Local Discontinuous Galerkin Methods for Phase Transition Problems

Lulu Tian

田
璐
璐

**LOCAL DISCONTINUOUS GALERKIN
METHODS FOR PHASE TRANSITION
PROBLEMS**

Lulu Tian

Graduation committee:

Chairman:

prof. dr. P.M.G. Apers University of Twente

Promotors:

prof. dr. ir. J.J.W. van der Vegt University of Twente
prof. dr. J.G.M. Kuerten Eindhoven University of Technology/
University of Twente

Members:

prof. dr. H.J. Zwart University of Twente
prof. dr. ir. H.W.M. Hoeijmakers University of Twente
prof. dr. ir. B. Koren Eindhoven University of Technology
prof. dr. ir. E.H. van Brummelen Eindhoven University of Technology
prof. dr. A.E.P. Veldman University of Groningen

UNIVERSITY OF TWENTE.

The research presented in this thesis was carried out at the Mathematics of Computational Science group, Department of Applied Mathematics, University of Twente, Enschede, The Netherlands.

This work was supported by the China Scholarship Council (CSC), project no. 2011634101.

ISBN: 978-90-365-3958-6 DOI: 10.3990/1.9789036539586
<http://dx.doi.org/10.3990/1.9789036539586>

Printed by Gildeprint, Enschede.

Copyright © 2015, Lulu Tian, Enschede, The Netherlands.

LOCAL DISCONTINUOUS GALERKIN METHODS FOR PHASE TRANSITION PROBLEMS

DISSERTATION

to obtain
the degree of doctor at the University of Twente,
on the authority of the rector magnificus,
prof. dr. H. Brinksma,
on account of the decision of the graduation committee,
to be publicly defended
on Friday 02 October 2015 at 14:45

by

Lulu Tian
born on 16 January 1987
in Shandong, China

This dissertation has been approved by:
prof. dr. ir. J.J.W. van der Vegt
prof. dr. J.G.M. Kuerten

Contents

1	Introduction	1
1.1	Motivation	1
1.2	Systems modeling phase transition	6
1.2.1	A system modeling phase transition in solids and Van der Waals fluids	6
1.2.2	The (non)-isothermal Navier-Stokes-Korteweg equations	7
1.2.3	Mesh adaptation	8
1.3	Outline	9
2	A Local Discontinuous Galerkin Method for the Propagation of Phase Transition in Solids and Fluids	11
2.1	Introduction	12
2.2	LDG Discretization using the Viscosity-Capillarity approach .	15
2.2.1	Notation	15
2.2.2	LDG discretization	15
2.2.3	Time discretization	17
2.3	L^2 – Stability of the LDG scheme	18
2.4	Error estimates	20
2.4.1	Projection operator	21
2.4.2	Notations and Lemmas for the LDG discretization . .	21

2.4.3	Error estimates of the initial conditions	23
2.4.4	A priori error estimate of the LDG discretization . . .	23
2.5	Linear stability analysis of the LDG scheme	30
2.6	Numerical experiments	33
2.7	Conclusion	39
3	A local discontinuous Galerkin method for the (non)-isothermal Navier-Stokes-Korteweg equations	47
3.1	Introduction	48
3.2	LDG Discretization of the NSK system	53
3.2.1	Notations	53
3.2.2	LDG discretization for the isothermal NSK equations	54
3.2.3	LDG Discretization for the non-isothermal NSK equations	57
3.3	Implicit time discretization method	59
3.3.1	Diagonally Implicit Runge-Kutta methods	60
3.3.2	Newton-Krylov methods	61
3.4	Numerical experiments	62
3.4.1	Interface width	64
3.4.2	Numerical tests for the isothermal NSK equations . .	64
3.4.3	Numerical experiments for the non-isothermal NSK equations	75
3.5	Conclusions	84
3.6	Appendix	87
4	An h-adaptive local discontinuous Galerkin method for liquid-vapor flows with phase change and solid wall boundaries	95
4.1	Introduction	96
4.2	LDG discretization of the NSK equations	100
4.2.1	Notations	100
4.2.2	LDG discretization for the non-isothermal NSK equations	101
4.2.3	Numerical fluxes	103
4.3	Mesh adaptation	104
4.3.1	Refinement and coarsening of quadrilaterals	104
4.3.2	Candidate elements for refinement and coarsening . .	106
4.3.3	Strategy for refinement and coarsening	107
4.3.4	Flow chart for mesh adaptation	108
4.4	Numerical examples	109
4.4.1	Coalescence of vapor bubbles in a liquid	110
4.4.2	DIRK time integration method on an adapted mesh .	115

4.4.3	Bubbles and droplets in contact with solid wall boundaries	119
4.5	Conclusions	129
5	Conclusions and Outlook	131
5.1	Conclusions	131
5.2	Outlook	132
	Summary	135
	Samenvatting	137
	Bibliography	139
	Acknowledgements	151
	List of publications	153

Introduction

1.1 Motivation

Phase transition occurs when a substance changes from a solid, liquid, or gas state to another state. Under a specific combination of temperature and pressure, every element or substance can transform from one phase to another. For example, phase transitions in argon and water are shown in Figure

Figure 1.1: Examples of phase transition, Left: rapidly melting solid argon undergoes transitions from solid to liquid and from liquid to gas, Right: boiling water undergoes phase transition from liquid to vapor.

1.1. Many materials, including various polymers [54], natural rubbers [55] and metals [75, 5], undergo phase transitions, where phase boundaries travel through the material. This kind of materials is desirable for applications in medical sensors, actuators, robots and refrigerators [84, 101], and has received significant attention in recent years [10, 6, 35]. Cavitation problems, which are associated with liquid-vapor flows with phase change, are of high industrial interest in turbines, pumps, ship propellers and nozzles [86, 40], since cavitation can lead to erosion of the material. As an example, Figure 1.2 shows the damage on the blades of a ship propeller by cavitation bubbles. If the flow caused by the propeller of a ship results in a local pressure below the saturation pressure, vapor bubbles appear, which collapse once they enter a region of higher pressure. The collapse of the cavitation bubbles might lead to erosion of the propeller, and to vibrations and sound [17, 40]. Phase transitions in liquid-vapor flows also occur in heat exchangers, nuclear reactors, boilers, etc. [58]. An experiment of steam injected into a cross flow of water [28] exhibiting condensation of vapor to liquid is shown in Figure 1.3.

Figure 1.2: Examples of cavitation. Left: Cavitation damage on the blades of a ship propeller. In 1917 Lord Rayleigh [86] explained that this effect is caused by small vapor bubbles that collapse at the surface of the propeller blades. Right: A model for a propeller with cavitation in a water tunnel experiment.

Understanding phase transitions in solids and fluids requires experimental investigations as well as analytical models. The first microscopic description of phase transition is due to Johannes Diderik van der Waals, who derived the Van der Waals equation for gases and liquids in 1873 and received the

Figure 1.3: Examples of injected steam bubbles at two different times [28]. A vapor bubble is injected into a liquid channel, and grows until a sudden collapse occurs.

Nobel prize in 1910 for his contribution to understanding gas-liquid flows. The Van der Waals equation is a molecular model and approximates the behavior of real fluids by considering the attractive and repulsive forces between the molecules. Because of its relatively simple form and the accurate approximation to the pressure in both liquid and vapor, the Van der Waals equation of state has been widely used [100, 99, 89, 81, 72, 46, 107, 39]. The interface width between the different phases can be predicted based on the Van der Waals equation of state and it becomes infinite when the temperature approaches the critical value [9]. Modifications and improvements of Van der Waals theory are discussed in [14]. Another important contribution to the understanding of phase transitions in fluids is due to Korteweg [63], who proposed that the stress tensor depends on the density and its spatial gradients because of capillary forces. The Korteweg theory was applied by Serrin [93] in order to find conditions for the equilibrium of liquid and vapor phases in a Van der Waals fluid. For more information about interfacial and capillary theory, see [90].

The technique of modeling the interface as a thin layer, instead of a sharp transition between the phases, also results in an important model to compute flows with phase transition, and is called diffuse interface model [9, 18, 124, 89]. In diffuse interface models, only a single set of governing equations needs to be solved on the entire flow domain, including the interface area. The location of the interface then follows from the solution,

for example as the surface where the mass density attains a certain value. Another important technique to deal with interface problems is the sharp-interface method. In the early 1800s, Young, Laplace and Gauss considered the interface between two fluids as a surface of zero thickness and physical quantities are discontinuous across the interface based on static or mechanical equilibrium arguments [9]. Sharp interface models have been used in many applications [11, 34, 32, 111]. They require, however, an extra evolution equation for the interface and face challenges in the reconstruction of the interface, leading to mathematical models that are solved by level-set [103, 79], front-tracking [111, 112], or volume of fluid methods [53, 68]. The sharp interface technique is, however, not valid in some situations. First, the interfacial thickness of the interface is comparable to the length of the examined domain in a near-critical fluid and becomes infinite at the critical point, which can not be neglected as is done in the sharp interface method. Moreover, some physical phenomena, such as the creation and coalescence of vapor bubbles in a liquid, can not be described by the sharp interface method. These processes can be simulated only if the interface is modeled as a continuous medium [9, 69, 38, 58], or if ad hoc models for the interfacial mass transfer are applied. In this work, we will focus on systems modeling phase transitions in solids and fluids, described by diffuse interface models.

Numerical methods for partial differential equations (PDEs) describing a diffuse interface model have received significant attention [67, 83, 102, 71]. When the solutions of the systems admit discontinuities, standard numerical methods like finite difference and finite volume methods, which are developed under the assumption of smooth solutions, lead to poor numerical results [71]. Either numerical viscosity is necessary, which artificially smooths the solution, or a dispersion error occurs, resulting in oscillations in the numerical solution. A popular approach is then the discontinuity tracking method that combines a standard finite difference or finite volume method in smooth regions with an explicit procedure for the tracking of the interface that may emerge in the flow during phase transition [45, 97, 73]. It is, however, complicated to apply these techniques for three-dimensional problems, where the curves or surfaces may interact as time evolves. An alternative technique is a discontinuity capturing method that produces accurate approximations to discontinuous solutions without the explicit tracking of the interface. This method has made great progress in the past years and is applicable to many problems [71, 104, 105, 95, 96, 88, 22]. Understanding the discontinuity capturing method requires a good understanding of the mathematical theory of conservation laws as well as the physical behavior of the solutions. When it comes to systems associated with phase transitions in solids and fluids, the

mathematical theory becomes increasingly difficult [4, 31, 33], and is still an area of active research.

The numerical approach taken in the present research is different from those cited above. We will use a local discontinuous Galerkin (LDG) finite element method to solve systems modeling phase transitions in solids, Van der Waals fluids and the Navier-Stokes-Korteweg equations. The LDG method is an extension of the discontinuous Galerkin (DG) method that aims to solve partial differential equations that contain higher than first order spatial derivatives and was originally developed by Cockburn and Shu in [30] for nonlinear convection-diffusion equations containing second-order spatial derivatives. The idea behind LDG methods is to rewrite equations with higher derivatives as a first order system, then apply the DG method to this extended system. The design of the numerical fluxes is the key ingredient for ensuring numerical stability. LDG techniques have been developed for convection-diffusion equations [30], nonlinear KdV type equations [123], the Camassa-Holm equation [119] and many other types of partial differential equations. For a review, see [121]. The LDG method results in an extremely local discretization, which offers great advantages in parallel computing and is well suited for *hp*-adaptation. In particular, the LDG method offers in many cases provable nonlinear stability.

Solving the systems modeling phase transitions in solids, Van der Waals fluids and the Navier-Stokes-Korteweg equations is, however, a challenge. First, for applications where the temperature is far below the critical temperature of the fluid, the liquid-vapor interface is very thin and an excessive number of points in a uniform mesh is required to capture the interface [58]. To alleviate this problem, we consider phase transitions when the temperature is below, but close to the critical temperature. Second, the coupled system of partial differential equations that describe two-phase flows are highly non-linear and require advanced numerical techniques to solve them. Examples are the Cahn-Hilliard equations, second gradient theory, and the (non)-isothermal Navier-Stokes-Korteweg equations that are used to describe liquid-vapor flows with phase change [9, 19]. Solving these systems numerically has shown significant progress [51, 52, 64, 89, 36, 50, 117, 42, 58, 59, 43, 61, 116, 118]. In the following section we will discuss several systems modeling phase transitions in solids and fluids that will be solved in the present work with the LDG method.

1.2 Systems modeling phase transition

1.2.1 A system modeling phase transition in solids and Van der Waals fluids

The first problem we focus on is a popular mathematical model for isothermal motion of phase transitions in elastic bars and in Van der Waals fluids. The system consists of conservation laws with a non-convex stress-strain relation or equation of state, and is a mixed hyperbolic-elliptic system [57, 94, 3, 92, 99, 109, 99, 93, 29, 35, 107]. The most obvious difficulty to solve mixed hyperbolic-elliptic initial value problems is that the system is unstable in the elliptic region. To deal with this difficulty we expect to find “weak” or “generalized” solutions of the mixed system taking values only in the stable hyperbolic domains if initial conditions are in the stable hyperbolic domains [100, 3]. The weak solutions of such systems exhibit propagating phase boundaries separating states in one hyperbolic domain from states in another hyperbolic domain [1, 5, 4, 99, 100, 110]. Such waves are not uniquely characterized by the entropy inequality and require an additional jump relation, called a kinetic relation [3, 2, 5, 71, 110]. The kinetic relation depends on the material and controls the initiation of the phase transition and the rate at which phase transition takes place.

To single out one physically correct solution, we use the viscosity-capillarity (VC) approach [100, 99, 47, 106]. In the viscosity-capillarity approach, the ignored diffusive and capillary terms are introduced into the conservation laws to obtain a system called VC system, and the limit of the coefficients of these terms going to zero is considered. The viscosity-capillarity criterion was thoroughly discussed in [47], where it was applied to isothermal motion of phase transitions in a Van der Waals fluid. Solving the VC system by finite difference and finite element methods has to be conducted in such a way that stable and high order accurate numerical solutions are obtained without spurious oscillations at phase boundaries, see e.g. [4, 22, 23, 31, 33].

In this work an LDG method will be proposed to solve the VC system. We will

- prove the stability and error analysis of the LDG scheme for the VC system,
- compute exact solutions for a Riemann problem of the conservation laws with a trilinear stress-strain relation, using the techniques presented in [3, 2],

- compare the numerical solutions for the Riemann problems of the corresponding VC system with the exact solutions,
- perform numerical experiments for the VC system with a Van der Waals type of equation of state.

1.2.2 The (non)-isothermal Navier-Stokes-Korteweg equations

The second problem we study are the Navier-Stokes-Korteweg (NSK) equations used as a diffuse interface model to compute phase transitions in liquid-vapor flows [46, 81, 16, 72, 9, 82]. The non-isothermal NSK equations, composed of the balance equations for mass, momentum and energy, model liquid-vapor flows with phase transition at a non-uniform temperature. Compared with the standard compressible Navier-Stokes equations, the NSK equations contain an additional stress tensor called Korteweg term, which is related to the capillary forces. The Van der Waals equation of state [100, 99, 89, 81, 72, 46, 72, 44] is used to describe the pressure in both the liquid and vapor state, especially close to the critical temperature. When the temperature is assumed constant, the isothermal NSK equations are obtained by removing the energy equation.

The theoretical solvability of the isothermal and non-isothermal NSK equations has received considerable attention [51, 52, 64, 89, 36, 50, 65, 66]. Numerically, in most articles so far only the isothermal NSK equations in non-conservative form are considered. Frequently, the isothermal NSK equations are rewritten into an extended system by introducing an extra variable [72, 44, 16, 89]. It is, however, not trivial to do this for the non-isothermal NSK equations, where the Van der Waals equation of state depends on both the density and the temperature. As an alternative, we will present an LDG method for both the isothermal and the non-isothermal NSK equations, while keeping the conservative form of the (non)-isothermal NSK equations.

To our knowledge, we are the first to use a discontinuous Galerkin method to solve the non-isothermal NSK equations. We will

- develop an LDG discretization for the isothermal NSK equations,
- perform several numerical tests, including accuracy and convergence rate tests for the LDG discretization of the isothermal NSK equations, several benchmark problems and a simulation of the coalescence of two dimensional vapor bubbles in a liquid,

- extend the LDG discretization for the isothermal NSK equations to the non-isothermal NSK equations,
- verify accuracy, stability and capabilities of the LDG discretization for the non-isothermal NSK equations by numerical examples.

1.2.3 Mesh adaptation

Since small mesh sizes are only required at the interface region and the LDG discretisation is well suited for a computational mesh with hanging nodes, we will consider adapted meshes to save computational costs and to capture the interface more accurately.

To start the mesh adaptation, we first need criteria to select candidate elements for refinement and coarsening in the computational mesh. Candidate elements for refinement will be refined, while the coarsening of elements depends on their neighboring elements. There are two main types of strategy to obtain these criteria in finite volume and finite element methods: error estimators and heuristic indicators. Error estimators are based on theoretical results, and they are only available when a posteriori error estimates hold locally [77, 78, 60, 114, 7, 87]. Heuristic indicators usually depend on local spatial gradients of thermodynamic variables, such as density, pressure, energy and entropy. Compared with an a posteriori error estimate, heuristic indicators are easy to compute and widely used in practical applications [13, 115, 40, 16], but they have a limited theoretical foundation. Since an a posteriori error estimate is currently out of scope for the LDG discretization of the (non)-isothermal NSK equations, we choose the density gradient as an heuristic indicator in the present work.

Mesh adaptation, together with LDG discretizations, will be developed for the (non)-isothermal NSK equations. We will

- present a criterion to choose candidate elements for refinement and coarsening,
- provide algorithms for mesh adaptation,
- perform two-dimensional numerical computations on an adaptive mesh and compare these results with the same test cases on a uniform mesh.
- consider two-dimensional simulations with solid wall boundaries, where vapor bubbles and liquid droplets are in contact with a solid wall.

1.3 Outline

The outline of this thesis is as follows. Chapter 2 focuses on a system based on the viscosity-capillarity approach to model phase transitions in solids and Van der Waals fluids. An LDG discretization is presented for the VC system with various viscous-capillary coefficients. The L^2 -stability and an a priori error estimate of the LDG scheme for the VC system will be discussed. Numerical experiments for phase transition in solids and fluids, including the Van der Waals model, will be performed to demonstrate the accuracy and stability of the LDG method. The LDG solutions of the VC system are compared with exact solutions of the original conservation laws.

In Chapter 3, LDG discretizations will be presented for the NSK equations modelling phase transitions in liquid-vapor flows. Accuracy and stability of the LDG discretizations will be verified by extensive numerical examples, including one-dimensional stationary and travelling waves, and the coalescence of two-dimensional vapor bubbles in a liquid. These numerical examples will be performed for both the isothermal and the non-isothermal NSK equations.

To save computing time and memory and to capture the interface more accurately, we develop mesh adaptation in Chapter 4. Criteria for selection of candidate elements are presented that depend on the locally largest density gradient. Then a strategy is provided for the refinement and coarsening of the candidate elements. The same numerical tests for the coalescence of vapor bubbles as discussed in Chapter 3 will be performed on a locally refined mesh. Also, bubbles and droplets in contact with a solid wall will be considered.

Finally, conclusions are drawn and an outlook for future research is given in Chapter 5.

A Local Discontinuous Galerkin Method for the Propagation of Phase Transition in Solids and Fluids

1

In this chapter a local discontinuous Galerkin (LDG) finite element method for the solution of a hyperbolic-elliptic system modeling the propagation of phase transition in solids and fluids is presented. Viscosity and capillarity terms are added to select the physically relevant solution. The L^2 -stability of the LDG method is proven for basis functions of arbitrary polynomial order. An a priori error estimate is provided for the LDG discretization of the phase transition model when the stress-strain relation is linear, assuming that the solution is sufficiently smooth and the system is hyperbolic. To obtain a reference exact solution we solved a Riemann problem for a trilinear strain-stress relation using a kinetic relation to select the unique admissible solution. The LDG method is demonstrated by computing several model problems representing phase transition in solids and in fluids with a Van der Waals equation of state.

¹The content of this chapter is published in the Journal of Scientific Computing [107], with co-authors: Y. Xu, J.G.M. Kuerten and J.J.W. Van der Vegt.

2.1 Introduction

The propagation of phase transition in solids and fluids can be modeled with hyperbolic-elliptic systems of partial differential equations. Examples are solid-solid transformations in elastic materials [3] and a homogeneous compressible fluid with liquid and vapor phases with a van der Waals equation of state [110]. A well-known one-dimensional hyperbolic-elliptic model that describes these phase transition phenomena is given by the following partial differential equations

$$\begin{aligned}\gamma_t - v_x &= 0, \\ v_t - (\sigma(\gamma))_x &= 0,\end{aligned}\tag{2.1}$$

where γ, v represent the deformation gradient (the strain) and velocity, respectively, and σ is the stress. We consider a stress-strain relation $\sigma(\gamma)$ as sketched in Fig 2.1. The system (2.1) is hyperbolic for $\sigma'(\gamma) > 0$ and elliptic for $\sigma'(\gamma) < 0$. This mixed type hyperbolic-elliptic system contains a rich mathematical structure. For example, the standard entropy condition for a hyperbolic system is insufficient to determine the unique solution. This has stimulated an extensive analysis to investigate conditions that ensure the uniqueness of solutions of hyperbolic-elliptic systems, in particular their Riemann solutions. For an overview of the general theory, we refer to [71].

Figure 2.1: Examples of strain-stress relation $\sigma(\gamma)$, general and trilinear case.

The need to impose additional conditions to ensure uniqueness of the solution originates from the fact that in the model equations small scale

mechanisms that are induced by viscosity, capillarity and heat conduction are neglected [4]. One way to reintroduce the neglected physical information is the viscosity-capillarity (VC) approach. In the VC approach, solutions of (2.1) are obtained by taking the limit of the solution of the system:

$$\begin{aligned}\tilde{\gamma}_t - \tilde{v}_x &= 0, \\ \tilde{v}_t - (\sigma(\tilde{\gamma}))_x &= \nu \tilde{v}_{xx} - \lambda \tilde{\gamma}_{xxx},\end{aligned}\tag{2.2}$$

when the parameters ν and λ tend to zero, while the number $\omega = 2\sqrt{\lambda}/\nu$ is fixed. The notion of VC solutions for the equations describing a Van der Waals fluid was first proposed by Slemrod [100] based on Korteweg's theory of capillarity.

The solution of hyperbolic-elliptic systems may contain nonclassical shock waves or subsonic propagating phase transitions. Such waves do not satisfy standard entropy criteria and require an additional kinetic relation to select the unique admissible solution. For details of the theory of both classical and nonclassical shock waves, we refer to [71]. In particular, for the trilinear approximation to the stress-strain curve $\sigma(\gamma)$, Abeyaratne and Knowles derived in [3] the exact solution of (2.1) containing both shock waves and phase boundaries. The kinetic relation and initiation criterion for the relevant phase transition must, however, be provided separately using physical modeling. Later, in [2], Abeyaratne and Knowles pointed out that a kinetic relation for (2.1) can also be obtained by considering traveling wave solutions for the augmented system (2.2) that includes viscosity and capillarity terms.

The numerical solution of mixed hyperbolic-elliptic systems, such as (2.1), is non-trivial. Standard numerical schemes smear out discontinuities and cause spurious solutions at the elliptic-hyperbolic boundary. Also, commonly used stabilization techniques, such as limiters, are counter productive for diffusive-dispersive regularization as given by the VC-equations (2.2).

One way to obtain accurate numerical discretizations for hyperbolic-elliptic systems is to use Glimm random choice methods [70] or front tracking techniques [12], [15], [21], [25], [26], [74], [125]. These methods use the exact solution of Riemann problems and resolve the phase boundary over one cell. They converge to the correct solutions of the non-classical Riemann problem. For complicated systems of hyperbolic-elliptic partial differential equations the use of an exact Riemann problem is, however, non-trivial, in particular in multiple dimensions.

An alternative is provided by finite difference and finite element discretizations of the VC-equations (2.2) using numerical methods that were originally developed to capture shocks and contact discontinuities in hyperbolic partial

differential equations. Both for finite difference and finite element methods extensive research has been conducted to ensure that stable and high order accurate numerical solutions are obtained without spurious oscillations at phase boundaries, see e.g. [4], [22], [31], [33]. This is non-trivial and still a topic of ongoing research.

In this chapter we will investigate the use of the local discontinuous Galerkin (LDG) finite element method for the solution of the VC-equations (2.2). The LDG method is an extension of the discontinuous Galerkin (DG) method that aims to solve partial differential equations (PDEs) that contain higher than first order spatial derivatives and was originally developed by Cockburn and Shu in [30] for solving nonlinear convection-diffusion equations containing second-order spatial derivatives. The idea behind LDG methods is to rewrite equations with higher order derivatives as a first order system, then apply the DG method to this extended system. The design of the numerical fluxes is the key ingredient for ensuring stability. LDG techniques have been developed for convection diffusion equations [30], nonlinear KdV type equations [123], the Camassa-Holm equation [119] and many other types of partial differential equations. For a review, see [121]. The LDG method results in an extremely local discretization, which offers great advantages in parallel computing and is well suited for *hp*-adaptation. In particular, the LDG method offers provable nonlinear stability. The LDG method for the VC-equations (2.2) that we describe in this chapter shares all these elegant properties.

Recently, the LDG method was also used in [48] for the solution of the VC-equations (2.2) including a non-local convolution type regularization of (2.1). For this non-local model discretized with piecewise constant basis functions and central numerical fluxes in the LDG discretization, Haink and Rohde proved in Theorem 3.1 in [48] a discrete energy estimate. In this chapter we will prove a general L^2 -stability estimate for the LDG discretization of (2.2) using alternating numerical fluxes and basis functions of arbitrary polynomial order. This L^2 -stability estimate is also crucial for the a priori error analysis in which we prove that the LDG discretization is of optimal order. Another important topic we address is a detailed comparison of the LDG solutions with exact solutions of Riemann problems containing both phase transitions and shocks. For this purpose, we use the detailed analysis provided in [2], [3].

The outline of the chapter is as follows. In Section 2 we present the LDG discretization for (2.2). Next, in Section 2.3 the L^2 -stability of the LDG scheme is proven and an error estimate of the semi-discrete LDG scheme is given in Section 2.4. In Section 2.5, we discuss a linear stability analysis of

the LDG method for the VC-equations. Numerical experiments for phase transition in solids and fluids, including the Van der Waals model [24], are described in Section 2.6. Special attention is given to demonstrate that solutions of the LDG method consistently converge to exact solutions of the phase transition model (2.1). Finally, conclusions are drawn in Section 2.7.

2.2 LDG Discretization using the Viscosity-Capillarity approach

2.2.1 Notation

We denote the mesh in the domain $\Omega \subset \mathbf{R}$ by $K_j = (x_{j-1/2}, x_{j+1/2})$, for $j = 1, \dots, M$. The center of an element is $x_j = \frac{1}{2}(x_{j-1/2} + x_{j+1/2})$ and the mesh size is denoted by $h_j = x_{j+1/2} - x_{j-1/2}$, with $h = \max_{1 \leq j \leq M} h_j$ being the maximum mesh size. We assume that the mesh is regular, namely the ratio between the maximum and the minimum mesh size stays bounded during mesh refinement. We define the space V_h^k as the space of polynomials of degree up to k in each element K_j , i.e.

$$V_h^k = \{v \in L^2(\Omega) : v(x) \in P^k(K_j) \text{ for } x \in K_j, j = 1, \dots, M\}.$$

Note that functions in V_h^k are allowed to be discontinuous across element faces. For $P^k(K_j)$, we use Legendre polynomials as basis functions in V_h^k throughout this chapter.

The numerical solution is denoted by u_h , and belongs to the finite element space V_h^k . We denote by $(u_h)_{j+1/2}^-$ and $(u_h)_{j+1/2}^+$ the traces of u_h at $x_{j+1/2}$, taken from the left element K_j , and the right element K_{j+1} , respectively. We use the standard notation $[u_h] = u_h^+ - u_h^-$ to denote the jump of u_h at each element boundary point.

2.2.2 LDG discretization

In this section, we present the LDG method for the VC-equations (2.2), which are defined as:

$$\begin{aligned} \gamma_t &= v_x, \\ v_t &= (\sigma(\gamma))_x + \nu v_{xx} - \lambda \gamma_{xxx}, \end{aligned} \tag{2.3}$$

with initial conditions:

$$\begin{aligned}\gamma(x, 0) &= \gamma_0(x), \\ v(x, 0) &= v_0(x).\end{aligned}\tag{2.4}$$

To define the LDG scheme, we first rewrite (2.3) as a first-order system:

$$\begin{aligned}\gamma_t &= v_x, \\ v_t &= f_x + \nu q_x - \lambda s_x,\end{aligned}\tag{2.5}$$

where we introduced the auxiliary variables f, s, p and q , which satisfy the equations:

$$\begin{cases} f = \sigma(\gamma), \\ s = p_x, \\ p = \gamma_x, \\ q = v_x. \end{cases}\tag{2.6}$$

The LDG method for (2.5), when f, q and s are assumed known, can be formulated as: find $\gamma_h, v_h \in V_h^k$, such that for all test functions $\phi, \varphi \in V_h^k$,

$$\begin{aligned}& \int_{K_j} (\gamma_h)_t \phi dx + \int_{K_j} v_h \phi_x dx - \widehat{v_h} \phi^-|_{j+1/2} + \widehat{v_h} \phi^+|_{j-1/2} = 0, \\& \int_{K_j} (v_h)_t \varphi dx + \int_{K_j} f_h \varphi_x dx - \widehat{f_h} \varphi^-|_{j+1/2} + \widehat{f_h} \varphi^+|_{j-1/2} \\& \quad - \lambda \int_{K_j} s_h \varphi_x dx + \lambda \widehat{s_h} \varphi^-|_{j+1/2} - \lambda \widehat{s_h} \varphi^+|_{j-1/2} + \nu \int_{K_j} q_h \varphi_x dx \\& \quad - \nu \widehat{q_h} \varphi^-|_{j+1/2} + \nu \widehat{q_h} \varphi^+|_{j-1/2} = 0, \quad j = 1, \dots, M.\end{aligned}\tag{2.7}$$

The “hat” terms in the cell boundary contributions in (2.7), resulting from integration by parts, are the so-called “numerical fluxes”, which are single-valued functions defined at the element boundaries and should be designed to ensure stability. Here we take the alternating numerical fluxes:

$$\widehat{v_h} = v_h^+, \quad \widehat{f_h} = f_h^-, \quad \widehat{s_h} = s_h^-, \quad \widehat{q_h} = q_h^-.\tag{2.8}$$

Similarly, we derive for the auxiliary equations (2.6) the following local discontinuous Galerkin discretization: find $f_h, s_h, p_h, q_h \in V_h^k$, such that for all

test functions $\zeta, \eta, \xi, \tau \in V_h^k$,

$$\int_{K_j} f_h \zeta dx - \int_{K_j} \sigma(\gamma_h) \zeta dx = 0, \quad (2.9a)$$

$$\int_{K_j} s_h \eta dx + \int_{K_j} p_h \eta_x dx - \widehat{p_h} \eta^-|_{j+1/2} + \widehat{p_h} \eta^+|_{j-1/2} = 0, \quad (2.9b)$$

$$\int_{K_j} p_h \xi dx + \int_{K_j} \gamma_h \xi_x dx - \widehat{\gamma_h} \xi^-|_{j+1/2} + \widehat{\gamma_h} \xi^+|_{j-1/2} = 0, \quad (2.9c)$$

$$\int_{K_j} q_h \tau dx + \int_{K_j} v_h \tau_x dx - \widehat{v_h} \tau^-|_{j+1/2} + \widehat{v_h} \tau^+|_{j-1/2} = 0. \quad (2.9d)$$

The numerical fluxes in (2.9) are chosen as:

$$\widehat{p_h} = p_h^+, \quad \widehat{\gamma_h} = \gamma_h^-, \quad \widehat{v_h} = v_h^+. \quad (2.10)$$

We remark that the choice of numerical fluxes in (2.8) and (2.10) is not unique. We can, for example, also choose the following numerical fluxes:

$$\widehat{v_h} = v_h^-, \quad \widehat{\gamma_h} = \gamma_h^+, \quad \widehat{s_h} = s_h^+, \quad \widehat{p_h} = p_h^-, \quad \widehat{q_h} = q_h^+, \quad \widehat{f_h} = f_h^+. \quad (2.11)$$

In Section 2.3 we will prove that both the numerical fluxes (2.8), (2.10) and (2.11) result in an LDG discretization which is L^2 -stable.

2.2.3 Time discretization

Suppose that the coefficients of the polynomial expansions of $\gamma_h(x, t)$ and $v_h(x, t)$ in each element are given by

$$(\gamma_0(t), \gamma_1(t), \dots, \gamma_k(t), v_0(t), v_1(t), \dots, v_k(t)) \equiv U(t).$$

The LDG discretization (2.7) for γ_h and v_h then can be written as the ODE system:

$$\begin{aligned} U_t &= F(U, t), \\ U(0) &= U_0, \end{aligned} \quad (2.12)$$

which we discretize in time by the third-order accurate explicit Runge-Kutta time stepping method [96], given as:

$$\begin{cases} V = U^n + \Delta t F(U^n, t^n), \\ W = \frac{3}{4}U^n + \frac{1}{4}V + \frac{1}{4}\Delta t F(V, t^n + \Delta t), \\ U^{n+1} = \frac{1}{3}U^n + \frac{2}{3}W + \frac{2}{3}\Delta t F(W, t^n + \frac{1}{2}\Delta t). \end{cases} \quad (2.13)$$

2.3 L^2 – Stability of the LDG scheme

The solution of the viscosity-capillarity equations (2.3) preserves energy. In [29] Cockburn and Gau proved that the related discrete energy is also preserved for the finite difference discretization they proposed. In this section, we will prove that the LDG scheme (2.7) - (2.10) also preserves a discrete energy. This implies L^2 – stability of the LDG discretization and it is an important and necessary property to obtain a stable and robust LDG scheme.

Theorem 2.1. (L^2 – stability of the LDG scheme)

Assume $\frac{\partial W(\gamma)}{\partial \gamma} = \sigma(\gamma)$, and define the discrete energy E_h as

$$E_h = \sum_{j=1}^M \left(\int_{K_j} W(\gamma_h) dx + \frac{1}{2} \int_{K_j} v_h^2 dx + \frac{\lambda}{2} \int_{K_j} p_h^2 dx \right).$$

Then the discrete energy E_h computed from the LDG discretization of the viscosity-capillarity equations given by (2.7)- (2.10) satisfies the relation

$$\frac{d}{dt} E_h = -\nu \sum_{j=1}^M \int_{K_j} (q_h)^2 dx, \quad (2.14)$$

when periodic boundary conditions are applied at the domain boundary.

Proof. We first take the time derivative of (2.9c),

$$\int_{K_j} (p_h)_t \xi dx + \int_{K_j} (\gamma_h)_t \xi_x dx - (\widehat{\gamma_h})_t \xi^-|_{j+1/2} + (\widehat{\gamma_h})_t \xi^+|_{j-1/2} = 0. \quad (2.15)$$

After choosing in (2.7), (2.9) and (2.15) the following test functions,

$$\phi = f_h - \lambda s_h, \quad \varphi = v_h, \quad \zeta = -(\gamma_h)_t, \quad \eta = \lambda(\gamma_h)_t, \quad \xi = \lambda p_h, \quad \tau = \nu q_h,$$

we get

$$\begin{aligned} \int_{K_j} (\gamma_h)_t (f_h - \lambda s_h) dx + \int_{K_j} v_h (f_h - \lambda s_h)_x dx - \widehat{v_h} (f_h - \lambda s_h)^-|_{j+1/2} \\ + \widehat{v_h} (f_h - \lambda s_h)^+|_{j-1/2} = 0, \end{aligned} \quad (2.16a)$$

$$\begin{aligned} \int_{K_j} (v_h)_t v_h dx + \int_{K_j} (f_h + \nu q_h - \lambda s_h) (v_h)_x dx \\ - (\widehat{f_h} + \nu \widehat{q_h} - \lambda \widehat{s_h}) v_h^-|_{j+1/2} + (\widehat{f_h} + \nu \widehat{q_h} - \lambda \widehat{s_h}) v_h^+|_{j-1/2} = 0, \end{aligned} \quad (2.16b)$$

$$- \int_{K_j} f_h (\gamma_h)_t dx + \int_{K_j} \sigma(\gamma_h) (\gamma_h)_t dx = 0, \quad (2.16c)$$

$$\begin{aligned} \lambda \int_{K_j} s_h (\gamma_h)_t dx + \lambda \int_{K_j} p_h ((\gamma_h)_t)_x dx - \lambda \widehat{p_h} (\gamma_h)_t^-|_{j+1/2} \\ + \lambda \widehat{p_h} (\gamma_h)_t^+|_{j-1/2} = 0, \end{aligned} \quad (2.16d)$$

$$\begin{aligned} \lambda \int_{K_j} (p_h)_t p_h dx + \lambda \int_{K_j} (\gamma_h)_t (p_h)_x dx - \lambda (\widehat{\gamma_h})_t p_h^-|_{j+1/2} \\ + \lambda (\widehat{\gamma_h})_t p_h^+|_{j-1/2} = 0, \end{aligned} \quad (2.16e)$$

$$\nu \int_{K_j} q_h^2 dx + \nu \int_{K_j} v_h (q_h)_x dx - \nu \widehat{v_h} q_h^-|_{j+1/2} + \nu \widehat{v_h} q_h^+|_{j-1/2} = 0. \quad (2.16f)$$

Adding (2.16a)-(2.16f), and integrating the divergence terms, we obtain:

$$\begin{aligned} \int_{K_j} ((\gamma_h)_t \sigma(\gamma_h) + (v_h)_t v_h + \lambda (p_h)_t p_h) dx + \nu \int_{K_j} q_h^2 dx \\ + F_{j+1/2} - F_{j-1/2} + \Theta_{j-1/2} = 0. \end{aligned} \quad (2.17)$$

The numerical entropy fluxes are given by:

$$\begin{aligned} F &= v_h^- f_h^- - \lambda s_h^- v_h^- + \lambda p_h^- (\gamma_h)_t^- + \nu q_h^- v_h^- - \widehat{v_h} f_h^- + \lambda \widehat{v_h} s_h^- \\ &\quad - \widehat{f_h} v_h^- - \nu \widehat{q_h} v_h^- + \lambda \widehat{s_h} v_h^- - \lambda \widehat{p_h} (\gamma_h)_t^- - \lambda (\widehat{\gamma_h})_t p_h^- - \nu \widehat{v_h} q_h^- \\ &= \lambda v_h^+ s_h^- - \lambda p_h^+ (\gamma_h)_t^- - \nu v_h^+ q_h^- - f_h^- v_h^+, \end{aligned}$$

where we used the numerical fluxes (2.8) and (2.10). The Θ term is given by

$$\begin{aligned} \Theta &= -[v_h f_h] + \lambda [s_h v_h] - \lambda [p_h (\gamma_h)_t] - \nu [q_h v_h] + \widehat{v_h} [f_h] - \lambda \widehat{v_h} [s_h] \\ &\quad + \widehat{f_h} [v_h] + \nu \widehat{q_h} [v_h] - \lambda \widehat{s_h} [v_h] + \lambda \widehat{p_h} [(\gamma_h)_t] + \lambda \widehat{\gamma_h}_t [p_h] + \nu \widehat{v_h} [q_h]. \end{aligned}$$

Using the definition of the numerical fluxes (2.8) and (2.10) and after some algebraic manipulation, we obtain:

$$\Theta = 0.$$

After summation of (2.17) over all j and applying periodic boundary conditions, all entropy fluxes cancel and we obtain the following expression for the rate of change of the discrete energy:

$$\begin{aligned} \frac{d}{dt} E_h(t) &\equiv \sum_{j=1}^M \int_{K_j} (\sigma(\gamma_h)(\gamma_h)_t + (v_h)_t v_h + \lambda (p_h)_t p_h) dx \\ &= -\nu \sum_{j=1}^M \int_{K_j} (q_h)^2 dx, \end{aligned} \tag{2.18}$$

which proves (2.14). $\square$

Remark 2.1. *From the proof of Theorem 1, we can see that it holds for a general nonlinear σ function, which is not always an increasing function. From the definition of $W(\gamma)$, it follows that the summation of $\sum_j \int_{K_j} W(\gamma_h)$ is in general not negative, since $\sigma(\gamma)$ is an increasing-decreasing-increasing function, thus $W(\gamma)$ is a double well function, the same definition of $W(\gamma)$ can be found in [29].*

2.4 Error estimates

In this section we will prove an error estimate for the LDG discretization of the phase transition model (2.1) and also for the VC-equations (2.3) when

ν, λ are finite and strictly positive. In the proof, the stress-strain relation is linear and we assume that the system is hyperbolic.

2.4.1 Projection operator

In what follows, we will use two projections $\pi^\pm$ from the Sobolev space $H^1(\Omega)$ onto the finite element space V_h^k ,

$$\pi^\pm : H^1(\Omega) \rightarrow V_h^k,$$

which are defined as follows. Given a function $\psi \in H^1(\Omega)$ and an arbitrary element $K_j \subset \Omega, j = 1, \dots, M$, the restriction of $\pi^\pm \psi$ to K_j is defined as the elements of $P^k(K_j)$ that satisfy:

$$\begin{aligned} \int_{K_j} (\pi^+ \psi - \psi) \omega dx &= 0, \\ \forall \omega \in P^{k-1}(K_j), \pi^+ \psi(x_{j-1/2}^+) &= \psi(x_{j-1/2}^+), \\ \int_{K_j} (\pi^- \psi - \psi) \omega dx &= 0, \\ \forall \omega \in P^{k-1}(K_j), \pi^- \psi(x_{j+1/2}^-) &= \psi(x_{j+1/2}^-). \end{aligned} \quad (2.19)$$

For the projections mentioned above, it is easy to see (c.f. [27]) that,

$$\|\pi^\pm \psi - \psi\|_\Omega \leq Ch^{k+1}, \quad (2.20)$$

with the positive constant C only depending on u and independent of h . We will denote the standard L^2 -inner product as $(\cdot, \cdot)_\Omega$ and the L^2 -norm as $\|\cdot\|_\Omega$.

2.4.2 Notations and Lemmas for the LDG discretization

The error analysis can be greatly simplified by introducing the DG discretization operator $\mathcal{D}$,

$$\mathcal{D}(\eta, \phi; \hat{\eta}) = \sum_j \mathcal{D}_{K_j}(\eta, \phi; \hat{\eta}), \quad (2.21)$$

where $\mathcal{D}_{K_j}(\eta, \phi; \hat{\eta})$ is defined in each element K_j as:

$$\mathcal{D}_{K_j}(\eta, \phi; \hat{\eta}) = -(\eta, \phi_x)_{K_j} + (\hat{\eta} \phi^-)_{j+1/2} - (\hat{\eta} \phi^+)_{j-1/2}. \quad (2.22)$$

The following lemma from [122] gives very useful relations for the operator $\mathcal{D}$.

Lemma 2.1.1. *The DG discretization operator (2.21) with periodic boundary conditions satisfies the following relations: for all $\phi \in V_h^k$,*

$$\mathcal{D}(\eta, \phi; \eta^-) + \mathcal{D}(\phi, \eta; \phi^+) = 0, \quad (2.23a)$$

$$\mathcal{D}(\eta, \phi; \eta^+) + \mathcal{D}(\phi, \eta; \phi^-) = 0, \quad (2.23b)$$

$$\mathcal{D}(\eta - \pi^- \eta, \phi; (\eta - \pi^- \eta)^-) = 0, \quad (2.23c)$$

$$\mathcal{D}(\eta - \pi^+ \eta, \phi; (\eta - \pi^+ \eta)^+) = 0. \quad (2.23d)$$

For the error analysis of the LDG scheme given by (2.7)-(2.10), we define the following two bilinear forms:

$$\begin{aligned} \mathcal{A}(\gamma, v, s, p, q; \phi, \varphi, \eta, \xi, \tau) &= \sum_j \mathcal{A}_{K_j}(\gamma, v, s, p, q; \phi, \varphi, \eta, \xi, \tau), \\ \mathcal{B}(\gamma, v, s, p, q; \phi, \varphi, \eta, \xi, \tau) &= \sum_j \mathcal{B}_{K_j}(\gamma, v, s, p, q; \phi, \varphi, \eta, \xi, \tau), \end{aligned} \quad (2.24)$$

with

$$\begin{aligned} \mathcal{A}_{K_j}(\gamma, v, s, p, q; \phi, \varphi, \eta, \xi, \tau) &= \\ &(\gamma_t, \phi)_{K_j} + (v_t, \varphi)_{K_j} + (s, \eta)_{K_j} + (p_t, \xi)_{K_j} + (q, \tau)_{K_j}, \\ \mathcal{B}_{K_j}(\gamma, v, s, p, q; \phi, \varphi, \eta, \xi, \tau) &= \\ &-\mathcal{D}_{K_j}(v, \phi; v^+) - \sigma' \mathcal{D}_{K_j}(\gamma, \varphi; \gamma^-) - \nu \mathcal{D}_{K_j}(q, \varphi; q^-) + \lambda \mathcal{D}_{K_j}(s, \varphi; s^-) \\ &-\mathcal{D}_{K_j}(p, \eta; p^+) - \mathcal{D}_{K_j}(\gamma_t, \xi; \gamma^-) - \mathcal{D}_{K_j}(v, \tau; v^+). \end{aligned}$$

The LDG scheme for the VC equations (2.3), given by (2.7), (2.9a), (2.9b), (2.9d) and (2.15) and numerical fluxes (2.8), (2.10) can now be expressed as: find $\gamma_h, v_h, s_h, p_h, q_h \in V_h^k$, such that for all test functions $\phi, \varphi, \eta, \xi, \tau \in V_h^k$, the following relation is satisfied.

$$\mathcal{A}(\gamma_h, v_h, s_h, p_h, q_h; \phi, \varphi, \eta, \xi, \tau) + \mathcal{B}(\gamma_h, v_h, s_h, p_h, q_h; \phi, \varphi, \eta, \xi, \tau) = 0, \quad (2.25)$$

where we use in this formulation the time derivative of (2.9c), given by (2.15).

We also define the following error contributions:

$$\begin{aligned} e_\gamma &= \gamma - \gamma_h = \gamma - \pi^- \gamma + \pi^- e_\gamma, \quad e_v = v - v_h = v - \pi^+ v + \pi^+ e_v, \\ e_s &= s - s_h = s - \pi^- s + \pi^- e_s, \quad e_p = p - p_h = p - \pi^+ p + \pi^+ e_p, \\ e_q &= q - q_h = q - \pi^- q + \pi^- e_q. \end{aligned} \quad (2.26)$$

2.4.3 Error estimates of the initial conditions

We choose the initial conditions as

$$\gamma_h(x, 0) = \pi^- \gamma(x, 0), \quad v_h(x, 0) = \pi^+ v(x, 0), \quad (2.27)$$

then (2.20) gives

$$\begin{aligned} \|v(\cdot, 0) - v_h(\cdot, 0)\|_\Omega &\leq Ch^{k+1}, \\ \|\gamma(\cdot, 0) - \gamma_h(\cdot, 0)\|_\Omega &\leq Ch^{k+1}, \end{aligned} \quad (2.28)$$

which means

$$\|\pi^+ e_v(t=0)\|_\Omega \leq Ch^{k+1}, \quad \|\pi^- e_\gamma(t=0)\|_\Omega \leq Ch^{k+1}. \quad (2.29)$$

From (2.9c), we can easily get

$$\begin{aligned} &\int_{K_j} (p(x, 0) - p_h(x, 0)) \xi dx + \int_{K_j} (\gamma(x, 0) - \gamma_h(x, 0)) \xi_x \\ &\quad - (\hat{\gamma}(x, 0) - \hat{\gamma}_h(x, 0)) \xi^-|_{j+1/2} + (\hat{\gamma}(x, 0) - \hat{\gamma}_h(x, 0)) \xi^+|_{j-1/2} \\ &= 0. \end{aligned} \quad (2.30)$$

For the choice $\hat{\gamma} = \gamma^-$ using (2.27), we have

$$\int_{K_j} (p(x, 0) - p_h(x, 0)) \xi dx = 0. \quad (2.31)$$

Choosing $\xi = \pi^- e_p(x, 0)$, we then easily get the relation

$$\|\pi^- e_p(t=0)\|_\Omega \leq Ch^{k+1}. \quad (2.32)$$

2.4.4 A priori error estimate of the LDG discretization

In the next theorem, we provide an error estimate for the LDG discretization (2.7) - (2.10) of the phase transition model (2.1) using the VC-equations (2.3) with ν, λ going to zero. We consider a linear stress-strain relation and assume that the system is hyperbolic.

Theorem 2.2. *Assume a linear stress-strain relation in the phase transition model (2.1) and the related VC-equations (2.3) with $\sigma(\gamma) = \gamma_0 + \sigma' \gamma$, where the constant σ' satisfies $\sigma' \geq C_\sigma^2 > 0$. Assume that the exact solution satisfies*

$\gamma(t) \in H^{k+2}(\Omega), v(t) \in H^{k+1}(\Omega)$ for $t \in (t_0, T]$ on a domain $\Omega \subset \mathbf{R}$ with periodic boundary conditions. Let $\gamma_h, v_h \in V_h^k$, the space of element wise discontinuous polynomials of degree up to k , be the numerical solution of the semi-discrete LDG scheme (2.7) - (2.10) and initial condition (2.27). If the parameters $\nu, \lambda \downarrow 0$, with the number $\omega = 2\sqrt{\lambda}/\nu$ constant and $\lambda \sim h$, then the following error estimate for the LDG solution of (2.1) holds:

$$\sigma' \|e_\gamma\|_\Omega^2 + 2 \|e_v\|_\Omega^2 \leq Ch^{2k+2}, \quad (2.33)$$

where C depends on the final time T , $\|\gamma\|_{L^\infty(0,T);H^{k+2}(\Omega)}$, $\|v\|_{L^\infty(0,T);H^{k+1}(\Omega)}$ and $\|\gamma_t\|_{L^\infty(0,T);H^{k+1}(\Omega)}$.

Proof. We give proof for the error estimates in the following steps.

• **Energy equation for the error estimates**

After choosing the test functions in (2.25) as

$$\phi = \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \varphi = \pi^+ e_v, \eta = \lambda \pi^- e_{\gamma_t}, \xi = \lambda \pi^+ e_p, \tau = \nu \pi^- e_q,$$

using the consistency of the LDG scheme and summation over all elements K_j , we obtain the following relation for the error

$$\begin{aligned} & \mathcal{A}(\gamma - \gamma_h, v - v_h, s - s_h, p - p_h, q - q_h; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \pi^+ e_v, \\ & \quad \lambda \pi^- e_{\gamma_t}, \lambda \pi^+ e_p, \nu \pi^- e_q) + \\ & \mathcal{B}(\gamma - \gamma_h, v - v_h, s - s_h, p - p_h, q - q_h; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \pi^+ e_v, \\ & \quad \lambda \pi^- e_{\gamma_t}, \lambda \pi^+ e_p, \nu \pi^- e_q) = 0. \end{aligned} \quad (2.34)$$

If we introduce now the relations for the error given by (2.26), we can express (2.34) as

$$\begin{aligned} & \mathcal{A}(\gamma - \pi^- \gamma, v - \pi^+ v, s - \pi^- s, p - \pi^+ p, q - \pi^- q; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \\ & \quad \pi^+ e_v, \lambda \pi^- e_{\gamma_t}, \lambda \pi^+ e_p, \nu \pi^- e_q) + \\ & \mathcal{B}(\gamma - \pi^- \gamma, v - \pi^+ v, s - \pi^- s, p - \pi^+ p, q - \pi^- q; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \\ & \quad \pi^+ e_v, \lambda \pi^- e_{\gamma_t}, \lambda \pi^+ e_p, \nu \pi^- e_q) + \\ & \mathcal{A}(\pi^- e_\gamma, \pi^+ e_v, \pi^- e_s, \pi^+ e_p, \pi^- e_q; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \pi^+ e_v, \lambda \pi^- e_{\gamma_t}, \\ & \quad \lambda \pi^+ e_p, \nu \pi^- e_q) + \\ & \mathcal{B}(\pi^- e_\gamma, \pi^+ e_v, \pi^- e_s, \pi^+ e_p, \pi^- e_q; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \pi^+ e_v, \lambda \pi^- e_{\gamma_t}, \\ & \quad \lambda \pi^+ e_p, \nu \pi^- e_q) = 0. \end{aligned} \quad (2.35)$$

Next, if we use the expressions for $\mathcal{A}$ and $\mathcal{B}$ given by (2.24) and the properties of the operator $\mathcal{D}$ defined in Lemma 1, we obtain after a lengthy but straightforward computation that

$$\begin{aligned}
 & \mathcal{A}(\pi^- e_\gamma, \pi^+ e_v, \pi^- e_s, \pi^+ e_p, \pi^- e_q; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \pi^+ e_v, \lambda \pi^- e_{\gamma_t}, \\
 & \quad \lambda \pi^+ e_p, \nu \pi^- e_q) + \\
 & \mathcal{B}(\pi^- e_\gamma, \pi^+ e_v, \pi^- e_s, \pi^+ e_p, \pi^- e_q; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \pi^+ e_v, \lambda \pi^- e_{\gamma_t}, \\
 & \quad \lambda \pi^+ e_p, \nu \pi^- e_q) = \\
 & \frac{1}{2} \frac{d}{dt} (\sigma' \|\pi^- e_\gamma\|_\Omega^2 + \|\pi^+ e_v\|_\Omega^2 + \lambda \|\pi^+ e_p\|_\Omega^2) + \nu \|\pi^- e_q\|_\Omega^2. \tag{2.36}
 \end{aligned}$$

Also, using (2.23c), (2.23d) in Lemma 1 and the properties of the projection operators $\pi^\pm$ given by (2.19), we obtain the relation

$$\begin{aligned}
 & \mathcal{B}(\gamma - \pi^- \gamma, v - \pi^+ v, s - \pi^- s, p - \pi^+ p, q - \pi^- q; \sigma' \pi^- e_\gamma - \lambda \pi^- e_s, \\
 & \quad \pi^+ e_v, \lambda \pi^- e_{\gamma_t}, \lambda \pi^+ e_p, \nu \pi^- e_q) \\
 & = -\lambda \mathcal{D}((\gamma - \pi^- \gamma)_t, \pi^+ e_p; (\gamma - \pi^- \gamma)_t^-) \\
 & \quad - \sigma' \mathcal{D}(\gamma - \pi^- \gamma, \pi^+ e_v; (\gamma - \pi^- \gamma)^-) \\
 & \quad - \mathcal{D}(v - \pi^+ v, \sigma' \pi^- e_\gamma - \lambda \pi^- e_s; (v - \pi^+ v)^+) \\
 & \quad - \nu \mathcal{D}((v - \pi^+ v), \pi^- e_q; (v - \pi^+ v)^+) \\
 & \quad + \lambda \mathcal{D}(s - \pi^- s, \pi^+ e_v; (s - \pi^- s)^-) \\
 & \quad - \lambda \mathcal{D}(p - \pi^+ p, \pi^- e_{\gamma_t}; (p - \pi^+ p)^+) \\
 & \quad - \nu \mathcal{D}(q - \pi^- q, \pi^+ e_v; (q - \pi^- q)^-) \\
 & = 0. \tag{2.37}
 \end{aligned}$$

If we introduce now relations (2.36)-(2.37) into (2.35), and use (2.24), the error equation (2.35) can be simplified as

$$\begin{aligned}
 & \frac{1}{2} \frac{d}{dt} (\sigma' \|\pi^- e_\gamma\|_\Omega^2 + \|\pi^+ e_v\|_\Omega^2 + \lambda \|\pi^+ e_p\|_\Omega^2) + \nu \|\pi^- e_q\|_\Omega^2 \\
 & + \mathcal{G} - \lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega + \lambda((s - \pi^- s), \pi^- e_{\gamma_t})_\Omega = 0, \tag{2.38}
 \end{aligned}$$

where we define the following contribution

$$\begin{aligned}
 \mathcal{G} = & \sigma'((\gamma - \pi^- \gamma)_t, \pi^- e_\gamma)_\Omega + ((v - \pi^+ v)_t, \pi^+ v)_\Omega \\
 & + \lambda((p - \pi^+ e_p)_t, \pi^+ e_p)_\Omega + \nu(q - \pi^- q, \pi^- e_q)_\Omega.
 \end{aligned}$$

In the following, we will give estimates for $\mathcal{G}$, $\lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega$ and $\lambda((s - \pi^- s), \pi^- e_{\gamma_t})_\Omega$ separately.

• **Error estimate for $\mathcal{G}$.**

Using Cauchy's inequality with ϵ and the interpolation estimate (2.20), we can estimate $\mathcal{G}$ as

$$\begin{aligned} \mathcal{G} &\leq \frac{\sigma'}{4\epsilon_1^2} \|\gamma_t - \pi^- \gamma_t\|_\Omega^2 + \sigma' \epsilon_1^2 \|\pi^- e_\gamma\|_\Omega^2 + \frac{1}{4\epsilon_2^2} \|v_t - \pi^+ v_t\|_\Omega^2 \\ &\quad + \epsilon_2^2 \|\pi^+ e_v\|_\Omega^2 + \frac{\lambda}{4\epsilon_3^2} \|p_t - \pi^+ p_t\|_\Omega^2 + \lambda \epsilon_3^2 \|\pi^+ e_p\|_\Omega^2 \\ &\quad + \frac{\nu}{4\epsilon_4^2} \|q - \pi^- q\|_\Omega^2 + \nu \epsilon_4^2 \|\pi^- e_q\|_\Omega^2 \\ &\leq Ch^{2k+2} + \sigma' \epsilon_1^2 \|\pi^- e_\gamma\|_\Omega^2 + \epsilon_2^2 \|\pi^+ e_v\|_\Omega^2 + \lambda \epsilon_3^2 \|\pi^+ e_p\|_\Omega^2 \\ &\quad + \nu \epsilon_4^2 \|\pi^- e_q\|_\Omega^2. \end{aligned} \quad (2.39)$$

with $\epsilon_i > 0$, ($i = 1, 2, 3, 4$). Introducing (2.39) into (2.38) gives:

$$\begin{aligned} &\frac{1}{2} \frac{d}{dt} (\sigma' \|\pi^- e_\gamma\|_\Omega^2 + \|\pi^+ e_v\|_\Omega^2 + \lambda \|\pi^+ e_p\|_\Omega^2) + \nu \|\pi^- e_q\|_\Omega^2 \\ &\quad - \lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega + \lambda(s - \pi^- s, \pi^- e_{\gamma_t})_\Omega \leq Ch^{2k+2} + \\ &\quad \sigma' \epsilon_1^2 \|\pi^- e_\gamma\|_\Omega^2 + \epsilon_2^2 \|\pi^+ e_v\|_\Omega^2 + \lambda \epsilon_3^2 \|\pi^+ e_p\|_\Omega^2 + \nu \epsilon_4^2 \|\pi^- e_q\|_\Omega^2. \end{aligned} \quad (2.40)$$

• **Error estimate for $\lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega$.**

Next, we consider the contribution $\lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega$. Using the Cauchy and Schwarz inequalities we obtain:

$$\lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega \leq \frac{1}{2} \|\gamma_t - \pi^- \gamma_t\|_\Omega^2 + \frac{\lambda^2}{2} \|\pi^- e_s\|_\Omega^2. \quad (2.41)$$

The upper bound in (2.41) contains, however, $\|\pi^- e_s\|_\Omega$, which can not be directly bounded in (2.38). We therefore use the LDG equation (2.16d) together with the numerical fluxes (2.10) to derive the following error equation

$$\begin{aligned} &(s - s_h, \eta)_{K_j} + (p - p_h, \eta_x)_{K_j} - ((p - p_h)^+ \eta^-)_{j+1/2} \\ &\quad + ((p - p_h)^+ \eta^+)_{j-1/2} = 0, \quad \forall \eta \in V_h^k. \end{aligned} \quad (2.42)$$

Using the error relations (2.26), we can transform (2.42) into

$$\begin{aligned} &(s - \pi^- s, \eta)_{K_j} + (\pi^- e_s, \eta)_{K_j} + (\pi^+ e_p, \eta_x)_{K_j} - (\pi^+ e_p)^+ \eta^-|_{j+1/2} \\ &\quad + (\pi^+ e_p)^+ \eta^+|_{j-1/2} = 0, \quad \forall \eta \in V_h^k. \end{aligned} \quad (2.43)$$

Here, we used that

$$(p - \pi^+ p, \eta_x)_{K_j} - (p - \pi^+ p)^+ \eta^-|_{j+1/2} + (p - \pi^+ p)^+ \eta^+|_{j-1/2} = 0,$$

for the projection operator π^+ defined in (2.19) and $\eta \in V_h^k$.

The error equation (2.43) can be further evaluated using the following trace and inverse inequalities

$$|\eta(x_{j\pm\frac{1}{2}})| \leq \frac{C_{trace}}{\sqrt{h}} \|\eta\|_{K_j}, \quad \|\eta_x\|_{K_j} \leq \frac{C_{inv}}{h} \|\eta\|_{K_j}, \quad \text{for } \eta \in V_h^k$$

and selecting $\eta = \pi^- e_s$. This provides an estimate for $\|\pi^- e_s\|_\Omega$ by summing over the elements K_j and introducing ϵ_5

$$\|\pi^- e_s\|_\Omega \leq \frac{1}{2\sqrt{\epsilon_5}} \|s - \pi^- s\|_\Omega + \frac{\sqrt{\epsilon_5}}{2h} (C_{inv} + C_{trace}) \|\pi^+ e_p\|_\Omega. \quad (2.44)$$

Collecting all contributions and using the interpolation estimate (2.20) then results in the following estimate for (2.41)

$$\begin{aligned} \lambda(\gamma_t - \pi^- \gamma_t, \pi^- e_s)_\Omega &\leq \frac{1}{2} \|\gamma_t - \pi^- \gamma_t\|_\Omega^2 + \frac{\lambda^2}{4\epsilon_5} \|s - \pi^- s\|_\Omega^2 \\ &\quad + \frac{\epsilon_5}{4h^2} \lambda^2 (C_{inv} + C_{trace})^2 \|\pi^+ e_p\|_\Omega^2. \end{aligned} \quad (2.45)$$

Note that the parameter λ in the VC system (2.3) goes to zero, so if we choose

$$\lambda \sim O(h), \quad \lambda = 2C_1 h, \quad (2.46)$$

(2.45) becomes

$$\lambda(\gamma_t - \pi^- \gamma_t, \pi^- e_s)_\Omega \leq Ch^{2k+2} + \epsilon_5 C_1^2 (C_{inv} + C_{trace})^2 \|\pi^+ e_p\|_\Omega^2. \quad (2.47)$$

Introducing (2.47) into (2.40) and after integration in time, we obtain,

$$\begin{aligned} &\frac{1}{2} (\sigma' \|\pi^- e_\gamma\|_\Omega^2 + \|\pi^+ e_v\|_\Omega^2 + \lambda \|\pi^+ e_p\|_\Omega^2) + \nu \int_0^t \|\pi^- e_q\|_\Omega^2 dt \\ &\quad + \lambda \int_0^t (s - \pi^- s, \pi^- e_{\gamma_t})_\Omega dt \\ &\leq Ch^{2k+2} + \frac{1}{2} \sigma' \|\pi^- e_\gamma(t=0)\|_\Omega^2 + \frac{1}{2} \|\pi^+ e_v(t=0)\|_\Omega^2 \\ &\quad + \frac{1}{2} \lambda \|\pi^+ e_p(t=0)\|_\Omega^2 + \int_0^t (\sigma' \epsilon_1^2 \|\pi^- e_\gamma\|_\Omega^2 + \epsilon_2^2 \|\pi^+ e_v\|_\Omega^2 \\ &\quad + \nu \epsilon_4^2 \|\pi^- e_q\|_\Omega^2 + (\lambda \epsilon_3^2 + \epsilon_5 C_1^2 (C_{inv} + C_{trace})^2) \|\pi^+ e_p\|_\Omega^2) dt. \end{aligned} \quad (2.48)$$

Finally, introducing the estimates of the initial conditions (2.29) and (2.32) into (2.48) results in the estimate

$$\begin{aligned}
 & \frac{1}{2} (\sigma' \|\pi^- e_\gamma\|_\Omega^2 + \|\pi^+ e_v\|_\Omega^2 + \lambda \|\pi^+ e_p\|_\Omega^2) + \nu \int_0^t \|\pi^- e_q\|_\Omega^2 dt \\
 & \quad + \lambda \int_0^t (s - \pi^- s, \pi^- e_{\gamma_t})_\Omega dt \\
 & \leq Ch^{2k+2} + \int_0^t (\sigma' \epsilon_1^2 \|\pi^- e_\gamma\|_\Omega^2 + \epsilon_2^2 \|\pi^+ e_v\|_\Omega^2 + \nu \epsilon_4^2 \|\pi^- e_q\|_\Omega^2 \\
 & \quad + (\lambda \epsilon_3^2 + \epsilon_5 C_1^2 (C_{inv} + C_{trace})^2) \|\pi^+ e_p\|_\Omega^2) dt.
 \end{aligned} \tag{2.49}$$

• **Error estimate for $\lambda \int_0^t (s - \pi^- s, \pi^- e_{\gamma_t})_\Omega dt$.**

Consider now $\lambda \int_0^t (s - \pi^- s, \pi^- e_{\gamma_t})_\Omega dt$. Using (2.29), this contribution can be estimated straightforwardly as

$$\begin{aligned}
 & \lambda \int_0^t (s - \pi^- s, \pi^- e_{\gamma_t})_\Omega dt \\
 & = \lambda (s - \pi^- s, \pi^- e_\gamma)|_0^t - \lambda \int_0^t (s_t - \pi^- s_t, \pi^- e_\gamma) dt \\
 & \leq \lambda \|s - \pi^- s\|_\Omega \|\pi^- e_\gamma\|_\Omega + \lambda \|(s - \pi^- s)(t=0)\|_\Omega \|\pi^- e_\gamma(t=0)\|_\Omega \\
 & \quad + \lambda \int_0^t \|s_t - \pi^- s_t\|_\Omega \|\pi^- e_\gamma\|_\Omega dt \\
 & \leq \frac{\lambda}{4\epsilon_6^2} \|s - \pi^- s\|_\Omega^2 + \lambda \epsilon_6^2 \|\pi^- e_\gamma\|_\Omega^2 + \frac{\lambda}{4\epsilon_7^2} \|(s - \pi^- s)(t=0)\|_\Omega^2 \\
 & \quad + \lambda \epsilon_7^2 \|\pi^- e_\gamma(t=0)\|_\Omega^2 \\
 & \quad + \frac{\lambda}{4\epsilon_8^2} \int_0^t \|(s_t - \pi^- s_t)\|_\Omega^2 dt + \lambda \epsilon_8^2 \int_0^t \|\pi^- e_\gamma\|_\Omega^2 dt \\
 & \leq Ch^{2k+2} + \lambda \epsilon_6^2 \|\pi^- e_\gamma\|_\Omega^2 + \lambda \epsilon_8^2 \int_0^t \|\pi^- e_\gamma\|_\Omega^2 dt.
 \end{aligned} \tag{2.50}$$

Introducing (2.50) into (2.49) gives

$$\begin{aligned}
 & \frac{1}{2} (\sigma' \|\pi^- e_\gamma\|_\Omega^2 + \|\pi^+ e_v\|_\Omega^2 + \lambda \|\pi^+ e_p\|_\Omega^2) + \nu \int_0^t \|\pi^- e_q\|_\Omega^2 dt \\
 & \leq Ch^{2k+2} + \int_0^t (\sigma' \epsilon_1^2 \|\pi^- e_\gamma\|_\Omega^2 + \epsilon_2^2 \|\pi^+ e_v\|_\Omega^2 + \nu \epsilon_4^2 \|\pi^- e_q\|_\Omega^2 \\
 & \quad + (\lambda \epsilon_3^2 + \epsilon_5 C_1^2 (C_{inv} + C_{trace})^2) \|\pi^+ e_p\|_\Omega^2 + \lambda \epsilon_8^2 \|\pi^- e_\gamma\|_\Omega^2) dt \\
 & \quad + \lambda \epsilon_6^2 \|\pi^- e_\gamma\|_\Omega^2,
 \end{aligned} \tag{2.51}$$

which is equivalent to

$$\begin{aligned}
 & \left(\frac{1}{2} \sigma' - \lambda \epsilon_6^2 \right) \|\pi^- e_\gamma\|_\Omega^2 + \frac{1}{2} \|\pi^+ e_v\|_\Omega^2 + \frac{\lambda}{2} \|\pi^+ e_p\|_\Omega^2 + \\
 & \quad \nu (1 - \epsilon_4^2) \int_0^t \|\pi^- e_q\|_\Omega^2 dt \\
 & \leq Ch^{2k+2} + \int_0^t \left((\sigma' \epsilon_1^2 + \lambda \epsilon_8^2) \|\pi^- e_\gamma\|_\Omega^2 + \epsilon_2^2 \|\pi^+ e_v\|_\Omega^2 + \right. \\
 & \quad \left. (\lambda \epsilon_3^2 + \epsilon_5 C_1^2 (C_{inv} + C_{trace})^2) \|\pi^+ e_p\|_\Omega^2 \right) dt. \tag{2.52}
 \end{aligned}$$

Choose now $\epsilon_1 = \frac{1}{2\sqrt{2}}$ and ϵ_6, ϵ_8 as

$$\begin{aligned}
 \epsilon_6 &= \frac{1}{2} \sqrt{\frac{\sigma'}{\lambda}}, \text{ then } \frac{1}{2} \sigma' - \lambda \epsilon_6^2 = \frac{1}{4} \sigma', \\
 \epsilon_8 &= \frac{1}{2} \sqrt{\frac{\sigma'}{2\lambda}}, \text{ then } \sigma' \epsilon_1^2 + \lambda \epsilon_8^2 = \frac{1}{4} \sigma'. \tag{2.53}
 \end{aligned}$$

Select $\epsilon_3 = \frac{1}{2}$ and ϵ_5 such that

$$\lambda \epsilon_3^2 + \epsilon_5 C_1^2 (C_{inv} + C_{trace})^2 = \frac{\lambda}{2}.$$

Finally, choosing $\epsilon_2 = \epsilon_4 = \frac{1}{\sqrt{2}}$, we obtain the inequality

$$\begin{aligned}
 & \frac{\sigma'}{4} \|\pi^- e_\gamma\|_\Omega^2 + \frac{1}{2} \|\pi^+ e_v\|_\Omega^2 + \frac{\lambda}{2} \|\pi^+ e_p\|_\Omega^2 \\
 & \leq Ch^{2k+2} + \int_0^t \left(\frac{\sigma'}{4} \|\pi^- e_\gamma\|_\Omega^2 + \frac{1}{2} \|\pi^+ e_v\|_\Omega^2 + \frac{\lambda}{2} \|\pi^+ e_p\|_\Omega^2 \right) dt. \tag{2.54}
 \end{aligned}$$

Since $\lambda \downarrow 0$, the final estimate for the error contributions is now obtained using Gronwall's Lemma for integrals, resulting in:

$$\max_t \frac{\sigma'}{4} \|\pi^- e_\gamma\|_\Omega^2 + \max_t \frac{1}{2} \|\pi^+ e_v\|_\Omega^2 \leq Ch^{2k+2}, \tag{2.55}$$

and using (2.26), (2.55) gives the result stated in Theorem 2.2. $\square$

Remark 2.2. For the case $\lambda, \nu \downarrow 0$ with $\omega = 2\sqrt{\lambda}/\nu$ constant we obtain by choosing $\lambda = 2C_1 h$, ϵ_6, ϵ_8 as (2.53) and $0 < \epsilon_4 < 1$, that the bounding constant C in (2.33) is independent of ν and λ .

Corollary 2.3. *Under the assumptions of Theorem 2.2 except, that $\lambda, \nu > 0$ have finite, strictly positive values, the following error estimate holds,*

$$\sigma' \|e_\gamma\|_\Omega^2 + 2\|e_v\|_\Omega^2 + 2\lambda\|e_p\|_\Omega^2 \leq Ch^{2k},$$

where C depends on the final time T , $\|\gamma\|_{L^\infty(0,T);H^{k+2}(\Omega)}$, $\|v\|_{L^\infty(0,T);H^{k+1}(\Omega)}$ and $\|\gamma_t\|_{L^\infty(0,T);H^{k+1}(\Omega)}$.

Proof. Since $\lambda > 0$ has a finite value, the term $\lambda(\gamma_t - \pi^- \gamma_t, \pi^- e_s)_\Omega$ in (2.45) should be estimated in a different way.

• **Error estimate for $\lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega$.**

Using the Cauchy and Schwarz inequalities we obtain:

$$\lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega \leq \frac{1}{2h^2} \|\gamma_t - \pi^- \gamma_t\|_\Omega^2 + \frac{\lambda^2 h^2}{2} \|\pi^- e_s\|_\Omega^2. \quad (2.56)$$

Using (2.44), (2.56) becomes

$$\lambda((\gamma - \pi^- \gamma)_t, \pi^- e_s)_\Omega \leq Ch^{2k} + \epsilon_5 \frac{\lambda^2}{4} (C_{inv} + C_{trace})^2 \|\pi^+ e_p\|_\Omega^2. \quad (2.57)$$

The rest proof is similar to the proof of Theorem 2.2, finally we obtain the result stated in Corollary 2.3. □

2.5 Linear stability analysis of the LDG scheme

In order to obtain a reasonable estimate for a stable time step for the third order accurate TVD Runge-Kutta scheme (2.13) applied to the LDG discretization, we perform in this section a linear stability analysis.

First, we explain the specific problem that we analyze. The parameters ν , λ in the VC-equations (2.3) are defined as in [29]:

$$\nu = 2\nu_0, \quad \lambda = \omega^2 \nu_0^2, \quad (2.58)$$

where

$$\nu_0 = \left(\sup_{\gamma \geq -1} \max\{0, \sigma'(\gamma)\} \right)^{1/2} (\Delta x)^\beta, \quad (2.59)$$

for $\beta \in (0, 1]$ and $\omega = 2\sqrt{\lambda}/\nu$ a fixed number. We assume that the stress-strain relation $\sigma(\gamma)$ in (2.3) is a trilinear function, defined as

$$\sigma(\gamma) = \begin{cases} \mu_1\gamma, & \gamma \in (-1, \gamma_M), \\ -\mu_2\gamma + b, & \gamma \in (\gamma_M, \gamma_m), \\ \mu_3\gamma, & \gamma \in (\gamma_m, \infty), \end{cases} \quad (2.60)$$

see also Figure 2.1. We thus consider locally a linear stress-strain relation $\sigma(\gamma) = \sigma'\gamma$, and assume that $\sigma' > 0$. In the elliptic part, where $\sigma' < 0$, the exact solution is unstable and γ will rapidly move to the hyperbolic part. The third order TVD Runge-Kutta time stepping method (2.13) has an amplification matrix Q , that is equal to

$$Q = Id + A + \frac{1}{2}A^2 + \frac{1}{6}A^3, \quad (2.61)$$

with $A = \Delta t B$ and $F(U(t)) = BU(t)$ after linearization of $\sigma(\gamma)$. For stability, the following condition on the operator norm of Q must hold

$$\|Q\| \leq 1, \quad (2.62)$$

which is equivalent in the hyperbolic part to

$$\left| 1 + \lambda_i + \frac{1}{2}\lambda_i^2 + \frac{1}{6}\lambda_i^3 \right| \leq 1, \quad (2.63)$$

with λ_i the eigenvalues of A for $i = 1, \dots, n$, and provides a restriction on the time step Δt . Since A depends on the polynomial order used in the LDG discretization, we will compute now the time step restriction for various polynomial orders.

Since the LDG matrix A has a block Toeplitz structure on a uniform mesh when periodic boundary conditions are applied, we can compute the eigenvalues using a discrete Fourier transform. For piecewise constant polynomials, we obtain the matrix

$$\hat{\mathbf{A}}(\theta) = \frac{\Delta t}{\Delta x} \begin{pmatrix} 0 & a \\ \sigma' b - \frac{\lambda}{\Delta x^2} ab^2 & \frac{\nu}{\Delta x} ab \end{pmatrix}, \quad (2.64)$$

with

$$a = e^{i\theta} - 1, \quad b = 1 - e^{-i\theta}, \quad c = ab = -4 \sin^2\left(\frac{\theta}{2}\right) \text{ and } \theta \in [-\pi, \pi).$$

The eigenvalues of $\hat{\mathbf{A}}$, taking (2.58) and (2.59) into account, are equal to

$$\begin{aligned}\lambda_{1,2} &= \frac{\Delta t}{\Delta x} \frac{\nu}{\Delta x} \left(\frac{c}{2} \pm \sqrt{(1 - \omega^2) \frac{c^2}{4} + \frac{\sigma' c}{(\nu/\Delta x)^2}} \right) \\ &= \Delta t \mu \left(c \pm \sqrt{(1 - \omega^2) c^2 + \frac{\sigma' c}{\mu}} \right),\end{aligned}\tag{2.65}$$

with $\mu = \frac{\nu}{2(\Delta x)^2}$. Given a value of ω, σ' and μ we can compute now the time step Δt such that $\lambda_{1,2}$ satisfy (2.63) for all $\theta \in [-\pi, \pi]$.

For linear basis functions, we obtain the matrix $\hat{\mathbf{A}}(\theta)$

$$\hat{\mathbf{A}}(\theta) = \Delta t \begin{pmatrix} \mathbf{0} & p \\ \sigma' q - \lambda q p q & \nu q p \end{pmatrix} \begin{pmatrix} \gamma_0 \\ \gamma_1 \\ v_0 \\ v_1 \end{pmatrix},\tag{2.66}$$

with

$$\begin{aligned}p &= \frac{1}{\Delta x} \begin{pmatrix} e^{i\theta} - 1 & 1 - e^{i\theta} \\ 3(e^{i\theta} - 1) & -3(e^{i\theta} + 1) \end{pmatrix}, \\ q &= \frac{1}{\Delta x} \begin{pmatrix} 1 - e^{-i\theta} & 1 - e^{-i\theta} \\ 3(e^{-i\theta} - 1) & 3(1 + e^{-i\theta}) \end{pmatrix}.\end{aligned}$$

The matrix $\hat{\mathbf{A}}(\theta)$ has eigenvalues $\lambda_i(\theta), i = 1, \dots, 4$, which can be used to compute the time step constraint using (2.63) in the same way as done for constant basis functions. Unfortunately, it is not possible to obtain completely analytic expressions for the time step. In the computations performed in the next section, we use the parameters $\max_{\gamma} \sigma' = 20$, $\beta = 1$ in (2.58), (2.59) and determine the time step $\Delta t = CFL \Delta x$ with

$$CFL \leq \begin{cases} 0.03, & \omega = 0.15, \\ 0.05, & \omega = 1.0, \\ 0.02, & \omega = 3.0, \end{cases}\tag{2.67}$$

for constant basis functions, and

$$CFL \leq \begin{cases} 0.006, & \omega = 0.15, \\ 0.008, & \omega = 1.0, \\ 0.01, & \omega = 3.0, \end{cases}\tag{2.68}$$

for linear basis functions. For quadratic basis functions, the numerical experiments show that the CFL bounds should be (2.68) divided by five.

2.6 Numerical experiments

In this section, we describe three numerical experiments to investigate the performance of the proposed LDG scheme. Examples 2.1 and 2.2 are model test cases for phase transition in an elastic solid. Numerical simulations for compressible fluids with a liquid and vapor phase and the Van der Waals equation of state are shown in Example 2.3. For the first test case, which has a trilinear σ function, we computed the exact solution by following the analysis in [3], with the kinetic relation specified in [2]. This model problem was also studied by Cockburn and Gau [29] using a finite difference method, but their calculations only showed convergence to the exact solution for certain values of the coefficients in the VC-equations. In all computations, we employ the LDG scheme (2.7), (2.9) with numerical fluxes given by (2.8) and (2.10).

Example 2.1. Piecewise linear stress-strain curve

For the trilinear stress-strain relation (2.60), we use the following parameters:

$$\gamma_M = 0.1, \quad \gamma_m = 0.2, \quad \mu_1 = 20, \quad \mu_2 = 10, \quad \mu_3 = 5, \quad b = 3.$$

These conditions were also studied in [29]. The parameters ν , λ are chosen as (2.58) and (2.59), and the initial conditions are given by:

$$A: \quad \gamma(x, 0) = \begin{cases} 0.3, & x < 0, \\ 0.4, & x > 0, \end{cases} \quad v(x, 0) = \begin{cases} 0, & x < 0, \\ -0.8, & x > 0, \end{cases} \quad (2.69)$$

which is the most challenging Riemann problem among all possible types of solutions, and includes two phase transitions and two shocks.

The computational domain $[-0.5, 0.5]$ is discretized uniformly by M elements, and we impose the following boundary conditions:

$$\begin{cases} \gamma_0^L = \gamma_0^R, & \gamma_M^R = \gamma_M^L, \\ v_0^L = v_0^R, & v_M^R = v_M^L. \end{cases}$$

We tested the LDG scheme for the solution of the VC-equations (2.3) with piecewise constant, linear and quadratic polynomial basis functions, and compared the results at time $T_{end} = 0.05$ with the exact solution. Here, we only present the results for quadratic polynomials.

First, we compare the exact solution and the numerical solutions in Figure 2.4 for piecewise quadratic basis functions and $\omega = 1.0$ using various mesh resolutions. From this figure, it is clear that the numerical solutions converge well to the exact solution. As expected, there are shock waves and phase

transitions in γ : for example, the left value of γ jumps from the hyperbolic state 0.3 (phase 3) to 0.25 (also in phase 3) with a shock wave, then goes through the elliptic region to 0.05 (phase 1), which gives a phase transition. Next, γ changes phase from phase 1 to phase 3, followed by a shock to the right initial γ state.

Note also that the solution at the phase boundaries remains monotonic without the use of a limiter. Figure 2.5 describes the numerical results of the LDG scheme with quadratic polynomial basis functions for $\omega = 0.15, 1.0$ and 3.0 , when initially both γ values are outside the elliptic region. The effect of changing ω on the solution near the phase boundary is rather small, but relatively large near the shock waves in the hyperbolic region. As can be seen by comparison with Figure 2.5, values $\omega \leq 1$ give better agreement with the exact solution.

If we compare our LDG results with the results of the finite difference method discussed in [29], then the LDG scheme shows the following improvements:

- for $\omega = 0.15$ and a fixed mesh resolution e.g. $M = 800$, the solutions of the LDG scheme in Figure 2.5 are more accurate than those obtained with the finite difference method presented in [29];
- for the parameter $\beta = 1.0$, the numerical solutions of the finite difference method [29] converge to a wrong solution, while the LDG results converge to the exact solution.

Apart from the initial condition (2.69), we also explore three other sets of initial conditions depending on whether the initial value of γ is in the elliptic or hyperbolic region.

B: Both initial γ -values are in the hyperbolic region, but close to the elliptic region,

$$\gamma(x, 0) = \begin{cases} 0.08, & x < 0, \\ 0.22, & x > 0. \end{cases} \quad (2.70)$$

C: One initial γ -value is inside the elliptic region,

$$\gamma(x, 0) = \begin{cases} 0.12, & x < 0, \\ 0.40, & x > 0. \end{cases} \quad (2.71)$$

D: Both initial γ -values are inside the elliptic region,

$$\gamma(x, 0) = \begin{cases} 0.120, & x < 0, \\ 0.125, & x > 0. \end{cases} \quad (2.72)$$

Figure 2.2: piecewise cubic strain-stress relation

We use the same initial condition (2.69) for the velocity in all these test cases.

The results of the LDG calculations of γ , v for the initial conditions B, C, D are shown in Figures 2.6. From these results, we observe that the solutions oscillate and dissipate most near the phase boundary when $\omega = 3.0$. We also plot the traces of the numerical solution (points connecting initial γ -values S_L and S_R) for various initial conditions in Figure 2.7. One important observation is that the solutions never stay inside the elliptic region:

- when an initial state is outside the elliptic region, or the solution evolves to the boundary of the hyperbolic region, the solution will immediately go through the elliptic region to another hyperbolic region;
- when the initial state is inside the elliptic region, the solution will move quickly to a hyperbolic region.

Example 2.2. Cubic stress-strain curve

In this section, we present results of the LDG scheme for the VC-equations (2.3) with a cubic stress-strain relation

$$\sigma(\gamma) = \gamma(\gamma - 0.5)(\gamma - 1), \quad (2.73)$$

see Figure 2.2.

The initial data are given as:

$$\gamma_0(x) = \begin{cases} 1.07265, & x < 0, \\ 0.15000, & x > 0, \end{cases} \quad v_0(x) \equiv 0. \quad (2.74)$$

From the numerical results in Figures 2.8 and 2.9, it is easy to see that:

1. the numerical results in Figures 2.8 and 2.9 are very similar to those of the trilinear stress-strain relation (Figures 2.4-2.6): both of these two test cases include shocks and phase transitions;
2. Figure 2.9 shows the results for quadratic polynomials using various ω values for a fixed mesh resolution $M = 1600$, which indicates that solutions with larger values of ω have more dissipation at the phase boundary;
3. comparing the LDG results with those of the finite difference method in [29], the LDG results are much closer to the exact solution. For example, we don't observe numerical oscillations around the first phase transition in the LDG scheme (see Figures 2.8 and 2.9), which exist in the velocity figures computed with the finite difference method [29].

Table 2.1: Accuracy test for modified VC-equations (2.76) with the exact solution (2.75). Periodic boundary condition. Uniform meshes with M cells at time $t = 0.2$.

	M	L^∞ - error	order	L^2 - error	order
P^0	20	7.33E-02	—	5.54E-02	—
	40	3.54E-02	1.05	2.67E-02	1.05
	80	1.73E-02	1.03	1.32E-02	1.02
	160	8.58E-03	1.01	6.55E-03	1.01
	320	4.28E-03	1.00	3.27E-03	1.00
P^1	20	8.11E-03	—	5.80E-03	—
	40	2.05E-03	1.98	1.45E-03	2.00
	80	5.14E-04	2.00	3.63E-04	2.00
	160	1.28E-04	2.00	9.09E-05	2.00
	320	3.21E-05	2.00	2.27E-05	2.00
P^2	20	2.57E-04	—	1.91E-04	—
	40	3.22E-05	2.99	2.34E-05	3.03
	80	4.04E-06	3.00	2.89E-06	3.02
	160	5.05E-07	3.00	3.59E-07	3.01
	320	6.31E-08	3.00	4.47E-08	3.00

In order to verify the a priori error analysis discussed in Section 2.4, we

also selected the following smooth exact solution,

$$\gamma(x, t) = 0.6 + 0.5 \sin(2\pi x + t), \quad v(x, t) = 0.1 \cos(2\pi x - t), \quad (2.75)$$

which satisfies the VC system (2.3) with source terms $a(x, t)$, $b(x, t)$.

$$\begin{cases} \gamma_t = v_x + a(x, t), \\ v_t = \sigma(\gamma)_x + \nu v_{xx} - \lambda \gamma_{xxx} + b(x, t). \end{cases} \quad (2.76)$$

We compute the error of γ in the L^∞ and L^2 norm, and obtain the order of accuracy. The results are presented in Table 2.1, which shows that for k -th order polynomials the LDG discretization has $k + 1$ -th order accuracy. We emphasize that the numerical results are better than the theoretical error estimate given in Section 2.4.

Example 2.3. General non-monotonic stress-strain curve

Next, we investigate the LDG scheme for (2.3) with a general non-monotonic stress-strain relation. In this part, we consider a viscosity-capillarity model

Figure 2.3: Example of Van der Waals pressure law.

for a compressible fluid with a liquid and vapor phase [24], given by

$$\begin{cases} v_t - u_x = 0, \\ u_t + P(v)_x = \nu u_{xx} - \lambda v_{xxx}, \end{cases} \quad (2.77)$$

where $v = 1/\rho$ is the specific volume, u the particle velocity. The Van der Waals equation of state is given by:

$$P(v, T) = \frac{RT}{v - b} - \frac{a}{v^2},$$

where a , b , R are constants with the temperature $T > 0$ fixed. We use the non-dimensional formulation in which:

$$a = 3, \quad b = \frac{1}{3}, \quad R = \frac{8}{3},$$

and take the relative temperature to be $T = 0.95$.

The system (2.77) under consideration is close to that for (2.2) except for the difference between $\sigma(\gamma)$ and $-P(v)$, which are both increasing-decreasing-increasing functions. With appropriate viscosity and capillarity coefficients, for example $\nu = h$, $\lambda = \omega\nu^2$ with $\omega = 0.5, 1.0$ and 3.0 , we can obtain the same results as those obtained in [24]. Two test cases are considered, both of them use meshes with 400, 800 and 1600 elements.

E: Propagating phase boundary with initial conditions:

$$v(x, 0) = \begin{cases} 0.6, & x < 0, \\ 1.5, & x > 0, \end{cases} \quad u(x, 0) = \begin{cases} -2.0, & x < 0, \\ 0.0, & x > 0. \end{cases}$$

The solutions of the LDG method are considered at time $T_{end} = 0.15$.

F: Stationary phase boundary with initial conditions:

$$v(x, 0) = \begin{cases} 0.684117091, & x < 0, \\ 1.72700257, & x > 0, \end{cases} \quad u(x, 0) \equiv 0. \quad (2.78)$$

This initial condition is very close to the Maxwell stationary phase boundary and the LDG method should keep the Maxwell discontinuity stationary. The numerical results are shown at $T_{end} = 0.2$.

Figures 2.10 and 2.11 show solutions obtained with the LDG method for various mesh resolutions $M = 400, 800, 1600$; Figures 2.12 and 2.13 show solutions with various values of ω . From these figures, we can draw several conclusions:

1. The numerical solutions converge consistently;

2. Figures 2.10 and 2.12 show that the propagating phase boundary case also includes both shock waves and phase transitions;
3. Figures 2.11 and 2.13 show that the LDG method keeps the Maxwell discontinuity stationary;
4. Figure 2.12 shows for various values of ω that the width of the jump in the specific volume v is larger for bigger ω .

From this test case, we conclude that the LDG method that we presented in this chapter also applies to the VC system (2.3) with general nonlinear stress-strain relations σ .

2.7 Conclusion

In this chapter, we have designed, analyzed and tested an LDG method for the numerical solution of the VC equations modeling the propagation of phase transitions in solids [29] and fluids [24]. L^2 -stability is proved for general solutions of the VC system. We also provide an a priori error estimate of the semi-discrete local discontinuous Galerkin method when the solutions are assumed to be sufficiently smooth and the stress-strain relation in (2.1) and (2.3) is linear. Also, a linear stability analysis is performed to obtain an estimate for a stable time step in the Runge-Kutta time integration method. Numerical experiments show that the results of the LDG scheme converge well to the exact solution of the phase transition model given by (2.1). Moreover, the LDG scheme can also be applied to a model of Van der Waals fluids [24] when the artificial viscosity is taken to be proportional to Δx . The error analysis for a linear stress-strain relation shows that the LDG discretization of the phase transition model (2.1) is of optimal order, when $\lambda \sim Ch$ and $\lambda, \nu \downarrow 0$, with $\omega = 2\sqrt{\lambda}/\nu$ fixed. For finite values of λ, ν , the error bound is suboptimal, but numerical results indicate that in practice still an optimal convergence rate is obtained.

In the future, we will consider the extension of the LDG scheme to the non-isothermal Navier-Stokes-Korteweg equations with a Van der Waals equation of state [82]. This will be a challenge because this non-isothermal flow model contains highly nonlinear high-order terms.

Figure 2.4: Phase transitions and shocks in an elastic solid model with tri-linear stress-strain relation σ , $\omega = 1.0$, initial condition A.

Figure 2.5: Phase transitions and shocks in an elastic solid model with tri-linear stress-strain relation σ , initial condition A, various ω , $M = 800$.

(a) Strain γ , initial condition B

(b) Velocity v , initial condition B

(c) Strain γ , initial condition C

(d) Velocity v , initial condition C

(e) Strain γ , initial condition D

(f) Velocity v , initial condition D

Figure 2.6: Phase transitions in an elastic solid model with trilinear stress-strain relation σ , initial condition B, C and D, various ω , $M = 800$.

(a) Initial condition A

(b) Initial condition B

(c) Initial condition C

(d) Initial condition D

Figure 2.7: Phase transitions in an elastic solid model with trilinear stress-strain relation σ , trace of the numerical solution, $\omega = 1.0$.

Figure 2.8: Phase transition in an elastic solid model with cubic stress-strain relation σ , $\omega = 1.0$.

Figure 2.9: Phase transition in an elastic solid model with cubic stress-strain relation σ , $M = 1600$.

Figure 2.10: Van der Waals fluid, initial condition E, $\omega = 1.0$, $T_{end} = 0.15$.

Figure 2.11: Van der Waals fluid, initial condition F, $\omega = 1.0$, $T_{end} = 0.2$.

Figure 2.12: Van der Waals fluid, initial condition E, $M = 800$, $T_{end} = 0.15$.

Figure 2.13: Van der Waals fluid, initial condition F, $M = 800$, $T_{end} = 0.2$.

A local discontinuous Galerkin method for the (non)-isothermal Navier-Stokes-Korteweg equations

2

In this chapter, we develop a local discontinuous Galerkin (LDG) discretization for the (non)-isothermal Navier-Stokes-Korteweg (NSK) equations. The NSK equations are used to model the dynamics of a compressible fluid exhibiting liquid-vapour phase transitions. These equations are closed with a Van der Waals equation of state and contain third order nonlinear derivative terms. These contributions frequently cause standard numerical methods to violate the energy dissipation relation and require additional stabilization terms to prevent numerical instabilities. To address these problems we develop an LDG method for the (non)-isothermal NSK equations combined with a time-implicit Runge-Kutta integration method. An important feature of the LDG discretizations presented in this chapter is that they are relatively simple, robust and do not require special regularization terms. Finally, computational experiments are provided to demonstrate the capabilities, accuracy and stability of the LDG discretizations.

²The content of this chapter is published in the Journal of Computational Physics [108], with co-authors: Y. Xu, J.G.M. Kuerten and J.J.W. Van der Vegt.

3.1 Introduction

In this chapter, we will present a local discontinuous Galerkin (LDG) method for the numerical solution of the Navier-Stokes-Korteweg (NS-K) equations that model liquid-vapor phase transitions. This research is motivated by our previous work [107], where we solved a mixed hyperbolic-elliptic system that models phase transitions in solids and fluids using an LDG method. In that chapter, L^2 -stability of the LDG discretization of the phase transition model was proved, and an error estimate for the LDG discretization for the viscosity-capillarity (VC) system with linear strain-stress relation was provided. The numerical experiments discussed in [107] show that the LDG method for the VC system is stable and the LDG solutions converge to the analytical solution of the original problem.

Two-phase flows can be treated either by sharp interface models or by diffuse interface models. Sharp interface models assume that the interface thickness is equal to zero and have successfully been applied to many two-phase flows [11, 34, 32, 111]. Sharp interface models require, however, an extra evolution equation for the interface and face challenges in the reconstruction of the interface, leading to mathematical models that are solved by a Level Set or a Volume of Fluid method [53]. In contrast, diffuse interface models [9, 18, 124, 89] regard the interface as thin layers of fluid where properties such as mass density, viscosity and pressure change smoothly. In the diffuse interface model, only a single set of governing equations needs to be solved on the entire flow domain, including the interface area. The Navier-Stokes-Korteweg (NSK) equations [46, 81, 82, 16, 72] contain an additional contribution to the stress tensor related to capillary forces and are an example of a diffuse interface model. The NSK equations are used in this chapter to model the dynamics of a compressible fluid exhibiting phase transitions between liquid and vapor.

We consider a fluid in a domain $\Omega \in \mathbb{R}^d$ with $d \leq 3$, and let ρ be the density of the fluid and $\mathbf{u}$ the velocity. The isothermal NSK equations with zero external forces, in dimensionless and conservative form, read

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) - \nabla \cdot \tau - \nabla \cdot \xi &= \mathbf{0}, \end{aligned} \quad (3.1)$$

in $\Omega \times (0, T]$, with p the pressure, $\otimes$ the tensor product and $\mathbf{I}$ the identity matrix. The viscous stress tensor τ and Korteweg stress tensor ξ are given

by

$$\begin{aligned}\tau &= \frac{1}{\mathbb{R}e} \left(\nabla \mathbf{u} + \nabla^T \mathbf{u} - \frac{2}{3} \nabla \cdot \mathbf{u} \mathbf{I} \right), \\ \xi &= \frac{1}{\mathbb{W}e} \left(\left(\rho \Delta \rho + \frac{1}{2} |\nabla \rho|^2 \right) \mathbf{I} - \nabla \rho \nabla^T \rho \right),\end{aligned}\tag{3.2}$$

where $\mathbb{R}e$, $\mathbb{W}e$ are the Reynolds number and Weber number. The definition of the dimensionless variables is summarized in the Appendix. To simulate phase transitions between liquid and vapor, which are distinguished by different values of the density ρ , we need an expression for the thermodynamic pressure that is valid in both liquid and vapor state. The van der Waals equation of state is an appropriate choice, especially close to the critical temperature. For the isothermal NSK equations, we use the following dimensionless form [72, 44]

$$p(\theta, \rho) = \frac{8}{27} \frac{\theta \rho}{(1 - \rho)} - \rho^2,\tag{3.3}$$

with θ the dimensionless temperature. Figure 3.1 describes the shape of the van der Waals type equation of state (3.3) for temperature $\theta = 0.85$.

Other relevant thermodynamic quantities for (non)-isothermal fluids [72, 40] are the free energy density

$$W(\rho, \theta) = R\theta \rho \log \left(\frac{\rho}{b - \rho} \right) - a\rho^2,$$

and the chemical potential

$$\mu(\rho, \theta) = R\theta \log \left(\frac{\rho}{b - \rho} \right) + R\theta \frac{b}{b - \rho} - 2a\rho.$$

For isothermal flows, the total energy can be defined as

$$\mathcal{E}(\rho, \rho \mathbf{u}) = \int_{\Omega} \left(W(\rho) + \frac{1}{2\mathbb{W}e} |\nabla \rho|^2 + \frac{1}{2} \frac{|\rho \mathbf{u}|^2}{\rho} \right) d\mathbf{x},\tag{3.4}$$

and satisfies for periodic boundary conditions the relation [72, 44, 16, 89]

$$\frac{d}{dt} \mathcal{E}(\rho(\cdot, t), \rho \mathbf{u}(\cdot, t)) = - \int_{\Omega} \nabla \mathbf{u} : \tau d\mathbf{x} \leq 0,\tag{3.5}$$

Figure 3.1: van der Waals type of pressure-density relation at the dimensionless temperature $\theta = 0.85$, gas constant $R = \frac{8}{27}$, and coefficients $a = 1.0$, $b = 1.0$.

for positive Re . Here “ $\cdot$ ” is summation of the element-wise product of two matrices. Suppose $A = (a_{ij}), B = (b_{ij}) \in \mathbb{R}^{d \times d}$, then $A : B = \sum_i \sum_j a_{ij} b_{ij}$.

An important question is the solvability of the isothermal NSK equations, which has received considerable attention. For isothermal NSK equations, local and global smooth solutions for Cauchy problems of (3.1) with constant coefficients and small, smooth initial data were discussed in [51, 52]; the extension to Lipschitz continuous viscous coefficients and more general initial conditions was presented in [64]. In [89] a mathematical model with physically relevant non-local energies was proposed instead of the van der Waals free energy and a short-time existence theorem for the Cauchy problem of the non-local NSK equations was proved. The existence of strong solutions and global weak solutions of the isothermal NSK system (3.1) modeling compressible fluids of Korteweg type was discussed in [36, 50].

As discussed in [3, 107], it is not trivial to obtain a numerical solution of mixed hyperbolic-elliptic systems. When it comes to the more complex mixed system (3.1), the non-monotonic van der Waals equation of state can induce instabilities in the numerical solution. And the third order spatial derivatives of the mass density, stemming from the divergence of the Korteweg tensor ξ , causes dispersive behaviour of the numerical solution. Therefore numerical methods for the isothermal NSK equations face several challenges. One difficulty is that standard numerical methods including finite difference, finite volume, and discontinuous Galerkin (DG) methods with poor numerical fluxes, may violate the energy dissipation relation (3.5) and suffer from an in-

crease in energy for multiphase flows [40]. Another problem is the occurrence of parasitic currents: unphysical velocities close to the interface. In particular, the velocity field does not tend to zero when equilibrium is approached [40, 44]. In [59], a method is presented to eliminate parasitic currents for finite volume methods, but this is still a topic of ongoing research. Moreover, to capture the interface accurately requires locally a fine mesh.

Many articles addressed the numerical solution of the isothermal Navier-Stokes-Korteweg equations modeling liquid-vapor flows with phase change. A detailed description of higher order schemes, including the local discontinuous Galerkin method, to solve the non-conservative form of the isothermal NSK equations was given in [40]. A finite element formulation based on an isogeometric analysis of the non-conservative form of the isothermal NSK equations was developed in [46]. This method can straightforwardly deal with the higher-order derivatives in the isothermal NSK equations. In [72] a semi-discrete Galerkin method based on entropy variables and a new time integration scheme was proposed for the non-conservative form of the isothermal NSK equations. A DG scheme for the non-conservative form of the isothermal NSK equations, obtained by choosing special numerical fluxes, was presented in [44]. Another way to obtain a stable numerical discretization of the isothermal NSK equations is by adding two vanishing regularization terms. This approach was successfully used in [16] in combination with globally continuous finite element spaces and a time-implicit discretization.

The non-isothermal NSK equations [9, 82] model two-phase flows involving phase transition at nonuniform temperatures. Besides the isothermal equations (3.1), the non-isothermal NSK equations also contain an equation for the total energy

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) - \nabla \cdot \boldsymbol{\tau} - \nabla \cdot \boldsymbol{\xi} &= \mathbf{0}, \\ \frac{\partial (\rho E)}{\partial t} + \nabla \cdot ((\rho E + p) \mathbf{u}) - \nabla \cdot ((\boldsymbol{\tau} + \boldsymbol{\xi}) \cdot \mathbf{u}) + \nabla \cdot \mathbf{q} + \nabla \cdot \mathbf{j}_E &= 0, \end{aligned} \quad (3.6)$$

where the total energy density is given by

$$\rho E = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{1}{2} \frac{1}{\mathbb{W}e} |\nabla \rho|^2. \quad (3.7)$$

For the non-isothermal NSK equations (4.1), the dimensionless van der Waals

equation of state is given by [82, 39]

$$p = \frac{8\theta\rho}{3-\rho} - 3\rho^2. \quad (3.8)$$

The specific internal energy e in (4.4) is given by

$$e = \frac{8}{3}C_v\theta - 3\rho,$$

with C_v the specific heat at constant volume. The total entropy is specified as $S = \rho s$ with s the entropy density

$$s = -\frac{8}{3}\log\left(\frac{\rho}{3-\rho}\right) + \frac{8}{3}C_v\log(\theta).$$

The heat flux $\mathbf{q}$ and energy flux $\mathbf{j}_E$ through the interface in (4.1) are defined as

$$\mathbf{q} = -\frac{8C_v}{3\mathbb{W}e\mathbb{P}r}\nabla\theta, \quad \mathbf{j}_E = \frac{1}{\mathbb{W}e}(\rho\nabla \cdot \mathbf{u})\nabla\rho, \quad (3.9)$$

where $\mathbb{P}r$ is the Prandtl number, see Appendix. Recently global existence and uniqueness of strong solutions to the non-isothermal NSK equations were proved for bounded domains in [65, 66].

Most articles so far only discuss the non-conservative form of the isothermal NSK equations (3.1). Frequently, the isothermal NSK equations (3.1) are rewritten into an extended system by adding an extra variable for the total energy equation [72, 44, 16, 89]. It is, however, not trivial to do this for the non-isothermal NSK equations, where the van der Waals equation of state depends on both the density and temperature, so the frequently used relation

$$\nabla p = \rho\nabla W'(\rho)$$

is no longer satisfied. The numerical methods for the isothermal NSK equations discussed in [72, 44, 16, 89] are therefore difficult to extend to the non-isothermal NSK equations. The great potential of the LDG method to solve phase transition problems, as shown in [48, 107], motivated us to develop an LDG method for systems (3.1) and (4.1), while keeping the conservative form of the (non)-isothermal NSK equations and obtain a stable numerical discretization without additional regularization terms. To our knowledge, we are the first to discuss an LDG method for the conservative form of the (non)-isothermal NSK equations.

The LDG method is an extension of the discontinuous Galerkin (DG) method that aims to solve partial differential equations (PDEs) containing higher order spatial derivatives and was originally developed by Cockburn and Shu in [30] for solving nonlinear convection-diffusion equations containing second-order spatial derivatives. The idea behind LDG methods is to rewrite the original equations as a first order system, and then apply the DG method to this first order system. The design of the numerical fluxes is the key ingredient to ensure stability. LDG techniques have been developed for convection-diffusion equations [30], nonlinear KdV type equations [123], the Camassa-Holm equation [120] and many other types of partial differential equations. For a review, see [121]. The LDG method results in an extremely local discretization, which offers great advantages in parallel computing and *hp*-adaptation.

The organization of this chapter is as follows. In Section 4.2 we present the LDG method for the (non)-isothermal NSK equations in detail. An important aspect of this discretization is that it preserves the conservative form of the NSK equations. Section 3.3 discusses an implicit Runge-Kutta time integration method, which is used to overcome the stiffness of the NSK equations. In Section 3.4, numerical experiments are presented to investigate the accuracy and stability of the LDG discretization of the (non)-isothermal NSK equations. For the isothermal NSK equations, discrete mass conservation and energy dissipation are verified for the LDG solutions, while the mass conservation and total entropy are verified for the non-isothermal NSK equations. Finally, we give conclusions in Section 3.5.

3.2 LDG Discretization of the NSK system

In this section, we develop an LDG method to solve the NSK system in $\Omega \in \mathbb{R}^d$ with $d \leq 3$. We restrict the numerical experiments to one and two dimensions in this chapter, but the LDG discretization described here can be easily extended to three dimensions. We first introduce notations used for the description of the LDG discretization.

3.2.1 Notations

We denote by $\mathcal{T}_h$ a tessellation of Ω with regular shaped elements K , Γ represents all boundary faces of $K \in \mathcal{T}_h$ and $\Gamma_0 = \Gamma \setminus \partial\Omega$. Suppose e is a face shared by the “left” and “right” elements K_L and K_R . The normal vectors $\mathbf{n}_L$ and $\mathbf{n}_R$ on e point, respectively, exterior to K_L and K_R . Let φ be a

function on K_L and K_R , which could be discontinuous across e , then the left and right trace are denoted as $\varphi_L = (\varphi|_{K_L})|_e$, $\varphi_R = (\varphi|_{K_R})|_e$, respectively. For more details about these definitions, we refer the reader to [121].

For the LDG discretization, we define the finite element spaces

$$\begin{aligned} V_h &= \{\phi \in L^2(\Omega) : \phi|_K \in \mathcal{P}^k(K), \forall K \in \mathcal{T}_h\}, \\ \Sigma_h^d &= \{\mathbf{\Phi} = (\phi^{(1)}, \phi^{(2)}, \dots, \phi^{(d)})^T \in (L^2(\Omega))^d : \phi^{(i)}|_K \in \mathcal{P}^k(K), \\ &\quad i = 1, \dots, d, \forall K \in \mathcal{T}_h\}, \end{aligned}$$

with $\mathcal{P}^k(K)$ the space of polynomials of degree up to $k \geq 0$ on $K \in \mathcal{T}_h$.

The numerical solution is denoted by $\mathbf{U}_h$, with each component of $\mathbf{U}_h$ belonging to the finite element space V_h , and can be written as

$$\mathbf{U}_h(\mathbf{x}, t)|_K = \sum_{l=0}^{N_p} \widehat{\mathbf{U}}_l^K(t) \phi_l(\mathbf{x}), \text{ for } \mathbf{x} \in K. \quad (3.10)$$

Here, $\widehat{\mathbf{U}}_l^K(t)$ are unknowns and Legendre polynomials are used for the basis functions $\phi_l(\mathbf{x})$. In the next two sections we will discuss a local discontinuous Galerkin discretization for both the isothermal and non-isothermal NSK equations. We first consider the isothermal NSK equations since they provide a simpler model for phase transitions and are frequently used in applications. The non-isothermal NSK equations are computationally more demanding, but provide a more realistic model of the complex physics of phase transition.

3.2.2 LDG discretization for the isothermal NSK equations

In this section, we propose an LDG discretization for the isothermal NSK equations, which are rewritten as a first order system, given by the primary equations

$$\begin{aligned} \rho_t + \nabla \cdot \mathbf{m} &= 0, \\ \mathbf{m}_t + \nabla \cdot \mathbf{F}(\mathbf{U}) - \nabla \cdot \tau(\mathbf{z}, s) - \nabla \cdot \xi(\rho, \mathbf{r}, g) &= \mathbf{0}, \end{aligned} \quad (3.11)$$

and auxiliary equations

$$\begin{aligned}
 \mathbf{z} &= \nabla \mathbf{u}, \\
 l &= \nabla \cdot \mathbf{u}, \\
 \mathbf{r} &= \nabla \rho, \\
 g &= \nabla \cdot \mathbf{r},
 \end{aligned} \tag{3.12}$$

where

$$\begin{aligned}
 \mathbf{u} &= \frac{\mathbf{m}}{\rho}, \\
 \tau &= \frac{1}{\mathbb{R}e} \left(\mathbf{z} + \mathbf{z}^T - \frac{2}{3} l \mathbf{I} \right), \\
 \xi &= \frac{1}{\mathbb{W}e} \left(\left(\rho g + \frac{1}{2} |\mathbf{r}|^2 \right) \mathbf{I} - \mathbf{r} \mathbf{r}^T \right),
 \end{aligned} \tag{3.13}$$

and

$$\mathbf{F}(\mathbf{U}) = \mathbf{m} \otimes \mathbf{u} + p(\rho) \mathbf{I}, \quad \mathbf{U} = \begin{pmatrix} \rho \\ \mathbf{m} \end{pmatrix}.$$

The LDG discretization for the isothermal NSK equations (3.11) - (4.11) is now as follows: find $\rho_h, l_h, g_h \in V_h$, and $\mathbf{m}_h, \mathbf{z}_h, \mathbf{r}_h \in \Sigma_h^d$, such that for all test functions $\phi, \varphi, \zeta \in V_h$ and $\psi, \eta, \varsigma \in \Sigma_h^d$, the following relations are satisfied

$$\begin{aligned}
 \int_K (\rho_h)_t \phi \, dK - \int_K \mathbf{m}_h \cdot \nabla \phi \, dK + \int_{\partial K} \widehat{\mathbf{m}_h} \cdot \mathbf{n} \phi \, ds &= 0, \\
 \int_K (\mathbf{m}_h)_t \psi \, dK - \int_K (\mathbf{F}_h - \tau_h - \xi_h) \cdot \nabla \psi \, dK + \\
 \int_{\partial K} (\widehat{\mathbf{F}_h} - \widehat{\tau_h} - \widehat{\xi_h}) \cdot \mathbf{n} \psi \, ds &= 0,
 \end{aligned} \tag{3.14}$$

and

$$\begin{aligned}
 \int_K \mathbf{z}_h \eta \, dK &= - \int_K \mathbf{u}_h \nabla \cdot \eta \, dK + \int_{\partial K} \widehat{\mathbf{u}}_h \eta \cdot \mathbf{n} \, ds, \\
 \int_K l_h \zeta \, dK &= - \int_K \mathbf{u}_h \cdot \nabla \zeta \, dK + \int_{\partial K} \widehat{\mathbf{u}}_h \cdot \mathbf{n} \zeta \, ds, \\
 \int_K \mathbf{r}_h \varsigma \, dK &= - \int_K \rho_h \nabla \cdot \varsigma \, dK + \int_{\partial K} \widehat{\rho}_h \varsigma \cdot \mathbf{n} \, ds, \\
 \int_K g_h \varphi \, dK &= - \int_K \mathbf{r}_h \cdot \nabla \varphi \, dK + \int_{\partial K} \widehat{\mathbf{r}}_h \cdot \mathbf{n} \varphi \, ds,
 \end{aligned} \tag{3.15}$$

where

$$\begin{aligned}
 \widehat{\mathbf{u}}_h &= \frac{\widehat{\mathbf{m}}_h}{\widehat{\rho}_h}, \\
 \widehat{\tau}_h &= \frac{1}{\mathbb{R}e} \left(\widehat{\mathbf{z}}_h + \widehat{\mathbf{z}}_h^T - \frac{2}{3} \widehat{l}_h \mathbf{I} \right), \\
 \widehat{\xi}_h &= \frac{1}{\mathbb{W}e} \left(\left(\widehat{\rho}_h g_h + \frac{1}{2} |\widehat{\mathbf{r}}_h|^2 \right) I - \widehat{\mathbf{r}}_h \widehat{\mathbf{r}}_h^T \right),
 \end{aligned} \tag{3.16}$$

and

$$\mathbf{F}_h = \mathbf{F}(\mathbf{U}_h), \quad \mathbf{U}_h = \begin{pmatrix} \rho_h \\ \mathbf{m}_h \end{pmatrix}.$$

For the numerical fluxes in (4.12), (4.13) and (4.14), denoted with a hat, we choose the Lax-Friedrich flux for the convective part and central numerical fluxes for the other terms,

$$\begin{aligned}
 \widehat{\mathcal{F}}_h|_e &= \frac{1}{2} (\mathcal{F}_h|_L + \mathcal{F}_h|_R - \alpha (\mathbf{U}_h|_R - \mathbf{U}_h|_L)), \\
 \widehat{\mathbf{m}}_h|_e &= \frac{1}{2} (\mathbf{m}_h|_L + \mathbf{m}_h|_R), \quad \widehat{\rho}_h|_e = \frac{1}{2} (\rho_h|_L + \rho_h|_R), \\
 \widehat{\mathbf{r}}_h|_e &= \frac{1}{2} (\mathbf{r}_h|_L + \mathbf{r}_h|_R), \quad \widehat{\mathbf{z}}_h|_e = \frac{1}{2} (\mathbf{z}_h|_L + \mathbf{z}_h|_R), \\
 \widehat{l}_h|_e &= \frac{1}{2} (l_h|_L + l_h|_R), \quad \widehat{g}_h|_e = \frac{1}{2} (g_h|_L + g_h|_R),
 \end{aligned} \tag{3.17}$$

with $\mathcal{F}_h = (\mathbf{m}_h, \mathbf{F}_h)^T$ and α a positive constant that is chosen as the maximum absolute eigenvalue of $\frac{\partial \mathcal{F}_h}{\partial \mathbf{U}_h}$ globally.

3.2.3 LDG Discretization for the non-isothermal NSK equations

The LDG discretization for the isothermal NSK equations presented in Section 3.2.2 can be extended to the non-isothermal NSK equations (4.1). The equations can also be rewritten as a first order system that includes Equations (3.11)-(4.11) and additional equations given by

$$\begin{aligned} (\rho E)_t + \nabla \cdot \mathbf{G}(\mathbf{U}) - \nabla \cdot ((\tau + \xi) \cdot \mathbf{u}) + \nabla \cdot \mathbf{q} + \nabla \cdot \mathbf{j}_E &= 0, \\ \mathbf{q} &= -\frac{8C_v}{3\mathbb{W}e\mathbb{P}r} \nabla \theta, \\ \mathbf{j}_E &= \frac{1}{\mathbb{W}e} \rho l \mathbf{r}, \quad \mathbf{G}(\mathbf{U}) = (\rho E + p) \mathbf{u}. \end{aligned} \quad (3.18)$$

The LDG discretization for the non-isothermal NSK equations contains (4.12)-(4.14), and the LDG discretization for the energy equation contributions, given by (3.18), can be written as

$$\begin{aligned} &\int_K ((\rho E)_h)_t \chi \, dK \\ &- \int_K (\mathbf{G}_h - (\tau_h + \xi_h) \cdot \mathbf{u}_h + \mathbf{q}_h + (\mathbf{j}_E)_h) \cdot \nabla \chi \, dK \\ &+ \int_{\partial K} \left(\widehat{\mathbf{G}}_h - (\widehat{\tau}_h + \widehat{\xi}_h) \cdot \widehat{\mathbf{u}}_h + \widehat{\mathbf{q}}_h + (\widehat{\mathbf{j}}_E)_h \right) \cdot \mathbf{n} \chi \, ds = 0. \end{aligned} \quad (3.19a)$$

$$\int_K \mathbf{q}_h \sigma \, dK - \frac{8C_v}{3\mathbb{W}e\mathbb{P}r} \int_K \theta_h \nabla \cdot \sigma \, dK + \frac{8C_v}{3\mathbb{W}e\mathbb{P}r} \int_{\partial K} \widehat{\theta}_h \sigma \cdot \mathbf{n} \, ds = 0, \quad (3.19b)$$

with

$$(\mathbf{j}_E)_h = \frac{1}{\mathbb{W}e} \rho_h l_h \mathbf{r}_h, \quad \mathbf{G}_h = \mathbf{G}(\mathbf{U}_h) \text{ and } \mathbf{U}_h = \begin{pmatrix} \rho_h \\ \mathbf{m}_h \\ (\rho E)_h \end{pmatrix}.$$

The same numerical fluxes (4.16) as used in the LDG discretization for the isothermal NSK equations are used in the non-isothermal equations. If we denote $\mathcal{G}_h(\mathbf{U}_h) = \begin{pmatrix} \mathcal{F}_h \\ \mathbf{G}_h \end{pmatrix}$, then the numerical flux for $\mathcal{G}_h$ is also the Lax-

Friedrichs flux, but now with the constant α the maximum absolute eigenvalue of $\frac{\partial \mathcal{G}_h}{\partial \mathbf{U}_h}$. For the one dimensional case the eigenvalues of $\frac{\partial \mathcal{G}_h}{\partial \mathbf{U}_h}$ are provided in [39]. For two dimensional case, u, v are additional eigenvalues in, respectively x and y direction. The additional numerical fluxes in the energy equation contributions (3.19) are chosen as

$$\widehat{\mathbf{q}}_h = \frac{1}{2}(\mathbf{q}_h|_L + \mathbf{q}_h|_R), \quad \widehat{\theta}_h = \frac{1}{2}(\theta_h|_L + \theta_h|_R), \quad (\widehat{\mathbf{j}}_E)_h = \frac{1}{W_e} \widehat{\rho}_h \widehat{l}_h \widehat{\mathbf{r}}_h. \quad (3.20)$$

Remark 3.1. *We emphasize that not only the (first-order) convective part of the isothermal NSK equations (3.11), but also the (first-order) convective part of the non-isothermal NSK equations is of mixed hyperbolic-elliptic type. The eigenvalues of the systems are given explicitly below.*

The convective part of the isothermal NSK equations is given by

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p) &= 0. \end{aligned} \quad (3.21)$$

In 2D, assuming $\mathbf{u} = (u, v)^T$, the Jacobian matrices are

$$A^1 = \begin{pmatrix} 0 & 1 & 0 \\ -u^2 + p'(\rho) & 2u & 0 \\ -uv & v & u \end{pmatrix}, \quad A^2 = \begin{pmatrix} 0 & 0 & 1 \\ -uv & v & u \\ -v^2 + p'(\rho) & 0 & 2v \end{pmatrix}$$

for, respectively, the x - and y -direction. The eigenvalues of A^1 are $\{u - \sqrt{p'(\rho)}, u, u + \sqrt{p'(\rho)}\}$ and those of A^2 are $\{v - \sqrt{p'(\rho)}, v, v + \sqrt{p'(\rho)}\}$. Consequently, (3.21) is a hyperbolic-elliptic system due to the non-monotonicity of the van der Waals equation of state, and it is elliptic when $p'(\rho) < 0$.

The eigenvalues of the convective part of the one dimensional non-isothermal NSK equations were studied in [39]. The eigenvalues of the 2D non-isothermal NSK equations are the extension of those of the 1D non-isothermal NSK equations, with one extra u, v , in the x, y direction respectively. In detail, the convective part of the non-isothermal NSK equations is rewritten, in primitive form, as

$$\mathbf{V}_t + \widetilde{F}(\mathbf{V})_x + \widetilde{G}(\mathbf{V})_y = 0, \quad \text{with } \mathbf{V} = (\rho, u, v, p) \text{ in } 2D.$$

The Jacobian matrices are given by

$$\frac{\partial \tilde{F}}{\partial \mathbf{V}} = \begin{pmatrix} u & \rho & 0 & 0 \\ 0 & u & 0 & 1/\rho \\ 0 & 0 & u & 0 \\ 0 & f(p, \rho) & 0 & u \end{pmatrix}, \quad \frac{\partial \tilde{G}}{\partial \mathbf{V}} = \begin{pmatrix} v & 0 & \rho & 0 \\ 0 & v & 0 & 0 \\ 0 & 0 & v & 1/\rho \\ 0 & 0 & f(p, \rho) & v \end{pmatrix},$$

where the function f is equal to

$$f(p, \rho) = \frac{3}{C_v(3 - \rho)} \left((1 + C_v p + \rho^2(3 - 3C_v + 2C_v \rho)) \right).$$

The eigenvalues of $\frac{\partial \tilde{F}}{\partial \mathbf{V}}$ are $\{u, u, u - \sqrt{\beta}, u + \sqrt{\beta}\}$, and those of $\frac{\partial \tilde{G}}{\partial \mathbf{V}}$ are $\{v, v, v - \sqrt{\beta}, v + \sqrt{\beta}\}$, with $\beta = 2 \left(\frac{p}{\rho} + \frac{4\theta(3+C_v(-3+2\rho))}{C_v(-3+\rho)^2} \right)$.

3.3 Implicit time discretization method

The equations for the DG expansion coefficients for each variable are obtained by introducing the polynomial representation (4.8) into the LDG discretizations (4.12)-(4.14) and (3.19). The coefficients of the polynomial expansions of $\rho_h(\mathbf{x}, t)$, $\mathbf{m}_h(\mathbf{x}, t)$ and $\rho E_h(\mathbf{x}, t)$ in the LDG discretization are collected in the vector $\hat{\mathbf{U}}(t)$. The LDG discretization, given by (4.12)-(4.14) and (3.19) with corresponding fluxes for $\rho_h(\mathbf{x}, t)$, $\mathbf{m}_h(\mathbf{x}, t)$ and $\rho E_h(\mathbf{x}, t)$, then results in a system of ordinary differential and algebraic equations (DAEs)

$$\begin{aligned} \frac{d\hat{\mathbf{U}}(t)}{dt} + \mathbf{L}(\hat{\mathbf{U}}(t), \hat{\mathbf{Z}}(t), \hat{\mathbf{G}}(t)) &= 0, \\ \hat{\mathbf{Z}}(t) - \mathbf{P}(\hat{\mathbf{U}}(t)) &= 0, \\ \hat{\mathbf{G}}(t) - \mathbf{Q}(\hat{\mathbf{U}}(t), \hat{\mathbf{Z}}(t)) &= 0, \end{aligned} \tag{3.22}$$

with $\hat{\mathbf{Z}}(t), \hat{\mathbf{G}}(t)$ the coefficients of the auxiliary variables, and $\mathbf{L}, \mathbf{P}, \mathbf{Q}$ non-linear functions of $\hat{\mathbf{U}}(t), \hat{\mathbf{Z}}(t)$, and $\hat{\mathbf{G}}(t)$. The initial values are

$$\hat{\mathbf{U}}(t_0) = \hat{\mathbf{U}}_0.$$

Note, in case of the isothermal NSK equations, the contributions from (3.19) are missing. Both explicit and implicit time integration methods [49] can

be applied to the DAE system (3.22). Due to the Korteweg stress tensor ξ , the NSK system is a third order nonlinear system of partial differential equations, and explicit time integration methods then require the time step to satisfy

$$\Delta t = O(h^2), \quad h = \min\{\Delta x, \Delta y\}, \quad (3.23)$$

for stability [39]. Moreover, when we would consider local mesh refinement near the interface, the time step restriction (3.23) becomes even more severe. Therefore, we consider an implicit time stepping method.

3.3.1 Diagonally Implicit Runge-Kutta methods

For the implicit time integration we use Diagonally Implicit Runge-Kutta (DIRK) methods, since they allow that the equations for each implicit stage are solved in a sequential manner. A class of Diagonally Implicit Runge-Kutta (DIRK) formulae, which are $A-$ stable and computationally efficient, was discussed in [8, 20, 49]. A special feature of the DIRK method in [20] is that it provides embedded DIRK formulae that allow a straightforward calculation of the local truncation error at each time step without extra computation. This provides an efficient way to estimate the time step required for a certain accuracy level. In [98] DIRK methods based on the minimization of certain error functions were considered, and several Butcher tables for specific DIRK formulae were given.

For the third order accurate LDG discretization in space, which uses quadratic basis functions, we use the third order Singly DIRK scheme from [98], given by

$$\begin{aligned} \hat{\mathbf{U}}^{n1} &= \hat{\mathbf{U}}^n + \Delta t a_{11} \mathbf{K}_1, \quad \hat{\mathbf{Z}}^{n1} = \mathbf{P}(\hat{\mathbf{U}}^{n1}), \quad \mathbf{G}^{n1} = \mathbf{Q}(\hat{\mathbf{U}}^{n1}, \hat{\mathbf{Z}}^{n1}), \\ \mathbf{K}_1 &= -\mathbf{L} \left(t_n + c_1 \Delta t, \hat{\mathbf{U}}^{n1}, \hat{\mathbf{Z}}^{n1}, \hat{\mathbf{G}}^{n1} \right), \\ \hat{\mathbf{U}}^{n2} &= \hat{\mathbf{U}}^n + \Delta t a_{21} \mathbf{K}_1 + \Delta t a_{22} \mathbf{K}_2, \\ \hat{\mathbf{Z}}^{n2} &= \mathbf{P}(\hat{\mathbf{U}}^{n2}), \quad \hat{\mathbf{G}}^{n2} = \hat{\mathbf{Q}}(\hat{\mathbf{U}}^{n2}, \hat{\mathbf{Z}}^{n2}), \\ \mathbf{K}_2 &= -\mathbf{L} \left(t_n + c_2 \Delta t, \hat{\mathbf{U}}^{n2}, \hat{\mathbf{Z}}^{n2}, \hat{\mathbf{G}}^{n2} \right), \end{aligned}$$

$$\begin{aligned}
 \hat{\mathbf{U}}^{n3} &= \hat{\mathbf{U}}^n + \Delta t a_{31} \mathbf{K}_1 + \Delta t a_{32} \mathbf{K}_2 + \Delta t a_{33} \mathbf{K}_3, \\
 \hat{\mathbf{Z}}^{n3} &= \mathbf{P}(\hat{\mathbf{U}}^{n3}), \quad \hat{\mathbf{G}}^{n3} = \mathbf{Q}(\hat{\mathbf{U}}^{n3}, \hat{\mathbf{Z}}^{n3}), \\
 \mathbf{K}_3 &= -\mathbf{L} \left(t_n + c_3 \Delta t, \hat{\mathbf{U}}^{n3}, \hat{\mathbf{Z}}^{n3}, \hat{\mathbf{G}}^{n3} \right), \\
 \hat{\mathbf{U}}^{n+1} &= \hat{\mathbf{U}}^n + \Delta t b_1 \mathbf{K}_1 + \Delta t b_2 \mathbf{K}_2 + \Delta t b_3 \mathbf{K}_3.
 \end{aligned}$$

The coefficients in the SDIRK scheme are defined in the Butcher table

$$\begin{array}{c|c}
 \mathbf{c} & \mathbf{A} \\
 \hline
 & \mathbf{b}^T
 \end{array} = \begin{array}{c|cc}
 \frac{\gamma}{2} & \frac{\gamma}{2} & \frac{\gamma}{2} \\
 \hline
 1 & 1 - b_2 - \gamma & b_2 \quad \gamma \\
 \hline
 & 1 - b_2 - \gamma & b_2 \quad \gamma
 \end{array}$$

with $b_2 = \frac{1}{4}(5 - 20\gamma + 6\gamma^2)$ and $\gamma = 0.43586652$. For the second order accurate LDG discretization in space, which uses linear polynomial basis functions, we use the second order accurate implicit Runge-Kutta time integration scheme

$$\begin{aligned}
 \hat{\mathbf{U}}^{n1} &= \hat{\mathbf{U}}^n + \Delta t \frac{1}{2} \mathbf{K}_1, \quad \hat{\mathbf{Z}}^{n1} = \mathbf{P}(\hat{\mathbf{U}}^{n1}), \quad \hat{\mathbf{G}}^{n1} = \mathbf{Q}(\hat{\mathbf{U}}^{n1}, \hat{\mathbf{Z}}^{n1}), \\
 \mathbf{K}_1 &= -\mathbf{L} \left(t_n + \frac{1}{2} \Delta t, \hat{\mathbf{U}}^{n1}, \hat{\mathbf{Z}}^{n1}, \hat{\mathbf{G}}^{n1} \right), \\
 \hat{\mathbf{U}}^{n+1} &= \hat{\mathbf{U}}^n + \Delta t \mathbf{K}_1.
 \end{aligned} \tag{3.24}$$

Note that the intermediate stages $\mathbf{K}_1, \mathbf{K}_2$ and $\mathbf{K}_3$ must be solved implicitly, i.e. three (or one) large-scale nonlinear problems need to be dealt with. In recent years, great progress has been made in solving large nonlinear algebraic systems using globalized inexact Newton methods [41, 80]. The main difficulty with classical Newton methods is that a large-scale linear system needs to be solved at each iteration, which can be costly with a direct solver. A popular alternative is a class of Newton-Krylov methods, which solve the large-scale nonlinear system iteratively. For more details, we refer to [62]. In the next section we describe the use of these methods to solve the nonlinear stage equations in the SDIRK method.

3.3.2 Newton-Krylov methods

Newton-Krylov methods solve the nonlinear equations

$$F(x) = 0, \quad \text{with } F \in \mathbb{R}^N, \tag{3.25}$$

in the following way: given an initial solution x_0 , iteratively compute

$$x_{k+1} = x_k + s, \quad \text{with } s \text{ a solution of } DF(x_k)s = -F(x_k), \quad (3.26)$$

where x_k is the current approximate solution and $DF(x_k)$ the Jacobian matrix of $F(x)$ at x_k . These methods combine outer nonlinear Newton iterations with inner linear Krylov iterations. The inner iteration stops when

$$\|F(x_k) + DF(x_k)s_k\| \leq \eta_k \|F(x_k)\|, \quad (3.27)$$

where the constant $\eta_k \in (0, 1)$ can be either fixed or specified dynamically.

We take the second order implicit Runge-Kutta time integration method (3.24) to explain the computation of the Jacobian matrix. System (3.24) can be rewritten as

$$\mathbf{F}_1 = \mathbf{K}_1 + \mathbf{L} \left(t_n + \frac{1}{2} \Delta t, \hat{\mathbf{U}}^{n1}, \hat{\mathbf{Z}}^{n1}, \hat{\mathbf{G}}^{n1} \right) = 0,$$

$$\mathbf{F}_2 = \hat{\mathbf{Z}}^{n1} - \mathbf{P}(\hat{\mathbf{U}}^{n1}) = 0,$$

$$\mathbf{F}_3 = \hat{\mathbf{G}}^{n1} - \mathbf{Q}(\hat{\mathbf{U}}^{n1}, \hat{\mathbf{Z}}^{n1}) = 0$$

with $\hat{\mathbf{U}}^{n1} = \hat{\mathbf{U}}^n + \Delta t \frac{1}{2} \mathbf{K}_1$. The Jacobian matrix $\mathbf{J}$ has the structure

$$\mathbf{J} = \begin{pmatrix} \frac{\partial \mathbf{F}_1}{\partial \mathbf{K}_1} & \frac{\partial \mathbf{F}_1}{\partial \hat{\mathbf{Z}}^{n1}} & \frac{\partial \mathbf{F}_1}{\partial \hat{\mathbf{G}}^{n1}} \\ \frac{\partial \mathbf{F}_2}{\partial \mathbf{K}_1} & \frac{\partial \mathbf{F}_2}{\partial \hat{\mathbf{Z}}^{n1}} & \mathbf{0} \\ \frac{\partial \mathbf{F}_3}{\partial \mathbf{K}_1} & \frac{\partial \mathbf{F}_3}{\partial \hat{\mathbf{Z}}^{n1}} & \frac{\partial \mathbf{F}_3}{\partial \hat{\mathbf{G}}^{n1}} \end{pmatrix}$$

which is shown in Figure 3.2. It is not practical to solve the linear system in (3.26), with $DF(x_k)$ as Jacobian matrix, using a direct method. The linear system is therefore solved using GMRES with an ILU(0) preconditioner in order to prevent a large fill-in of the matrix.

3.4 Numerical experiments

In this section, we perform several numerical experiments to investigate the stability and accuracy of the LDG schemes for the (non)-isothermal NSK equations proposed in Sections 3.2.2 and 3.2.3. The examples in Section 3.4.2 are test cases for the isothermal NSK equations, including an investigation of the order of accuracy, a few one-dimensional benchmark problems and

Figure 3.2: Non-zeros in the Jacobian matrix for the LDG discretization of the two-dimensional non-isothermal NSK equations on a mesh with 20^2 elements.

a two-dimensional simulation of the coalescence of two bubbles. These model problems were recently also (partly) studied in [72, 16] using a semi-discrete Galerkin method and a continuous finite element method, together with special time integration schemes. Compared to these methods the LDG schemes that we present in this chapter are relatively simple, robust and do not require additional regularization terms. The simulations of the non-isothermal NSK equations (4.1) are presented in Section 3.4.3, including accuracy verification, a static Riemann problem and a two-dimensional simulation of bubble coalescence. Note that we did not use any limiter in the computations. Periodic boundary conditions and a uniform mesh are applied for all test cases.

We use implicit Runge-Kutta(RK) time integration methods to solve the ODE system resulting from the LDG discretization for the accuracy tests and two dimensional bubble coalescence simulations. In the accuracy tests, the time step is chosen as $dt = 0.8h$ for the third order implicit RK time method, with h the length of an element. The time step $dt = 1.5h$ is chosen for the second order implicit RK time method for the two dimensional bubble coalescence tests.

In several numerical examples, an equilibrium state with an interface between liquid and vapor is used to verify the capabilities of the proposed LDG scheme, described in Section 3.2.2. The velocity is denoted by u in 1D,

while $\mathbf{u} = (u, v)^T$ in 2D. At a certain dimensionless temperature $\theta < 1$ in the van der Waals equation of state, the densities in the equilibrium state ρ_v, ρ_l that satisfy the following relations for the pressure and chemical potential

$$\begin{aligned} p(\theta, \rho_v) &= p(\theta, \rho_l), \\ \mu(\theta, \rho_v) &= \mu(\theta, \rho_l), \end{aligned} \tag{3.28}$$

are called Maxwell states.

3.4.1 Interface width

To resolve the diffuse interface accurately, a sufficiently fine mesh is required in a simulation of a phase-field problem, otherwise the numerical solution will contain non-physical oscillations [72]. Suppose that the Helmholtz free energy is denoted by f , and that Δf is the difference in Helmholtz free energy between the phase mixture and the separate phases:

$$\Delta f = f - f_0.$$

Here $f_0(\rho) = f(\rho_v, \theta_0) + (\rho - \rho_v) \frac{f(\rho_l, \theta_0) - f(\rho_v, \theta_0)}{\rho_l - \rho_v}$ for the given temperature θ_0 . The interface thickness [19] is then given by

$$d = 2 \frac{L}{\sqrt{\mathbb{W}e}} \frac{\rho_l - \rho_v}{\sqrt{\Delta f_{max}}}, \tag{3.29}$$

with Δf_{max} the maximum value of Δf , L the reference length scale and ρ_l, ρ_v the critical densities at a given temperature. From the numerical tests, we found that at least 10 mesh nodes are required inside the interface to capture the interface accurately and guarantee the stability of the energy or entropy. This gives the relation $d = \alpha h$, $\alpha > 10$ with h the mesh size in the interface region.

3.4.2 Numerical tests for the isothermal NSK equations

Similar to [16, 72], choosing the temperature as $\theta = 0.85$ and the van der Waals equation of state (3.3), the critical vapor and liquid densities are equal to $\rho_v = 0.106576655$, $\rho_l = 0.602380109$.

Accuracy test

In this section, we will study the accuracy of the LDG discretization for the isothermal NSK equations. To investigate the accuracy of the one-

dimensional LDG discretization, we select an exact smooth solution as

$$\begin{aligned}\rho &= 0.6 + 0.1 \sin(5\pi t) \cos(2\pi x), \\ u &= \sin(3\pi t) \sin(2\pi x),\end{aligned}\tag{3.30}$$

which satisfies (3.1) with an additional source term $\mathbf{S}$. The source terms are added artificially and obtained by inserting the chosen exact smooth solution (3.32) into (3.11). The computational domain is $\Omega = (0, 1)$, and the coefficients in (3.1) are

$$\mathbb{R}e = 20, \quad \mathbb{W}e = 100.\tag{3.31}$$

The solutions are obtained using the LDG discretization with piecewise linear and quadratic polynomials, combined with the third order implicit Runge-Kutta time integration method with stopping parameter η_k in (3.27) chosen as $\eta_k = 10^{-9}$. Table 3.1 shows the accuracy of the LDG scheme for the one-dimensional isothermal NSK equations. From this table, we can see that the LDG discretizations have optimal order of accuracy for the different polynomial orders.

Table 3.1: Accuracy test of the LDG discretization for the one-dimensional isothermal NSK equations (3.1) with exact solution (3.30). The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters in the isothermal NSK equations (3.1) are set as (3.31). The LDG discretization uses linear and quadratic basis functions and periodic boundary conditions. Results are for uniform meshes with M cells at time $t = 0.1$.

	M	$\ \rho - \rho_h\ _{L^2(\Omega)}$	order	$\ u - u_h\ _{L^2(\Omega)}$	order
P^1	16	1.65E-03	—	8.91E-03	—
	32	4.06E-04	2.03	2.27E-03	1.97
	64	1.08E-05	1.90	6.02E-04	1.92
	128	2.83E-05	1.94	1.56E-04	1.95
	256	7.25E-06	1.96	4.00E-05	1.97
P^2	16	1.21E-04	—	7.20E-04	—
	32	1.58E-05	2.95	9.64E-05	2.90
	64	2.18E-06	2.86	1.30E-05	2.90
	128	2.92E-07	2.90	1.70E-06	2.93
	256	3.81E-08	2.94	2.18E-07	2.96

To investigate the accuracy of the LDG discretization for the two-dimensional

isothermal NSK equations, we choose an exact smooth solution

$$\begin{aligned}\rho &= 0.6 + 0.1 \sin(5\pi t) \cos(2\pi x) \cos(2\pi y), \\ u &= \sin(3\pi t) \sin(2\pi x) \sin(2\pi y), \\ v &= \sin(\pi t) \sin(4\pi x) \sin(4\pi y),\end{aligned}\tag{3.32}$$

which satisfies (3.11) with additional source terms. The computational domain is $\Omega = (0, 1) \times (0, 1)$ and square quadrilateral elements are used. Table 3.2 shows the results of the LDG scheme for the two-dimensional isothermal NSK equations using piecewise linear and quadratic polynomials, indicating that the LDG discretization in Section 3.2.2 has optimal order of accuracy.

Table 3.2: Accuracy test of the LDG discretization for the two-dimensional isothermal NSK equations (3.11) with exact solution (3.32). The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters in the isothermal NSK equations (3.1) are set as (3.31). The LDG discretization uses piecewise linear and quadratic polynomials and periodic boundary conditions. Results are for uniform meshes with square elements at time $t = 0.1$.

	Mesh	$\ \rho - \rho_h\ _{L_2}$	order	$\ u - u_h\ _{L_2}$	order	$\ v - v_h\ _{L_2}$	order
P^1	16^2	1.82E-03	—	3.95E-03	—	1.53E-02	—
	32^2	3.74E-04	1.85	9.42E-04	2.07	3.67E-03	2.06
	64^2	1.49E-04	1.95	2.36E-04	2.00	9.08E-04	2.01
	128^2	3.77E-05	1.98	5.91E-05	2.00	2.26E-04	2.00
P^2	16^2	3.38E-4	—	3.08E-4	—	1.81E-3	—
	32^2	3.35E-5	3.33	3.33E-5	3.21	2.22E-4	3.01
	64^2	3.85E-6	3.12	3.89E-6	3.10	2.81E-5	3.00
	128^2	4.80E-7	3.00	4.80E-7	3.02	3.51E-6	3.00

One-dimensional interface problem

As a further verification of the accuracy and robustness of the LDG discretization, we solve two traveling wave problems for isothermal NSK equations in 1D. It is known that some numerical discretizations produce solutions with overshoots, or incorrect wave speeds at discontinuities for this test case, see

Figure 3.3: One-dimensional stationary wave problem. LDG solutions with piecewise linear and quadratic polynomials at $t = 0.1$ on a mesh containing 400 elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters in the isothermal NSK equations (3.1) are set as $Re = 200$ and $We = 10000$.

e.g. [72]. First, we consider a stationary wave problem with initial conditions

$$\begin{aligned}\rho_0(x) &= \frac{\rho_R + \rho_L}{2} + \frac{\rho_R - \rho_L}{2} \tanh\left(\frac{x - 0.5}{2} \sqrt{We}\right), \\ u_0(x) &= \frac{u_R + u_L}{2} + \frac{u_R - u_L}{2} \tanh\left(\frac{x - 0.5}{2} \sqrt{We}\right).\end{aligned}\quad (3.33)$$

The coefficients in the initial conditions (3.33) are taken as

$$(\rho_L, u_L) = (0.107, 0), \quad (\rho_R, u_R) = (0.602, 0).$$

We extend the domain $(0, 1)$ to $[-1, 1]$ with reflection symmetry at $x = 0$ and use periodic boundary conditions. The physical parameters in (3.11) are set as $Re = 200$ and $We = 10000$ and the mesh contains 400 elements. We plot the solutions of the LDG scheme for the isothermal NSK equations with piecewise linear and quadratic polynomials at time $t = 0.1$ in Figure 3.3. Figure 3.3 shows that all numerical solutions are smooth without large oscillations, and the solutions resulting from linear and quadratic basis functions are indistinguishable at this mesh resolution. Since the initial condition is close to, but not exactly an equilibrium solution of the governing equations, the solution slightly changes in time and the velocity is small, but not equal to zero at the time shown in Figure 3.3.

Figure 3.4: One-dimensional propagating wave problem. LDG solutions with piecewise linear and quadratic polynomials at $t = 0.2$ on a mesh containing 400 elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters in the isothermal NSK equations (3.1) are set as $\mathbb{R}e = 200$ and $\mathbb{W}e = 10000$.

Next, we study a wave propagation problem. The initial conditions are set as (3.33) with

$$(\rho_R, u_R) = (0.107, 1.0), \quad (\rho_L, u_L) = (0.602, 1.0).$$

The LDG solution for the isothermal NSK equations with this initial condition results in a propagating traveling wave solution moving from the left to the right at speed 1.0. Again, stable numerical solutions are obtained as shown in Figure 3.4.

Coalescence of two bubbles

An important test case is the simulation of the coalescence of two bubbles, which was also studied in [16, 72]. The computational domain is $[0, 1]^2$. The parameters are $\mathbb{R}e = 512$, $\mathbb{W}e = 65500$. We consider two vapor bubbles of different radii, which are initially close to each other and at rest. The initial conditions are

$$\rho_0(\mathbf{x}) = \rho_1 + \frac{1}{2}(\rho_2 - \rho_1) \sum_{i=1}^2 \tanh\left(\frac{d_i(\mathbf{x}) - r_i}{2} \sqrt{\mathbb{W}e}\right), \quad \mathbf{u} \equiv \mathbf{0}, \quad (3.34)$$

with ρ_1, ρ_2 close to an equilibrium given a fixed constant temperature. Here $d_i(\mathbf{x}) = \|\mathbf{x} - \mathbf{x}_i\|$ is the Euclidean distance and the points $\mathbf{x}_i$ are equal to

$\mathbf{x}_1 = (0.4, 0.5)$ and $\mathbf{x}_2 = (0.78, 0.5)$, respectively. The radii of the two bubbles are $r_1 = 0.25$ and $r_2 = 0.1$. After some time, the bubbles will merge into one vapor bubble by capillarity and pressure forces.

Mass conservation and energy dissipation are critical parameters to investigate whether a numerical discretization for the NSK equations is suitable. To verify the mass conservation and energy dissipation properties of our LDG scheme, we denote the discrete mass and energy at time t , respectively, by

$$m_h(t) = \int_{\Omega} \rho_h(t) d\mathbf{x},$$

$$\mathcal{E}_h(t) = \int_{\Omega} \left(W(\rho_h(t)) + \frac{1}{2\mathbb{W}e} |\nabla \rho_h(t)|^2 + \frac{1}{2} \frac{|(\rho \mathbf{u})_h(t)|^2}{\rho_h(t)} \right) d\mathbf{x}.$$

The initial mass is $m_h(t_0) = \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x}$.

Before using the LDG discretization, we will discuss the mesh required for this method to capture the interface and to represent the solution accurately. For the isothermal NSK equations with equation of state (3.3), (3.29), we obtain the following results:

- Given the temperature $\theta = 0.85$, the critical densities are $\rho_v = 0.107$ and $\rho_l = 0.602$. The interface width then is equal to

$$d = \frac{2(\rho_l - \rho_v)}{\sqrt{\Delta f_{max}}} \frac{1}{\sqrt{\mathbb{W}e}} = 14.04 \frac{1}{\sqrt{\mathbb{W}e}}.$$

Consequently $h = \frac{1}{\sqrt{\mathbb{W}e}}$ is a reasonable choice.

- Given the temperature $\theta = 0.8$, the critical densities are $\rho_v = 0.080$ and $\rho_l = 0.644$. The interface width then is equal to

$$d = \frac{2(\rho_l - \rho_v)}{\sqrt{\Delta f_{max}}} \frac{1}{\sqrt{\mathbb{W}e}} = 12.00 \frac{1}{\sqrt{\mathbb{W}e}}.$$

Consequently $h = \frac{1}{\sqrt{\mathbb{W}e}}$ is a reasonable choice also for this case.

We use the LDG discretization with piecewise linear and quadratic polynomials for the isothermal NSK equations and the second order implicit Runge-Kutta time integration method (3.24) with stopping parameter $\eta_k = 10^{-6}$ in the Newton method. Given $\theta = 0.85$, the initial condition is set as (4.20) with $\rho_1 = 0.1, \rho_2 = 0.6$. We choose a mesh of 256^2 square elements. Figure 3.7 presents the evolution for the mass loss and energy, showing that

the mass is conserved, and the energy decreases monotonically in time. The evolution of the bubble coalescence process is shown in Figures 3.5 and 3.6. These figures show that the two bubbles, which are below the critical temperature and initially close to each other and at rest, merge into one bubble during the simulation because of surface tension. After coalescence the resulting bubble slowly reaches an equilibrium state, in which the interface has a constant radius of curvature due to surface tension and the velocity field approaches zero.

The method for the isothermal NSK equations with $\theta = 0.85$ was also tested on a coarser mesh with 128^2 elements. Figure 3.8 shows the density profiles at various times, indicating that stable results are still obtained on this coarser mesh. The density and pressure along the line $y = 0.5$ are displayed in Figure 3.9, which shows that the diffuse interface has only 8 nodes in this test. The evolution of the energy is displayed in Figure 3.10, showing that the energy is slightly increasing on a mesh with 128^2 elements for the isothermal NSK equations with $We = 65500$. On meshes coarser with less than 8 nodes in the diffuse interface no stable results are obtained for this Weber number.

Choosing $\theta = 0.8$, (3.28) results in critical densities $\rho_l = 0.6442, \rho_v = 0.0800$ with a larger density ratio. When the LDG discretization is applied to the isothermal NSK equations with $\theta = 0.8$ and initial condition (4.20) with $\rho_1 = 0.08, \rho_2 = 0.64$, stable results are still obtained on a mesh of 256^2 elements, as can be seen from Figure 3.12. Figure 3.11 shows that the mass is conserved, and the energy is only slightly increasing in time.

We also study the behaviour of the numerical scheme for the isothermal NSK equations when the initial densities are further away from the equilibrium densities ρ_l, ρ_v . For example, given a fixed temperature $\theta = 0.85$, $\rho_1 = 0.05, \rho_2 = 0.65$ were chosen in (4.20). We choose the parameters in (3.1) as $Re = 500$, $We = 10000$, and the mesh of 100^2 elements. Mass and energy properties are presented in Figure 3.13, which shows that the mass is conserved and the energy is decreasing in time. Figure 3.14 shows the coalescence of bubbles for the isothermal NSK equations with $Re = 200, We = 10000$ when the initial density is far away from an equilibrium on a mesh of 100^2 elements. Figure 3.15 shows the results for the isothermal NSK equations with $Re = 512, We = 65500$ when the initial density is far away from equilibrium on a mesh of 256^2 elements. Because of the non-equilibrium initial condition we get sound waves traveling to the boundaries of the domain and transported back into the domain on the opposite side due to the periodic boundary conditions. For the isothermal NSK equations with $Re = 512, We = 65500$ on a mesh of 256^2 elements, the amplitude of these sound waves is so large that

Figure 3.5: Density ρ for two coalescing bubbles computed with the LDG discretization of the isothermal NSK equations (3.1) using piecewise linear polynomials on a mesh with 256^2 square elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters are set as $\mathbb{R}e = 512$, $We = 65500$. The initial condition is (4.20) with $\rho_1 = 0.1, \rho_2 = 0.6$.

Figure 3.6: Density ρ for two coalescing bubbles computed with the LDG discretization of the isothermal NSK equations (3.1) using piecewise linear polynomials on a mesh with 256^2 square elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters are set as $\mathbb{R}e = 512$, $We = 65500$. The initial condition is (4.20) with $\rho_1 = 0.1, \rho_2 = 0.6$.

Figure 3.7: Evolution of mass loss and energy as a function of time during the coalescence of two bubbles computed with the LDG discretization of the isothermal NSK equations (3.1) using piecewise linear polynomials on a mesh with 256^2 square elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters are set as $\mathbb{R}e = 512$, $We = 65500$. The initial condition is (4.20) with $\rho_1 = 0.1, \rho_2 = 0.6$.

Figure 3.8: Density ρ for two coalescing bubbles computed with the LDG discretization of the isothermal NSK equations (3.1) using piecewise linear polynomials on a mesh with 128^2 square elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters are set as $\text{Re} = 512$, $\text{We} = 65500$. The initial condition is (4.20) with $\rho_1 = 0.1$, $\rho_2 = 0.6$.

Figure 3.9: Density and pressure along $y = 0.5$ at time $t = 5.0$ for the coalescence of two bubbles for the isothermal NSK equations (3.1) using piecewise linear polynomials on a mesh with 128^2 square elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$, and the physical parameters are set as $Re = 512$, $We = 65500$. The initial condition is (4.20) with $\rho_1 = 0.1$, $\rho_2 = 0.6$.

Figure 3.10: Evolution of mass loss and energy as a function of time during the coalescence of two bubbles computed with the LDG discretization of the isothermal NSK equations using piecewise linear polynomials on a mesh with 128^2 square elements. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$ and the physical parameters are set as $Re = 512$, $We = 65500$. The initial condition is (4.20) with $\rho_1 = 0.1$, $\rho_2 = 0.6$.

Figure 3.11: Evolution of mass loss and energy as a function of time during the simulation of two bubbles for the isothermal NSK equations with $\mathbb{R}e = 512$, $We = 65500$ on a mesh of 256^2 elements using piecewise linear polynomials. The van der Waals EOS is chosen as (3.3), $\theta = 0.8$. The initial condition is (4.20) with $\rho_1 = 0.08$, $\rho_2 = 0.64$.

this results in regions where the density is so low that a bubble occurs there. Since the simulations are isothermal, there is no latent heat that prevents this. The large Weber number also helps the formation of a bubble, since the surface tension is rather low.

3.4.3 Numerical experiments for the non-isothermal NSK equations

Choosing the temperature $\theta = 0.989$ and the van der Waals equation of state (3.8), the Maxwell states are

$$\rho_v = 0.79525689, \quad \rho_l = 1.21357862. \quad (3.35)$$

Accuracy test

For the accuracy test of the LDG discretization of the one-dimensional non-isothermal NSK equations (4.1), a smooth exact solution is chosen as

$$\begin{cases} \rho(x, t) = 0.6 + 0.1 \sin(5\pi t) \cos(2\pi x), \\ v(x, t) = \sin(3\pi t) \sin(2\pi x), \\ \theta(x, t) = 0.8 + 0.1 \sin(\pi t) \sin(2\pi x), \end{cases} \quad (3.36)$$

Figure 3.12: Density ρ for two bubbles computed with the LDG discretization of the isothermal NSK equations with $\mathbb{R}e = 512$, $\mathbb{W}e = 65500$ on a mesh of 256^2 elements using piecewise linear polynomials. The van der Waals EOS is chosen as (3.3), $\theta = 0.8$. The initial condition is (4.20) with $\rho_1 = 0.08, \rho_2 = 0.64$.

Figure 3.13: Evolution of mass loss and energy as a function of time during the coalescence of two bubbles computed with the LDG discretization of the isothermal NSK equations with $\mathbb{R}e = 200$, $We = 10000$ on a mesh with 100^2 square elements. Piecewise linear polynomials are used. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$. The initial condition is (4.20) with $\rho_1 = 0.05, \rho_2 = 0.65$.

which satisfies the non-isothermal NSK equations (4.1) with a properly chosen source term $\mathbf{S}$. The Prandtl number $\mathbb{P}r$ in (4.1) is chosen as $\mathbb{P}r = 0.843$, and $C_v = 5.375$.

In order to verify the accuracy of the LDG scheme for the two-dimensional non-isothermal NSK equations (4.1), we select the exact smooth solution

$$\begin{cases} \rho(x, t) = 0.6 + 0.1 \sin(5\pi t) \cos(2\pi x) \cos(2\pi y), \\ u(x, t) = \sin(3\pi t) \sin(2\pi x) \sin(2\pi y), \\ v(x, t) = \sin(3\pi t) \sin(4\pi x) \sin(4\pi y), \\ \theta(x, t) = 0.8 + 0.1 \sin(\pi t) \sin(2\pi x) \cos(2\pi y), \end{cases} \quad (3.37)$$

which satisfies the non-isothermal NSK equations (4.1) with a properly chosen source term.

The results of the accuracy tests of the LDG discretization for the 1D and 2D non-isothermal NSK equations are given in Tables 3.3 and 3.4, respectively. From these results, we can see that the LDG discretization for the non-isothermal NSK equations has optimal order of accuracy.

Figure 3.14: Coalescence of two bubbles for the isothermal NSK equations with $\mathbb{R}e = 200$, $\mathbb{W}e = 10000$ on a mesh of 100^2 elements. Piecewise linear polynomials are used. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$. The initial condition is (4.20) with $\rho_1 = 0.05$, $\rho_2 = 0.65$.

Figure 3.15: Coalescence of two bubbles for the isothermal NSK equations with $\mathbb{R}e = 512$, $\mathbb{W}e = 65500$ on a mesh of 256^2 elements. Piecewise linear polynomials are used. The van der Waals EOS is chosen as (3.3), $\theta = 0.85$. The initial condition is (4.20) with $\rho_1 = 0.05$, $\rho_2 = 0.65$.

Table 3.3: Accuracy test of the LDG discretization for the one-dimensional non-isothermal NSK equations (4.1) with exact solution (3.36). The physical parameters are chosen as $\mathbb{R}e = 50$, $We = 1000$, $Pr = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8). LDG discretization with piecewise linear and quadratic polynomials, periodic boundary conditions, uniform meshes and time $t = 0.1$.

	Mesh	$\ \rho - \rho_h\ _{L_2}$	order	$\ u - u_h\ _{L_2}$	order	$\ \theta - \theta_h\ _{L_2}$	order
P^1	16	1.43E-03	–	3.65E-03	–	2.88E-04	–
	32	3.551E-04	2.01	9.32E-04	1.97	7.44E-05	1.95
	64	8.89E-05	2.00	2.36E-04	1.98	1.90E-05	1.97
	128	2.22E-05	2.00	5.96E-05	1.99	4.80E-06	1.99
	256	5.56E-06	2.00	1.50E-05	1.99	1.20E-06	2.00
P^2	16	2.71E-5	–	1.35E-4	–	1.21E-5	–
	32	2.14E-6	3.66	1.71E-5	2.68	1.33E-6	3.18
	64	2.42E-7	3.14	2.18E-6	2.97	1.54E-7	3.11
	128	2.96E-8	3.03	2.77E-7	2.98	1.86E-8	3.04
	256	3.70E-9	3.00	3.50E-8	2.96	2.31E-9	3.01

One-dimensional interface problem

In this section we consider a one-dimensional interface problem to investigate the accuracy and robustness of the LDG discretization of the non-isothermal NSK equations. The initial conditions are set as a similar form as (3.33) with

$$\begin{aligned}
 (\rho_L, u_L, \theta_L) &= (0.795, 0.0, 0.989), \\
 (\rho_R, u_R, \theta_R) &= (1.213, 0.0, 0.989).
 \end{aligned} \tag{3.38}$$

The domain is $[-5, 5]$.

Figure 3.16 shows that the LDG scheme for the non-isothermal NSK equations results in accurate and stable solutions. Figure 3.17 compares the LDG solutions for the isothermal and non-isothermal NSK equations with the van der Waals equation of state (3.8). The dimensionless numbers are equal to $\mathbb{R}e = 128.6$, $We = 968.6$ and the initial conditions are defined in (3.38). Figure 3.17 shows that, compared to the isothermal NSK equations, the LDG solutions for the non-isothermal NSK equations result in less oscillations in the density near the interface.

Coalescence of two bubbles

Next, we simulate the coalescence of two bubbles. The parameters are $\mathbb{R}e = 950$, $We = 34455$. The computational domain is $[0, 1]^2$. We consider two

Table 3.4: Accuracy test of the LDG discretization for the two-dimensional non-isothermal NSK equations (4.1) with exact solution (3.37). The physical parameters are chosen as $\mathbb{R}e = 50$, $We = 1000$, $Pr = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8). LDG discretization with piecewise linear and quadratic polynomials, periodic boundary conditions, and uniform meshes with square elements at time $t = 0.1$.

	Mesh	$\ \rho - \rho_h\ _{L_2}$	order	$\ u - u_h\ _{L_2}$	order	$\ \theta - \theta_h\ _{L_2}$	order
P^1	16^2	2.08E-03	—	3.72E-02	—	9.85E-4	—
	32^2	5.61E-04	1.88	9.36E-04	1.99	2.63E-4	1.90
	64^2	1.47E-04	1.94	2.34E-04	2.00	6.91E-5	1.94
	128^2	3.76E-05	1.97	5.85E-05	2.00	1.76E-5	1.97
P^2	16^2	5.11E-4	—	6.66E-4	—	7.36E-4	—
	32^2	5.57E-5	3.19	6.94E-5	3.21	1.28E-4	2.51
	64^2	6.93E-6	3.01	7.99E-6	3.11	1.56E-5	3.04
	128^2	8.74E-7	2.98	9.70E-7	3.04	1.78E-6	3.13

Figure 3.16: One-dimensional static interface problem for the non-isothermal NSK equations. Numerical solutions obtained with the LDG scheme with piecewise quadratic polynomials at $t = 2.0$ on a mesh containing 400 elements. The physical parameters are chosen as $\mathbb{R}e = 128.6$, $We = 968.6$, $Pr = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8).

Figure 3.17: One-dimensional static interface problem for the isothermal and non-isothermal NSK equations, numerical solutions obtained with the piecewise quadratic polynomials at $t = 2.0$ on a mesh containing 400 elements. The physical parameters are chosen as $\mathbb{R}e = 128.6$, $\mathbb{W}e = 968.6$, $\mathbb{P}r = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8).

vapor bubbles of different radii, which are initially close to each other and at rest. The initial conditions are

$$\rho_0(\mathbf{x}) = \rho_1 + \frac{1}{2}(\rho_2 - \rho_1) \sum_{i=1}^2 \tanh\left(\frac{d_i(\mathbf{x}) - r_i}{2} \sqrt{\mathbb{W}e}\right),$$

$$\mathbf{u} \equiv \mathbf{0}, \quad \theta = \theta_0 \quad (3.39)$$

where θ_0 is a chosen constant, and ρ_1, ρ_2 are constants close to the critical densities for given θ_0 . These values will be specified in each test. The points $\mathbf{x}_i$ are equal to $\mathbf{x}_1 = (0.4, 0.5)$ and $\mathbf{x}_2 = (0.78, 0.5)$. The radii of the two bubbles are $r_1 = 0.25$ and $r_2 = 0.1$.

For the non-isothermal NSK equations with equation of state (3.8), the interface width (3.29) shows the following results:

- Given the initial temperature $\theta = 0.989$, the critical densities are $\rho_v = 0.7952$, $\rho_l = 1.2135$, and the interface width follows as

$$d = \frac{2(\rho_l - \rho_v)}{\sqrt{\Delta f_{max}}} \frac{1}{\sqrt{\mathbb{W}e}} = 31.05 \frac{1}{\sqrt{\mathbb{W}e}}.$$

Then the mesh size $h = \frac{2}{\sqrt{\mathbb{W}e}}$ can be chosen.

- Given the initial temperature $\theta = 0.95$, the critical densities are $\rho_v = 0.5790$, $\rho_l = 1.4617$, and the interface width follows as

$$d = \frac{2(\rho_l - \rho_v)}{\sqrt{\Delta f_{max}}} \frac{1}{\sqrt{\mathbb{W}e}} = 14.42 \frac{1}{\sqrt{\mathbb{W}e}}.$$

Then the mesh size $h = \frac{1}{\sqrt{\mathbb{W}e}}$ is a reasonable choice.

We use the LDG discretization for the non-isothermal NSK equations with bi-linear basis functions and the second order implicit Runge-Kutta time integration method (3.24) with stopping parameter $\eta_k = 10^{-6}$ in (3.27). Similar to the isothermal case, the bubbles merge into one vapor bubble, which tends to be of circular shape later in time by capillarity and pressure forces. Choosing $\theta_0 = 0.989$, the initial condition is set as (4.22) with $\rho_1 = 0.795$, $\rho_2 = 1.213$. The LDG discretizations is used for the non-isothermal NSK equations with $\mathbb{W}e = 34455$ on a mesh of 200^2 square elements and a mesh of 100^2 square elements. These two meshes lead to very similar results for mass conservation and entropy increase, see Figure 3.18. The process of coalescence computed for the non-isothermal NSK equations with initial condition (4.22) and $\rho_1 = 0.795$, $\rho_2 = 1.213$, $\theta_0 = 0.989$ on a mesh of 200^2 elements is shown in Figures 3.19. Density and pressure along the line $y = 0.5$ for two coalescing bubbles are computed with the LDG discretization of the non-isothermal NSK equations on a mesh with 100^2 square elements, shown in Figure 3.20.

Given $\theta_0 = 0.95$, critical densities $\rho_v = 0.5790$, $\rho_l = 1.4617$ with a larger density ratio are found by (3.28) with equations of state (3.8). The initial condition is set as (4.22) with $\rho_1 = 0.579$, $\rho_2 = 1.462$ and $\theta_0 = 0.95$. The time evolution of the bubbles, mass and entropy are shown in Figures 3.21 and 3.23. The mass is conserved, and the entropy is a non-decreasing function of time apart from a small interval in which it is almost constant. For $\theta_0 = 0.92$, the critical densities are $\rho_v = 0.479$, $\rho_l = 1.587$. The initial condition is set as (4.22) with $\rho_1 = 0.479$, $\rho_2 = 1.587$. Figure 3.22 shows that stable results are obtained although the entropy does not increase during part of the calculation. A finer mesh is required to guarantee an increasing entropy in this case.

The behaviour of the numerical scheme for the Non-isothermal NSK equations is also studied when the initial densities are further away from the equilibrium densities ρ_l, ρ_v . Given $\theta_0 = 0.989$, $\rho_1 = 0.6$, $\rho_2 = 1.4$ is set in (4.22). Figures 3.24 shows the mass is conserved and entropy is increasing in time. The momentum in both directions and energy are conserved, as shown

Figure 3.18: Evolution of mass loss on a mesh of 100^2 elements and entropy on meshes of 100^2 and 200^2 square elements as a function of time during the coalescence of two bubbles for the non-isothermal NSK equations with $\text{Re} = 950$, $\text{We} = 34455$, $\text{Pr} = 0.843$, $C_v = 5.375$. The initial condition is set as (4.22) with $\rho_1 = 0.795$, $\rho_2 = 1.213$ and $\theta_0 = 0.989$.

in Figures 3.24. Figure 3.25 presents the coalescence, similar results with Figure 3.19.

3.5 Conclusions

We developed local discontinuous Galerkin methods for the solution of the (non)-isothermal Navier-Stokes-Korteweg equations containing the van der Waals equation of state and nonlinear third order density derivatives. The LDG methods are based on the conservative form of the NSK equations and are relatively simple compared to other available numerical discretizations for the NSK equations. A diagonally implicit Runge-Kutta integration time method is used to integrate in time in order to deal with the severe time step restriction encountered for explicit time integration methods. The Jacobian matrix for the implicit Runge-Kutta method includes the extra variables for the higher order derivatives. The numerical experiments demonstrate the capabilities, accuracy and stability of the proposed LDG discretizations of the NSK equations. It is worthwhile to point out that the proposed LDG discretization is straightforward and works well for larger density ratios, but has limitations in the mesh required to obtain stable solutions and the correct

Figure 3.19: Density ρ for two coalescing bubbles computed with the LDG discretization of the non-isothermal NSK equations using piecewise linear polynomials on a mesh with 200^2 square elements. The physical parameters are chosen as $\text{Re} = 950$, $\text{We} = 34455$, $\text{Pr} = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8). The initial condition is set as (4.22) with $\rho_1 = 0.795$, $\rho_2 = 1.213$ and $\theta_0 = 0.989$.

(a) time $t = 5, \rho$ along $y = 0.5$.

(b) time $t = 10, \rho$ along $y = 0.5$.

(c) time $t = 5, p$ along $y = 0.5$.

(d) time $t = 10, p$ along $y = 0.5$.

Figure 3.20: Density and pressure along $y = 0.5$ for two coalescing bubbles computed with the LDG discretization of the non-isothermal NSK equations using piecewise linear polynomials on a mesh with 100^2 square elements. The physical parameters are chosen as $\mathbb{R}e = 950$, $\mathbb{W}e = 34455$, $\mathbb{P}r = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8). The initial condition is set as (4.22) with $\rho_1 = 0.795$, $\rho_2 = 1.213$ and $\theta_0 = 0.989$.

Figure 3.21: Evolution of mass loss and entropy as a function of time during the coalescence of two bubbles for the non-isothermal NSK equations. The initial condition is set as (4.22) with $\rho_1 = 0.579, \rho_2 = 1.462$ and $\theta_0 = 0.95$. The mesh contains 200^2 square elements. The physical parameters are chosen as $\mathbb{R}e = 950$, $\mathbb{W}e = 34455$, $\mathbb{P}r = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8).

energy or entropy behaviour.

In future research we will also consider the (non)-isothermal NSK equations for initial conditions that result in a larger elliptic region in the phase transition area. This will be combined with local mesh refinement to capture the interface more efficiently.

3.6 Appendix

In this Appendix we briefly discuss the derivation of the dimensionless form of the NSK equations and the definition of the dimensionless variables.

Dimensionless form of the isothermal NSK equations

The isothermal NSK equations are given by [72, 16, 40]

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
 \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) - \nabla \cdot \boldsymbol{\tau} - \nabla \cdot \boldsymbol{\xi} &= \mathbf{0},
 \end{aligned}
 \tag{3.40}$$

Figure 3.22: Density profile at $t = 5.0$ and entropy as a function of time during the coalescence of two bubbles for the non-isothermal NSK equations. The initial condition is set as (4.22) with $\rho_1 = 0.479, \rho_2 = 1.587, \theta_0 = 0.92$. A mesh contains 200^2 square elements. The physical parameters are chosen as $\mathbb{R}e = 950$, $\mathbb{W}e = 34455$, $\mathbb{P}r = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8).

where ρ is the mass density, $\mathbf{u}$ the velocity. The viscous stress tensor τ and the Korteweg stress tensor are defined as

$$\begin{aligned} \tau &= \mu \left(\nabla \mathbf{u} + \nabla^T \mathbf{u} - \frac{2}{3} \nabla \cdot \mathbf{u} \mathbf{I} \right), \\ \xi &= \lambda \left(\left(\rho \triangle \rho + \frac{1}{2} |\nabla \rho|^2 \right) \mathbf{I} - \nabla \rho \nabla^T \rho \right), \end{aligned} \quad (3.41)$$

with μ the viscosity coefficient and λ the capillary coefficient. The thermodynamic pressure is defined as

$$p = Rb \frac{\rho \theta}{b - \rho} - a \rho^2, \quad (3.42)$$

with θ the temperature, R the universal gas constant, a, b positive constants depending on the fluid.

The equations are made dimensionless using the following reference variables for the mass density, temperature and pressure

$$\rho_c = b, \quad \theta_c = \frac{8ab}{27R}, \quad p_c = ab^2,$$

Figure 3.23: Density ρ for two coalescing bubbles computed with the LDG discretization of the non-isothermal NSK equations using piecewise linear polynomials on a mesh with 200^2 square elements. The physical parameters are chosen as $\mathbb{R}e = 950$, $We = 34455$, $\mathbb{P}r = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8). The initial condition is set as (4.22) with $\rho_1 = 0.579$, $\rho_2 = 1.462$ and $\theta_0 = 0.95$

(a) mass loss

(b) entropy increase

(c) momentum loss in x direction

(d) momentum loss in y direction

(e) energy loss

Figure 3.24: Evolution of mass loss and entropy on a mesh of 200^2 square elements as a function of time during the coalescence of two bubbles for the non-isothermal NSK equations. The parameters are $\mathbb{R}e = 950$, $\mathbb{W}e = 34455$, $\mathbb{P}r = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8). The initial condition is set as (4.22) with $\theta_0 = 0.989$, $\rho_1 = 0.6$, $\rho_2 = 1.4$.

Figure 3.25: Density ρ for two coalescing bubbles computed with the LDG discretization of the non-isothermal NSK equations using piecewise linear polynomials on a mesh with 200^2 square elements. The physical parameters are chosen as $Re = 950$, $We = 34455$, $Pr = 0.843$, $C_v = 5.375$, and the van der Waals EOS is set as (3.8). The initial condition is set as (4.22) with $\theta_0 = 0.989$, $\rho_1 = 0.6$, $\rho_2 = 1.4$.

The reference variable for the velocity is the average sound speed in the system $u_c = \sqrt{p_c/\rho_c}$ and the reference variable for time is $\frac{L}{u_c}$, with L the reference length. The Reynolds and Weber numbers are then defined as

$$\mathbb{R}e = \rho_c u_c L / \mu, \quad \mathbb{W}e = u_c^2 L^2 / (\rho_c \lambda).$$

Letting

$$\rho = \rho_c \tilde{\rho}, \quad \mathbf{u} = u_c \tilde{\mathbf{u}}, \quad p = p_c \tilde{p}, \quad \theta = \theta_c \tilde{\theta},$$

the governing equations (3.40) and (3.42) then can be transformed into their dimensionless form, resulting in (3.1)-(3.3).

Dimensionless form of the non-isothermal NSK equations

The non-isothermal NSK equations are given by [39, 82]

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) - \nabla \cdot \boldsymbol{\tau} - \nabla \cdot \boldsymbol{\xi} &= \mathbf{0}, \\ \frac{\partial (\rho E)}{\partial t} + \nabla \cdot ((\rho E + p) \mathbf{u}) - \nabla \cdot ((\boldsymbol{\tau} + \boldsymbol{\xi}) \cdot \mathbf{u}) + \nabla \cdot \mathbf{q} + \nabla \cdot \mathbf{j}_E &= 0, \end{aligned} \tag{3.43}$$

with the definition of viscous stress tensor $\boldsymbol{\tau}$ and the Korteweg stress tensor defined in (3.41). The total energy density is given by

$$\rho E = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{1}{2} \lambda |\nabla \rho|^2, \tag{3.44}$$

with the specific internal energy e defined as

$$e = C_v \theta - \frac{a}{M^2} \rho.$$

The van der Waals equation of state for the non-isothermal NSK equations (3.43) is given by

$$p = \frac{R \theta \rho}{M - b \rho} - \frac{a}{M^2} \rho^2, \tag{3.45}$$

where C_v is the specific heat at constant volume, R the perfect gas constant, M the molar mass of the fluid, b the molar volume and a a constant modelling

the interactions between the fluid particles. The heat flux $\mathbf{q}$ and energy flux $\mathbf{j}_E$ through the interface in (3.43) are defined as

$$\mathbf{q} = -K\nabla\theta, \quad \mathbf{j}_E = \lambda(\rho\nabla \cdot \mathbf{u})\nabla\rho, \quad (3.46)$$

with K the thermal conductivity.

Note that the form of the equation of state (3.45) for the non-isothermal NSK equations is different from (3.42) for the isothermal NSK equations, though they have a similar shape.

The reference variables for the mass density, temperature and pressure are, respectively,

$$\rho_c = M/(3b), \quad \theta_c = \frac{8a}{27Rb}, \quad p_c = a/(27b^2).$$

The reference variable for the velocity is defined as $u_c = \sqrt{p_c/\rho_c}$ and the reference variable for time is $\frac{L}{u_c}$, with L the reference length. The Reynolds and Weber numbers are then equal to

$$\text{Re} = \rho_c u_c L / \mu, \quad \text{We} = u_c^2 L^2 / (\rho_c \lambda).$$

The Prandtl number and the reduced heat capacity are defined as $\text{Pr} = \mu C_v / K$, $\widetilde{C_v} = MC_v / R$.

The governing equations (3.43)-(3.46) then can be transformed into their dimensionless form, resulting in (4.1)-(3.9).

An h -adaptive local discontinuous Galerkin method for liquid-vapor flows with phase change and solid wall boundaries

3

In this chapter, we develop a mesh adaptation algorithm for a local discontinuous Galerkin (LDG) discretization of the (non)-isothermal Navier-Stokes-Korteweg (NSK) equations modeling liquid-vapor flows with phase change. This work is a continuation of Chapter 3, where we proposed LDG discretizations for the (non)-isothermal NSK equations with a time-implicit Runge-Kutta method. To save computing time and to capture the thin interfaces more accurately, we extend the LDG discretization with a mesh adaptation method. We emphasize that the adaptive LDG discretization is relatively simple and does not require additional stabilization. The use of a locally refined mesh in combination with an implicit Runge-Kutta time method is, however, non-trivial, but results in an efficient time integration method for the NSK equations. Computations, including cases with solid wall boundaries, are provided to demonstrate the accuracy, efficiency and capabilities of the adaptive LDG discretizations.

³The content of this chapter is joint work with Y. Xu, J.G.M. Kuerten and J.J.W. Van der Vegt, and will be submitted as a journal article.

4.1 Introduction

In this chapter, we present a mesh adaptation algorithm for a local discontinuous Galerkin (LDG) method of the (non)-isothermal Navier-Stokes-Korteweg (NSK) equations. The NSK equations, containing the Korteweg expression for the capillary forces together with the Van der Waals equation of state, model the dynamics of compressible flows with liquid-vapor phase transition. This research follows on our previous work [108], where we solved the (non)-isothermal NSK equations in conservative form with an LDG method. We emphasize that the proposed LDG discretizations are relatively simple, robust and do not require special regularization terms. Extensive numerical studies in [108] demonstrate the capabilities, accuracy and stability of the LDG discretizations. These numerical examples were performed for the (non)-isothermal NSK equations with periodic boundary conditions and on a uniform mesh.

Solving the NSK equations with phase transition takes large computing memory and time. First, according to the theory of the diffuse interface model [19] and computational examples in [40, 72, 108], the mesh needs to be sufficiently fine such that several mesh nodes lay inside the width of the interface in order to capture the solution in the interface region accurately. Otherwise, relations for the decay of the energy in case of the isothermal NSK equations and the growth of the entropy in case of the non-isothermal NSK equations will be violated. Second, the third order derivatives of the density, which appear in the NSK equations, require a strict time step limitation in case explicit integration time methods are adopted. When an implicit integration time method is used for the NSK equations, in particular for a large Weber number, a large nonlinear system of ordinary differential equations (ODEs) needs to be solved.

Small mesh sizes are, however, required only in the interface region. Since the LDG method is well suited to deal with hanging nodes, a locally refined mesh can be combined with the LDG discretizations for the (non)-isothermal NSK equations. This will significantly enhance the accuracy and efficiency of the LDG method. In the remaining part of the introduction, we briefly present the non-isothermal NSK equations with solid wall boundary conditions that will be treated in this chapter. Then we will discuss mesh adaptation.

Consider a fluid in a domain $\Omega \subset \mathbb{R}^d$ with $d \leq 3$, and let ρ be the density of the fluid, $\mathbf{u}$ the velocity and θ the temperature. The non-isothermal NSK

equations, in dimensionless and conservative form, read

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
 \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) - \nabla \cdot \tau - \nabla \cdot \xi &= \rho \mathbf{g}, \\
 \frac{\partial (\rho E)}{\partial t} + \nabla \cdot ((\rho E + p) \mathbf{u}) - \nabla \cdot ((\tau + \xi) \cdot \mathbf{u}) + \nabla \cdot \mathbf{q} + \nabla \cdot \mathbf{j}_E \\
 &= \rho \mathbf{g} \cdot \mathbf{u},
 \end{aligned} \tag{4.1}$$

in $\Omega \times (0, T]$, with p the pressure, $\mathbf{g}$ the dimensionless acceleration of the gravity and $\otimes$ the tensor product. The viscous stress tensor τ and Korteweg stress tensor ξ are given by

$$\begin{aligned}
 \tau &= \frac{1}{\mathbb{R}e} \left(\nabla \mathbf{u} + \nabla^T \mathbf{u} - \frac{2}{3} \nabla \cdot \mathbf{u} \mathbf{I} \right), \\
 \xi &= \frac{1}{\mathbb{W}e} \left(\left(\rho \triangle \rho + \frac{1}{2} |\nabla \rho|^2 \right) \mathbf{I} - \nabla \rho \nabla^T \rho \right),
 \end{aligned} \tag{4.2}$$

with constant Reynolds number $\mathbb{R}e$ and Weber number $\mathbb{W}e$ [72, 39]. Here $\mathbf{I}$ is the identity matrix. The Van der Waals equation of state [89, 72, 39, 44] is used to represent the pressure in both the liquid and vapor state (characterized by different values of the density ρ), and is given in dimensionless form by

$$p(\theta, \rho) = Rb \frac{\theta \rho}{b - \rho} - a \rho^2 \quad (a, b > 0), \tag{4.3}$$

where R, a and b are constants. The total energy density is given by

$$\rho E = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{1}{2} \frac{1}{\mathbb{W}e} |\nabla \rho|^2. \tag{4.4}$$

The specific internal energy e in (4.4) is given by

$$e = \frac{8}{3} C_v \theta - 3\rho,$$

with C_v the non-dimensional specific heat at constant volume. The heat flux $\mathbf{q}$ and energy flux $\mathbf{j}_E$ through the interface in (4.1) are defined as

$$\mathbf{q} = -\frac{8C_v}{3\mathbb{W}e\mathbb{P}r} \nabla \theta, \quad \mathbf{j}_E = \frac{1}{\mathbb{W}e} (\rho \nabla \cdot \mathbf{u}) \nabla \rho, \tag{4.5}$$

with Prandtl number $\mathbb{Pr}$.

Initial and boundary conditions have to be set for the NSK equations in non-isothermal case. The initial conditions are given by

$$\rho(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \theta(\mathbf{x}, 0) = \theta_0(\mathbf{x}). \quad (4.6)$$

For the boundary conditions, we consider at a solid surface a contact angle for the density, the no-slip boundary condition for the velocity and a Dirichlet or Neumann boundary condition for the temperature:

$$\begin{aligned} & -\frac{\nabla \rho}{\|\nabla \rho\|} \cdot \mathbf{n} = \cos(\phi), \\ & \mathbf{u} = \mathbf{0}, \\ & \theta = \theta_d(\mathbf{x}), \text{ or } \nabla \theta \cdot \mathbf{n} = \theta_n(\mathbf{x}), \end{aligned} \quad (4.7)$$

at $\mathbf{x} \in \partial\Omega, t > 0$. Here ϕ is the contact angle, and $\mathbf{n}$ is the unit outward normal to the boundary. For simplicity, the contact angle ϕ is fixed to $\pi/2$, and the boundary condition for the temperature is set as $\nabla \theta \cdot \mathbf{n} = 0$ in the present work.

When the temperature is considered constant, system (4.1) reduces to the isothermal NSK equations [72, 44, 16, 89, 108]. A review of theoretical and numerical methods to solve the (non)-isothermal NSK equations has been presented in our previous work [108]. Due to the Van der Waals equation of state and the nonlinear third order derivative of the mass density, it is a challenge to develop efficient and accurate methods for the (non)-isothermal NSK equations. Recently, important progress has been made to solve the isothermal NSK equations, examples are: [58] for a finite volume method with second gradient techniques, [44] for a Galerkin method with carefully chosen numerical fluxes, [16] for a finite element method with additional stabilization terms, and [72] for a Galerkin method with functional entropy variables. See also [40] for a discontinuous Galerkin method for the NSK equations in non-conservative form. Very few articles in the literature so far considered numerical methods for the non-isothermal NSK equations. Also, the isothermal NSK equations are frequently solved in a non-conservative form and an additional term is introduced to the total energy, which makes it difficult to extend the numerical discretization to the non-isothermal NSK equations. In contrast, we developed a simple LDG discretization for the isothermal NSK equations in conservative form and extended it in a straightforward way to the non-isothermal case [108]. In the current chapter, we focus on mesh adaptation for this method and the effects of solid wall boundaries.

The two commonly used adaptation methods are h -adaptation and p -adaptation [40]. Here h -adaptation refers to the local refinement and coarsening of the computational mesh, and in p -adaptation the polynomial degree can be adjusted in each element. We focus on h -adaptation in the present work. To start the mesh adaptation, we first need a criterion to decide whether an element in the computational mesh needs to be refined or coarsened. The candidate elements for refinement will be refined, and the coarsening of elements depends on their neighbors.

There are two main types of criteria for refinement and coarsening in finite volume and finite element methods: error estimators and heuristic indicators. Error estimators are based on theoretical results, and they are only available when a posteriori error estimates hold. For example, a posteriori error estimates can be found for first order finite volume schemes for scalar conservation laws and nonlinear hyperbolic systems of conservation laws [77, 78, 60]. A posteriori error estimates for finite element methods can be found in [7, 76, 113, 114] and for higher order Runge-Kutta discontinuous Galerkin methods for multidimensional nonlinear scalar conservation laws in [37]. Heuristic indicators usually depend on local gradients of thermodynamic variables like density, pressure, energy and entropy. Compared with a posteriori error estimates, heuristic indicators are easy to compute, and are widely used in practical applications [13, 115, 40, 16], but they have a limited theoretical foundation. Several indicators for adaptive Runge-Kutta discontinuous Galerkin methods for hyperbolic conservation laws can be found in [85, 126, 127]. Since a reliable a posteriori error estimate is currently out of scope for LDG discretizations of the (non)-isothermal NSK equations, a heuristic indicator is chosen in this chapter, which is based on the density gradient $|\nabla\rho|$.

The outline of this chapter can be summarized as follows. In Section 4.2, we briefly discuss an LDG discretization for the (non)-isothermal NSK equations in conservative form and without additional stabilization terms. Boundary conditions are treated in a special way in the LDG discretization. The mesh adaptation method is presented in Section 4.3. An adaptation criterion is proposed to select candidate elements for refinement and coarsening in the computational mesh. Also, a strategy for refining and coarsening of the candidate elements is discussed. In Section 4.4 computational experiments, including simulations with solid wall boundaries, are presented to verify the adaptive LDG method for the (non)-isothermal NSK equations. Finally, we give conclusions and recommendations for future research in Section 4.5.

4.2 LDG discretization of the NSK equations

In this section, we will present an LDG method to solve the (non)-isothermal NSK system in $\Omega \subset \mathbb{R}^d$ with $d \leq 3$. Special attention is given to the solid wall boundary conditions (4.7). We restrict the numerical experiments to one and two dimensions in this paper, but the LDG discretization described here can be easily extended to three dimensions. We first introduce some notations used for the description of the LDG discretization.

4.2.1 Notations

We denote by $\mathcal{T}_h$ a tessellation of Ω with regular shaped elements K , Γ represents all boundary faces of $K \in \mathcal{T}_h$ and $\Gamma_0 = \Gamma \setminus \partial\Omega$. Suppose e is a face shared by the “left” and “right” elements K_L and K_R . The normal vectors $\mathbf{n}_L$ and $\mathbf{n}_R$ on e point, respectively, exterior to K_L and K_R . Let φ be a function on K_L and K_R , which could be discontinuous across e , then the left and right trace are denoted as $\varphi_L = (\varphi|_{K_L})|_e$, $\varphi_R = (\varphi|_{K_R})|_e$, respectively. For more details about these definitions, we refer the reader to [121].

To get the LDG discretization, we define the finite element spaces

$$\begin{aligned} V_h &= \{\phi \in L^2(\Omega) : \phi|_K \in \mathcal{P}^k(K), \forall K \in \mathcal{T}_h\}, \\ \Sigma_h^d &= \{\Phi = (\phi^{(1)}, \phi^{(2)}, \dots, \phi^{(d)})^T \in (L^2(\Omega))^d : \phi^{(i)}|_K \in \mathcal{P}^k(K), \\ &\quad i = 1, \dots, d, \forall K \in \mathcal{T}_h\}, \end{aligned}$$

with $\mathcal{P}^k(K)$ the space of polynomials of degree up to $k \geq 0$ on $K \in \mathcal{T}_h$. In the present work, the computational mesh is composed of rectangular cells for simplicity, and tensor products of the one-dimensional orthogonal Legendre polynomials are used as basis functions.

The numerical solution is denoted by $\mathbf{U}_h$, with each component of $\mathbf{U}_h$ belonging to the finite element space V_h , and can be written as

$$\mathbf{U}_h(\mathbf{x}, t)|_K = \sum_{l=0}^{N_p} \hat{\mathbf{U}}_l^K(t) \phi_l^K(\mathbf{x}), \text{ for } \mathbf{x} \in K. \quad (4.8)$$

Here, $\hat{\mathbf{U}}_l^K(t)$ are the unknowns in element K and $\phi_l^K(\mathbf{x})$ the basis functions in K .

4.2.2 LDG discretization for the non-isothermal NSK equations

In this section we will present an LDG discretization for the non-isothermal NSK equations with solid boundaries (4.7). For details and a similar LDG discretization for the isothermal NSK equations, see [108].

To start with the LDG discretization, we first write the NSK equations (4.1) as a first-order system and keep the conservative form, given by

$$\begin{aligned}\rho_t + \nabla \cdot \mathbf{m} &= 0, \\ \mathbf{m}_t + \nabla \cdot \mathbf{F}(\mathbf{U}) - \nabla \cdot \tau(\mathbf{z}, l) - \nabla \cdot \xi(\rho, \mathbf{r}, g) &= \rho \mathbf{g}, \\ (\rho E)_t + \nabla \cdot \mathbf{G}(\mathbf{U}) - \nabla \cdot ((\tau + \xi) \cdot \mathbf{u}) + \nabla \cdot \mathbf{q} + \nabla \cdot \mathbf{j}_E &= \mathbf{g} \cdot \mathbf{m},\end{aligned}\quad (4.9)$$

and auxiliary equations

$$\begin{aligned}\mathbf{z} &= \nabla \mathbf{u}, \\ l &= \nabla \cdot \mathbf{u}, \\ \mathbf{r} &= \nabla \rho, \\ g &= \nabla \cdot \mathbf{r}, \\ \mathbf{q} &= -\frac{8C_v}{3\mathbb{W}e\mathbb{P}r} \nabla \theta,\end{aligned}\quad (4.10)$$

where

$$\begin{aligned}\mathbf{u} &= \frac{\mathbf{m}}{\rho}, \\ \tau &= \frac{1}{\mathbb{R}e} \left(\mathbf{z} + \mathbf{z}^T - \frac{2}{3} l \mathbf{I} \right), \\ \xi &= \frac{1}{\mathbb{W}e} \left(\left(\rho g + \frac{1}{2} |\mathbf{r}|^2 \right) \mathbf{I} - \mathbf{r} \mathbf{r}^T \right), \\ \theta &= \left(\frac{\rho E - \frac{1}{2} \mathbf{m}^2 / \rho - \frac{1}{2\mathbb{W}e} g^2}{\rho} + 3\rho \right) \frac{3}{8C_v}, \\ \mathbf{j}_E &= \frac{1}{\mathbb{W}e} \rho l \mathbf{r},\end{aligned}\quad (4.11)$$

and

$$\mathbf{F}(\mathbf{U}) = \mathbf{m} \otimes \mathbf{u} + p(\rho)\mathbf{I}, \quad \mathbf{G}(\mathbf{U}) = (\rho E + p)\mathbf{u}, \quad \mathbf{U} = \begin{pmatrix} \rho \\ \mathbf{m} \\ \rho E \end{pmatrix}.$$

The LDG discretization for the non-isothermal NSK equations (4.9) - (4.10) is now as follows: find $\rho_h, (\rho E)_h, l_h, g_h \in V_h$, and $\mathbf{m}_h, \mathbf{z}_h, \mathbf{r}_h, \mathbf{q}_h \in \Sigma_h^d$, such that for all test functions $\phi, \chi, \varphi, \zeta \in V_h$ and $\psi, \eta, \varsigma \in \Sigma_h^d$, the following relations are satisfied

$$\begin{aligned} & \int_K (\rho_h)_t \phi \, dK - \int_K \mathbf{m}_h \cdot \nabla \phi \, dK + \int_{\partial K} \widehat{\mathbf{m}}_h \cdot \mathbf{n} \phi \, ds = 0, \\ & \int_K (\mathbf{m}_h)_t \psi \, dK - \int_K (\mathbf{F}_h - \tau_h - \xi_h) \cdot \nabla \psi \, dK + \\ & \quad \int_{\partial K} (\widehat{\mathbf{F}}_h - \widehat{\tau}_h - \widehat{\xi}_h) \cdot \mathbf{n} \psi \, ds = \int_K \rho_h \mathbf{g} \psi \, dK, \\ & \int_K ((\rho E)_h)_t \chi \, dK - \int_K (\mathbf{G}_h - (\tau_h + \xi_h) \cdot \mathbf{u}_h + \mathbf{q}_h + (\mathbf{j}_E)_h) \cdot \nabla \chi \, dK \\ & \quad + \int_{\partial K} (\widehat{\mathbf{G}}_h - (\widehat{\tau}_h + \widehat{\xi}_h) \cdot \widehat{\mathbf{u}}_h + \widehat{\mathbf{q}}_h + (\widehat{\mathbf{j}}_E)_h) \cdot \mathbf{n} \chi \, ds \\ & \quad = \int_K \mathbf{g} \cdot \mathbf{m}_h \chi \, dK, \end{aligned} \tag{4.12}$$

and

$$\begin{aligned} & \int_K \mathbf{z}_h \eta \, dK = - \int_K \mathbf{u}_h \nabla \cdot \eta \, dK + \int_{\partial K} \widehat{\mathbf{u}}_h \eta \cdot \mathbf{n} \, ds, \\ & \int_K l_h \zeta \, dK = - \int_K \mathbf{u}_h \cdot \nabla \zeta \, dK + \int_{\partial K} \widehat{\mathbf{u}}_h \cdot \mathbf{n} \zeta \, ds, \\ & \int_K \mathbf{r}_h \varsigma \, dK = - \int_K \rho_h \nabla \cdot \varsigma \, dK + \int_{\partial K} \widehat{\rho}_h \varsigma \cdot \mathbf{n} \, ds, \end{aligned}$$

$$\begin{aligned}
 \int_K g_h \varphi \, dK &= - \int_K \mathbf{r}_h \cdot \nabla \varphi \, dK + \int_{\partial K} \widehat{\mathbf{r}}_h \cdot \mathbf{n} \varphi \, ds, \\
 \int_K \mathbf{q}_h \sigma \, dK - \frac{8C_v}{3\mathbb{W}e\mathbb{P}r} \int_K \theta_h \nabla \cdot \sigma \, dK + \frac{8C_v}{3\mathbb{W}e\mathbb{P}r} \int_{\partial K} \widehat{\theta}_h \sigma \cdot \mathbf{n} \, ds &= 0,
 \end{aligned} \tag{4.13}$$

where

$$\begin{aligned}
 \widehat{\mathbf{u}}_h &= \frac{\widehat{\mathbf{m}}_h}{\widehat{\rho}_h}, \\
 \widehat{\tau}_h &= \frac{1}{\mathbb{R}e} \left(\widehat{\mathbf{z}}_h + \widehat{\mathbf{z}}_h^T - \frac{2}{3} \widehat{l}_h \mathbf{I} \right), \\
 \widehat{\xi}_h &= \frac{1}{\mathbb{W}e} \left(\left(\widehat{\rho}_h \widehat{g}_h + \frac{1}{2} |\widehat{\mathbf{r}}_h|^2 \right) I - \widehat{\mathbf{r}}_h \widehat{\mathbf{r}}_h^T \right), \\
 \theta_h &= \left(\frac{(\rho E)_h - \frac{1}{2} \mathbf{m}_h^2 / \rho_h - \frac{1}{2\mathbb{W}e} g_h^2}{\rho_h} + 3\rho_h \right) \frac{3}{8C_v}, \\
 (\widehat{\mathbf{j}}_E)_h &= \frac{1}{\mathbb{W}e} \widehat{\rho}_h \widehat{l}_h \widehat{\mathbf{r}}_h,
 \end{aligned} \tag{4.14}$$

and

$$\mathbf{F}_h = \mathbf{F}(\mathbf{U}_h), \quad \mathbf{G}_h = \mathbf{G}(\mathbf{U}_h), \quad \mathbf{U}_h = \begin{pmatrix} \rho_h \\ \mathbf{m}_h \\ (\rho E)_h \end{pmatrix}.$$

The terms denoted with a hat in (4.12), (4.13)-(4.14) are single valued functions on each edge of element K , and are called numerical fluxes. We discuss the choices of the numerical fluxes in the next section.

4.2.3 Numerical fluxes

For the numerical fluxes in the LDG discretizations, solid wall boundaries (4.7) should be accounted for. Consider an edge $e \in \partial K$.

- If e is an interior edge, we choose the Lax-Friedrichs flux for the convective part and central numerical fluxes for the other flux terms. This

means

$$\begin{aligned}
 \widehat{\mathcal{F}}_h|_e &= \frac{1}{2}(\mathcal{F}_h|_L + \mathcal{F}_h|_R - \alpha(\mathbf{U}_h|_R - \mathbf{U}_h|_L)), \\
 \widehat{\mathbf{m}}_h|_e &= \frac{1}{2}(\mathbf{m}_h|_L + \mathbf{m}_h|_R), \quad \widehat{\rho}_h|_e = \frac{1}{2}(\rho_h|_L + \rho_h|_R), \\
 \widehat{\mathbf{r}}_h|_e &= \frac{1}{2}(\mathbf{r}_h|_L + \mathbf{r}_h|_R), \quad \widehat{\mathbf{z}}_h|_e = \frac{1}{2}(\mathbf{z}_h|_L + \mathbf{z}_h|_R), \\
 \widehat{l}_h|_e &= \frac{1}{2}(l_h|_L + l_h|_R), \quad \widehat{g}_h|_e = \frac{1}{2}(g_h|_L + g_h|_R), \\
 \widehat{\theta}_h|_e &= \frac{1}{2}(\theta_h|_L + \theta_h|_R), \quad \widehat{\mathbf{q}}_h|_e = \frac{1}{2}(\mathbf{q}_h|_L + \mathbf{q}_h|_R).
 \end{aligned} \tag{4.15}$$

with $\mathcal{F}_h^T = (\mathbf{m}_h^T, \mathbf{F}_h^T, \mathbf{G}_h^T)$ and α the global maximum of the absolute eigenvalue of $\frac{\partial \mathcal{F}_h}{\partial \mathbf{U}_h}$ [108].

- If e is an edge at the solid wall boundary of the domain, the numerical fluxes for the density, momentum and temperature on e are given by

$$\mathbf{n} \cdot (\widehat{\nabla \rho})_h|_e = -\|\nabla \rho\| \cos(\phi), \quad \widehat{\mathbf{m}}_h|_e = \mathbf{0}, \quad \mathbf{n} \cdot (\widehat{\nabla \theta})_h|_e = \theta_n|_e, \tag{4.16}$$

and the numerical fluxes for the remaining terms use data from the interior of the domain.

4.3 Mesh adaptation

In this section mesh adaptation for two-dimensional phase transition problems will be considered. We will first discuss refinement and coarsening of quadrilaterals, then present a criterion to select candidate elements in the computational mesh for refinement and coarsening, and finally we will discuss the mesh adaptation procedure. A flow chart of the mesh adaptation algorithm will be given at the end of this section.

4.3.1 Refinement and coarsening of quadrilaterals

In this section we will discuss the refinement of a single quadrilateral and the coarsening of children quadrilaterals. We assume that

Figure 4.1: Refinement of quadrilaterals.

- a background mesh with rectangular elements is used in the computational mesh,
- an element (called parent element) is always divided into 4 child elements with equal size,
- 4 child elements obtained from the same parent element can be coarsened to the parent element.

A description of the refinement of a parent quadrilateral and the coarsening of the child quadrilaterals is shown in Figure 4.1. During mesh adaptation, the L^2 -projection is used to compute the LDG coefficients, $\hat{\mathbf{U}}_l^K$ in (4.8). For example in Figure 4.1, L^2 -projection in the refinement process means that the degrees of freedom on sub-element Ki are obtained by L^2 -projection from the parent element K onto element Ki for $i = 1, \dots, 4$,

$$\int_{Ki} \mathbf{U}_h^{Ki}(\mathbf{x}) \phi_l^{Ki}(\mathbf{x}) d\mathbf{x} = \int_{Ki} \mathbf{U}_h^K(\mathbf{x}) \phi_l^{Ki}(\mathbf{x}) d\mathbf{x}, \quad l = 0, \dots, N_p - 1.$$

Here ϕ_l^{Ki} is the l -th basis function on element Ki . L^2 -projection in the coarsening step requires that the degrees of freedom on the parent element

K are obtained by L^2 -projection from sub-elements Ki onto element K ,

$$\int_K \mathbf{U}_h^K(\mathbf{x}) \phi_l^K(\mathbf{x}) d\mathbf{x} = \sum_{i=1}^4 \int_{Ki} \mathbf{U}_h^{Ki}(\mathbf{x}) \phi_l^K|_{Ki}(\mathbf{x}) d\mathbf{x}, \quad l = 0, \dots, N_p - 1,$$

where $\phi_l^K|_{Ki}$ is the basis function ϕ_l^K restricted to the child element Ki . For detailed procedures for refinement of quadrilaterals and the required L^2 -projection, see [40, 127].

4.3.2 Candidate elements for refinement and coarsening

In this section, we will provide a criterion to select candidate elements in the computational mesh for refinement and coarsening based on the locally largest value of the density gradient. Since the density changes rapidly at the interfacial region, the elements near the interface need to be refined. As the topology of the flow field changes, elements which were refined from a parent element and are not close to the interface anymore, need to be coarsened.

In this adaptation criterion, an indicator η_ρ^K for each element K is defined based on the gradients of the density on element K , and its direct and indirect neighbors [40]

$$\eta_\rho^K = \max \left\{ \frac{\text{diam}(K^j)}{|K^j|} \|\nabla \rho\|_{L^2(K^j)} \mid K^j \text{ is neighbor of } K \text{ of degree at most } m \right\}. \quad (4.17)$$

Here $\text{diam}(K^j)$ and $|K^j|$ represent the longest edge and the area of element K^j , respectively. The element K^j is a neighbor of element K of degree at most m if there exist $m + 1$ cells in the computational mesh with

$$K = K^0,$$

$$K^l \text{ is a neighbor of } K^{l+1}, \quad l = 0, 1, \dots, m.$$

Here $m = 0$ means only a contribution of element K and $m = 1$ contributions of K and its direct neighbours. Note that the computation of η_ρ^K for all cells is expensive for large m , but for $m = 0$ it leads to unstable results or slows down the iterative linear solvers [40]. We choose $m = 1$ throughout the present work.

Based on the indicators for the elements in the computational mesh, we select candidate elements for refinement and coarsening. We define the refinement level of the initial coarse elements by 0. An initial coarse element

can be refined at most LEV times. For each element K in the computational mesh,

$$\begin{aligned}
 &\text{if } \eta_\rho^K > \eta_{upp} \text{ and the refinement level of } K < LEV \\
 &\quad \text{then we mark } K \text{ as a candidate element for refinement,} \\
 &\text{else if } \eta_\rho^K < \eta_{low} \text{ and the refinement level of } K > 0 \\
 &\quad \text{then we mark } K \text{ as a candidate element for coarsening,} \quad (4.18)
 \end{aligned}$$

with problem dependent parameters η_{upp}, η_{low} and

$$\eta_{upp} > \eta_{low} > 0.$$

4.3.3 Strategy for refinement and coarsening

In this section we will present a refinement and coarsening algorithm for the LDG discretization, given candidate elements selected through the adaptation criterion (4.18). Although the LDG method allows locally many refinement levels, we impose that the difference in refinement levels between two neighbouring elements is less than one to improve the stability and accuracy of the LDG method.

To guarantee the difference in refinement levels between two neighbouring elements less than one, we use the “refinement must, coarsening can” strategy in the mesh adaptation. This strategy means that a candidate refinement cell is definitely refined and coarsening of a candidate element K depends on the neighbors of element K .

Algorithm 1 Refinement of candidate elements

```

call candidate elements for refinement by criterion (4.18)  $Cells_{refine}$ 
for each element  $K$  in  $Cells_{refine}$  do
  for each neighbor  $\tilde{K}$  of  $K$  do
    if  $\tilde{K}$  is not in  $Cells_{refine}$  and the refinement level of  $\tilde{K} <$  the
      refinement level of  $K$  then
      add  $\tilde{K}$  to  $Cells_{refine}$ 
    end if
  end for
end for

```

Algorithm 1 and 2 result in lists for refinement and coarsening, respectively. In Algorithm 1, all candidate refinement elements will be refined, and

Algorithm 2 Coarsening of candidate elements

```

call candidate elements for coarsening by criterion (4.18)  $Cells_{coarse}$ 
for each element  $K$  in  $Cells_{coarse}$  do
  set  $K_p$  as the parent cell of  $K$ 
  if all the children of  $K_p$  are in  $Cells_{coarse}$  then
    if the refinement level of all the neighbors of  $\tilde{K}_p <$  the
      refinement level of  $K$  then
      keep  $K$  in  $Cells_{coarse}$ 
    else
      delete  $K$  from  $Cells_{coarse}$ 
    end if
  else
    delete  $K$  from  $Cells_{coarse}$ 
  end if
end for

```

some neighbors of these elements are added to the refinement list to ensure mesh quality. In Algorithm 2, a candidate coarsening element K may not be coarsened due to the refinement level difference with the neighbors.

4.3.4 Flow chart for mesh adaptation

Next, we provide a flow chart to illustrate the adaptive LDG method. Given the maximum refinement level LEV and the final time T ,

- Step 1. Partition the domain into uniform rectangles, compute the degrees of freedom on each element K by projecting the initial solution on element K , and set the level of element K to be 0. An initial computational mesh $\mathcal{T}_h(t_0)$, the level of the elements in $\mathcal{T}_h(0)$ and the degrees of freedom $\{\hat{\mathbf{U}}^K(0), K \in \mathcal{T}_h(0)\}$ are obtained.
- Step 2. Given a computational mesh $\mathcal{T}_h(t_n)$ at time $t = t_n$, the refinement level of the elements in the mesh $\mathcal{T}_h(t_n)$ and the degrees of freedom $\{\hat{\mathbf{U}}^K(t_n), K \in \mathcal{T}_h(t_n)\}$
 - detect candidate elements for refinement and coarsening in the computational mesh through adaptation criterion (4.18),
 - create lists of elements for refinement and coarsening with Algorithm 1 and 2, respectively,

- for each element K in the refinement list, divide element K into four uniform child elements Ki , $i = 1, 2, 3, 4$, increase the refinement level of elements Ki by one, and get the degrees of freedom on elements Ki from element K by L^2 projection,
- when four cells in the coarsening list are all children of the same parent element K_p , merge them and get the degrees of freedom on K_p from its children elements by L^2 projection.

A new adapted mesh $\mathcal{T}_h(t_{n+1})$ and the refinement level of the elements in $\mathcal{T}_h(t_{n+1})$ are obtained.

- Step 3. Evolve the solution from t_n to t_{n+1} with the LDG method: i.e. solve a system of ODEs resulting from the LDG discretizations through an implicit RK time method, and obtain $\{\hat{\mathbf{U}}^K(t_{n+1}), K \in \mathcal{T}_h(t_{n+1})\}$.
- Step 4. If $t_{n+1} < T$, go to Step 2.

Note that the initial coarse mesh is uniform, we perform Step 2 therefore LEV times to capture the initial interface accurately. The degrees of freedom on the refined elements in the initial mesh are obtained by L^2 projection from the initial solution. Since it is not necessary to change the adapted mesh every time step during a simulation for the (non)-isothermal NSK equations, we apply Step 2 every 10 time steps in the numerical simulations discussed in the next section.

4.4 Numerical examples

In this section, numerical simulations will be presented to demonstrate the adaptive LDG discretizations for the (non)-isothermal NSK equations. First, we will consider simulations of the coalescence of vapor bubbles in a liquid. In our previous work we performed these simulations on a uniform mesh [108]. The same examples are computed here on an adaptive mesh, and the results will be compared with those in a uniform mesh. Second, we will discuss the structure of the Jacobi matrix for an adapted mesh for the non-isothermal NSK equations. Finally, we will study the shape of a vapor bubble and a liquid droplet in a domain with solid wall boundaries and prescribed contact angles, which are challenging problems in fluid mechanics. One example, representing a vapor bubble in contact with a solid wall, was studied in [58] by a finite difference scheme and an explicit time integration method on a uniform mesh. The last example describes a liquid droplet on a solid surface,

which was recently studied in [72] by a semi-discrete Galerkin method and a special time integration method on a uniform mesh.

We use a relatively simple LDG method to solve the NSK equations in conservative form on the adapted mesh. The adapted mesh is obtained using adaptation criterion (4.18), Algorithm 1 and Algorithm 2 in Section 4.3. Note that for the selection criterion given by (4.18), $m = 1$ is chosen in (4.17) to compute the indicator η_ρ^K for each element K . This means only contributions of element K and its direct neighbors are used, which saves many computations compared to [40], where $m = 4, 8$ was chosen. The computational domain in all simulations is $[0, 1]^2$.

Due to the third derivative of the density in the NSK equations, a diagonally implicit Runge-Kutta (DIRK) time integration method [8] is adopted to solve the ODEs resulting from the LDG discretizations. In particular, a second order DIRK scheme is used for all the numerical examples discussed in this section.

4.4.1 Coalescence of vapor bubbles in a liquid

An important test case is a simulation of the coalescence of two vapor bubbles in a liquid. We simulate the coalescence of vapor bubbles in a liquid for both the isothermal and non-isothermal NSK equations on adapted meshes.

Example 4.4.1. *Coalescence of vapor bubbles in a liquid, isothermal case*

This example was also studied with a Galerkin method on a uniform mesh [72], and with a finite element method including additional stabilization terms on an adaptive mesh [16]. In this example, the Van der Waals equation of state (4.3) is chosen for the isothermal NSK equations as [16, 72, 108]

$$p(\rho) = \frac{8\theta\rho}{27(1-\rho)} - \rho^2, \quad (4.19)$$

with a dimensionless temperature $\theta = 0.85$. The parameters of the isothermal NSK equations are set as $\mathbb{R}e = 512$, $\mathbb{W}e = 65500$.

The initial conditions are

$$\rho_0(\mathbf{x}) = \rho_1 + \frac{1}{2}(\rho_2 - \rho_1) \sum_{i=1}^2 \tanh\left(\frac{(d_i(\mathbf{x}) - r_i)}{2} \sqrt{\mathbb{W}e}\right), \quad \mathbf{u} \equiv \mathbf{0}, \quad (4.20)$$

with $\rho_1 = 0.1, \rho_2 = 0.6$. Here $d_i(\mathbf{x}) = \|\mathbf{x} - \mathbf{x}_i\|$ is the Euclidean distance and the points $\mathbf{x}_i$ are equal to $\mathbf{x}_1 = (0.4, 0.5)$ and $\mathbf{x}_2 = (0.78, 0.5)$, respectively.

The radii of the two bubbles are $r_1 = 0.25$ and $r_2 = 0.1$. Similar to [108], periodic boundary conditions are used for all variables .

The initial coarse mesh is set at 32×32 elements with three levels of refinement in the interface region. Then the adapted mesh has the same resolution in the interfacial region as for the computations on the uniform mesh in [108]. The parameters in (4.18) are chosen as $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$.

The results of the adaptive LDG method for Example 4.4.1 are shown in Figures 4.2-4.4. Figures 4.2-4.3 describe the coalescence of bubbles, showing that the bubbles merge into one vapor bubble by capillarity and pressure forces. Figure 4.4 shows the evolution of mass and energy during the simulation on the adapted mesh, indicating that the mass is conserved and the energy is decreasing in time. It is noticeable that the results for the mass loss on the adapted mesh have a larger accuracy than the results in Figure 4.5 for the uniform mesh used in [108].

The numbers of elements in the adapted mesh at the initial, average and final time are shown in Table 4.1. These numbers are much less than 256^2 , the number of elements in the uniform mesh used in [108]. Compared with the uniform mesh with equivalent mesh resolution in the interface region, the adaptive LDG method leads to a considerably smaller nonlinear system of algebraic equations that is solved by the Newton-GMRES method. Note that the computing time for the simulation of the coalescence of bubbles on the adaptive mesh reduces to about $1/3$ of the simulation time on a uniform mesh.

Example 4.4.2. *Coalescence of vapor bubbles in a liquid, non-isothermal case*

In this example we compute the coalescence of vapor bubbles in a liquid for the non-isothermal NSK equations. The parameters of the non-isothermal NSK equations are set as $\mathbb{Re} = 950$, $\mathbb{We} = 34455$. The Van der Waals equation of state (4.3) is chosen as in [108, 39, 82]

$$p(\rho) = \frac{8\theta\rho}{(3-\rho)} - 3\rho^2. \quad (4.21)$$

The initial conditions are

$$\begin{aligned} \rho_0(\mathbf{x}) &= \rho_1 + \frac{1}{2}(\rho_2 - \rho_1) \sum_{i=1}^2 \tanh\left(\frac{(d_i(\mathbf{x}) - r_i)}{2} \sqrt{\mathbb{We}}\right), \\ \mathbf{u} &\equiv \mathbf{0}, \quad \theta(\mathbf{x}) = 0.989, \end{aligned} \quad (4.22)$$

Figure 4.2: Example 4.4.1: time sequence of the coalescence of vapor bubbles. Isothermal NSK equations with $\text{Re} = 512$, $\text{We} = 65500$ and pressure formulation (4.19) at $\theta = 0.85$. Initial conditions (4.20) and periodic boundaries. Initially uniform mesh of 32^2 elements with $LEV = 3$, $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$ in adaptation criterion (4.18). Left: density profile, Right: computational mesh.

Figure 4.3: Example 4.4.1: time sequence of the coalescence of vapor bubbles. Isothermal NSK equations with $\mathbb{R}e = 512$, $We = 65500$ and pressure formulation (4.19) at $\theta = 0.85$. Initial conditions (4.20) and periodic boundaries. Initially uniform mesh of 32^2 elements with $LEV = 3$, $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$ in adaptation criterion (4.18). Left: density profile, Right: computational mesh.

Figure 4.4: Example 4.4.3: evolution of mass and energy during the coalescence of vapor bubbles. Isothermal NSK equations with $\mathbb{R}e = 512$, $We = 65500$ and pressure formulation (4.19) at $\theta = 0.85$. Initial conditions (4.20) and periodic boundaries. Initially uniform mesh of 32×32 elements with three levels of refinement, $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$ in adaptation criterion (4.18).

Figure 4.5: Example 4.4.3: evolution of mass loss and energy during the coalescence of vapor bubbles on a uniform mesh of 256×256 elements. Isothermal NSK equations with $\mathbb{R}e = 512$, $We = 65500$ and pressure formulation (4.19) at $\theta = 0.85$. Initial conditions (4.20) and periodic boundaries.

with $\rho_1 = 0.795, \rho_2 = 1.213$. Here $d_i(\mathbf{x}) = \|\mathbf{x} - \mathbf{x}_i\|$ is the Euclidean distance and the points $\mathbf{x}_i$ are equal to $\mathbf{x}_1 = (0.4, 0.5)$ and $\mathbf{x}_2 = (0.78, 0.5)$, respectively. The radii of the two bubbles are $r_1 = 0.25$ and $r_2 = 0.1$.

The initial uniform mesh is set at 25×25 elements with three levels of refinement in the interface region. The parameters in adaptation criterion (4.18) are chosen as $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$. The adapted mesh then has the same resolution in the interfacial region as the uniform mesh used in [108].

The results of the adaptive LDG method for Example 4.4.2 are shown in Figures 4.6-4.7. Similar to the results for the isothermal case in Example 4.4.1, Figures 4.6-4.7 describe the process of the coalescence of the vapor bubbles, showing that the bubbles merge into one vapor bubble by capillarity and pressure forces. Figure 4.8 shows the evolution of mass, entropy, momentum along one direction and energy, indicating that the numerical mass, momentum and energy are conserved and the entropy is generally increasing in time. The small oscillations in the entropy can be eliminated by choosing different parameters in adaptation criterion (4.18).

4.4.2 DIRK time integration method on an adapted mesh

In this section we will consider a diagonally implicit Runge-Kutta time method on an adapted mesh. In particular, we will present the Jacobi matrix for an example of the non-isothermal NSK equations in a uniform and an adapted mesh, respectively. For the implementation of the DIRK method and the computation of the Jacobi matrix, see [108].

Figure 4.9 shows the distribution of the non-zeros in the Jacobi matrix for Example 4.4.2 for both a uniform and an adapted mesh. For the sake of the ability to plot the Jacobi matrix, we choose the uniform mesh of 20×20 square elements and the adapted mesh as an initially uniform mesh of 10×10 elements with one level of refinement. These two meshes have the same resolution in the interface region. From Figure 4.9, we see that the Jacobi matrix of the adapted mesh contains less non-zeros than the one of the uniform mesh. This phenomena will be more obvious when a fine mesh resolution is used in the interface region, then the adapted mesh contains far less elements than the uniform mesh as shown in Table 4.1.

It is noticeable that some new branches of non-zeros are present in the Jacobi matrix for the adapted mesh, which are caused by the local mesh refinement. We observe that in the Newton method, which is used to solve the non-linear algebraic equations resulting from the DIRK time integration method, the number of GMRES iterations for the adapted mesh (which is 2)

Figure 4.6: Example 4.4.2: time sequence of the coalescence of bubbles. Non-isothermal NSK equations with $\mathbb{R}e = 950$, $We = 34455$ and pressure formulation (4.21). Initial condition (4.22) and periodic boundaries. Initially uniform mesh of 25^2 elements with $LEV = 3$, $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$ in (4.18). Left: density profile, Right: corresponding computational mesh.

Figure 4.7: Example 4.4.2: time sequence of the coalescence of bubbles. Non-isothermal NSK equations with $\mathbb{R}e = 950$, $\mathbb{W}e = 34455$ and pressure formulation (4.21). Initial condition (4.22) and periodic boundaries. Initially uniform mesh of 25^2 elements with $LEV = 3$. $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$ in (4.18). Left: density profile, Right: computational mesh.

Figure 4.8: Evolution of changes in numerical variables during the coalescence of vapor bubbles. Non-isothermal NSK equations with $\mathbb{R}e = 950$, $\mathbb{W}e = 34455$ and pressure formulation (4.21). Initial condition (4.22) and periodic boundaries. Initially uniform mesh of 25×25 elements with $LEV = 3$. $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$ in (4.18).

is less than the number required for the uniform mesh (which is 4). Although the implementation of a DIRK method in combination with a locally refined mesh is non-trivial, we see from the examples discussed in this section that the DIRK method results in an efficient time integration method to solve the NSK equations on a locally refined mesh in combination with an LDG discretization.

4.4.3 Bubbles and droplets in contact with solid wall boundaries

In the next two numerical examples, we study a vapor bubble rising towards a solid wall and a liquid droplet on a solid substrate. It is pointed out that the shape of the vapor bubble and the liquid droplet depends on two factors [72]: (1) the contact angle and (2) the Bond number $\mathbb{Bo}$. The contact angle is a parameter to model the physical interactions between the surface and the fluids, and is determined by whether the surface is hydrophilic or hydrophobic to the fluid. The contact angle has been studied theoretically [91] and numerically [58, 56]. In the present simulation, the contact angle is imposed by the first equation in the boundary conditions (4.7) and ϕ is fixed to be $\pi/2$ for simplicity. The Bond number quantifies the relative importance of gravity against surface tension, and is defined as

$$\mathbb{Bo} = \frac{\Delta\rho|\mathbf{g}|r^2}{\sigma}. \quad (4.23)$$

Here $\Delta\rho$ is the difference between the liquid and vapor mass density, $\mathbf{g}$ is the dimensionless gravity, r is the radius of the droplet or bubble and σ is the surface tension. The importance of the Bond number will be studied in the following numerical examples.

Since the initial temperature is chosen as constant close to the critical temperature, and the temperature does not vary much in time [108], we consider the isothermal NSK equations for simplicity. The Van der Waals equations of state is set as in (4.21), and the temperature is chosen as $\theta = 0.9497$ in the following examples. The parameters for the isothermal NSK equations are $\mathbb{Re} = 500$, $\mathbb{We} = 34455$. For adaptation criterion (4.18) in the mesh adaptation algorithm, the parameters are chosen as $\eta_{upp} = 0.1$, $\eta_{low} = 0.02$.

Example 4.4.3. *Vapor bubble in contact with a solid wall* In this example, we will investigate the shape of a vapor bubble rising towards a solid wall, while accounting for the contact angle at the solid surface and the gravity.

(a) Jacobi matrix for a uniform mesh

(b) Jacobi matrix for an adapted mesh

Figure 4.9: Shape of Jacobi matrix for Example 4.4.2 of the non-isothermal NSK equations on a uniform and an adapted mesh. Both meshes have the same resolution in the interface region. Initial conditions (4.22). Left matrix for a uniform mesh of 20×20 elements; Right matrix for an initially uniform mesh of 10×10 elements with one level of refinement. Adaptation criterion (4.18) with $\eta_{upp} = 0.05$, $\eta_{low} = 0.01$.

This example was studied in [58] by a model based on the second gradient theory on a uniform mesh.

The initial conditions are set as

$$\begin{aligned}\rho(\mathbf{x}, 0) &= \frac{\rho_1 + \rho_2}{2} + \frac{\rho_2 - \rho_1}{2} \tanh\left(\frac{d(\mathbf{x}) - r}{2} \sqrt{\mathbb{W}e}\right), \\ \mathbf{u} &= 0,\end{aligned}\tag{4.24}$$

with $d(\mathbf{x}) = \sqrt{(x - 0.5)^2 + (y - 0.5)^2}$, $r = 0.2$ and $\rho_1 = 0.578, \rho_2 = 1.463$. The dimensionless gravity points in the negative y -direction with magnitudes $|\mathbf{g}| = 0.006, 0.02$. Because of relation (4.23), the Bond numbers are 0.18 and 0.6, respectively.

The time evolution of the bubble rising towards a wall under different values of gravity is presented in Figures 4.10-4.14. From these figures, we see that

- the adaptive mesh is consistent with the motion of the vapor bubble,
- the vapor bubble starts rising under the action of gravity, then attaches to the upper wall, and finally reaches an equilibrium state,
- the contact line moves rapidly after the contact of the bubble with the solid wall, as pointed out by [58],
- the gravity has an important impact on the shape of the bubble. Figures 4.10-4.12 show that when the Bond number is large, the gravity makes the vapor bubble move to the upper solid wall and obtain a flattened shape in equilibrium. When the Bond number is relatively small, due to a smaller value of the gravitational acceleration, the bubble moves more slowly to the upper wall and obtains a spherical cap in equilibrium, as shown in Figures 4.13 - 4.14.

Example 4.4.4. A liquid droplet on a solid wall In this example the shape of a liquid droplet on a solid substrate, as used in wetting problems, is studied. This example was investigated using a (discontinuous) Galerkin method for the isothermal NSK equations in non-conservative form and on a uniform mesh [40, 72].

The initial conditions are set as

$$\begin{aligned}\rho(\mathbf{x}, 0) &= \frac{\rho_1 + \rho_2}{2} - \frac{\rho_2 - \rho_1}{2} \tanh\left(\frac{d(\mathbf{x}) - r}{2} \sqrt{\mathbb{W}e}\right), \\ \mathbf{u} &= 0,\end{aligned}\tag{4.25}$$

Figure 4.10: Example 4.4.3: time sequence and adapted mesh of a vapor bubble rising towards a solid wall. Initial conditions (4.24) and solid boundaries (4.7). Initially uniform mesh of 25^2 elements with $LEV = 3$. $\eta_{upp} = 0.1$, $\eta_{low} = 0.02$ in (4.18). $Re = 500$, $We = 34455$, $|\mathbf{g}| = 0.02$. Left: density profile, Right: computational mesh.

(a) $t = 8$.

(b) $t = 8$.

(c) $t = 10$.

(d) $t = 10$.

(e) $t = 12$.

(f) $t = 12$.

Figure 4.11: Example 4.4.3: time sequence and adapted mesh of a vapor bubble rising towards a solid wall. Initial conditions (4.24) and solid boundaries (4.7). Initially uniform mesh of 25^2 elements with $LEV = 3$, $\eta_{upp} = 0.1$, $\eta_{low} = 0.02$ in (4.18). $Re = 500$, $We = 34455$, $|\mathbf{g}| = 0.02$. Left: density profile, Right: computational mesh.

(a) $t = 14$.

(b) $t = 14$.

(c) $t = 25$.

(d) $t = 25$.

Figure 4.12: Example 4.4.3: time sequence and adapted mesh of a vapor bubble rising towards a solid wall. Initial conditions (4.24) and solid boundaries (4.7). Initially uniform mesh of 25^2 elements with $LEV = 3$, $Re = 500$, $We = 34455$, $|\mathbf{g}| = 0.02$. Left: density profile, Right: computational mesh.

Figure 4.13: Example 4.4.3: time sequence and adapted mesh of a vapor bubble rising towards a solid wall. Initial conditions (4.24) and solid boundaries (4.7). Initially uniform mesh of 25^2 elements with $LEV = 3$, $\eta_{upp} = 0.1$, $\eta_{low} = 0.02$ in (4.18). $\mathbb{R}e = 500$, $\mathbb{W}e = 34455$, $|\mathbf{g}| = 0.006$. Left: density profile, Right: computational mesh.

(a) $t = 20$. (b) $t = 20$. (c) $t = 22$. (d) $t = 22$. (e) $t = 25$. (f) $t = 25$.

Figure 4.14: Example 4.4.3: time sequence and adapted mesh of a vapor bubble rising towards a solid wall. Initial conditions (4.24) and solid boundaries (4.7). Initially uniform mesh of 25^2 elements with $LEV = 3$, $\eta_{upp} = 0.1$, $\eta_{low} = 0.02$ in (4.18). $\text{Re} = 500$, $\text{We} = 34455$, $|\mathbf{g}| = 0.006$. Left: density profile, Right: computational mesh.

Figure 4.15: Example 4.4.4: initial state of a droplet on a solid substrate with initial condition (4.25). Initially uniform mesh of 25×25 elements with three levels of refinement, $\eta_{upp} = 0.1$, $\eta_{low} = 0.02$ in adaptation criterion (4.18). Left: density profile, Right: computational mesh.

with $d(\mathbf{x}) = \sqrt{(x - 0.5)^2 + y^2}$, $r = 0.2$ and $\rho_1 = 0.578, \rho_2 = 1.463$. At the initial time, a half spherical liquid droplet rests on a solid wall as shown in Figure 4.15. The dimensionless gravity points in the negative y -direction with magnitude $|\mathbf{g}| = 0.008, 0.02, 0.05$. Recalling relation (4.23), the corresponding Bond numbers are 0.24, 0.60 and 1.49, respectively.

We perform the computations until time $t = 15.0$ and present the density profiles for different values of the dimensionless gravity in Figure 4.16. Figure 4.16 shows that the magnitude of the Bond number has an important effect on the shape of the droplet:

- when the Bond number is relatively small, the surface tension dominates and the droplet has the shape of a spherical cap in an equilibrium,
- when the Bond number is relatively large, the gravity, as the dominant force, flattens the droplet.

Table 4.1 shows the number of elements used in the adaptive mesh for Examples 4.4.3 and 4.4.4, which are much smaller than the number of elements required for a uniform mesh. Therefore, computing time and memory are saved when the adaptive LDG method is applied, compared to computations on a uniform mesh.

 (a) $t = 15$, $|\mathbf{g}| = 0.008$.

 (b) $t = 15$, $|\mathbf{g}| = 0.008$.

 (c) $t = 15$, $|\mathbf{g}| = 0.02$.

 (d) $t = 15$, $|\mathbf{g}| = 0.02$.

 (e) $t = 15$, $|\mathbf{g}| = 0.05$.

 (f) $t = 15$, $|\mathbf{g}| = 0.05$.

Figure 4.16: Example 4.4.4: an equilibrium of a droplet on a solid substrate with initial condition (4.25) at the various gravity. Initially uniform mesh of 25^2 elements with $LEV = 3$, $\eta_{upp} = 0.1$, $\eta_{low} = 0.02$ in (4.18). Left: density profile, Right: computational mesh.

Table 4.1: Adaptive mesh for the simulations of the examples. (a) N_0 : initial number of elements; (b) TDT total refinement and coarsening times; (c) N_T : number of elements at the final time; (d) $\bar{N}$: average number of elements, defined by $\bar{N} = (\sum_{q=0}^{TOT} N_q)/TOT$ where N_q is the number of elements at the q -th time level and TOT is the total number of time levels; and (e) PR : the percentage ratio of $\bar{N}$ to the number of elements if a uniform mesh would be used, i.e. $PR = 100\bar{N}/M^2$ with M the number of elements in one direction in a uniform mesh. The uniform mesh has the same resolution in the interfacial region as the adapted mesh.

Case	N_0	TDT	N_T	N	PR
Example 4.4.1	9736	196	7570	8250	12.60
Example 4.4.3	4297	154	3097	3851	9.63
Example 4.4.4	2467	30	2488	2484	6.21

4.5 Conclusions

In this chapter, an h -adaptive local discontinuous Galerkin method was presented for the (non)-isothermal NSK equations. In order to select candidate elements for refinement and coarsening, a criterion is provided to compute an indicator for the elements in the computational mesh based on the locally largest value of the density gradient. A strategy called “refinement must, coarsening can” is adopted in refining and coarsening the candidate cells. Numerical experiments demonstrate the accuracy, efficiency and capabilities of the local discontinuous Galerkin method for the (non)-isothermal NSK equations on an adapted mesh. In particular, contact angles and solid wall boundaries were considered in the simulations. We emphasize that only direct neighbors are used in the computation of the indicators for the elements in the adapted mesh, and the coarsening procedure is relatively simple. The implicit Runge-Kutta time integration method in combination with an adapted mesh results in an efficient time integration method for the NSK equations, which does not suffer from the severe time step restriction $dt \leq Ch^2$, with h the smallest element size and C a constant, as occurs for explicit time integration methods. This is particularly important when using a locally refined mesh, since the locally small mesh resolution would further reduce the allowable time-step for explicit integration methods.

Future research will investigate suitable criteria for mesh adaptation. Apart from the jump in the magnitude of the density, other indicators discussed in [85, 127], a posteriori error estimates and residual analysis are also interesting options as criteria for refinement or coarsening. These latter ap-

proaches require, however, a significant theoretical effort.

Conclusions and Outlook

5.1 Conclusions

In this thesis several local discontinuous Galerkin (LDG) discretizations are presented to solve higher-order partial differential equations modeling phase transitions in solids and fluids. We summarize our contributions as follows. For a viscosity-capillarity (VC) system associated with isothermal motion of phase transitions in elastic bars and in Van der Waals fluids, we have developed and analyzed an LDG discretization. L^2 -stability of the LDG discretization was proved for the VC system with a general stress-strain relation. An a priori error estimate of the LDG discretization was provided for the VC system with a trilinear stress-strain relation in the hyperbolic region, assuming that the solution is sufficiently smooth. As a reference solution for the VC system with a trilinear stress-strain relation, we computed an exact solution for the Riemann problem of the corresponding conservation laws using the techniques provided in [2, 3]. Computations were also performed for the VC system with the Van der Waals equation of state.

The (non)-isothermal Navier-Stokes-Korteweg equations model the dynamics of compressible flows with liquid-vapor phase change. We solved the (non)-isothermal NSK equations in conservative form with the LDG method without adding additional stabilization terms. The LDG discretizations lead to coupled nonlinear systems of ordinary differential and algebraic equations, which are solved by an implicit time integration method. To investigate the performance of the LDG discretizations for the (non)-isothermal NSK equa-

tions, we presented several numerical examples, including one-dimensional benchmark problems and two-dimensional simulations of the coalescence of vapor bubbles in a liquid. It is shown that for stability a mesh needs to satisfy a relation $d = \alpha h$, $\alpha > 10$, with d the diffuse interface width and h the mesh size at the interfacial region. The numerical results verified the accuracy, stability and capability of the LDG discretization for the mathematical models considered in this thesis.

Furthermore, LDG discretizations on an adapted, locally refined mesh were considered for the (non)-isothermal NSK equations. The locally largest value of the density gradient was used as a criterion to detect whether an element in the computational mesh needs to be refined or coarsened. Numerical examples demonstrated the accuracy, stability and capabilities of the adaptive LDG method. In particular, the non-isothermal NSK equations with solid wall boundary conditions have been solved on an adapted mesh.

It should be pointed out that the (non)-isothermal NSK equations were solved when the dimensionless temperature is below, but close to the critical temperature, so that the interface has a relatively large width. The mathematical models we tackled in this monograph are restricted to one and two dimensions, although the proposed LDG discretizations can be extended to three-dimensional problems straightforwardly.

5.2 Outlook

In this section we present some suggestions and ideas for future work based on the results of the research presented in this thesis. One future direction of research will be concerned with the theoretical proof of convergence and stability of the LDG discretizations for the (non)-isothermal NSK equations. First, we will consider a one-dimensional system with linear higher order derivatives in a Van der Waals fluid [100], given by

$$\omega_t = u_x, \quad (5.1)$$

$$u_t = (-p + \mu u_x - \mu^2 A w_{xx})_x, \quad (5.2)$$

$$E_t = (u(-p + \mu u_x - \mu^2 A \omega_{xx}))_x + \alpha \theta_{xx} + \mu^2 A (u_x \omega_x)_x, \quad (5.3)$$

where ω is the specific volume, u the velocity and E the specific energy, defined as

$$E \equiv \frac{u^2}{2} + e + \frac{C \omega_x^2}{2}.$$

Here e is the specific internal energy, and μ, α, A and C are constants. In our work [107], L^2 -stability was proved for the LDG discretization of a system composed by the first two equations (5.1)-(5.2). For system (5.1)-(5.3), one obvious question is how to define the total energy in the proof since the energy equation is already present in (5.3). The coupling relation between the specific energy, the specific internal energy and entropy also adds to the difficulty of the proof.

A theoretical investigation of the mesh adaptation criteria in Chapter 4 is another interesting and useful direction of research. Currently, as an adaptation criterion the locally largest density gradient, together with two problem-dependent constants, is used to detect whether a cell in the mesh needs to be refined or coarsened. Other indicators, discussed in [85, 126, 127], such as a posteriori error estimates and residual analysis are also interesting options as criteria for refinement or coarsening of cells. These latter approaches require, however, a significant theoretical effort.

Moreover, the computational efficiency of the current code can be improved by parallelization. Especially for three-dimensional problems, parallelization will reduce the computing time of simulations. Since a discontinuous Galerkin method only requires local information, parallelization can be combined with the LDG discretizations using a block decomposition of the computational mesh.

Finally, when the temperature is far below the critical temperature, very thin interfaces arise. Then the diffuse interface model, such as the NSK equations, requires a very fine resolution at the interfacial region, which becomes difficult even with mesh adaptation. Efficient techniques, such as a multi-scale method, are then indispensable in order to be able to deal with these very thin interfaces. Meanwhile, the Van der Waals equation of state is not accurate to model the pressure at various states when the temperature is low. Instead, other types of equations of state have to be considered.

The scope of current research also expands to faster iterative solvers for the implicit time integration, the NSK equations with proper inflow-outflow boundary conditions, and real life applications.

Summary

In this thesis we develop a local discontinuous Galerkin (LDG) finite element method to solve mathematical models for phase transitions in solids and fluids. The first model we study is called a viscosity-capillarity (VC) system associated with phase transitions in elastic bars and Van der Waals fluids. We develop and analyze an LDG discretization for the VC system. We prove L^2 -stability for the VC system with a general stress-strain relation. Using a priori error analysis, we provide an error estimate for the LDG discretization of the VC system when the stress-strain relation is linear, assuming that the solution is sufficiently smooth and the system is in a hyperbolic region. To obtain a reference solution for the VC system with a trilinear stress-strain relation, we solve a Riemann problem of the conservation laws using a kinetic relation. Numerical examples are also provided to verify the LDG discretization of the VC system with the Van der Waals equation of state.

Secondly, we consider the Navier-Stokes-Korteweg (NSK) equations describing the dynamics of a compressible fluid with liquid-vapor phase change. Compared with the classical Navier-Stokes equations, the NSK equations contain an additional stress tensor related to the capillarity forces. The Van der Waals equation of state is used in the NSK equations to describe the pressure as a function of temperature and density in both liquid and vapor states. We solve the isothermal NSK equations with the LDG method in conservative form without additional stabilization. In solving the ordinary differential equations (ODEs) resulting from the LDG discretization, a severe

time restriction is required for an explicit time method due to the third order derivative of the density in the Korteweg tensor. To circumvent this, we use a time-implicit Runge-Kutta method. Next, we extend the LDG discretization for the isothermal NSK equations to the non-isothermal case, retaining the conservative formulation. Computations, including one-dimensional benchmark problems and two-dimensional simulations of the coalescence of vapor bubbles in a liquid, demonstrate the accuracy, convergence and stability of the proposed LDG discretizations, provided the mesh is sufficiently fine to accurately capture the interface between the two phases.

Finally, a mesh adaptation algorithm is studied for the LDG discretization of the (non)-isothermal NSK equations to save computing time and memory and to capture the interface more accurately. The motivation is the fact that a fine resolution is only required in the interfacial region and that the LDG method is suited to deal with hanging nodes. As an adaptation criterion, the locally largest value of the density gradient is used to select candidate elements for refinement and coarsening. A time-implicit Runge-Kutta method is used to solve the ODEs resulting from the LDG discretizations on an adapted mesh. The same numerical examples for the two-dimensional (non)-isothermal NSK equations are computed on adaptive meshes, and compared with those on uniform meshes. Boundary conditions where vapor bubbles and a liquid droplet are in contact with a solid wall are also considered.

We emphasize that an important feature of the LDG discretizations for the mathematical models presented in this thesis is that they are relatively simple and robust, and do not require special regularization terms. The use of the time-implicit Runge-Kutta method in combination with the mesh adaptation is non-trivial, but results in an efficient and accurate method for the NSK equations. Computational experiments show the accuracy, stability and capabilities of the (adaptive) LDG method.

Samenvatting

Dit proefschrift beschrijft de ontwikkeling van een lokale discontinue Galerkin (LDG) eindige elementen methode om wiskundige modellen voor faseovergangen in vaste stoffen en vloeistoffen op te lossen. Het eerste model dat we bestuderen wordt een viscosity-capillarity (VC) systeem genoemd dat gebruikt wordt voor faseovergangen in elastische staven en Van der Waals vloeistoffen. We bewijzen de L^2 -stabiliteit van een VC systeem met een algemeen verband tussen spanning en deformatie. Met behulp van een a priori foutenanalyse geven we een schatting van de fout voor de LDG discretisatie van het VC systeem in het geval dat het verband tussen spanning en deformatie lineair is en onder de aanname dat de oplossing voldoende glad is en zich in het hyperbolische gebied bevindt. Om een referentieoplossing van het VC systeem met een trilineair verband tussen spanning en deformatie te verkrijgen, lossen we een Riemann probleem voor de behoudswetten op met behulp van een kinetische relatie. We geven ook numerieke voorbeelden om de LDG discretisatie van het VC systeem met een Van der Waals toestandsvergelijking te verifiëren.

Als tweedebeschuwen we de (niet-)isotherme Navier-Stokes-Korteweg (NSK) vergelijkingen, die de dynamica van een compressibele vloeistof die faseovergangen tussen vloeistof en damp kan ondergaan beschrijft. Vergeleken met de klassieke Navier-Stokes vergelijkingen bevatten de NSK vergelijkingen een extra spanningstensor ten gevolge van capillaire krachten. Om de druk als functie van dichtheid en temperatuur in zowel de vloeistof- als de damp-

fase te beschrijven wordt de Van der Waals toestandsvergelijking gebruikt. We lossen de isotherme NSK vergelijkingen op met de LDG methode in behoudsvorm zonder extra stabilisatie. Het stelsel gewone differentiaalvergelijkingen dat resulteert uit de LDG discretisatie kan alleen met een expliciete tijdstapmethode opgelost worden als aan een strenge tijdstaprestrictie voldaan is. Dit is onder meer een gevolg van de derde orde afgeleide van de dichtheid in de Kortewegtensor. Om dit probleem te omzeilen gebruiken we een impliciete Runge-Kutta tijdintegratie.

Vervolgens breiden we de LDG discretisatie voor de isotherme NSK vergelijkingen uit naar het niet-isotherme geval, met behoud van de behoudsvorm. Berekeningen, onder andere eendimensionale standaardproblemen en tweedimensionale simulaties van de coalescentie van dampbellen in een vloeistof, laten zien dat de voorgestelde LDG discretisatie nauwkeurig en stabiel is en convergeert, als het rekenrooster voldoende fijn is om het interface tussen de twee fasen nauwkeurig te beschrijven.

Tenslotte wordt een roosteradaptatiealgoritme voor de LDG discretisatie van de (niet-)isotherme NSK vergelijkingen bestudeerd dat bedoeld is om rekentijd en geheugen te besparen en het interface nauwkeuriger te beschrijven. De motivatie hiervoor is dat een grote resolutie alleen nodig is in de buurt van het interface en dat de LDG methode geschikt is voor zwevende roosterpunten. Als adaptatiecriterium wordt de lokaal grootste waarde van de dichtheidgradiënt gebruikt voor de selectie van kandidaat elementen voor verfijning en vergroving. Een impliciete Runge-Kutta tijdintegratiemethode wordt gebruikt om het stelsel gewone differentiaalvergelijkingen op te lossen dat volgt uit de LDG discretisatie op een aangepast rekenrooster. Dezelfde numerieke voorbeelden van de tweedimensionale (niet-)isotherme NSK vergelijkingen worden berekend op adaptieve roosters en vergeleken met de oplossingen op uniforme roosters. Ook worden randvoorwaarden voor dampbellen en druppels in contact met een vaste wand bestudeerd.

We benadrukken dat de betrekkelijke eenvoud en robuustheid belangrijke eigenschappen zijn van de LDG discretisaties die in dit proefschrift gepresenteerd worden. Bovendien hebben ze geen speciale regularisatietermen nodig. Toepassing van de impliciete Runge-Kutta tijdintegratiemethode is niet triviaal in combinatie met roosteradaptatie, maar leidt tot een efficiënte en nauwkeurige methode voor de NSK vergelijkingen. Numerieke experimenten laten zien dat de (adaptieve) LDG methode nauwkeurig en stabiel is en veel toepassingsmogelijkheden heeft.

Bibliography

- [1] R. Abeyaratne and J.K. Knowles. On the driving traction acting on a surface of strain discontinuity in a continuum. *J. Mech. Phys. Solids*, 38:345–360, 1990.
- [2] R. Abeyaratne and J.K. Knowles. Implications of viscosity and strain-gradient effects for the kinetics of propagating phase boundaries in solids. *SIAM J. Appl. Math.*, 51:1205 – 1221, 1991.
- [3] R. Abeyaratne and J.K. Knowles. Kinetic relations and the propagation of phase boundaries in solids. *Arch. Rational Mech. Anal.*, 114:119 – 154, 1991.
- [4] R. Abeyaratne and J.K. Knowles. *Evolution of phase transitions: a continuum theory*. Cambridge University Press, 2006.
- [5] R. Abeyaratne, K. Sang-Joo, and J.K. Knowles. A one-dimensional continuum model for shape-memory alloys. *Internat. J. Solids Structures*, 31:2229–2249, 1994.
- [6] R. Ahluwalia and G. Ananthakrishna. Power-law statistics for avalanches in a martensitic transformation. *Phys. Rev. Lett.*, 86:4076–4079, 2001.
- [7] M. Ainsworth and J.T. Oden. A posteriori error estimation in finite element analysis. *Comput. Methods Appl. Mech. Engrg.*, 142:1–88, 1997.

-
- [8] R. Alexander. Diagonally implicit Runge-Kutta methods for stiff ODE's. *SIAM J. Numer. Anal.*, 14:1006–1021, 1977.
 - [9] D.M. Anderson, G.B. McFadden, and A.A. Wheeler. Diffuse-interface methods in fluid mechanics. *Annu. Rev. Fluid Mech.*, 30:139–165, 1998.
 - [10] G.S. Bales and R.J. Gooding. Interfacial dynamics at a first-order phase transition involving strain: dynamical twin formation. *Phys. Rev. Lett.*, 67:3412–3415, 1991.
 - [11] G.K. Batchelor. *An Introduction to Fluid Dynamics*. Cambridge University Press, 1967.
 - [12] A. Berezovski and G.A. Maugin. Numerical simulation of phase-transition front propagation in thermoelastic solids. In *Numerical mathematics and advanced applications*, pages 703 – 711, Berlin Heidelberg, 2006. Springer.
 - [13] M.J. Berger and P. Colella. Local adaptive mesh refinement for shock hydrodynamics. *J. Comput. Phys.*, 82:64–84, 1989.
 - [14] V. Bongiorno and H.T. Davis. Modified van der Waals theory of fluid interfaces. *Phys. Rev. A*, 12:2213, 1975.
 - [15] B. Boutin, C. Chalons, F. Lagoutiere, and P.G. LeFloch. Convergent and conservative schemes for nonclassical solutions based on kinetic relations. *Interfaces Free Bound.*, 10:399 – 421, 2008.
 - [16] M. Braack and P. Andreas. Stable discretization of a diffuse interface model for liquid-vapor flows with surface tension. *ESAIM Math. Model. Numer. Anal.*, 47:401–420, 2013.
 - [17] C.E. Brennen. *Cavitation and bubble dynamics*. Cambridge University Press, 2013.
 - [18] D. Bresch, B. Desjardins, and C.K. Lin. On some compressible fluid models: Korteweg, lubrication, and shallow water systems. *Comm. Partial Differential Equations*, 28:843–868, 2003.
 - [19] J.W. Cahn and J.E. Hilliard. Free energy of a nonuniform system. I. Interfacial free energy. *J. Chem. Phys.*, 28:258 – 267, 1958.
 - [20] J.R. Cash. Diagonally implicit Runge-Kutta formulae with error estimates. *IMA J. Appl. Math.*, 24:293–301, 1979.

- [21] C. Chalons. Transport-equilibrium schemes for computing nonclassical shocks. *Numer. Methods Partial Differential Equations*, 24:11271147, 2006.
- [22] C. Chalons and J.F. Coulombel. Relaxation approximation of the Euler equations. *J. Math. Anal. Appl.*, 348:872 – 893, 2008.
- [23] C. Chalons and P. Goatin. Godunov scheme and sampling technique for computing phase transitions in traffic flow modeling. *Interfaces Free Bound.*, 10:197 – 221, 2008.
- [24] C. Chalons and P.G. LeFloch. High-order entropy-conservative schemes and kinetic relations for van der Waals fluids. *J. Comput. Phys.*, 168:184 – 206, 2001.
- [25] C. Chalons and P.G. LeFloch. Computing under-compressive waves with the random choice scheme. Nonclassical shock waves. *Interfaces Free Bound.*, 5:129 – 158, 2003.
- [26] Ch. Chalons, F. Coquel, P. Engel, and Ch. Rohde. Fast relaxation solvers for hyperbolic-elliptic phase transition problems. *SIAM J. Sci. Comput.*, 34:1753 – 1776, 2012.
- [27] P.G. Ciarlet. *The finite element method for elliptic problems*, volume 4. North Holland, 1978.
- [28] N. Clerx, L.G.M. van Deurzen, A. Pecenko, R. Liew, C.W.M. van der Geld, and J.G.M. Kuerten. Temperature fields induced by direct contact condensation of steam in a cross-flow in a channel. *Heat and mass transfer*, 47:981–990, 2011.
- [29] B. Cockburn and H. Gau. A model numerical scheme for the propagation of phase transitions in solids. *SIAM J. Sci. Comput.*, 17:1092 – 1121, 1996.
- [30] B. Cockburn and C.W. Shu. The local discontinuous Galerkin method for time-dependent convection-diffusion systems. *SIAM J. Numer. Anal.*, 141:2440 – 2463, 1998.
- [31] R.M. Colombo and A. Corli. Sonic and kinetic phase transitions with applications to Chapman-Jouguet deflagrations. *Math. Methods Appl. Sci.*, 27:843 – 864, 2004.

-
- [32] F. Coquel, D. Diehl, C. Merkle, and C. Rohde. Sharp and diffuse interface methods for phase transition problems in liquid-vapour flows. *IRMA Lect. Math. Theor. Phys.*, 7:239–270, 2005.
- [33] F. Coquel and B. Perthame. Relaxation of energy and approximate Riemann solvers for general pressure laws in fluid dynamics. *SIAM J. Numer. Anal.*, 35:2223 – 2249, 1998.
- [34] J. Crank. *Free and Moving Boundary Problems*. Oxford University Press, 1997.
- [35] H.H. Dai and D.X. Kong. The propagation of impact-induced tensile waves in a kind of phase-transforming materials. *J. Comput. Appl. Math.*, 190:57–73, 2006.
- [36] R. Danchina and B. Desjardinsb. Existence of solutions for compressible fluid models of Korteweg type. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 18:97–133, 2001.
- [37] A. Dedner, C. Makridakis, and M. Oehlberger. Error control for a class of Runge-Kutta discontinuous Galerkin methods for nonlinear conservation laws. *SIAM J. Numer. Anal.*, 45:514–538, 2007.
- [38] F. Dell’Isola, H. Gouin, and G. Rotoli. Nucleation of spherical shell-like interfaces by second gradient theory: numerical simulations. *Eur. J. Mech. B/Fluids*, 15:545–568, 1996.
- [39] J.L. Desmarais and J.G.M. Kuerten. Open boundary conditions for the Diffuse Interface Model in 1-D. *J. Comput. Phys.*, 163:393–418, 2014.
- [40] D. Diehl. *Higher order schemes for simulation of compressible liquid-vapor flows with phase change*. PhD thesis, Universität Freiburg, 2007.
- [41] S.C. Eisenstat and H.F. Walker. Globally convergent inexact Newton methods. *SIAM Journal on Optimization*, 4:393–422, 1994.
- [42] C.M. Elliott and D.A. French. A nonconforming finite-element method for the two-dimensional Cahn-Hilliard equation. *SIAM J. Numer. Anal.*, 26:884–903, 1989.
- [43] D. Furihata. A stable and conservative finite difference scheme for the Cahn-Hilliard equation. *Numer. Math.*, 87:675–699, 2001.

- [44] J. Giesselmann, C. Makridakis, and T. Pryer. Energy consistent discontinuous Galerkin methods for the Navier-Stokes-Korteweg system. *Math. Comp.*, 83:2071–2099, 2014.
- [45] J. Glimm, D. Marchesin, E. Isaacson, and O. McBryan. A shock tracking method for hyperbolic systems. In *Army Numerical Analysis and Computers Conference (NASA Res. Center, Moffett Field, Calif., 1980)*, 1980.
- [46] H. Gomez, T.J. Hughes, X. Nogueira, and V.M. Calo. Isogeometric analysis of the isothermal Navier–Stokes–Korteweg equations. *Comput. Methods Appl. Mech. Engrg.*, 199:1828 – 1840, 2010.
- [47] R. Hagan and M. Slemrod. The viscosity-capillarity criterion for shocks and phase transitions. *Arch. Rational Mech. Anal.*, 83:333 – 361, 1983.
- [48] J. Haink and C. Rohde. Local discontinuous Galerkin schemes for model problems in phase transition theory. *Commun. Comput. Phys.*, 4:860 – 893, 2008.
- [49] E. Hairer and G. Wanner. *Solving ordinary differential equation II. Stiff and differential-algebraic problems*. Springer, 2002.
- [50] B. Haspot. Existence of global weak solution for compressible fluid models of Korteweg type. *J. Math. Fluid Mech.*, 13:223 – 249, 2011.
- [51] H. Hattori and D. Li. Solutions for two-dimensional system for materials of Korteweg type. *SIAM J. Math. Anal.*, 25:85 – 98, 1994.
- [52] H. Hattori and D. Li. The existence of global solutions to a fluid dynamic model for materials for Korteweg type. *J. Partial Differential Equations*, 9:323 – 342, 1996.
- [53] C.W. Hirt and B.D. Nichols. Volume of fluid (VOF) method for the dynamics of free boundaries. *J. Comput. Phys.*, 39:201 – 225, 1981.
- [54] L. Holliday and I.M. Ward. *A general introduction to the structure and properties of oriented polymers*, chapter Structure and Properties of Oriented Polymers, pages 1–35. Springer Netherlands, 1975.
- [55] R. Houwink and H.K. De Decker. *Elasticity, plasticity and structure of matter*. Cambridge University Press, 1971.

-
- [56] D. Jacqmin. Contact-line dynamics of a diffuse fluid interface. *J. Fluid Mech.*, 402:57–88, 2000.
 - [57] R.D. James. The propagation of phase boundaries in elastic bars. *Arch. Rational Mech. Anal.*, 73:125–158, 1980.
 - [58] D. Jamet, O. Lebaigue, N. Coutris, and J.M. Delhay. The second gradient method for the direct numerical simulation of liquid-vapor flows with phase change. *J. Comput. Phys.*, 169:624–651, 2001.
 - [59] D. Jamet, D. Torres, and J.U. Brackbill. On the theory and computation of surface tension: the elimination of parasitic currents through energy conservation in the second-gradient method. *J. Comput. Phys.*, 182:262 – 276, 2002.
 - [60] V. Jovanovic and C. Rohde. Error estimates for finite volume approximations of classical solutions for nonlinear systems of hyperbolic balance laws. *SIAM J. Numer. Anal.*, 43:2423–2449, 2006.
 - [61] D. Kay and R. Welford. A multigrid finite element solver for the Cahn-Hilliard equation. *J. Comput. Phys.*, 212:288–304, 2006.
 - [62] C.T. Kelley. *Iterative methods for linear and nonlinear equations*. Society for Industrial and Applied Mathematics, 1995.
 - [63] D.J. Korteweg. Sur la forme que prennent les équations du mouvement des fluides si l’on tient compte des forces capillaires causées par des variations de densité considérables mais continues et sur la théorie de la capillarité dans l’hypothèse d’une variation continue de la densité. *Archives Néerlandaises des Sciences exactes et naturelles*, 6:1–24, 1901.
 - [64] M. Kotschote. Strong solutions for a compressible fluid model of Korteweg type. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 25:679 – 696, 2008.
 - [65] M. Kotschote. Strong solutions to the compressible non-isothermal Navier-Stokes equations. *Adv. Math. Sci. Appl.*, 22:319 – 347, 2012.
 - [66] M. Kotschote. Dynamical Stability of Non-Constant Equilibria for the Compressible Navier-Stokes Equations in Eulerian Coordinates. *Commun. Math. Phys.*, 328:809 – 847, 2014.
 - [67] H.O. Kreiss and J. Lorenz. *Initial-boundary value problems and the Navier-Stokes equations*. Academic press, 1989.

- [68] B. Lafaurie, C. Nardone, R. Scardovelli, S. Zaleski, and G. Zanetti. Modelling merging and fragmentation in multiphase flows with SURFER. *J. Comput. Phys.*, 113:134–147, 1994.
- [69] H.G. Lee, J.S. Lowengrub, and J. Goodman. Modeling pinchoff and reconnection in a Hele-Shaw cell. I. The models and their calibration. *Phys. Fluids*, 14:492–513, 2002.
- [70] P.G. LeFloch. Propagating phase boundaries: Formulation of the problem and existence via the Glimm method. *Arch. Rational Mech. Anal.*, 123:153 – 197, 1993.
- [71] P.G. LeFloch. *Hyperbolic Systems of Conservation Laws: The theory of classical and nonclassical shock waves*, volume 35. Birkhäuser, 2002.
- [72] J. Liu, H. Gomez, J.A. Evans, T.J. Hughes, and C.M. Landis. Functional entropy variables: A new methodology for deriving thermodynamically consistent algorithms for complex fluids, with particular reference to the isothermal Navier–Stokes–Korteweg equations. *J. Comput. Phys.*, 248:47 – 86, 2013.
- [73] De-Kang Mao. A shock tracking technique based on conservation in one space dimension. *SIAM J. Numer. Anal.*, 32:1677–1703, 1995.
- [74] C. Merkle and C. Rohde. The sharp-interface approach for fluids with phase change: Riemann problems and ghost fluid techniques. *Math. Model. Numer. Anal.*, 41:1089 – 1123, 2007.
- [75] A. Nadai and P.G. Hodge. Theory of Flow and Fracture of Solids. *J. Appl. Math.*, 30:640, 1963.
- [76] J.T. Oden, W. Wu, and M. Ainsworth. An a posteriori error estimate for finite element approximations of the Navier-Stokes equations. *Comput. Methods Appl. Mech. Engrg.*, 111:185–202, 1994.
- [77] M. Ohlberger. A posteriori error estimate for finite volume approximations to singularly perturbed nonlinear convection-diffusion equations. *Numer. Math.*, 87:737–761, 2001.
- [78] M. Ohlberger and J. Vovelle. Error estimate for the approximation of nonlinear conservation laws on bounded domains by the finite volume method. *Math. Comp.*, 75:113–150, 2006.

-
- [79] S. Osher. *Level set methods. In Geometric level set methods in imaging, vision, and graphics*. Springer New York, 2003.
- [80] R.P. Pawlowski, J.N. Shadid, J.P. Simonis, and H.F. Walker. Globalization techniques for Newton-Krylov methods and applications to the fully coupled solution of the Navier-Stokes equations. *SIAM Rev.*, 48:700 – 721, 2006.
- [81] A. Pecencko, J.G.M. Kuerten, and C.W.M. van der Geld. A diffuse-interface approach to two-phase isothermal flow of a Van der Waals fluid near the critical point. *Int. J. Multiphase Flow*, 36:558 – 569, 2010.
- [82] A. Pecencko, L.G.M. Van Deurzen, J.G.M. Kuerten, and C.W.M. van der Geld. Non-isothermal two-phase flow with a diffuse-interface model. *Int. J. Multiphase Flow*, 37:149 – 165, 2011.
- [83] R. Peyret and T.D. Taylor. *Computational methods for fluid flow*. New York, Springer-Verlag, 1985.
- [84] P.K. Purohit and K. Bhattacharya. On beams made of a phase-transforming material. *Int. J. Solids Struc.*, 39:3907–3929, 2002.
- [85] J. Qiu and C.W. Shu. A Comparison of Troubled-Cell Indicators for Runge–Kutta Discontinuous Galerkin Methods Using Weighted Essentially Nonoscillatory Limiters. *SIAM J. Sci. Comput.*, 27:995–1013, 2005.
- [86] L. Rayleigh. On the pressure developed in a liquid during the collapse of a spherical cavity. *Philosophical Magazine and Journal of Science*, 34:94–98, 1917.
- [87] S.I. Repin. A posteriori error estimation for nonlinear variational problems by duality theory. *J. Math. Sci.*, 99:927–935, 2000.
- [88] P.L. Roe. Approximate Riemann solvers, parameter vectors, and difference schemes. *J. Comput. Phys.*, 43:357–372, 1981.
- [89] C. Rohde. On local and non-local Navier–Stokes–Korteweg systems for liquid-vapour phase transitions. *ZAMM Z. Angew. Math. Mech.*, 85:839 – 857, 2005.
- [90] J.S. Rowlinson and B. Widom. *Molecular theory of capillarity*. Courier Corporation, 2013.

- [91] P. Seppecher. Moving contact lines in the Cahn-Hilliard theory. *Int. J. Engin. Sci.*, 34:977–992, 1996.
- [92] D. Serre. *Systems of Conservation Laws 1: Hyperbolicity, entropies, shock waves*. Cambridge University Press, 1999.
- [93] J. Serrin. Phase transitions and interfacial layers for van der Waals fluids. In *Recent Methods in Nonlinear Analysis and Applications*, pages 21–28, 1980.
- [94] M. Shearer. The Riemann problem for a class of conservation laws of mixed type. *J. Differential Equations*, 46:426–443, 1982.
- [95] C.W. Shu. TVB uniformly high-order schemes for conservation laws. *Math. Comp.*, 49:105–121, 1987.
- [96] C.W. Shu and S. Osher. Efficient implementation of essentially non-oscillatory shock-capturing schemes. *J. Comput. Phys.*, 77:439 – 471, 1988.
- [97] G.R. Shubin, A.B. Stephens, and H.M. Glaz. Steady shock tracking and Newton’s method applied to one-dimensional duct flow. *J. Comput. Phys.*, 39:364–374, 1981.
- [98] L.M. Skvortsov. Diagonally implicit Runge-Kutta methods for stiff problems. *Comput. Math. Math. Phys.*, 46:2110 – 2123, 2006.
- [99] M. Slemrod. Admissibility criteria for propagating phase boundaries in a van der Waals fluid. *Arch. Rational Mech. Anal.*, 81:301–315, 1983.
- [100] M. Slemrod. Dynamic phase transitions in a van der Waals fluid. *J. Differential Equations*, 52:1 – 23, 1984.
- [101] Y. Song, X. Chen, V. Dabade, T.W. Shield, and R.D. James. Enhanced reversibility and unusual microstructure of a phase-transforming material. *Nature*, 502:85 – 88, 2013.
- [102] J.C. Strikwerda. *Finite difference schemes and partial differential equations*. Siam, 2004.
- [103] M. Sussman, P. Smereka, and S. Osher. A level set approach for computing solutions to incompressible two-phase flow. *J. Comput. Phys.*, 114:146–159, 1994.

- [104] P.K. Sweby. High resolution schemes using flux limiters for hyperbolic conservation laws. *SIAM J. Numer. Anal.*, 21:995–1011, 1984.
- [105] E. Tadmor. Numerical viscosity and the entropy condition for conservative difference schemes. *Math. Comp.*, 43:369–381, 1984.
- [106] M.D. Thanh. Traveling waves of an elliptichyperbolic model of phase transitions via varying viscositycapillarity. *J. Differential Equations*, 251:439–456, 2011.
- [107] L. Tian, Y. Xu, J.G.M. Kuerten, and J.J.W. Van der Vegt. A local discontinuous Galerkin method for the propagation of phase transition in solids and fluids. *J. Sci. Comput.*, 59:688 – 720, 2014.
- [108] L. Tian, Y. Xu, J.G.M. Kuerten, and J.J.W. Van der Vegt. A local discontinuous Galerkin method for the (non)-isothermal NavierStokesKorteweg equations. *J. Comput. Phys.*, 295:685–714, 2015.
- [109] L. M. Truskinovskii. Dynamics of non-equilibrium phase boundaries in a heat conducting non-linearly elastic medium. *J. Appl. Math. Mech.*, 51:777 – 784, 1987.
- [110] L. Truskinovsky. *Shock induced transitions and phase structures in general media*, chapter Kinks versus shocks, pages 185–229. Springer New York, 1993.
- [111] G. Tryggvason, B. Bernard, E. Asghar, J. Damir, N. Al-Rawahi, W. Tauber, J. Han, S. Nas, and Y-J. Jan. A front-tracking method for the computations of multiphase flow. *J. Comput. Phys.*, 169:708 – 759, 2001.
- [112] S.O. Unverdi and G. Tryggvason. A front-tracking method for viscous, incompressible, multi-fluid flows. *J. Comput. Phys.*, 100:25–37, 1992.
- [113] R. Verfürth. A posteriori error estimators for the Stokes equations. *Numer. Math.*, 55:309–325, 1989.
- [114] R. Verfürth. A review of a posteriori error estimation techniques for elasticity problems. *Comput. Methods Appl. Mech. Engrg.*, 176:419–440, 1999.
- [115] R. Vilsmeier and D. Hänel. Adaptive methods on unstructured grids for Euler and Navier-Stokes equations. *Computers & Fluids*, 22:485–499, 1993.

- [116] G.N. Wells, E. Kuhl, and K. Garikipati. A discontinuous Galerkin method for the CahnHilliard equation. *J. Comput. Phys.*, 218:860–877, 2006.
- [117] A.A. Wheeler, W.J. Boettinger, and G.B. McFadden. Phase-field model for isothermal phase transitions in binary alloys. *Phy. Rev. A*, 45:7424, 1992.
- [118] Y. Xia, Y. Xu, and C.W. Shu. Local discontinuous Galerkin methods for the Cahn-Hilliard type equations. *J. Comput. Phys.*, 227:472–491, 2007.
- [119] Y. Xu and C.W. Shu. Error estimates of the semi-discrete local discontinuous Galerkin method for nonlinear convection-diffusion and KdV equations. *Comput. Methods Appl. Mech. Engrg.*, 196:3805–3822, 2007.
- [120] Y. Xu and C.W. Shu. A local discontinuous Galerkin method for the Camassa-Holm equation. *SIAM J. Numer. Anal.*, 46:1998 – 2021, 2008.
- [121] Y. Xu and C.W. Shu. Local discontinuous Galerkin methods for high-order time-dependent partial differential equations. *Commun. Comput. Phys.*, 7:1 – 46, 2010.
- [122] Y. Xu and C.W. Shu. Optimal error estimates of the semi-discrete local discontinuous Galerkin methods for high order wave equations. *SIAM J. Numer. Anal.*, 50:79 – 104, 2012.
- [123] J. Yan and C.W. Shu. A local discontinuous Galerkin method for KdV type equations. *SIAM J. Numer. Anal.*, 40:769 – 791, 2002.
- [124] P. Yue, J.J. Feng, C. Liu, and J. Shen. A diffuse-interface method for simulating two-phase flows of complex fluids. *J. Fluid Mech.*, 515:293 – 317, 2004.
- [125] X.G. Zhong, T.Y. Hou, and P.G. LeFloch. Computational methods for propagating phase boundaries. *J. Comput. Phys.*, 124:192 – 216, 1996.
- [126] H. Zhu and J. Qiu. Adaptive Runge-Kutta discontinuous Galerkin methods using different indicators: one-dimensional case. *J. Comput. Phys.*, 228:6957–6976, 2009.
- [127] H. Zhu and J. Qiu. An h-adaptive RKDG method with troubled-cell indicator for two-dimensional hyperbolic conservation laws. *Adv. Comput. Math.*, 39:445–463, 2013.

Acknowledgements

This dissertation is the outcome of my research performed at the Department of Applied Mathematics at the University of Twente. It is impossible without inspirations and encouragements from my supervisors, family, friends and colleagues, and I would like to take this opportunity to thank them.

First of all, my most sincere gratitude goes to my supervisors: Jaap van der Vegt and Hans Kuerten. During the PhD study, we have regular meetings and they give me inspiration, useful advice and constant support. They always encourage me to try new things and give me a lot of confidence, which are enormous important to me. It has been my honor to work with them. Thank you very much, Jaap, for your patience and dedication these years. Besides research, you and your wife Phing help me to adapt the life in the Netherlands. Thanks a lot, Hans, for your fresh ideas and fruitful discussions which made me improve the work from physical side of my project.

I would like to pronounce my sincere thanks to Prof. Yan Xu at University of Science and Technology of China for giving me the foundation in finite element method and for introducing me to Jaap. I appreciate her insightful suggestions in my research, and valuable help with various issues in my life.

I would like to thank my graduation committee for taking their time to evaluate this thesis and provide helpful comments.

A special word of thanks goes to the secretaries Marielle, Linda who helped me with many issues at Twente. I would like to thank Mathematics of Computational Science group and collaborators Tatyana, Mike, Deepak,

Freekjan, Sjoerd, Poorvi, Devashish, Elena, Irana, Wenny, Tito and Anthony for the research assistance and interesting seminars. I also thank other colleagues Huan, Anastasia, Bettina, Edo, Edson, Felix, Koen, Ruddy, Arnida, Leonie, Henk, Paola, Julia and many others who create a nice atmosphere to work.

Being far away from my family and country is not easy, yet I am really grateful for being surrounded by warmhearted people. I am particularly grateful for all the assistance and support given by Lei and Ying. I thank Meiru, Hainan, La for sharing so many happy moments with me, I will miss you girls. Thanks also go to Li, Yanting, Fei, Honglin, Lantian, Yong, Jiahui, Junwen, Shuang, Long, Xinwei, Jiajia, Hairong, Leilei, Jingwei, etc.

I owe sincere thankfulness to Lissy for delightful talking and countless invitation to her house. I also thank Necane, Loreto, Leo and Ivan. I will miss the parties we had which helped me a lot to relieve the pressure from my research.

Many thanks are due to Xiuer, Fei, Yang, Fang and Hui for your continuous support and care. You girls are source of my joy. I thank Jinfeng, Ruihan, Kangkang and Lan for your help in many ways.

I am greatly indebted to my parents and younger sister for your love, support and patience for all these years. Finally, I would like to express special gratitude to my fiancé for his love, understanding and encouragement during all the ups and downs of this journey. Thank you for being there for me.

Lulu Tian,
Enschede, September, 2015

List of publications

Journal papers

- L. Tian, Y. Xu, J. G. M. Kuerten and J. J. W. Van der Vegt, A local discontinuous Galerkin method for the propagation of phase transition in solids and fluids, *Journal of Scientific Computing* 59 (2014), pp.688-720.
- L. Tian, Y. Xu, J. G. M. Kuerten and J. J. W. Van der Vegt, A local discontinuous Galerkin method for the (non)-isothermal Navier-Stokes-Korteweg equations, *Journal of Computational Physics* 295 (2015), pp.685-714.
- L. Tian, Y. Xu, J. G. M. Kuerten and J. J. W. Van der Vegt, An h-adaptive local discontinuous Galerkin method for liquid-vapor flows with phase change and solid wall boundaries, to submit to *Journal of Computational Physics*.