博 士 論 文

Mathematical analysis and numerical computation of volume-constrained evolutionary problems, involving free boundaries

(自由境界を含む体積保存条件つき発展問題の解析と数値計算)

金沢大学大学院自然科学研究科

数物科学専攻

計算科学講座

学籍番号: 0523102011

氏名: Karel Švadlenka （カレル シュワドレンカ）

主任指導教員名: 小俣 正朗

Contents

Abstract

The object of study of the present thesis are evolutionary problems satisfying volume preservation condition, i.e., problems whose solution have a constant value of the integral of their graph. In particular, the following types of problems with volume constraint are dealt with: parabolic problem (heat-type), hyperbolic problem (wave-type), parabolic free-boundary problem (heat-type with obstacle) and hyperbolic free-boundary problem (degenerate wave-type with obstacle). The key points are design of equations, proof of existence of weak solutions to them and development of numerical methods and algorithms for such problems. The main tool in both the theoretical analysis and the numerical computation is the discrete Morse flow, a variational method consisting in discretizing time and stating a minimization problem on each time-level. The volume constraint appears in the equation as a nonlocal nonlinear Lagrange multiplier but it can be handled elegantly in discrete Morse flow method by restraining the set of admissible functions for minimization. The theory is illustrated with results of numerical experiments.

Chapter 1

Introduction

1.1 Introductory notes

In this work, we deal with the evolution of objects of a constant volume, in particular, of surfaces that can be expressed as a graph of a scalar function. The necessity of volume constraint arose in various models of physical phenomena. A typical example is an elastic membrane filled with incompressible fluid. When an outer force is applied on the membrane, it changes its shape while preserving the volume. The model equation for the membrane then has to account for this constraint.

Volume conservation in our research was first introduced in the model for a soap-film bubble moving on a flat surface. Deformations of the surface of the bubble are written in terms of a degenerate free-boundary hyperbolic equation (see [41]). However, if no condition on the volume is posed, the solution of the equation tends to zero, which means that the bubble shrinks and vanishes. In order to prevent the bubble from shrinking, the volume constraint has to be added.

The adding of the constraint is to be done at the level of deriving the model equation on the basis of physical considerations. We achieve this by imposing an appropriate limitation on the set of functions among which we look for stationary points of the Lagrangian of the system. We shall see that this results in the appearance of a new nonlocal term in the model equation. This interprets the volume constraint as an outer force acting on the whole surface.

The soap bubble model became a starting point for other models, such as motion of droplets on surfaces. On the interface of the liquid forming the drop and the surrounding gas a strong layer is formed due to tension forces, and it is natural to regard the droplet as consisting of two parts: a film and liquid filling the film. In such a case, the film must preserve volume, i.e., the volume of the region between the film and the underlying surface has to be constant in time. The fluid is described by standard equations of fluid dynamics and interacts with the film via pressure forces.

We could try to model the motion of the drop by just considering the Navier-Stokes equations for the fluid. However, with this approach it is impossible to incorporate aspects like the positive contact angle of the drop or motion of dripping drops. We remark that although we have a mass-preservation condition (continuity equation) for the liquid, the film needs its own independent constraint since it determines the boundary of the domain, where the fluid is moving.

We believe that such type of models combining a volume-preserving film and fluid surrounded by the film, are applicable to a wide range of phenomena. Some examples could be the flow of blood in vessels or the circulatory system as a whole, collision of objects with inner structure, propagation of waves in the sea etc. Of course, according to necessity, the coupled models may be simplified by considering the equation for the film only.

The primary aim of the present thesis is to provide mathematical analysis of such volume-preserving equations, i.e., show the existence of certain kind of solutions, their uniqueness and, if possible, regularity. However, we were able to do so for only some classes of problems by this time, leaving more complex problems for future research. One example of such unsolved problems is modelling of a droplet dripping from a ceiling, which amounts to solving a vector-valued degenerate-hyperbolic free-boundary problem.

The thesis is organized in the following way. In the beginning, we formally discuss the derivation of equations for volume-preserving phenomena from the principles of physics and hint at the relation with constrained elliptic problems. Next we introduce the main tool of this thesis, the discrete Morse flow, and show its basic properties. Chapters 4 and 5 are devoted to the analysis of basic evolutionary problems with volume constraint, considering problems without and with free boundaries, respectively. We prove existence of weak solutions and in some cases also their regularity. In the end, we make some comments on the numerical solution of these problems and present results of computational experiments.

1.2 Notation and function spaces

We provide a list of notations and function spaces used in the thesis.

Generally used symbols. If not stated otherwise, the symbols listed below have the following meaning:

$\mathbb{N}$	natural numbers (often $i, j, k, l, m, n \in \mathbb{N}$),
$\mathbb{R}^m$	m-dimensional real Euclidean space ($\mathbb{R} = \mathbb{R}^1$),
Ω	bounded domain in $\mathbb{R}^m$ with Lipschitz boundary, corresponding to the spatial region, where the equation is solved,
$\partial\Omega$	boundary of domain Ω,
$\lvert\Omega\rvert$	the Lebesgue measure of Ω,
$\bar{\Omega}$	closure of the set Ω,
T	a positive real value representing the final time,
Q_T	the open time-space cylinder $(0, T) \times \Omega$,
V	positive real value representing the volume,
$\mathcal{K}, \mathcal{K}_V$	sets of functions from certain spaces satisfying the volume constraint,
u	unknown function,
u_t	partial derivative of u with respect to time ($= \frac{\partial u}{\partial t}$),
∇u	gradient of u with respect to spatial variables ($= (u_{x_1}, u_{x_2}, \ldots, u_{x_m})$),
Δu	the Laplace operator with respect to space ($= \frac{\partial^2 u}{\partial x_1^2} + \cdots + \frac{\partial^2 u}{\partial x_m^2}$),

$u\|_{\partial\Omega}$	the trace of u on $\partial\Omega$,
u_0, v_0	initial data (shape and velocity, respectively),
λ	Lagrange multiplier, nonlocal term originating in the volume constraint,
h	positive real value, time step of the discretization in time,
N	natural number expressing the total number of time steps,
a.e.	means "almost everywhere" or "almost every",
$\{u > 0\}$	set of points (t, x) from Q_T, for which $u(t, x) > 0$,
$\chi_{u>0}$	characteristic (or indicator) function of the set $\{u > 0\}$,
C	denotes a generic positive constant, independent of parameters in question.

Function spaces. The following function spaces and their corresponding norms are used in the study (we mention only the norms used in the text). Let Ω be an open domain, $k \in \mathbb{N}$, $p \geq 1$, $T > 0$ and X a real Banach space with norm $\|\cdot\|_X$.

$C(\Omega)$	continuous functions $u : \Omega \to \mathbb{R}$,
$C^k(\Omega)$	functions $u : \Omega \to \mathbb{R}$ that are k-times continuously differentiable,
$C^\infty(\Omega)$	functions $u : \Omega \to \mathbb{R}$ that are infinitely differentiable ($= \bigcap_{k=0}^\infty C^k(\Omega)$),
$C_0^\infty(\Omega)$	functions from $C^\infty(\Omega)$ with compact support,
$L^p(\Omega)$	functions $u : \Omega \to \mathbb{R}$ that are Lebesgue measurable and $\|u\|_{L^p(\Omega)} < \infty$, where $\|u\|_{L^p(\Omega)} = \left(\int_\Omega \|u\|^p \, dx\right)^{1/p}$,
$L^\infty(\Omega)$	functions $u : \Omega \to \mathbb{R}$ that are Lebesgue measurable and $\|u\|_{L^\infty(\Omega)} < \infty$, where $\|u\|_{L^\infty(\Omega)} = \text{ess sup}_\Omega \|u\|$,
$W^{k,p}(\Omega)$	locally summable functions $u : \Omega \to \mathbb{R}$ such that for each multiindex α with $\|\alpha\| \leq k$, $D^\alpha u$ exists in the weak sense and belongs to $L^p(\Omega)$. The norm is defined as follows: $\|u\|_{W^{k,p}(\Omega)} = \left(\sum_{\|\alpha\| \leq k} \int_\Omega \|D^\alpha u\|^p \, dx\right)^{1/p}$, $\|u\|_{W^{k,\infty}(\Omega)} = \sum_{\|\alpha\| \leq k} \text{ess sup}_\Omega \|D^\alpha u\|$,
$H^k(\Omega)$	$= W^{k,2}(\Omega)$,
$H_0^1(\Omega)$	the closure of $C_0^\infty(\Omega)$ in $H^1(\Omega)$,
$L^p(0, T; X)$	measurable functions $u : [0, T] \to X$ with $\|u\|_{L^p(0,T;X)} < \infty$, where $\|u\|_{L^p(0,T;X)} = \left(\int_0^T \|u\|_X^p \, dt\right)^{1/p}$,
$L^\infty(0, T; X)$	measurable functions $u : [0, T] \to X$ with $\|u\|_{L^\infty(0,T;X)} < \infty$, where $\|u\|_{L^\infty(0,T;X)} = \text{ess sup}_{0 \leq t \leq T} \|u\|_X$,
$W^{1,p}(0, T; X)$	functions $u \in L^p(0, T; X)$ such that u_t exists in the weak sense and belongs to $L^p(0, T; X)$. The norm is $\|u\|_{W^{1,p}(0,T;X)} = \left(\int_0^T \|u(t)\|_X^p + \|u_t(t)\|_X^p \, dt\right)^{1/p}$,
$W^{1,\infty}(0, T; X)$	functions $u \in L^\infty(0, T; X)$ such that u_t exists in the weak sense and belongs to $L^\infty(0, T; X)$. The norm is $\|u\|_{W^{1,\infty}(0,T;X)} = \text{ess sup}_{0 \leq t \leq T} \left(\|u(t)\|_X + \|u_t(t)\|_X\right)$,
$H^1(0, T; X)$	$= W^{1,2}(0, T; X)$,
$C_0^\infty(\Omega; \mathbb{R}^m)$	functions $u : \Omega \to \mathbb{R}^m$ with $u_i \in C_0^\infty(\Omega)$, $i = 1, \ldots, m$.

The above spaces are used also for other domains of definition, such as $(0, T)$ or Q_T. We often use $C_0^\infty(Q_T)$, $L^2(0, T)$, $L^2(\partial\Omega)$, $L^2(Q_T)$, $L^\infty(Q_T)$, $H^1(Q_T)$, etc. The space

$C_0^\infty([0,T) \times \Omega)$ consists of functions from $C^\infty([0,T] \times \bar{\Omega})$ that have compact support in $[0,T) \times \Omega$, i.e., they need not vanish on $\{0\} \times \Omega$. We often use the norms of gradients in the following sense:

$$\|\nabla u\|_{L^p(\Omega)} = \| \, |\nabla u| \, \|_{L^p(\Omega)}.$$

Chapter 2

Mathematical aspects of volume preservation

In this Chapter, a typical equation of volume-preserving surface is formally derived and problems treated in the thesis are classified.

2.1 Lagrange multiplier

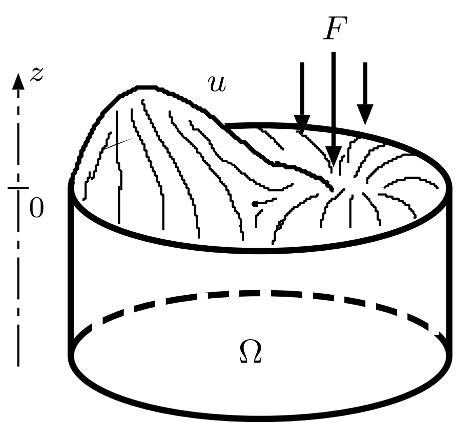


Figure 2.1: Motion of a constrained film.

We study the situation depicted in Figure 2.1 from the viewpoint of scalar functions. A membrane is fixed on the boundary of a vessel filled with fluid. We want to know the motion of the membrane when an outer force F with potential P is applied on it. We denote by u the function expressing the shape of the membrane over a domain Ω, by ρ the area density of the membrane and by γ its elastic modulus. We assume that ρ and γ are constant, and neglect the action of the fluid on the membrane. Then the Lagrangian for the membrane can be written in the following form:

$$L(u) = \int_{\Omega} \big(\frac{1}{2}\rho(u_t)^2 - \frac{1}{2}\gamma|\nabla u|^2 + P(u)\big)\, dx. \tag{2.1.1}$$

The equation of motion within time interval $(0,T)$ is given by stationary point(s) of the action

$$S(u) = \int_0^T L(u)\,dt,$$

that satisfy certain initial conditions, boundary condition and the volume constraint with volume V:

$$\int_\Omega u(t,x)\,dx = V \qquad \forall\, t \in [0,T]. \tag{2.1.2}$$

This means that we look for a stationary point inside the set

$$\mathcal{K} := \{u;\;\; u(0,x) = u_0(x),\, u_t(0,x) = v_0(x),\, u|_{\partial\Omega} = 0,\, \int_\Omega u\,dx = V\},$$

where u_0 is the initial shape and v_0 is the initial velocity of the membrane. For simplicity, we have prescribed homogeneous Dirichlet boundary condition.

We compute the first variation of $S(u)$. For that purpose, it is necessary to construct perturbations that belong to $\mathcal{K}$. We select a test function $\varphi \in C_0^\infty((0,T)\times\Omega)$ and use the following notation for its volume

$$\Phi(t) = \int_\Omega \varphi(t,x)\,dx.$$

Setting

$$u_\varepsilon = \frac{u + \varepsilon\varphi}{1 + \frac{\varepsilon}{V}\Phi},$$

we see that this perturbation is well defined, since for small values of ε the denominator is positive, and that it belongs to $\mathcal{K}$ because the boundary and initial conditions are satisfied and

$$\int_\Omega (u + \varepsilon\varphi)\,dx = V + \varepsilon\Phi.$$

Stationary points then satisfy the identity

$$\frac{d}{d\varepsilon} S(u_\varepsilon)|_{\varepsilon=0} = 0 \quad \text{or equivalently} \quad \lim_{\varepsilon\to 0} \frac{S(u_\varepsilon) - S(u)}{\varepsilon} = 0.$$

We find that

$$
\begin{aligned}
0 &= \lim_{\varepsilon\to 0} \frac{S(u_\varepsilon)-S(u)}{\varepsilon}\\
&= \lim_{\varepsilon\to 0} \frac{\rho}{2\varepsilon}\int_0^T\int_\Omega \Big[\Big(\frac{(u_t+\varepsilon\varphi_t)(1+\frac{\varepsilon}{V}\Phi)-(u+\varepsilon\varphi)\frac{\varepsilon}{V}\Phi_t}{(1+\frac{\varepsilon}{V}\Phi)^2}\Big)^2-(u_t)^2\Big]\,dx\,dt\\
&\quad -\lim_{\varepsilon\to 0} \frac{\gamma}{2\varepsilon}\int_0^T\int_\Omega \Big[\Big(\frac{|\nabla u+\varepsilon\nabla\varphi|}{1+\frac{\varepsilon}{V}\Phi}\Big)^2-|\nabla u|^2\Big]\,dx\,dt\\
&\quad +\lim_{\varepsilon\to 0} \frac{1}{\varepsilon}\int_0^T\int_\Omega \Big[P\Big(\frac{u+\varepsilon\varphi}{1+\frac{\varepsilon}{V}\Phi}\Big)-P(u)\Big]\,dx\,dt\\
&= \lim_{\varepsilon\to 0} \frac{\rho}{2\varepsilon}\int_0^T\int_\Omega \frac{(u_t+\varepsilon\varphi_t+\frac{\varepsilon}{V}\Phi u_t-\frac{\varepsilon}{V}\Phi_t u)^2-(u_t)^2(1+\frac{\varepsilon}{V}\Phi)^4+o(\varepsilon)}{(1+\frac{\varepsilon}{V}\Phi)^4}\,dx\,dt\\
&\quad -\lim_{\varepsilon\to 0} \frac{\gamma}{2\varepsilon}\int_0^T\int_\Omega \frac{|\nabla u|^2+2\varepsilon\nabla u\nabla\varphi+\varepsilon^2|\nabla\varphi|^2-(1+2\frac{\varepsilon}{V}\Phi+\frac{\varepsilon^2}{V^2}\Phi^2)|\nabla u|^2}{(1+\frac{\varepsilon}{V}\Phi)^2}\,dx\,dt\\
&\quad +\lim_{\varepsilon\to 0} \frac{1}{\varepsilon}\int_0^T\int_\Omega P'(u)\Big(\frac{u+\varepsilon\varphi}{1+\frac{\varepsilon}{V}\Phi}-u\Big)\,dx\,dt\\
&= \lim_{\varepsilon\to 0} \frac{\rho}{2\varepsilon}\int_0^T\int_\Omega \frac{2\varepsilon u_t\varphi_t+2\frac{\varepsilon}{V}\Phi(u_t)^2-2\frac{\varepsilon}{V}\Phi_t u u_t-4\frac{\varepsilon}{V}\Phi(u_t)^2+o(\varepsilon)}{(1+\frac{\varepsilon}{V}\Phi)^4}\,dx\,dt\\
&\quad -\lim_{\varepsilon\to 0} \frac{\gamma}{2\varepsilon}\int_0^T\int_\Omega \frac{2\varepsilon\nabla u\nabla\varphi-2\frac{\varepsilon}{V}\Phi|\nabla u|^2+o(\varepsilon)}{(1+\frac{\varepsilon}{V}\Phi)^2}\,dx\,dt\\
&\quad +\int_0^T\int_\Omega P'(u)\big(\varphi-\frac{1}{V}\Phi u\big)\,dx\,dt\\
&= \int_0^T\int_\Omega \Big[\rho\big(u_t\varphi_t-\frac{1}{V}u_t(\Phi u)_t\big)-\gamma\big(\nabla u\nabla\varphi-\frac{1}{V}\Phi|\nabla u|^2\big)+P'(u)\big(\varphi-\frac{1}{V}\Phi u\big)\Big]\,dx\,dt\\
&= \int_0^T\int_\Omega \Big[\rho u_t\varphi_t-\gamma\nabla u\nabla\varphi+P'(u)\varphi\Big]\,dx\,dt\\
&\quad +\frac{1}{V}\int_0^T\int_\Omega \Big[-\rho u_t(u\Phi)_t+\gamma|\nabla u|^2\Phi-P'(u)u\Phi\Big]\,dx\,dt.
\end{aligned}
$$

Let us study the term in the last line above. If we assume that the shape of the film is smooth, we can integrate this term by parts in time, obtaining

$$
\begin{aligned}
&\frac{1}{V}\int_0^T\int_\Omega \Big[-\rho u_t(u\Phi)_t+\gamma|\nabla u|^2\Phi-P'(u)u\Phi\Big]\,dx\,dt\\
&=\frac{1}{V}\int_0^T\int_\Omega \big(\rho u_{tt}u+\gamma|\nabla u|^2-F(u)u\big)\Phi\,dx\,dt.
\end{aligned}
$$

Thus, denoting

$$
\lambda=\frac{1}{V}\int_\Omega \big(\rho u_{tt}u+\gamma|\nabla u|^2-F(u)u\big)\,dx, \tag{2.1.3}
$$

we arrive at the relation

$$
\int_0^T\int_\Omega \big(-\rho u_t\varphi_t+\gamma\nabla u\nabla\varphi-F(u)\varphi-\lambda\varphi\big)\,dx\,dt=0 \qquad \forall\varphi\in C_0^\infty((0,T)\times\Omega).
$$

The strong version of the above is

$$\rho u_{tt} = \gamma \Delta u + F(u) + \lambda(u). \tag{2.1.4}$$

The analysis of this type of equations is the main object of the present thesis. We can see that we got the usual wave equation with an additional nonlocal term. This new term represents a uniform outer force on the membrane originating in the volume constraint. It may be called a *Lagrange multiplier*, since the same equation can be derived by a formal application of the theory of Lagrange multipliers. To see this, we consider the extremum problem for the Lagrangian once more. Since the constraint has to hold independently of time, one can judge that the Lagrange multiplier λ for the volume constraint $\int_\Omega u\,dx = V$ should depend on time only. Then we get the following unconstrained problem: find a stationary point of

$$\tilde{S}(u) = \int_0^T L(u)\,dt + \int_0^T \lambda(t)\Big(\int_\Omega u\,dx\Big)\,dt$$

among functions satisfying initial and boundary conditions. The first variation of this functional gives the same equation (2.1.4).

The usage of Lagrange multipliers is established for elliptic problems. We have, for example, the following theorem (see [8], Section 8.4).

Theorem 2.1.1. *Let*

$$\mathcal{K} = \{w \in H_0^1(\Omega);\ \int_\Omega G(w)\,dx = 0\},$$

where $G : \mathbb{R} \to \mathbb{R}$ is a given, smooth function with derivative $g = G'$. Let $u \in \mathcal{K}$ satisfy

$$\int_\Omega |\nabla u|^2\,dx = \min_{w\in\mathcal{K}} \int_\Omega |\nabla w|^2\,dx.$$

Then there exists a real number λ such that

$$\int_\Omega \nabla u \nabla v\,dx = \lambda \int_\Omega g(u) v\,dx$$

for all $v \in H_0^1(\Omega)$.

This means that u is a weak solution of the boundary-value problem

$$\begin{aligned} -\Delta u &= \lambda g(u) && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega. \end{aligned}$$

In our case $G(u) = u - V/|\Omega|$ and $g(u) = 1$, which shows the correspondence of this equation to (2.1.4).

In proving the above theorem, one finds the Lagrange multiplier has the form

$$\lambda = \frac{\int_\Omega \nabla u \nabla w\,dx}{\int_\Omega g(u) w\,dx},$$

for any function $w \in H_0^1(\Omega)$, which gives a nonzero denominator. If we take $w = u$ and consider our case, we get

$$\lambda = \frac{\int_\Omega \nabla u \nabla u \, dx}{\int_\Omega g(u) u \, dx} = \frac{\int_\Omega |\nabla u|^2 \, dx}{\int_\Omega u \, dx} = \frac{1}{V} \int_\Omega |\nabla u|^2 \, dx,$$

again corresponding to (2.1.3).

We would like to extend the theory from Theorem 2.1.1 to evolutionary equations of parabolic and hyperbolic type. Generalization of the volume constraint to general integral constraints is also a matter of interest. In order to achieve this, we approximate the evolutionary problem by a sequence of elliptic minimization problems. For the elliptic problems, we can use Theorem 2.1.1, which gives time-discrete Lagrange multipliers and time-discrete weak formulation. Taking the discretization parameter to zero, we obtain a weak solution of target equation (2.1.4). This method is called the discrete Morse flow and its basic features are explained in the next Chapter 3. Before doing so, we summarize and sort various types of problems studied in this work.

2.2 Classification of problems

Problem (2.1.4) is of hyperbolic type but we are going to consider also other classes of problems. Although, as mentioned in the Introduction, the final aim are vector-valued problems, here we confine ourselves to problems for scalar functions. We divide them into parabolic and hyperbolic problems. Inside these groups we consider problems without and with free boundary. The parabolic problems are represented by a heat-type problem, whereas we chose a wave-type problem as an example of hyperbolic problems. A term standing for a solution-dependent outer force is added in both cases. Free-boundary problems are represented by an obstacle-type problem. The classification is featured in Table 2.1, including physical examples for each case.

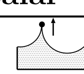
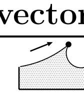
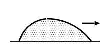
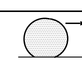
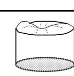
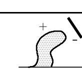
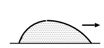
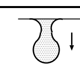
		scalar		**vector**	
parabolic	**without free b.**		lifting of a lid		lifting of a lid
	with free b.		slow motion of a bubble		slow motion of a bubble
hyperbolic	**without free b.**		beating a drum		pulling of charged film
	with free b.		fast motion of a bubble		falling droplet

Table 2.1: Classification of problems.

The example for the parabolic problem without free boundary imagines a glass filled to the brim with water and tightly covered by an elastic membrane like a lid. This lid is picked at some place and slowly lifted. We are then interested in the evolution of the shape of the membrane.

Parabolic free boundary problems are represented by an example of slow motion of a droplet (or a bubble), caused, for example, by chemical nonhomogeneity of the underlying surface (see Section 5.3).

Examples for hyperbolic problems can be taken the same as in the parabolic case, but with greater speed causing oscillations. We have also included two different examples for the vector-valued case: one describes the deformation and motion of a soap film caused by static electricity (sugar can be added to the soapy water in order to make it electrically active), and the other deals with a water droplet dripping from a horizontal plane.

The model for moving droplet is explained in some more detail in Section 5.3 and additional information on some of the other examples can be found in Chapter 7.

Chapter 3

Discrete Morse flow method

In this Chapter we explain the basic ideas and properties of the variational method called *discrete Morse flow*, reflecting upon its applicability to volume-constrained problems and, eventually, to free-boundary problems. This method solves time-dependent problems with differential operators concerning space variables in divergence form by discretizing time and defining a sequence of minimization problems approximating the original problem. The corresponding minimizers are then interpolated with respect to time and discretization parameter is sent to zero.

The method was first introduced in [20] by N. Kikuchi for parabolic problems and applied to hyperbolic problems in [15], [18], [21], [27], [29], [31], [39] and other papers. It was also applied to numerical solutions of free-boundary problems, e.g., in [28], [30] and [43]. Extension to volume-preserving problems is addressed in [36], [37], [41] or [35]. We did not find any references to volume-constrained hyperbolic problems in the literature, which would be close to our approach. Representative works dealing with the problem of volume constraint in evolution equations include, for example, [3] and [16]. However, the approaches to the problems used there are fundamentally different than our own. A completely different approach that was successful in analyzing large classes of constrained evolutionary problems is the subdifferential technique using Yosida approximations (see [2], [5], [26], etc.). Nevertheless, this method works only on the abstract level, having no possibility to be applied in numerical computations. Moreover, it strongly relies on convex structure of solved problems. We shall discuss the features of this method more in detail in Section 5.1.

3.1 Mathematical formulation

We shall explain the details on the example of the wave equation. It is considered in a bounded domain $\Omega \subset \mathbb{R}^m$ with smooth boundary $\partial\Omega$, on which homogeneous Dirichlet boundary condition is given.

Initial position $u_0 \in H_0^1(\Omega)$ and initial velocity $v_0 \in H_0^1(\Omega)$ are prescribed. Therefore, we have the following problem:

$$
\begin{aligned}
u_{tt}(t,x) &= \Delta u(t,x) \quad \text{in } Q_T = (0,T)\times\Omega, && (3.1.1)\\
u(t,x) &= 0 \quad \text{on } (0,T)\times\partial\Omega, && (3.1.2)\\
u(0,x) &= u_0(x) \quad \text{in } \Omega, && (3.1.3)\\
u_t(0,x) &= v_0(x) \quad \text{in } \Omega. && (3.1.4)
\end{aligned}
$$

First, we fix a natural number $N > 0$, determine the time step $h = T/N$ and put $u_1(x) = u_0(x) + hv_0(x)$. Function u_0 corresponds to the approximate solution at time level $t = 0$, while function u_1 is the approximate solution at time level $t = h$. We define the approximate solution u_n on further time levels $t = nh$ for $n = 2, 3, \ldots, N$, to be the minimizer of the following functional in $H_0^1(\Omega)$:

$$
J_n(u) = \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\, dx + \frac{1}{2}\int_\Omega |\nabla u|^2\, dx. \tag{3.1.5}
$$

We observe that the second term of the functional is lower-semicontinuous with respect to sequentially weak convergence in $H^1(\Omega)$ and the first term is continuous in $L^2(\Omega)$. The existence of minimizers then follows immediately from the fact that the functionals are bounded from below for each $n = 2, 3, \ldots, N$. This is a crucial advantage over the continuous version of this functional, the Lagrangian introduced in (2.1.1). Of course, if other terms, representing outer forces etc. are present, we have to make certain assumptions concerning these terms in order to get the existence of a minimizer.

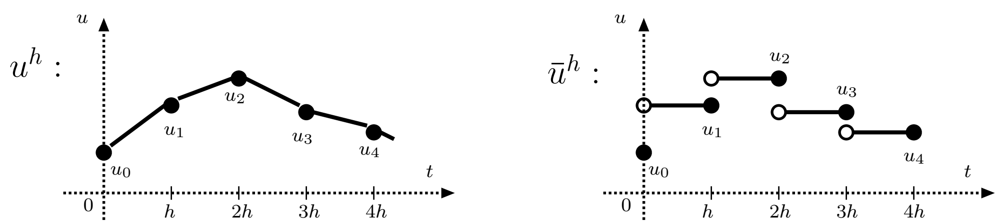


Figure 3.1: Interpolation of minimizers.

As the next step, we define the approximate solutions $\bar{u}^h$ and u^h through interpolation of the minimizers $\{u_n\}_{n=0}^N$ in time. The interpolation is schematically demonstrated in Figure 3.1 and precisely given by

$$
\bar{u}^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ u_n(x), & t \in ((n-1)h, nh],\ n = 1,\ldots,N, \end{cases} \tag{3.1.6}
$$

$$
u^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ \frac{t-(n-1)h}{h} u_n(x) + \frac{nh-t}{h} u_{n-1}(x), & t \in ((n-1)h, nh], n = 1,\ldots,N. \end{cases}
$$

Since u_n is a minimizer of J_n, the first variation of J_n at u_n vanishes. Thus, for any

$\varphi \in H_0^1(\Omega)$ we have

$$\begin{aligned} 0 &= \frac{d}{d\varepsilon} J_n(u_n + \varepsilon\varphi)|_{\varepsilon=0} = \lim_{\varepsilon\to 0} \frac{J_n(u_n+\varepsilon\varphi) - J_n(u_n)}{\varepsilon} \\ &= \lim_{\varepsilon\to 0} \frac{1}{\varepsilon} \int_\Omega \frac{|u_n + \varepsilon\varphi - 2u_{n-1} + u_{n-2}|^2 - |u_n - 2u_{n-1} + u_{n-2}|^2}{2h^2}\, dx \\ &\quad + \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon} \int_\Omega \left(|\nabla u_n + \varepsilon \nabla\varphi|^2 - |\nabla u_n|^2 \right) dx \\ &= \lim_{\varepsilon\to 0} \int_\Omega \frac{(2u_n + \varepsilon\varphi - 4u_{n-1} + 2u_{n-2})\varphi}{2h^2}\, dx + \lim_{\varepsilon\to 0} \frac{1}{2} \int_\Omega \left(2\nabla u_n \nabla\varphi + \varepsilon|\nabla\varphi|^2 \right) dx \\ &= \int_\Omega \frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} \varphi\, dx + \int_\Omega \nabla u_n \nabla\varphi\, dx. \end{aligned} \tag{3.1.7}$$

Using the definition of $\bar{u}^h$ and u^h in (3.1.6), this can be rewritten as

$$\int_\Omega \Big[\frac{u_t^h(t) - u_t^h(t-h)}{h} \varphi + \nabla\bar{u}^h(t)\nabla\varphi \Big]\, dx = 0 \qquad \text{for a.e. } t \in (h,T) \quad \forall\varphi \in H_0^1(\Omega).$$

We note that the above relation holds also when multiplied by any function $\tilde{\varphi} \in C([0,T])$. Hence, integrating over the time interval (h,T) and using a standard density argument, we arrive at

$$\int_h^T \int_\Omega \Big[\frac{u_t^h(t) - u_t^h(t-h)}{h} \varphi + \nabla\bar{u}^h \nabla\varphi \Big]\, dx\, dt = 0 \qquad \forall\varphi \in L^2(0,T; H_0^1(\Omega)). \tag{3.1.8}$$

Now, we would like to take the time step to zero. To be able to do so, some estimate on the approximate solutions is needed. We state it in the following Lemma.

Lemma 3.1.1. *Suppose Ω is a bounded domain with smooth boundary. Let J_n, $n = 2,\dots,N$, be the functionals defined by (3.1.5) and let u_n be corresponding minimizers in $H_0^1(\Omega)$. Define functions $\bar{u}^h$ and u^h by (3.1.6) and assume $h \le 1$. Then the following estimate holds*

$$\|u_t^h(t)\|_{L^2(\Omega)} + \|\nabla\bar{u}^h(t)\|_{L^2(\Omega)} \le C_E \qquad \textit{for a.e. } t \in (0,T), \tag{3.1.9}$$

where constant C_E depends on H^1-norms of the initial data but is independent of h.

Proof. Estimate of such kind is usually derived by testing the equation by the time-derivative of solution. Here it amounts to setting $\varphi := u_n - u_{n-1}$ in (3.1.7). This yields

$$\int_\Omega \frac{u_n - 2u_{n-1} + u_{n-2}}{h^2}(u_n - u_{n-1})\, dx + \int_\Omega (\nabla u_n - \nabla u_{n-1})\nabla u_n\, dx = 0.$$

We employ the inequality

$$\frac{a^2}{2} - \frac{b^2}{2} \le (a-b)a, \qquad \forall a,\, b \in \mathbb{R}, \tag{3.1.10}$$

to find that for each $n = 2, 3, \dots, N$, the following holds:

$$\int_\Omega \left[\left(\frac{u_n - u_{n-1}}{h}\right)^2 - \left(\frac{u_{n-1} - u_{n-2}}{h}\right)^2 + |\nabla u_n|^2 - |\nabla u_{n-1}|^2\right] dx \le 0$$
$$\int_\Omega \left[\left(\frac{u_n - u_{n-1}}{h}\right)^2 + |\nabla u_n|^2\right] dx \le \int_\Omega \left[\left(\frac{u_{n-1} - u_{n-2}}{h}\right)^2 + |\nabla u_{n-1}|^2\right] dx.$$

These inequalities are summed from $n = 2$ to an arbitrary integer $k \le N$. Since the terms in between cancel, we obtain

$$\begin{aligned}
\int_\Omega \left[\left(\frac{u_k - u_{k-1}}{h}\right)^2 + |\nabla u_k|^2\right] dx &\le \int_\Omega \left[\left(\frac{u_1 - u_0}{h}\right)^2 + |\nabla u_1|^2\right] dx \\
&= \int_\Omega \left[(v_0)^2 + |\nabla u_0 + h\nabla v_0|^2\right] dx \\
&\le \int_\Omega \left[(v_0)^2 + 2|\nabla u_0|^2 + 2h^2|\nabla v_0|^2\right] dx \\
&\le 2\|u_0\|^2_{H^1(\Omega)} + 2\|v_0\|^2_{H^1(\Omega)}.
\end{aligned}$$

This is already the desired estimate (3.1.9), because

$$u_t^h(t) = \frac{u_k - u_{k-1}}{h} \qquad \text{for } t \in ((k-1)h, kh), \quad k = 1, 2, \dots, N.$$

□

Thanks to estimate (3.1.9), we can apply the theorem by Eberlein and Shmulyan (see [42], Appendix to Chapter V) to extract a subsequence $\{\nabla \bar{u}^{h_k}\}_{k\in\mathbb{N}}$ which converges weakly in $L^2(Q_T)$ to a function $\mathbf{v}$. From the sequence $\{h_k\}_{k\in\mathbb{N}}$ obtained in this way, we can extract another subsequence $\{h_{k_l}\}_{l\in\mathbb{N}}$ so that $\{u_t^{h_{k_l}}\}_{l\in\mathbb{N}}$ converges weakly in $L^2(Q_T)$ to a function U. In the sequel, we often use this logic but we shall omit this lengthy explanation and subscripts and simply write

$$\nabla \bar{u}^h \rightharpoonup \mathbf{v} \qquad \text{in } (L^2(Q_T))^m, \tag{3.1.11}$$
$$u_t^h \rightharpoonup U \qquad \text{in } L^2(Q_T). \tag{3.1.12}$$

We should now show that there is a function $u \in L^2(0, T; H_0^1(\Omega))$ such that $\mathbf{v} = \nabla u$ and $U = u_t$ in $L^2(Q_T)$. To this end, a more detailed analysis is needed. First, we estimate the norm of the difference of the approximate functions $\bar{u}^h$ and u^h. Let $t \in ((n-1)h, nh)$. Then

$$\begin{aligned}
\|\bar{u}^h(t) - u^h(t)\|^2_{L^2(\Omega)} &= \int_\Omega (\bar{u}^h - u^h)^2\, dx \\
&= \int_\Omega \left(u_n - \frac{t-(n-1)h}{h}u_n - \frac{nh-t}{h}u_{n-1}\right)^2 dx \\
&= \int_\Omega \left(\frac{nh-t}{h}\right)^2 (u_n - u_{n-1})^2\, dx \\
&\le \int_\Omega (u_n - u_{n-1})^2\, dx = h^2 \int_\Omega (u_t^h)^2\, dx \\
&\le C_E^2 h^2.
\end{aligned}$$

This means that

$$\|\bar{u}^h(t) - u^h(t)\|_{L^2(\Omega)} \le Ch \qquad \text{for a.e. } t \in (0,T).$$

We have further

$$\begin{aligned}
\|u^h\|^2_{L^2(Q_T)} - \|\bar{u}^h\|^2_{L^2(Q_T)} &= \int_0^T \int_\Omega \big((u^h)^2 - (\bar{u}^h)^2\big)\,dx\,dt \\
&= \sum_{n=1}^N \int_{(n-1)h}^{nh} \int_\Omega \Big[\Big(\frac{t-(n-1)h}{h}u_n - \frac{nh-t}{h}u_{n-1}\Big)^2 - u_n^2\Big]\,dx\,dt \\
&= \sum_{n=1}^N \int_{(n-1)h}^{nh} \int_\Omega \Big[\frac{(t-(n-1)h)^2 - h^2}{h^2}u_n^2 \\
&\qquad + 2\frac{(t-(n-1)h)(nh-t)}{h^2}u_n u_{n-1} + \frac{(nh-t)^2}{h^2}u_{n-1}^2\Big]\,dx\,dt \\
&= \sum_{n=1}^N \int_\Omega \big[-\frac{2h}{3}u_n^2 + \frac{h}{3}u_n u_{n-1} + \frac{h}{3}u_{n-1}^2\big]\,dx \\
&\le \frac{h}{6}\sum_{n=1}^N \int_\Omega \big[-4u_n^2 + u_n^2 + u_{n-1}^2 + 2u_{n-1}^2\big]\,dx \\
&= \frac{h}{2}\sum_{n=1}^N \int_\Omega (-u_n^2 + u_{n-1}^2)\,dx = \frac{h}{2}\int_\Omega (u_0^2 - u_N^2)\,dx \\
&\le \frac{h}{2}\|u_0\|^2_{L^2(\Omega)}.
\end{aligned}$$

In the same way we get also

$$\|\nabla u^h\|^2_{L^2(Q_T)} - \|\nabla \bar{u}^h\|^2_{L^2(Q_T)} \le \frac{h}{2}\|\nabla u_0\|^2_{L^2(\Omega)}.$$

Finally, from Poincaré's inequality (see [8], Section 5.6) we know that there is a universal constant C_P so that

$$\|u^h\|_{L^2(Q_T)} \le C_P \|\nabla u^h\|_{L^2(Q_T)} \qquad \text{for all } h \in (0,1). \tag{3.1.13}$$

We summarize the results for future use. We remark that the results of the following Lemma rely only on the interpolation (3.1.6) and are independent of the problem under consideration, a fact frequently used later on.

Lemma 3.1.2. *Let $\bar{u}^h$ and u^h be defined by (3.1.6). Then the following relations hold.*

$$\|\bar{u}^h(t) - u^h(t)\|_{L^2(\Omega)} \le h\|u^h_t(t)\|_{L^2(\Omega)} \qquad \text{for a.e. } t \in (0,T), \tag{3.1.14}$$

$$\|u^h\|^2_{L^2(Q_T)} \le \|\bar{u}^h\|^2_{L^2(Q_T)} + \frac{h}{2}\|u_0\|^2_{L^2(\Omega)}, \tag{3.1.15}$$

$$\|\nabla u^h\|^2_{L^2(Q_T)} \le \|\nabla \bar{u}^h\|^2_{L^2(Q_T)} + \frac{h}{2}\|\nabla u_0\|^2_{L^2(\Omega)}. \tag{3.1.16}$$

Now, (3.1.9), (3.1.16) and (3.1.13) imply that u^h is uniformly bounded in $H^1(Q_T)$. Therefore, there is a weakly convergent subsequence in $H^1(Q_T)$ and, by Rellich theorem (see [8], Section 5.7), a strongly converging subsequence in $L^2(Q_T)$ (we always mean "subsequence of the last obtained sequence"). Let us denote the cluster function as u:

$$u^h \rightharpoonup u \qquad \text{weakly in } H^1(Q_T). \tag{3.1.17}$$

Because of (3.1.12), $U = u_t$ holds almost everywhere. Moreover, from (3.1.11) for any $\varphi \in C_0^\infty(Q_T)$

$$\int_0^T \int_\Omega \Big(\frac{\partial \bar{u}^h}{\partial x_i} - \frac{\partial u^h}{\partial x_i}\Big)\varphi \, dx\, dt \to \int_0^T \int_\Omega \Big(\mathbf{v}_i - \frac{\partial u}{\partial x_i}\Big)\varphi \, dx\, dt \qquad \text{as } h \to 0+,$$

while at the same time

$$\int_0^T \int_\Omega \Big(\frac{\partial \bar{u}^h}{\partial x_i} - \frac{\partial u^h}{\partial x_i}\Big)\varphi \, dx\, dt = -\int_0^T \int_\Omega (\bar{u}^h - u^h)\frac{\partial \varphi}{\partial x_i} \, dx\, dt \to 0 \qquad \text{as } h \to 0+$$

by (3.1.14). This means that $\mathbf{v} = \nabla u$ almost everywhere in Q_T.

We have shown in this way that there is a function $u \in H^1(Q_T)$, such that

$$\nabla \bar{u}^h \rightharpoonup \nabla u \qquad \text{in } (L^2(Q_T))^m, \tag{3.1.18}$$

$$u_t^h \rightharpoonup u_t \qquad \text{in } L^2(Q_T). \tag{3.1.19}$$

Now, we can pass to limit in (3.1.8) as $h \to 0+$. We shall, for the time being, consider a test function φ belonging to $C_0^\infty([0,T) \times \Omega)$. To begin with, we have

$$\begin{aligned}\int_h^T \int_\Omega \nabla \bar{u}^h \nabla \varphi \, dx\, dt &= \int_0^T \int_\Omega \nabla \bar{u}^h \nabla \varphi \, dx\, dt - \int_0^h \int_\Omega \nabla \bar{u}^h \nabla \varphi \, dx\, dt \\ &\to \int_0^T \int_\Omega \nabla u \nabla \varphi \, dx\, dt \qquad \text{as } h \to 0+, \end{aligned} \tag{3.1.20}$$

because of the boundedness (3.1.9) of $\nabla \bar{u}^h$:

$$\begin{aligned}\Big|\int_0^h \int_\Omega \nabla \bar{u}^h \nabla \varphi \, dx\, dt\Big| &\le \int_0^h \Big(\int_\Omega |\nabla \bar{u}^h|^2 \, dx\Big)^{1/2} \Big(\int_\Omega |\nabla \varphi|^2 \, dx\Big)^{1/2} dt \\ &\le \int_0^h \sqrt{C_E}\, C \, dt = Ch \to 0 \qquad \text{as } h \to 0+. \end{aligned}$$

Moreover, we have

$$\begin{aligned}&\int_h^T \int_\Omega \frac{u_t^h(t) - u_t^h(t-h)}{h}\varphi \, dx\, dt \\ &\quad = \int_h^T \int_\Omega \frac{u_t^h(t)}{h}\varphi(t) \, dx\, dt - \int_0^{T-h} \int_\Omega \frac{u_t^h(t)}{h}\varphi(t+h) \, dx\, dt \\ &\quad = \int_0^T \int_\Omega u_t^h(t) \frac{\varphi(t) - \varphi(t+h)}{h} \, dx\, dt - \int_0^h \int_\Omega \frac{u_t^h(t)}{h}\varphi(t) \, dx\, dt \\ &\qquad + \int_{T-h}^T \int_\Omega \frac{u_t^h(t)}{h}\varphi(t+h) \, dx\, dt \qquad (3.1.21) \\ &\to -\int_0^T \int_\Omega u_t \varphi_t \, dx\, dt - \int_\Omega v_0 \varphi(0) \, dx \qquad \text{as } h \to 0+. \end{aligned}$$

The convergence is deduced from the following facts: (i) in the first term of (3.1.21), u_t^h converges weakly and $(\varphi(t) - \varphi(t+h))/h$ converges strongly in $L^2(Q_T)$; (ii) in the second term, $u_t^h = (u_1 - u_0)/h = v_0$ for $t \in (0, h)$; (iii) in the third term, $\varphi(t + h) = 0$ for $t \in (T - h, T)$. Thus, we can finally state that

$$\int_0^T \int_\Omega (-u_t \varphi_t + \nabla u \nabla \varphi)\, dx\, dt - \int_\Omega v_0 \varphi(0, x)\, dx = 0 \quad \forall \varphi \in C_0^\infty([0, T) \times \Omega). \tag{3.1.22}$$

Noting that the space of functions from $H^1(Q_T)$ with zero trace on $(\{0\} \times \Omega) \cup ([0, T] \times \partial\Omega)$ is a closed linear subspace of $H^1(Q_T)$ and, therefore, weakly closed by Mazur's theorem (see [8], Appendix D), we conclude by (3.1.17) that u belongs to this space. Consequently, u satisfies boundary condition (3.1.2) and initial condition (3.1.3) in the sense of traces. We remark that the convergence of traces follows also from the compactness of the trace operator $T : H^1(\Omega) \to L^2(\partial\Omega)$. Moreover, from [8] (Section 5.9), it follows that u, as a function from $H^1(0, T; L^2(\Omega))$, belongs to $C([0, T]; L^2(\Omega))$. Thus, the initial condition (3.1.3) is satisfied even in the strong sense.

To summarize, we have proved by the discrete Morse flow method that there exists a weak solution $u \in H^1(Q_T)$ to problem (3.1.1) – (3.1.4) in the sense of (3.1.22), satisfying boundary and initial conditions (3.1.2), (3.1.3) in the sense of traces.

3.2 Advantages and extensions of the method

There are certainly many different and easier ways how to achieve this result. Nevertheless, the method of discrete Morse flow can be naturally applied to problems with volume constraint and extends even to free-boundary problems, as we shall gradually show in the following pages.

The advantage of this approach regarding volume-constrained problems, and the reason we have adopted it, lies in the fact that a semi-discretization of time allows us to use results from elliptic theory. Moreover, the variational principle enables us to deal with the volume constraint by incorporating the condition in the set of admissible functions.

We considered using standard methods to solve this problem, but the nonlinear and nonlocal character of the multiplier term (see (2.1.3)) complicates the situation greatly. For example, the Galerkin approximation method yields a system of nonlinear ordinary differential equations and the existence of its solution on the whole time interval is not clear. Likewise, applying fixed point methods requires stronger assumptions on the data and fails to guarantee that the volume is preserved for approximate solutions, which makes it difficult to obtain necessary estimates. As such, these approaches do not easily yield the existence of a (weak) solution to our problem. What is more, unlike the Morse flow method, they are not suitable for numerical computations. The relation to subdifferential methods was mentioned in the beginning of this chapter.

As already intimated, we add the volume constraint into the set of admissible functions for minimization of the time-discrete functional when solving problems with preservation of volume. In other words, we minimize the same functional (3.1.5) in the set

$$\mathcal{K} = \{u \in H_0^1(\Omega); \int_\Omega u\,dx = V\},$$

instead of minimizing in $H_0^1(\Omega)$. The details of the analysis and results are presented in the following Chapter 4 for both parabolic and hyperbolic problems.

The situation becomes somewhat complicated for free-boundary problems. Let us consider an obstacle problem with a plane obstacle corresponding to the level $u = 0$ (think of a soap bubble on the surface of water). Assuming that there is no reflection when the soap film touches the plane (i.e., energy is lost), we show that the degenerate hyperbolic equation

$$\chi_{u>0} u_{tt} = \Delta u + \gamma \chi_\varepsilon'(u) + \lambda(u)\chi_{u>0}, \quad \text{with } \lambda(u) = \frac{1}{V}\int_\Omega \left(u_{tt}u + |\nabla u|^2 + \gamma u \chi_\varepsilon'(u)\right)\,dx,$$

is a reasonable description of the motion of the bubble. Here $\chi_{u>0}$ is the characteristic function of the set $\{(t,x); u(t,x) > 0\}$ (the region where the bubble sits), χ_ε is its appropriate smoothing and γ depends on the various gas/liquid/solid surface tensions. The discrete Morse flow can be applied to this problem, too, and amounts to minimizing of

$$J_n(u) = \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\chi_{u>0}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx + \int_\Omega \gamma\chi_\varepsilon(u)\,dx$$

$$\text{in} \qquad \mathcal{K} = \{u \in H_0^1(\Omega); \int_\Omega u\chi_{u>0}\,dx = V\}.$$

The obstacle condition is achieved through the characteristic functions appearing in the admissible function set and at the discretized term of the functional. Parabolic and hyperbolic free-boundary problems of this type are studied in Chapter 5.

Chapter 4

Problems without free boundary

In this Chapter, we deal with the simplest version of volume-constrained problems - parabolic problems of heat type with an 'heat source' term and hyperbolic problems corresponding to wave equation.

4.1 Parabolic problem

4.1.1 Setting

In this part, which paraphrases paper [36], we consider the problem of finding a scalar function $u : [0,T) \times \Omega \to \mathbb{R}$ subject to the following constraints:

$$\begin{array}{rcll} u_t(t,x) - \Delta u(t,x) &=& f(t,x,u) + \lambda(t) & (t,x) \in Q_T, \\ u(t,x) &=& g(x) & t \in (0,T),\ x \in \partial\Omega, \\ u(0,x) &=& u_0(x) & x \in \Omega. \end{array} \tag{4.1.1}$$

Throughout this section, Ω is a bounded domain in $\mathbb{R}^m$ with piecewise smooth boundary $\partial\Omega$, $Q_T = (0,T) \times \Omega$, $T > 0$, and $\lambda(t)$ is the Lagrange multiplier determined by the volume-preserving condition:

$$\int_\Omega u(t,x)\,dx = V \tag{4.1.2}$$

for all t in the interval $(0,T)$ and a given volume V. The multiplier is independent of x and has the form

$$\lambda(t) = \frac{1}{V} \int_\Omega (u_t u + |\nabla u|^2 - f(u)u)\,dx. \tag{4.1.3}$$

Such equations can appear in the case of slow motion or large resistance to the motion when we adopt the same derivation process as in Section 2.1. For numerical simulations using this equation, we refer to Section 7.1.

When the first equation in (4.1.1) is multiplied by u and integrated over Ω, one deduces that λ must be of the form (4.1.3). On the contrary, if (4.1.3) holds, volume condition (4.1.2) turns out to be satisfied by the same calculation.

We assume that $g \in L^2((0,T) \times \partial\Omega)$ and $u_0 \in H^1(\Omega)$ satisfy $g(x) = u_0(x)$ on the boundary of Ω. See Section 4.1.5 for remarks on the corresponding problem with Neumann boundary conditions.

Further, we assume that $f(t,x,s)$ is measurable and differentiable in t, satisfying

$$\begin{aligned} |f(t,x,s)| &\le 2C_f|s| + \gamma(t,x), \qquad \gamma \in L^\infty(Q_T), && (4.1.4)\\ |f_t(t,x,s)| &\le 2C'_f|s| + \Gamma(t,x), \qquad \Gamma \in L^\infty(0,T;L^2(\Omega)), && (4.1.5)\end{aligned}$$

with $C'_f, \gamma, \Gamma \ge 0$ and

$$0 \le C_f \le \frac{1}{4C_S^2}. \tag{4.1.6}$$

Here C_S is a constant depending only on m and $|\Omega|$, which is derived from Poincaré's inequality:

$$\|u\|_{L^2(\Omega)} \le C_S \|\nabla u\|_{L^2(\Omega)} \tag{4.1.7}$$

for all u in $H_0^1(\Omega)$.

We also require that $f(t,x,s)$ be continuous in s. Therefore, there exists a primitive function $F(t,x,s)$ such that

$$\frac{\partial}{\partial s}F(t,x,s) = f(t,x,s).$$

Note that F can be chosen such that

$$|F(t,x,s)| \le C_f s^2 + \gamma(t,x)|s|, \quad |F_t(t,x,s)| \le C'_f s^2 + \Gamma(t,x)|s|. \tag{4.1.8}$$

4.1.2 Variational method

To simplify the calculations in what follows, we take $V = 1$ and consider the homogeneous Dirichlet boundary condition, i.e., $g \equiv 0$. (See Section 4.1.5 for notes on nonhomogeneous boundary conditions.)

We invoke the method of discrete Morse flow in solving problem (4.1.1). Using this approach we construct a partition of the interval $(0,T)$ into N equal subintervals and take $h = T/N$. Next, starting with the initial value u_0 and using the notation

$$F_n(x,u) = \frac{1}{h}\int_{(n-1)h}^{nh} F(t,x,u)dt, \qquad f_n(x,u) = \frac{1}{h}\int_{(n-1)h}^{nh} f(t,x,u)dt,$$

we seek a sequence of minimizers $\{u_n\}$ from the convex set

$$\mathcal{K}_V = \{u \in H^1(\Omega); u|_{\partial\Omega} = 0, \int_\Omega u\,dx = 1\}, \tag{4.1.9}$$

such that each u_n minimizes the functional

$$J_n(u) = \int_\Omega \frac{|u-u_{n-1}|^2}{2h}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx - \int_\Omega F_n(u)\,dx. \tag{4.1.10}$$

The existence of minimizers can be shown by the direct method. Using assumption (4.1.8), we have for any minimizing sequence $\{u^k\} \subset \mathcal{K}_V$ the estimate

$$\begin{aligned} -\int_\Omega F_n(u^k)\,dx &= -\frac{1}{h}\int_\Omega \int_{(n-1)h}^{nh} F(t,x,u^k)\,dx\,dt \\ &\geq -\frac{1}{h}\int_\Omega \int_{(n-1)h}^{nh} \Big(C_f|u^k|^2 + \gamma(t,x)|u^k|\Big)\,dx\,dt \\ &\geq -\int_\Omega \big(C_f|u^k|^2 + \sup_{t\in(0,T)} |\gamma(t,x)||u^k|\big)\,dx. \end{aligned}$$

The last expression is for $C_f > 0$ greater or equal to

$$-\big(C_f + \frac{C_f}{2}\big)\int_\Omega |u^k|^2\,dx - \frac{1}{2C_f}\int_\Omega \sup_{t\in(0,T)} \gamma^2(t,x)\,dx,$$

and for $C_f = 0$ it is greater or equal to

$$-\frac{3}{8C_S^2}\int_\Omega |u^k|^2\,dx - \frac{2C_S^2}{3}\int_\Omega \sup_{t\in(0,T)} \gamma^2(t,x)\,dx.$$

In either case, by (4.1.6) and (4.1.7) we find that

$$\begin{aligned} -\int_\Omega F_n(u^k)\,dx &\geq -\frac{3}{8C_S^2}\int_\Omega |u^k|^2\,dx - \bar{C}\|\gamma\|^2_{L^\infty(0,T;L^2(\Omega))} \\ &\geq -\frac{3}{8}\int_\Omega |\nabla u^k|^2\,dx - \bar{C}\|\gamma\|^2_{L^\infty(0,T;L^2(\Omega))}. \end{aligned}$$

Hence, we get the boundedness of gradients of the minimizing sequence in $L^2(\Omega)$:

$$\begin{aligned} C &\geq J_n(u^k) \geq \frac{1}{2}\int_\Omega |\nabla u^k|^2\,dx - \int_\Omega F_n(u^k)\,dx \\ &\geq \frac{1}{8}\int_\Omega |\nabla u^k|^2\,dx - \bar{C}\|\gamma\|^2_{L^\infty(0,T;L^2(\Omega))}. \end{aligned}$$

Remembering the fact that the usual norm of $H^1(\Omega)$ for functions with zero trace is equivalent to the seminorm (see (4.1.7)), we can extract a subsequence converging weakly in $H^1(\Omega)$ and strongly in $L^2(\Omega)$ to a function $u \in H^1_0(\Omega)$. Because of the strong convergence, the function u obviously has volume $V(=1)$ and, thus, belongs to $\mathcal{K}_V$. If we can show lower semicontinuity of J_n with respect to weak convergence in $H^1(\Omega)$, it becomes clear that $u_n = u$ is a minimizer of J_n. The lower semicontinuity is established by employing condition (4.1.8) and the continuity of $F_n(x,u^k)$ in u^k.

To ensure that this method corresponds to equation (4.1.1), we introduce a Lagrange multiplier λ_n for each n, which is a fixed real number. Due to (an extension) of Theorem 2.1.1, we know that for each $n = 1,\dots,N$, there is λ_n complying with

$$\frac{d}{d\varepsilon}J_n(u_n+\varepsilon\zeta)|_{\varepsilon=0} = \lambda_n\int_\Omega \frac{d}{du}(u - V/|\Omega|)\zeta\,dx = \lambda_n\int_\Omega \zeta\,dx$$

for all $\zeta \in C_0^\infty(\Omega)$. Upon computing the variation we obtain

$$\int_\Omega \Big(\frac{u_n - u_{n-1}}{h}\zeta + \nabla u_n \nabla \zeta - f_n(u_n)\zeta \Big)\, dx = \lambda_n \int_\Omega \zeta \, dx, \tag{4.1.11}$$

which is the weak formulation for

$$\frac{u_n - u_{n-1}}{h} = \Delta u_n + f_n(u_n) + \lambda_n,$$

a time-discretized formulation of (4.1.1).

The explicit form of the Lagrange multiplier is found by considering volume-preserving perturbations:

$$v^\varepsilon = V \frac{u_n + \varepsilon\zeta}{\int_\Omega (u_n + \varepsilon\zeta)\, dx} \in \mathcal{K}_V,$$

where again $\zeta \in C_0^\infty(\Omega)$. Here we use exceptionally the general volume V to show the way of dependence. Upon denoting $Z = \int_\Omega \zeta \, dx$, the variation can be expressed

$$\begin{aligned}
0 \;&=\; \frac{d}{d\varepsilon} J_n(v^\varepsilon)|_{\varepsilon=0} = \lim_{\varepsilon\to 0} \frac{J_n\big(\frac{u_n+\varepsilon\zeta}{1+\varepsilon\frac{Z}{V}}\big) - J_n(u_n)}{\varepsilon} \\
&=\; \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon h} \int_\Omega \Big(\big|\frac{u_n+\varepsilon\zeta}{1+\varepsilon\frac{Z}{V}} - u_{n-1}\big|^2 - |u_n - u_{n-1}|^2 \Big)\, dx \\
&\quad + \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon} \int_\Omega \Big(\big|\frac{\nabla u_n + \varepsilon\zeta}{1+\varepsilon\frac{Z}{V}}\big|^2 - |\nabla u_n|^2 \Big)\, dx - \lim_{\varepsilon\to 0} \frac{1}{\varepsilon} \int_\Omega \Big(F_n\big(\frac{u_n+\varepsilon\zeta}{1+\varepsilon\frac{Z}{V}}\big) - F_n(u_n) \Big)\, dx \\
&=\; \lim_{\varepsilon\to 0} \frac{1}{2\varepsilon h} \int_\Omega \Big(\frac{u_n+\varepsilon\zeta}{1+\varepsilon\frac{Z}{V}} + u_n - 2u_{n-1} \Big)\big(\zeta - \frac{Z}{V}u_n\big)\, dx + \lim_{\varepsilon\to 0} \int_\Omega \frac{\nabla u_n \nabla\zeta - \frac{Z}{V}|\nabla u_n|^2}{(1+\varepsilon\frac{Z}{V})^2} \\
&\quad - \int_\Omega f_n(u_n)\big(\zeta - \frac{Z}{V}u_n\big)\, dx \\
&=\; \int_\Omega \Big(\frac{u_n - u_{n-1}}{h}\zeta + \nabla u_n \nabla\zeta - f_n(u_n)\zeta \Big)\, dx \\
&\quad - \frac{Z}{V} \int_\Omega \Big(\frac{u_n - u_{n-1}}{h} u_n + |\nabla u_n|^2 - f_n(u_n)u_n \Big)\, dx,
\end{aligned}$$

which, compared with (4.1.11), implies

$$\lambda_n = \int_\Omega \Big[\frac{u_n - u_{n-1}}{h} u_n + |\nabla u_n|^2 - f_n(u_n)u_n \Big]\, dx. \tag{4.1.12}$$

We see that the discretized multiplier λ_n from (4.1.12) corresponds well to the form of λ from (4.1.3). Actually, as will be shown below, the approximate weak solutions defined in terms of u_n and λ_n converge to a weak solution of (4.1.1). For definiteness, we introduce the following definition:

Definition 4.1.1. *A function $u \in L^\infty(0,T;H_0^1(\Omega)) \cap H^1(0,T;L^2(\Omega))$ is said to be a weak solution of (4.1.1) if it satisfies*

$$\int_0^T \int_\Omega (u_t\phi + \nabla u \nabla\phi - f(u)\phi)\, dx\, dt = \int_0^T \int_\Omega \lambda\phi \, dx\, dt \tag{4.1.13}$$

for each $\phi \in L^2(0,T;H_0^1(\Omega))$ with λ given by (4.1.3), and the initial condition $u(0) = u_0$.

Note that the integral $\int_0^T \int_\Omega \lambda\phi\, dx\, dt$ makes sense for u with the stated regularity.

We introduce the approximate weak solution via an interpolation in time of the minimizers u_n obtained above. Namely, for $(t, x) \in ((n-1)h, nh] \times \Omega,\ n = 1, ..., N\ \ (T = Nh)$, we set

$$\begin{aligned} \bar{u}^h(t,x) &= u_n(x), \\ u^h(t,x) &= \frac{t-(n-1)h}{h} u_n(x) + \frac{nh-t}{h} u_{n-1}(x), \\ \bar{\lambda}^h(t) &= \lambda_n, \\ \bar{f}^h(t,x,\bar{u}^h) &= f_n(x,u_n), \end{aligned} \tag{4.1.14}$$

and for $t = 0$ we define $\bar{u}^h(0, x) = u_0(x)$ and $u^h(0, x) = u_0(x)$. We see that these functions satisfy the conditions $u^h(0) = u_0$ and

$$\int_0^T \int_\Omega \left(u_t^h \phi + \nabla \bar{u}^h \nabla \phi - \bar{f}^h(\bar{u}^h)\phi \right) dx\, dt = \int_0^T \int_\Omega \bar{\lambda}^h \phi\, dx\, dt \tag{4.1.15}$$

for all $\phi \in L^2(0, T; H_0^1(\Omega))$. Let us call functions u^h and $\bar{u}^h$, defined by the sequence $\{u_n\}_{n=0}^N$, *approximate weak solution* to problem (4.1.1).

4.1.3 The limit process

Our goal is to prove approximation properties of the weak solutions u^h and $\bar{u}^h$. Specifically, we want to prove that by passing to the limit as $h \to 0+$, we obtain a weak solution to the original problem (4.1.1) as defined in (4.1.13). To this end, we must first derive an energy estimate.

Lemma 4.1.1. *We have the following bound for the approximate solution:*

$$\int_0^t \|u_t^h(\tau)\|^2_{L^2(\Omega)}\, d\tau + \|\nabla \bar{u}^h(t)\|^2_{L^2(\Omega)} \le C_E \qquad \forall t \in (0, T), \tag{4.1.16}$$

where the constant C_E depends on $\|u_0\|_{H^1(\Omega)}$, $\|\gamma\|_{L^\infty(0,T;L^2(\Omega))}$, $\|\Gamma\|_{L^\infty(0,T;L^2(\Omega))}$, C_f, C_f', C_S and T, but is independent of h.

Proof. We first carry out some auxiliary estimates. By (4.1.8),

$$\begin{aligned} &|\int_\Omega F_1(u_0)\, dx| = \left| \frac{1}{h} \int_0^h \int_\Omega F(t, x, u_0)\, dx\, dt \right| \\ &\le C_f \int_\Omega u_0^2\, dx + \frac{1}{h} \int_0^h \int_\Omega \gamma |u_0|\, dx\, dt \le (C_f + \frac{1}{2}) \int_\Omega u_0^2\, dx + \frac{1}{2h} \int_0^h \int_\Omega \gamma^2\, dx\, dt. \end{aligned}$$

Our next calculation makes use of Young's inequality, Poincaré's inequality (4.1.7), and assumption (4.1.6):

$$\begin{aligned} &|\int_\Omega F_n(u_n)\, dx| = \left| \frac{1}{h} \int_{(n-1)h}^{nh} \int_\Omega F(t, x, u_n)\, dx\, dt \right| \\ &\le C_f \int_\Omega u_n^2\, dx + \frac{1}{h} \int_{(n-1)h}^{nh} \int_\Omega |\gamma u_n|\, dx\, dt \le \frac{3}{8} \int_\Omega |\nabla u_n|^2\, dx + \frac{C_1}{h} \int_{(n-1)h}^{nh} \int_\Omega \gamma^2\, dx\, dt, \end{aligned}$$

where $C_1 = 2C_S^2$. Further,

$$
\begin{aligned}
|\int_\Omega F_{n-1}(u_{n-1}) - F_n(u_{n-1})\,dx| &= \left|\frac{1}{h}\int_{(n-1)h}^{nh}\int_\Omega F(t-h,x,u_{n-1}) - F(t,x,u_{n-1})\,dx\,dt\right| \\
&\le \int_\Omega\int_{(n-1)h}^{nh}\left(C'_f u_{n-1}^2 + \max_{t\in(0,T)}\Gamma(t)|u_{n-1}|\right)dx\,dt \\
&\le (C'_f + \frac{1}{2})h\int_\Omega u_{n-1}^2\,dx + \frac{h}{2}\|\Gamma\|^2_{L^\infty(0,T;L^2(\Omega))}.
\end{aligned}
$$

For ease of interpretation in what follows, we denote A_1 to be the expression

$$
A_1 = \|\nabla u_0\|^2_{L^2(\Omega)} + (2C_f+1)\int_\Omega u_0^2\,dx + (2C_1+1)\|\gamma\|^2_{L^\infty(0,T;L^2(\Omega))} + T\|\Gamma\|^2_{L^\infty(0,T;L^2(\Omega))}.
$$

We calculate the sum with respect to n from 1 to l of the inequalities $J_n(u_n) \le J_n(u_{n-1})$. Applying the above estimates, for $l=1$ we have

$$
\begin{aligned}
&h\|\frac{u_1-u_0}{h}\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)} \le \|\nabla u_0\|^2_{L^2(\Omega)} + 2\int_\Omega F_1(u_1)\,dx - 2\int_\Omega F_1(u_0)\,dx \\
&\le \|\nabla u_0\|^2_{L^2(\Omega)} + \frac{3}{4}\|\nabla u_1\|^2_{L^2(\Omega)} + (2C_1+1)\|\gamma\|^2_{L^\infty(0,T;L^2(\Omega))} + (2C_f+1)\int_\Omega u_0^2\,dx,
\end{aligned}
$$

therefore,

$$
h\|\frac{u_1-u_0}{h}\|^2_{L^2(\Omega)} + \frac{1}{4}\|\nabla u_1\|^2_{L^2(\Omega)} \le A_1.
$$

From the last inequality, since $u_n \in H_0^1(\Omega)$, $n = 0,\dots,N$, we also find

$$
\|u_1\|^2_{L^2(\Omega)} \le \tilde{C}A_1 \tag{4.1.17}
$$

for some constant $\tilde{C}$ ($\tilde{C} = 4C_S^2$). For $l > 1$ the calculation becomes

$$
\begin{aligned}
&h\sum_{n=1}^{l}\|\frac{u_n-u_{n-1}}{h}\|^2_{L^2(\Omega)} + \|\nabla u_l\|^2_{L^2(\Omega)} \qquad (4.1.18)\\
&\le \|\nabla u_0\|^2_{L^2(\Omega)} + 2\int_\Omega F_l(u_l)\,dx + 2\sum_{n=2}^{l}\int_\Omega (F_{n-1}(u_{n-1}) - F_n(u_{n-1}))\,dx - 2\int_\Omega F_1(u_0)\,dx \\
&\le \|\nabla u_0\|^2_{L^2(\Omega)} + \frac{3}{4}\|\nabla u_l\|^2_{L^2(\Omega)} + (2C_1+1)\|\gamma\|^2_{L^\infty(0,T;L^2(\Omega))} + (2C_f+1)\int_\Omega u_0^2\,dx \\
&\quad +(2C'_f+1)h\sum_{n=2}^{l}\int_\Omega u_{n-1}^2\,dx + lh\|\Gamma\|^2_{L^\infty(0,T;L^2(\Omega))}.
\end{aligned}
$$

Thus,

$$
h\sum_{n=1}^{l}\|\frac{u_n-u_{n-1}}{h}\|^2_{L^2(\Omega)} + \frac{1}{4}\|\nabla u_l\|^2_{L^2(\Omega)} \le A_1 + (2C'_f+1)h\sum_{n=2}^{l}\int_\Omega u_{n-1}^2\,dx.
$$

If we denote the last expression on the right-hand side as A_l, we have $\|u_l\|^2_{L^2(\Omega)} \leq \tilde{C}\|\nabla u_l\|^2_{L^2(\Omega)}/4 \leq \tilde{C}A_l$ and

$$A_{l+1} = A_l + (2C'_f + 1)h \int_\Omega u_l^2 \, dx \leq A_l(1 + (2C'_f + 1)\tilde{C}h).$$

For simplicity, we use the notation $B = (2C'_f + 1)\tilde{C}$ and obtain

$$h \sum_{n=1}^{l} \| \frac{u_n - u_{n-1}}{h} \|^2_{L^2(\Omega)} + \frac{1}{4}\|\nabla u_l\|^2_{L^2(\Omega)} \leq A_l \leq (1 + Bh)^{l-1} A_1.$$

Taking $t = hl$, we immediately arrive at an estimate implying (4.1.16):

$$h \sum_{n=1}^{l} \| \frac{u_n - u_{n-1}}{h} \|^2_{L^2(\Omega)} + \frac{1}{4}\|\nabla u_l\|^2_{L^2(\Omega)} \leq A_1 e^{Bt}.$$

□

From this proof one can see, that there are several possibilities how to weaken the assumptions on the outer force f. For instance, if the outer force does not explicitly depend on time, which is often the case (gravitation etc.), it can have much faster growth in the negative direction than that assigned by (4.1.4).

By the energy estimate, we have a converging subsequence of $\{u^h\}_{h>0}$. We slightly abuse the notation, as explained in Chapter 3.

Lemma 4.1.2. *There exists a shared subsequence of* $\{u^h\}_{h>0}$ *and* $\{\bar{u}^h\}_{h>0}$ *and a function* $u \in H^1(Q_T)$ *such that*

$$u_t^h \to u_t \quad \text{weakly in } L^2(Q_T), \tag{4.1.19}$$
$$\nabla \bar{u}^h \to \nabla u \quad \text{weakly in } (L^2(Q_T))^m, \tag{4.1.20}$$
$$\nabla u^h \to \nabla u \quad \text{weakly in } (L^2(Q_T))^m, \tag{4.1.21}$$
$$u^h \to u \quad \text{strongly in } L^2(Q_T), \tag{4.1.22}$$
$$\bar{u}^h \to u \quad \text{strongly in } L^2(Q_T). \tag{4.1.23}$$

Proof. As in Chapter 3, (4.1.19) and (4.1.20) follow from the energy estimate (4.1.16) and (4.1.21) follows from (3.1.16).

Since $H^1(Q_T) \subset L^2(Q_T)$ compactly, there exists a subsequence such that $u^h \to u$ strongly in $L^2(Q_T)$. Last relation (4.1.23) is a consequence of (3.1.14). □

We immediately obtain

Lemma 4.1.3. *The limit function u from the previous Lemma satisfies homogeneous boundary condition, the initial condition and the volume constraint (4.1.2).*

Proof. Obviously, $u \in L^2(0,T;H_0^1(\Omega))$. Since $u \in H^1(0,T;L^2(\Omega))$, we deduce by [8], Section 5.9, that $u \in C([0,T];L^2(\Omega))$ after suitable redefining on a set of measure zero.

Let us consider the function $u^h - u_0$. It vanishes on the parabolic boundary of the cylinder $([0,T]\times\partial\Omega)\cup(\{0\}\times\Omega)$ and converges weakly in $H^1(Q_T)$ to $u-u_0$. Hence, by Mazur's theorem, the trace of $u-u_0$ on the parabolic boundary is zero.

We also get

$$\int_\Omega u(t)\,dx = 1 \qquad \text{for a.e. } t\in[0,T]. \tag{4.1.24}$$

Indeed, u^h converges strongly to u in $L^2(Q_T)$ and $\int_\Omega u^h(t)\,dx = 1$ for every $h>0$ and $t\in(0,T)$. Therefore,

$$\int_0^T \Big(1-\int_\Omega u\,dx\Big)^2 dt = \int_0^T \Big(\int_\Omega (u^h-u)\,dx\Big)^2 dt \le |\Omega|\,\|u^h-u\|^2_{L^2(Q_T)} \to 0 \quad \text{as } h\to 0+\,.$$

□

Now we would like to pass to the limit in (4.1.15). Due to Lemma 4.1.2, the limit process in the left-hand side is standard. However, it is not immediately clear whether it is possible to pass to the limit in the nonlocal nonlinear term $\bar\lambda^h$. As such, we prove the following theorem.

Theorem 4.1.1. *There exists a limit function $u\in H^1(Q_T)$ corresponding to the subsequence u^h from Lemma 4.2, satisfying the boundary and initial conditions of (4.1.1) and the volume constraint (4.1.2) such that*

$$\int_0^T\int_\Omega (u_t\phi+\nabla u\nabla\phi - f(u)\phi)\,dx\,dt = \int_0^T\int_\Omega \lambda\phi\,dx\,dt, \tag{4.1.25}$$

for each $\phi\in L^2(0,T;H_0^1(\Omega))$ and with λ from (4.1.3).

Proof. We have (see (4.1.12))

$$\bar\lambda^h = \int_\Omega (u_t^h\bar u^h + |\nabla\bar u^h|^2 - \bar f^h(\bar u^h)\bar u^h)\,dx,$$

and since

$$\|\bar u^h(t)\|^2_{L^2(\Omega)} \le C_S^2\|\nabla\bar u^h(t)\|^2_{L^2(\Omega)} \le C_S^2 C_E \qquad \forall t\in[0,T],$$

we obtain by Lemma 4.1.1

$$
\begin{aligned}
\int_0^T (\bar\lambda^h)^2\,dt &\le 3\int_0^T \Big(\int_\Omega u_t^h \bar u^h\,dx\Big)^2 dt + 3\int_0^T \Big(\int_\Omega |\nabla \bar u^h|^2\,dx\Big)^2 dt \qquad (4.1.26)\\
&\quad +3\int_0^T \Big(\int_\Omega \bar f^h(\bar u^h)\bar u^h\,dx\Big)^2 dt\\
&\le 3\int_0^T \Big(\int_\Omega (u_t^h)^2\,dx\Big)\Big(\int_\Omega (\bar u^h)^2\,dx\Big) dt + 3\int_0^T \Big(\int_\Omega |\nabla \bar u^h|^2\,dx\Big)^2 dt\\
&\quad +3\int_0^T \Big(\int_\Omega (\bar f^h(\bar u^h))^2\,dx\Big)\Big(\int_\Omega (\bar u^h)^2\,dx\Big) dt\\
&\le 3C_S^2 C_E \int_0^T \int_\Omega (u_t^h)^2\,dx\,dt + 3\int_0^T C_E^2\,dt\\
&\quad +24 C_f^2 C_S^2 C_E \int_0^T \int_\Omega (\bar u^h)^2\,dx\,dt + 2C_S^2 C_E \|\gamma\|^2_{L^2(Q_T)}\\
&\le C(T, C_S, C_E, C_f, \|\gamma\|_{L^2(Q_T)}) < \infty.
\end{aligned}
$$

Therefore, there exists a function $\kappa(t) \in L^2(0,T)$ such that a subsequence of the right-hand side of (4.1.15) converges in the following sense:

$$
\int_0^T \int_\Omega \bar\lambda^h \phi\,dx\,dt = \int_0^T \bar\lambda^h (\int_\Omega \phi\,dx)\,dt \to \int_0^T \kappa(t)(\int_\Omega \phi\,dx)\,dt,
$$

which yields the equality

$$
\int_0^T \int_\Omega (u_t\phi + \nabla u \nabla \phi - f(u)\phi)\,dx\,dt = \int_0^T \kappa(t) \int_\Omega \phi\,dx\,dt, \qquad (4.1.27)
$$

for each $\phi \in L^2(0,T; H_0^1(\Omega))$.

To be precise, we mention also the limit process in the left-hand side of (4.1.15), yielding (4.1.27). In the last term corresponding to the outer force, it is necessary to take, by the density argument, test functions $\bar\phi^h$ which are piecewise constant on corresponding partitions of $(0,T)$ and which converge strongly to ϕ in $L^2(0,T; H_0^1(\Omega))$. In such a case, we have

$$
\int_\Omega \int_0^T \bar f^h(\bar u^h)\bar\phi^h\,dt\,dx = \int_\Omega \int_0^T f(\bar u^h)\bar\phi^h\,dt\,dx
$$

and we can pass to the limit because f is continuous in u, satisfies the bound (4.1.4) necessary for the application of dominated convergence theorem (together with the boundedness of $\bar u^h$ shown in Proposition 4.1.1), and $\bar u^h \to u$ almost everywhere. The limit of first two terms is clear because of the weak convergence given in Lemma 4.1.2 and the strong convergence of $\bar\phi^h$ in $L^2(0,T; H_0^1(\Omega))$.

It remains to show that $\kappa = \lambda$ a.e., in order to achieve (4.1.13). By appealing to (4.1.27), we choose $\phi(\tilde t, x) = u(\tilde t, x)$ for $\tilde t \in [0,t]$, and $\phi(\tilde t, x) = 0$ for $\tilde t \in (t,T]$. Thus, for every $t \in [0,T]$ we have

$$
\int_0^t \int_\Omega (u_t u + |\nabla u|^2 - f(u)u)\,dx\,d\tau = \int_0^t \kappa(\tau)\Big(\int_\Omega u\,dx\Big)\,d\tau = \int_0^t \kappa(\tau)\,d\tau,
$$

which concludes the proof. □

Remark 4.1.1. (On the uniqueness of weak solution)
Let $u, v \in H^1(Q_T)$ be two weak solutions and let us subtract identity (4.1.25) written for v from the same identity written for u and put $\phi = u - v \in L^2(0, T; H_0^1(\Omega))$. We get

$$\int_0^T \int_\Omega \big((u-v)_t(u-v) + |\nabla(u-v)|^2 - [f(u) - f(v)](u-v)\big)\, dx\, dt$$
$$= \int_0^T \int_\Omega [\lambda(u) - \lambda(v)](u-v)\, dx\, dt.$$

Since both u and v preserve the volume, the right-hand side vanishes and we have

$$\frac{1}{2}\|(u-v)(T)\|^2_{L^2(\Omega)} + \|\nabla(u-v)\|^2_{L^2(Q_T)} = \int_0^T \int_\Omega [f(u) - f(v)](u-v)\, dx\, dt.$$

This identity gives uniqueness for a relatively wide choice of the right-hand side function f. For example, we have uniqueness for $f = 0$, f nonincreasing in u, and for any Lipschitz continuous function (in u) with sufficiently small Lipschitz constant (smaller than or equal to $1/C_P^2$, where C_P is the constant from Poincaré's inequality (3.1.13), see also (4.1.6)).

4.1.4 Hölder continuity of weak solution

In this Section, we prove a theorem on the interior regularity of the limit weak solution from Theorem 4.1.1. Under stronger assumptions on f, it is possible to prove an a priori estimate corresponding to (4.1.16) for any weak solution introduced in Definition 4.1.1. In this way, one can show the boundedness and obtain the same regularity result for all such weak solutions. Nevertheless, as indicated in Chapter 3, we are not able to prove the existence of a weak solution without constructing approximate weak solutions by the discrete Morse flow method.

Since we do not study regularity near the boundary, the homogeneous and nonhomogeneous boundary conditions can be treated in the same way. For simplicity, we shall only consider the homogeneous case. On the other hand, by the same arguments as below, section 2.8 of [22] would assure Hölder continuity up to the boundary of Q_T, if we assumed that the initial condition u_0 is Hölder continuous.

Theorem 4.1.2. *For all $\tilde{Q}_T \subset\subset Q_T$ (compact subset), there exists a constant $\alpha > 0$, such that the weak solution u belongs to $C^\alpha(\tilde{Q}_T)$.*

We first introduce a "de Giorgi" class of functions corresponding to weak solutions of the parabolic problem.

Definition 4.1.2. *A function u with finite norm*

$$|u|_{Q_T} = \max_{0 \le t \le T} \|u(t)\|_{L^2(\Omega)} + \|\nabla u\|_{L^2(Q_T)}$$

belongs to the class $\mathcal{B}_2(Q_T, M, \beta, r, d, \kappa)$ if

(1) $M = \operatorname{ess\,sup}_{Q_T} |u| < \infty$,
(2) there exist $\beta, q, r, d, \kappa > 0$ *so that for* $w = \pm u$

$$\max_{t_0 \le t \le t_0+\tau} \int_{B_{\rho-\sigma_1\rho}} (w^{(k)}(t))^2\,dx \le \int_{B_\rho} (w^{(k)}(t_0))^2\,dx \tag{4.1.28}$$
$$+\beta\left[(\sigma_1\rho)^{-2}\int_{t_0}^{t_0+\tau}\int_{B_\rho}(w^{(k)})^2\,dx\,dt + \left(\int_{t_0}^{t_0+\tau}|A_{k,\rho}(t)|^{\frac{r}{q}}\,dt\right)^{\frac{2}{r}(1+\kappa)}\right]$$

and

$$\max_{t_0 \le t \le t_0+\tau-\sigma_2\tau} \int_{B_{\rho-\sigma_1\rho}} (w^{(k)})^2\,dx + \int_{t_0}^{t_0+\tau-\sigma_2\tau}\int_{B_{\rho-\sigma_1\rho}} |\nabla w^{(k)}|^2\,dx\,dt \tag{4.1.29}$$
$$\le \beta\left[[(\sigma_1\rho)^{-2} + (\sigma_2\tau)^{-1}]\int_{t_0}^{t_0+\tau}\int_{B_\rho}(w^{(k)})^2\,dx\,dt + \left(\int_{t_0}^{t_0+\tau}|A_{k,\rho}(t)|^{\frac{r}{q}}\,dt\right)^{\frac{2}{r}(1+\kappa)}\right],$$

for all $\sigma_1, \sigma_2 \in (0,1)$, $Q(\rho,\tau) \subset Q_T$ *and* k *with* $k \ge \operatorname{ess\,sup}_{Q(\rho,\tau)} w - d$. *Here* $w^{(k)} = \max\{w-k, 0\}$, $Q(\rho,\tau) = B_\rho \times (t_0, t_0+\tau) = \{|x-x_0| < \rho, t_0 < t < t_0+\tau\}$ *and* $A_{k,\rho}(t) = \{x \in B_\rho; w(x,t) > k\}$. *Constants* q *and* r *should satisfy*

$$\frac{1}{r} + \frac{m}{2q} = \frac{m}{4}. \tag{4.1.30}$$

Before proving the regularity theorem, we must first establish the boundedness of the weak solution which is required in the above definition. In the course of the proof, we shall use an auxiliary result stated in the subsequent Lemma.

Lemma 4.1.4. *For functions* $\bar{u}^h$ *and* u^h *defined in (4.1.14) and any* $k \in \mathbb{R}$, *we have*

$$\int_0^T \int_\Omega u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt \ge 0.$$

Proof. First we write

$$\int_0^T \int_\Omega u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt = \sum_{n=1}^N \int_{(n-1)h}^{nh}\int_\Omega u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt$$

and for each n we divide Ω into four parts:

$$\begin{aligned} \Omega_1^n &= \{x : u_{n-1}(x) > k \;\&\; u_n(x) > k\}, & \Omega_2^n &= \{x : u_{n-1}(x) > k \;\&\; u_n(x) \le k\}, \\ \Omega_3^n &= \{x : u_{n-1}(x) \le k \;\&\; u_n(x) > k\}, & \Omega_4^n &= \{x : u_{n-1}(x) \le k \;\&\; u_n(x) \le k\}. \end{aligned}$$

We consider the integrals over each domain in turn. For Ω_1^n we have $\bar{u}^{h(k)} - u^{h(k)} = \bar{u}^h - u^h$ and therefore

$$\begin{aligned} &\int_{(n-1)h}^{nh}\int_{\Omega_1^n} u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt \\ &= \int_{(n-1)h}^{nh}\int_{\Omega_1^n} \frac{u_n - u_{n-1}}{h}\left(u_n - \frac{t-(n-1)h}{h}u_n - \frac{nh-t}{h}u_{n-1}\right)dx\,dt \\ &= \int_{\Omega_1^n}\int_{(n-1)h}^{nh} \frac{(u_n - u_{n-1})^2}{h}\frac{nh-t}{h}\,dt\,dx = \frac{1}{2}\int_{\Omega_1^n}(u_n - u_{n-1})^2\,dx \ge 0. \end{aligned}$$

In Ω_2^n, $u_n - u_{n-1} < 0$ and $\bar{u}^{h(k)} = 0$, thus,

$$\int_{(n-1)h}^{nh}\int_{\Omega_2^n} u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt = \int_{(n-1)h}^{nh}\int_{\Omega_2^n} -u_t^h u^{h(k)}\,dx\,dt$$
$$= -\int_{(n-1)h}^{nh}\int_{\Omega_2^n} \frac{u_n - u_{n-1}}{h}\max\{u^h - k, 0\}\,dx\,dt \geq 0.$$

For Ω_3^n, $u_n - u_{n-1} > 0$ and for each $x \in \Omega_3^n$ there exists $\tau(x) \in ((n-1)h, nh)$ such that $u^{h(k)} = 0$ in $((n-1)h, \tau(x))$ and $u^{h(k)} = u^h - k$ in $(\tau(x), nh)$. Hence,

$$\int_{(n-1)h}^{nh}\int_{\Omega_3^n} u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt$$
$$= \int_{\Omega_3^n}\int_{(n-1)h}^{\tau(x)} \frac{u_n - u_{n-1}}{h}\bar{u}^{h(k)}\,dt\,dx + \int_{\Omega_3^n}\int_{\tau(x)}^{nh} \frac{(u_n - u_{n-1})^2}{h}\frac{nh - t}{h}\,dt\,dx$$
$$= \int_{\Omega_3^n}\int_{(n-1)h}^{\tau(x)} \frac{u_n - u_{n-1}}{h}\bar{u}^{h(k)}\,dt\,dx + \frac{1}{2}\int_{\Omega_3^n}(u_n - u_{n-1})^2\left(\frac{nh - \tau(x)}{h}\right)^2 dx \geq 0.$$

Finally, the integral over Ω_4^n vanishes and this concludes the proof of the Lemma. □

Now we can present and prove a result on the boundedness of weak solutions. In fact, we prove the uniform boundedness of $\bar{u}^h$ with respect to h, which implies the boundedness of the limit, weak solution u.

Proposition 4.1.1. *If a function f fulfills condition (4.1.4), then any weak solution is bounded in $L^\infty(Q_T)$.*

Proof. By the definition of an approximate weak solution (see (4.1.15), we know

$$\int_0^T\int_\Omega \left(u_t^h\phi + \nabla\bar{u}^h\nabla\phi - \bar{f}^h(\bar{u}^h)\phi\right)\,dx\,dt = \int_0^T\int_\Omega \bar{\lambda}^h\phi\,dx\,dt.$$

Thus, upon choosing the test function $\phi = \bar{u}^{h(k)} = \max\{\bar{u}^h - k, 0\}$ the above becomes

$$\int_0^T\int_\Omega \left(u_t^h\bar{u}^{h(k)} + \nabla\bar{u}^h\nabla\bar{u}^{h(k)} - \bar{f}^h(\bar{u}^h)\bar{u}^{h(k)}\right)\,dx\,dt = \int_0^T\int_\Omega \bar{\lambda}^h\bar{u}^{h(k)}\,dx\,dt. \tag{4.1.31}$$

Noting the result of the following computation:

$$\int_0^T\int_\Omega u_t^h u^{h(k)}\,dx\,dt = \int_0^T\int_\Omega \frac{1}{2}\frac{d}{dt}(u^{h(k)})^2\,dx\,dt$$
$$= \int_\Omega \frac{1}{2}\left((u^{h(k)})^2(T) - (u^{h(k)})^2(0)\right)\,dx = \int_\Omega \frac{1}{2}(u^{h(k)})^2(T)\,dx = \int_\Omega \frac{1}{2}(\bar{u}^{h(k)})^2(T)\,dx,$$

if we assume $u(0,x) < k$ a.e., and the statement of Lemma 4.1.4:

$$\int_0^T\int_\Omega u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt \geq 0,$$

we can rearrange the first term on the left-hand side of (4.1.31) to write

$$\int_0^T \int_\Omega u_t^h \bar{u}^{h(k)}\,dx\,dt = \int_0^T \int_\Omega u_t^h u^{h(k)}\,dx\,dt + \int_0^T \int_\Omega u_t^h(\bar{u}^{h(k)} - u^{h(k)})\,dx\,dt$$
$$\geq \frac{1}{2}\int_\Omega (\bar{u}^{h(k)})^2(T)\,dx.$$

For the gradient term in (4.1.31) we have

$$\int_0^T \int_\Omega \nabla\bar{u}^h \nabla\bar{u}^{h(k)}\,dx\,dt = \int_0^T \int_\Omega |\nabla\bar{u}^{h(k)}|^2\,dx\,dt.$$

Denoting the norm

$$|u|_{Q_T} = \left(\frac{1}{2}\int_\Omega u^2(T)\,dx + \int_0^T \int_\Omega |\nabla u|^2\,dx\,dt\right)^{1/2},$$

we arrive at the inequality

$$|\bar{u}^{h(k)}|^2_{Q_T} \leq \int_0^T \int_\Omega \left(\bar{\lambda}^h \bar{u}^{h(k)} + \bar{f}^h(\bar{u}^h)\bar{u}^{h(k)}\right)\,dx\,dt. \tag{4.1.32}$$

We now proceed to investigate the first term on the right-hand side of (4.1.32) for $m > 2$. Namely, we apply Young's inequality (see [8], Appendix B) with exponents $2^* = \frac{2m}{m-2} \in (2, 6]$ and $2^{*\prime} = \frac{2m}{m+2} \in [\frac{6}{5}, 2)$ to obtain

$$\int_0^T \int_\Omega \bar{\lambda}^h \bar{u}^{h(k)}\,dx\,dt \leq C_\varepsilon \int_0^T (\bar{\lambda}^h)^{2^{*\prime}} |A_k|\,dt + \varepsilon \int_0^T \int_{A_k} (\bar{u}^{h(k)})^{2^*}\,dx\,dt, \tag{4.1.33}$$

where $A_k(t) = \{x : \bar{u}^h(x,t) > k\}$, $|A_k|$ denotes the measure of A_k, and C_ε is a constant independent of h. The second term is estimated by the Sobolev imbedding theorem with $H^1(\Omega) \subset L^{2^*}(\Omega)$ (see [8], Section 5.6) and can be absorbed into the left-hand side if ε is chosen small enough. In this estimate, we make use of energy estimate (4.1.16) and the fact that $2^*/2 \in (1, 3]$ to derive

$$\int_0^T \int_{A_k} (\bar{u}^{h(k)})^{2^*}\,dx\,dt \leq C'_S \int_0^T \left(\int_{A_k} |\nabla\bar{u}^{h(k)}|^2\,dx\right)^{2^*/2} dt \tag{4.1.34}$$
$$\leq C_E^{\frac{2^*}{2}-1} C'_S \int_0^T \int_{A_k} |\nabla\bar{u}^{h(k)}|^2\,dx\,dt,$$

where C'_S is a constant (independent of h) obtained from the Sobolev imbedding.

We apply Hölder's inequality on the first term in (4.1.33) with exponents $2/2^{*\prime} = \frac{m+2}{m} \in (1, \frac{5}{3}]$ and $(2/2^{*\prime})' = \frac{m+2}{2} \geq \frac{5}{2}$. This, together with estimate (4.1.26) of $\bar{\lambda}^h$, yields

$$\int_0^T (\bar{\lambda}^h)^{2^{*\prime}} |A_k|\,dt \leq \left(\int_0^T (\bar{\lambda}^h)^2\,dt\right)^{\frac{2^{*\prime}}{2}} \left(\int_0^T |A_k|^{(2/2^{*\prime})'}\,dt\right)^{\frac{1}{(2/2^{*\prime})'}}$$
$$= \left(\int_0^T (\bar{\lambda}^h)^2\,dt\right)^{\frac{m}{m+2}} \left(\int_0^T |A_k|^{\frac{m+2}{2}}\,dt\right)^{\frac{2}{m+2}} \leq C\left(\int_0^T |A_k|^{\frac{m+2}{2}}\,dt\right)^{\frac{2}{m+2}}.$$

Next, we estimate the second term in (4.1.32). According to assumption (4.1.4), we can write

$$\begin{aligned}
&\int_0^T \int_{A_k} \bar{f}^h(\bar{u}^h)\bar{u}^{h(k)}\,dx\,dt \le 2C_f \int_0^T \int_{A_k} |\bar{u}^h|\bar{u}^{h(k)}\,dx\,dt + \int_0^T \int_{A_k} \gamma\bar{u}^{h(k)}\,dx\,dt \\
&\le 2C_f \int_0^T \int_{A_k} (|\bar{u}^h - k|\bar{u}^{h(k)} + k\bar{u}^{h(k)})\,dx\,dt + \int_0^T \int_{A_k} \gamma\bar{u}^{h(k)}\,dx\,dt \\
&\le C \int_0^T \int_{A_k} ((\bar{u}^{h(k)})^2 + k^2 + \gamma^2)\,dx\,dt.
\end{aligned}$$

This last expression can be estimated from above by Young's inequality to give

$$\begin{aligned}
&\int_0^T \int_{A_k} ((\bar{u}^{h(k)})^2 + k^2 + \gamma^2)\,dx\,dt \\
&\qquad \le \varepsilon \int_0^T \int_{A_k} (\bar{u}^{h(k)})^{2^*}\,dx\,dt + C_\varepsilon \int_0^T |A_k|\,dt + (k^2 + \|\gamma\|^2_{L^\infty(Q_T)}) \int_0^T |A_k|\,dt \\
&\qquad \le \varepsilon \int_0^T \int_{A_k} (\bar{u}^{h(k)})^{2^*}\,dx\,dt + C(T)k^2 \left(\int_0^T |A_k|^{\frac{m+2}{2}}\,dt\right)^{\frac{2}{m+2}},
\end{aligned}$$

for sufficiently large k. Here we again see that the first term can be absorbed into the left-hand side, as in (4.1.34).

Therefore, having started this investigation from (4.1.32), we have acquired the inequality

$$|\bar{u}^{h(k)}|_{Q_T} \le Ck \left(\int_0^T |A_k|^{\frac{m+2}{2}}\,dt\right)^{\frac{1}{m+2}},$$

where C is a constant independent of h. At this point we introduce Theorem 6.1 in Chapter II of [22] and apply it to the above inequality. This will provide us with a bound for the weak solution.

Theorem. *Suppose that* $\max_\Omega u_0 \le \hat{k}$, $\hat{k} \ge 0$, *and that the inequalities*

$$|u^k|_{Q_T} \le \nu k \left(\int_0^T |A_k(t)|^{\frac{r}{q}}\,dt\right)^{\frac{1+\kappa}{r}} \tag{4.1.35}$$

hold for $k \ge \hat{k}$ *with certain positive constants* ν *and* κ. *Here* q *and* r *are arbitrary numbers satisfying conditions*

$$\frac{1}{r} + \frac{m}{2q} = \frac{m}{4}, \tag{4.1.36}$$

$$r \in [2,\infty], \quad q \in \left[2, \frac{2m}{m-2}\right]. \tag{4.1.37}$$

Then

$$\max_{Q_T} u(x,t) \le 2\hat{k}\left[1 + 2^{\frac{2}{\kappa}+\frac{1}{\kappa^2}}(C_Y\nu)^{1+\frac{1}{\kappa}} T^{\frac{1+\kappa}{r}} |\Omega|^{\frac{1+\kappa}{q}}\right], \tag{4.1.38}$$

where C_Y is a constant from Young's inequality.

Having stated this theorem, we are now ready to complete the proof of Proposition 4.1.1. Indeed, by taking

$$r = (1+\kappa)(m+2), \qquad q = 2(1+\kappa), \qquad \kappa = \frac{4}{m(m+2)},$$

we see that

$$\frac{1+\kappa}{r} = \frac{1}{m+2}, \quad \frac{r}{q} = \frac{m+2}{2}, \quad r > 2, \quad 2 < q < \frac{2m}{m-2},$$

and so (4.1.35), (4.1.36) and (4.1.37) hold. Thus, the Theorem applies to yield our bound:

$$\max_{(t,x)\in Q_T} \bar{u}^h(t,x) \leq C.$$

Since the constant which bounds $\bar{u}^h$ is independent of h, we also deduce that the limit function – the weak solution u – is bounded by the same constant.

For $m = 1$ the boundedness follows directly from the energy estimate (4.1.16) and the imbedding $H^1(\Omega) \subset C(\Omega)$:

$$\max_{\bar{Q}_T} |\bar{u}^h| = \max_{t\in[0,T]} \max_{x\in\bar{\Omega}} |\bar{u}^h(t,x)| \leq \max_{t\in[0,T]} C\|\bar{u}^h(t)\|_{H^1(\Omega)} \leq C.$$

For the case $m = 2$ we can carry out a calculation similar to the above, making use of the imbedding theorem for $H_0^1(\Omega) \subset L^p(\Omega)$, and $p \in [1,\infty)$. For instance, we can use exponents 3 and 3/2 instead of 2^* and $(2^*)'$ in (4.1.33) and estimate the second term on the right-hand side by the mentioned imbedding. The first term then gives

$$|\bar{u}^{h(k)}|_{Q_T} \leq Ck\Big(\int_0^T |A_k|^4\,dt\Big)^{1/8},$$

which is enough to deduce boundedness along the lines of the above Theorem (with $r = 10$ and $q = 5/2$).

We repeat the same process for the function $\bar{w}^h := -\bar{u}^h$. This function satisfies

$$\int_0^T\int_\Omega \big(w_t^h\phi + \nabla\bar{w}^h\nabla\phi + \bar{f}^h(-\bar{w}^h)\phi\big)\,dx\,dt = -\int_0^T\int_\Omega \bar{\lambda}^h\phi\,dx\,dt,$$

whence by setting $\phi = \bar{w}^h$ and proceeding as above, we obtain

$$|\bar{w}^{h(k)}|_{Q_T}^2 \leq -\int_0^T\int_\Omega \big(\bar{\lambda}^h\bar{w}^{h(k)} + \bar{f}^h(-\bar{w}^h)\bar{w}^{h(k)}\big)\,dx\,dt.$$

The estimate for the right-hand side does not differ from the one for (4.1.32), since we worked all the time in absolute values. □

Proof of Theorem 4.1.2. Let us show the Hölder continuity of u. It is sufficient to check that u belongs to $\mathcal{B}_2(Q_T, M, \beta, r, d, \kappa)$ (see [22]). One can see that this follows if the condition below is satisfied for any piecewise smooth continuous function ζ with $0 \le \zeta \le 1$ which vanishes on the lateral surface of the cylinder $Q(\rho,\tau)$,

$$\begin{aligned}
&\int_{B_\rho} (w^{(k)}(x,t_0+\tau))^2\zeta^2(x,t_0+\tau)\,dx + C\int_{t_0}^{t_0+\tau}\int_{B_\rho} |\nabla w^{(k)}|^2\zeta^2\,dx\,dt \\
&\le \int_{B_\rho} (w^{(k)}(x,t_0))^2\zeta^2(x,t_0)\,dx \\
&+\beta_1\left[\int_{Q(\rho,\tau)} (|\nabla\zeta|^2+\zeta|\zeta_t|)(w^{(k)})^2\,dx\,dt + \left(\int_{t_0}^{t_0+\tau}(\int_{A_{k,\rho}(t)}\zeta\,dx)^{\frac{r}{q}}\,dt\right)^{\frac{2}{r}(1+\kappa)}\right].
\end{aligned} \tag{4.1.39}$$

By (4.1.25), for every $\phi \in L^2(0,T;H_0^1(\Omega))$ we have

$$\int_{Q_T} (u_t\phi + \nabla u\nabla\phi - \lambda\phi - f(u)\phi)\,dx\,dt = 0.$$

We choose $\phi = \zeta^2 u^{(k)}$ with ζ supported in $Q(\rho,\tau)$ as in (4.1.39), and obtain

$$\begin{aligned}
&\int_{Q(\rho,\tau)} u_t u^{(k)}\zeta^2\,dx\,dt + \int_{Q(\rho,\tau)} \nabla u^{(k)}\nabla(\zeta^2 u^{(k)})\,dx\,dt \\
&\qquad - \int_{Q(\rho,\tau)} \lambda\zeta^2 u^{(k)}\,dx\,dt - \int_{Q(\rho,\tau)} f(u)u^{(k)}\zeta^2\,dx\,dt = 0.
\end{aligned} \tag{4.1.40}$$

The first term in (4.1.40) becomes

$$\begin{aligned}
&\int_{Q(\rho,\tau)} u_t u^{(k)}\zeta^2\,dx\,dt = \frac{1}{2}\int_{Q(\rho,\tau)} \frac{\partial}{\partial t}\left((u^{(k)})^2\right)\zeta^2\,dx\,dt \\
&= -\frac{1}{2}\int_{Q(\rho,\tau)} (u^{(k)})^2(\zeta^2)_t\,dx\,dt + \frac{1}{2}\int_{B_\rho}\left\{\left[(u^{(k)})^2\zeta^2\right](x,t_0+\tau) - \left[(u^{(k)})^2\zeta^2\right](x,t_0)\right\}\,dx \\
&= -\int_{Q(\rho,\tau)} (u^{(k)})^2\zeta\zeta_t\,dx\,dt + \frac{1}{2}\int_{B_\rho}[(u^{(k)})^2\zeta^2](x,t_0+\tau)\,dx - \frac{1}{2}\int_{B_\rho}[(u^{(k)})^2\zeta^2](x,t_0)\,dx.
\end{aligned}$$

The second term in (4.1.40) gives

$$\int_{Q(\rho,\tau)} \nabla u^{(k)}\nabla(\zeta^2 u^{(k)})\,dx\,dt = \int_{Q(\rho,\tau)} |\nabla u^{(k)}|^2\zeta^2\,dx\,dt + 2\int_{Q(\rho,\tau)} \nabla u^{(k)}\nabla\zeta u^{(k)}\zeta\,dx\,dt,$$

where

$$-2\int_{Q(\rho,\tau)} \nabla u^{(k)}\nabla\zeta u^{(k)}\zeta\,dx\,dt \le \frac{1}{2}\int_{Q(\rho,\tau)} |\nabla u^{(k)}|^2\zeta^2\,dx\,dt + 2\int_{Q(\rho,\tau)} (u^{(k)})^2|\nabla\zeta|^2\,dx\,dt. \tag{4.1.41}$$

Since u and γ are bounded, assumption (4.1.4) implies

$$\begin{aligned}
\left|\int_{Q(\rho,\tau)} f(u)u^{(k)}\zeta^2\,dx\,dt\right| &\le \int_{t_0}^{t_0+\tau}\int_{A_{k,\rho}} (2C_f|u|+\gamma)u^{(k)}\zeta^2\,dx\,dt \\
&\le \left(2C_f M + \|\gamma\|_{L^\infty(Q_T)}\right)\int_{t_0}^{t_0+\tau}\int_{A_{k,\rho}} \zeta\,dx\,dt \\
&\le C\Big(\int_{t_0}^{t_0+\tau}\big(\int_{A_{k,\rho}}\zeta\,dx\big)^2\,dt\Big)^{1/2}.
\end{aligned}$$

Estimates (4.1.40) and (4.1.41) yield (4.1.39) if we can handle the term with the Lagrange multiplier. This is achieved by using the weak convergence of $\bar{\lambda}^h$ to λ in $L^2(0,T)$:

$$\begin{aligned}
\int_{Q(\rho,\tau)} \lambda\zeta^2 u^{(k)}\,dx\,dt &= \int_{t_0}^{t_0+\tau} \big(\lambda \int_{B_\rho} \zeta^2 u^{(k)}\,dx\big)\,dt \le M \int_{t_0}^{t_0+\tau} \big(|\lambda| \int_{A_{k,\rho}} \zeta\,dx\big)\,dt \\
&\le M\Big(\int_{t_0}^{t_0+\tau} \lambda^2\,dt\Big)^{1/2}\Big(\int_{t_0}^{t_0+\tau} \big(\int_{A_{k,\rho}} \zeta\,dx\big)^2\,dt\Big)^{1/2} \\
&\le C\Big(\int_{t_0}^{t_0+\tau} \big(\int_{A_{k,\rho}} \zeta\,dx\big)^2\,dt\Big)^{1/2}. \qquad (4.1.42)
\end{aligned}$$

Again it is necessary to determine constants q, r and κ. We set

$$\kappa = 1/m, \quad q = 2(1+\kappa), \quad r = 4(1+\kappa).$$

Then $r/q = 2$ and $2(1+\kappa)/r = 1/2$. Moreover, q and r satisfy (4.1.30):

$$\frac{1}{r} + \frac{m}{2q} = \frac{1}{4(1+\kappa)} + \frac{m}{4(1+\kappa)} = \frac{m}{4}.$$

The estimate for $-u$ is derived analogously, as we did not make use of any sign properties in the above proof. □

If we assume that boundary and initial data are Hölder continuous, the regularity of weak solutions can be extended up to the boundary applying the theory from [22], Section 2.8, because estimates similar to those derived above hold also for cylinders intersecting the boundary of Q_T.

4.1.5 Remarks on boundary conditions

Here we touch problems with boundary conditions that were not analyzed in the main text, i.e., conditions other then homogeneous Dirichlet condition.

First we consider nonhomogeneous Dirichlet boundary conditions, independent of t:

$$u|_{\partial\Omega} = g.$$

Assume g is chosen in such a way that $g \in H^1(\Omega)$, $\int_\Omega g dx = 0$, and that $u_0 = g$ on the boundary of Ω.

Using volume-preserving perturbations ($\zeta \in C_0^\infty(\Omega)$, $Z = \int_\Omega \zeta\,dx$)

$$u^\varepsilon = \frac{u + \varepsilon\left(\zeta + \frac{Z}{V}g\right)}{1 + \varepsilon\frac{Z}{V}},$$

the Lagrange multiplier can formally be computed to be

$$\lambda_n = \frac{1}{V}\int_\Omega \left[\frac{u_n - u_{n-1}}{h}u_n + |\nabla u_n|^2 - f_n(u_n)u_n\right]\,dx + \frac{1}{V}\int_{\partial\Omega} \frac{\partial u_n}{\partial \boldsymbol{n}} g\,dS,$$

where $\boldsymbol{n}$ is the interior normal. However, this form is not convenient for passing to the limit since we have no information about the behaviour of the gradient on the boundary. Therefore, we introduce a new function v by $u = v + g$ (analogously $u_n = v_n + g$). It is easy to see that this function satisfies $v|_{\partial\Omega} = 0$, and $\int_\Omega v\,dx = V$. Consequently, we can transform the problem into that of finding a minimizer $v_n \in \mathcal{K}_V$ of the functional

$$J_n^g(v) = \int_\Omega \frac{|v - v_{n-1}|^2}{2h}\,dx + \frac{1}{2}\int_\Omega |\nabla v + \nabla g|^2\,dx - \int_\Omega F_n(v+g)\,dx,$$

where

$$\mathcal{K}_V = \{v \in H^1(\Omega); v|_{\partial\Omega} = 0, \int_\Omega v\,dx = V\}.$$

The corresponding Lagrange multiplier can be calculated the same way as in the case of homogeneous boundary conditions:

$$\lambda_n = \frac{1}{V}\int_\Omega \left[\frac{v_n - v_{n-1}}{h} v + \nabla(v_n + g)\nabla v_n - f(v_n + g)v_n\right] dx. \tag{4.1.43}$$

Again, we get the same estimates for the functions $v_n + g$ as above in (4.1.16) and consequently also for v_n. Thus passing to the limit as $h \to 0$ introduces no further problems. We also note that multiplying (4.1.1) by $u - g$ and integrating over Ω produces a convenient form of λ, corresponding to that of (4.1.43).

Second remark concerns Neumann boundary conditions. Let $\boldsymbol{n}$ be the interior normal vector and consider the boundary condition

$$\frac{\partial u}{\partial \boldsymbol{n}} = p \qquad \text{on } \partial\Omega.$$

We assume that $p \in L^2(\partial\Omega)$ and that the initial value satisfies the given Neumann condition.

If outer force is not present or if it preserves volume in the sense $\int_\Omega f\,dx = 0$ for all $t \in [0, T]$, and if the Neumann boundary condition is homogeneous, the volume preserving condition is automatically satisfied (i.e., we can put $\lambda = 0$). This can be shown by integrating the equation over Ω:

$$\frac{d}{dt}\int_\Omega u\,dx = \int_\Omega (\Delta u + f)\,dx = -\int_{\partial\Omega} \frac{\partial u}{\partial \boldsymbol{n}}\,dS = 0.$$

Otherwise, we define the discretized functional by

$$J_n(u) = \int_\Omega \frac{|u - u_{n-1}|^2}{2h}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx - \int_\Omega F_n(u)\,dx + \int_{\partial\Omega} pu\,dS$$

and look for its minimizer in the set

$$\mathcal{K}'_V = \{u \in H^1(\Omega); \int_\Omega u\,dx = V\}.$$

Computed by our standard technique, the Lagrange multiplier becomes

$$\lambda_n = \frac{1}{V}\int_\Omega \left[\frac{u_n - u_{n-1}}{h}u_n + |\nabla u_n|^2 - f_n(u_n)u_n\right] dx + \frac{1}{V}\int_{\partial\Omega} p u_n \, dS.$$

However, by simply integrating the original equation in space we obtain

$$\lambda = \frac{1}{|\Omega|}\left(\int_{\partial\Omega} p\, dS - \int_\Omega f(u)\, dx\right)$$

In the discretized case this corresponds to perturbations of the type $u+\varepsilon$ of the functional $I_n(u) = J_n(u) - \lambda_n \int_\Omega u\, dx$ (see also Remark 4.2.4). Note that the multiplier therefore only depends on time via f. Thus, if f is continuous in u, the limit process of λ_n becomes obvious. Here the weak solution is defined in the following sense

$$\int_0^T \int_\Omega (u_t\phi + \nabla u \nabla\phi - f(u)\phi)\, dx\, dt + \int_0^T \int_{\partial\Omega} p\phi\, dt\, dS = \int_0^T \int_\Omega \lambda\phi\, dx\, dt,$$

for each $\phi \in L^2(0, T; H^1(\Omega))$.

4.2 Hyperbolic problem

4.2.1 Setting

In this part of the work, we consider a hyperbolic problem with volume conservation condition. Such equations can model, e.g., a fast, vibrating motion of a membrane containing a liquid of fixed volume. This section presents the contents of paper [37]. Since much of the calculations and reasoning is similar to the parabolic case, we omit the details in such cases and elaborate only on the new aspects.

We shall study the following volume-constrained hyperbolic initial-boundary-value problem:

$$\begin{aligned} u_{tt}(t,x) &= \Delta u(t,x) + \lambda(u) && \text{in } Q_T, && (4.2.1)\\ u(t,x) &= g(x) && \text{on } (0,T)\times\partial\Omega, && (4.2.2)\\ u(0,x) &= u_0(x) && \text{in } \Omega, && (4.2.3)\\ u_t(0,x) &= v_0(x) && \text{in } \Omega, && (4.2.4) \end{aligned}$$

where λ takes the form

$$\lambda(t) = \frac{1}{V}\int_\Omega (u_{tt}u + |\nabla u|^2)\, dx. \tag{4.2.5}$$

Here $Q_T = (0,T)\times\Omega$, where $T > 0$ and Ω is a bounded domain in $\mathbb{R}^m$ with Lipschitz continuous boundary $\partial\Omega$. Further, u is a scalar function: $Q_T \to \mathbb{R}$ and V is a positive real number representing the volume. We assume that $g \in L^2(\partial\Omega)$ and $u_0, v_0 \in H^1(\Omega)$ satisfy the compatibility conditions $u_0(x) = g(x)$, $v_0(x) = 0$ for $x \in \partial\Omega$ and $\int_\Omega u_0\, dx = V$, $\int_\Omega v_0\, dx = 0$. These conditions are necessary for the setting to make sense physically, while being essential also in the subsequent mathematical analysis.

A solution u of this problem has a constant volume $\int_\Omega u\,dx$. Indeed, by multiplying (4.2.1) by u and integrating over Ω, we see that due to the definition of λ in (4.2.5), any solution u fulfils the volume-preservation condition

$$\int_\Omega u(t,x)\,dx = V \qquad \forall t \in (0,T). \tag{4.2.6}$$

Model equation (4.2.1) can be derived formally by considering the Lagrangian of the physical system in the form

$$L(u) = \frac{1}{2}\int_\Omega \left[(u_t)^2 - |\nabla u|^2\right]\,dx \tag{4.2.7}$$

and searching for stationary points of its action among all functions satisfying (4.2.6). Let us suppose that there is a stationary point u. A heuristic use of the theory of Lagrange multipliers, explained in Chapter 2, suggests that there should be a function of time $\lambda(t)$ such that u is a stationary point of

$$\int_0^T L(u)\,dt + \int_0^T \lambda\Big(\int_\Omega u\,dx\Big)\,dt$$

and, thus, satisfies

$$\int_0^T\int_\Omega [-u_t\phi_t + \nabla u \nabla\phi]\,dx\,dt = \int_0^T \left(\lambda\int_\Omega \phi\,dx\right)dt \qquad \forall \phi \in C_0^\infty(Q_T),$$

which is a weak formulation for (4.2.1).

The aim of this section is to provide a rigorous mathematical justification of this formal derivation and to prove the existence of a weak solution. We shall see that one obtains weak solutions of various kinds depending on the regularity of the initial functions u_0 and v_0.

The variational method used here to accomplish this aim is again the discrete Morse flow of hyperbolic type, introduced already in Chapter 3. It consists in replacing the original problem by a sequence of minimization problems at discrete time levels (see (4.2.8) below). The discretized functional is nonnegative, thus, the existence of a minimizer can be shown, which is at crucial advantage over the functional (4.2.7).

In the sequel, we shall simplify the calculations by setting $g \equiv 0$. For remarks on nonhomogeneous boundary condition, see Section 4.2.4. Moreover, we do not consider any outer force term in the equation because it simplifies the exposition greatly. This issue is also dealt with in a remark in Section 4.2.4.

4.2.2 Approximate weak solution

In this section we present the time-discretized variational scheme defining approximate weak solutions. We divide the time interval $(0,T)$ into N parts and set $h = T/N$. The discretized functional reads

$$J_n(u) = \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx. \tag{4.2.8}$$

We search for a minimizer u_n in the convex set

$$\mathcal{K} = \{u \in H^1(\Omega);\ u|_{\partial\Omega} = 0, \int_\Omega u\,dx = V\},$$

where u_0 and $u_1 := u_0 + hv_0$ are given by the initial conditions (4.2.3), (4.2.4). We remark that u_0 and u_1 belong to $\mathcal{K}$ because of the compatibility conditions mentioned in the preceding subsection. By minimizing $J_n : \mathcal{K} \to \mathbb{R}$, $n = 2, 3, ..., N$, a sequence $\{u_n\}_{n=0}^N \subset \mathcal{K}$ can be obtained inductively. The second term of the functional is lower semi-continuous with respect to sequentially weak convergence in $H^1(\Omega)$ and its first term is continuous in $L^2(\Omega)$ due to Rellich theorem. Therefore, the existence of minimizers follows immediately, taking into account the boundedness from below of J_n.

In order to derive a weak formulation, we choose a function $\zeta \in C_0^\infty(\Omega)$ and consider a variation of the functional J_n using volume-preserving perturbations

$$u_n^\varepsilon = V \frac{u_n + \varepsilon\zeta}{\int_\Omega (u_n + \varepsilon\zeta)dx} \in \mathcal{K}.$$

We note by (4.2.6) that the denominator is equal to $V + \varepsilon \int_\Omega \zeta\,dx$, which implies that it is positive for sufficiently small values of ε. Then we have

$$\begin{aligned}
&\frac{d}{d\varepsilon} J_n(u_n^\varepsilon)|_{\varepsilon=0} \\
&= \int_\Omega \frac{u_n - 2u_{n-1} + u_{n-2}}{h^2}\zeta\,dx + \int_\Omega \nabla u_n \nabla\zeta\,dx \\
&\qquad - \Big(\int_\Omega \big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} u_n + |\nabla u_n|^2\big)\,dx \Big) \big(\int_\Omega \zeta\,dx \big) \\
&= 0.
\end{aligned}$$

Hence, we can write

$$\int_\Omega \frac{u_n - 2u_{n-1} + u_{n-2}}{h^2}\zeta\,dx + \int_\Omega \nabla u_n \nabla\zeta\,dx = \int_\Omega \lambda_n \zeta\,dx, \tag{4.2.9}$$

where λ_n is given by

$$\lambda_n = \frac{1}{V} \int_\Omega \Big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} u_n + |\nabla u_n|^2 \Big)\,dx. \tag{4.2.10}$$

We may call the value λ_n a discrete Lagrange multiplier (see Chapter 2).

We define two approximate functions $u^h, \bar{u}^h$ and an approximate Lagrange multiplier $\bar{\lambda}^h$ by time-interpolation of the sequence $\{u_n\}_{n=0}^N$ of minimizers:

$$\bar{u}^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ u_n(x), & t \in ((n-1)h, nh],\ n = 1, \dots, N \end{cases} \tag{4.2.11}$$

$$u^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ \frac{t-(n-1)h}{h} u_n(x) + \frac{nh-t}{h} u_{n-1}(x), & t \in ((n-1)h, nh], \\ & \qquad n = 1, \dots, N \end{cases}$$

$$\bar{\lambda}^h(t) = \lambda_n, \quad t \in ((n-1)h, nh],\ n = 2, \dots, N.$$

Integrating over the time interval (h,T), we obtain from (4.2.9) the identity

$$\int_h^T \int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h} \phi + \nabla \bar{u}^h \nabla \phi \Big)\, dx\, dt = \int_h^T \int_\Omega \bar{\lambda}^h \phi \, dx\, dt \qquad (4.2.12)$$
$$\forall \phi \in L^2(0,T; H_0^1(\Omega)).$$

Further, $u^h(0) = u_0$ and $u^h(h) = u_0 + hv_0$ hold. It is natural to call u^h and $\bar{u}^h$ defined by the sequence $\{u_n\}_{n=0}^N$ an *approximate weak solution* of (4.2.1)–(4.2.4).

One of our goals is to show that the approximate solutions defined above converge, as $h \to 0+$, to a weak solution of the original problem. We define two types of weak solutions.

Definition 4.2.1. *(1) A function $u \in W^{2,\infty}(0,T; L^2(\Omega)) \cap L^\infty(0,T; H_0^1(\Omega))$ is said to be a* ***weak in space solution*** *to (4.2.1)–(4.2.4) provided that for every $\phi \in C_0^\infty(\Omega)$*

$$\int_\Omega (u_{tt}\phi + \nabla u \nabla \phi)\, dx = \int_\Omega \lambda \phi \, dx \qquad (4.2.13)$$

holds for a.e. $t \in (0,T)$, with λ from (4.2.5). Moreover, we require that $u(0) = u_0$ and $u_t(0) = v_0$ be satisfied.

(2) A function $u \in H^1(0,T; L^2(\Omega)) \cap L^\infty(0,T; H_0^1(\Omega))$ is called a ***weak solution*** *to (4.2.1)–(4.2.4) if $u(0) = u_0$ is satisfied and the following identity holds for all test functions $\phi \in C_0^\infty([0,T) \times \Omega)$*

$$\int_0^T \int_\Omega (-u_t\phi_t + \nabla u \nabla \phi)\, dx\, dt - \int_\Omega v_0 \phi(0)\, dx \qquad (4.2.14)$$
$$= \frac{1}{V} \int_0^T \int_\Omega (-u_t (u\Phi)_t + |\nabla u|^2 \Phi)\, dx\, dt - \frac{1}{V} \int_\Omega u_0 v_0 \Phi(0)\, dx.$$

Here $\Phi = \int_\Omega \phi \, dx$ is a function of time only.

Note that on the right-hand side of (4.2.14) stands actually the expression $\int_0^T \int_\Omega \lambda \phi \, dx\, dt$ but it is integrated by parts with respect to time.

4.2.3 Limit process

We show that under the assumption $u_0, v_0 \in H^1(\Omega)$ the approximate solutions converge to a weak solution, whereas assuming $u_0, v_0 \in H^2(\Omega)$ yields a weak in space solution. The stepping stone in the proof of the convergence is the following energy estimate.

Proposition 4.2.1. *Let $h < 1$ and $u_0, v_0 \in H^1(\Omega)$. Then under the assumptions of Section 4.2.1, the approximate solution satisfies*

$$\|u_t^h(t)\|_{L^2(\Omega)}^2 + \|\nabla \bar{u}^h(t)\|_{L^2(\Omega)}^2 \le 2(1+h^2) \left(\|v_0\|_{H^1(\Omega)}^2 + \|\nabla u_0\|_{L^2(\Omega)}^2 \right) \le C_E \qquad (4.2.15)$$

for almost every $t \in (0,T)$, where C_E is a constant independent of h.

Proof. We select the test function $\psi_n = (1-\theta)u_n + \theta u_{n-1}$, $\theta \in (0,1)$. Noting that $\psi_n \in \mathcal{K}$ and by the minimality property we get

$$\begin{aligned} 0 &\leq \frac{1}{\theta}(J_n(\psi_n) - J_n(u_n)) \\ &= \frac{1}{2h^2}\int_\Omega \left(2(u_{n-1}-u_n)(u_n - 2u_{n-1} + u_{n-2}) + \theta(u_n - u_{n-1})^2\right) dx \\ &\quad + \frac{1}{2}\int_\Omega \left(2\nabla u_n \nabla(u_{n-1}-u_n) + \theta|\nabla(u_{n-1}-u_n)|^2\right) dx. \end{aligned}$$

Passing to the limit as $\theta \to 0+$,

$$\begin{aligned} 0 &\leq -\frac{1}{h^2}\int_\Omega (u_n - u_{n-1})(u_n - 2u_{n-1} + u_{n-2})\,dx + \int_\Omega \nabla u_n \nabla(u_{n-1}-u_n)\,dx \\ &\leq \frac{1}{2h^2}\int_\Omega (u_{n-1}-u_{n-2})^2 - (u_n - u_{n-1})^2\,dx + \int_\Omega \frac{|\nabla u_{n-1}|^2 - |\nabla u_n|^2}{2}\,dx. \end{aligned}$$

Thus, after summing up from $n = 2$ to $k = 2, 3, \ldots, N$, we arrive at

$$\frac{1}{h^2}\|u_k - u_{k-1}\|^2_{L^2(\Omega)} + \|\nabla u_k\|^2_{L^2(\Omega)} \leq \frac{1}{h^2}\|u_1 - u_0\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)}.$$

Recollecting (4.2.11) and $u_1 = u_0 + hv_0$, this is already the desired estimate. □

Using this result, we can derive a subsequence h_i, such that u^{h_i} converges in a certain topology to be mentioned in Lemma 4.2.1. Using the simplified notation without indeces of h (see Chapter 3), we thus have

Lemma 4.2.1. *There exists a subsequence of $\{h \to 0+\}$ and a function u belonging to $L^\infty(0,T;H^1_0(\Omega)) \cap W^{1,\infty}(0,T;L^2(\Omega))$ such that*

$$\begin{aligned} u^h_t &\rightharpoonup u_t \text{ weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)), \\ \nabla \bar{u}^h &\rightharpoonup \nabla u \text{ weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)), \\ u^h, \bar{u}^h &\to u \text{ strongly in } L^2(Q_T). \end{aligned}$$

Proof. First two convergences are an immediate consequence of estimate (4.2.15). The last convergence for u^h holds by Rellich theorem because $u^h - u_0 \in H^1(Q_T)$ vanishes on $([0,T]\times\partial\Omega) \cup (\{0\}\times\Omega)$, and $\|\nabla u^h\|_{L^2(\Omega)}$ and $\|u^h_t\|_{L^2(\Omega)}$ are uniformly bounded (see (3.1.16)). Since

$$\|\bar{u}^h - u^h\|_{L^2(Q_T)} \leq h\|u^h_t\|_{L^2(Q_T)},$$

(see (3.1.14)), we conclude that $\bar{u}^h$ and u^h converge to the same function. □

A finer estimate for more regular initial data is stated in the following lemma.

Lemma 4.2.2. *Let $u_0, v_0 \in H^2(\Omega)$. Then the approximate weak solution u^h obeys the estimate*

$$\int_\Omega \left|\frac{u^h_t(t) - u^h_t(t-h)}{h}\right|^2 dx + \int_\Omega |\nabla u^h_t(t)|^2\,dx \leq C'_E \qquad \textit{for a.e. } t \in (h,T), \tag{4.2.16}$$

where constant C'_E is independent of h.

Moreover, there is a $u_{tt} \in L^\infty(0,T;L^2(\Omega))$ and a subsequence to the sequence from Lemma 4.2.1 such that

$$\frac{u_t^h(t) - u_t^h(t-h)}{h} \rightharpoonup u_{tt} \quad \textit{weakly}^* \textit{ in } L^\infty(0,T;L^2(\Omega)). \tag{4.2.17}$$

Proof. We recall the identity $u_1 = u_0 + hv_0$. Let us further set $u_{-1} = u_0 - hv_0 + h^2\Delta u_1 \in L^2(\Omega)$. This function may not satisfy the volume constraint but since

$$\frac{u_1 - 2u_0 + u_{-1}}{h^2} = \Delta u_1,$$

we have for every $\zeta \in H_0^1(\Omega)$ the relation

$$\int_\Omega \frac{u_1 - 2u_0 + u_{-1}}{h^2}\zeta\,dx + \int_\Omega \nabla u_1 \nabla\zeta\,dx = 0 = \int_\Omega \lambda_1\zeta\,dx.$$

The last equality follows from

$$\lambda_1 = \int_\Omega \big(\frac{u_1 - 2u_0 + u_{-1}}{h^2}u_1 + |\nabla u_1|^2\big)\,dx = \int_\Omega (\Delta u_1\, u_1 + |\nabla u_1|^2)\,dx = 0.$$

Let us use the notation $d_n = u_n - u_{n-1}$, $n = 0, 1, ..., N$, and subtract equation (4.2.9) with n replaced by $n-1$ from (4.2.9) itself. This corresponds to discrete differentiation of the equation with respect to time. We get

$$\int_\Omega \frac{d_n - 2d_{n-1} + d_{n-2}}{h^2}\zeta\,dx + \int_\Omega \nabla d_n \nabla\zeta\,dx = \int_\Omega (\lambda_n - \lambda_{n-1})\zeta\,dx, \qquad n = 2, 3, \dots, N.$$

We choose $\zeta = d_n - d_{n-1}$ and since this function has zero volume, that is,

$$\int_\Omega \zeta\,dx = \int_\Omega (d_n - d_{n-1})\,dx = \int_\Omega (u_n - 2u_{n-1} + u_{n-2})\,dx = 0, \tag{4.2.18}$$

we find that

$$\int_\Omega \frac{d_n - 2d_{n-1} + d_{n-2}}{h^2}(d_n - d_{n-1})\,dx + \int_\Omega \nabla d_n \nabla(d_n - d_{n-1})\,dx = 0, \qquad n = 2, 3, \dots, N. \tag{4.2.19}$$

Note that the property (4.2.18) is very important because it enables us to get rid of the nonlinear terms λ_n.

After summing up from $n = 2$ to $k = 2, 3, \dots, N$, and applying (3.1.10), this yields

$$\frac{1}{h^2}\int_\Omega (d_k - d_{k-1})^2\,dx + \int_\Omega |\nabla d_k|^2\,dx \le \frac{1}{h^2}\int_\Omega (d_1 - d_0)^2\,dx + \int_\Omega |\nabla d_1|^2\,dx,$$

for $k = 2, \dots, N$, which is, after dividing by h^2, the same as

$$\int_\Omega \Big|\frac{u_t^h(t) - u_t^h(t-h)}{h}\Big|^2\,dx + \int_\Omega |\nabla u_t^h(t)|^2\,dx \le \int_\Omega |\Delta u_1|^2\,dx + \int_\Omega |\nabla v_0|^2\,dx$$

for a.e. $t \in (h,T)$. If we extend the definition (4.2.11) of approximate functions for $t \in (-h,0)$, (4.2.16) holds for a.e. $t \in (0,T)$. Hence, there is a function $v \in L^\infty(0,T;L^2(\Omega))$ so that

$$\frac{u_t^h(t) - u_t^h(t-h)}{h} \rightharpoonup v \quad \text{weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)).$$

On the other hand, taking $\varphi \in C_0^\infty(Q_T)$, which is an allowed test function for the above weak*-convergence, we have

$$\begin{aligned}
&\int_0^T \int_\Omega \frac{u_t^h(t) - u_t^h(t-h)}{h} \varphi \, dx \, dt \\
&\qquad = \int_0^T \int_\Omega \frac{u_t^h(t)}{h} \varphi \, dx \, dt - \int_{-h}^{T-h} \int_\Omega \frac{u_t^h(t)}{h} \varphi(t+h) \, dx \, dt \\
&\qquad = \int_0^T \int_\Omega u_t^h(t) \frac{\varphi(t) - \varphi(t+h)}{h} \, dx \, dt - \int_{-h}^0 \int_\Omega \frac{u_t^h(t)}{h} \varphi(t+h) \, dx \, dt \\
&\qquad\quad + \int_{T-h}^T \int_\Omega \frac{u_t^h(t)}{h} \varphi(t+h) \, dx \, dt \\
&\qquad = \int_0^T \int_\Omega u_t^h(t) \frac{\varphi(t) - \varphi(t+h)}{h} \, dx \, dt - \int_0^h \int_\Omega (v_0 - h\Delta u_1) \varphi \, dx \, dt \\
&\quad \to - \int_0^T \int_\Omega u_t \varphi_t \, dx \, dt \qquad \text{as } h \to 0+ .
\end{aligned}$$

This shows that $v = u_{tt}$ in the sense of distributions, and (4.2.17) follows. □

Remark 4.2.1. *The proof of Lemma 4.2.2 suggests that we can get any regularity of u with respect to t, if only the initial conditions are sufficiently regular. The regularity of initial conditions allows to define appropriate approximations u_{-n} for negative times $t \in (-nh, -(n-1)h)$ satisfying the approximate equation. Then we obtain relation (4.2.19) for difference quotients d_n of arbitrary order.*

By energy estimate (4.2.15) and the strong convergence of u^h we immediately get

Lemma 4.2.3. *The limit function u from Lemma 4.2.1 satisfies the homogeneous boundary condition (in the sense of traces) and the volume constraint (4.2.6).*

Now, we prove the main result for initial functions from $H^2(\Omega)$.

Theorem 4.2.1. *Let u_0, v_0 belong to $H^2(\Omega)$. Then the approximate weak solutions defined by (4.2.11) converge to the unique weak in space solution of the original problem (4.2.1)-(4.2.4).*

Proof. Let $\phi \in C^\infty((0,T);C_0^\infty(\Omega))$. Then

$$\int_h^T \int_\Omega \nabla \bar{u}^h \nabla \phi \, dx \, dt \to \int_0^T \int_\Omega \nabla u \nabla \phi \, dx \, dt \qquad \text{as } h \to 0+ . \tag{4.2.20}$$

Moreover, we have

$$\int_h^T \int_\Omega \frac{u_t^h(t) - u_t^h(t-h)}{h} \phi \, dx \, dt \to \int_0^T \int_\Omega u_{tt} \phi \, dx \, dt, \qquad \text{as } h \to 0+ . \tag{4.2.21}$$

If the right-hand side of (4.2.12) converges to $\int_0^T \int_\Omega \lambda \phi \, dx \, dt$, we arrive at the definition of weak in space solution to our problem. The multiplier $\bar{\lambda}^h$ has the form

$$\bar{\lambda}^h = \frac{1}{V} \int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h} \bar{u}^h + |\nabla \bar{u}^h|^2 \Big) \, dx. \tag{4.2.22}$$

It can be extended to $t \in (0, h)$, when one uses the definition of u_{-1} introduced in the proof of Lemma 4.2.2. By the estimates (4.2.15) and (4.2.16) we find that the approximate Lagrange multipliers are bounded in $L^2(0,T)$ independently of h:

$$\begin{aligned} \int_0^T (\bar{\lambda}^h)^2 \, dt &\le \frac{2}{V^2} \int_0^T \Big[\int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h} \Big)^2 \, dx \cdot \int_\Omega (\bar{u}^h)^2 \, dx \Big] \, dt \\ &\quad + \frac{2}{V^2} \int_0^T \Big(\int_\Omega |\nabla \bar{u}^h|^2 \, dx \Big)^2 \, dt \\ &\le C(T). \end{aligned}$$

In fact, by the same reason, we have even the uniform estimate $\bar{\lambda}^h(t) \le C$ for a.e. $t \in (0,T)$. The above estimate shows that there exists a function $\kappa \in L^2(0,T)$, such that $\bar{\lambda}^h \rightharpoonup \kappa$ weakly in $L^2(0,T)$. Passing to the limit as $h \to 0+$ in (4.2.12), we have by (4.2.20) and (4.2.21),

$$\int_0^T \int_\Omega (u_{tt} \phi + \nabla u \nabla \phi) \, dx \, dt = \int_0^T \int_\Omega \kappa \phi \, dx \, dt \qquad \text{for } \phi \in L^2(0,T; H_0^1(\Omega)).$$

For every $t \in (0,T)$ we select

$$\phi(t,x) = \begin{cases} u(t,x), & t \in [0,t), \ x \in \Omega, \\ 0 & t \in [t,T], \ x \in \Omega, \end{cases}$$

to obtain

$$\int_0^t \kappa \, dt = \frac{1}{V} \int_0^t \int_\Omega (u_{tt} u + |\nabla u|^2) \, dx \, dt = \int_0^t \lambda \, dt \qquad \forall t \in (0,T).$$

This shows that $\kappa = \lambda$ almost everywhere in $(0,T)$. Hence,

$$\int_0^T \int_\Omega (u_{tt} \phi + \nabla u \nabla \phi) \, dx \, dt = \int_0^T \int_\Omega \lambda \phi \, dx \, dt.$$

Thus, in particular,

$$\int_\Omega (u_{tt} \phi + \nabla u \nabla \phi) \, dx = \int_\Omega \lambda \phi \, dx \qquad \forall \phi \in H_0^1(\Omega), \ \text{ for a.e. } \ t \in (0,T).$$

The function u belongs to $W^{2,\infty}(0,T;L^2(\Omega))$ and thus also to $C^1([0,T];L^2(\Omega))$, justifying the strong formulation of initial conditions. Applying Mazur's theorem to $u-u_0$ and u_t-v_0, we infer that the initial conditions are satisfied.

The uniqueness follows, as in Remark 4.1.1, from the fact that after subtracting the above equation corresponding to two different solutions and testing by the difference of the solutions, the multiplier term disappears. Then we can use standard technique for uniqueness of solutions to hyperbolic equations (see, e.g., [8], Section 7.2). $\square$

We now explain how to obtain a weak solution for initial data belonging only to $H^1(\Omega)$. In the sequel, we shall need the following identity.

Lemma 4.2.4. *Let v be any smooth function independent of t, satisfying boundary conditions and volume constraint (4.2.6). Let ξ belong to $L^2(0,T;H^1_0(\Omega))$. By X we denote the integral $\int_\Omega \xi\,dx$, which is a function of time only. Then it holds*

$$\int_h^T\int_\Omega\left(\frac{u_t^h(t)-u_t^h(t-h)}{h}\bar{u}^hX+|\nabla\bar{u}^h|^2X\right)dx\,dt \tag{4.2.23}$$
$$=\int_h^T\int_\Omega\left(\frac{u_t^h(t)-u_t^h(t-h)}{h}vX+\nabla\bar{u}^h\nabla vX\right)dx\,dt.$$

Proof. The equation is obtained from (4.2.12) by putting $\phi=(\bar{u}^h-v)X$, which is a function from $L^2(0,T;H^1_0(\Omega))$. $\square$

Theorem 4.2.2. *Let $u_0,v_0\in H^1(\Omega)$. Then the approximate weak solutions defined by (4.2.11) converge to the unique weak solution u of the original problem (4.2.1)-(4.2.4).*

Proof. We can pass to limit in the left-hand side of (4.2.12). Selecting an arbitrary $\phi\in C_0^\infty([0,T)\times\Omega)$, we find that

$$\int_h^T\int_\Omega\nabla\bar{u}^h\nabla\phi\,dx\,dt=\int_0^T\int_\Omega\nabla\bar{u}^h\nabla\phi\,dx\,dt-\int_0^h\int_\Omega\nabla\bar{u}^h\nabla\phi\,dx\,dt$$
$$\to\int_0^T\int_\Omega\nabla u\nabla\phi\,dx\,dt\qquad\text{as } h\to0+\,. \tag{4.2.24}$$

Moreover, we have (see Chapter 3 for details)

$$\int_h^T\int_\Omega\frac{u_t^h(t)-u_t^h(t-h)}{h}\phi\,dx\,dt$$
$$=\int_h^T\int_\Omega\frac{u_t^h(t)}{h}\phi\,dx\,dt-\int_0^{T-h}\int_\Omega\frac{u_t^h(t)}{h}\phi(t+h)\,dx\,dt$$
$$=\int_0^T\int_\Omega u_t^h(t)\frac{\phi(t)-\phi(t+h)}{h}\,dx\,dt-\int_0^h\int_\Omega\frac{u_t^h(t)}{h}\phi\,dx\,dt$$
$$+\int_{T-h}^T\int_\Omega\frac{u_t^h(t)}{h}\phi(t+h)\,dx\,dt$$
$$\to-\int_0^T\int_\Omega u_t\phi_t\,dx\,dt-\int_\Omega v_0\phi(0)\,dx\qquad\text{as } h\to0+\,. \tag{4.2.25}$$

The convergence of $\bar{\lambda}^h$ is not obvious and is proven below by the application of Lemma 4.2.4. Let $\Phi = \int_\Omega \phi\, dx$. Then, due to (4.2.23), we have

$$\begin{aligned}
\int_h^T \bar{\lambda}^h \left(\int_\Omega \phi\, dx \right) dt &= \int_h^T \bar{\lambda}^h \Phi dt \\
&= \frac{1}{V} \int_h^T \int_\Omega \left(\frac{u_t^h(t) - u_t^h(t-h)}{h} \bar{u}^h \Phi + |\nabla \bar{u}^h|^2 \Phi \right) dx\, dt \\
&= \frac{1}{V} \int_h^T \int_\Omega \left(\frac{u_t^h(t) - u_t^h(t-h)}{h} v \Phi + \nabla \bar{u}^h \nabla v \Phi \right) dx\, dt.
\end{aligned}$$

Here we proceed similarly as in (4.2.24) and (4.2.25), writing $v\Phi$ instead of ϕ :

$$\int_h^T \bar{\lambda}^h \Phi dt \to \frac{1}{V} \int_0^T \int_\Omega (-u_t v \Phi_t + \nabla u \nabla v \Phi)\, dx\, dt - \frac{1}{V} \int_\Omega v_0 v \Phi(0)\, dx. \tag{4.2.26}$$

Using (4.2.24)–(4.2.26), we can pass to limit in (4.2.12) to arrive at

$$\begin{aligned}
&\int_0^T \int_\Omega (-u_t \phi_t + \nabla u \nabla \phi)\, dx\, dt - \int_\Omega v_0 \phi(0)\, dx \\
&\qquad = \int_0^T \int_\Omega (-u_t v \Phi_t + \nabla u \nabla v \Phi)\, dx\, dt - \int_\Omega v_0 v \Phi(0)\, dx.
\end{aligned}$$

By density argument, we see that in the above equation we can choose again $\phi = (u - v)\Psi$ with v as in Lemma 4.2.4 and $\Psi = \int_\Omega \psi\, dx$, $\psi \in C_0^\infty([0, T) \times \Omega)$ arbitrary. We get

$$\begin{aligned}
&\int_0^T \int_\Omega \left(-u_t (u\Psi)_t + |\nabla u|^2 \Psi \right) dx\, dt - \int_\Omega v_0 u(0) \Psi(0)\, dx \\
&\qquad = \int_0^T \int_\Omega (-u_t v \Psi_t + \nabla u \nabla v \Psi)\, dx\, dt - \int_\Omega v_0 v \Psi(0)\, dx.
\end{aligned} \tag{4.2.27}$$

We have used the fact that the limit function u satisfies the volume condition. Using (4.2.26) and (4.2.27) for the test function $\phi \in C_0^\infty([0, T) \times \Omega)$ introduced in (4.2.24) instead of ψ, we obtain

$$\int_h^T \bar{\lambda}^h \Phi dt \to \frac{1}{V} \int_0^T \int_\Omega (-u_t (u\Phi)_t + |\nabla u|^2 \Phi)\, dx\, dt - \frac{1}{V} \int_\Omega v_0 u(0) \Phi(0)\, dx.$$

Combining this fact with (4.2.24) and (4.2.25), together with standard technique for initial condition $u(0) = u_0$ (see Chapter 3) proves our statement. The uniqueness follows by the same reasoning as in the proof of Theorem 4.2.1. □

In this section, a mathematical model for surface vibration preserving volume was derived strictly from the mathematical point of view by introducing a series of variational functionals and making use of the essential properties of their minimizers. Mathematical analysis of the convergence of approximate solution is also given, leading to the proof of existence of weak solutions to a hyperbolic partial differential equation and the derivation of concrete expression for Lagrange multiplier. We realized the approximate solution by numerical computation for a physical phenomenon of lifting a film, comparing the volume-preserving and non-preserving cases (see Section 7.2).

4.2.4 Remarks

In this subsection, we provide several remarks touching the problem with a force term and other types of boundary conditions.

Remark 4.2.2. *(On outer force)*
In this remark, we would like to deal briefly with the problem having an outer force term: instead of (4.2.1) we consider

$$u_{tt}(t,x) = \Delta u(t,x) + f(t,x,u) + \lambda(t) \quad \text{ in } Q_T, \tag{4.2.28}$$

where we assume that function f is continuous in u and satisfies

$$|f(t,x,s)| \le C_f|s| + \gamma(t,x), \qquad \gamma \in L^2(Q_T). \tag{4.2.29}$$

In this case, setting again $g \equiv 0$, the Lagrange multiplier becomes

$$\lambda(t) = \frac{1}{V}\int_\Omega (u_{tt}u + |\nabla u|^2 - f(u)u)\,dx. \tag{4.2.30}$$

For functions f, F and γ, where F is a primitive function to f with respect to the third variable, we introduce on each time level $n = 1, 2, \ldots, N$ a time-independent variant in the following way:

$$f_n(x,s) = \frac{1}{h}\int_{(n-1)h}^{nh} f(t,x,s)\,dt, \quad F_n(x,s) = \frac{1}{h}\int_{(n-1)h}^{nh} F(t,x,s)\,dt,$$
$$\gamma_n(x,s) = \frac{1}{h}\int_{(n-1)h}^{nh} \gamma(t,x,s)\,dt.$$

The discretized functional then reads

$$J_n(u) = \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx - \int_\Omega F_n(u)\,dx. \tag{4.2.31}$$

We now prove that we can obtain the same energy estimate as in (4.2.15):

$$\|u_t^h(t)\|^2_{L^2(\Omega)} + \|\nabla \bar{u}^h(t)\|^2_{L^2(\Omega)} \le C_E(u_0, v_0, C_f, \|\gamma\|_{L^2(Q_T)}, T)$$

for a.e. $t \in (0,T)$, where C_E is a constant independent of h.

Proof. Again, we select the test function $\psi = (1-\theta)u_n + \theta u_{n-1}$, $\theta \in (0,1)$. By the minimality property $0 \le \frac{1}{\theta}(J_n(\psi) - J_n(u_n))$, passing to the limit as $\theta \to 0+$ and using (4.2.29), we get

$$\begin{aligned}
0 \quad &\le \quad -\frac{1}{h^2}\int_\Omega (u_n - u_{n-1})(u_n - 2u_{n-1} + u_{n-2})\,dx + \int_\Omega \nabla u_n \nabla(u_{n-1} - u_n)\,dx \\
&\quad\quad + \int_\Omega f_n(u_n)(u_n - u_{n-1})\,dx \\
&\le \quad \frac{1}{2h^2}\int_\Omega \big((u_{n-1} - u_{n-2})^2 - (u_n - u_{n-1})^2\big)\,dx + \int_\Omega \frac{|\nabla u_{n-1}|^2 - |\nabla u_n|^2}{2}\,dx \\
&\quad\quad + C_f^2 h \int_\Omega u_n^2\,dx + h\int_\Omega \gamma_n^2\,dx + \frac{h}{2}\int_\Omega \left(\frac{u_n - u_{n-1}}{h}\right)^2\,dx.
\end{aligned}$$

Thus, after summing up, we arrive at

$$\|\frac{u_n - u_{n-1}}{h}\|^2_{L^2(\Omega)} + \|\nabla u_n\|^2_{L^2(\Omega)} \leq \|v_0\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)} + 2\|\gamma\|^2_{L^2(Q_T)} + \sum_{k=1}^{n} h \left[2C_f^2 \|u_k\|^2_{L^2(\Omega)} + \|\frac{u_k - u_{k-1}}{h}\|^2_{L^2(\Omega)} \right].$$

Since $u_n \in H_0^1(\Omega)$, we have a constant $0 < C_P < 1$ independent of n such that

$$\|\nabla u_n\|^2_{L^2(\Omega)} \geq C_P \left(\|\nabla u_n\|^2_{L^2(\Omega)} + \|u_n\|^2_{L^2(\Omega)} \right).$$

Denoting

$$a_n = \|\frac{u_n - u_{n-1}}{h}\|^2_{L^2(\Omega)} + C_P \|\nabla u_n\|^2_{L^2(\Omega)} + C_P \|u_n\|^2_{L^2(\Omega)},$$

we get

$$a_n \leq \|v_0\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)} + 2\|\gamma\|^2_{L^2(Q_T)} + \max\{2C_f^2/C_P, 1\} h \sum_{k=1}^{n} a_k.$$

The discrete Gronwall lemma (see [13]) finally yields

$$a_n \leq \left(\|v_0\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)} + 2\|\gamma\|^2_{L^2(Q_T)} \right) e^{2T \max\{2C_f^2/C_P, 1\}}.$$

This is already the desired estimate. □

However, under assumption (4.2.29) we are not able to prove an estimate analogous to Lemma 4.2.2. Further assumptions, such as a condition on the behaviour of the time derivative of f, would be necessary. Also, in order to show the existence of minimizers to (4.2.31), we have to assume that either C_f from (4.2.29) is small enough or that f is bounded (see estimates in Section 4.1.2).

Remark 4.2.3. *(Nonhomogeneous boundary condition, independent of time)*
Consider the boundary condition

$$u|_{\partial\Omega} = g.$$

Assume g is chosen in such a way that $g \in H^2(\Omega)$, $\int_\Omega g\, dx = 0$ and that $u_0|_{\partial\Omega} = g|_{\partial\Omega}$. We introduce a new function v by $u = v + g$ (analogously $u_n = v_n + g$). Then $v|_{\partial\Omega} = 0$ and $\int_\Omega v\, dx = V$ and we can transform the problem to: find a minimizer v_n of the functional

$$J_n^g(v) = \int_\Omega \frac{|v - 2v_{n-1} + v_{n-2}|^2}{2h^2}\, dx + \frac{1}{2} \int_\Omega |\nabla v + \nabla g|^2\, dx$$

in

$$\mathcal{K} = \{v \in H^1(\Omega);\ v|_{\partial\Omega} = 0, \int_\Omega v\, dx = V\}.$$

The Lagrange multiplier in terms of v is calculated in the same way as in the case of homogeneous boundary condition:

$$\lambda_n = \frac{1}{V}\int_\Omega \Big[\frac{v_n - 2v_{n-1} + v_{n-2}}{h^2} v_n + \nabla(v_n + g)\nabla v_n\Big]\,dx. \tag{4.2.32}$$

Since the test function $(1-\theta)v_n + \theta v_{n-1}$ again belongs to $\mathcal{K}$, we get the same estimates for the functions v_n as above and, using the properties of g, also for the functions u_n. Hence, passing to the limit as $h \to 0+$ can be done in the same way as explained in the previous Section. We should note that by multiplying (4.2.1) by $u - g$ and integrating over Ω we obtain a convenient form of the Lagrange multiplier corresponding to (4.2.32), i.e., instead of (4.2.5) we have

$$\lambda = \frac{1}{V}\int_\Omega \big[u_{tt}(u-g) + \nabla u \nabla(u-g)\big]\,dx = \frac{1}{V}\int_\Omega \big[v_{tt} v + \nabla(v+g)\nabla v\big]\,dx.$$

Remark 4.2.4. *(Neumann boundary condition, independent of time)*
Here we deal with the condition

$$\frac{\partial u}{\partial \boldsymbol{n}} = p \qquad \text{on } \partial\Omega,$$

where $\boldsymbol{n}$ is the unit inner normal to $\partial\Omega$. We assume that $p \in L^2(\partial\Omega)$ and that the initial value satisfies the given Neumann condition. We define the discretized functional by

$$J_n(u) = \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx + \int_{\partial\Omega} pu\,dS$$

and look for its minimizer in the space

$$\mathcal{K}' = \{u \in H^1(\Omega); \int_\Omega u\,dx = V\}.$$

The Lagrange multiplier computed by the standard technique becomes

$$\lambda_n = \frac{1}{V}\int_\Omega \Big[\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} u_n + |\nabla u_n|^2\Big]\,dx + \frac{1}{V}\int_{\partial\Omega} pu_n\,dS.$$

However, by simply integrating the original equation in space we obtain

$$\lambda = \lambda_n = \frac{1}{|\Omega|}\int_{\partial\Omega} p\,dS. \tag{4.2.33}$$

In the discretized case this corresponds to perturbations of the type

$$u_n^\varepsilon = \frac{u_n + \varepsilon}{1 + \varepsilon\frac{|\Omega|}{V}} \in \mathcal{K}'$$

of the functional J_n:

$$\begin{aligned}
0 &= \lim_{\varepsilon \to 0} \frac{J_n(u_n^\varepsilon) - J_n(u_n)}{\varepsilon} \\
&= \int_\Omega \Big(\big(1 - \frac{|\Omega|}{V} u_n\big)(u_n - 2u_{n-1} + u_{n-2}) - \frac{|\Omega|}{V} |\nabla u_n|^2 \Big)\, dx + \int_{\partial\Omega} \big(1 - \frac{|\Omega|}{V} u_n\big) p\, dS \\
&= -\frac{|\Omega|}{V} \Big(\int_\Omega \big(u_n(u_n - 2u_{n-1} + u_{n-2}) + |\nabla u_n|^2\big)\, dx + \int_{\partial\Omega} p u_n\, dS \Big) + \int_{\partial\Omega} p\, dS \\
&= -|\Omega| \lambda_n + \int_{\partial\Omega} p\, dS.
\end{aligned}$$

The weak solution is obtained immediately in the following sense:

$$\int_0^T \int_\Omega (-u_t \phi_t + \nabla u \nabla \phi)\, dx\, dt - \int_\Omega v_0 \phi(0)\, dx + \int_0^T \int_{\partial\Omega} p\phi\, dS\, dt = \int_0^T \int_\Omega \lambda \phi\, dx\, dt$$

for each $\phi \in C_0^\infty([0,T); C^\infty(\Omega))$, with λ from (4.2.33).

Chapter 5

Problems with free boundary

In this Chapter, we study problems with volume preservation, where a free boundary appears. The equation models the motion of droplets on surfaces – the parabolic equation is considered as a model for small, viscous, slowly moving drops, and the hyperbolic one for the faster motion of larger drops. The main idea of the model is to divide the drop into two interacting parts: a film representing the surface of the drop, and the fluid inside. The film, which determines a (moving) boundary for the liquid inside, is considered to be the graph of a scalar function. The motion of the liquid is described by equations of fluid dynamics. Some more details of the model are given in the Appendix to this Chapter (see Section 5.3). Here we are concerned especially with the mathematical analysis of the problem for the film.

The key features of the phenomenon, described by the model equation, are the free boundary, volume constraint and contact angle. The underlying surface, on which the droplet rests, plays the role of an obstacle to the motion and gives rise to free boundary. Moreover, we assume that the volume of the drop does not change, obtaining the volume constraint. Finally, there is a nonzero contact angle on the boundary of the region where the drop touches the surface. This adds a delta-function term into the equation. In this work, we consider only smooth approximations to this term.

Our approach to free-boundary problems avoids direct analysis of the properties of the free boundary itself. This is a challenging task left for future research. Particularly, in our definition weak solutions are tested only by functions with support not intersecting the free boundary.

We propose construction of approximate solutions by a variational method and show their convergence to a unique weak solution. Application of variational principles to constrained problems of this type is effective. Another method that was successful in abstract analysis of constrained evolutionary problems relies on the technique of subdifferentials and Yosida approximation (see [2], [5], [26], etc.). Although this framework is able to solve a large class of problems, there are some disadvantages which we try to overcome by introducing a different approach. The most substantial contribution of the new proof is that, contrary to subdifferential approach, it is repruducible in numerical computations (for an example of numerical results, see [19] or Sections 7.3 and 7.4). Another feature of our method is the absence of assumptions on convexity, which are in essence indispensable for the definition of subdifferentials. This fact is significant in regard of future consideration of sharp contact angles. Moreover, the type of regularity results presented here is new, as far as we know.

5.1 Parabolic problem

First, we attack a problem of parabolic type. We show the existence of a weak solution. The main tool will again be the discrete Morse flow (see Chapter 3) combined with smoothing. The contents of this subsection are taken from the preprint [38].

5.1.1 Model equation and its properties

In the Appendix, we have obtained a model equation for droplet motion. Imposing appropriate initial and boundary conditions, we have the following problem:

$$\begin{aligned} u_t(t,x) &= \Delta u(t,x) - \gamma(x)\chi_\varepsilon'(u(t,x)) + \chi_{u>0}\lambda(t) \quad \text{in } Q_T, && (5.1.1)\\ u(0,x) &= u_0(x) \qquad \text{for } x\in\Omega, && (5.1.2)\\ u(t,x) &= 0 \qquad \text{on } (0,T)\times\partial\Omega. && (5.1.3)\end{aligned}$$

Here $T>0$ is the time up to which the motion is considered, Ω is a bounded domain in $\mathbb{R}^m$ with smooth boundary $\partial\Omega$ and $Q_T=(0,T)\times\Omega$. The unknown function u represents the shape of the drop. The initial shape u_0 is assumed to be a function belonging to $L^\infty(\Omega)\cap H_0^1(\Omega)$. The Laplacian comes from an approximation of the minimal surface operator, when we assume hydrophilic surfaces:

$$\sqrt{1+|\nabla u|^2}\approx\frac{1}{2}|\nabla u|^2. \tag{5.1.4}$$

Further, $\gamma\in L^\infty(\Omega)$ is a coefficient describing the surface tensions of the three phases: liquid (drop), solid (underlying surface) and gas (air). The dependence on the space variable expresses the fact that we consider chemically nonhomogeneous underlying surface. The symbol $\chi_{u>0}$ stands for the characteristic function of the set $\{u>0\}=\{(t,x):u(t,x)>0\}$ and χ_ε is its nondecreasing smoothing (see Figure 5.1) with the property $\chi_\varepsilon'(x)\le C/\varepsilon$ for $x\in(0,\varepsilon)$. The term comes from the requirement of fixed contact angle at the free boundary of the drop. The contact angle θ depends on the various surface tensions and is given by Young's equation

$$\cos\theta = 1-\gamma. \tag{5.1.5}$$

In order to satisfy this relation, it would be necessary to insert a delta function term $\gamma\delta_{\partial\{u>0\}}$ into the equation. We have simplified the problem mathematically by smoothing the delta function. A formal justification of the approximation is presented at the end of this subsection.
Finally, λ is a Lagrange multiplier defined by

$$\lambda=\frac{1}{V}\int_\Omega\left[uu_t+|\nabla u|^2+\gamma u\chi_\varepsilon'(u)\right]\,dx. \tag{5.1.6}$$

This is a parabolic problem with free-boundary $\partial\{u>0\}$ and a complicated term λ having the form of the integral of the unknown function. The solution of this nonlocal

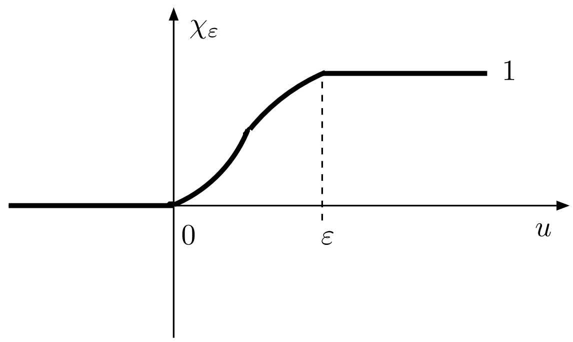


Figure 5.1: Smoothing of characteristic function.

equation as it is, seems very difficult. However, it is possible to solve the problem by the variational method called the *discrete Morse flow*, which is presented in the subsequent paragraphs. In this method we use the minimality property of a time-discretized functional, and insert the volume constraint, which gives rise to the nonlocal term, into the admissible function set. Thus, we can handle the constraint without considering it explicitly. This method is identical to the case without free boundary (Section 4.1).

Remark 5.1.1. *It is possible to add also a general outer force term $f(t, x, u)$ to the right-hand side of model equation (5.1.1). However, this would only complicate the formulas, so we keep only the smoothing of the delta function representing the contact angle condition, in order to emphasize its features important for later deliberations on the sharp contact angle case ($\varepsilon = 0$).*

Here we confine ourselves to stating assumptions on outer force term, which guarantee the correctness of all proofs below, even with the outer force term present. The function f should be continuous in the variable u and satisfy $f(u) = 0$ for $u \leq 0$. If $m \leq 3$ and f does not depend on time, the following condition is sufficient:

$$-C_1 u^5 - \Gamma_1(x) \leq f(x, u) \leq C_2 u + \Gamma_2(x),$$

where $\Gamma_1 \geq 0$ and $\Gamma_2 \geq 0$ belong to $L^\infty(\Omega)$, $C_1 > 0$ and C_2 is a constant smaller than a certain value. Otherwise, for time-dependent outer forces a more involved assumptions would be necessary. See [36] for details of the outer force treatment.

For example, gravity acting on a drop on a tilted plane with inclination angle ω would give the form $f(x, u) = -gu\cos\omega + gx\sin\omega$. This function satisfies the above assumptions. In a coupled model considering also the motion of the fluid, this term would also include the force exerted on the film by the fluid.

In the present subsection, we mention some features of the model equation (5.1.1), especially the relation that holds on the free boundary when the smoothing parameter ε is taken to zero.

First, we shall formally discuss the maximum principle for our equation. Let us consider the set $Q_T \cap \{u < 0\}$. If u is smooth, then it is an open set with smooth boundary.

Moreover, from the definition of χ_ε we see that $u_t = \Delta u$ holds in this set. Since u is zero on its boundary and $u_0 \geq 0$, from the maximum principle we have that u must vanish inside the set $\{u \leq 0\}$. This means that the solution of (5.1.1)–(5.1.3) is either zero or positive satisfying $u_t = \Delta u - \gamma\chi_\varepsilon'(u) + \lambda$. We see that the characteristic function in front of the Lagrange multiplier realizes the obstacle and gives rise to a free boundary. Moreover, reasoning from the maximum principle, it appears that it will be convenient to set up the volume preservation condition in the form

$$\int_\Omega \chi_{u(t,x)>0} u(t,x)\,dx = V \qquad \forall t \in [0,T], \tag{5.1.7}$$

so that we can make use of the "cut-off at zero" argument.

Next, we shall formally compute the free boundary condition for the free boundary problem corresponding to (5.1.1)– (5.1.3) for $\varepsilon \to 0+$. The obtained identity compared to (5.1.5) shows the adequacy of this ε-approximation.

Proposition 5.1.1. *Let us suppose there exists a classical solution u^ε to (5.1.1)–(5.1.3) and that for $\varepsilon \to 0+$ it converges in a sufficiently strong sense, which will be clarified in the proof, to a function v satisfying $v_t = \Delta v + \Lambda$, $\Lambda = \frac{1}{V}\int_\Omega (vv_t + |\nabla v|^2)\,dx$ in $Q_T \cap \{v > 0\}$ and $v \equiv 0$ in $Q_T \cap \{v \leq 0\}$. Then $|\nabla v|^2 = 2\gamma$ holds on $\partial\{v > 0\}$ for almost all $t \in (0,T)$.*

Proof. We select an arbitrary $\zeta \in C_0^\infty(Q_T)$ and multiply equation (5.1.1) by the function $\zeta u_k^\varepsilon \left(\equiv \zeta \frac{\partial u^\varepsilon}{\partial x_k}\right)$, $k = 1, ..., m$. Next, we integrate the resulting identity over $Q_T = (0,T) \times \Omega$ and obtain (see [4])

$$\int_{Q_T} \zeta u_k^\varepsilon \left(\Delta u^\varepsilon - u_t^\varepsilon + \lambda \chi_{u^\varepsilon>0}\right) dz = \int_{Q_T} \gamma\zeta u_k^\varepsilon \chi_\varepsilon'\left(u^\varepsilon\right) dz. \tag{5.1.8}$$

The simplifying notation $z = (x_1, ..., x_m, t)$ is used here. Applying Green's formula, we derive an equation with only first order derivatives of u^ε and then take ε to zero. Noting that $[\chi_\varepsilon(u^\varepsilon)]_{x_k} = \chi_\varepsilon'(u^\varepsilon)\,u_k^\varepsilon$, and assuming that $\chi_\varepsilon(u^\varepsilon) \to \chi_{v>0}$ a.e., we have for the right-hand side of (5.1.8)

$$\begin{aligned}
\int_{Q_T} \gamma\zeta u_k^\varepsilon \chi_\varepsilon'\left(u^\varepsilon\right) dz &= -\int_{Q_T} (\gamma\zeta)_k \chi_\varepsilon\left(u^\varepsilon\right) dz \\
&\xrightarrow[\varepsilon\to 0]{} -\int_{Q_T\cap\{v>0\}} (\gamma\zeta)_k \,dz \\
&= -\int_{Q_T\cap\partial\{v>0\}} \gamma\zeta\nu_k \,dS.
\end{aligned}$$

The symbol ν_k stands for the k-th component of the outer normal vector $\nu = (\nu_1, \ldots, \nu_{m+1})$ to the set $\{v > 0\} \subset Q_T$, ν_{m+1} being the time-direction component. Since $\gamma \in L^\infty(\Omega)$ only, we should mollify it, but we can assume $\gamma \in C^1(\Omega)$ in this formal setting.

As for the left-hand side of (5.1.8), we can proceed in the following way:

$$\begin{aligned}
&\int_{Q_T} \zeta u_k^\varepsilon \left(\Delta u^\varepsilon - u_t^\varepsilon + \lambda \chi_{u^\varepsilon>0}\right) dz \\
&= -\int_{Q_T} \left[\nabla\left(\zeta u_k^\varepsilon\right)\nabla u^\varepsilon + \zeta u_k^\varepsilon u_t^\varepsilon - \zeta u_k^\varepsilon \lambda\right] \chi_{u^\varepsilon>0}\, dz \\
&= -\int_{Q_T} \left(u_k^\varepsilon \nabla\zeta\nabla u^\varepsilon - \frac{1}{2}|\nabla u^\varepsilon|^2 \zeta_k + \zeta u_k^\varepsilon u_t^\varepsilon - \zeta u_k^\varepsilon \lambda\right)\chi_{u^\varepsilon>0}\, dz \\
&\xrightarrow[\varepsilon\to 0]{} -\int_{Q_T} \left(v_k \nabla\zeta\nabla v - \frac{1}{2}|\nabla v|^2 \zeta_k + \zeta v_k v_t - \zeta v_k \Lambda\right)\chi_{v>0}\, dz \\
&= \int_{Q_T\cap\{v>0\}} \zeta v_k (\Delta v - v_t + \Lambda)\, dz \\
&\qquad - \int_{Q_T\cap\partial\{v>0\}} \left(\zeta v_k \left(\nabla v, 0\right)\cdot\nu - \frac{1}{2}|\nabla v|^2 \zeta \nu_k\right) dS \\
&= -\int_{Q_T\cap\partial\{v>0\}} \left(\zeta v_k \left(\nabla v, 0\right)\cdot\nu - \frac{1}{2}|\nabla v|^2 \zeta \nu_k\right) dS.
\end{aligned}$$

Under the notation $Dv = (v_{x_1}, \cdots, v_{x_n}, v_t)$, the outer unit normal can be expressed as $\nu = -Dv/\left|Dv\right|$. Hence, on $\partial\{v>0\}$ we get $v_k = -\nu_k \left|Dv\right|$ and

$$-\int_{Q_T\cap\partial\{v>0\}} \left(\zeta v_k \left(\nabla v, 0\right)\cdot\nu - \frac{1}{2}|\nabla v|^2 \zeta \nu_k\right) dS = -\frac{1}{2}\int_{Q_T\cap\partial\{v>0\}} \left|\nabla v\right|^2 \zeta\nu_k\, dS.$$

The above calculations yield

$$2\int_{Q_T\cap\partial\{v>0\}} \gamma\zeta\nu_k\, dS = \int_{Q_T\cap\partial\{v>0\}} \left|\nabla v\right|^2 \zeta\nu_k\, dS,$$

which means that for almost all times $t \in (0, T)$,

$$\left|\nabla v\right|^2 = 2\gamma \quad \text{on } \partial\{v>0\}. \tag{5.1.9}$$

□

Let us study the relation between the free boundary condition (5.1.9), which we have just formally derived, and Young's equation (5.1.5). Using (5.1.5), we find

$$2\gamma = 2(1-\cos\theta) = \theta^2 + O(\theta^4).$$

On the other hand,

$$|\nabla v|^2 = \tan^2\theta = \theta^2 + O(\theta^4).$$

We see that the smoothing χ_ε of the characteristic function in (5.1.1) is reasonable and also that by the approximation (5.1.4) we have introduced an error of order $O(\theta^4)$ in the contact angle.

5.1.2 Existence of weak solution

Here we show the main result concerning our problem – the existence of a weak solution to (5.1.1)–(5.1.3) that is nonnegative and satisfies the volume conservation identity (5.1.7). We assume that $\gamma \in L^\infty(\Omega)$ and $u_0 \in L^\infty(\Omega) \cap H^1_0(\Omega)$ are nonnegative. We also assume that u_0 is Hölder continuous and satisfies (5.1.7).

The main idea of the proof is to state and solve a minimization problem corresponding to a smoothing of the original problem. Specifically, we regularize the volume constraint (5.1.7) by smoothing the characteristic function. We show the existence and several important properties of the solution to the smoothed problem using the discrete Morse flow variational technique. Since we also obtain the uniform convergence of solutions to the smooth problem with respect to δ, we shall finally be able to construct a weak solution to the original problem.

First, we introduce the approximate problem parametrized by $\delta > 0$:

$$\begin{aligned} & u^\delta_t = \Delta u^\delta - \gamma\chi'_\varepsilon(u^\delta) + \left(\tilde{\chi}_\delta(u^\delta) + u^\delta\tilde{\chi}'_\delta(u^\delta)\right)\lambda^\delta && \text{in } \ Q_T, \\ & u^\delta(0,x) = u_0(x) && \text{in } \Omega, \\ & u^\delta(t,x) = 0 && \text{on } \ \partial\Omega, \end{aligned} \tag{5.1.10}$$

where

$$\lambda^\delta = \frac{\int_\Omega \left(u^\delta_t u^\delta + |\nabla u^\delta|^2 + \gamma\chi'_\varepsilon(u^\delta)u^\delta\right)\,dx}{V + \int_\Omega \tilde{\chi}'_\delta(u^\delta)(u^\delta)^2\,dx}, \tag{5.1.11}$$

and $\tilde{\chi}_\delta(u)$ is a smoothing of the characteristic function $\chi_{u>0}$ (see Figure 5.2):

$$\tilde{\chi}_\delta(u) = \begin{cases} 0, & u \le -\delta \\ 1, & u \ge 0, \end{cases}$$

interpolating in $(-\delta, 0)$ by a smooth increasing function so that

$$\tilde{\chi}'_\delta(u) \le C/\delta \quad \text{for } \ u \in (-\delta, 0). \tag{5.1.12}$$

Note that the denominator in (5.1.11) is positive.

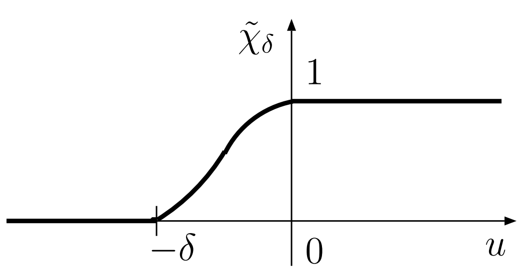


Figure 5.2: Smoothing of characteristic function.

A weak solution is defined in the following way.

Definition 5.1.1. *A function $u^\delta \in H^1(Q_T)\cap L^\infty(0,T;H_0^1(\Omega))$ is called a weak solution of (5.1.10), if it satisfies the initial condition and*

$$\int_0^T \int_\Omega \Big(u_t^\delta\varphi + \nabla u^\delta \nabla\varphi + \gamma\chi_\varepsilon'(u^\delta)\varphi\Big)\,dx\,dt \tag{5.1.13}$$
$$= \int_0^T \lambda^\delta \int_\Omega \big(\tilde\chi_\delta(u^\delta) + u^\delta\tilde\chi_\delta'(u^\delta)\big)\,\varphi\,dx\,dt \quad \forall\varphi\in L^2(0,T;H_0^1(\Omega)),$$

where λ^δ is given by (5.1.11).

We remark that $\lambda^\delta\in L^2(0,T)$ and all the integrals in the above equation have sense for u^δ with the stated regularity.

To solve this problem, we make use of the mentioned variational method. The results are summarized in the following theorem.

Theorem 5.1.1. *There exists a weak solution of the above approximate problem satisfying*

$$u^\delta \geq -\delta, \tag{5.1.14}$$

the perturbed volume constraint

$$\int_\Omega \tilde\chi_\delta(u^\delta)u^\delta\,dx = V \tag{5.1.15}$$

and the following estimate

$$\|u_t^\delta\|^2_{L^2(Q_T)} + \|\nabla u^\delta(t)\|^2_{L^2(\Omega)} + \int_\Omega \gamma\chi_\varepsilon(u^\delta)(t)\,dx \leq C(u_0) \tag{5.1.16}$$

for a.e. $t\in(0,T)$, where $C(u_0)$ does not depend on δ.

Moreover, the solutions are uniformly bounded in $[0,T]\times\bar\Omega$ and uniformly Hölder continuous on $\bar Q_T$ with respect to the parameter δ.

The rough structure of the proof, based on the result [36], is to use a minimizing method for a time-discretized functional in order to construct approximate solutions and show that these approximations converge to a weak solution. We divide the time interval $(0,T)$ equidistantly into N subintervals of length $h=T/N$, $N\in\mathbb{N}$, and for each $h>0$ we construct an approximate solution $u^{\delta,h}$ in the following manner.

First of all, put $u^{\delta,0}=u_0$, and for $n=1,2,\dots,N$, find a minimizer $u^{\delta,n}$ of the functional

$$J_n^\delta(u) = \int_\Omega \Big(\frac{|u-u^{\delta,n-1}|^2}{2h} + \frac{1}{2}|\nabla u|^2 + \gamma\chi_\varepsilon(u)\Big)\,dx \tag{5.1.17}$$

in the admissible function set

$$\mathcal{K}_V^\delta = \Big\{u\in H_0^1(\Omega);\int_\Omega \tilde\chi_\delta(u)u\,dx = V\Big\}. \tag{5.1.18}$$

This functional is called the discrete Morse flow corresponding to (5.1.10). We remark that neither in (5.1.10) nor in (5.1.17), any penalty term is present, although one would expect it for obstacle problems, having the method from [26] in mind. The role of the penalty here is played by the smoothed characteristic function modifying the volume constraint in the set $\mathcal{K}_V^\delta$. The maximum principle then yields the estimate (5.1.14), as proved in Lemma 5.1.2. Therefore, a penalty of the type $-1/\delta(u^\delta)^-$ on the right-hand side of (5.1.10) is unnecessary, though all the proofs would hold true also with such penalty present.

Next, we interpolate the minimizers $u^{\delta,n}$, $n = 0, 1, 2, \dots, N$ in time, i.e., we introduce the following functions (see Figure 3.1):

$$\bar{u}^{\delta,h}(t,x) = \begin{cases} u_0(x), & t = 0 \\ u^{\delta,n}(x), & t \in ((n-1)h, nh],\ n = 1, \dots, N \end{cases} \tag{5.1.19}$$

$$u^{\delta,h}(t,x) = \begin{cases} u_0(x), & t = 0 \\ \frac{t-(n-1)h}{h} u^{\delta,n}(x) + \frac{nh-t}{h} u^{\delta,n-1}(x), & t \in ((n-1)h, nh], n = 1, \dots, N \end{cases}$$

$$\bar{\lambda}^{\delta,h}(t) = \lambda^{\delta,n}, \quad t \in ((n-1)h, nh],\ n = 1, \dots, N$$

The values $\lambda^{\delta,n}$ are defined later.

We prove Theorem 5.1.1 by sending h to zero in the following lemmata. Above all, we have to show that there exists a minimizer of J_n^δ, that the functions $u^{\delta,h}$ are bounded in a certain norm and that they converge to a weak solution of the approximate problem (5.1.10).

Lemma 5.1.1. *There exists a minimizer $u^{\delta,n} \in \mathcal{K}_V^\delta$ of the functional J_n^δ from (5.1.17) for each $n = 1, 2, \dots, N$.*

Proof. Let $\{u_k\}_{k=1}^\infty \subset \mathcal{K}_V^\delta$ be a minimizing sequence: $J_n^\delta(u_k) \searrow \inf_{\mathcal{K}_V^\delta} J_n^\delta$. Since $J_n^\delta \neq \infty$ on $\mathcal{K}_V^\delta$, there is a function $u_1 \in \mathcal{K}_V^\delta$ such that $J_n^\delta(u_1) < \infty$. Then we have the estimate

$$\int_\Omega \Big(\frac{|u_k - u^{\delta,n-1}|^2}{2h} + \frac{1}{2}|\nabla u_k|^2 + \gamma\chi_\varepsilon(u_k) \Big)\, dx \le J_n^\delta(u_1) < \infty$$

and we immediately see that the minimizing sequence is bounded in $H_0^1(\Omega)$. Hence, there is a subsequence (denoted again by u_k) and a function $u \in H_0^1(\Omega)$ such that

$$\begin{aligned} u_k &\rightharpoonup u \quad \text{weakly in } H^1(\Omega), \\ u_k &\to u \quad \text{strongly in } L^2(\Omega). \end{aligned}$$

Moreover, u belongs to $\mathcal{K}_V^\delta$, which is seen from the following relations:

$$\Big| \frac{d}{du}(\tilde{\chi}_\delta(u)u) \Big| = |\tilde{\chi}_\delta'(u)u + \tilde{\chi}_\delta(u)| \le C(|u| + 1) \tag{5.1.20}$$

and, therefore,

$$\begin{aligned} \Big| \int_\Omega \tilde{\chi}_\delta(u)u\, dx - V \Big| &\le \int_\Omega |\tilde{\chi}_\delta(u)u - \tilde{\chi}_\delta(u_k)u_k|\ dx \\ &\le C \int_\Omega |u - u_k|\, (1 + |u| + |u_k|)\ dx \to 0 \qquad \text{as } k \to \infty. \end{aligned}$$

Since functional J_n^δ is lower-semicontinuous with respect to the sequentially weak convergence in $H^1(\Omega)$, we have

$$J_n^\delta(u) \le \liminf_{k\to\infty} J_n^\delta(u_k) = \inf_{\mathcal{K}_V^\delta} J_n^\delta,$$

confirming that u is a minimizer. □

Lemma 5.1.2. *The approximate solution is bounded from below:*

$$u^{\delta,n} \ge -\delta \qquad a.e.\ in\ \Omega, \tag{5.1.21}$$

and satisfies for almost every $t \in (0,T)$ the estimate

$$\|u_t^{\delta,h}\|^2_{L^2(Q_t)} + \|\nabla \bar{u}^{\delta,h}(t)\|^2_{L^2(\Omega)} + 2\int_\Omega \gamma\chi_\varepsilon(\bar{u}^{\delta,h}(t))\,dx \le C, \tag{5.1.22}$$

where C depends on $\|u_0\|_{H_0^1(\Omega)}$ and $\|\gamma\|_{L^1(\Omega)}$ but is independent of h and δ.

Proof. We prove the first assertion by mathematical induction. For $n=0$, we have $u^{\delta,0} = u_0 \ge 0$. It remains to show that if $u^{\delta,n-1} \ge -\delta$ a.e. in Ω, then (5.1.21) holds. If $u^{\delta,n}$ belongs to $\mathcal{K}_V^\delta$, then setting

$$\tilde{u}^{\delta,n} = (u^{\delta,n} + \delta)\chi_{u^{\delta,n} > -\delta} - \delta$$

(i.e., cutting at $-\delta$), we find that $\tilde{u}^{\delta,n} \in \mathcal{K}_V^\delta$ (see [12], Chapter 7.4) and

$$J_n^\delta(\tilde{u}^{\delta,n}) \le J_n^\delta(u^{\delta,n}).$$

This is because the first and last terms of the functional (5.1.17) do not increase by the cutting, the gradient term also does not increase (see again [12]) and the χ_ε-term does not change.

Thus, there is at least a minimizer satisfying (5.1.21). In addition, if the set of $x \in \Omega$ where $u^{\delta,n}(x) < -\delta$ has positive measure, we have $J_n^\delta(\tilde{u}^{\delta,n}) < J_n^\delta(u^{\delta,n})$ because the first and last terms of the functional increase sharply.

From the relation $J_n^\delta(u^{\delta,n}) \le J_n^\delta(u^{\delta,n-1})$ we derive

$$\int_\Omega \Big(\frac{|u^{\delta,n} - u^{\delta,n-1}|^2}{2h} + \frac{1}{2}|\nabla u^{\delta,n}|^2 + \chi_\varepsilon(u^{\delta,n})\Big)\,dx \le \int_\Omega \Big(\frac{1}{2}|\nabla u^{\delta,n-1}|^2 + \chi_\varepsilon(u^{\delta,n-1})\Big)\,dx.$$

Summing from $n=1$ to l, we obtain

$$\begin{aligned} h\sum_{n=1}^{l} \Big\|\frac{u^{\delta,n} - u^{\delta,n-1}}{h}\Big\|^2_{L^2(\Omega)} &+ \|\nabla u^{\delta,l}\|^2_{L^2(\Omega)} + 2\int_\Omega \gamma\chi_\varepsilon(u^{\delta,l})\,dx \\ &\le \|\nabla u_0\|^2_{L^2(\Omega)} + 2\int_\Omega \gamma\chi_\varepsilon(u_0)\,dx \\ &\le \|\nabla u_0\|^2_{L^2(\Omega)} + 2\|\gamma\|_{L^1(\Omega)} = C(u_0,\gamma). \end{aligned}$$

This readily yields (5.1.22). □

Lemma 5.1.3. *The minimizer $u^{\delta,n}$ satisfies the following weak formula*

$$\int_\Omega \Big(\frac{u^{\delta,n}-u^{\delta,n-1}}{h}\varphi + \nabla u^{\delta,n}\nabla\varphi + \gamma\chi_\varepsilon'(u^{\delta,n})\varphi\Big)\,dx \tag{5.1.23}$$
$$= \lambda^{\delta,n}\int_\Omega \big(\tilde\chi_\delta(u^{\delta,n}) + \tilde\chi_\delta'(u^{\delta,n})u^{\delta,n}\big)\,\varphi\,dx \qquad \forall\varphi\in H_0^1(\Omega),$$

where

$$\lambda^{\delta,n} = \frac{\int_\Omega \big(\frac{u^{\delta,n}-u^{\delta,n-1}}{h}u^{\delta,n} + |\nabla u^{\delta,n}|^2 + \gamma\chi_\varepsilon'(u^{\delta,n})u^{\delta,n}\big)\,dx}{V + \int_\Omega \tilde\chi_\delta'(u^{\delta,n})(u^{\delta,n})^2\,dx}. \tag{5.1.24}$$

Proof. We derive the weak formulation corresponding to the minimizing problem (5.1.17). It is possible to introduce Lagrange multipliers $\lambda^{\delta,n}$ (see [8], Chapter 8.4, or Chapter 3 of this thesis) and compute the first variation of the functional

$$I_n^\delta(u) = J_n^\delta(u) - \lambda^{\delta,n}\int_\Omega \tilde\chi_\delta(u)u\,dx$$

to obtain (5.1.23) for test functions $\varphi\in C_0^\infty(\Omega)$. Using the density argument, we note that (5.1.23) holds, indeed, for all $\varphi\in H_0^1(\Omega)$. The form of $\lambda^{\delta,n}$ is derived by putting $\varphi = u^{\delta,n}$ in (5.1.23). □

Lemma 5.1.4. *Let u_0 be bounded in Ω. Then the approximate solutions $u^{\delta,h}$ are uniformly bounded in $L^\infty(Q_T)$ with respect to h and δ.*

Proof. Rewriting (5.1.23) in terms of $u^{\delta,h}$ and integrating with respect to time, we have

$$\int_0^T\int_\Omega \Big(u_t^{\delta,h}\varphi + \nabla\bar u^{\delta,h}\nabla\varphi + \gamma\chi_\varepsilon'(\bar u^{\delta,h})\varphi\Big)\,dx\,dt \tag{5.1.25}$$
$$= \int_0^T \bar\lambda^{\delta,h}\int_\Omega \big(\tilde\chi_\delta(\bar u^{\delta,h}) + \tilde\chi_\delta'(\bar u^{\delta,h})\bar u^{\delta,h}\big)\,\varphi\,dx\,dt \quad \forall\varphi\in L^2(0,T;H_0^1(\Omega)),$$

where $\bar\lambda^{\delta,h}$ is defined in (5.1.19). We remark that owing to (5.1.22) and (5.1.31) below it is, indeed, possible to allow test functions from $L^2(0,T;H_0^1(\Omega))$.

Thus, upon choosing the test function $\varphi = \bar u^{\delta,h}_{(k)} = \max\{\bar u^{\delta,h}-k,0\}$ for some $k>0$, the above becomes

$$\int_0^T\int_\Omega \Big(u_t^{\delta,h}\bar u^{\delta,h}_{(k)} + \nabla\bar u^{\delta,h}\nabla\bar u^{\delta,h}_{(k)} + \gamma\chi_\varepsilon'(\bar u^{\delta,h})\bar u^{\delta,h}_{(k)}\Big)\,dx\,dt$$
$$= \int_0^T \bar\lambda^{\delta,h}\int_\Omega \big(\tilde\chi_\delta(\bar u^{\delta,h}) + \tilde\chi_\delta'(\bar u^{\delta,h})\bar u^{\delta,h}\big)\,\bar u^{\delta,h}_{(k)}\,dx\,dt. \tag{5.1.26}$$

Since we have a parabolic problem without free boundary, we can proceed similarly as in

Section 4.1 using the results of [22]. We compute

$$\begin{aligned}
\int_0^T \int_\Omega u_t^{\delta,h} u_{(k)}^{\delta,h}\, dx\, dt &= \int_0^T \int_\Omega \frac{1}{2}\frac{d}{dt}(u_{(k)}^{\delta,h})^2\, dx\, dt \\
&= \int_\Omega \frac{1}{2}\left((u_{(k)}^{\delta,h})^2(T) - (u_{(k)}^{\delta,h})^2(0)\right)\, dx \\
&= \int_\Omega \frac{1}{2}(u_{(k)}^{\delta,h})^2(T)\, dx \\
&= \int_\Omega \frac{1}{2}(\bar{u}_{(k)}^{\delta,h})^2(T)\, dx,
\end{aligned}$$

where we assume that k is chosen large enough for $u(0,x) < k$ to hold almost everywhere. Then, remembering from Lemma 4.1.4 that

$$\int_0^T \int_\Omega u_t^{\delta,h}(\bar{u}_{(k)}^{\delta,h} - u_{(k)}^{\delta,h})\, dx\, dt \geq 0,$$

we can rearrange the first term on the left-hand side of (5.1.26) to write

$$\begin{aligned}
\int_0^T \int_\Omega u_t^{\delta,h} \bar{u}_{(k)}^{\delta,h}\, dx\, dt &= \int_0^T \int_\Omega u_t^{\delta,h} u_{(k)}^{\delta,h}\, dx\, dt + \int_0^T \int_\Omega u_t^{\delta,h}(\bar{u}_{(k)}^{\delta,h} - u_{(k)}^{\delta,h})\, dx\, dt \\
&\geq \frac{1}{2}\int_\Omega (\bar{u}_{(k)}^{\delta,h})^2(T)\, dx.
\end{aligned}$$

For the gradient term we have

$$\int_0^T \int_\Omega \nabla \bar{u}^{\delta,h} \nabla \bar{u}_{(k)}^{\delta,h}\, dx\, dt = \int_0^T \int_\Omega |\nabla \bar{u}_{(k)}^{\delta,h}|^2\, dx\, dt.$$

Finally, we see that

$$\int_0^T \int_\Omega \gamma \chi_\varepsilon'(\bar{u}^{\delta,h}) \bar{u}_{(k)}^{\delta,h}\, dx\, dt \geq 0.$$

Denoting the norm

$$|u|_{Q_T} = \left(\frac{1}{2}\int_\Omega u^2(T)\, dx + \int_0^T \int_\Omega |\nabla u|^2\, dx\, dt\right)^{1/2},$$

we arrive at the inequality

$$|\bar{u}_{(k)}^{\delta,h}|_{Q_T}^2 \leq \int_0^T \bar{\lambda}^{\delta,h} \int_\Omega \left(\tilde{\chi}_\delta(\bar{u}^{\delta,h}) + \tilde{\chi}_\delta'(\bar{u}^{\delta,h})\bar{u}^{\delta,h}\right) \bar{u}_{(k)}^{\delta,h}\, dx\, dt. \tag{5.1.27}$$

Since $\tilde{\chi}_\delta'$ is nonzero only for negative arguments and $|\tilde{\chi}_\delta|$ is bounded by the constant 1, (5.1.27) implies

$$|\bar{u}_{(k)}^{\delta,h}|_{Q_T}^2 \leq \int_0^T \int_\Omega |\bar{\lambda}^{\delta,h} \bar{u}_{(k)}^{\delta,h}|\, dx\, dt. \tag{5.1.28}$$

We now proceed to investigate the term on the right-hand side of (5.1.28) for space dimension $m > 2$. Specifically, we apply Young's inequality with exponents $2^* = \frac{2m}{m-2} \in (2,6]$ and $2^{*\prime} = \frac{2m}{m+2} \in [\frac{6}{5}, 2)$ to obtain

$$\int_0^T \int_\Omega |\bar{\lambda}^{\delta,h} \bar{u}^{\delta,h}_{(k)}|\, dx\, dt \le C_\epsilon \int_0^T (\bar{\lambda}^{\delta,h})^{2^{*\prime}} |A_k|\, dt + \epsilon \int_0^T \int_{A_k} (\bar{u}^{\delta,h}_{(k)})^{2^*}\, dx\, dt, \tag{5.1.29}$$

where $A_k(t) = \{x : \bar{u}^{\delta,h}(x,t) > k\}$, $|A_k|$ denotes the Lebesgue measure of A_k, and C_ϵ is a constant independent of h and δ. The second term is estimated by the Sobolev imbedding theorem $H^1(\Omega) \subset L^{2^*}(\Omega)$ and can be absorbed into the left-hand side if ϵ is chosen small enough. In this estimate, we utilise the estimate (5.1.22) and the fact that $2^*/2 \in (1,3]$ to find

$$\int_0^T \int_{A_k} (\bar{u}^{\delta,h}_{(k)})^{2^*}\, dx\, dt \le C'_S \int_0^T \left(\int_{A_k} |\nabla \bar{u}^{\delta,h}_{(k)}|^2\, dx \right)^{2^*/2} dt \le C \int_0^T \int_{A_k} |\nabla \bar{u}^{\delta,h}_{(k)}|^2\, dx\, dt,$$

where C'_S is a constant (independent of h and δ) obtained from the Sobolev imbedding.

In order to estimate the remaining term on the right-hand side of (5.1.29), we provide some auxiliary results. Since $\tilde{\chi}_\delta$ is nondecreasing, we see that

$$\frac{1}{V + \int_\Omega \tilde{\chi}'_\delta(u^{\delta,n})(u^{\delta,n})^2\, dx} \le \frac{1}{V}. \tag{5.1.30}$$

Employing (5.1.24), (5.1.22) and (5.1.30),

$$\begin{aligned}
\int_0^T (\bar{\lambda}^{\delta,h})^2\, dt &\le \frac{1}{V^2} \int_0^T \left[\int_\Omega \left(u^{\delta,h}_t \bar{u}^{\delta,h} + |\nabla \bar{u}^{\delta,h}|^2 + \gamma \chi'_\varepsilon(\bar{u}^{\delta,h}) \bar{u}^{\delta,h} \right) dx \right]^2 dt \\
&\le \frac{1}{V^2} \int_0^T \left[C + 2 \left(\int_\Omega (\bar{u}^{\delta,h})^2\, dx \right) \left(\int_\Omega (u^{\delta,h}_t)^2\, dx \right) \right] dt \\
&\le C \left(1 + \int_0^T \int_\Omega (u^{\delta,h}_t)^2\, dx\, dt \right) \\
&\le C.
\end{aligned} \tag{5.1.31}$$

Note that the last constant C depends neither on h nor on δ.

Now, we can apply Hölder's inequality on the first term in (5.1.29) with exponents $2/2^{*\prime} = \frac{m+2}{m} \in (1, \frac{5}{3}]$ and $(2/2^{*\prime})' = \frac{m+2}{2} \ge \frac{5}{2}$. This, together with estimate (5.1.31), yields

$$\begin{aligned}
\int_0^T (\bar{\lambda}^{\delta,h})^{2^{*\prime}} |A_k|\, dt &\le \left(\int_0^T (\bar{\lambda}^{\delta,h})^2\, dt \right)^{\frac{2^{*\prime}}{2}} \left(\int_0^T |A_k|^{(2/2^{*\prime})'}\, dt \right)^{\frac{1}{(2/2^{*\prime})'}} \\
= \left(\int_0^T (\bar{\lambda}^{\delta,h})^2\, dt \right)^{\frac{m}{m+2}} &\left(\int_0^T |A_k|^{\frac{m+2}{2}}\, dt \right)^{\frac{2}{m+2}} \le C \left(\int_0^T |A_k|^{\frac{m+2}{2}}\, dt \right)^{\frac{2}{m+2}}.
\end{aligned}$$

Therefore, having started this investigation from (5.1.28), we have acquired the inequality

$$|\bar{u}^{\delta,h}_{(k)}|_{Q_T} \le C \left(\int_0^T |A_k|^{\frac{m+2}{2}}\, dt \right)^{\frac{1}{m+2}},$$

where C is a constant independent of h and δ. We apply the result from [22] (see Section 4.1.3) to the above inequality. This provides us with the following bound for the weak solution:

$$\max_{Q_T} u^{\delta,h} \leq C, \tag{5.1.32}$$

with C independent of h and δ. Combining this result with (5.1.21), we conclude that the statement of the Lemma is proved for $m > 2$.

For $m = 1$ the uniform boundedness follows directly from the Sobolev imbedding $H^1(\Omega) \subset C(\Omega)$ and (5.1.22):

$$\max_{Q_T} |\bar{u}^{\delta,h}(t,x)| \leq \max_{t\in[0,T]} \max_{x\in\Omega} |\bar{u}^{\delta,h}(t,x)| \leq \max_{t\in[0,T]} C\|\bar{u}^{\delta,h}(t)\|_{H^1(\Omega)} \leq C.$$

For the case $m = 2$ we use the imbedding $H_0^1(\Omega) \subset L^p(\Omega)$ for all $p \in [1,\infty)$. For example, we can use exponents 3, 3/2, instead of 2^*, $(2^*)'$ in (5.1.29) and estimate the second term on the right-hand side by the mentioned imbedding. The first term then gives

$$|\bar{u}_{(k)}^{\delta,h}|_{Q_T} \leq C\left(\int_0^T |A_k|^4\,dt\right)^{1/8},$$

which is an estimate yielding the boundedness according to [22]. □

Lemma 5.1.5. *There is a subsequence of $u^{\delta,h}$ converging to a weak solution of the approximate problem (5.1.10) defined in (5.1.13), which satisfies volume condition (5.1.15).*

Proof. From (5.1.22) we obtain the uniform boundedness of $u^{\delta,h}$ in $H_0^1(Q_T)$. Therefore, there is a subsequence $u^{\delta,h}$ and a function $u^\delta \in H^1(Q_T) \cap L^\infty(0,T;H_0^1(\Omega))$ such that

$$u_t^{\delta,h} \rightharpoonup u_t^\delta \quad \text{weakly in } L^2(Q_T) \tag{5.1.33}$$

$$\nabla\bar{u}^{\delta,h} \rightharpoonup \nabla u^\delta \quad \text{weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)) \tag{5.1.34}$$

$$u^{\delta,h} \rightharpoonup u^\delta \quad \text{weakly in } H^1(Q_T) \tag{5.1.35}$$

$$\bar{u}^{\delta,h}, u^{\delta,h} \to u^\delta \quad \text{strongly in } L^2(Q_T). \tag{5.1.36}$$

First two convergences follow immediately from estimate (5.1.22). Since it can be checked (see Lemma 3.1.2) that

$$\|\nabla u^{\delta,h}\|_{L^2(Q_T)}^2 \leq \|\nabla\bar{u}^{\delta,h}\|_{L^2(Q_T)}^2 + \frac{h}{2}\|\nabla u_0\|_{L^2(\Omega)}^2,$$

we have also the boundedness of $\nabla u^{\delta,h}$ in $L^2(Q_T)$ and (5.1.35) follows. Rellich's imbedding theorem gives the strong convergence of $u^{\delta,h}$ in $L^2(Q_T)$, and the identity

$$\|u^{\delta,h} - \bar{u}^{\delta,h}\|_{L^2(Q_T)} = \frac{h}{\sqrt{3}}\|u_t^{\delta,h}\|_{L^2(Q_T)}$$

assures that both $u^{\delta,h}$ and $\bar{u}^{\delta,h}$ converge to the same function. Moreover, we can prove that the volume condition (5.1.15) holds for u^δ by the same arguments as in (5.1.20).

It remains to prove that u^δ is a weak solution of (5.1.10). Let $\varphi \in C^\infty([0,T]; C_0^\infty(\Omega))$. Since $\gamma\chi_\varepsilon' \le C\gamma \in L^1(\Omega)$ and (5.1.36) holds, we get

$$\int_0^T \int_\Omega \gamma\chi_\varepsilon'(\bar{u}^{\delta,h})\varphi\,dx\,dt \to \int_0^T \int_\Omega \gamma\chi_\varepsilon'(u^\delta)\varphi\,dx\,dt.$$

Using (5.1.33)–(5.1.36) again, we can pass to the limit as $h \to 0+$ in the left-hand side of (5.1.25).

We shall study the limit process in the right-hand side. First, we provide some preparatory results. Noting that

$$\left|\frac{d}{du}(\tilde{\chi}_\delta(u) + \tilde{\chi}_\delta'(u)u)\right| = |2\tilde{\chi}_\delta'(u) + \tilde{\chi}_\delta''(u)u| \le C(|u|+1),$$

we have for any $\varphi \in C^\infty(\bar{Q}_T)$

$$\begin{aligned}
&\int_0^T \left[\int_\Omega \left(\tilde{\chi}_\delta(u^{\delta,h}) + \tilde{\chi}_\delta'(u^{\delta,h})u^{\delta,h} - \tilde{\chi}_\delta(u^\delta) - \tilde{\chi}_\delta'(u^\delta)u^\delta\right)\varphi\,dx\right]^2 dt \\
&\le C\int_0^T \left(\int_\Omega (u^{\delta,h} - u^\delta)^2\,dx\right)\left(\int_\Omega (1+|u^\delta| + |u^{\delta,h}|)^2\varphi^2\,dx\right) dt \\
&\le C\int_0^T \int_\Omega (u^{\delta,h} - u^\delta)^2\,dx\,dt \to 0 \qquad \text{as } h \to 0+,
\end{aligned}$$

which shows that

$$\int_\Omega \left(\tilde{\chi}_\delta(u^{\delta,h}) + \tilde{\chi}_\delta'(u^{\delta,h})u^{\delta,h}\right)\varphi\,dx \ \to \ \int_\Omega \left(\tilde{\chi}_\delta(u^\delta) + \tilde{\chi}_\delta'(u^\delta)u^\delta\right)\varphi\,dx$$

in $L^2(0,T)$. Further, (5.1.31) implies that (after taking a subsequence) there is a $\kappa^\delta \in L^2(0,T)$ such that

$$\bar{\lambda}^{\delta,h} \rightharpoonup \kappa^\delta \qquad \text{weakly in } L^2(0,T).$$

Now, we can pass to the limit as $h \to 0+$ in (5.1.25) getting an identity similar to the weak formulation of (5.1.10): for all $\varphi \in C^\infty([0,T]; C_0^\infty(\Omega))$

$$\begin{aligned}
\int_0^T \int_\Omega \Big(u_t^\delta\varphi + \nabla u^\delta \nabla\varphi + \gamma\chi_\varepsilon'(u^\delta)\varphi\Big)\,dx\,dt& \\
= \int_0^T \kappa^\delta \int_\Omega \left(\tilde{\chi}_\delta(u^\delta) + u^\delta\tilde{\chi}_\delta'(u^\delta)\right)\varphi\,dx\,dt.&
\end{aligned} \tag{5.1.37}$$

By a density argument, (5.1.37) holds for all functions $\varphi \in L^2(0,T; H_0^1(\Omega))$. It suffices to put here

$$\varphi(t,x) = \begin{cases} u^\delta(t,x), & t \le t_0 \\ 0, & t > t_0, \end{cases}$$

for arbitrary $t_0 \in (0,T)$ in order to check that κ^δ has the form (5.1.11).

The validity of initial condition can be proved by the use of Mazur's theorem as in the previous proofs. We present here another simple proof. Let $\varphi = \zeta\psi_h$ in (5.1.23), where $\zeta \in H_0^1(\Omega)$ and ψ_h is a piecewise constant function on the time partition (i.e., $\psi(t) = \psi(nh-h)$ for $t \in [nh-h, nh))$ converging strongly in $L^2(0,T)$ to some $\psi \in C([0,T])$ (for each such ψ there exists the mentioned approximation). Integration over time in (5.1.23) is equivalent to multiplication by h and summation from $n = 1$ to N. Since for the first term we have

$$\begin{aligned} h \sum_{n=1}^{N} \int_\Omega & \frac{u^{\delta,n} - u^{\delta,n-1}}{h} \zeta \psi_h(nh-h)\, dx \\ &= -h \sum_{n=1}^{N} \int_\Omega u^{\delta,n} \zeta \frac{\psi_h(nh) - \psi_h(nh-h)}{h}\, dx + \int_\Omega \big(u^{\delta,N} \zeta \psi_h(Nh) - u^{\delta,0} \zeta \psi_h(0) \big)\, dx \\ &= -h \sum_{n=1}^{N} \int_\Omega u^{\delta,n} \zeta \frac{\psi_h(nh) - \psi_h(nh-h)}{h}\, dx + \int_\Omega \big(u^{\delta,N} \zeta \psi_h(T) - u_0 \zeta \psi_h(0) \big)\, dx, \end{aligned}$$

we obtain from (5.1.23) in the limit the identity

$$\begin{aligned} \int_0^T \int_\Omega & \Big(- u^\delta \zeta \psi_t + \nabla u^\delta \nabla \zeta \psi + \gamma \chi'_\varepsilon(u^\delta) \zeta \psi \Big)\, dx\, dt \\ &= \int_0^T \lambda^\delta \int_\Omega \big(\tilde{\chi}_\delta(u^\delta) + u^\delta \tilde{\chi}'_\delta(u^\delta) \big) \zeta \psi\, dx\, dt + \int_\Omega \big(- u^\delta(T) \zeta \psi(T) + u_0 \zeta \psi(0) \big)\, dx, \end{aligned}$$

which implies

$$\begin{aligned} \int_0^T \int_\Omega & \Big(- u^\delta \varphi_t + \nabla u^\delta \nabla \varphi + \gamma \chi'_\varepsilon(u^\delta) \varphi \Big)\, dx\, dt \\ &= \int_0^T \lambda^\delta \int_\Omega \big(\tilde{\chi}_\delta(u^\delta) + u^\delta \tilde{\chi}'_\delta(u^\delta) \big) \varphi\, dx\, dt + \int_\Omega u_0 \varphi(0)\, dx \end{aligned}$$

for all $\varphi \in L^2(0,T; H_0^1(\Omega))$ with $\varphi_t \in L^2(0,T; H^{-1}(\Omega))$ and $\varphi(T) = 0$. Comparing the above result to (5.1.13) yields $u^\delta(0) = u_0$.

Thus, we have proved that u^δ complies with the definition of a weak solution. □

Lemma 5.1.6. *The constructed weak solution to the approximate problem (5.1.10) satisfies estimates (5.1.14) and (5.1.16).*

Proof: Estimate (5.1.14) follows immediately from (5.1.21) and the strong convergence of $u^{\delta,h}$. Estimate (5.1.16) might be derived by putting $\varphi = u_t$ in the weak equation (5.1.13). However, for this kind of proof we need the regularity $u^\delta \in H^1(0,T; H_0^1(\Omega))$ which would be necessary to prove. Nevertheless, we may use directly (5.1.22). From the properties of weak convergence, we immediately obtain the desired estimate, since the constant in (5.1.22) does not depend on δ. □

Lemma 5.1.7. *Weak solutions to the approximate problems (5.1.10) are uniformly Hölder continuous with respect to δ on $\bar{Q}_T$.*

Proof. It is sufficient to check that u^δ belongs to a class $\mathcal{B}_2(Q_T, M, \beta, r, d, \kappa)$, where all the constants describing the class are independent of δ. This class is introduced in Definition 4.1.2 of Section 4.1.

One can see that $u \in \mathcal{B}_2(Q_T, M, \beta, r, d, \kappa)$ follows if the condition below is satisfied for any piecewise smooth continuous function ζ with $0 \le \zeta \le 1$ which vanishes on the lateral surface of the cylinder $Q(\rho, \tau) = \{(t, x) \in Q_T : t \in (t, t + \tau_0),\ x \in B_\rho\}$.

$$\begin{aligned} &\int_{B_\rho} (w_{(k)}(x, t_0 + \tau))^2 \zeta^2(x, t_0 + \tau)\, dx + C \int_{t_0}^{t_0+\tau} \int_{B_\rho} |\nabla w_{(k)}|^2 \zeta^2\, dx\, dt \\ &\le \int_{B_\rho} (w_{(k)}(x, t_0))^2 \zeta^2(x, t_0)\, dx \\ &+ \tilde{\beta} \left[\int_{Q(\rho,\tau)} (|\nabla \zeta|^2 + \zeta |\zeta_t|) w_{(k)}^2\, dx\, dt + \Big(\int_{t_0}^{t_0+\tau} \big(\int_{A_{k,\rho}(t)} \zeta\, dx \big)^{\frac{r}{q}} dt \Big)^{\frac{2}{r}(1+\kappa)} \right]. \end{aligned} \tag{5.1.38}$$

By (5.1.13), we have for every $\varphi \in L^2(0, T; H_0^1(\Omega))$

$$\int_0^T \int_\Omega \Big(u_t^\delta \varphi + \nabla u^\delta \nabla \varphi + \gamma \chi_\varepsilon'(u^\delta) \varphi \Big) = \int_0^T \lambda^\delta \int_\Omega \big(\tilde{\chi}_\delta(u^\delta) + u^\delta \tilde{\chi}_\delta'(u^\delta) \big)\, \varphi.$$

We choose $\varphi = \zeta^2 u_{(k)}^\delta$ with ζ supported in $Q(\rho, \tau)$ as in (5.1.38), and we obtain

$$\begin{aligned} &\int_{Q(\rho,\tau)} \Big(u_t^\delta u_{(k)}^\delta \zeta^2 + \nabla u_{(k)}^\delta \nabla (\zeta^2 u_{(k)}^\delta) \Big)\, dx\, dt \\ &\quad = \int_{Q(\rho,\tau)} \Big(\lambda^\delta \big(\tilde{\chi}_\delta(u^\delta) u_{(k)}^\delta + \tilde{\chi}_\delta'(u^\delta) u^\delta u_{(k)}^\delta \big) \zeta^2 - \gamma \chi_\varepsilon'(u^\delta) u_{(k)}^\delta \zeta^2 \Big)\, dx\, dt. \end{aligned} \tag{5.1.39}$$

The first term in (5.1.39) becomes

$$\begin{aligned} \int_{Q(\rho,\tau)} u_t^\delta u_{(k)}^\delta \zeta^2\, dx\, dt &= \frac{1}{2} \int_{Q(\rho,\tau)} \frac{\partial}{\partial t} \big((u_{(k)}^\delta)^2 \big) \zeta^2\, dx\, dt \\ &= - \int_{Q(\rho,\tau)} (u_{(k)}^\delta)^2 \zeta \zeta_t\, dx\, dt \\ &\quad + \frac{1}{2} \int_{B_\rho} [(u_{(k)}^\delta)^2 \zeta^2](x, t_0 + \tau)\, dx - \frac{1}{2} \int_{B_\rho} [(u_{(k)}^\delta)^2 \zeta^2](x, t_0)\, dx. \end{aligned}$$

The second term in (5.1.39) gives

$$\begin{aligned} &\int_{Q(\rho,\tau)} \nabla u_{(k)}^\delta \nabla (\zeta^2 u_{(k)}^\delta)\, dx\, dt \\ &\qquad = \int_{Q(\rho,\tau)} |\nabla u_{(k)}^\delta|^2 \zeta^2\, dx\, dt + 2 \int_{Q(\rho,\tau)} \nabla u_{(k)}^\delta \nabla \zeta u_{(k)}^\delta \zeta\, dx\, dt, \end{aligned}$$

where we estimate

$$-2 \int_{Q(\rho,\tau)} \nabla u_{(k)}^\delta \nabla \zeta u_{(k)}^\delta \zeta\, dx\, dt \le \frac{1}{2} \int_{Q(\rho,\tau)} |\nabla u_{(k)}^\delta|^2 \zeta^2\, dx\, dt + 2 \int_{Q(\rho,\tau)} (u_{(k)}^\delta)^2 |\nabla \zeta|^2\, dx\, dt. \tag{5.1.40}$$

Since $u^\delta_{(k)}$, γ and χ'_ε are nonnegative, we have

$$-\int_{Q(\rho,\tau)} \gamma\chi'_\varepsilon(u^\delta)u^\delta_{(k)}\zeta^2\,dx\,dt \le 0. \tag{5.1.41}$$

The estimate of the term with Lagrange multiplier is achieved by using (5.1.14), (5.1.31) and the properties of $\tilde\chi_\delta$:

$$\begin{aligned}
&\int_{Q(\rho,\tau)} \lambda^\delta\left(\tilde\chi_\delta(u^\delta)u^\delta_{(k)} + \tilde\chi'_\delta(u^\delta)u^\delta u^\delta_{(k)}\right)\zeta^2\,dx\,dt \\
&\quad\le C\int_{t_0}^{t_0+\tau}\Big(|\lambda^\delta|\int_{B_\rho} u^\delta_{(k)}\zeta^2\,dx\Big)\,dt \le C(M)\int_{t_0}^{t_0+\tau}\Big(|\lambda^\delta|\int_{A_{k,\rho}}\zeta\,dx\Big)\,dt \\
&\quad\le C\Big(\int_{t_0}^{t_0+\tau}(\lambda^\delta)^2\,dt\Big)^{1/2}\Big(\int_{t_0}^{t_0+\tau}\big(\int_{A_{k,\rho}}\zeta\,dx\big)^2\,dt\Big)^{1/2} \\
&\quad\le C\Big(\int_{t_0}^{t_0+\tau}\big(\int_{A_{k,\rho}}\zeta\,dx\big)^2\,dt\Big)^{1/2}.
\end{aligned} \tag{5.1.42}$$

Estimates (5.1.39)–(5.1.42) yield (5.1.38) if we can appropriately determine the constants q, r and κ. We set

$$\kappa = 1/m, \quad q = 2(1+\kappa), \quad r = 4(1+\kappa).$$

Then $r/q = 2$ and $2(1+\kappa)/r = 1/2$. Moreover, q and r satisfy (4.1.30):

$$\frac{1}{r} + \frac{m}{2q} = \frac{1}{4(1+\kappa)} + \frac{m}{4(1+\kappa)} = \frac{m}{4}.$$

The estimate for $w^\delta := -u^\delta$ is derived analogously. The weak equation multiplied by -1 gives

$$\int_0^T\int_\Omega w^\delta_t\varphi + \nabla w^\delta\nabla\varphi - \gamma\chi'_\varepsilon(-w^\delta)\varphi = \int_0^T\lambda^\delta\int_\Omega\left(-\tilde\chi_\delta(-w^\delta) + w^\delta\tilde\chi'_\delta(-w^\delta)\right)\varphi.$$

Again, we consider the test function $\zeta^2 w^\delta_{(k)}$. The nonlinear lower order terms can be estimated in a similar way, except (5.1.41), where we use the boundedness of the functions:

$$\int_{Q(\rho,\tau)}\gamma\chi'_\varepsilon(-w^\delta)w^\delta_{(k)}\zeta^2\,dx\,dt \le C\Big(\int_{t_0}^{t_0+\tau}\big(\int_{A_{k,\rho}}\zeta\,dx\big)^2\,dt\Big)^{1/2}.$$

Since u_0 is assumed to be Hölder continuous and identities (5.1.38) hold for $\pm u^\delta$ by the same calculations also for cylinders $Q(\rho,\tau)$ intersecting the boundary of Q_T, we can use the results from [22] (Chapter 2.8) to say that functions u^δ are uniformly Hölder continuous in $[0,T]\times\bar\Omega$. □

Lemma 5.1.8. *There exists a δ_0 such that the functions u^δ satisfy for $\delta \le \delta_0$ the following estimate:*

$$\int_\Omega (u^{\delta-})^2(T)\,dx + \int_0^T\int_\Omega |\nabla u^{\delta-}|^2\,dx\,dt \le C\delta. \tag{5.1.43}$$

Proof. The estimate is shown by setting $\varphi = u^{\delta -}$ in (5.1.13). Inserting the form of λ^δ we obtain

$$\int_0^T \int_\Omega \Big(u_t^\delta u^{\delta -} + |\nabla u^{\delta -}|^2 + \gamma \chi_\varepsilon'(u^\delta) u^{\delta -} \Big)\, dx\, dt =$$
$$\int_0^T \frac{\int_\Omega \big(\tilde\chi_\delta(u^\delta) u^{\delta -} + \tilde\chi_\delta'(u^\delta)(u^{\delta -})^2 \big)}{V + \int_\Omega \tilde\chi_\delta'(u^\delta)(u^{\delta -})^2} \int_\Omega \Big(u_t^\delta u^\delta + |\nabla u^\delta|^2 + \gamma \chi_\varepsilon'(u^\delta) u^\delta \Big)\, dx\, dt.$$

Since

$$\Big|\int_\Omega \tilde\chi_\delta(u^\delta) u^{\delta -}\, dx\Big| \le \int_{\{x : u^\delta(x) \in (-\delta, 0)\}} |u^{\delta -}|\, dx \le |\Omega| \delta, \tag{5.1.44}$$
$$\Big|\int_\Omega \tilde\chi_\delta'(u^\delta)(u^{\delta -})^2\, dx\Big| \le \int_{\{x : u^\delta(x) \in (-\delta, 0)\}} \frac{C}{\delta}(u^{\delta -})^2\, dx \le C|\Omega|\delta, \tag{5.1.45}$$

we have for δ small enough the estimate

$$\Big|\frac{\int_\Omega \big(\tilde\chi_\delta(u^\delta) u^{\delta -} + \tilde\chi_\delta'(u^\delta)(u^{\delta -})^2 \big)\ dx}{V + \int_\Omega \tilde\chi_\delta'(u^\delta)(u^{\delta -})^2\ \ dx}\Big| \le \tilde C \delta.$$

We also note that

$$\int_\Omega f^2(x)\, dx = \int_\Omega [(f^-)^2(x) + (f^+)^2(x)]\, dx,$$

and, therefore, we get

$$\int_0^T \int_\Omega u_t^\delta u^{\delta -}\, dx\, dt + (1 - \tilde C \delta) \int_0^T \int_\Omega |\nabla u^{\delta -}|^2\, dx\, dt$$
$$\le \tilde C \delta \int_0^T \int_\Omega \big(|u_t^\delta u^\delta| + |\nabla u^{\delta +}|^2 + \gamma \chi_\varepsilon'(u^\delta) u^\delta \big)\ dx.$$

This gives by (5.1.16) the desired estimate (5.1.43). □

Now we prove the main result - existence of weak solution to (5.1.1)–(5.1.3), the meaning of which is explained in the following Definition.

Definition 5.1.2. *A function belonging to the space $u \in H^1(Q_T) \cap L^\infty(0, T; H_0^1(\Omega))$ is called a weak solution to (5.1.1), provided it satisfies the initial condition (5.1.2) and the identities*

$$\int_0^T \int_\Omega (u_t \varphi + \nabla u \nabla \varphi + \gamma \chi_\varepsilon'(u) \varphi)\ dx\, dt = \int_0^T \int_\Omega \lambda \varphi\, dx\, dt \quad \forall \varphi \in C_0^\infty(Q_T \cap \{u > 0\}),$$
$$u \equiv 0 \qquad in \quad Q_T \setminus \{u > 0\}, \tag{5.1.46}$$

with λ defined in (5.1.6).

Theorem 5.1.2. *There exists a unique weak solution to the problem (5.1.1)–(5.1.3) that is Hölder continuous in $[0, T] \times \bar\Omega$.*

Proof. Recollecting (5.1.16) provides us with a subsequence of $\{u^\delta\}_{\delta>0}$ converging weakly in $H^1(Q_T)$:

$$u_t^\delta \rightharpoonup u_t \qquad \text{weakly in } L^2(Q_T), \tag{5.1.47}$$

$$\nabla u^\delta \rightharpoonup \nabla u \qquad \text{weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)), \tag{5.1.48}$$

$$u^\delta \to u \qquad \text{strongly in } L^2(Q_T). \tag{5.1.49}$$

Moreover, in virtue of the uniform Hölder continuity (see Lemma 5.1.7) and boundedness (see Lemma 5.1.4), we can use the Arzelà-Ascoli theorem to extract another subsequence converging uniformly on Q_T.

We fix an arbitrary function $\varphi \in C_0^\infty(Q_T \cap \{u>0\})$ and denote its support as S_φ. Then we have

$$u^\delta \rightrightarrows u \qquad \text{uniformly in } S_\varphi. \tag{5.1.50}$$

Our goal is to show (5.1.46) for this u and φ by passing to the limit as $\delta \to 0+$ in (5.1.13). First, we have by (5.1.47) and (5.1.48)

$$\int_0^T \int_\Omega \left(u_t^\delta \varphi + \nabla u^\delta \nabla \varphi\right)\, dx\, dt \to \int_0^T \int_\Omega \left(u_t \varphi + \nabla u \nabla \varphi\right)\, dx\, dt.$$

Since χ'_ε is continuous and bounded and $|\gamma \chi'_\varepsilon(u^\delta)\varphi| \le C\gamma \in L^1(\Omega)$, we obtain

$$\int_0^T \int_\Omega \gamma \chi'_\varepsilon(u^\delta)\varphi\, dx\, dt \to \int_0^T \int_\Omega \gamma \chi'_\varepsilon(u)\varphi\, dx\, dt.$$

Also, by the uniform convergence (5.1.50), we see that $u^\delta > 0$ on S_φ for δ small enough. Consequently, we have for small δ the key identity

$$\int_\Omega \left(\tilde\chi_\delta(u^\delta) + u^\delta \tilde\chi'_\delta(u^\delta)\right)\varphi\, dx = \int_\Omega \tilde\chi_\delta(u^\delta)\varphi\, dx = \int_\Omega \varphi\, dx.$$

The support of test functions φ becomes relevant here, reminding us of the role of the characteristic function in (5.1.1). Finally, due to (5.1.31), we have the uniform boundedness of λ^δ in $L^2(0,T)$. Thus, reselecting a subsequence, there is a function $\tilde\lambda \in L^2(0,T)$ such that

$$\lambda^\delta \rightharpoonup \tilde\lambda \qquad \text{weakly in } L^2(0,T).$$

We have arrived at the following identity:

$$\int_0^T \int_\Omega \left(u_t\varphi + \nabla u \nabla \varphi + \gamma \chi'_\varepsilon(u)\varphi\right)\, dx\, dt = \int_0^T \tilde\lambda \int_\Omega \varphi\, dx\, dt. \tag{5.1.51}$$

It remains to show that $\tilde\lambda$ corresponds to the form of λ from (5.1.6), that u is nonnegative and that it satisfies the volume condition (5.1.7). The nonnegativity of u is seen from (5.1.14) and the uniform convergence. Volume preservation is shown, for example, in the following way (compare with the proof of Lemma 5.1.5)

$$\begin{aligned}
\left|\int_\Omega u\chi_{u>0}\, dx - V\right| &= \left|\int_\Omega \left(u\chi_{u>0} - u^\delta \tilde\chi_\delta(u^\delta)\right)\, dx\right| \\
&= \left|\int_\Omega \left(u\tilde\chi_\delta(u) - u^\delta \tilde\chi_\delta(u^\delta)\right)\, dx\right| \\
&\le C\int_\Omega |u-u^\delta|\, dx \to 0 \quad \text{for } \delta \to 0+\,.
\end{aligned}$$

Now, the form of $\tilde{\lambda}$ would be ensured if we could put

$$\varphi(t,x) = \begin{cases} u(t,x), & t \le t_0 \\ 0, & t > t_0 \end{cases} \tag{5.1.52}$$

in (5.1.51). We cannot do so directly because this function does not have compact support inside $\{u > 0\}$. We also cannot apply any approximation technique. Indeed, we only know that function u is a Hölder continuous H^1-function, which is not good enough information to get necessary regularity (Lipschitz continuity) of the boundary of $\{u > 0\}$. Thus, we cannot use approximations by functions from $C_0^\infty(\{u > 0\})$. Still, we notice that (5.1.52) is an admissible function in (5.1.13). Then we get

$$\int_0^{t_0} \int_\Omega \big(u_t^\delta u + \nabla u^\delta \nabla u + \gamma \chi_\varepsilon'(u^\delta) u\big)\, dx\, dt = \int_0^{t_0} \lambda^\delta \int_\Omega \big(\tilde{\chi}_\delta(u^\delta) + u^\delta \tilde{\chi}_\delta'(u^\delta)\big)\, u\, dx\, dt. \tag{5.1.53}$$

For the first three terms on the left-hand side of (5.1.53), the convergences from (5.1.47)–(5.1.49) are sufficient. In the remaining terms, we use the uniform convergence, boundedness of u^δ from below (see (5.1.14)), properties of the function $\tilde{\chi}_\delta$ and the following estimates:

$$\begin{aligned} \Big|\int_\Omega \tilde{\chi}_\delta(u^\delta) u\, dx - V\Big| &= \Big|\int_\Omega \big(\tilde{\chi}_\delta(u^\delta) u^\delta + \tilde{\chi}_\delta(u^\delta)(u - u^\delta)\big)\, dx - V\Big| \\ &= \Big|\int_\Omega \tilde{\chi}_\delta(u^\delta)(u - u^\delta)\, dx\Big| \\ &\le C \max_{Q_T} |u - u^\delta| \to 0 \quad \text{as } \delta \to 0, \end{aligned}$$

$$\begin{aligned} \Big|\int_\Omega u^\delta \tilde{\chi}_\delta'(u^\delta) u\, dx\Big| &= \Big|\int_\Omega \big((u^{\delta-})^2 \tilde{\chi}_\delta'(u^\delta) + u^{\delta-} \tilde{\chi}_\delta'(u^\delta)(u - u^\delta)\big)\, dx\Big| \\ &\le C\delta + C \max_{Q_T} |u - u^\delta| \to 0 \quad \text{as } \delta \to 0. \end{aligned}$$

Hence, taking δ to zero in (5.1.53) yields

$$\int_0^{t_0} \tilde{\lambda}\, dt = \frac{1}{V} \int_0^{t_0} \int_\Omega \big(u_t u + |\nabla u|^2 + \gamma \chi_\varepsilon'(u) u\big)\, dx\, dt,$$

which immediately implies $\tilde{\lambda}(t) = \lambda(t)$ almost everywhere in $(0,T)$.

The uniqueness follows from the uniqueness of the solution obtained by the method of subdifferentials (see Remark 5.1.2). □

Remark 5.1.2. *We show that the weak solution constructed above is the same as the solution obtained by subdifferential technique. More precisely, we prove that our solution satisfies the relation*

$$\int_0^T \int_\Omega \Big[(-u_t - \gamma \chi_\varepsilon'(u))(z - u) - \nabla u \nabla (z - u)\Big]\, dx\, dt \le 0 \qquad \forall z \in \mathcal{K}, \tag{5.1.54}$$

where

$$\mathcal{K} = \{u \in L^2(0,T;H_0^1(\Omega));\ u \geq 0,\ \int_\Omega u\,dx = V\}.$$

Since solution of (5.1.54) is unique (this can be seen taking two solutions $u, v \in \mathcal{K}$, setting $z = v$ in (5.1.54) and $z = u$ in the corresponding relation for v, adding the resulting inequalities and using Gronwall's lemma), we conclude that there is a unique weak solution in the sense of Definition 5.1.2, which is identical to the unique solution in the sense of Yosida approximation.

To start with, take any $z \in \mathcal{K} \cap C(0,T;H_0^1(\Omega))$ and define function $\bar{z}^h$ by

$$\bar{z}^h(t,x)|_{t\in(nh,nh+h)} = z^n(x) = z(nh,x), \qquad x \in \Omega.$$

Then for $\epsilon \in (0,1)$ the function $u^{\delta,n} + \epsilon(z^n - u^{\delta,n})$ is nonnegative and has volume V, thus is an admissible variation for the functional (5.1.17), yielding

$$\frac{1}{\epsilon}\big(J_n^\delta(u^{\delta,n}) - J_n^\delta(u^{\delta,n} + \epsilon(z^n - u^{\delta,n}))\big) \leq 0.$$

Letting $\epsilon \to 0+$ gives

$$\int_0^T \int_\Omega \Big[\big(-u_t^{\delta,h} - \gamma\chi_\varepsilon'(\bar{u}^{\delta,h})\big)(\bar{z}^h - \bar{u}^{\delta,h}) - \nabla\bar{u}^{\delta,h}\nabla(\bar{z}^h - \bar{u}^{\delta,h})\Big]\,dx\,dt \leq 0.$$

Using (5.1.33)–(5.1.36) in the limit as $h \to 0+$, we find

$$\int_0^T \int_\Omega \Big[\big(-u_t^\delta - \gamma\chi_\varepsilon'(u^\delta)\big)(z - u^\delta) - \nabla u^\delta\nabla z\Big]\,dx\,dt + \liminf_{h\to 0}\int_0^T\int_\Omega |\nabla\bar{u}^{\delta,h}|^2\,dx\,dt \leq 0.$$

Hence, by the lower semicontinuity of the Dirichlet integral, we obtain

$$\int_0^T \int_\Omega \Big[\big(-u_t^\delta - \gamma\chi_\varepsilon'(u^\delta)\big)(z - u^\delta) - \nabla u^\delta\nabla(z - u^\delta)\Big]\,dx\,dt \leq 0.$$

Results (5.1.47)–(5.1.49) and the same reasoning as above finally give (5.1.54).

Remark 5.1.3. *In order to show that the problem is indeed a free boundary problem, i.e., that the solution does not "spread" into the whole domain Ω, we employ the term $\gamma\chi_\varepsilon(u)$ to argue as follows. Let us assume that for some time $t \in (0,T)$ the solution is positive in the whole domain Ω. We shall show that for a sufficiently large domain Ω, sufficiently small $\varepsilon > 0$ and for nondegenerate γ (i.e., $\gamma \geq \gamma_0 > 0$ in Ω), this leads to a contradiction.*

Choosing Ω large enough, there exists a compact subset $\Omega_c \subset \Omega$ such that $|\Omega_c| > C/\gamma_0$, where C is the constant from estimate (5.1.16). As one can see from the proof of Lemma 5.1.2, we can put

$$\|\nabla u_0\|_{L^2(\Omega)}^2 + 2\int_\Omega \gamma\chi_\varepsilon(u_0)\,dx \leq \|\nabla u_0\|_{L^2(\Omega)}^2 + 2\int_{u_0>0}\gamma\,dx =: C,$$

in particular, C does not depend on Ω but only on the support of u_0 which is naturally assumed to be compact. Since Ω_c is compact, there are real numbers $\eta > 0$ and $\delta_0 > 0$ so *that* $u^\delta \geq \eta$ *in* Ω_c *for* $\delta \in (0, \delta_0)$*. Further, we set* ε *so small that* $\chi_\varepsilon(\eta) = 1$*. Then we have from (5.1.16) the inequality*

$$C \geq \int_{\Omega_c} \gamma \chi_\varepsilon(u^\delta)\, dx = \int_{\Omega_c} \gamma\, dx \geq |\Omega_c| \gamma_0,$$

which contradicts the assumed measure of Ω_c*.*

In this section, we have proved the existence, uniqueness and certain regularity of a weak solution to a parabolic free boundary problem with integral constraint. The equation can describe slow motion of drops on surfaces, where the contact angles are smoothed. The volume constraint results in a time-dependent outer force term having a nonlocal form depending on the solution. The problem was solved by the discrete Morse flow method, which is a variational method based on the minimization of a time-discretized functional. The constraints can then be included in the set of functions admissible for minimization. The possibility of direct application to numerical schemes and independence of convexity of the problem distinguishes the construction of approximate solutions in the present proof from the subdifferential technique using Yosida approximation. It remains a future task to employ the independence of convexity and study constrained evolutionary equations with delta function terms, corresponding to sharp contact angles in the droplet model.

5.2 Hyperbolic problem

In this Section, we discuss a hyperbolic free-boundary problem with volume conservation. The equation can model motion of a soap-film bubble on water surface and is explained in the Appendix to this Chapter (Section 5.3). The disappearance of energy when the film touches the surface causes the degeneracy of the equation.

We attempt to analyze the problem once again by the discrete Morse flow method. However, we are not able to prove a sufficient estimate on the approximate solutions. Therefore, we modify the method by implementing the technique of subdifferentials. Then we obtain an energy estimate and try to show the existence of a weak solution in the case of one space dimension. The text is thus divided into two parts: in the first part we introduce standard discrete Morse flow approximations, which form the base for numerical computations, and show that they are well-defined. This part is based on the paper [41]. In the latter part we prove the existence of a weak solution to our problem by the combination of discrete Morse flow and subdifferential technique.

5.2.1 Construction of approximate solutions

Here we construct well-defined approximate solutions to the problem for bubble motion using the discrete Morse flow method. We use the graph of a scalar function $u : [0, T] \times \bar{\Omega} \to \mathbb{R}$ to describe the shape of the bubble. Here $T > 0$ and Ω is a bounded connected domain in $\mathbb{R}^m$ with smooth boundary. The zero level set of u coincides with water surface where the bubble rests. The set of points where the bubble touches the water surface is called *free boundary*. We also assume that the volume of air which is surrounded by the bubble is preserved at any time, that is, the movement can be described by wave equation with volume constraint, i.e., $\int_\Omega u\,dx = V$ (V is a positive number representing the volume). The following equations describe the motion (see Section 5.3 for details):

$$\begin{aligned}
\chi_{u>0}\, u_{tt}(t,x) &= \Delta u(t,x) - \gamma(x)\chi'_\varepsilon(u) + \lambda(t)\chi_{u>0} \quad \text{in } Q_T = (0,T)\times\Omega,\\
u(t,x) &= 0 \qquad\qquad\qquad \text{on } (0,T)\times\partial\Omega,\\
u(0,x) &= u_0(x) \qquad\qquad\quad \text{in } \Omega,\\
u_t(0,x) &= v_0(x) \qquad\qquad\quad \text{in } \Omega.
\end{aligned} \tag{5.2.1}$$

Here $\chi_{u>0}$ is the characteristic function of the set $\{(t,x)\in[0,T]\times\Omega : u(t,x)>0\}$ and $\chi_\varepsilon \in C^2(\mathbb{R})$ is a smoothing of χ satisfying

$$\chi_\varepsilon(s) = \begin{cases} 0, & s \le 0 \\ 1, & s \ge \varepsilon \end{cases}$$

with interpolating in $0 < s < \varepsilon$ in such a way that $\chi'_\varepsilon(s) \le C/\varepsilon$ (see Figure 5.1). The term $\chi'_\varepsilon(u)$ describes the adhesive force which generates new surface against surface tension of water. It is due to this term that oscillation of solution in the whole domain does not occur. The specificity of this equation lies in the coefficient $\chi_{u>0}$ on the left-hand side. Because of this coefficient, non-negativity of the solution is guaranteed.

We assume that $\gamma \in L^\infty(\Omega)$ and that $u_0, v_0 \in H^1(\Omega)\cap L^\infty(\Omega)$ satisfy the compatibility conditions $u_0(x) = 0$, $v_0(x) = 0$ for $x \in \partial\Omega$ and $\int_\Omega u_0\,dx = V$, $\int_\Omega v_0\,dx = 0$. We obtain the explicit form of the Lagrange multiplier λ as

$$\lambda = \frac{1}{V}\int_\Omega \left(u_{tt}u + |\nabla u|^2 + \gamma\chi'_\varepsilon(u)u\right)\,dx \tag{5.2.2}$$

by formal calculation of the first variation of the Lagrangian with volume constraint condition (see Chapter 2). The integral representation above makes the problem more difficult. However, we can calculate an approximate solution to (5.2.1) by use of a time-semidiscretized functional which is called *the discrete Morse flow of hyperbolic type* (see Chapter 3).

We can formally derive the free boundary condition for the problem which is obtained when ε is taken to zero in (5.2.1).

Lemma 5.2.1. *Let us assume the existence of u^ε, the classical solution to (5.2.1), and the existence of v so that $u^\varepsilon \longrightarrow v$ ($\varepsilon \to 0$) in a suitable sense (assumptions are shown in the calculation) with v satisfying $v_{tt} = \Delta v + \lambda$ in $Q_T \cap \{v>0\}$, where $\lambda = \int_\Omega (v_{tt}v + |\nabla v|^2)\,dx$. Then the equality $|\nabla v|^2 - (v_t)^2 = 2\gamma$ holds on $\partial\{v>0\}$.*

Proof. We multiply $\zeta u_k^\varepsilon \big(\equiv \zeta \frac{\partial u^\varepsilon}{\partial x_k},\ \zeta \in C_0^\infty(Q_T)\big)$ to both sides of (5.2.1) and integrate on Q_T. We get the following identity (see [4]):

$$\int_{Q_T} \zeta u_k^\varepsilon \left(\Delta u^\varepsilon - \chi_{u^\varepsilon>0}u_{tt}^\varepsilon + \lambda^\varepsilon \chi_{u^\varepsilon>0}\right)\,dz = \int_{Q_T} \gamma\zeta u_k^\varepsilon \chi'_\varepsilon(u^\varepsilon)\,dz. \tag{5.2.3}$$

Noting that $[\chi_\varepsilon(u)]_{x_k} = \chi'_\varepsilon(u)\, u_k$ and by the integration by parts, the right-hand side of (5.2.3) can be calculated in the following way:

$$\begin{aligned}\int_{Q_T} \gamma\zeta u^\varepsilon_k \chi'_\varepsilon(u^\varepsilon)\, dz \quad &= -\int_{Q_T} (\gamma\zeta)_k \chi_\varepsilon(u^\varepsilon)\, dz \\ &\xrightarrow[\varepsilon\to 0]{} -\int_{Q_T\cap\{v>0\}} (\gamma\zeta)_k\, dz \quad (\chi_\varepsilon(u^\varepsilon) \to \chi_{v>0} \text{ a.e. is assumed}) \\ &= -\int_{Q_T\cap\partial\{v>0\}} \gamma\zeta\nu_k\, dS,\end{aligned}$$

where ν_k is the k-th element of the outer normal $\nu = (\nu_1 \cdots \nu_{m+1})$ to the set $\{v > 0\} \subset Q_T$ with ν_{m+1} being the t-direction.

On the other hand, the left-hand side of (5.2.3) can be calculated as follows:

$$\begin{aligned}&\int_{Q_T} \zeta u^\varepsilon_k \left(\Delta u^\varepsilon - \chi_{u^\varepsilon>0} u^\varepsilon_{tt} + \lambda^\varepsilon \chi_{u^\varepsilon>0}\right)\, dz \\ &= -\int_{Q_T} \left(\nabla(\zeta u^\varepsilon_k)\nabla u^\varepsilon - (\zeta u^\varepsilon_k)_t u^\varepsilon_t \chi_{u^\varepsilon>0} - \zeta u^\varepsilon_k \lambda^\varepsilon \chi_{u^\varepsilon>0}\right)\, dz \\ &= -\int_{Q_T} \Big([\nabla u^\varepsilon \nabla\zeta - u^\varepsilon_t \zeta_t]\, u^\varepsilon_k - \frac{1}{2}\zeta_k \left[|\nabla u^\varepsilon|^2 - (u^\varepsilon_t)^2\right] - \zeta u^\varepsilon_k \lambda^\varepsilon \Big) \chi_{u^\varepsilon>0}\, dz \\ &\xrightarrow[\varepsilon\to 0]{} -\int_{Q_T} \Big([\nabla v \nabla\zeta - v_t\zeta_t]\, v_k - \frac{1}{2}\zeta_k \left[|\nabla v|^2 - (v_t)^2\right] - \zeta v_k \lambda \Big) \chi_{v>0}\, dz \\ &= -\int_{Q_T} \Big(\nabla(\zeta v_k)\nabla v - (\zeta v)_t v_t - \zeta v_k \lambda\Big) \chi_{v>0}\, dz \\ &\qquad\qquad + \frac{1}{2}\int_{Q_T\cap\partial\{v>0\}} \big(|\nabla v|^2 - (v_t)^2\big)\zeta\nu_k\, dS \\ &= \int_{Q_T\cap\{v>0\}} \zeta v_k(\Delta v - v_{tt} + \lambda)\, dz - \int_{Q_T\cap\partial\{v>0\}} \zeta v_k\, (\nabla v, -v_t)\cdot\nu\, dS \\ &\qquad\qquad + \frac{1}{2}\int_{Q_T\cap\partial\{v>0\}} \big(|\nabla v|^2 - (v_t)^2\big)\zeta\nu_k\, dS \\ &= -\int_{Q_T\cap\partial\{v>0\}} \zeta v_k(\nabla v, -v_t)\cdot\nu\, dS + \frac{1}{2}\int_{Q_T\cap\partial\{v>0\}} \big(|\nabla v|^2 - (v_t)^2\big)\zeta\nu_k\, dS.\end{aligned}$$

Note that outer normal to $\{v > 0\}$ is $\nu = -Dv/|Dv|$, where $Dv = (v_{x_1}, \cdots, v_{x_m}, v_t)$. Therefore, we can see that $v_k = -\nu_k |Dv|$ on $\partial\{v > 0\}$. Then, eventually, the left hand side of (5.2.3) becomes

$$-\frac{1}{2}\int_{Q_T\cap\partial\{v>0\}} \left[|\nabla v|^2 - (v_t)^2\right] \zeta\nu_k\, dS.$$

Thus we get the equation

$$\int_{Q_T\cap\partial\{v>0\}} \gamma\zeta\nu_k\, dS = \frac{1}{2}\int_{Q_T\cap\partial\{v>0\}} \left[|\nabla v|^2 - (v_t)^2\right] \zeta\nu_k\, dS,$$

which shows that

$$|\nabla v|^2 - (v_t)^2 = 2\gamma \quad \text{on } \partial\{v > 0\}. \tag{5.2.4}$$

The limit boundary condition (5.2.4) is the same as the one obtained for the hyperbolic free boundary problem introduced in [21]. □

Now we introduce an approximation problem to (5.2.1). We add the volume constraint in the admissible space for finding a minimizer of a discretized functional corresponding to the Lagrangian.

Problem 5.2.1. *Let functions $u_0, v_0 \in H^1_0(\Omega)$ be given and define $u_1 = u_0 + hv_0$. Divide the time interval $(0,T)$ equidistantly into N subintervals of length $h = T/N$. For each such subinterval $((n-1)h, nh)$, $n = 2, 3, \ldots, N$, find a minimizer u_n of the following functional*

$$J_n(u) := \int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\chi_{u>0}\, dx + \frac{1}{2}\int_\Omega |\nabla u|^2\, dx + \int_\Omega \gamma\chi_\varepsilon(u)\, dx \tag{5.2.5}$$

in the function set

$$\mathcal{K}_V = \Big\{ u \in H^1(\Omega);\ u = 0 \text{ on } \partial\Omega,\ \int_\Omega u\chi_{u>0}\, dx = V \Big\}.$$

Let us check that a minimizer is nonnegative (almost everywhere). If $0 \le K_1 \le K_2$ and $u \in \mathcal{K}_V$, then also $\max\{u, -K_1\})$ and $\max\{u, -K_2\}$ belong to $\mathcal{K}_V$. Due to the presence of the characteristic function in the discretized term in (5.2.5), we find that $J_n(\max\{u, -K_1\}) \le J_n(\max\{u, -K_2\})$. We have used the fact that $\nabla \max\{u, -K\}(x) = 0$ for $\{x : u(x) \le -K\}$ (see [12], Chapter 7.4). Thus,

$$J_n(u\chi_{u>0}) \le J_n(u).$$

To show the sharp inequality requires finer analysis but it is enough for us to know that there is a nonnegative minimizer. This deliberation makes clear the importance of the characteristic function in the constraint in $\mathcal{K}_V$.

In the following theorems, we shall show the existence and regularity of the minimizers.

Theorem 5.2.1. *There exists a nonnegative minimizer u_n of the functional J_n in $\mathcal{K}_V$.*

Proof. For given u_{n-1} and u_{n-2}, we shall show the existence of u_n. We prove the lower semicontinuity of J_n which automatically leads to existence. Since the minimizer is supposed to be nonnegative, it is enough to show the existence in $\{u \in \mathcal{K}_V; u \ge 0\}$, which is a convex closed set. Let $\{u^k\}$ be a minimizing sequence of J_n. Then $u^k - u_0$ are uniformly bounded in $H^1(\Omega)$. Therefore, there is a subsequence, denoted by $\{u^k\}$ again, and a limit function $u \in \mathcal{K}_V$ such that

$$\begin{aligned} \nabla u^k &\to \nabla u && \text{weakly in } L^2(\Omega), \\ u^k &\to u && \text{almost everywhere in } \Omega. \end{aligned}$$

Moreover, there is a function $\gamma \in L^p(\Omega)$ for any $p \in [1,\infty)$ with $0 \le \gamma \le 1$, such that

$$\chi_{u^k>0} \to \gamma \qquad \text{weakly in } L^p(\Omega).$$

Then, by the lower semicontinuity of Dirichlet integral, we have

$$\begin{aligned}
&\int_\Omega \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2}\gamma\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx + \int_\Omega \gamma\chi_\varepsilon(u)\,dx \\
&\le \liminf_{k\to\infty}\left[\int_\Omega \frac{\left|u^k - 2u_{n-1} + u_{n-2}\right|^2}{2h^2}\chi_{u^k>0}\,dx + \frac{1}{2}\int_\Omega \left|\nabla u^k\right|^2\,dx + \int_\Omega \gamma\chi_\varepsilon(u^k)\,dx\right].
\end{aligned}$$

Since $\gamma = 1$ almost everywhere in $\{u > 0\}$, the value of $J_n(u)$ is less than or equal to the left-hand side of the above inequality. Thus we have

$$J_n(u) \le \liminf_{k\to\infty} J_n(u^k),$$

which completes the proof. □

In the following, we show the continuity of minimizers u_n, which implies that the sets $\{u_n > 0\}$ are relatively open in $\bar{Q}_T$. This fact is indispensable in the definition of approximate weak solutions (Definition 5.2.3). First, we recall the definition of classes de Giorgi.

Definition 5.2.1. *A function $u \in H^1(\Omega)$ belongs to the class $\mathcal{B}_2(\Omega, M, \gamma, d)$ if*
(1) $M = \sup_\Omega |u| < \infty$,
(2) *there is a $\gamma > 0$ so that for $w = \pm u$*

$$\int_{A_{k,r-\sigma r}} |\nabla w|^2\,dx \le \gamma\left[\frac{1}{(\sigma r)^2}\sup_{B_r}(w-k)^2 + 1\right]|A_{k,r}|, \tag{5.2.6}$$

for all $\sigma \in (0,1)$, $B_r \subset \Omega$ and k with $k \ge \max_{B_r} w - d$, for any $d > 0$, where $A_{k,r} = \{x \in B_r;\ u(x) > k\}$. The symbol B_r means a ball of radius r.

Theorem 5.2.2. *For all compact subsets $\tilde\Omega \subset\subset \Omega$, there exists a positive constant α (depending on h) with $0 < \alpha < 1$, such that minimizers u_n belong to $C^\alpha(\tilde\Omega)$.*

Proof. We shall show that the minimizer belongs to the space $\mathcal{B}_2(\Omega, M, \gamma, d)$. Results from Chapter 2.6 in [23] then ensure Hölder continuity of the minimizer.

Without loss of generality, we can set $V = 1$. Condition (1) from the above definition is proven by a standard elliptic technique from [23], we have only to consider a test function belonging to $\mathcal{K}_V$, particularly of the form

$$\psi_\delta(u) = \frac{u - \delta(u-k)^+}{\int_\Omega (u - \delta(u-k)^+)\,dx}, \qquad \delta \to 0+,$$

where $(u-k)^+ = \max\{u-k, 0\}$. We use mathematical induction. For $n = 2$, functions $u_{n-1} = u_0 + hv_0$ and $u_{n-2} = u_0$ are bounded, so we assume that we have the boundedness of u_k for $k = 1, \dots, n-1$, and prove the boundedness of u_n. The minimality property $(J_n(\psi_\delta(u_n)) - J_n(u_n))/\delta \geq 0$ yields after taking $\delta > 0$ to zero the relation

$$\int_\Omega \Big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2}(u_n - k)^+ + \nabla u_n \nabla (u_n - k)^+ + \gamma \chi'_\varepsilon(u_n)(u_n - k)^+\Big)\,dx \tag{5.2.7}$$
$$\leq \Big(\int_\Omega (u_n - k)^+\,dx\Big) \int_\Omega \Big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} u_n + |\nabla u_n|^2 + \gamma \chi'_\varepsilon(u_n) u_n\Big)\,dx.$$

The last integral on the right-hand side of the above inequality can be rearranged in the following way:

$$\begin{aligned}
&\int_\Omega \Big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} u_n + |\nabla u_n|^2 + \gamma \chi'_\varepsilon(u_n) u_n\Big)\,dx \\
\leq\ & \frac{1}{2} J_n(u_n) + \int_\Omega \frac{2u_{n-1} - u_{n-2}}{2h^2} u_n\,dx + \int_\Omega \frac{C}{\varepsilon} \gamma u_n\,dx \\
\leq\ & \frac{1}{2} J_n(u_n) + \int_\Omega \frac{|2u_{n-1} - u_{n-2}|}{2h^2}\big((u_n - k) + k\big)\,dx + C\int_\Omega u_n\,dx \\
\leq\ & \frac{1}{2} J_n(u_n) + \int_{u_n > k} \frac{|2u_{n-1} - u_{n-2}|}{2h^2}(u_n - k)\,dx + k\int_\Omega \frac{|2u_{n-1} - u_{n-2}|}{2h^2}\,dx + C.
\end{aligned}$$

Neglecting terms with accordant sign and noting that $(u_n - k)^+ = 0$ on $\Omega \setminus A_k$, where $A_k = \{x \in \Omega : u_n(x) > k\}$, we have from (5.2.7),

$$\begin{aligned}
\int_{A_k} |\nabla u_n|^2\,dx \leq & \int_{A_k} \frac{|2u_{n-1} - u_{n-2}|}{2h^2}(u_n - k)\,dx \\
&+ \Big(\int_{A_k} (u_n - k)\,dx\Big)\Big(\int_{A_k} \frac{|2u_{n-1} - u_{n-2}|}{2h^2}(u_n - k)\,dx + k\int_\Omega \frac{|2u_{n-1} - u_{n-2}|}{2h^2}\,dx + C\Big),
\end{aligned}$$

where C depends on h but not on n. As u_{n-1} and u_{n-2} are bounded, we get

$$\begin{aligned}
\int_{A_k} |\nabla u_n|^2\,dx &\leq C\Big(\int_{A_k} (u_n - k)\,dx\Big)\Big(1 + k + \int_{A_k} (u_n - k)\,dx\Big) \\
&\leq C\Big[\int_{A_k} (u_n - k)^2\,dx + k^2 |A_k|\Big].
\end{aligned}$$

This inequality gives the estimate assumed in Theorem 2.5.1 from [23] to obtain the bound for u_n.

Let us now derive estimate (5.2.6) for $w = +u$. Later, we will show that it holds also for $w = -u$. First we prove that the minimizer of J_n satisfies the following inequality for $\zeta \geq 0$, $\zeta \in H^1_0(\Omega)$:

$$\begin{aligned}
0 \leq\ & \int_\Omega \Big(\frac{|u_n - 2u_{n-1} + u_{n-2}|}{h^2} u_n + |\nabla u_n|^2 + \gamma \chi'_\varepsilon(u_n) u_n\Big)\,dx \Big(\int_\Omega \zeta\,dx\Big) \\
&+ \int_\Omega \frac{|u_n - 2u_{n-1} + u_{n-2}|}{h^2} \zeta\,dx - \int_\Omega \nabla u_n \nabla \zeta\,dx.
\end{aligned} \tag{5.2.8}$$

We shall write u instead of u_n and assume $u \geq 0$. Let us set

$$\psi_\delta = \frac{u-\delta\zeta}{I_\delta}\chi_{u-\delta\zeta>0}, \tag{5.2.9}$$

where $\delta > 0$ and $I_\delta = \int_\Omega (u-\delta\zeta)\chi_{u-\delta\zeta>0}\,dx$. We have $I_\delta \leq 1$ by the volume condition $\int_\Omega u\,dx = V$ with $V = 1$, while

$$\begin{aligned} I_\delta &= \int_\Omega u\chi_{u-\delta\zeta>0}\,dx - \delta\int_\Omega \zeta\chi_{u-\delta\zeta>0}\,dx \\ &= \int_\Omega u\,dx - \int_{u\leq\delta\zeta} u\,dx - \delta\int_{u>\delta\zeta}\zeta\,dx \\ &\geq 1 - \delta\int_{u\leq\delta\zeta}\zeta\,dx - \delta\int_{u>\delta\zeta}\zeta\,dx \\ &= 1-\delta\int_\Omega \zeta\,dx. \end{aligned} \tag{5.2.10}$$

As $\psi_\delta \in \mathcal{K}_V$, we have $(J_n(\psi_\delta) - J_n(u))/\delta \geq 0$ by the minimizing property of u. Passing to the limit as $\delta \to 0+$ and using the relation (5.2.10), we get after technical computations the inequality (5.2.8).

Using (5.2.8) for a suitable function ζ we now show that u satisfies estimate (5.2.6). Choose r and $s = r - \sigma r$ ($\sigma \in (0,1)$) to be arbitrary numbers with $0 < s < r$. Take $\zeta = \eta^2\max\{u-k,0\}$, where η is a function with support in B_r satisfying $0 \leq \eta \leq 1$, $\eta = 1$ in B_s (concentric with B_r) and $|\nabla\eta| \leq 2/(r-s)$ in $B_r \setminus B_s$. In this way, we obtain from (5.2.8) the estimate

$$0 \leq C|A_{k,r}| - \int_\Omega \nabla u_n \nabla\zeta\,dx, \tag{5.2.11}$$

with the constant C depending only on h, ε, M, $|\Omega|$ and $J_n(u_n)$. The gradient term is estimated using Young's inequality:

$$\begin{aligned} -\int_\Omega \nabla u_n\nabla\zeta\,dx &= -\int_{A_{k,r}} |\nabla u_n|^2\eta^2\,dx - \int_{A_{k,r}} \nabla u_n\nabla\eta 2\eta(u_n-k)\,dx \\ &\leq -\int_{A_{k,r}} |\nabla u_n|^2\eta^2\,dx + \frac{1}{2}\int_{A_{k,r}} |\nabla u_n|^2\eta^2\,dx + 2\int_{A_{k,r}} |\nabla\eta|^2(u_n-k)^2\,dx \\ &\leq -\frac{1}{2}\int_{A_{k,s}} |\nabla u_n|^2\,dx + \frac{8}{(\sigma r)^2}\sup_{B_r}(u_n-k)^2|A_{k,r}|. \end{aligned}$$

The above estimate together with (5.2.11) gives the desired result (5.2.6).

Let us turn to the case of $-u$. We set $w = -u$ and note that w minimizes the following functional

$$J_n(w) := \int_\Omega \frac{|w+2u_{n-1}-u_{n-2}|^2}{2h^2}\chi_{w<0}\,dx + \frac{1}{2}\int_\Omega |\nabla w|^2 dx + \int_\Omega \gamma\chi_\varepsilon(-w)\,dx \tag{5.2.12}$$

in the admissible function set $\mathcal{K}_{-V} := \{w \in H^1(\Omega);\ w = 0 \text{ on } \partial\Omega,\ \int_\Omega w\,dx = -1, w \leq 0\}$. We introduce function φ by the formula

$$\varphi = -\frac{w-\zeta}{\int_\Omega (w-\zeta)\,dx}, \tag{5.2.13}$$

where $\zeta = \eta \max\{w-k,0\}$. Here, k is a negative real number and η is a smooth cut-off function chosen in the same way as above. For the sake of simplicity, let us denote $K = 1/\int_\Omega (w-\zeta)\,dx = 1/(-1-\int_\Omega \zeta\,dx)$. Checking that φ belongs to $\mathcal{K}_{-V}$, we can write $0 \le J_n(\varphi) - J_n(w)$ and, thus,

$$\begin{aligned}
0 \;\le\; & \frac{1}{2h^2}\int_\Omega \left(|K(-w+\zeta)+2u_{n-1}-u_{n-2}|^2 - |w+2u_{n-1}-u_{n-2}|^2\right)\chi_{\{K(-w+\zeta)<0\}}\,dx \\
& + \frac{1}{2h^2}\int_\Omega |w+2u_{n-1}-u_{n-2}|^2\left(\chi_{\{K(-w+\zeta)<0\}} - \chi_{w<0}\right)\,dx \\
& + \int_\Omega \gamma\chi_\varepsilon(-K(-w+\zeta))\,dx - \int_\Omega \gamma\chi_\varepsilon(-w)\,dx \\
& + \frac{K^2}{2}\int_\Omega |\nabla(-w+\zeta)|^2\,dx - \frac{1}{2}\int_\Omega |\nabla w|^2\,dx. \qquad (5.2.14)
\end{aligned}$$

We estimate the expression on the right-hand side of the above inequality. The term in the second line is less than or equal to $\frac{1}{2h^2}\int_{\mathrm{supp}\zeta} |w+2u_{n-1}-u_{n-2}|^2\,dx$, since $\chi_{\{K(-w+\zeta)<0\}} - \chi_{w<0} = \chi_{w<\zeta} - \chi_{w<0}$ is positive only for x such that $0 \le w(x) < \zeta(x)$. Noting that $K^2 < 1$ we can write

$$\begin{aligned}
& \frac{K^2}{2}\int_\Omega |\nabla(-w+\zeta)|^2\,dx - \frac{1}{2}\int_\Omega |\nabla w|^2\,dx \qquad (5.2.15) \\
\le\; & K^2 \int_{A_{k,r}} \left(|\nabla w|^2(1-\eta)^2 + |\nabla\eta|^2(w-k)^2\right)\,dx - \frac{1}{2}\int_{A_{k,r}} |\nabla w|^2\,dx \\
\le\; & K^2 \int_{A_{k,r}} |\nabla w|^2\,dx + K^2\int_{A_{k,r}} |\nabla\eta|^2(w-k)^2\,dx - \left(\frac{1}{2}+K^2\right)\int_{A_{k,s}} |\nabla w|^2\,dx.
\end{aligned}$$

The estimates of the terms in first and third line of (5.2.14) are straightforward. Since $\mathrm{supp}\,\zeta \subset A_{k,r}$, we have by (5.2.14)

$$\int_{A_{k,s}} |\nabla w|^2\,dx \le 2C|A_{k,r}| + \theta\int_{A_{k,r}} |\nabla w|^2\,dx + \frac{4}{(r-s)^2}\int_{A_{k,r}} (w-k)^2\,dx,$$

where the constant C again depends only on M, $|\Omega|$, ε and h. Here, we denoted $\theta = \frac{K^2}{1/2+K^2} < 1$. Applying Lemma V.3.1 from [11], we obtain the desired estimate (5.2.6). □

By use of the above theorem, we can choose the support of test functions in the set $\{u_n > 0\}$. Then the first variation formula of $J_n(u)$ is

$$\begin{aligned}
& \int_\Omega \left(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2}\phi + \nabla u_n \nabla\phi + \gamma\chi_\varepsilon'(u_n)\phi\right)dx = \int_\Omega \lambda_n \phi\,dx \\
& \qquad\qquad \forall \phi \in C_0^\infty(\Omega \cap \{u_n > 0\}), \\
& \int_\Omega \nabla u_n \nabla\phi dx = 0 \qquad \forall\phi \in C_0^\infty(\Omega \cap \{u_n \le 0\}^\circ).
\end{aligned}$$

Here,

$$\lambda_n = \frac{1}{V}\int_\Omega \left(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2}u_n + |\nabla u_n|^2 + \gamma\chi_\varepsilon'(u_n)u_n\right)dx$$

is the Lagrange multiplier coming from the volume constraint. From the second identity, we can conclude that $u_n \equiv 0$ outside the set $\{u_n > 0\}$.

We are ready to carry out interpolation in time of minimizers $\{u_n\}$ and introduce the approximate weak solution. First we state the definition of a *weak solution*.

Definition 5.2.2. *We call $u \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H_0^1(\Omega))$ a weak solution to (5.2.1), if $u(0,x) = u_0(x)$ in Ω and u satisfies the following:*

$$\int_0^T \int_\Omega (-u_t\phi_t + \nabla u \nabla \phi + \gamma\chi_\varepsilon'(u)\phi)\, dx\, dt - \int_\Omega v_0\phi(0,x)\, dx \tag{5.2.16}$$
$$= \frac{1}{V}\int_0^T \int_\Omega \big(-u_t(u\Phi)_t + |\nabla u|^2\Phi + \gamma\chi_\varepsilon'(u)u\Phi\big)\, dx\, dt - \frac{1}{V}\int_\Omega u_0 v_0 \Phi(0)\, dx$$
$$\forall \phi \in C_0^\infty([0,T) \times \Omega \cap \{u > 0\}),$$
$$u \equiv 0 \quad \text{outside } \{u > 0\}, \tag{5.2.17}$$

where $\Phi(t) = \int_\Omega \phi(t,x)\, dx$.

Now, we consider the approximate solutions. We define $\bar{u}^h$, u^h and $\bar{\lambda}^h$ on $(0,T) \times \Omega$ by

$$\begin{aligned} \bar{u}^h(t,x) &= u_n(x), \\ u^h(t,x) &= \frac{t-(n-1)h}{h}u_n(x) + \frac{nh-t}{h}u_{n-1}(x), \\ \bar{\lambda}^h(t) &= \lambda_n, \end{aligned}$$

for $(t,x) \in ((n-1)h, nh] \times \Omega$, $n = 1,2,\ldots,N$. Further, we set $\bar{u}^h(0,x) = u^h(0,x) = u_0(x)$. We can construct *approximate weak solution* to our problem in terms of $\bar{u}^h$ and u^h:

Definition 5.2.3. *Let $\{u_n\} \subset \mathcal{K}_V$ and let $\bar{u}^h$ and u^h be defined as above. If the following conditions*

$$\int_h^T \int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h}\phi + \nabla\bar{u}^h\nabla\phi + \gamma\chi_\varepsilon'(\bar{u}^h)\phi\Big)\, dx\, dt = \int_h^T \int_\Omega \bar{\lambda}^h\phi\, dx\, dt,$$
$$\forall \phi \in C_0^\infty([0,T) \times \Omega \cap \{u^h > 0\}),$$
$$u^h \equiv 0 \quad \text{in} \quad Q_T \setminus \{u^h > 0\},$$

and the initial conditions $u^h(0) = u_0$, $u^h(h) = u_0 + hv_0$ are satisfied, then we call $\bar{u}^h$ and u^h approximate solutions to (5.2.1).

If one can pass to the limit as $h \to 0$, then the above approximate solutions are expected to converge to the solution of (5.2.16)–(5.2.17). However, we were not able to derive estimates for the approximate solution that would guarantee a sufficient regularity and convergence. The main hurdle in finding the estimates is the characteristic function appearing with the time-discretized term in (5.2.5).

This difficulty is overcome in the following subsection by introducing certain penalties and using the subdifferential theory. Still, the approximate solution defined above can be used to carry out effective numerical computations, which is not directly possible for the penalized approximations.

5.2.2 Existence of solutions in one space dimension

In this part of the thesis, we try to prove the existence of weak solutions to problem (5.2.1), i.e.,

$$\begin{aligned} \chi_{u>0}\, u_{tt}(t,x) &= \Delta u(t,x) - \gamma(x)\chi_\varepsilon'(u) + \lambda(t)\chi_{u>0} \quad \text{in } Q_T = (0,T)\times\Omega, \\ u(t,x) &= 0 \qquad\qquad\qquad \text{on } (0,T)\times\partial\Omega, \\ u(0,x) &= u_0(x) \qquad\qquad\quad \text{in } \Omega, \\ u_t(0,x) &= v_0(x) \qquad\qquad\quad \text{in } \Omega, \end{aligned} \tag{5.2.18}$$

in the following sense (compare with Definition 4.2.1):

Definition 5.2.4. *A function $u \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H_0^1(\Omega))$ is called a weak solution to (5.2.18) if $u(0) = u_0$ is satisfied and the following identity holds for all test functions $\psi \in C_0^\infty\big(([0,T)\times\Omega)\cap\{u>0\}\big)$:*

$$\begin{aligned} &\int_0^T \int_\Omega \big(-u_t\psi_t + \nabla u\nabla\psi + \gamma\chi_\varepsilon'(u)\psi\big)\,dx\,dt - \int_\Omega v_0\psi(0)\,dx \\ &\quad = \frac{1}{V}\int_0^T\int_\Omega \big(-u_t(u\Psi)_t + |\nabla u|^2\Psi + \gamma\chi_\varepsilon'(u)u\Psi\big)\,dx\,dt - \frac{1}{V}\int_\Omega u_0v_0\Psi(0)\,dx, \end{aligned} \tag{5.2.19}$$

where the notation $\Psi = \int_\Omega \psi\,dx$ is used.

We put the same assumptions on Ω, T and all the functions appearing above as in Section 5.2.1. However, we are able to construct only a solution which is still weaker with respect to the nonlinearity in the right-hand side of (5.2.19).

The method of proof is based on the idea of K. Kikuchi (minimizing movement) and uses penalties for the constraints and uniform convergence which can be obtained, when we restrict the space dimension to $m = 1$. It is worth noting that this method is different from Yosida approximation method and, thus, is more suitable for numerical schemes. Unlike in (5.2.5), we define the approximate solution on n-th time level t_n ($h = T/N$, $t_n = nh$, $n = 2,\ldots,N$) as a minimizer of

$$J_n(u) = \int_\Omega \frac{|u-2u_{n-1}+u_{n-2}|^2}{2h^2}\,dx + \frac{1}{2}\int_\Omega |\nabla u|^2\,dx + \int_\Omega \gamma\chi_\varepsilon(u)\,dx + \Phi_1(u) + \Phi_2(u) \tag{5.2.20}$$

in the space $H_0^1(\Omega)$. The penalties Φ_1 and Φ_2 are functionals $H^1(\Omega) \to \{0,\infty\}$ defined as follows:

$$\Phi_1(u) = \begin{cases} 0, & \text{if } u \geq 0 \text{ a.e. in } \Omega \\ \infty, & \text{otherwise,} \end{cases} \tag{5.2.21}$$

$$\Phi_2(u) = \begin{cases} 0, & \text{if } \int_\Omega u\,dx = V \\ \infty, & \text{otherwise.} \end{cases} \tag{5.2.22}$$

Starting functions u_0 and $u_1 = u_0 + hv_0$ are determined from the initial conditions and remaining approximations $u_2, u_3, \ldots, u_N$ are computed inductively.

We prove that J_n is weakly lower semicontinuous in $H_0^1(\Omega)$ and that Φ_1 and Φ_2 are convex, in order to ensure the existence of corresponding subdifferentials (see [8], Section 9.6). Since the sum of convex, lower semicontinuous functions is again convex and lower semicontinuous, it is enough to show convexity and lower semicontinuity of Φ_1 and Φ_2 separately. We want to show for $\theta \in (0,1)$ and $u, v \in H^1(\Omega)$ that

$$\Phi_1(\theta u + (1-\theta)v) \leq \theta\Phi_1(u) + (1-\theta)\Phi_1(v).$$

If either $\Phi_1(u)$ or $\Phi_1(v)$ is infinite, the inequality is trivially fulfilled, so we consider the remaining case $\Phi_1(u) = \Phi_1(v) = 0$. This means that $u \geq 0$ and $v \geq 0$ a.e. in Ω. Hence, $\theta u + (1-\theta)v \geq 0$ a.e. in Ω and $\Phi_1(\theta u + (1-\theta)v) = 0$.

The proof for Φ_2 is analogous: if $\Phi_2(u) = \Phi_2(v) = 0$, then $\int_\Omega u\,dx = V$, $\int_\Omega v\,dx = V$ and $\int_\Omega (\theta u + (1-\theta)v)\,dx = V$. Thus $\Phi_2(\theta u + (1-\theta)v) = 0 = \theta\Phi_2(u) + (1-\theta)\Phi_2(v)$.

Let $u^k \rightharpoonup u$ weakly in $H_0^1(\Omega)$. We are supposed to show that

$$\Phi_1(u) \leq \liminf_{k\to\infty} \Phi_1(u^k). \tag{5.2.23}$$

Since both sides of the inequality can have only two values (0 and ∞), it is sufficient to show that if the right-hand side is zero, then the left-hand side is zero, too. Assume the contrary, i.e., that the right-hand side of (5.2.23) is zero but the left-hand side is infinity. This implies that for each $k \in \mathbb{N}$, there is a $K > k$ so that $u^K \geq 0$ a.e. in Ω and that there is a set $S \subset \Omega$ of positive measure, so that $u \leq 0$ in S. In particular,

$$j = \int_S u^2\,dx > 0.$$

From Rellich's theorem we have

$$\int_\Omega (u - u^k)^2\,dx \to 0 \tag{5.2.24}$$

but for each $k \in \mathbb{N}$, there is a $K > k$ such that $u^K \geq 0$ a.e. in Ω, especially in S. Hence,

$$\int_\Omega (u - u^K)^2\,dx \geq \int_S (u - u^K)^2\,dx \geq \int_S u^2\,dx = j > 0,$$

which is a contradiction.

The proof of lower semicontinuity for Φ_2 is similar. Assuming $\Phi_2(u) = \infty$ and $\liminf \Phi_2(u^k) = 0$, we have for any $k \in \mathbb{N}$ the existence of $K > k$ so that

$$\Big|\int_\Omega (u - u^K)\,dx\Big|^2 = \Big|\int_\Omega u\,dx - V\Big|^2 = j' > 0.$$

However,

$$\int_\Omega |u - u^k|^2\,dx \geq \frac{1}{|\Omega|}\Big(\int_\Omega |u - u^k|\,dx\Big)^2 \geq \frac{1}{|\Omega|}\Big|\int_\Omega (u - u^k)\,dx\Big|^2,$$

so the left-hand side in the above cannot go to zero as $k \to \infty$, which is in contradiction to (5.2.24).

We are ready to prove the existence of minimizers.

Lemma 5.2.2. *For each $n = 2, \dots, N$, there is a minimizer of J_n in $H_0^1(\Omega)$.*

Proof. Choose a minimizing sequence $\{u^k\}_{k=1}^{\infty} \subset H_0^1(\Omega)$ so that

$$J_n(u^k) \to \inf_{u \in H_0^1(\Omega)} J_n(u) = m.$$

Functionals J_n are proper and nonnegative, so m is a finite number. Thus we deduce that the sequence $\{u^k\}$ is bounded in $H_0^1(\Omega)$. We can then extract a weakly convergent subsequence $u^{k_j} \rightharpoonup u$. Since J_n is weakly lower semicontinuous, u is a minimum of J_n. $\square$

Remark 5.2.1. *Since for any function $u \in H_0^1(\Omega)$ satisfying $u \geq 0$ a.e. in Ω and $\int_\Omega u\,dx = V$, the value $J_n(u)$ is finite, any minimizer u_n of J_n must satisfy*

$$\begin{aligned} u_n &\geq 0 \qquad a.e.\ in\ \Omega, \\ \int_\Omega u_n\,dx &= V. \end{aligned}$$

We denote the set of functions complying with the conditions from the above remark as $\mathcal{K}$:

$$\mathcal{K} := \Big\{u \in H_0^1(\Omega);\ u \geq 0 \text{ a.e. in } \Omega,\ \int_\Omega u\,dx = V\Big\}.$$

We derive an estimate for approximate solutions.

Lemma 5.2.3. *There is a constant C independent of n so that minimizers u_n satisfy*

$$\Big\|\frac{u_n - u_{n-1}}{h}\Big\|_{L^2(\Omega)}^2 + \|\nabla u_n\|_{L^2(\Omega)}^2 \leq C. \tag{5.2.25}$$

Proof. As the set $\mathcal{K}$ is convex, the function $(1-\theta)u_n + \theta u_{n-1}$ belongs to $\mathcal{K}$ for all $\theta \in (0,1)$. A function u_n is a minimizer of J_n if and only if 0 belongs to the subdifferential ∂J_n at u_n (see [8], Chapter 9.6). This means that $J_n(u_n) \leq J_n(v)$ for all $v \in H_0^1(\Omega)$. Therefore, by the minimality property we have

$$0 \leq \frac{1}{\theta}\big(J_n((1-\theta)u_n + \theta u_{n-1}) - J_n(u_n)\big).$$

Since the terms Φ_1 and Φ_2 drop away, passing to the limit as $\theta \to 0+$, we get

$$\begin{aligned} 0 \;&\leq\; -\frac{1}{h^2}\int_\Omega (u_n - u_{n-1})(u_n - 2u_{n-1} + u_{n-2})\,dx + \int_\Omega \nabla u_n \nabla(u_{n-1} - u_n)\,dx \\ &\qquad + \int_\Omega \gamma \chi_\varepsilon'(u_n)(u_n - u_{n-1})\,dx \\ &\leq\; \frac{1}{2h^2}\int_\Omega \big((u_{n-1} - u_{n-2})^2 - (u_n - u_{n-1})^2\big)\,dx + \frac{1}{2}\int_\Omega \big(|\nabla u_{n-1}|^2 - |\nabla u_n|^2\big)\,dx \\ &\quad + h\int_\Omega \gamma^2 \frac{C^2}{\varepsilon^2}\,dx + \frac{h}{2}\int_\Omega \Big(\frac{u_n - u_{n-1}}{h}\Big)^2\,dx. \end{aligned}$$

Thus, after summing up, we arrive at

$$\Big\|\frac{u_n - u_{n-1}}{h}\Big\|^2_{L^2(\Omega)} + \|\nabla u_n\|^2_{L^2(\Omega)} \leq \|v_0\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)} + C\|\gamma\|^2_{L^2(\Omega)} + h\sum_{k=1}^{n}\Big\|\frac{u_k - u_{k-1}}{h}\Big\|^2_{L^2(\Omega)}.$$

Defining

$$a_n = \Big\|\frac{u_n - u_{n-1}}{h}\Big\|^2_{L^2(\Omega)} + \|\nabla u_n\|^2_{L^2(\Omega)},$$

we get

$$a_n \leq \|v_0\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)} + C\|\gamma\|^2_{L^2(\Omega)} + h\sum_{k=1}^{n} a_k.$$

The discrete Gronwall lemma (see [13]) implies

$$a_n \leq \big(\|v_0\|^2_{L^2(\Omega)} + \|\nabla u_1\|^2_{L^2(\Omega)} + C\|\gamma\|^2_{L^2(\Omega)}\big)e^{2T}.$$

This is already the desired estimate. □

As in the previous Sections, we interpolate minimizers in time:

$$\bar{u}^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ u_n(x), & t \in ((n-1)h, nh],\ n = 1,\dots,N \end{cases} \tag{5.2.26}$$

$$u^h(t,x) = \begin{cases} u_0(x), & t = 0 \\ \frac{t-(n-1)h}{h}u_n(x) + \frac{nh-t}{h}u_{n-1}(x), & t \in ((n-1)h, nh], n = 1,\dots,N \end{cases}$$

Rewritten in terms of $\bar{u}^h$ and u^h, (5.2.25) becomes

$$\|u^h_t(t)\|^2_{L^2(\Omega)} + \|\nabla\bar{u}^h(t)\|^2_{L^2(\Omega)} \leq C \qquad \text{for a.e. } t \in (0,T). \tag{5.2.27}$$

Our next step is to show the Hölder continuity of u_n.

Lemma 5.2.4. *Minimizers u_n of J_n are Hölder continuous on compact subsets of Ω.*

Proof. Notice that all the test functions from the proof of Theorem 5.2.2 belong to $\mathcal{K}$. Therefore, we can carry out the proof exactly in the same way because the penalties Φ_1 and Φ_2 have no influence. □

Thanks to the continuity of minimizers, it is guaranteed that $\{u_n > 0\}$ is relatively open in Ω for $n = 2,\dots,N$. Thus, it makes sense to consider test functions with compact support in $\Omega\cap\{u_n > 0\}$. For such a test function $\psi \in C_0^\infty(\Omega\cap\{u_n > 0\})$ with $\Psi = \int_\Omega \psi\, dx$, we define the perturbation

$$u_n^\epsilon = \frac{u_n + \epsilon\psi}{1 + \frac{\epsilon}{V}\Psi}, \qquad \epsilon > 0,$$

and compute the limit

$$\lim_{\epsilon\to 0+}\frac{J_n(u_n^\epsilon) - J_n(u_n)}{\epsilon} \geq 0. \tag{5.2.28}$$

Note that $u_n^\epsilon \in \mathcal{K}$ for ϵ sufficiently small, which implies $\Phi_1(u_n^\epsilon) = \Phi_2(u_n^\epsilon) = 0$ if $\epsilon < \epsilon_0$ for some $\epsilon_0 > 0$. Hence, from (5.2.28) we get

$$\int_\Omega \Big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} \psi + \nabla u_n \nabla \psi + \gamma \chi_\varepsilon'(u_n)\psi \Big)\, dx \geq \lambda_n \Psi,$$

where

$$\lambda_n = \frac{1}{V} \int_\Omega \Big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} u_n + |\nabla u_n|^2 + \gamma \chi_\varepsilon'(u_n) u_n \Big)\, dx.$$

Replacing ψ with $-\psi$, we obtain the reverse inequality, whence the equality

$$\int_\Omega \Big(\frac{u_n - 2u_{n-1} + u_{n-2}}{h^2} \psi + \nabla u_n \nabla \psi + \gamma \chi_\varepsilon'(u_n)\psi \Big)\, dx = \lambda_n \Psi, \quad \forall \psi \in C_0^\infty(\Omega \cap \{u_n > 0\}). \tag{5.2.29}$$

Using the definition of $\bar{u}^h$ and u^h, this is the same as

$$\int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h} \psi + \nabla \bar{u}^h \nabla \psi + \gamma \chi_\varepsilon'(\bar{u}^h)\psi \Big)\, dx = \bar{\lambda}^h \Psi,$$

for all $t \in (h, T)$ and for all $\psi \in C_0^\infty(\Omega \cap \{\bar{u}^h(t) > 0\})$, where $\bar{\lambda}^h$ is the interpolated multiplier

$$\bar{\lambda}^h(t) = \frac{1}{V} \int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h} \bar{u}^h(t) + |\nabla \bar{u}^h(t)|^2 + \gamma \chi_\varepsilon'(\bar{u}^h(t)) \bar{u}^h(t) \Big)\, dx, \quad t \in (h, T).$$

Integrating over (h, T) and extending the test functions to time-dependent domains, we have

$$\int_h^T \int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h} \psi + \nabla \bar{u}^h \nabla \psi + \gamma \chi_\varepsilon'(\bar{u}^h)\psi \Big)\, dx\, dt = \int_h^T \bar{\lambda}^h \Psi\, dt, \tag{5.2.30}$$

for all $\psi \in C_0^\infty\big(([0,T) \times \Omega) \cap \{\bar{u}^h > 0\}\big)$.

In passing to the limit as $h \to 0+$, we use a method, which gets rid of the term with $\bar{\lambda}^h$ by considering only test functions of zero volume and restores the multiplier term after carrying out the limit. Therefore, we introduce the following space of test functions:

$$\mathcal{C}(v) = \Big\{ \psi \in C_0^\infty\big(([0,T) \times \Omega) \cap \{v > 0\}\big);\ \int_\Omega \psi = 0 \Big\}.$$

Relation (5.2.30) then implies

$$\int_h^T \int_\Omega \Big(\frac{u_t^h(t) - u_t^h(t-h)}{h} \psi + \nabla \bar{u}^h \nabla \psi + \gamma \chi_\varepsilon'(\bar{u}^h)\psi \Big)\, dx\, dt = 0 \qquad \forall \psi \in \mathcal{C}(\bar{u}^h). \tag{5.2.31}$$

In order to be able to pass to the limit as $h \to 0+$ in (5.2.31), we need besides a standard energy estimate (see (5.2.27)) also uniform convergence of u^h because the space $\mathcal{C}_h$ depends on the unknown function $\bar{u}^h$. We are able to get the uniform convergence only for $m = 1$, and that is why we confine ourselves to the one-dimensional case from now on.

Lemma 5.2.5. *Let Ω be an open interval in $\mathbb{R}$. Then there is a decreasing sequence $\{h_j\}_{j=1}^\infty$ with limit zero (we write only $h \to 0+$) and a function $u \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H_0^1(\Omega))$ such that*

$$
\begin{aligned}
u_t^h &\to u_t && \text{weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)), && (5.2.32)\\
\nabla \bar{u}^h &\to \nabla u && \text{weakly}^* \text{ in } L^\infty(0,T;L^2(\Omega)), && (5.2.33)\\
u^h &\rightrightarrows u && \text{uniformly in } Q_T. && (5.2.34)
\end{aligned}
$$

The cluster function u is continuous and nonnegative in Q_T and satisfies the volume condition $\int_\Omega u\,dx = V$. Moreover, it satisfies the initial condition $u(0,x) = u_0(x)$ in Ω.

Proof. First two statements follow from the estimate (5.2.27). We shall prove uniform equicontinuity of u^h with respect to h. First, we see by (5.2.27) that

$$
\|u^h(s) - u^h(t)\|_{L^2(\Omega)}^2 = \int_\Omega \Big(\int_t^s u_t^h(\tau)\,d\tau \Big)^2 dx \le C(s-t)^2.
$$

with C independent of h. Further, using the inequality

$$
\|f\|_{L^\infty(\Omega)} \le C \|f\|_{L^2(\Omega)}^{1/2} \Big\| \frac{df}{dx} \Big\|_{L^2(\Omega)}^{1/2},
$$

which holds for one dimension and $f \in H_0^1(\Omega)$, we find again by (5.2.27) that

$$
\|u^h(s) - u^h(t)\|_{L^\infty(\Omega)} \le C \|u^h(s) - u^h(t)\|_{L^2(\Omega)}^{1/2} \|u_x(s) - u_x(t)\|_{L^2(\Omega)}^{1/2} \le C|s-t|^{1/2}.
$$

With these estimates at hand, the proof of equicontinuity is immediate:

$$
\begin{aligned}
|u^h(s,y) - u^h(t,x)| &\le |u^h(s,y) - u^h(s,x)| + |u^h(s,x) - u^h(t,x)|\\
&= \Big| \int_x^y u_x^h(s,\xi)\,d\xi \Big| + |u^h(s,x) - u^h(t,x)|\\
&\le |y-x|^{1/2} \Big(\int_\Omega |u_x^h(s,\xi)|^2\,d\xi \Big)^{1/2} + C|s-t|^{1/2}\\
&\le C\big(|y-x|^{1/2} + |s-t|^{1/2} \big).
\end{aligned}
$$

Moreover, from this estimate we get the uniform boundedness in $L^\infty(Q_T)$ by setting $s = 0$ and $y = 0$. Therefore, by Arzelà-Ascoli theorem there is a subsequence $\{u^h\}$ converging to u uniformly in Q_T. □

Now, we take h to zero in (5.2.31). We aim at obtaining a weak solution according to Definition 5.2.4, so we fix an arbitrary $\varphi \in \mathcal{C}(u)$. Since u is continuous on Q_T, there is a constant $\eta > 0$ such that $u \ge \eta$ on the support of φ. Subsequence $\{u^h\}$ from Lemma 5.2.5 converges to u uniformly, granting a positive h_0 so that

$$
\max_{(t,x)\in Q_T} |u^h(t,x) - u(t,x)| \le \frac{\eta}{2} \qquad \text{for } h < h_0.
$$

Hereby, $u^h \geq u - |u^h - u| \geq \eta/2$ on the support of φ for $h \in (0, h_0)$. Noting that $\bar{u}^h$ acquires only a subset of values of u^h (i.e., $\bar{u}^h(t,x) = u^h(kh,x)$ for $t \in ((k-1)h, kh])$, we have also

$$\bar{u}^h \geq \frac{\eta}{2} > 0 \qquad \text{on } \operatorname{supp}\varphi \quad \text{for } h \in (0, h_0).$$

This means that relation (5.2.31) holds for our test function φ, if $h < h_0$. The limit as $h \to 0+$ is calculated in the same way as in the proof of Theorem 4.2.2. We arrive at

$$\int_0^T \int_\Omega (-u_t\varphi_t + \nabla u \nabla \varphi + \gamma \chi'_\varepsilon(u)\varphi)\, dx\, dt - \int_\Omega v_0 \varphi(0)\, dx = 0 \qquad \forall \varphi \in \mathcal{C}(u). \tag{5.2.35}$$

The last task is to eliminate the vanishing volume condition imposed on the test functions in $\mathcal{C}(u)$. The fundamental idea is to put

$$\varphi := V\psi - \Big(\int_\Omega \psi\, dx\Big) u \qquad \text{for arbitrary } \psi \in C_0^\infty\big(([0,T) \times \Omega) \cap \{u > 0\}\big).$$

Integrating such φ over Ω, we check that it has zero volume and is, in this sense, an admissible test function for (5.2.35). However, it is not smooth enough and it does not exactly have compact support inside $([0,T) \times \Omega) \cap \{u > 0\}$, as required. Hence, we have to use an approximation $\tilde{u} \in C_0^\infty(\{u > 0\})$ to u with volume V. Setting $\varphi := V\psi - (\int_\Omega \psi\, dx)\tilde{u}$ in (5.2.35), we have

$$\begin{aligned} &\int_0^T \int_\Omega \big(-u_t\psi_t + \nabla u \nabla \psi + \gamma \chi'_\varepsilon(u)\psi\big)\, dx\, dt - \int_\Omega v_0 \psi(0)\, dx \\ &\qquad = \int_0^T \int_\Omega \big(-u_t(\tilde{u}\Psi)_t + \nabla u \nabla \tilde{u}\Psi + \gamma \chi'_\varepsilon(u)\tilde{u}\Psi\big)\, dx\, dt - \int_\Omega v_0 \tilde{u}(0)\Psi(0)\, dx. \end{aligned} \tag{5.2.36}$$

It turns out that we have obtained a solution weaker than the solution introduced in Definition 5.2.4. If we could put $\tilde{u} = u$ in the above, we would arrive at the desired identity (5.2.19). In order to do so, further investigation concerning the free boundary would be necessary.

5.3 Appendix

We derive a model for the motion of a droplet on a plane, driven by the nonuniform surface properties of the plane. The changing surface tension of the substrate results in different contact angles in different parts of the drop contour and the instability of the droplet. The droplet changes its shape leaning towards the area with smaller surface tension. We suggest that such a motion can be approximately modeled by a parabolic or hyperbolic equation for the surface of the drop with volume constraint. The resulting problem is a free boundary equation with a complicated nonlocal term.

In this setting, there is no outer force present. The drop moves purely by the chemical gradient on the surface of the substrate. We adopted this model in order to avoid complications with an outer force term representing gravity, stress etc. However, one of the aims of this modelling is to treat moving droplets on inclined surfaces, where an outer force is indispensable. In such modelling, we are planning to combine the equations of motion of the liquid (Navier-Stokes equations) with an equation for the surface of the drop (the equation mentioned above). It is natural to consider the surface of the drop separately because, as it is known, a film with characteristic properties develops on the interface between any liquid and gas (see Figure 5.3). Moreover, this approach is in a sense inevitable if we aim at realizing a positive contact angle. The liquid and the film interact in the model via pressure forces, and that is why the outer force term in the equation for the film becomes important.

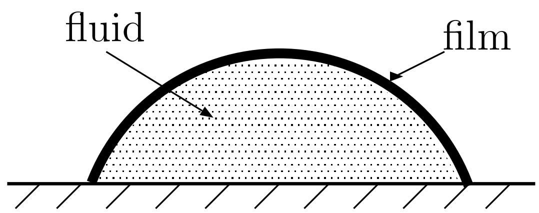


Figure 5.3: Coupled model.

One of the most typical features of drops on surfaces is the positive contact angle (the angle of the surface and the edge of the drop). The equilibrium contact angle θ of the droplet depends on the properties of the liquid and the material on which the droplet is lying ([24], [44]) and is described by Young's equation

$$\gamma_{SG} - \gamma_{SL} = \gamma_{LG} \cos\theta, \tag{5.3.1}$$

where γ_{SG} is the solid surface tension, γ_{LG} the liquid surface tension and γ_{SL} the solid/ liquid interfacial surface tension. Certain materials, like ethanol on glass or silicon, make the droplet spread completely (total wetting), while other materials, as water on plastic or lotus leaves, make the droplet rest on the substrate in the form of a spherical cap close to a sphere (non-wetting). In this study, we deal with the case of partial wetting with relatively small contact angles.

Although many experiments and measurements of moving drops have been done, there is no well-established analytic model to describe the dynamical aspects of drop motion. Many papers have been devoted to analyzing the shape of steady drops on horizontal and inclined surfaces. Works dealing with the motion of droplets generally make some kind of steady or quasisteady assumptions. The authors of [34] take a similar approach as [6] and develop a model for a drop that does not change its shape and moves steadily overcoming shear exerted by the solid surface. They consider a thin 'pancake' droplet and rely on the lubrication approximation of de Gennes ([10]). We would like to show a different approach that we consider to be more appropriate for slow motion of drops caused by nonuniform properties of the underlying surface.

Taking into account the principles of surface tension and the main feature of the drop - positive contact angle, we think that a reasonable design for the model of moving drop is to approximate the drop by a film, representing the surface of the drop. Then there

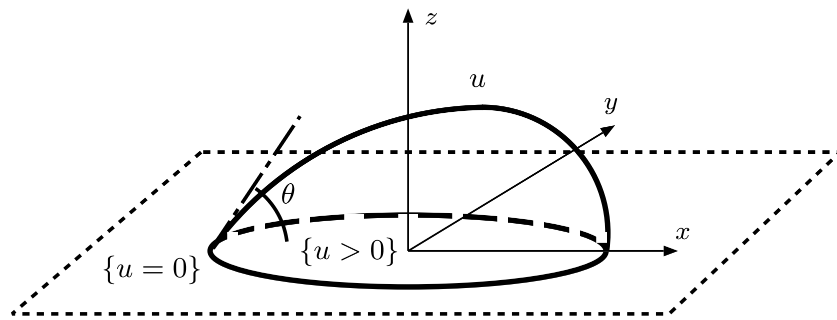


Figure 5.4: Droplet attached to a plane.

is also the option left to fill this film with fluid behaving in accordance to a model of fluid dynamics, and couple these two models. In the case of the film, we have to develop a model for a volume-preserving membrane with an obstacle and positive contact angle that is moving in the horizontal direction. As already Frenkel ([9]) observes, the motion of the fluid inside the droplet is not a mere translation - the fluid is pouring from the rear edge of the drop towards the front edge. This led us to the thought that it is plausible to assume that the film moves in the vertical direction. Moreover, this assumption is inevitable in a scalar model.

The model, derived here along the lines of these examinations, is very simple and does not include all the properties that moving drops exhibit. For example, it is known that moving drops show hysteresis in the contact angle. The contact angle in the front is larger than the expected value (advancing contact angle) and the angle in the rear becomes smaller (receding contact angle). This hysteresis leads to stick-slip behaviour (i.e., sudden large-scale change of the equilibrium shape of the drop caused by a small perturbation of a parameter of the system) and jerky movements ([17]). It has been ascribed to surface inhomogeinities but models explaining this phenomenon in different ways have been developed recently. For instance, in [32] it is shown that a theory considering a thin film, which is left after the droplet moves away, gives a good agreement with experiments for hydrophilic surfaces. This explanation would make it possible to include this phenomenon in our coupled model and actually fits very well in it. See also [7] for a mathematical model of contact angle hysteresis. In this work, we do not consider secondary properties, since we are aiming at the development of a general model. To add aspects such as hysteresis of the contact angle into the basic model will be our future goal.

We start the derivation of the model by reviewing the equilibrium shape of the drop. From the assumption of partial wetting ($\theta < 90^o$), we can describe the film as a scalar function $u : Q_T = (0,T) \times \Omega \to \mathbb{R}$, where $(0,T)$ is the time interval and Ω is the domain where the motion is considered (see Figure 5.4). The plane, on which the drop rests, corresponds to 0-level set of the function u. The domain $\Omega \subset \mathbb{R}^m$ is taken bounded but large enough so that the drop does not touch its boundary during the motion. Homogeneous Dirichlet condition is prescribed on its boundary $\partial\Omega$, which is assumed to be Lipschitz.

The main features determining the shape of the drop are surface tension, contact angle and volume preservation. The boundary of the drop, i.e., the place where the contact angle can be observed, agrees with the boundary of the set $\{u > 0\}$ and will be called *free boundary.* We have three types of surfaces in this situation. By γ_{SG} we denote the surface tension between the solid underlying plane and air, by γ_{LG} the surface tension between the drop and air and by γ_{SL} the interfacial surface tension on the solid/liquid boundary. We assume that the surface tension of the drop is homogeneous and constant.

Let us use the symbol $\chi_{u>0}$ for the characteristic function of the set $\{u > 0\}$ and simplify the notation for surface tensions:

$$\gamma_g = \gamma_{LG}, \qquad \gamma_s = \gamma_{LS} - \gamma_{SG}.$$

Under the above simplifications, the surface energy of the drop can be written in the following way:

$$E = \gamma_g \int_\Omega \left(\sqrt{1 + |\nabla u|^2}\right) \chi_{u>0}\, dx + \int_\Omega \gamma_s \chi_{u>0}\, dx. \tag{5.3.2}$$

The drop assumes the shape which minimizes the energy E under the volume constraint

$$\int_\Omega u \chi_{u>0}\, dx = V, \tag{5.3.3}$$

where $V > 0$ is the volume of the drop. There is obviously no condition on the behaviour of the minimizer in the region where it is nonpositive which leads us to adding the extra condition $u \geq 0$. Then the minimization of (5.3.2) under condition (5.3.3) is equivalent to the minimization under the same constraint of the functional

$$E = \gamma_g \int_\Omega \sqrt{1 + |\nabla u|^2}\, dx + \int_\Omega (\gamma_g + \gamma_s) \chi_{u>0}\, dx, \tag{5.3.4}$$

the form analyzed in [14] and [40], where, among other results, the existence of minimizers is shown.

If γ_g and γ_s are constant and the drop is small so that it is not influenced by gravitation forces, the drop has the shape of a spherical cap (see [6]). This can be shown using Schwarz symmetrization and isoperimetric inequality in the framework of BV functions (see, e.g., [7]). In this case, we can derive the well-known Young's equation for the contact angle θ ([33], [44])

$$\gamma_s = -\gamma_g \cos\theta \tag{5.3.5}$$

by explicitly minimizing functional (5.3.2) under condition (5.3.3).

Lemma 5.3.1. *Let γ_s be a constant. Then the contact angle θ of the spherical cap, which minimizes the expression (5.3.2) among all spherical caps with the same volume, satisfies relation (5.3.5).*

Proof. Since the proof is just technical, we mention briefly only the case $m = 2$. Let the radius of the spherical cap be denoted by r and the angle of the cap by θ, as in Figure 5.5.

The value of (5.3.2) then becomes

$$E(\theta, r) = 2\gamma_g \theta r + 2\gamma_s r \sin\theta. \tag{5.3.6}$$

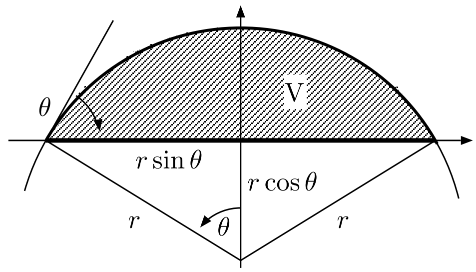


Figure 5.5: Proof of Young's equation.

Since the volume of the liquid does not change, we have

$$\theta r^2 - r^2 \cos\theta \sin\theta = V.$$

Extracting r from this equation and substituting into (5.3.6) gives

$$E(\theta) = 2(\gamma_g \theta + \gamma_s \sin\theta)\sqrt{\frac{V}{\theta - \cos\theta\sin\theta}}.$$

We can see that this function is convex when $\theta > 0$, hence the angle θ yielding the minimum of $E(\theta)$ satisfies

$$\frac{dE}{d\theta} = \frac{2(\gamma_g \cos\theta + \gamma_s)(\theta\cos\theta - \sin\theta)}{(\theta - \cos\theta\sin\theta)^{3/2}} = 0.$$

Because for positive values of θ we have $\theta\cos\theta - \sin\theta < 0$, we conclude that the desired relation (5.3.5) holds. $\square$

If we assume that the minimizer exists and is smooth, we derive also the following more general result, which holds for nonuniform distribution of γ_s (i.e., nonspherical drops).

Lemma 5.3.2. *Let the minimizer of (5.3.2) be smooth in $\overline{\{u > 0\}}$. Then Young's equation (5.3.5) holds on $\partial\{u > 0\}$.*

Proof. First, we derive the relation satisfied by the minimizer inside $\{u > 0\}$. For this purpose, we fix an arbitrary function $\varphi \in C_0^\infty(\Omega \cap \{u > 0\})$, denote its volume $\int_\Omega \varphi\, dx$ by Φ and introduce the volume preserving perturbation

$$u_\varepsilon = V\frac{u + \varepsilon\varphi}{V + \varepsilon\Phi}.$$

Then we have

$$\begin{aligned}
0 &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\big(E(u_\varepsilon)-E(u)\big)\\
&= \lim_{\varepsilon\to 0}\frac{\gamma_g}{\varepsilon}\int_\Omega\Big(\sqrt{1+\frac{|\nabla u+\varepsilon\nabla\varphi|^2}{(1+\varepsilon\Phi/V)^2}}\chi_{u+\varepsilon\varphi>0}-\sqrt{1+|\nabla u|^2}\chi_{u>0}\Big)\,dx\\
&\qquad +\frac{1}{\varepsilon}\int_\Omega\gamma_s(\chi_{u+\varepsilon\varphi>0}-\chi_{u>0})\,dx\\
&= \lim_{\varepsilon\to 0}\frac{\gamma_g}{\varepsilon}\int_\Omega\Big(\sqrt{1+\frac{|\nabla u+\varepsilon\nabla\varphi|^2}{(1+\varepsilon\Phi/V)^2}}-\sqrt{1+|\nabla u|^2}\Big)\chi_{u>0}\,dx\\
&= \gamma_g\int_\Omega\frac{\nabla u\nabla\varphi-\frac{1}{V}|\nabla u|^2\Phi}{\sqrt{1+|\nabla u|^2}}\chi_{u>0}\,dx\\
&= \gamma_g\int_\Omega\Big(\frac{\nabla u\nabla\varphi}{\sqrt{1+|\nabla u|^2}}-\lambda\varphi\Big)\,dx,
\end{aligned}$$

where we have put

$$\lambda=\frac{1}{V}\int_{\{u>0\}}\frac{|\nabla u|^2}{\sqrt{1+|\nabla u|^2}}\,dx.$$

Using Green's theorem we obtain the relation

$$\gamma_g\int_\Omega\Big(\frac{\Delta u(1+|\nabla u|^2)-\nabla u^T D^2u\nabla u}{(1+|\nabla u|^2)^{3/2}}-\lambda\Big)\varphi\,dx=0\qquad\forall\varphi\in C_0^\infty(\Omega\cap\{u>0\}).\quad(5.3.7)$$

On the other hand, we can carry out the so-called inner variation of (5.3.2), which uses the perturbation

$$u_\varepsilon=\frac{V}{V_\varepsilon}u(\tau_\varepsilon^{-1}(x)),$$

where

$$\tau_\varepsilon(x)=x+\varepsilon\eta(x),\qquad \eta\in C_0^\infty(\Omega,\mathbb{R}^m)$$

with Jacobian

$$|D\tau_\varepsilon|=1+\varepsilon\,\mathrm{div}\eta+o(\varepsilon),\qquad\varepsilon\to 0,$$

and V_ε is determined so that the perturbation preserves volume:

$$V_\varepsilon=\int_\Omega u(\tau_\varepsilon^{-1}(x))\,dx=\int_\Omega u(y)\,|D\tau_\varepsilon(y)|\,dy=V+\varepsilon\int_\Omega u\,\mathrm{div}\eta\,dx+o(\varepsilon),\quad\varepsilon\to 0.$$

Noting that

$$\begin{aligned}
\frac{\partial u_\varepsilon}{\partial x_i}(x) &= \frac{V}{V_\varepsilon}\sum_j\frac{\partial u}{\partial x_j}(\tau_\varepsilon^{-1}(x))\frac{\partial(\tau_\varepsilon^{-1})_j}{\partial x_i}(x)\\
&= \frac{V}{V_\varepsilon}\sum_j\frac{\partial u}{\partial x_j}(\tau_\varepsilon^{-1}(x))(D\tau_\varepsilon)^{-1}_{ji}(\tau_\varepsilon^{-1}(x))\\
&= \frac{V}{V_\varepsilon}\sum_j\frac{\partial u}{\partial x_j}(\tau_\varepsilon^{-1}(x))\Big(\delta_{ij}-\varepsilon\frac{\partial\eta_j}{\partial x_i}(\tau_\varepsilon^{-1}(x))+o(\varepsilon)\Big),
\end{aligned}$$

and employing the substitution $y = \tau_\varepsilon^{-1}(x)$, we have

$$\begin{aligned}
0 &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\big(E(u_\varepsilon) - E(u)\big)\\
&= \lim_{\varepsilon\to 0}\frac{\gamma_g}{\varepsilon}\int_\Omega \Big[\sqrt{1+\frac{V^2}{V_\varepsilon^2}\sum_i\Big(\frac{\partial u}{\partial x_i} - \varepsilon\sum_j \frac{\partial u}{\partial x_j}\frac{\partial \eta_j}{\partial x_i}\Big)^2}(1+\varepsilon\,\mathrm{div}\eta)\\
&\qquad -\sqrt{1+|\nabla u|^2}\Big]\chi_{u>0}\,dx + \frac{1}{\varepsilon}\int_\Omega (\gamma_s(\tau_\varepsilon)(1+\varepsilon\,\mathrm{div}\eta) - \gamma_s)\,\chi_{u>0}\,dx\\
&= \lim_{\varepsilon\to 0}\frac{\gamma_g}{\varepsilon}\int_\Omega \frac{2\varepsilon\,\mathrm{div}\eta + \frac{V^2}{V_\varepsilon^2}\Big(|\nabla u|^2 - 2\varepsilon\sum_{i,j}\frac{\partial u}{\partial x_i}\frac{\partial u}{\partial x_j}\frac{\partial \eta_j}{\partial x_i}\Big)(1+2\varepsilon\,\mathrm{div}\eta) - |\nabla u|^2}{2\sqrt{1+|\nabla u|^2}}\chi_{u>0}\,dx\\
&\qquad + \int_\Omega\Big(\frac{\gamma_s(\tau_\varepsilon)-\gamma_s}{\varepsilon} + \gamma_s(\tau_\varepsilon)\,\mathrm{div}\eta\Big)\chi_{u>0}\,dx\\
&= \gamma_g\int_{\{u>0\}}\Big(\frac{(1+|\nabla u|^2)\,\mathrm{div}\eta - \nabla u^T D\eta\nabla u}{\sqrt{1+|\nabla u|^2}} - \lambda u\,\mathrm{div}\eta\Big)\,dx + \int_{\{u>0\}}\mathrm{div}(\gamma_s\eta)\,dx.
\end{aligned}$$

Using Green's theorem and result (5.3.7), we find that

$$\begin{aligned}
0 &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\,(E(u_\varepsilon) - E(u))\\
&= \gamma_g\int_{\{u>0\}}\Big(-\frac{\nabla u^T D^2 u\eta}{\sqrt{1+|\nabla u|^2}} + \frac{\Delta u(\nabla u\cdot\eta) + \nabla u^T D^2 u\eta}{\sqrt{1+|\nabla u|^2}}\\
&\qquad -\frac{(\nabla u^T D^2 u\nabla u)(\nabla u\cdot\eta)}{(1+|\nabla u|^2)^{3/2}} + \lambda(\nabla u\cdot\eta)\Big)\,dx\\
&\quad + \int_{\partial\{u>0\}}\Big(\gamma_g\sqrt{1+|\nabla u|^2}(\eta\cdot\nu) - \gamma_g\frac{(\nabla u\cdot\eta)(\nabla u\cdot\nu)}{\sqrt{1+|\nabla u|^2}} + \gamma_s(\eta\cdot\nu)\Big)\,dS\\
&= \int_{\partial\{u>0\}}\Big(\gamma_g\frac{(1+|\nabla u|^2)(\eta\cdot\nu) - (\nabla u\cdot\nu)(\nabla u\cdot\eta)}{\sqrt{1+|\nabla u|^2}} + \gamma_s(\eta\cdot\nu)\Big)\,dS,
\end{aligned}$$

where ν denotes the unit outer normal to $\partial\{u > 0\}$ and has actually the form $\nu = -\nabla u/|\nabla u|$, which yields

$$0 = \int_{\partial\{u>0\}}\Big(\frac{\gamma_g}{\sqrt{1+|\nabla u|^2}} + \gamma_s\Big)(\nu\cdot\eta)\,dS \qquad \forall\eta\in C_0^\infty(\Omega,\mathbb{R}^m).$$

We conclude that

$$\gamma_s = -\frac{1}{\sqrt{1+|\nabla u|^2}}\gamma_g \qquad \text{on } \partial\{u>0\},$$

meaning that the Young's equation (5.3.5) holds. □

Besides supposing that $0 < -\gamma_s < \gamma_g$, i.e., $0 < \theta < \pi/2$, which enables us to handle the problem in terms of scalar functions, we additionally suppose that γ_s is close to the value $-\gamma_g$, i.e., that the drop has a relatively small contact angle (hydrophilic surfaces). This assumption is made only to be able to linearize the minimal surface operator and thus to get theoretical results concerning existence of solution. However, in numerical computation, we can use the full operator and the assumption becomes irrelevant. Making this assumption, the gradient of u remains small and the following approximation is possible:

$$\sqrt{1+|\nabla u|^2} \approx 1 + \frac{1}{2}|\nabla u|^2. \tag{5.3.8}$$

Putting finally

$$\gamma := 1 + \frac{\gamma_s}{\gamma_g} \;\in\; (0,1),$$

we can rewrite the approximation of the surface energy (5.3.4) in the form

$$\tilde{E} = \gamma_g \left[\frac{1}{2} \int_\Omega |\nabla u|^2 \, dx + \int_\Omega \gamma(x) \chi_{u>0} \, dx \right]. \tag{5.3.9}$$

We have omitted the characteristic function in the first term. This is possible due to the fact that the minimizer of (5.3.9) satisfying condition (5.3.3) can be shown to be nonnegative. Indeed, the positive part v^+ of a function $v \in H^1(\Omega)$ satisfying (5.3.3) still fulfils (5.3.3) and $\tilde{E}(v^+) \le \tilde{E}(v)$. This fact is connected to the maximum principle for the corresponding differential equation. Functionals of the form (5.3.9) are studied in [1], where it is shown that their minimizers without volume constraint are Lipschitz continuous.

In the derivation of a dynamical model for the motion of a droplet driven by the changing contact angle, we do not start from equation (5.3.5), as is a common practice, but from the minimization problem for the energy functional (5.3.9). Let us now consider the situation when γ_s is not constant. Then the contact angle becomes also a function of space, as is apparent from (5.3.5). Setting a drop on a surface with nonhomogeneous surface tension, the drop starts moving in order to find its stationary position. If the surface tension is monotonely decreasing in a certain direction, the drop stretches itself towards the area with smaller tension and possibly starts moving in this direction, trying to make its contact angle as small as possible. On the other hand, the surface tension on the drop/air boundary inhibits this motion, trying to form the drop into a ball. These two motions, restricted by the volume conservation, result in the change of shape and/or translation of the drop.

Unlike [34], in the case of motion driven by the changing contact angle, the movements are relatively slow and the shape is transforming little by little by pouring of the liquid towards the front edge. Therefore, the influence of inertial forces and friction can be assumed negligible. In such situation, it seems acceptable to consider the motion as a result of vertical displacement of the film. Here we have adopted the scalar description which inevitably allows only the variation in the vertical direction. Nevertheless, the comparison of numerical results with experimental photographs (see Section 7.3) suggests that it is an adequate approximation.

Now we derive an equation of motion along the lines mentioned above. Using (5.3.9) as the potential energy for the surface of the drop and considering the kinetic energy proportional to $\chi_{u>0} u_t^2$, we find that the Lagrangian becomes

$$L(u) = \int_0^T \int_\Omega \left(\beta u_t^2 - \gamma_g |\nabla u|^2 - (\gamma_g + \gamma_s) \chi_\varepsilon(u) \right) \, dx \, dt.$$

Assuming the existence of a stationary point, we can compute the variation of the Lagrangian using test functions

$$u_\varepsilon = V \frac{u + \varepsilon\varphi}{V + \varepsilon \int_\Omega \varphi \, dx}, \qquad \varphi \in C_0^\infty((0,T) \times \Omega \cap \{u > 0\})$$

as in the proof of Lemma 5.3.2. This procedure is formally equivalent to introducing a time-dependent Lagrange multiplier $\lambda(t)$ and calculating the variation of the functional $L(u) - \int_0^T \lambda \int_\Omega u \, dx \, dt$ without the constraint. Noting that the resistance force acting against the vertical motion of the film is proportional to the speed of the film, we get a weak formulation for the following relation

$$\beta \chi_{u>0} u_{tt} + \mu u_t = \gamma_g \left(\Delta u - \gamma \chi_\varepsilon'(u) + \chi_{u>0} \lambda \right), \tag{5.3.10}$$

where

$$\lambda = \frac{1}{V} \int_\Omega \left[\beta u_{tt} u + \mu u_t u + \gamma_g |\nabla u|^2 + \gamma_g \gamma u \chi_\varepsilon'(u) \right] dx.$$

This is the type of equation studied in Section 5.2. Here, β is proportional to area density of the region constituting the membrane, μ is a drag coefficient and λ is a Lagrange multiplier originating in the volume constraint (see the similar derivation of (5.3.7)). The characteristic function in front of u_{tt} expresses the fact that energy is lost when the film touches the surface. Refer to the paper [43] for more detailed explanation of the equation.

We have replaced the characteristic function in the second term of (5.3.9) by a function $\chi_\varepsilon \in C^2(\mathbb{R})$ satisfying

$$\chi_\varepsilon(s) = \begin{cases} 0, & s \le 0 \\ 1, & \varepsilon \le s \end{cases}$$

and $|\chi_\varepsilon'(s)| \le C/\varepsilon$ for $s \in (0, \varepsilon)$. The purpose of the smoothing is to avert the appearance of delta function in the equation.

If we consider a motion with a long time-scale without oscillations ($|\beta u_{tt}| << |\mu u_t|$), it can be sufficiently expressed by the following parabolic partial differential equation

$$u_t = \Delta u - \gamma \chi_\varepsilon'(u) + \chi_{u>0} \lambda, \tag{5.3.11}$$

where we have put $\mu/\gamma_g = 1$. The specific form of the time-dependent function $\lambda(t)$ is

$$\lambda = \frac{1}{V} \int_\Omega \left[u u_t + |\nabla u|^2 + \gamma u \chi_\varepsilon'(u) \right] dx. \tag{5.3.12}$$

This is the model equation analyzed in Section 5.1.

Chapter 6

Numerical algorithms

For constrained problems, the discrete Morse flow is not only an effective tool of theoretical analysis but also a very practical method of numerical computation. As the evolution problem is approximated by minimization on discrete time levels, the constraint is taken care of just by restricting the set of admissible functions for the minimization. Here we deliberate on the practical aspects of the method in numerical computation and introduce the basic algorithm.

6.1 General comments

The discrete Morse flow method consists in partitioning the time interval $(0, T)$ into N subintervals of length $h = T/N$ and with given initial functions u_0 (and u_1 for hyperbolic problems) computing the minimizer of the functional

$$J_n(u) = \int_\Omega \Big(D(u, u_{n-1}, u_{n-2}) + \frac{1}{2}|\nabla u|^2 + F_n(u) \Big)\, dx \tag{6.1.1}$$

for $n = 1, 2, \ldots, N$, in the admissible function set

$$\mathcal{K}_V = \begin{cases} \big\{u \in H^1_0(\Omega);\ \int_\Omega u\, dx = V\big\} & \text{for problems without obstacle,} \\ \big\{u \in H^1_0(\Omega);\ \int_\Omega \chi_{u>0} u\, dx = V\big\} & \text{for problems with obstacle.} \end{cases} \tag{6.1.2}$$

The term $F_n(u)$ in (6.1.1) includes, e.g., outer force terms or the term $\gamma \chi_\varepsilon(u)$ expressing contact angle in the model for droplets. The discretized term $D(u, u_{n-1}, u_{n-2})$ has the form

$$D = \begin{cases} |u - u_{n-1}|^2/(2h) & \text{for parabolic problems,} \\ |u - 2u_{n-1} + u_{n-2}|^2/(2h^2) & \text{for hyperbolic problems without obstacle,} \\ |u - 2u_{n-1} + u_{n-2}|^2 \chi_{u>0}/(2h^2) & \text{for hyperbolic problems with obstacle.} \end{cases} \tag{6.1.3}$$

We would like to bring to notice the fact that the way of computing approximations to a solution of a parabolic free-boundary problem, as stated above, is different from the definition of approximate solutions used in Section 5.1 to prove the existence of weak solutions.

To rectify this, we add an Appendix to this Chapter (see Section 6.3), where we introduce approximate solutions for the parabolic obstacle problem applicable in numerical computation and show that they are well-defined.

In numerical computations, the space is discretized as in the standard finite element method, usually with triangular meshes and standard basis functions $\{\varphi_i\}_{i=1}^M$. Apart from the outer-force term, functional (6.1.1) is then a quadratic function of coefficients a_i^n corresponding to individual basis functions in the expansion of the approximate solution, i.e.,

$$u_n(x) = \sum_{i=1}^M a_i^n \varphi_i(x), \qquad n = 0, 1, \ldots, N.$$

On the other hand, the volume condition represents a linear constraint, most typically (in the case of Dirichlet boundary conditions) of the form

$$\sum_{i=1}^M a_i^n = \frac{V}{\Delta} = \text{const}, \qquad n = 0, 1, \ldots, N,$$

where Δ is the area of one element. Here we assume that all elements are identical because dropping this assumption has no substantial influence on the character of the situation. Thus, the functional is constrained to a hyperplane S giving again quadratic function and a (unique) minimum. The question is how to find this minimum in praxis.

The direct but often not practical way is to first find the explicit form of the constrained functional and then minimize it. One of the disadvantages of this approach is that the resulting stiffness matrix loses its good properties, in particular, symmetry and sparsity.

Other possibility is to apply gradient minimizing method with simultaneous projecting on the volume-constraint hyperplane. In one step of this method we compute the minimum in the direction of steepest descent starting from a point on the volume hyperplane and project it back on the constraint hyperplane (see Figure 6.1). As in the usual gradient method, the speed of convergence depends on how near are the level curves of the functional to a circle (that is, how much clustered are the eigenvalues of the corresponding matrix), which leads to the usage of preconditioners.

When solving problems without obstacles, we can use the orthogonal projection on the constraint hyperplane. However, when we compute an obstacle problem, we have the lower admissible set from (6.1.2). This set is not convex, but since we have shown in Chapter 5 that the minimizers are nonnegative, we can use the following convex set in its place:

$$\mathcal{K}'_V = \big\{u \in H_0^1(\Omega);\ u \geq 0,\ \int_\Omega u\, dx = V\big\}.$$

The condition $u \geq 0$ written in terms of the coefficients a_i is

$$a_i \geq 0, \qquad i = 1, 2, \ldots, M,$$

which again designates a convex subset of the hyperplane:

$$\mathcal{K}_V^M = \big\{[a_1, \ldots, a_M] \in \mathbb{R}^M;\ \sum_{i=1}^M a_i = V/\Delta,\ a_i \geq 0,\ i = 1, \ldots, M\big\}.$$

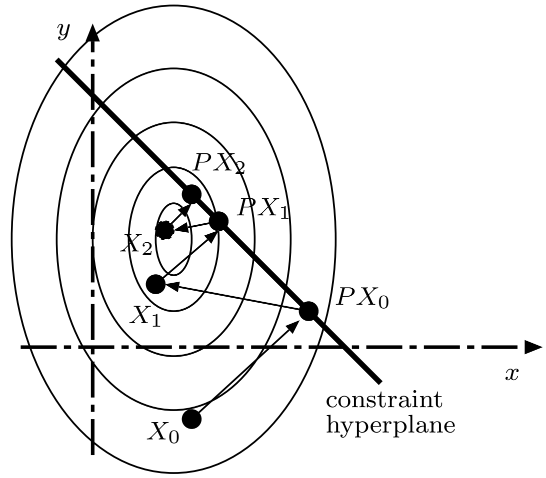


Figure 6.1: Constrained gradient method.

We can define the projection of a point X on $\mathcal{K}_V^M$ as the nearest point to PX in $\mathcal{K}_V^M$, where PX is the orthogonal projection of X on the hyperplane S (see point X' in Figure 6.2).

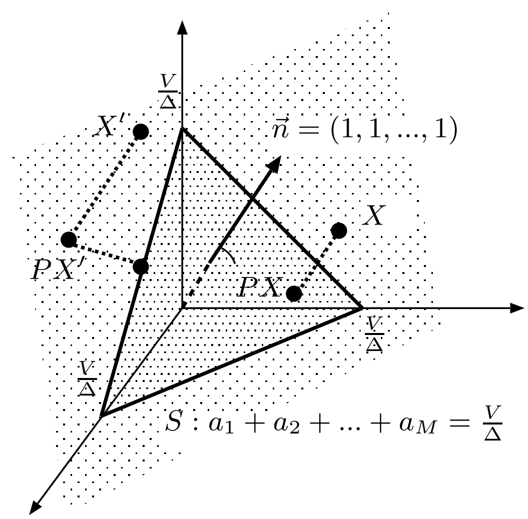


Figure 6.2: Projection on the admissible set.

Since the set $\mathcal{K}_V^M$ in the discretized setting is a polytope, the projection is well-defined. The orthogonal projection P amounts to adding a fixed value to each component a_i because the normal vector to S is the vector $\frac{1}{M}[1, 1, \ldots, 1]$:

$$P([a_1, \ldots, a_M]) = [a_1, \ldots, a_M] + \frac{V/\Delta - \sum_{i=1}^{M} a_i}{M} [1, \ldots, 1].$$

If the projection PX of X already is a point of $\mathcal{K}_V^M$, the free boundary does not appear. On the other hand, if PX falls outside of $\mathcal{K}_V^M$, the nearest point in $\mathcal{K}_V^M$ will have at least one vanishing component, which means that the free boundary is realized. Figure (6.3) shows the hyperplane and the set $\mathcal{K}_V^M$ (hatched region) in the case of three dimensions (4 elements).

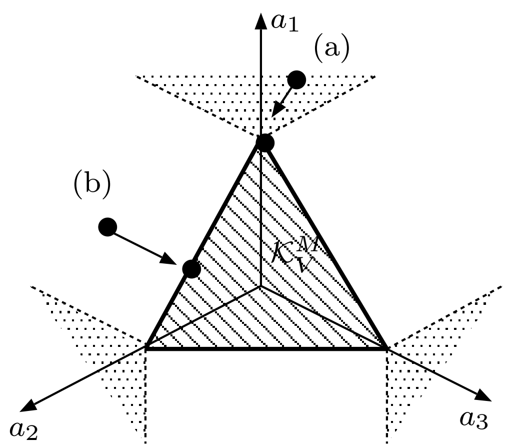


Figure 6.3: Volume constraint hyperplane.

If PX is in one of the dotted cones, the final projection will have two vanishing components and the corresponding function looks like Figure 6.4 (a), while the projection of points from the white region results in functions of the shape in Figure 6.4 (b).

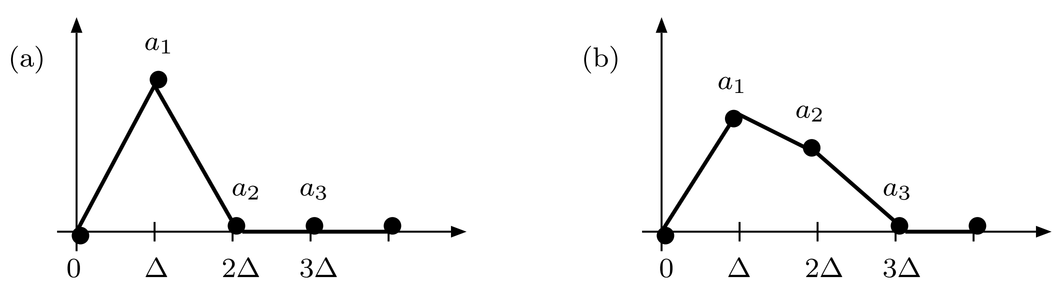


Figure 6.4: Discretized functions with free boundary.

Nonetheless, besides this type of projection, in real computations we often adopt easier ways of "projecting", such as the "cut and adjust" method. In this method, we compute the unconstrained minimizer, cut it at the obstacle and correct the volume by multiplying the whole function by a suitable value.

A completely different approach, using a modification of the finite element method with special basis functions of zero volume, is proposed in the following Section 6.2.

In the end, we briefly explain the general algorithm for numerical computations of volume-constrained obstacle problems. However, a detailed analysis is beyond the scope of the thesis. Our numerical method uses finite element discretization of space and searches for a minimizer of the functional (6.1.1) in this discretized space. The minimizer is determined by the steepest descent method combined with bisection method. In each step of the search, the resulting function is projected on the volume-constraint hyperplane and, if need be, on the set satisfying the obstacle condition. The rough scheme of the algorithm is presented in Figure 6.5 for the parabolic case.

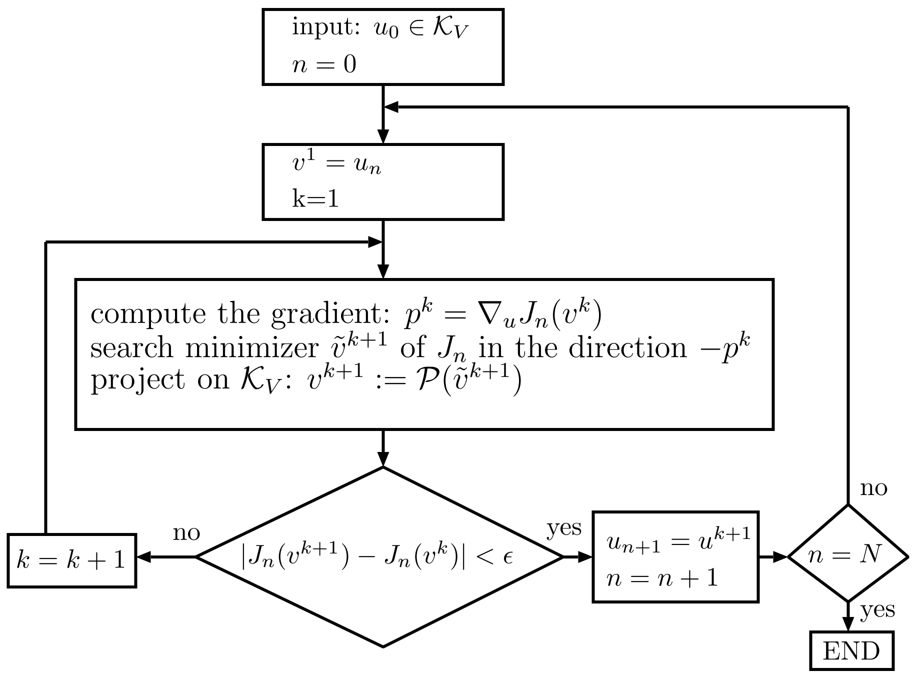


Figure 6.5: Numerical algorithm.

The time step h and diameter of each finite element are chosen small enough related to the smoothing parameter ε in the contact angle term, if present. As minimization methods are of implicit type, there is theoretically no restriction on the relation between the time step h and the smallest diameter of the space-mesh.

6.2 Finite elements with zero volume

Here we propose a version of finite element method suitable for volume-preserving problems. The proposed method differs from standard FEM in the definition of basis functions. Instead of "hat" functions ψ_i, we shall use basis functions φ_i with zero volume, having the shape of a wavelet (see Figure 6.6).

First, we have to change the formulation of the problem, so that we get a constraint of zero volume. This can be done by subtracting a suitable function, having the originally

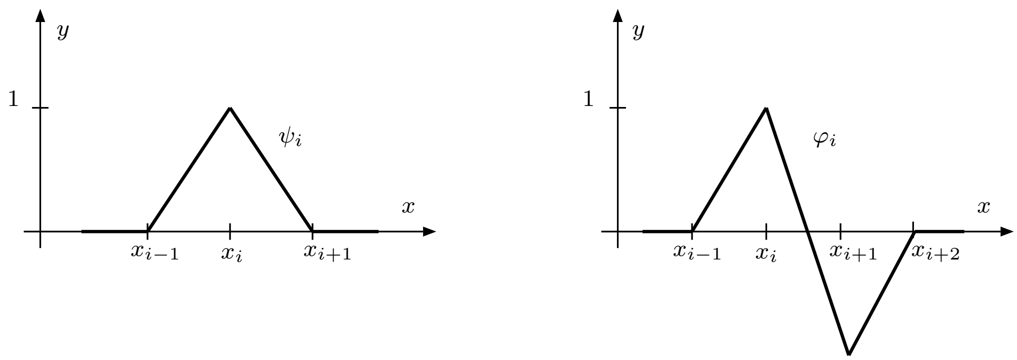


Figure 6.6: Standard and modified basis functions.

required volume V, from the solution (for example, the initial condition). This may be sometimes difficult with obstacle problems, where it may be necessary to adjust the subtracted function in each time step.

We present the main aspects of the new method on the example of a constrained heat equation in one dimension. Let us consider the problem in the space interval $\Omega = (0, l)$, $l > 0$. We define a triangulation $\mathscr{T}_h$ of $(0, l)$ as the equidistant partition $\{x_i\}_{i=0}^{N+1}$ with space step $h = l/(N+1)$: $x_0 = 0$, $x_1 = h, \ldots, x_{N+1} = l$. Only in this subsection the symbol h will have a different meaning than in the preceding text because we do not want to change the established notation in the FEM. The time step is denoted by τ. We shall solve the problem with linear finite elements, so the standard and modified finite element spaces are defined as

$$\begin{aligned} V_h &= \big\{u_h \in C([0,l]);\ u_h \text{ is piecewise linear on } \mathscr{T}_h,\ u_h(0) = u_h(l) = 0\big\}, \\ \mathscr{V}_h &= \big\{u_h \in C([0,l]);\ u_h \text{ is piecewise linear on } \mathscr{T}_h,\ u_h(0) = u_h(l) = 0,\ \sum_{i=1}^{N} u_h(x_i) = 0\big\}. \end{aligned}$$

Note that the condition

$$\sum_{i=1}^{N} u_h(x_i) = 0 \tag{6.2.1}$$

and the condition $\int_0^l u_h\, dx = 0$ are equivalent for $u_h \in V_h$.

The basis of $\mathscr{V}_h$ consists of $\{\varphi_i\}_{i=1}^{N-1}$, where (see Figure 6.6)

$$\varphi_i(x) = \begin{cases} (x - x_{i-1})/h & x \in [x_{i-1}, x_i] \\ -2(x - x_i)/h + 1 & x \in [x_i, x_{i+1}] \\ (x - x_{i+1})/h - 1 & x \in [x_{i+1}, x_{i+2}] \\ 0 & \text{otherwise.} \end{cases} \tag{6.2.2}$$

Lemma 6.2.1. *Every function u_h from $\mathscr{V}_h$ can be expressed as a linear combination of functions $\varphi_1, \ldots, \varphi_{N-1}$.*

Proof. We are looking for the coefficients a_i, $i = 1, \dots, N-1$, in the expansion

$$u_h(x) = \sum_{i=1}^{N-1} a_i \varphi_i(x). \tag{6.2.3}$$

The above holds if and only if it holds for x_j, $j = 0, \dots, N+1$. This gives the relations

$$\begin{aligned}
u_h(x_1) &= a_1 \\
u_h(x_2) &= a_2 - u_h(x_1) \\
u_h(x_3) &= a_3 - u_h(x_2) \\
&. \\
&. \\
u_h(x_{N-1}) &= a_{N-1} - u_h(x_{N-2}).
\end{aligned}$$

The solution is

$$a_i = \sum_{j=1}^{i} u_h(x_j).$$

However, we have to check that (6.2.3) holds also for $x = x_N$ because this condition is not considered in the above system of equations in order not to make it overdetermined. We have

$$\sum_{i=1}^{N-1} a_i \varphi_i(x_N) = a_{N-1}\varphi_{N-1}(x_N) = -a_{N-1} = -\sum_{j=1}^{N-1} u_h(x_j) = u_h(x_N),$$

due to (6.2.1). □

The volume constrained heat equation is reduced (see Section 4.1 for details) to the minimization of the following functional

$$J_n(u) = \int_0^l \frac{|u - u^{n-1}|^2}{2\tau}\, dx + \frac{1}{2}\int_0^l |\nabla u|^2\, dx$$

in the set

$$\mathcal{K} = \left\{ u \in H_0^1(\Omega);\ \int_0^l u\, dx = V \right\}.$$

Here u^{n-1} is the solution on the previous time-level and u^0 is a given initial function from $\mathcal{K}$. We use the transformation $v = u - u^0$ (analogously $v^n = u^n - u^0$), whereby the problem changes to minimizing of

$$\tilde{J}_n(v) = \int_0^l \frac{|v - v^{n-1}|^2}{2\tau}\, dx + \frac{1}{2}\int_0^l |\nabla v + \nabla u^0|^2\, dx$$

in the space

$$V = \left\{ u \in H_0^1(\Omega);\ \int_0^l u\, dx = 0 \right\}.$$

A variation of $\tilde{J}_n$ gives the following identity:

$$\int_0^l \frac{v - v^{n-1}}{\tau}\varphi\,dx + \int_0^l (\nabla v + \nabla u^0)\nabla\varphi\,dx = 0 \qquad \forall\varphi \in V.$$

The finite element approximation consists in searching for the solution $v_h \in \mathscr{V}_h$ of

$$\int_0^l \frac{v_h - v_h^{n-1}}{\tau}\varphi_h\,dx + \int_0^l (\nabla v_h + \nabla u_h^0)\nabla\varphi_h\,dx = 0 \qquad \forall\varphi_h \in \mathscr{V}_h,$$

or, equivalently, minimizing $\tilde{J}_n$ in $\mathscr{V}_h$. Here, $u_h^0 \in \mathscr{V}_h$ is an appropriate interpolation of u^0.

Define the bilinear form B and functionals f^n, f_h^n as follows:

$$\begin{aligned}
B(v,\varphi) &= \frac{1}{\tau}\int_0^l v\varphi\,dx + \int_0^l \nabla v\nabla\varphi\,dx,\\
f^n(\varphi) &= \frac{1}{\tau}\int_0^l v^{n-1}\varphi\,dx - \int_0^l \nabla u^0\nabla\varphi\,dx,\\
f_h^n(\varphi) &= \frac{1}{\tau}\int_0^l v_h^{n-1}\varphi\,dx - \int_0^l \nabla u_h^0\nabla\varphi\,dx.
\end{aligned}$$

Since V is a Hilbert space, $\mathscr{V}_h$ is its finite-dimensional subspace, the form B is continuous and coercive on V and functionals f^n and f_h^n are bounded and linear, Lax-Milgram theorem gives a unique solution to each of the following problems:

$$B(v,\varphi) = f^n(\varphi) \qquad \text{for all } \varphi \in V, \tag{6.2.4}$$

$$B(v_h,\varphi_h) = f_h^n(\varphi_h) \qquad \text{for all } \varphi_h \in \mathscr{V}_h. \tag{6.2.5}$$

Problem (6.2.5) is solved by the finite element method with modified basis functions $\{\varphi_i\}$. Using (6.2.3), we have the system for coefficients a_i^n:

$$\frac{1}{\tau}\int_0^l \sum_{i=1}^{N-1} a_i^n\varphi_i\varphi_j\,dx + \int_0^l \sum_{i=1}^{N-1} a_i^n\nabla\varphi_i\nabla\varphi_j\,dx = \mathbf{b}^n, \qquad j = 1,2,\ldots,N-1,$$

where $\mathbf{b}^n$ is the corresponding force vector. This can be rewritten as

$$\big(\frac{1}{\tau}\mathbf{A} + \mathbf{B}\big)\mathbf{a}^n = \mathbf{b}^n,$$

where the stiffness matrix $\mathbf{A}$ with elements $\alpha_{ij} = \int_0^l \varphi_i\varphi_j\,dx$ and the stiffness matrix $\mathbf{B}$ with elements $\beta_{ij} = \int_0^l \nabla\varphi_i\nabla\varphi_j\,dx$ are given by

$$\mathbf{A} = \frac{h}{6}\begin{pmatrix}
6 & -2 & -1 & 0 & . & . & . & . & . & 0\\
-2 & 6 & -2 & -1 & 0 & . & . & 0 & . & 0\\
-1 & -2 & 6 & -2 & -1 & 0 & . & . & . & 0\\
0 & -1 & -2 & 6 & -2 & -1 & 0 & . & . & 0\\
. & . & . & . & . & . & . & . & . & .\\
. & . & . & . & . & . & . & . & . & .\\
. & . & . & . & 0 & -1 & -2 & 6 & -2 & -1\\
. & 0 & . & . & . & 0 & -1 & -2 & 6 & -2\\
. & . & . & . & . & . & 0 & -1 & -2 & 6
\end{pmatrix}$$

and

$$\mathbf{B} = \frac{1}{h}\begin{pmatrix} 6 & -4 & 1 & 0 & . & . & . & . & . & 0 \\ -4 & 6 & -4 & 1 & 0 & . & . & 0 & . & 0 \\ 1 & -4 & 6 & -4 & 1 & 0 & . & . & . & 0 \\ 0 & 1 & -4 & 6 & -4 & 1 & 0 & . & . & 0 \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & 0 & 1 & -4 & 6 & -4 & 1 \\ . & 0 & . & . & . & 0 & 1 & -4 & 6 & -4 \\ . & . & . & . & . & . & 0 & 1 & -4 & 6 \end{pmatrix}.$$

We can see that we have obtained a system with pentadiagonal symmetric matrix. Compared with the tridiagonal matrix in the usual finite element method it is somewhat more computationally demanding but this is the price paid for the constraint. If we apply the volume condition (6.2.1) directly, we get a matrix which is neither a band matrix nor a symmetric matrix because a full row $(1, 1, 1, \ldots, 1)$ appears there.

Since the discrete Morse flow is a minimization method, we usually do not solve systems with the above matrices but use an iterative minimization method. Mostly, a gradient method is used, which amounts to searching for the minimum in the direction of the gradient of $\tilde{J}_n$ with respect to the coefficients a_i. The gradient is an $(N-1)$-dimensional vector, in contrast with the N-component vector for the unconstrained case. Nevertheless, the algorithm of the minimization is the same.

Now, we are concerned with the convergence of the approximation as $h \to 0$, that is, with error estimates. By Céa's lemma we have

$$\|v_h^n - v^n\|_V \leq C \operatorname{dist}(v^n, \mathscr{V}_h).$$

Hence, to get an error estimate, it is sufficient to find a good approximation of a function $v^n \in V$ in $\mathscr{V}_h$. In the sequel, we write Ω instead of $(0, l)$.

Lemma 6.2.2. *Let $v \in V \cap H^2(\Omega)$. Then there exists a function $v_h \in \mathscr{V}_h$ such that*

$$\begin{aligned} \|v - v_h\|_{L^2(\Omega)} &\leq Ch^2 \|v_{xx}\|_{L^2(\Omega)}, \\ \|v - v_h\|_{H^1(\Omega)} &\leq Ch\, \|v_{xx}\|_{L^2(\Omega)}, \end{aligned} \tag{6.2.6}$$

for h less than some fixed h_0.

Proof. We define two types of projections. Projection $P_h : V \to V_h$ takes the same values at nodes:

$$P_h v \in V_h, \qquad P_h v(x_i) = v(x_i), \quad i = 0, 1, \ldots, N+1.$$

On the other hand, projection $\Pi_h : V \to \mathscr{V}_h$ adjusts the volume by subtracting a fixed value at nodes $x_1, x_2, \ldots, x_N$:

$$\Pi_h v \in \mathscr{V}_h, \quad \Pi_h v(x_i) = v(x_i) - \frac{1}{N}\sum_{i=1}^{N} v(x_i), \;\; i = 1, \ldots, N, \quad \Pi_h v(x_0) = \Pi_h v(x_{N+1}) = 0.$$

Then we have

$$\|v - \Pi_h v\|_{H^1(\Omega)} \leq \|v - P_h v\|_{H^1(\Omega)} + \|P_h v - \Pi_h v\|_{H^1(\Omega)}. \tag{6.2.7}$$

The estimate for the first term is a well-known result of the interpolation theory:

$$\|v - P_h v\|_{H^1(\Omega)} \le Ch\|v_{xx}\|_{L^2(\Omega)}.$$

We estimate the second term on the right-hand side of (6.2.7). Function $P_h v - \Pi_h v$ vanishes at the end nodes and has a constant value $s := 1/N \sum_{i=1}^N v(x_i)$ at all other nodes (see Figure 6.7).

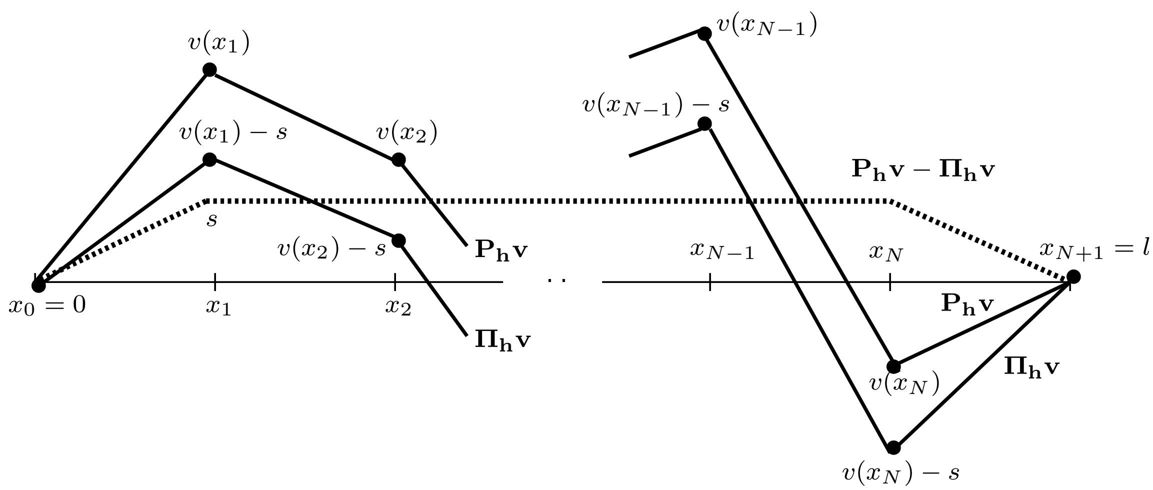


Figure 6.7: Projections P_h and Π_h.

This leads to the estimates

$$\begin{aligned}
\|P_h v - \Pi_h v\|^2_{L^2(\Omega)} &= \int_{x_0}^{x_1} \big(\frac{s}{h}x\big)^2\,dx + \sum_{i=1}^{N-1} s^2\,dx + \int_{x_N}^{x_{N+1}} \big(\frac{s}{h}(x - x_N)\big)^2\,dx \\
&= \big(N - \frac{1}{3}\big)hs^2 \le ls^2 \qquad (6.2.8)\\
\|(P_h v)_x - (\Pi_h v)_x\|^2_{L^2(\Omega)} &= \int_{x_0}^{x_1} \big(\frac{s}{h}\big)^2\,dx + \int_{x_N}^{x_{N+1}} \big(\frac{s}{h}\big)^2\,dx \\
&= \frac{2}{h}s^2. \qquad (6.2.9)
\end{aligned}$$

It remains to estimate the sum $\sum_{i=1}^N v(x_i)$, which should be small for small h, since v has zero volume. We write

$$\sum_{i=1}^N v(x_i) = \sum_{i=1}^N v(x_i) - \frac{1}{h}\int_0^l v\,dx = \sum_{i=1}^{N+1} \Big(\frac{v(x_{i-1}) + v(x_i)}{2} - \frac{1}{h}\int_{x_{i-1}}^{x_i} v\,dx\Big) \qquad (6.2.10)$$

and use Taylor's theorem for v on each interval (x_{i-1}, x_i):

$$\begin{aligned}
v(x) &= v(x_{i-1}) + v_x(x_{i-1})(x - x_{i-1}) + \int_{x_{i-1}}^{x} (x - t)v_{xx}(t)\,dt, \\
v(x) &= v(x_i) - v_x(x_i)(x_i - x) - \int_{x}^{x_i} (x - t)v_{xx}(t)\,dt.
\end{aligned}$$

Adding the above identities, dividing by $2h$ and integrating over (x_{i-1}, x_i) we obtain

$$\begin{aligned}
\frac{1}{h}\int_{x_{i-1}}^{x_i} v\,dx &= \int_{x_{i-1}}^{x_i} \frac{v(x_{i-1})+v(x_i)}{2h}\,dx + \int_{x_{i-1}}^{x_i} \frac{v_x(x_{i-1})(x-x_{i-1}) - v_x(x_i)(x_i-x)}{2h}\,dx \\
&\qquad + \frac{1}{2h}\int_{x_{i-1}}^{x_i}\int_{x_{i-1}}^{x_i} |x-t| v_{xx}(t)\,dt\,dx \\
&= \frac{v(x_{i-1})+v(x_i)}{2} + \frac{h}{4}\big(v_x(x_{i-1}) - v_x(x_i)\big) \\
&\qquad + \frac{1}{4h}\int_{x_{i-1}}^{x_i} \big((t-x_{i-1})^2 + (x_i-t)^2\big) v_{xx}(t)\,dt.
\end{aligned}$$

Inserting this form into (6.2.10),

$$\begin{aligned}
\Big|\sum_{i=1}^{N} v(x_i)\Big| &= \frac{h}{4}\Big|\sum_{i=1}^{N+1}\big(v_x(x_{i-1}) - v_x(x_i)\big)\Big| \\
&\qquad + \frac{1}{4h}\sum_{i=1}^{N+1}\int_{x_{i-1}}^{x_i} \big((t-x_{i-1})^2 + (x_i-t)^2\big)|v_{xx}(t)|\,dt \\
&\le \frac{h}{4}|v_x(l) - v_x(0)| \\
&\qquad + \frac{1}{4h}\Big(\sum_{i=1}^{N+1}\int_{x_{i-1}}^{x_i} \big((t-x_{i-1})^2 + (x_i-t)^2\big)^2\,dt\Big)^{1/2}\Big(\sum_{i=1}^{N+1}\int_{x_{i-1}}^{x_i} v_{xx}(t)^2\,dt\Big)^{1/2} \\
&= \frac{h}{4}\Big|\int_0^l v_{xx}(t)\,dt\Big| + \frac{1}{4}\sqrt{\frac{7l}{15}}\,h\|v_{xx}\|_{L^2(0,l)} \\
&\le C\sqrt{l}h\|v_{xx}\|_{L^2(\Omega)}.
\end{aligned}$$

Thus, $|s| \le Ch^2\|v_{xx}\|_{L^2(\Omega)}$ and (6.2.8) plus (6.2.9) immediately yield the announced error estimates. $\square$

One can see that error estimates (6.2.6) are of the same optimal order as estimates for standard finite element approximation.

The presented method is likely to be extendable to higher dimensions and approximations by polynomials of higher degrees, with error estimates for higher order norms. We shall not study such extensions here. We only remark that the numerical example in Section 7.2 was computed using two-dimensional volume-free basis functions, essentially of the shape illustrated in Figure 6.8. To construct modified bases in higher dimensions seems rather difficult but it is not too restrictive because the two-dimensional case corresponds to a surface in 3d space. Unfortunately, the application of the modified basis to obstacle problems is not straightforward.

In the end, we shall discuss an application of volume-free basis functions to problems with pinned points or points whose motion is prescribed. An example of such problems is given in the second part of Section 7.1. We solve the motion of an elastic volume-preserving string, which is fixed on both ends and picked and lifted with prescribed velocity at one

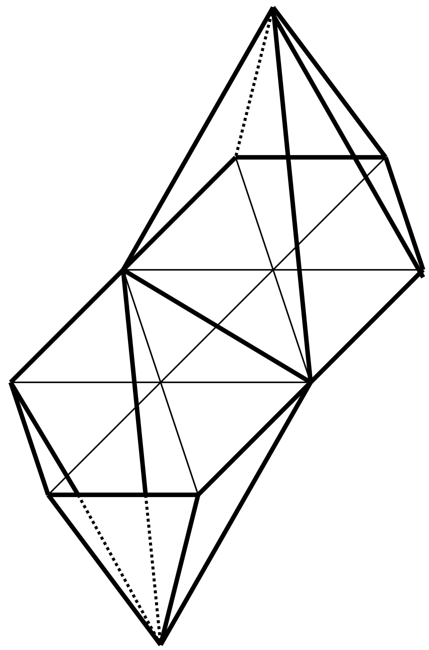


Figure 6.8: Basis functions for 2d domains supported on 10 elements of mesh.

point inside the domain. The direct way of solution would mean to split the domain into two subdomains with boundary at the pinned point. In each subdomain one would solve the model equation with time-dependent boundary condition. However, the solutions in respective subdomains are correlated by the overall volume preservation.

In the standard finite element method, it would be enough to fix the coefficient of the basis function corresponding to the moving point to be the prescribed value. In the case of modified basis functions, there are two basis functions that do not vanish at a node, so the same method does not work. The problem can be solved by a simple change of the basis functions having support in the neighbourhood of the moving point so that there is only one basis function that does not vanish at the concerned node. The new basis for a pinned point x_i is depicted in Figure 6.9.

We can see that basis functions φ_{i-1} and φ_i were replaced by new volume-free functions φ'_{i-1} and φ'_i, where only function φ'_i has a nonzero value at x_i. Hence, we can fix the coefficient of this basis function according to the prescribed value and solve for the remaining coefficients $a_1, \dots, a_{i-1}, a_{i+1}, \dots, a_{N-1}$. The same procedure can be done with any number of pinned points.

6.3 Appendix

Here we define and justify approximate solutions of parabolic free-boundary problem (5.1.1)–(5.1.3), suitable for practical computations. The construction of an approximate solution for computational purposes is based on the minimization of the following time-

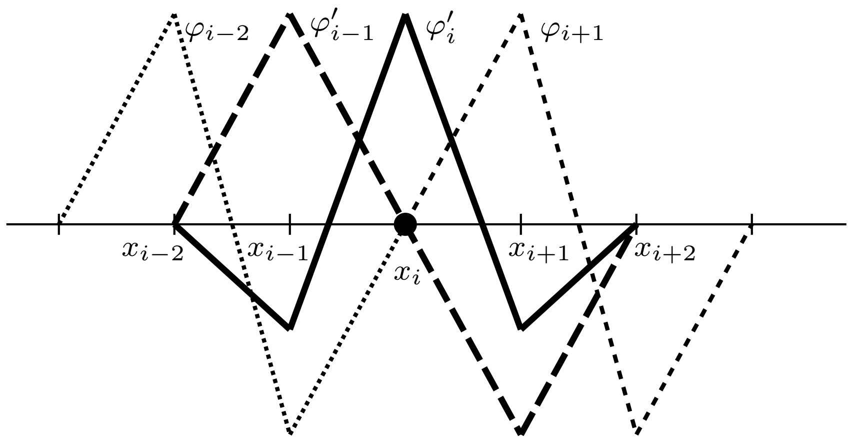


Figure 6.9: Basis functions for a problem with pinned nodes.

discretized functional:

$$J_n(u) = \int_\Omega \Big(\frac{|u - u_{n-1}|^2}{2h} + \frac{1}{2}|\nabla u|^2 + \gamma \chi_\varepsilon(u) - F(u) \Big)\, dx \tag{6.3.1}$$

in the admissible function set

$$\mathcal{K}_V = \Big\{ u \in H_0^1(\Omega);\, \int_\Omega \chi_{u>0} u \, dx = V \Big\}. \tag{6.3.2}$$

Compared to (5.1.17), we see two differences. One is that a sharp characteristic function appears in (6.3.2) to accomplish the effect of the obstacle. In numerical computation, the solution is projected on $\mathcal{K}_V$ every time a new approximation of the solution is computed. The other difference is the presence of the new term $F(u)$ representing the action of outer forces. We have not considered this term until now in order to simplify the formulas. For example, the corresponding form for gravitation force would be

$$F(u) = -\frac{1}{2} g u^2,$$

or gravity for a drop on a tilted plane with inclination angle α would give

$$F(u) = -\frac{1}{2} g u^2 \cos\alpha + g x u \sin\alpha.$$

For simplicity, we assume that $F(x, s)$ (where s represents u) is independent of time and has the form $F(x, s) = (a(x)s^2 + b(x)s)\chi_{s>0}$, where $a, b \in L^\infty(\Omega)$, $a(x) \leq 0$ and $b(x) \geq 0$. By $f(x, s)$ we denote the derivative with respect to s, i.e., $f(x, s) = (2a(x)s + b(x))\chi_{s>0}$. For a more general approach regarding the outer force, see Section 4.1.

We start the computation from the function u_0 that is given as the initial condition and inductively calculate u_n, $n = 1, \dots, N$. The characteristic function in the volume condition in (6.3.2) ensures that the minimizer is nonnegative and, therefore, satisfies the obstacle condition. Indeed, should the minimizer u_n be negative in a region of positive measure, the function $\chi_{u_n>0}u_n$ still belongs to $\mathcal{K}_V$ and the value $J_n(\chi_{u_n>0}u_n)$ is less than for the original function, which is a contradiction.

As in the proof of existence of a weak solution, we interpolate the minimizers in time producing a piecewise constant function $\bar{u}^h$ and a continuous piecewise linear function u^h (see (5.1.19)).

In what follows, we shall briefly mention the main properties of the approximate solutions and show they are well-defined. Our assumptions are the same as in Section 5.1. The following theorems show that there exists a Hölder continuous minimizer. The regularity is indispensable for obtaining an equality from the first variation of our functional by considering only test functions with support inside the open set $\{u > 0\}$. Otherwise, taking general test functions would yield only an inequality.

Theorem 6.3.1. *There exists a minimizer of J_n for each $n = 1, \dots, N$.*

Proof. The proof is similar to the proof of Theorem 5.2.1 in Section 5.2. □

Theorem 6.3.2. *For each compact subset $\tilde{\Omega}$ of Ω, there is a positive number $\alpha < 1$, depending on h, such that the minimizers u_n of J_n for $n = 1, \dots, N$, belong to the Hölder space $C^\alpha(\tilde{\Omega})$.*

Proof. If a function u belongs to the class $\mathcal{B}_2(\Omega, M, \gamma, d)$ defined in Definition 5.2.1, Theorem 2.6.1 of [23] tells us that u is Hölder continuous.

Without loss of generality, let us suppose that $V = 1$. The condition (1) from Definition 5.2.1 (boundedness of u_n) can be proved by the technique for elliptic equations of [23]. We won't go into details here, referring to the proof of Theorem 5.2.2. We study the condition (2) in the case $w = +u$ and $w = -u$, respectively. For a nonnegative function $\zeta \in H_0^1(\Omega)$ we select a volume-preserving test function

$$\psi_\delta = \frac{1}{I_\delta}(u - \delta\zeta)\,\chi_{u-\delta\zeta>0}, \quad \delta > 0, \quad I_\delta = \int_\Omega (u - \delta\zeta)\chi_{u-\delta\zeta>0}\,dx.$$

The minimality of u gives $(J_n(\psi_\delta) - J_n(u))/\delta \geq 0$, where we take $\delta \to 0+$, while employing the estimate $1 - \delta \int_\Omega \zeta\,dx \leq I_\delta \leq 1$:

$$\begin{aligned} 0 \leq &\int_\Omega \Big(\frac{u - u_{n-1}}{h}u + |\nabla u|^2 + \gamma\chi_\varepsilon'(u)\,u - 2au^2\Big)\,dx\,\Big(\int_\Omega \zeta\,dx\Big) \\ &+ \int_\Omega \Big(-\frac{u - u_{n-1}}{h} - \gamma\chi_\varepsilon'(u) + b\Big)\zeta\,dx - \int_\Omega \nabla u\,\nabla\zeta\,dx. \end{aligned} \tag{6.3.3}$$

Specifying the form of ζ in (6.3.3) provides us with (5.2.6) for $+u$. Let us take any smooth function η, $0 \leq \eta \leq 1$, supported in the ball B_r, valued $\eta = 1$ in the concentric ball B_s for $s = r - \sigma r$, $\sigma \in (0, 1)$ and satisfying $|\nabla\eta| \leq 2/(r - s)$ in $B_r \setminus B_s$. Setting $\zeta = \eta^2 \max\{u - k, 0\}$, we obtain the estimate

$$0 \leq C\,|A_{k,r}| - \int_\Omega \nabla u\nabla\zeta\,dx.$$

The constant C depends only on $h, \varepsilon, M, |\Omega|$ and $J_n(u)$. The application of Young's inequality gives

$$\begin{aligned}
-\int_\Omega \nabla u \nabla \zeta \, dx &\leq -\int_{A_{k,r}} |\nabla u|^2 \eta^2 \, dx + \frac{1}{2}\int_{A_{k,r}} |\nabla u|^2 \eta^2 \, dx + 2\int_{A_{k,r}} |\nabla \eta|^2 (u-k)^2 \, dx \\
&\leq -\frac{1}{2}\int_{A_{k,s}} |\nabla u|^2 \, dx + \frac{8}{(\sigma r)^2} \sup_{B_r}(u-k)^2 \, |A_{k,r}| \, ,
\end{aligned}$$

which is the desired estimate. The calculations for $-u$ are similar. □

Now, we can select test functions with support in $\{u_n > 0\}$ and compute the first variation of J_n. We find that the interpolated functions u^h and $\bar{u}^h$ comply with the following definition.

Definition 6.3.1. *A function $u^h \in H^1(Q_T) \cap L^\infty(0,T; H_0^1(\Omega))$ is an approximate solution to (5.1.1)–(5.1.3), if it satisfies*

$$\begin{aligned}
\int_0^T \int_\Omega \left(u_t^h \phi + \nabla \bar{u}^h \nabla \phi + \gamma \chi_\varepsilon' \left(\bar{u}^h\right) \phi - f(\bar{u}^h)\phi\right) \, dx \, dt &= \int_0^T \int_\Omega \bar{\lambda}^h \phi \, dx \, dt \\
\forall \phi \in C_0^\infty(Q_T \cap \{u^h > 0\}), \\
u^h = 0 \quad \text{in } \; Q_T \setminus \{u^h > 0\}, \qquad \qquad \qquad \qquad (6.3.4)
\end{aligned}$$

and the initial condition $u^h(0) = u_0$. Here, $\bar{\lambda}^h$ is defined as

$$\bar{\lambda}^h = \int_\Omega \left(u_t^h \bar{u}^h + |\nabla \bar{u}^h|^2 + \gamma \chi_\varepsilon'(\bar{u}^h)\bar{u}^h - f(\bar{u}^h)\bar{u}^h\right) \, dx.$$

For the approximate solution, we get the following energy estimate.

Proposition 6.3.1. *There is a constant C depending on $\|\gamma\|_{L^\infty(\Omega)}$, $\|a\|_{L^\infty(\Omega)}$, ε, $\|u_0\|_{H^1(\Omega)}$, $\|b\|_{L^2(\Omega)}$ and T, such that*

$$\|u_t^h\|^2_{L^2(Q_T)} + \|\nabla \bar{u}^h(t)\|^2_{L^2(\Omega)} + \|\sqrt{-a}\, \bar{u}^h(t)\|^2_{L^2(\Omega)} \leq C \qquad \text{for a.e. } t \in (0,T).$$

Proof. We use the perturbation $(1-\delta)u_n + \delta u_{n-1}$ in the minimization of J_n. □

Unlike the hyperbolic case, we got the energy estimate without having to resort to singular penalties. It also turns out that from this estimate we can show the existence of a weak solution for one space dimension by similar method as in the hyperbolic case (Section 5.2.2), including the correct form of the limit Lagrange multiplier (i.e., corresponding to $\tilde{u} = u$ in (5.2.36)). As the limit process in Lagrange multiplier for the hyperbolic case is still missing, the difference in difficulty of analysis between parabolic and hyperbolic problems becomes apparent.

Chapter 7

Numerical experiments

In this Chapter we present some examples of numerical experiments for each type of problem, as classified in Section 2.2. As we have already emphasized, the discrete Morse flow method, being a minimization method, is highly suitable for constrained problems. This Chapter has the purpose of illustrating the real usage of the method but does not aim at constructing accurate models. The models presented here are very simple and, in fact, often far from being exact, though we claim they capture the features of the phenomena well. To develop more reliable models, it would be necessary to couple the presented model in each case with another complicated model (usually for the fluid, as was, e.g., hinted at in Section 5.3 when deriving a model for moving droplet). However, this would far surpass the primarily theoretical scope of the thesis. First results in this direction were presented in [19].

For each type of equation from the range studied in Chapters 4 and 5, we choose one or two examples of physical phenomena and carry out numerical simulations with concrete data. The results are presented in figures and are not further analyzed from the numerical point of view.

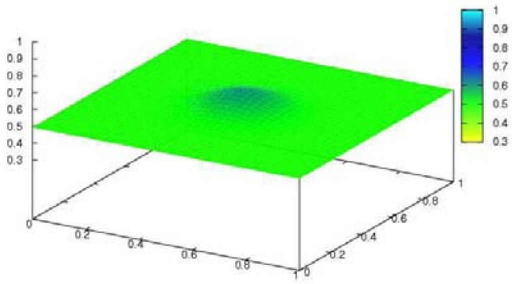
7.1 Parabolic problem without free boundary

Here we present two applications of the theory from Section 4.1, i.e., volume-constrained parabolic equations without free boundary. These results are taken from [36]. Equation (4.1.1) is used. One cannot readily see if structural conditions (4.1.4) – (4.1.6) are satisfied in these examples. However, the numerical experiments suggest that these assumptions are not necessarily essential to the computation.

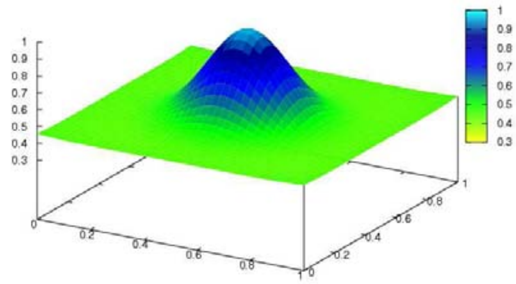
Our first application uses Neumann boundary conditions and concerns the motion of an electrolyte. An electrolytic suspension is kept in a container covered by a plate electrode. A small perturbation in the solution causes the liquid to move in the direction of the electrode. After touching the electrode, the discharged electrolyte returns to its initial position.

We consider equation (4.1.1) in a rectangular domain $(0, 1) \times (0, 1)$, with initial condition $u_0(x) = 0.5$ and the electrode positioned at height 1.0. The outer force depends linearly on the value of u (with coefficient of order 10^3) and becomes zero when the electrolyte touches the electrode. A small perturbation is created at the center of the domain.

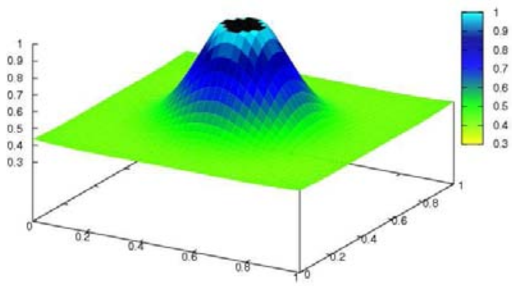
In the program, the discharge is delayed by smoothing the dependence of f on u. We use 400 elements and time step 0.001. The situation at four distinct time points is shown in Figure 7.1.



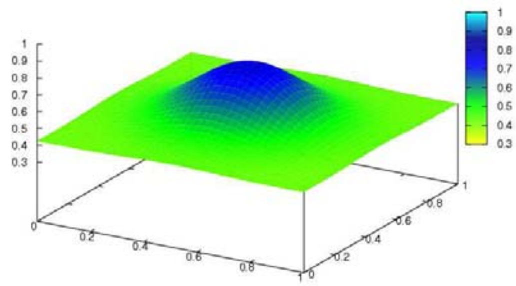
$t = 1.9 \cdot 10^{-4}$



$t = 2.5 \cdot 10^{-4}$

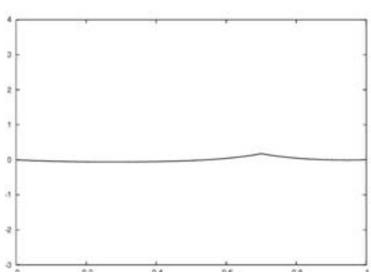


$t = 2.6 \cdot 10^{-4}$

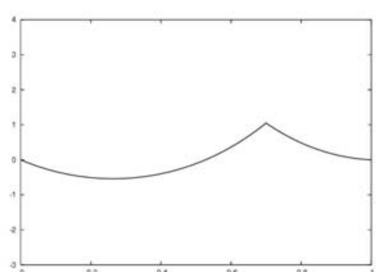


$t = 5 \cdot 10^{-4}$

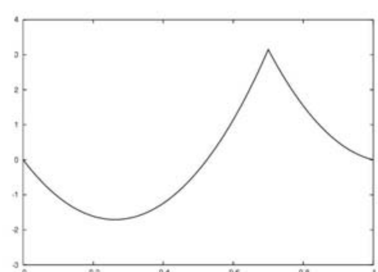
Figure 7.1: Motion of electrolyte.



$t = 0.025$



$t = 0.15$



$t = 0.45$

Figure 7.2: Raising an elastic lid from a single point.

Our second example deals with an experiment where we raise part of a film which, like a lid, covers a container filled with an incompressible fluid. Since the amount of fluid inside the container is preserved, the film must sink in certain parts.

We consider the one-dimensional case where the set of points being lifted contains only one point. The domain Ω is the interval $(0, 1)$, $u_0(x) = 0$, and we lift the point $x = 0.7$ in such a way that it moves up with a constant velocity. The boundary values are fixed, i.e., the homogeneous Dirichlet condition is used.

The domain is divided into 200 elements and time step is chosen as $0.5 \cdot 10^{-4}$. In the program, we use special volume-preserving basis functions which enable us to consider the problem as a whole (see Chapter 6 for details). We thus avoid the necessity of solving two problems in two domains with time-dependent boundary conditions, which are interrelated by means of the volume constraint. The results can be seen in Figure 7.2.

7.2 Hyperbolic problem without free boundary

In this Section, we present numerical results for a two-dimensional volume-constrained hyperbolic problem with outer force term and compare them with the nonpreserving case, paraphrasing the paper [37]. Equation (4.2.1) is solved. As a numerical example, we have chosen the phenomenon of lifting a membrane under Dirichlet boundary conditions. This is similar to the example in preceding Section, the differences being the dimension, the way of lifting and the type of equation. The real experiment can be carried out by filling a container to the brim with water and covering the water surface by a film which is then fixed at the boundary. The film lid is then picked at a certain place and raised.

In the numerical computation, we used a square domain $(0, 1) \times (0, 1)$ triangulated into 3200 elements, time step 0.025, diffusion coefficient 0.01 and a constant outer force of the magnitude 60.0 applied at a circular subdomain with center $[0.4, 0.5]$ and radius 0.27.

In the minimizing of the functional, we used special volume-preserving basis functions. This simplifies the computation in the sense that we do not have to project the minimizers on the volume-conservation hyperplane. Moreover, the computation is reliable and accurate (see Section 6.2).

The results at time 0.35 are shown in Figure 7.3 for the volume-preserving case and for the problem without volume constraint, respectively. It is observed that in both cases the film oscillates for a certain time until it reaches a stable state where the outer force and the surface tension expressed by the Laplacian are in balance. This state is depicted in the Figure.

The most important difference between the volume-preserving and nonpreserving cases lies in the fact that in the volume-preserving case the membrane caves in downwards in the region between the lifted subdomain and the boundary. We also solved the Neumann problem, where the membrane which is not volume-constrained moves upward without any obstruction while the volume constrained membrane merely caves in. Therefore, if we neglect gravity, the volume-constraint acts in a similar way as air pressure. We suppose that this fact could be useful in the solution of multiple-factor coupled problems, where the influence of outer pressure is commonly ignored, although it plays an important role.

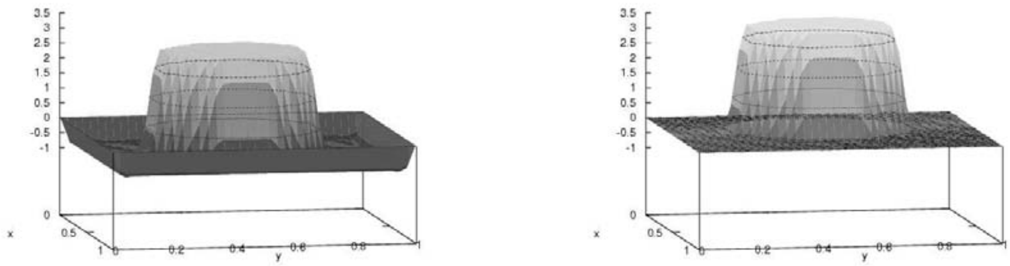


Figure 7.3: Lifting of a film - comparison of the volume-preserving and nonpreserving cases.

7.3 Parabolic problem with free boundary

We made the first attempt to realize numerically the following experiment: A surfactant is spread on the left part of a horizontally fixed plastic foil while the right part is left untreated. In this way, the surface tension in the left part of the foil decreases. A drop of coloured water is placed with a syringe on the right part of the foil, so that it touches the left part just enough to be influenced by the difference of equilibrium contact angles on both sides. The drop was created as slowly as possible in order to surpress the influence of acceleration of the liquid. The motion of the drop is recorded by a camera with 3 shots per second. Selected five shots starting from the time short after the drop started leaning to the left are shown in Figure 7.4.

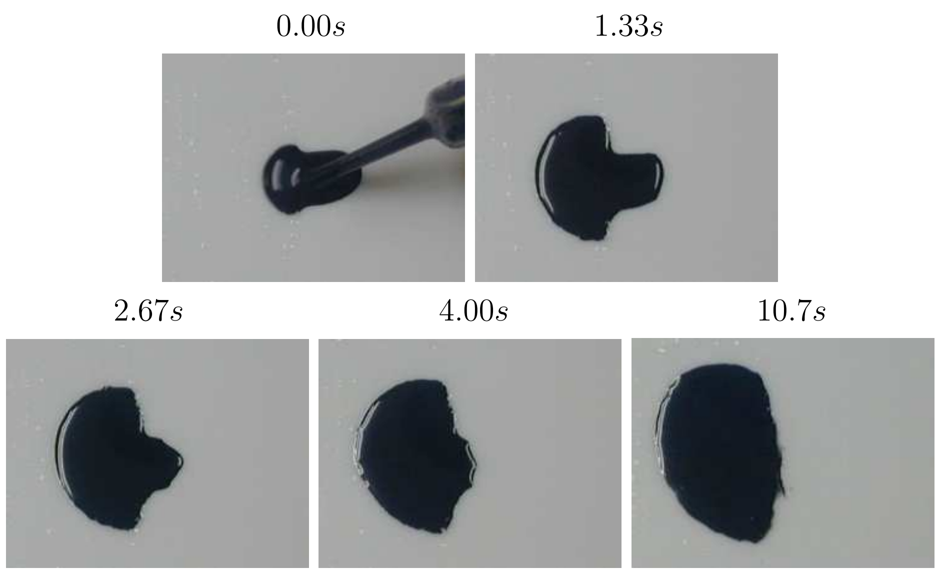


Figure 7.4: Laboratory experiment.

The model equation (5.1.1) is derived in Section 5.3. The numerical computation was performed with the use of the algorithm explained previously in Chapter 6. In order to reproduce the practical experiment, we chose the values of the parameters as

$$\begin{aligned} \gamma_L &= 0.05 \quad \text{(left side)}, \\ \gamma_R &= 0.35 \quad \text{(right side)}, \\ h &= 0.001, \\ \varepsilon &= 0.02. \end{aligned}$$

Here h is the time step. The nonuniform distribution of the surface active agent is reflected in the function γ in equation (5.1.1). In the laboratory experiment, it was necessary to contact an area greater than several points with the treated surface in order to make the drop move. We, therefore, chose a stage of the drop short after it started moving to the left as the reference state. This is possible, since with parabolic equations one can choose the initial time freely. However, it is essential to control the creation of the drop and avoid the consequences of liquid acceleration. The first and second shots of the experiment were matched with the numerical results and the relative time for the numerical computation was determined. The following pictures in Figure 7.5 are selected so that they correspond to the experimental ones with respect to this relative time. The numerical results were obtained by H. Nakagawa.

The domain is the rectangle $(-2,1)\times(-1.5,1.5)$, the "left part" being the rectangle $(-2,0)\times(-1.5,1.5)$. The domain is partitioned into 300×300 squares with sides of length $\Delta x = 0.01$ and each square is divided into two triangular elements. Then we have set $h = 0.001$ and $\varepsilon = 2\Delta x$. A precomputed stationary solution of the equation (5.1.1) with $\gamma \equiv \gamma_R$ is set as the initial shape. It is positioned in the right side of the domain but impinges on several elements of the left side. The boundary conditions are homogeneous Dirichlet because the drop is not supposed to touch the boundary.

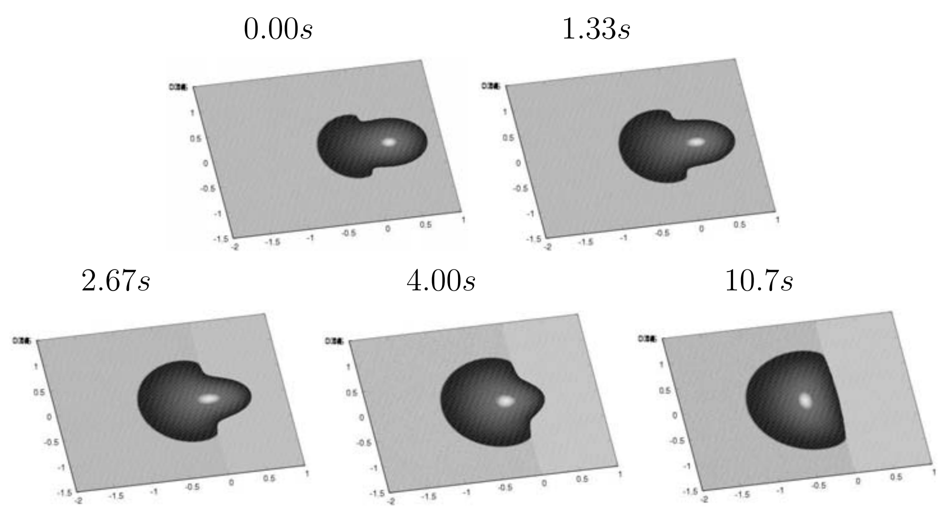


Figure 7.5: Numerical results.

One can observe a good agreement of the shape evolution, including the final stationary state. However, more precise experimental measurements and comparison with results of numerical computations with corresponding data are still to be done.

7.4 Hyperbolic problem with free boundary

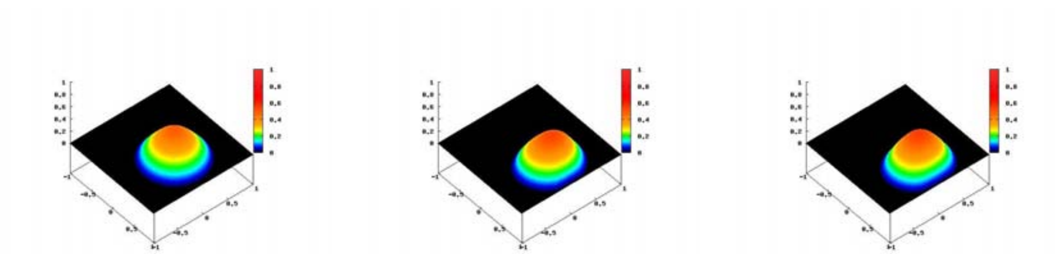
Here we present computational results for a hyperbolic free-boundary problem obtained by T. Yamazaki and published in the paper [41]. The equation can model, as mentioned in Section 5.2, the motion of a soap bubble on water surface. We consider several different types of bubble motion.

In the following simulations, we use equation (5.2.1) with a damping term μu_t, i.e.,

$$\chi_{u>0} u_{tt} + \mu u_t = \Delta u - \gamma \chi'_\varepsilon(u) - \lambda \chi_{u>0}.$$

We choose the parameters as follows: $h = 0.005$ (time step), $\varepsilon = 0.05$ (parameter of smoothing of the characteristic function in the contact-angle term), $\mu = 0.5$ and $\gamma = 0.5$.

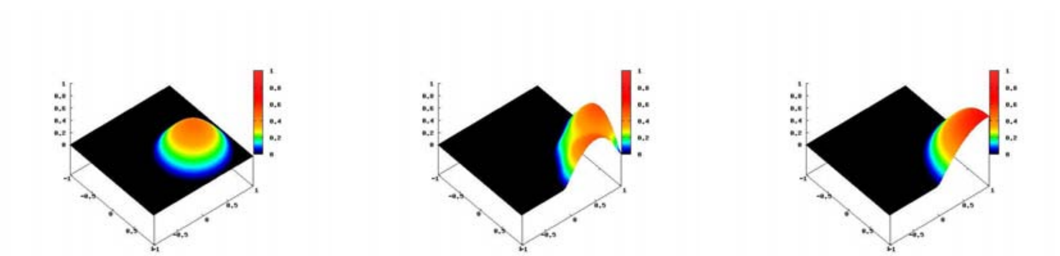
The first example is calculated under Dirichlet boundary conditions (see Figure 7.6). An initial velocity is imparted to the bubble through defining the shape on the first time level by shifting the initial shape in a suitable direction. The bubble approaches the boundary of Ω, reflects on the boundary and stops in a certain position.



$t = 0.000$ $t = 0.190$ $t = 2.500$

Figure 7.6: Bubble motion under Dirichlet boundary conditions.

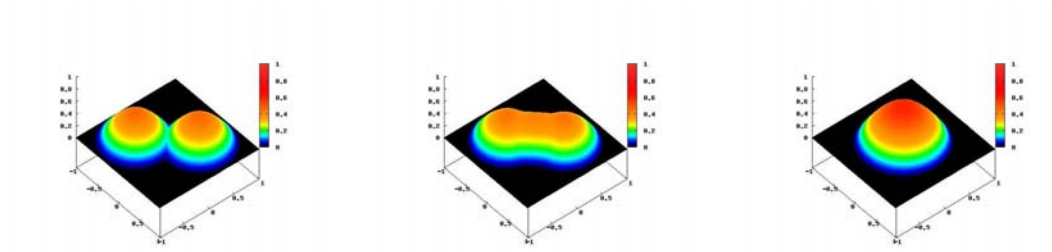
The second example uses Neumann boundary conditions. The results are shown in Figure 7.7. In this case, after touching the boundary, the bubble stops and keeps the smallest surface. This means that the bubble settles itself in the corner of the boundary $\partial\Omega$.



$t = 0.000$ $t = 0.350$ $t = 2.500$

Figure 7.7: Bubble motion under Neumann boundary conditions.

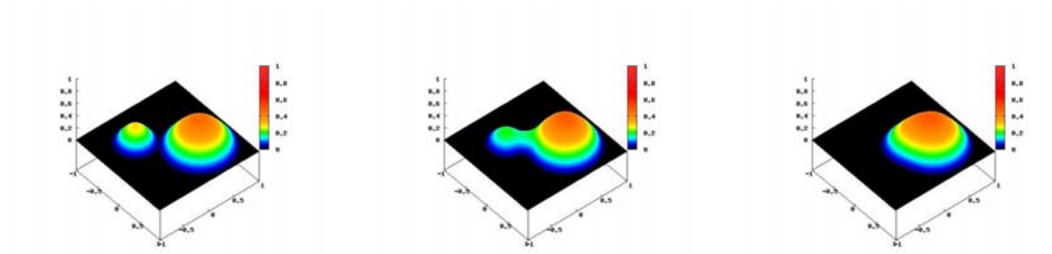
The third example treats a collision of two bubbles with the same volume. After the collision, the bubbles merge. The resulting volume is the sum of volumes of the original bubbles (Figure 7.8).



$t = 0.000$ $t = 0.175$ $t = 2.500$

Figure 7.8: Collision of two bubbles with the same volume.

The last example is similar to the third one. In this case, however, the bubbles have different volumes. One can see in Figure 7.9 that during the collision, the small bubble is absorbed into the big one.



$t = 0.000$ $t = 0.150$ $t = 1.500$

Figure 7.9: Collision of two bubbles with different volumes.

Chapter 8

Conclusion

The present thesis attempts to comprehensively study evolutionary problems with volume constraint (i.e. with constant area under the graph of the solution), starting from the derivation of suitable equations, continuing with their analysis and ending with development of numerical schemes and obtaining numerical results. The goal has been achieved partially because we were not able to cover all the aspects in detail, the core part of the study being the mathematical analysis of the problem. We proved the existence of weak solutions for a heat-type parabolic problem, wave-type hyperbolic problem and parabolic problem with an obstacle. Partial results were found for a degenerate hyperbolic obstacle problem.

The variational method called discrete Morse flow proved to be a powerful tool both in the theoretical analysis and the numerical computation. Since it is a time-discrete minimization method, the volume constraint reduces to "trimming" of the set of functions admissible for minimization on discrete time levels.

We propose numerical algorithms for solving volume preserving problems, believing that they will be useful in numerical solution of coupled models, for example, models for interaction of a volume-preserving membrane and a fluid. Such kind of models have wide applications, and interesting numerical results for the motion of drop on surfaces and simple simulation of heart motion have been obtained recently. These simulations use the discrete Morse flow minimization method for the membrane and particle method for the fluid.

The investigation of volume-constrained problems is not closed. There are many interesting problems yet to be solved. We mention some of the main items:

- proof of existence of a weak solution to the hyperbolic obstacle problem in higher dimensions
- analysis of free-boundary problems with sharp contact angles (this means to take ε to zero in the term χ_ε in (5.2.1), to study solutions near the free boundary and the properties of the free boundary itself)
- generalization to arbitrary integral constraints
- analysis of evolutionary (free-boundary) problems with minimal surface operator, as mentioned in Section 5.3

- treatment of vector-valued problems (e.g., “overhanging” droplets with contact angles greater than 90° or the case of a drop dripping from a horizontal plane)
- error analysis of numerical schemes
- posing well-defined systems for the coupled problems and their mathematical analysis
- comparison of numerical results with real experiments.

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My thanks go to all of my schoolmates in the laboratory, especially to Mr. Takashi Yamazaki who was tirelessly helping me at school during my first year in Japan. He is the creator of the program for computation of bubble motion from Section 7.4.

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