extended diffusion equation (8.5) by a DG method is significantly more elaborate than the discretization of the conserved form of the convective transport. The discretization scheme needs to be able to handle variable coefficients given by the variable surface area element. Furthermore, a tensor product of the gradient given by the extended surface gradient replaces the standard gradient. The LDG scheme developed by Cockburn and Dawson (2000), which is described in detail in section 4.1.3, is suitable for these characteristics of the diffusive term in equation (8.5).

From the numerical point of view, the solution of the extended diffusion equation (8.5), equipped a suitable initial value, requires the specification of additional boundary conditions. However, on closed surfaces (or interfaces), the surface diffusion problem is not exposed to any boundary conditions.

Due to the lack of physical boundary conditions, artificial boundary conditions need to be introduced for treating the extended problem numerically. The fact that the surface gradient of the solution is always perpendicular to interface, i.e. condition

$$\nabla^{(\mathfrak{s})} c^{\mathfrak{s}} \cdot \boldsymbol{n}^{(\mathfrak{s})} = 0 \text{ on } \mathfrak{S}$$
(8.13)

needs to hold, has been employed by Dziuk and Elliott (2009) as a **natural boundary condition**. The above condition may be generalized to the embedded surface gradient which is perpendicular to isocontours of the Level Set function, i.e.

$$(\boldsymbol{P}^{(\mathfrak{s})} \nabla c) \cdot \boldsymbol{n}^{(\mathfrak{s})} = 0 \text{ in } \Sigma_h^{\gamma}. \tag{8.14}$$

Equation (8.5) is considered as an equation in the density variable Ψ , which is discretized by a linear combination of DG polynomials

$$\Psi_{h}(t,x) = \sum_{j=1}^{J} \sum_{i=1}^{N_{p}} \Psi^{j,i}(t) \varphi_{i}^{j}(\boldsymbol{x})$$

such that for each discrete point in time t^k

$$\Psi_h(t^k) \in V_h^p = \left\{ v \in L^2\left(\Sigma_h^\gamma\right) \colon v|_K \in P^p(K), \forall K \in \mathfrak{I}_{h,\gamma} \right\},\tag{8.15}$$

where $\mathfrak{I}_{h,\gamma} \subset \mathfrak{T}_h$ denotes the set of all cells contained in the Narrow Band Σ_h^{γ} associated with the Level Set function Φ_h at time t^k . Utilizing a set of auxiliary variables

$$\boldsymbol{q_h} \in \boldsymbol{W}_h^k = \left\{ \boldsymbol{w} \in \left(L^2 \left(\Sigma_h^{\gamma} \right) \right)^D : v|_K \in P^k(K)^D, K \in \mathfrak{I}_{h,\gamma} \right\},$$

one seeks to find Ψ_h which solves a modified Brezzi scheme

$$\int_{K_j} \frac{\partial \Psi_h}{\partial t} \varphi_i^j d\boldsymbol{x} - \frac{1}{\operatorname{Pe}^{(\mathfrak{s})}} \int_{K_j} \|\nabla \Phi_h\| \boldsymbol{\theta}_h \cdot \nabla \varphi_i^j d\boldsymbol{x} + \frac{1}{\operatorname{Pe}^{(\mathfrak{s})}} \int_{\partial \Sigma_h^{\gamma}} F_{\boldsymbol{\theta}} \left(\boldsymbol{\theta}_h^+, \boldsymbol{\theta}_h^-, c_h^+, c_h^- \right) d\boldsymbol{x} = 0$$
$$\int_{K_j} \boldsymbol{\theta}_h \cdot \boldsymbol{\tau}_i^j d\boldsymbol{x} = \int_{K_j} P_h^{\mathfrak{s}} \boldsymbol{q}_h \cdot \boldsymbol{\tau}_i^j d\boldsymbol{x}$$
$$\int_{K_j} \boldsymbol{q}_h \cdot \boldsymbol{\tau}_i^j d\boldsymbol{x} = -\int_{K_j} c_h \nabla \cdot \boldsymbol{\tau}_i^j d\boldsymbol{x} + \int_{\partial \Sigma_h^{\gamma}} F_{q_h} (c_h^+, c_h^-) \boldsymbol{n}^j \cdot \boldsymbol{\tau}_i^j d\boldsymbol{s}$$

holds for all cells $K_j \in \mathfrak{I}_{h,\gamma}$ and all basis polynomials

$$\varphi_i^j \in V_h^p \text{ and } \boldsymbol{\tau}_i^j \in \boldsymbol{W}_h^k \quad i = 1, \dots, N_p$$

and where c_h is replaced by identity

$$c_h = \frac{1}{\|\nabla \Phi_h\|} \Psi_h.$$

The scheme uses a central flux in $P_h^s q_h$, penalized by c_h , and a central flux in c_h for the auxiliary differential equations as follows

$$\begin{split} &\int_{\partial \Sigma_h^{\gamma}} F_{\theta} \left(\boldsymbol{\theta}_h^{+}, \boldsymbol{\theta}_h^{-}, c_h^{+}, c_h^{-} \right) \, d\boldsymbol{x} = -\int_{\Gamma_h} c_h^{-} \, \varphi_i^j \, d\boldsymbol{s} - \sum_{e \in E^j} \int_e \left\{ \tau \left[\left[c_h \right] \right] - \left\{ \left\{ \boldsymbol{\theta}_h \right\} \right\} \right) \cdot \boldsymbol{n}^{(\mathfrak{s})} \, \varphi_i^j \, d\boldsymbol{s} \\ &\int_{\partial \Sigma_h^{\gamma}} F_{q_h}(c_h^{+}, c_h^{-}) \, \boldsymbol{n}^j \cdot \boldsymbol{\tau}_i^j \, d\boldsymbol{s} = \sum_{e \in E^j} \int_e \left\{ \left\{ c_h \right\} \right\} \, \boldsymbol{n}^j \cdot \boldsymbol{\tau}_i^j \, d\boldsymbol{s} + \int_{\Gamma_h} c_h^{+} \, \boldsymbol{n}^j \cdot \boldsymbol{\tau}_i^j \, d\boldsymbol{s} \end{split}$$

Furthermore, the initial value has to be fulfilled for $t^0 = 0$.

8.3.1 Details of the numerical method

When the boundaries' normal vector coincides with the normal vector to the level set isocontours $n^{(s)}$ boundary condition (8.14) is incorporated weakly in the scheme and

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Figure 8.5: Illustration of inner and outer boundaries of a Narrow Band around a circle in 2D and a sphere in 3D, respectively. The cells of the Narrow Band are marked in grey.

only the surface integrals depending on c_h need to be discretized. This requires the use of curved boundaries that are aligned with isocontours of the Level Set function when designing the Narrow Band. An example of curved boundaries for the case of a circle and a sphere is illustrated by figure 8.5. The blue isocontour marks the outer boundary, while the red isocontour gives the inner boundary. As another important aspect, when employing curved boundaries, the boundary of the Narrow Band does not include cusps and corners, which would restrict the order of convergence. However, the numerical treatment of curved boundaries is a highly complex topic that is a separate field of research. Recently, it has become increasingly popular to embed complex domains in fixed, usually structured grids. Ficticious domain methods, generally attributed to Glowinski, Pan, and Periaux (1994), form the most original class of these methods as well as its variants, the immersed boundary (Peskin, 2002) or immersed interface methods (LeVeque and Li, 1994). One also refers to unfitted methods, when the underlying mesh does not resolve the considered subdomain and its boundaries. The use of unfitted elements has by now been introduced both in the context of FE by Hansbo and Hansbo (2002) as well as DG by Bastian and Engwer (2009). On a Cartesian structured mesh, a cut cell method is used to cut out complex subdomains and derive suitable quadrature rules. In order to avoid any explicit representation and approximation of the curved boundaries, a DG approach based on unfitted elements is employed, exploiting suitable quadrature rules. Within the context of DG, Müller, Kummer, and Oberlack (2013) have derived highly accurate quadrature rules for implicit domains, using simplified moment fitting equations.

Quadrature rules for implicit domains (Müller, Kummer, and Oberlack, 2013) Considering a convex, *D*-dimensional polytope K_j in a very general grid Ω_h , quadrature rules for integrating over zero-isocontours $I_j = \{x \in K_j : \Phi(x) = 0\}$ and partial volumes

$$A_j = \{ \boldsymbol{x} \in K_j : \Phi(\boldsymbol{x}) < 0 \}$$
 or $B_j = \{ \boldsymbol{x} \in K_j : \Phi(\boldsymbol{x}) > 0 \}$ respectively,

are constructed hierarchically. In the one-dimensional case, the roots of the Level Set function Φ are determined on the line element K_j . A standard Gaussian quadrature rule of order N is then applied to each of the induced subsections, assuming the integral to be given by a polynomial basis of order N. In the two-dimensional case, surface integrals are deduced from the intersected line integrals by means of a divergence-free basis, yielding a simplified system of moment fitting equations. Integrals over partial volumes, in turn, can be reconstructed by means of defining anti-derivatives of the polynomial basis functions in a similar fashion. Finally, the three-dimensional case is reduced to two-dimensional boundary elements. The interested reader may refer to Müller, Kummer, and Oberlack (2013) for further details.

Dealing with partial cell volumes Integration over partial cell volumes leads to ill-conditioned mass and operator matrices if cells contain relatively small volume fractions only, i.e. within this context small fractions of the Narrow Band. In fact, this case becomes inevitable when moving the interface and simultaneously the boundaries of the Narrow Band.

Numerical tests indicate that by preconditioning only, this problem cannot be resolved. However, a method developed by Kummer (2016) is adopted here, by which critical cells are agglomerated to neighbouring cells and cells with critical volumes are eliminated. Defining the fractional species volume by

$$\mathfrak{f}_{\mathfrak{A}}(K_j) = \frac{\int_{K_j \cap \mathfrak{A}} 1 d\boldsymbol{x}}{\int_{K_j} 1 d\boldsymbol{x}},$$

and setting a treshhold $0 \le \alpha < 1$ for critical cells, a list A_{α} of cell-pairs to agglomerate is identified according to the following algorithm (Kummer, 2016):

Algorithm	2 Cell	agglor	neration	algorithm	(Kummer	. 2016)
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set $A_{\alpha} \coloneqq \{\}$ for all cells $K_j \in \Sigma_h^{\gamma}$, with $\mathfrak{f}_{\mathfrak{A}}(K_j) > 0$ do if $\mathfrak{f}_{\mathfrak{A}}(K_j) < \alpha$ then select cell L_{\max}^e from all edge-neighbors L_j^e of K_j , where $\mathfrak{f}_{\mathfrak{A}}(L_j^e)$ is maximal. $A_{\alpha} \leftarrow A_{\alpha} \cup \{\{K_j, L_{\max}^e\}\}$, i.e. add the pair $\{K_j, L_{\max}^e\}$ to A_{α} end if end for Q

The polynomial space for discretizing the diffusion problem is modified on the respective pairs of cells such that the discretization is based on the finite element space

$$V_{h,\alpha}^{k} = \left\{ v \in L^{2}(\Omega_{h}) : v|_{K} \in P^{k}(K), K \in \mathfrak{T}_{h}, v|_{K \cup L} \in P^{k}(K \cup L) \text{ for } (K,L) \in A_{\alpha} \right\}.$$

Due the above requirements, the modified polynomials can be obtained by a linear combination of original basis polynomials, i.e.

$$\varphi_i = \widetilde{\varphi}_i + q(\boldsymbol{x}) \, \widetilde{\widetilde{\varphi}}_i, \text{ where } \widetilde{\varphi}_i \in P^k(L), \, \widetilde{\widetilde{\varphi}}_i \in P^k(K).$$

Thus, for linear operators, changing to the modified basis is a purely algebraic operation. Furthermore, it should be remarked that the given polynomial basis does not form an orthonormal set with respect to partial cell volumes. Kummer (2016) showed that, with respect to the linear case, a transformation to an orthonormal basis can be achieved by a simple Jacobi preconditioning.

Within the present work the extended transport equation without diffusion in conserved form (8.5) is discretized by an Eulerian DG scheme on a Narrow Band with implicitly defined boundaries. The constructed method takes advantage of the aforementioned elements when creating and processing operator and mass matrices. Quadrature rules for partial cell volumes based on hierarchical moment fitting (Müller, Kummer, and Oberlack, 2013) are exploited when implementing artificial boundary conditions on these implicit boundaries. Cells with critical volumes are eliminated by the cell agglomeration algorithm. In this way, operator matrices achieve condition numbers that admit the solution of the matrix system.

A code library for discretizing and solving the extended form of the surface diffusion problem has been developed within this thesis and is integrated in the software framework Bosss. Figure 8.6 gives and overview of the structure and functionality of the new classes.

8.3.2 Numerical Results

This section accounts for numerical results of solving the interfacial diffusion equation by the Eulerian algorithm developed in this work.

In the two-dimensional problems that are analysed, the polynomial basis that is used for discretizing the Level Set function Φ is always chosen one degree higher than the polynomial basis used to approximate the density variable Ψ . Tests are given for polynomial orders 1 and 2, as for zero-order polynomials, the boundaries cannot be accurately resolved,

The subsequent computations are based on different polynomial degrees on equidistant Cartesian meshes. Numerical errors are computed for the actual concentration variable c with respect to exact solutions c_{ex} of the surface concentration by formula (8.6). Here, both L^2 error estimates on the Level Set isocontour as well as the surface integrals on the inner and outer boundary isocontours are constructed using hierarchical moment



Figure 8.6: Structure of the Bosss application by which the diffusion problem is solved and discretized.

fitting quadrature rules of order eight, which have been provided by Müller, Kummer, and Oberlack (2013).

As the curved domain of the extended problem is resolved by a cut cell approach, small fractions of the cells at the boundaries of the Narrow Band lead to severely high condition numbers of the mass and operator matrices, in particular for a second order polynomial basis. Condition numbers are improved by employing a cell agglomeration treshhold of five percent. But nevertheless, it is a trade off by which accurary is lost with eliminated quadrature nodes. Finally, the resulting matrix system is preconditioned by a Jacobi preconditioner and solved by means of the sparse direct solver Schenk and Gärtner (2014).

The penalty parameter τ is chosen dependent on the grid size *h*:

$$\tau = \kappa/h, \kappa > 0,$$

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For a given initial concentration, sets of solutions to the purely diffusive equation can be generated in a similar fashion as in the three-dimensional case. In polar coordinates (r, φ) the surface diffusion equation in non-dimensional form on a circle of radius r_0 is given by

which is suggested for example by Arnold, Brezzi, Cockburn, and Marini (2002). Numerical experiments indicated an optimal performance for $\kappa = 10.0$ for the following

$$\frac{\partial c}{\partial t} - \frac{1}{\operatorname{Pe}^{(\mathfrak{s})}} \frac{\partial^2 c}{\partial \varphi^2} = 0.$$
(8.16)

Applying separation of variables, it is assumed that

$$c(t,\varphi) = \sum_{k} T_{k}(t) F_{k}(\varphi), \qquad (8.17)$$

where T_k and F_k are solutions of the ODEs

$$\frac{T'_k(t)}{T_k(t)} = -\lambda_k^2 = \frac{1}{\operatorname{Pe}^{(\mathfrak{s})}} \frac{F''_k(\varphi)}{F_k(\varphi)}.$$
(8.18)

In fact, the functions F_k represent Eigenfunctions of the surface Laplacian. Their general form is, on r_0 ,

$$F_k(\varphi) = C_{1,k} \sin\left(\lambda_k \sqrt{\operatorname{Pe}^{(\mathfrak{s})}}\varphi\right) + C_{2,k} \cos\left(\lambda_k \sqrt{\operatorname{Pe}^{(\mathfrak{s})}}\varphi\right), \tag{8.19}$$

with suitable constants $C_{1,k}$ and $C_{2,k}$. The functions T_k are simply provided by $T_k(t) = \exp(-\lambda_k^2 t)$. Requiring that $\lambda_k \sqrt{\operatorname{Pe}^{(\mathfrak{s})}}$ is an integer, one can apply angular summation rules to the trigonometric functions which yields a polynomial basis on the circle. For this reason, arbitrary initial values can be decomposed by a set of suitable eigenfunctions F_k .

An initial (dimensionless) distribution provided by $c(\varphi) = \cos^2(\varphi)$ can be decomposed using the Eigenfunctions

$$F_1(\varphi) = C_{1,1}$$
 and $F_2(\varphi) = C_{2,2} \cos(2\varphi) = C_{2,2} \left(\cos^2(\varphi) - \sin^2(\varphi)\right)$

with $\lambda_k \sqrt{\operatorname{Pe}^{(s)}} = 2$ and requiring $C_{1,1} = C_{2,2}$.

This yields the solution

$$c(\varphi,t) = \frac{C_{1,1}}{2} + \frac{C_{1,1}}{2} \left(\cos^2(\varphi) - \sin^2(\varphi)\right) \exp\left(-4t/\operatorname{Pe}^{(\mathfrak{s})}\right)$$

with a constant to be determined from the total saturation as follows:

$$\int_0^{2\pi} c(\varphi, t) r_0 \, d\varphi = r_0 \, \pi \, C_{1,1} \stackrel{!}{=} \pi \, r_0 \Rightarrow C_{1,1} = 1.$$

computations presented.



Figure 8.7: Relative surface L^2 -errors and order of convergence for the diffusion on a circle without signed distance property. The initial extended concentration is x^2 , the error is measured after 10000 timesteps of size 0.00001. On the left, the same polynomial basis has been used for both the density variable and its derivatives of the concentration variable. On the right, the derivatives of *c* are resolved by polynomials of one degree less. The width of the Narrow Band is 3 *h*.

This sample problem has been employed to compute the order of convergence of the method developed, when the Level Set function is polynomial and the Narrow Band defined as suggested above. The upper row in figure 8.7 illustrates the relative errors, evaluated at time $\overline{T} = 0.1$, for polynomial degrees 1 and 2, when starting with an initial concentration of x^2 .

On the left, the same polynomial order has been employed both for the density variable, and for the derivatives of the original concentration. This choice has been motivated by the fact that the derivative is linked to the density variable by scaling with the surface area element, which is not necessarily polynomial. The slopes of the resulting linear regression lines are 1.67 for a first order discretization, and 2.53 for second order polynomials. Results for mixed order polynomials are displayed on the right, and the slopes of regression lines are 1.62 for first order polynomials, and 2.6 for second order polynomials. As a second test case, the diffusion of a constant initial concentration on an ellipse is investigated, i.e. a problem with a steady solution over all time steps. The problem is discretized by polynomial bases of degree 1 and 2 and the Narrow Band has width 3 h.

The relative errors after 1000 time steps of size 0.0001 are depicted by figure 8.8. The diagram illustrates the numerical error when the initial concentration is given by the Level Set function itself, i.e. by a second order polynomial $c_0 = 2.0 - x^2/a^2 - y^2/b^2$. The



Figure 8.8: Results of the diffusive problem on an ellipse for the steady solution $c_0 = 2.0 - x^2/a^2 - y^2/b^2$. The width of the Narrow Band is given by 3 h.

resulting slopes of the computed regression lines are 1.44 for polynomial degree 1, and 3.62 for degree 2. To conclude, some examples of three-dimensional computations of unsteady surface transport without convection are illustrated by figures 8.10 and 8.9.

Figure 8.10 depicts the numerical solution of the unsteady transport problem without convection on a slightly modified Enzensberg star surface, showing how the developed method can be easily applied to topologically more complex surfaces. The surface is embedded by the Level Set function

$$\Phi = 75\left(x^2y^2 + y^2z^2 + x^2z^2\right) - \left(0.5 - x^2 - y^2 - z^2\right)^3 - 40,$$

scaled by a factor 0.01. The density variable is discretized by first order polynomials, while the Level Set function is resolved by fifth order polynomials. Starting with an initial distribution of $c_0(x) = x^2/(x^2 + y^2 + z^2)$, with evolving time, the solution diffuses uniformly on the surface, as expected.

Figure 8.9 illustrates the numerical solution of the purely diffusive problem on a cube for various timesteps, indicating that the presented method is even suitable for surfaces with edges. The implicit time stepping scheme starts from an initial distribution that is given by the Level Set function of the previous problem, i.e. $c_0 = 75 (x^2y^2 + y^2z^2 + x^2z^2) - (0.5 - x^2 - y^2 - z^2)^3 - 40$, and generates a concentration that diffuses uniformly with proceeding time.

The presented results show that the diffusive surface transport problem is successfully discretized and numerically solved by the method developed in the context of the present work. The method has been investigated for first and second order polynomial bases with respect to the density variable. The method has also proven suitable for the

numerical solution of the diffusive transport on complex surfaces and surfaces with corners. With respect to accuracy, in the two-dimensional results presented, raising the polynomial degree by one results in an increase of the order of convergence by one, which meets the expectations of a DG scheme.

Orders of convergence of most of the computed numerical errors are suboptimal, though. This can be explained by different influence factors.

First, numerical accuracy is of interest on the surface itself where the grid refinement imposes a proportional increase in degrees of freedom. Correspondingly, L^2 -errors on the surface itself have been considered in the present investigation. On the Narrow Band, however, where the extended equation is solved numerically, a grid refinement does not impose the same proportional increase. For this reason, convergence rates based on the error on the surface may be lower than errors measured in the Narrow Band cells. In fact, the contraction of the Narrow Band for each grid size influences the band width and condition number of the computational matrix. The impact factor both of cells with partial volumes and of artifical boundaries increases. At the same time, the relation of the total number of degrees of freedom employed in the computation to the degrees of freedom that can be associated with the zero-isocontour of the Level Set decreases.

Second, the cell agglomoration introduces a certain inaccuracy with all of the test problems. As the boundaries of the Narrow Band are distinct for each grid partitioning, this inaccuracy is unevenly distributed for different grid sizes, in particular for second order polynomials. This fact causes a notable deviation of data points from the regression lines. The presence of partial cell volumina has another negative impact. The penalty parameter employed in the Brezzi scheme depends on the grid size, which cannot be accurately determined for cells with partial volumina.

Futhermore, when approximating the problem by second order polynomials, accuracy is notably higher for the steady settings. This behavior may be attributed to the simple first order time stepping scheme. A second order multistep method ought to raise accuracy for the unsteady case. Nevertheless, in the presence of variable coefficients and an alternating and evolving computational domain, multistep methods are intricate to implement.

Surface Transport Equations including both Convec-8.4 tion and Diffusion

The complete convection-diffusion equation is treated by a first order differential operator splitting scheme. Its implementation is based on the simplest form of the conservation laws constructed in Chapter 5, i.e. on equation (5.27), given by

$$\frac{\partial}{\partial t} \left(c \| \nabla \Phi \| \right) + \nabla \cdot \left(\boldsymbol{u} \, c \| \nabla \Phi \| \right) = \frac{1}{\operatorname{Pe}^{(s)}} \nabla \left(\| \nabla \Phi \| \left(\boldsymbol{P}^{(s)} \nabla c \right) \right) \text{ in } \Sigma_h^{\gamma}.$$
(8.20)

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The operator splitting discretizes the diffusive part by an implicit scheme, and the convective part by an explicit scheme. Both methods presented in the previous sections are essential to the operator splitting, as they constitute the fundamental tools for treating the split equation. The algorithm for performing timestep k + 1, i.e. computing the numerical solution at time t^{k+1} is structured as follows:

- 1. The Level Set equation is solved first, yielding $\Phi_h(t^{k+1})$ from $\Phi_h(t^k)$. Based on the updated Level Set function $\Phi_h(t^{k+1})$ of the interface, the Level Set functions embedding the implicit boundaries, $\Phi_h^{In}(t^{k+1})$, $\Phi_h^{Out}(t^{k+1})$ are computed, by shifting the function $\Phi_h(t^{k+1})$ by the band width. In this way, the new Narrow Band is obtained.
- 2. As the underlying curved domain of the diffusive part of the equation has been updated within the current timestep, an extension of the density variable $\Psi_h(t^k)$ is necessary. Values in the outer cells of the Narrow Band are deleted before performing an extension of the interfacial values to the entire Narrow Band. The extension is obtained by performing a suitable number of pseudo-timesteps in the PTM.
- 3. The convective part of the equation, given by equation (8.4), discretized by an explicit scheme, is solved for the density variable $\Psi_h(t^{k+1/2})$ by applying the scheme presented in Section 8.2 and using $\Psi(t^k)$ as an initial value. Note that, for the temporal discretization, the time step size is still given by $dt = t^{k+1} t^k$.
- 4. The diffusive part, given by equation (8.5), is discretized in time by an implicit scheme, is solved for the density variable $\Psi(t_{k+1})$ by the algorithm presented in Section 8.3. The density variable yields the concentration variable $c(t_{n+1})$ of the current timestep. As a remark, note that the Level Set function of the surface, as well as quantities depending on the Level Set function are not updated in the intermediate step, as only the diffusion operator depends on the updated Level Set function.

This chapter on numerical results is rounded off by some 2D-examples of the convectiondiffusion problem. The first example is illustrated by figure 8.11. A tangential velocity field imposes a counterclockwise rotation of the circle, i.e. the surface remains steady. The computation starts with an initial concentration

$$c(x,y) = 4.0 x y \frac{(x^2 - y^2)}{(x^2 + y^2)},$$

with a diffusion coefficient of 0.1 and 50 pseudo-timesteps of re-extension after each timestep. With proceeding time, the concentration profile is rotated in counterclockwise direction and diffuses continuously.

In a second example illustrated by figure 8.12 a small deformation is imposed on the initially circular surface by the velocity field $u = (\cos(x), y \sin(x))$. The computation starts from the initial concentration

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$$c(x,y) = r - 0.75 + \left(8.0 x y(x^2 - y^2) \frac{((x^2 - y^2)^2 - 4.0 x^2 y^2)}{r^8}\right) \sin(1.0)(r - 0.5)(1.0 - r),$$

where $r = \sqrt{x^2 + y^2}$ and is performed 150 timesteps of size dt = 0.001. The underlying domain is discretized by a Cartesian mesh consisting of 30×30 grid cells, the density variable by third order polynomials and the Level Set function by forth order polynomials. After the computation of each time step, a re-extension is achieved by performing 10 timesteps. This example shows that the method also supports the use of polynomial bases of degrees higher than two. Furthermore, the method may indeed applied to problems that include convection and diffusion on an unsteady, deforming surface. A numerical error analysis has not been performed yet and should be employed in order to investigate the influence of different factors, such as width of the band, choice of the penalty parameter and the influence of the pseudo-timestepping scheme.

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Figure 8.9: The purely diffusive problem on a cube is solved by the Eulerian DG approach, indicating that the presented method is even suitable for surfaces with edges. Starting from an initial distribution $c_0 = 75 (x^2y^2 + y^2z^2 + x^2z^2) - (0.5 - x^2 - y^2 - z^2)^3 - 40$, the concentration diffuses uniformly on the non-smooth surface. The cube itself is represented by a Level Set function, resolved by polynomials of degree five. The illustrated solution is based on first order polynomials, a grid resolution given by 2700 cells.



(c) Solution at t = 0.2

(d) Solution at t = 0.5

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Figure 8.10: The purely diffusive problem on Enzensberg's stern surface is numerically solved by the Eulerian DG approach. For the discretization of the density variable, first order polynomials are employed, the Level Set function is resolved by fifth order polynomials. The computational grid given by 2700 cells and a diffusion coefficient equal to one. Starting with an initial distribution of $x^2/(x^2 + y^2 + z^2)$, with evolving time, the solution diffuses uniformly on the surface, as expected.



(e) Concentration after 200 timesteps

(f) Concentration after 250 timesteps

Figure 8.11: Solution of the surface convection-diffusion problem on a Narrow Band around a circle, which is indicated by the isocontour in black. The tangential velocity field causes a counter-clockwise rotation, the diffusion coefficient is given by 0.1. The equation is discretized by second order polynomials for the density variable on 900 grid cells.



(e) Concentration after 120 timesteps (f) Concentration after 150 timesteps

Figure 8.12: Solution of the surface convection-diffusion problem on a Narrow Band around a circle, which is indicated by the isocontour in black. The velocity field causes a slight deformation of the circle, the diffusion coefficient is given by 0.05. The equation is discretized by third order polynomials for the density variable on 900 grid cells.

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8.5 Interfacial transport Stokes flow around a spherical droplet

To conclude this work, the presented forms of interfacial surfactant transport equations are solved numerically for a Stokes flow around a spherical bubble. This corresponds to the setting described in chapter 6. In the results presented, a steady flow field is prescribed, i.e. the problem is not coupled to any numerical solution of the Stokes equations. Both the exchange of surfactant with the bulks and the influence on surface tension are neglected, i.e. the flow field given by identities (6.3) and (6.2) is assumed to remain unchanged. The viscosities have been chosen to present an air bubble in water (at a temperature of 20° and a pressure of 1 bar), i.e. $\eta^i = 0.018m \operatorname{Pa} s$ and $\eta^o = 1.0m \operatorname{Pa} s$.

8.5.1 Purely diffusive transport

The first numerical example is given by the diffusion-dominated form of the interfacial transport problem. A diffusion coefficient equal to one is assumed. Figure 8.13 illustrates a numerical solution at different time steps which has been obtained by a first order polynomial approximation on a computational computational grid of 2700 Cartesian cells. Figure 8.13 visualizes the evolution of the surfactant concentration profile along the θ -coordinate for a fixed value of the azimuthal angle $\varphi = 0$. The numeric solution for an initial distribution of $\cos(\theta)^2$ is plotted in blue, while the black dotted line indicates the numerical solution presented in section 6.3.3.

The numeric solution remains symmetric with respect to the axis given by $\theta = 0$, i.e. the equator of the sphere, where it assumes its minimum. The curves of the exact and the numerically computed solutions appear to be nearly identical for different time steps. With evolving time, the curve flattens and the numerical solution approaches the neighbourhood of 1/3, which is the exact steady solution derived in section 6.3.3.

8.5.2 Surfactant transport including advection

Next, the interfacial transport problem is considered for large Péclet numbers due to a low diffusion coefficient. In this case, the diffusivity of the surfactant can be neglected and the transport equation is purely convective.

This is a setting characteristically assumed in stagnant cap models, considered, for instance, by Sadhal and Johnson (1983), Johnson and Sadhal (1983), or Harper (1982). The transport problem is numerically discretized by the scheme presented in section 8.4, using second order polynomials in a domain of $30 \times 30 \times 30$ Cartesian grid cells.

Figure 8.14 illustrates how the surfactant is driven to the cap opposed to the inflow, starting with a uniform and constant initial distribution. For illustration, the surface of the drop is colored by the computed surface excess concentration. More in detail, figure 8.15 depicts the evolution of the surfactant concentration profile along the θ -coordinate for a fixed value of the azimuthal angle $\varphi = \pi/4$.



Figure 8.13: The purely diffusive problem is solved by the Eulerian DG approach presented in this thesis, starting with an initial distribution of $\cos(\theta)^2$. The numerical solution along the θ -coordinate is represented by the blue plot. It fits well with the exact solution derived in section 6.3.3, which is indicated by the black dotted line for comparison.

The concentration develops a profile which is also characteristic in stagnant cap models. Surfactant molecules are swept from the inlet to the back of the droplet, i.e. its minimum is found at the inlet ($\theta = \pi$). It accumulates around the rear end of the drop (i.e. $\theta = 0$) where it obtains its maximum. This setting is computationally important when intending to solve the stagnant cap model by considering additional surfactant exchange with the bulks. To conclude, the surface diffusion coefficient is modified with a resulting Péclet number of 0.2, such that the interfacial surfactant transport including both advection and diffusion is solved numerically. The problem has been discretized by first order polynomials in a domain of $30 \times 30 \times 30$ grid cells and second order polynomials for the Level Set function. A re-extension of 10 pseudo-timesteps (with a step size of 0.001) is performed after each time step.

The numerical solution is depicted by figure 8.16 illustrates the characteristic surfactant distribution in the given setting which has been described in 6. As in the previous

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Figure 8.14: Surfactant transport without diffusion on a rigid sphere in a Stokes flow setting without exchange with the bulks. Characteristically, starting from a uniform distribution, the surfactant is driven to the pole opposed to the inlet of the flow. The problem has been discretized by second order polynomials in a domain of $30 \times 30 \times 30$ grid cells.



Figure 8.15: Numerical solution of the interfacial transport on a rigid sphere in a creeping flow setting without diffusion. The plot shows the profile of the surface excess concentration at $\varphi = \pi/2$, along the polar angle using a cubic interpolation.

example, starting from a uniform distribution, the surfactant molecules are swept to the rear end of the droplet, i.e. to the pole opposed to the inlet of the flow, where surfactant concentration attains its maximum. With evolving time, it approaches the steady solution that has been derived in Chapter 6, marked by the black dotted line.

Comparing this setting (Pe = 50) with the previously shown case of Pe = 0, it can be clearly noticed that the extremal points of surface excess concentration of the surfactant are less distant from the curve, which is attributed to the effects of diffusion.

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Figure 8.16: Numerical solution of the interfacial transport on a rigid sphere in a creeping flow setting without exchange with the bulks. The plot shows the profile of the surface excess concentration at $\varphi = \pi/2$, along the polar angle using a cubic interpolation.

9 Conclusion

Processes that are governed by PDEs on surfaces, or on more general submanifolds, appear in various areas of research. The need to numerically simulate these processes motivates the computational solution of surface differential equations, and hence, the subject of this work. Examples may be found in image processing, biochemistry, and fluid mechanics and other fields of research. With a focus on fluid mechanics, the interest of the present work is motivated by transport processes on phase interfaces, for instance, the transport of surface active substances, such as soaps or emulsifiers.

The transport of solute on two-phase interfaces requires a specific numerical treatment of convection-diffusion equations defined on surfaces that may change rapidly with respect to geometry or topology. In the numerical context, this is the most complex type of surface differential equation, as the problem domain may be both moving and deforming. The surface differential operators involved in the interfacial transport equation require a thoughtful approximation that is distinct from the available discretizations of standard differential operators. Evolving interfacial physical quantities, such as surfactant concentration, along a moving deformable surface is a highly challenging task.

For some decades, numerical algorithms for discretizing and solving surface differential equations have mimicked the numerical algorithms available for the solution of standard differential equations in topologically simple domains. Surfaces have been tracked by Lagrangian grids and surface differential equations resolved in a locally parametric form by all standard methods ranging from finite differences over finite volume to finite element methods. However, it has been realized that algorithms based on Lagrangian methods reach their limits in fluid mechanical applications. Against this background, in recent years, research on solving surface or interfacial problems has entered new paths, attempting to pursue an Eulerian discretization. As a striking advantage of this Eulerian approach, an implicit representation of the interface by a Level Set function can be maintained. Traditional Lagrangian methods, in contrast, require a tedious reconstruction of the interfacial mesh and, when considering additional exchange with the bulk phases, a resolution of an adapted mesh for the bulk phases that is aligned with the interface.

The method developed in the present thesis does **not** hold on to traditional Lagrangian approaches and does **not** treat interfacial transport problems by establishing an interfacial grid. Instead, it is inspired by these novel ideas and attempts to treat interfacial

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problems on the basis of the given Eulerian grid. To the author's knowledge, in this context, it is the first Eulerian method that uses a Discontinuous Galerkin (DG) scheme for solving interfacial convection-diffusion equations. In this way, it incorporates favorable features of both the Finite Element (FE) and the Finite Volume (FVM) methods by combining polynomial approximations of arbitrary order with the use of numerical fluxes to approximate integrals over the cell boundaries.

In the Eulerian approach employed here, surface differential operators are expressed in terms of global derivatives. The surface differential operators are identified with the parts of standard differential operators tangential to the surface, or interface, respectively, using the surface projection tensor. All interfacial physical quantities, such as the surfactant concentration, which are only defined along the interface, are extended off the interface into a higher dimensional domain. The interface \mathfrak{S} itself is captured implicitly as the zero-isocontour of a Level Set function Φ , which is advected by the fluid flow. In this context, the surface normal $n^{(s)}$ is obtained by the normalized gradient of the Level Set function.

To reduce the amount of computational cost caused by the additional dimension, computations are restricted to a small subgrid only. These selected cells form a tube around the interface, which is called the Narrow Band. In this way, sufficient regularity of the Level Set function ($\nabla \Phi \neq 0$) is assured. The extended physical quantities are then evolved in this Narrow Band. Thus, the evolution of the physical quantity investigated along the interface (zero level-set contour) is embedded in the evolution of the extended quantity in the Narrow Band. As an advantage of this approach, the evolution of the extended physical quantity can be easily performed using standard numerical methods on the same Eulerian grid that is used for the computation of the flow field. No further explicit discretization of the interface is necessary.

The Narrow Band itself continuously moves or deforms along with the Level Set function, and therefore, it is not created as an independent physical grid, but it is rather induced from the full computational domain. In the method presented, the restriction of discrete quantities is achieved through a selective storage allocation and extraction of the degrees of freedom associated with the cells that are included in the Narrow Band. In particular, this approach takes advantage of the local band structure of the matrices in a DG approximation. Provided that numerical fluxes are suitably defined, for each cell in the Narrow Band, only those matrix blocks of the operator matrix need to be considered that are associated with the cell itself, or with its neighbouring cells.

In the Eulerian formulation, however, the conserved form of the interfacial balance law is destroyed by the extension of the interfacial differential equation to the threedimensional domain. This fact has been identified as an obstacle at the initial project phase. From the viewpoint of numerical accuracy, the conserved form of a differential equation is always favorable to reduce numerical errors and preserve the quantity numerically. As one achievement of the present work, infinite sets of conservation laws have been discovered by using the direct construction method, i.e. by applying local conservation law multipliers (Kallendorf, Cheviakov, Oberlack, and Wang, 2012). The obtained families of conservation laws yield a fully conserved form of the system

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of equations under consideration. This involves the continuity equation and the Level Set equation, which are naturally in conserved form for incompressible flows, and the surface transport equation in extended form, both with and without diffusion. In particular, each equation becomes a divergence-type conservation law. The conserved forms obtained for surfactant transport dynamics equations were further generalized in section 5.3.3 to provide conserved forms of the source-free transport equation (5.5) of any excess surface physical quantity, where the non-convective flux is tangential to the surface.

These conserved forms constitute a well-suited basis for discretizing the interfacial transport equation by a DG scheme, while maintaining an implicit representation of the interface. Within the scope of this work, simplest forms of the conservation laws discovered replace the interfacial transport problem and are then treated by an Eulerian DG approach. The convection-diffusion equation is discretized by a simple operator splitting scheme, which motivates to solve the purely convective and the purely diffusive parts of the conserved form independently. In fact, both the convective and the diffusive part of the conservation law correspond to the conserved forms of the purely convective and purely diffusive interfacial equations.

In the present work, an MPI parallelized and modular package for the numerical simulation of interfacial transport problems has been designed. The library, developed in C#, discretizes interfacial convection, diffusion as well as convection-diffusion equations by a DG method, and is integrated into the existing software framework *BoSSS* Kummer (2012).

Subsequently, computational examples of all of the three forms of surface transport equation are developed and solved for both two-and three-dimensional underlying domains. Based on exact solutions to the two-dimensional examples, a study of convergence is presented for first and second order polynomial bases, where the purely convective equation, both on a steady and on a moving surface, as well as the purely diffusive equation on a steady surface are considered. In addition, in the case without diffusion, a study of convergence is also provided for zeroth order polynomials. Illustrations of sample problems are provided for problems of all mentioned complexities, i.e. for steady, but complex, moving as well as moving and deforming surfaces.

Against the background of the numerically computed results, the constructed Eulerian DG method can be assessed in detail as follows.

New opportunities have opened to treat purely convective surface transport problems easily, by discretizing a plain convection equation on the basis of the Eulerian grid. The concentration is then linked to the computed density variable by scaling with the surface area element, obtained from the Level Set function. The purely convective interfacial transport is of practical relevance in applications where diffusion is generally neglected, for instance, in case of the stagnant cap model. Furthermore, operator splitting techniques generally require the solution of the convective part of the problem in the explicit time step. The DG method, in contrast, is not only able to handle purely convective equations, but also supports using polynomial bases of arbitrarily high polynomial degrees. Errors computed for the test cases considered indicate that the presented scheme achieves optimal order of convergence ($\mathcal{O}(h^{p+1})$) for zero, first and second order polynomial bases.

The implementation of the diffusive part, in contrast, is a more challenging task. For one part, the constructed conservation laws additionally involve the tangential gradient of the concentration, which requires a treatment of variable coefficients in a second order problem and additionally causes the problem to degenerate in normal direction. Furthermore, the lack of physical boundary conditions constitutes a clear challenge. Inspired by a method presented by Dziuk and Elliott (2009), the author utilised a natural boundary condition, demanding that the tangential gradient does not yield any flow in orthogonal direction to the Level Set isocontours. This simple requirement, however, involves curved boundaries, given by isocontours of the Level Set function, parallel to the actual surface, or interface, respectively. The solution of the purely diffusive problem has been discretized by basis polynomials up to second order. It needs to be remarked that, in a similar fashion, Dziuk and Elliott (2009) use unfitted finite elements that adapt with a moving, three-dimensional Narrow Band around the interface for discretizing the Eulerian form of the interfacial transport equation. Deckelnick, Dziuk, Elliott, and Heine (2010), however, fail to generalize their approach to polynomial degrees greater than one. The authors point out to the fact that the degenerate conditioning of the matrices can be removed by diagonal preconditioning only for piecewise linear basis polynomials, while it is not as easily treated in the case of higher order unfitted elements. In this respect, the method developed within the present work constitutes a significant improvement. Furthermore, although both approaches employ the same boundary conditions, the discretization by unfitted finite elements presented by Elliott and Dziuk approximates the boundaries of the Narrow Band only linearly, while arbitrary polynomial orders may be used for resolving boundaries in the method presented in this thesis. When discretizing by first order polynomials, numerical tests indicate optimal order of convergence, while for some of the examples, an approximation by second order polynomials is slightly suboptimal. It may be concluded that in this case, further effort needs to be invested in order to optimize condition numbers of the operator matrix in presence of the partial cell volumina. Nevertheless, it should be pointed out that a second order discretization of the surface transport is an accomplishment not achieved by other authors. Beyond, it is illustrated that the method can be applied to surfaces with kinks, such as a cube, and surfaces of more intricate topology.

Finally, the complete convection-diffusion equation can be treated by employing a first order differential operator splitting, where the diffusive and convective parts of the equation are discretized by the previous schemes. Some 2D-examples are given for the performance of the method; an error analysis is yet to be performed. As the Level Set function moves and deforms with each time step, both the implicit boundaries of the curved, computational domain and the Narrow Band move and deform. For this reason, the computational, i.e. the density, variable, needs to be extrapolated to new grid cells in the Narrow Band, or re-extended within the boundary cells, respectively, while being conserved on the interface itself. For this purpose, a pseudo-timestepping scheme is adopted, and a new LDG fashioned DG discretization is presented. In contrast to a constructive extrapolation of interfacial values, for instance, by a closest point approach, this method is suitable in a multi-processing environment. With respect to the conservation of the variable on the interface, numerical experiments indicate a nearly optimal order of convergence for zero, first and second order polynomial bases with respect to the conservation of the variable on the interface. The pseudotimestepping scheme achieves a slightly better order of convergence than a Closest Point approach. In contrast, it is suitable for variable widths of the Narrow Band, and most importantly, it can be easily applied in a multi-processing computation. Numerical results are concluded by a simulation of the interfacial convection-diffusion transport on a spherical surface in a two-phase immiscible incompressible Stokes flow are developed.

Within this context, exact solutions are developed (Kallendorf, Fath, Oberlack, and Wang, 2015). In the present investigation, the deformation of the droplet, the Marangoni effect as well as surfactant exchange with the bulks have been neglected. In contrast to known previous results, unsteady surfactant transport on the interface that includes diffusion, or is even dominated by diffusion, is covered. With respect to the most general form of the equation, the surface excess concentration derived here combines exponential functions with Heun's confluent functions. Consequently, general properties can be concluded, as, in particular, the steady state solution to the problem. Furthermore, solutions to the purely diffusive equation can be constructed using Legendre polynomials. In a potential further investigation, when the Marangoni effect, i.e. the influence of surfactant on surface tension and thereby on the flow field, is taken into account, the set of solutions to the unsteady interfacial transport obtained in the present study can be employed as the base state. In a setting with large Biot numbers, i.e. when the ratio of surfactant exchange with the bulk phases is high, or when the Marangoni number is small, approximative analytic solutions can be achieved by a perturbation analysis.

Like other research works pioneering a new method, the present work is focussed on the construction and performance of the numerical algorithm and cannot cover the application that has motivated its development. From the practical point of view, interfacial transport equations, for instance, of surfactant, can be successfully discretized and solved by the Eulerian DG method introduced. For physical relevance, a coupling to a two-phase DG solver by considering a surfactant dependent surface tension is still necessary. In fact, the numerical simulation of two-phase flows by a Level Set DG method is still a topic of on-going research. In a first step towards the physical model, the present method may be applied to models of soluble surfactants, i.e. by coupling the interfacial transport equation (2.46) to the transport equation in the bulks (2.45) through the source term (2.47) and identity (2.48). The transport problem in the bulk itself can be discretized by standard DG methods (i.e. LDG or IP-methods for the diffusive part), while boundary condition (2.48) on the Level Set isocontour can be incorporated in the same fashion as condition (8.14) on the boundary of the Narrow Band.

Other processes which are governed by surface PDEs have been stated in the introduction, such as denoising, deblurring and smoothing in image processing or morQ

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phogenesis in biochemistry. Processing image data obtained from 3D scans involves the solution of surface differential equations. For instance, smoothing of image data can be achieved by solving a surface diffusion equation, which describes the gradient descent flow of harmonic energy. In recent years, there has been some research on this topic based on a Level Set representation of the interface, for example, in brain imaging, see also Mémoli, Sapiro, and Thompson (2004). In this context, the present method may be applied. Models of morphogenesis have been used to investigate the growth of distinct organisms' structures. In the simplest model developed by Cummings (1989), an axisymmetric growth, starting from an initial spherical shape is considered and has been further developed by Leung and Berzins (2003b). The surface evolution of the pair of morphogenes is given by surface reaction-diffusion equations with linear source terms. These equations can be treated by the method presented here, as the simplest conservation law of the purely diffusive problem holds for unsteady surfaces, even in absence of the convective term. Changes in the concentration of these chemical compounds then induce a growth of the surface structure because Gauss and mean curvatures are assumed to be functions of the morphogene concentrations. With respect to the present method, the surface evolution needs to be resolved by finding an intelligent way for constructing a Gauss and mean-curvature dependent Level Set.

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A Appendix

A.1 Point Symmetries of the Surfactant Transport Equations

In the current section, standard notation is used to denote symmetries. For details, see Bluman, Cheviakov, and Anco, 2010 or any text on symmetries of differential equations. These results have been given by A.Cheviakov in Kallendorf, Cheviakov, Oberlack, and Wang, 2012.

1. The case of no diffusion, $\alpha = 0$. In this case, the surfactant transport equations (5.14) have an infinite set of point symmetries spanned by the following families of infinitesimal generators.

• Translations in space and time:

$$X_j = \frac{\partial}{\partial x^j}, \quad j = 1, 2, 3; \qquad X_4 = \frac{\partial}{\partial t}$$

• Dilations

$$\mathbf{X}_5 = t\frac{\partial}{\partial t} + x^i \frac{\partial}{\partial x^i}.$$

• Generalized scalings

$$X_6 = h_1(\Phi) \frac{\partial}{\partial \Phi}, \quad X_7 = h_2(\Phi) c \frac{\partial}{\partial c}, \quad X_8 = f(t) \frac{\partial}{\partial t} - f'(t) u^i \frac{\partial}{\partial u^i}.$$

• The Galilean group

$$X_9 = g_1(t)\frac{\partial}{\partial x^1} + g_1'(t)\frac{\partial}{\partial u^1}, \quad X_{10} = g_2(t)\frac{\partial}{\partial x^2} + g_2'(t)\frac{\partial}{\partial u^2}, \quad X_{11} = g_3(t)\frac{\partial}{\partial x^3} + g_3'(t)\frac{\partial}{\partial u^3}$$

• The generalized rotation around the x^3 axis , given by

$$X_{12} = k_1(t) \left(x^2 \frac{\partial}{\partial x^1} - x^1 \frac{\partial}{\partial x^2} + u^2 \frac{\partial}{\partial u^1} - u^1 \frac{\partial}{\partial u^2} \right) + k_1'(t) \left(x^2 \frac{\partial}{\partial u^1} - x^1 \frac{\partial}{\partial u^2} \right),$$

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and the corresponding generalized rotations around the axes of x^1, x^2 given by X_{13}, X_{14} involving arbitrary functions $k_2(t), k_3(t)$ and cyclic index permutations $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$. [The generalized rotations X_{12}, X_{13}, X_{14} include usual rotations when the corresponding $k_i(t) = 1, i = 1, 2, 3$.]

In the above generators, f(t), $g_i(t)$, $h_i(t)$, $k_i(t)$ are arbitrary functions.

2. The case of nonzero diffusion, $\alpha \neq 0.$

In the case when the surface diffusion is present, $1/\text{Pe} = \alpha \neq 0$, the surfactant transport equations (5.23) also have an infinite set of point symmetries, spanned by the following infinitesimal generators:

$$X_1, X_2, X_3, X_4, X_6, X_7, X_9, X_{10}, X_{11}, X_{12}, X_{13}, X_{14},$$

from above, and an additional scaling symmetry

$$\mathbf{X}_{15} = 2t\frac{\partial}{\partial t} + x^i\frac{\partial}{\partial x^i} - u^i\frac{\partial}{\partial u^i}.$$

[Note that symmetries X_5 and X_8 hold when $\alpha = 0$ but do not hold when $\alpha \neq 0$.]

Curriculum Vitae

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