Applications of Mathematics

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Numerical methods for fourth order nonlinear degenerate diffusion problems

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NUMERICAL METHODS FOR FOURTH ORDER NONLINEAR DEGENERATE DIFFUSION PROBLEMS

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Abstract. Numerical schemes are presented for a class of fourth order diffusion problems. These problems arise in lubrication theory for thin films of viscous fluids on surfaces. The equations being in general fourth order degenerate parabolic, additional singular terms of second order may occur to model effects of gravity, molecular interactions or thermocapillarity. Furthermore, we incorporate nonlinear surface tension terms. Finally, in the case of a thin film flow driven by a surface active agent (surfactant), the coupling of the thin film equation with an evolution equation for the surfactant density has to be considered.

Discretizing the arising nonlinearities in a subtle way enables us to establish discrete counterparts of the essential integral estimates found in the continuous setting. As a consequence, the resulting algorithms are efficient, and results on convergence and nonnegativity or even strict positivity of discrete solutions follow in a natural way. The paper presents a finite element and a finite volume scheme and compares both approaches. Furthermore, an overview over qualitative properties of solutions is given, and various applications show the potential of the proposed approach.

Keywords: thin film, fourth order degenerate parabolic equation, nonnegativity preserving scheme, surfactant driven flow, finite element method, finite volume method

MSC 2000: 35K35, 35K55, 35K65, 65M12, 65M50, 65M60, 76D08

1. INTRODUCTION

In this paper we will discuss numerical approximation of certain fourth order degenerate parabolic equations and systems. The basic model is the following. Find a pair of functions $u, p\colon \Omega \times (0, T) \to \mathbb{R}$ where Ω is a domain in $\mathbb{R}^d$ $(d = 1, 2)$ such

that

(1)
$$\partial_t u - \operatorname{div}(\mathcal{M}(u)\nabla p) = 0 \qquad \text{in } \Omega \times (0,T),$$
$$p = -\Delta u \quad \text{in } \Omega \times (0,T),$$
$$\frac{\partial}{\partial \nu} u = \frac{\partial}{\partial \nu} p = 0 \qquad \text{on } \partial\Omega \times (0,T),$$
$$u(0,\cdot) = u_0(\cdot) \quad \text{in } \Omega.$$

Here u represents the height of the film and p stands for the pressure. We assume that the nonnegative mobility $\mathcal{M} \in C(\mathbb{R})$ vanishes at zero and has at most polynomial growth. By $n := \sup\{s \in \mathbb{R}^+ : \lim_{u \to 0} \mathcal{M}(u)/u^s < \infty\}$ we denote its growth exponent near zero. Equation (1) models the height of thin films of viscous fluids which—driven solely by surface tension—spread on plain, solid surfaces. It can be derived by lubrication approximation from the Navier-Stokes equations for incompressible fluids (cf. Section 2 and [31]).

Physically, the explicit form of the nonlinear mobility $\mathcal{M}(u)$ depends on the boundary condition at the liquid-solid interface. A *no-slip* condition entails $\mathcal{M}(u) = u^3$, various *slip* conditions (cf. [6]) yield $\mathcal{M}(u) = u^3 + \beta u^n$, $\beta > 0$, $n \in (0,3)$. Mathematically, the smoothness of $\mathcal{M}(\cdot)$ at zero determines the qualitative behaviour of solutions (cf. Figs. 1, 2). Combined with *no-flux* boundary conditions and nonnegative initial data, (1) is an initial-boundary-value problem which shows from the analytical point of view a rather peculiar behaviour already in the most basic model case:

- In contrast to solutions of nondegenerate fourth order parabolic equations, initially nonnegative solutions to (1) preserve nonnegativity (cf. [9], [13], [19]).
- If $n \in (0,3)$, there exist solutions to (1) exhibiting for $t > 0$ a zero contact angle at the contact line between liquid, solid and gas (cf. [5], [10], [13], [20]). Moreover, this contact line propagates with finite speed, i.e. we are dealing with a free boundary problem (cf. [7], [8], [11], [22], [20] and Fig. 1). However, if initial data have a non-zero contact angle, the propagation speed may be singular for $t = 0$.
- If $n \geqslant 3$, it is conjectured (and proven for $d = 1$ and $n > 4$, see [5]) that the support of the solution is constant in time (cf. Fig. 2).
- No maximum or comparison principles hold true.

Numerical analysis of fourth order degenerate parabolic problems is a young field. J. Barrett, J. Blowey, and H. Garcke [1] proved convergence results for equation (1) in one space dimension and stability results in arbitrary dimensions. Their approach is based on variational inequalities to guarantee nonnegativity of discrete solutions.
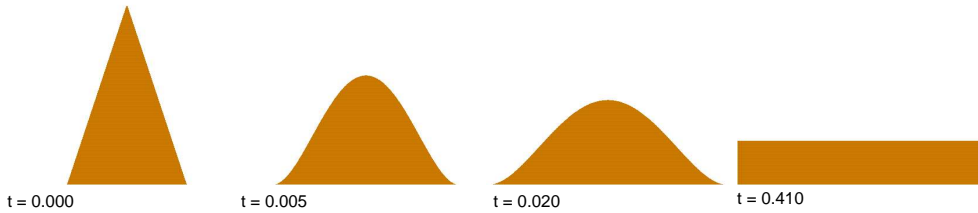
Figure 1. Instantaneous development of zero contact angle for initial data with non-zero contact angle illustrated for $n = 1$ and hat-shaped initial datum on the interval.
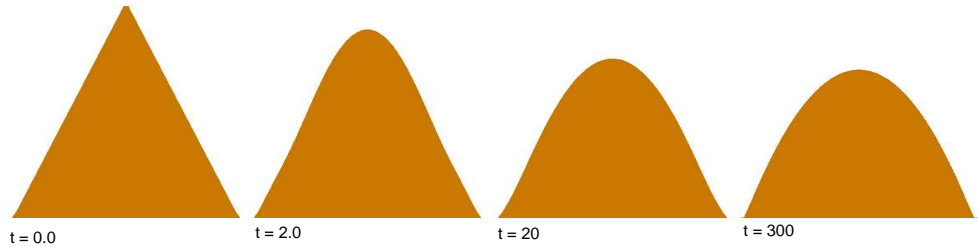

Figure 2. No spreading of support, but convergence to a parabolic profile, illustrated for $n = 4$ and the same initial datum as in Fig. 1.

In [2] they applied their technique to the Cahn-Hilliard equation with degenerate mobility which has some similarity with (1).

A different approach to the discretization of (1) has been pursued by Grün and Rumpf [25] and generalized in the presence of additional terms in [23] and [26] (cf. also the paper by L. Zhornitskaya and A. Bertozzi [32] for a related strategy devoted to finite difference schemes and strictly positive solutions). In arbitrary space dimensions, results on nonnegativity (in some cases even on positivity) and convergence of discrete solutions follow in a natural way [18]. The numerical cost consists of solving in each time step a system of linear equations involving a sparse matrix. Moreover, a time-step control based on an explicit formula for the normal velocity of the free boundary allows us to trace its propagation very precisely.

Here we give an overview over the results and especially emphasize the relations between a finite element (cf. Section 4) and a finite volume (cf. Section 5) discretization, respectively. Both have their special advantages. The finite volume scheme comes along with a simple definition of the numerical mobility and is especially well-suited for a coupling with transport phenomena. The finite element scheme is based on a Galerkin discretization and hence better to treat analytically. But they both share the same fundamental characteristics. Furthermore, we discuss generalizations in various directions. In Section 7, we present a modification of the basic problem taking into account the mean curvature to model surface tension more appropri-

ately. In Section 6 additional nonlinear terms are introduced to model effects such as evaporation and condensation, gravity, or thermocapillarity. Finally, various examples show the range of application and illustrate the rich qualitative behaviour of solutions.

2. Derivation of the basic thin film model

Before we consider numerical approximations of the thin film equation, let us have a look at a derivation of the model. Our starting point are the Navier-Stokes equations equipped with suitable boundary conditions at the liquid-gas and the liquid-solid interface, respectively. Scaling arguments in this framework will indicate that to leading order the horizontal flow is of Poiseuille-type, i.e. parabolic in profile. Assuming the free energy to be dissipated solely due to viscous friction, averaging horizontal flow components over the vertical axis, and taking the incompressibility of the liquid into account, Equation (1) will be derived. In principle, we follow here the derivation by Oron et al. [31]. For a different approach we refer to [17], [20].

Let us assume the following configuration: A thin film is supposed to sit on the plane $P = \{x \in \mathbb{R}^{d+1} \mid x_0 = 0\}$ where $x_0, \ldots, x_d$ are the coordinates in $\mathbb{R}^{d+1}$. We suppose $x^\perp = x_0$ to be the vertical component perpendicular to the plane P and $\overline{x} = (x_1, \ldots, x_d)$ to be the tangential component within P. Let us denote by D the liquid domain. Hence, the boundary of D consists of two components: a planar one $\underline{\partial}D$ representing the solid-liquid interface and being a subset of P, and a free boundary $\overline{\partial}D$ representing the liquid-gas interface. We suppose $\overline{\partial}D$ to be a graph over P, its height function being denoted by u. Suppose $v \colon D \to \mathbb{R}^{d+1}$ is the velocity field of the fluid flow and $q \colon D \to \mathbb{R}$ the corresponding pressure. Again we split v into a tangential component $\overline{v} = (v_1, \ldots, v_d)$ and a vertical component $v^\perp = v_0$. The velocity and the pressure are supposed to be governed by the incompressible Navier-Stokes equations

$$\partial_t v + (v \cdot \nabla)v - \nu \Delta v + \nabla q = -\nabla w',$$
$$\operatorname{div} v = 0,$$

where ν is the viscosity and w' the derivative of an external potential w. By $S = 2\nu D(v) - q\mathrm{Id}$ we denote the usual stress tensor where $D(v) = \frac{1}{2}[(\nabla v)^T + \nabla v]$. The Navier-Stokes equations are completed by appropriate boundary conditions on ∂D. On $\underline{\partial}D$ we suppose Navier slip conditions for a constant $\beta > 0$

$$v^\perp = 0,$$
$$\overline{v} \cdot r = 2\beta\nu\, D(v)n \cdot r$$

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for any tangent vector r on $\underline{\partial}D$, whereas on the free boundary $\overline{\partial}D$ we have the usual surface tension condition

$$Sn \cdot n = -\sigma h$$

for the mean curvature h and a surface tension coefficient $\sigma > 0$. By the definition of the evolving D we obtain the relation $v^\perp = \frac{d}{dt} u(t, \overline{x}(t))$ between velocity and height on $\overline{\partial}D$ and thus by differentiation one finds

$$v^\perp = \partial_t u + \overline{v} \cdot \nabla_{\overline{x}} u.$$

Now, let us consider the configuration of a thin film. We assume a characteristic scaling of height and length:

$$\varepsilon = \frac{\text{height}}{\text{length}} \ll 1.$$

This motivates the introduction of rescaled dependent and independent variables (which throughout this section we denote by uppercase characters):

$$X = (x^\perp, \varepsilon\overline{x}) = (X^\perp, \overline{X}),$$
$$T = \varepsilon t,$$
$$U = u,$$
$$\Sigma = \varepsilon\sigma, \ H = h,$$
$$V = \frac{d}{dt}X = \frac{1}{\varepsilon}\frac{d}{dt}(x^\perp, \varepsilon\overline{x}) = \left(\frac{1}{\varepsilon}v^\perp, \overline{v}\right) = (V^\perp, \overline{V}),$$
$$\partial_{x^\perp} = \partial_{X^\perp}, \ \partial_{\overline{x}} = \varepsilon\partial_{\overline{X}}, \ \partial_t = \varepsilon\partial_T,$$
$$Q = \varepsilon q, \ W = \varepsilon w.$$

Here we make use of the fact that the pressure q as the Lagrange multiplier with respect to the incompressibility condition and the additional potential w as a comparable term should scale like $\text{div } v$. Writing now the Navier-Stokes equations in the scaled variables, we get

$$0 = \varepsilon^2 \partial_T V^\perp + \varepsilon^2 (V \cdot \nabla_X) V^\perp - \varepsilon(\partial_{X^\perp}^2 + \varepsilon^2 \Delta_{\overline{X}})V^\perp + \frac{1}{\varepsilon}\partial_{X^\perp}(Q + W'),$$
$$0 = \varepsilon \partial_T \overline{V} + \varepsilon(V \cdot \nabla_X)\overline{V} - (\partial_{X^\perp}^2 + \varepsilon^2 \Delta_{\overline{X}})\overline{V} + \nabla_{\overline{X}}(Q + W'),$$
$$0 = \varepsilon \operatorname{div}_X V,$$

where we have set $\nu = 1$. We confine ourselves to the highest order terms and end up with

$$\operatorname{div}_X V = 0,$$
$$\partial_{X^\perp}(Q + W') = 0,$$
$$\nabla_{\overline{X}}(Q + W') = \partial_{X^\perp}^2 \overline{V}.$$

This is completed by the corresponding boundary conditions in scaled variables, i.e., on $\overline{\partial}D$ we obtain

$$V^\perp(U) = \partial_T U + (\overline{V} \cdot \nabla_{\overline{X}})U$$

and on $\underline{\partial}D$ the Navier slip conditions transforms to

$$\overline{V} = \beta\left(\varepsilon^2 \nabla_{\overline{X}} V^\perp + \partial_{X^\perp}\overline{V}\right).$$

Thus restricting ourselves the highest order terms we get on $\underline{\partial}D$

$$V^\perp = 0,$$
$$\overline{V} = \beta\partial_{X^\perp}\overline{V}.$$

Furthermore, we consider the scaling with respect to the stress tensor S and achieve

$$S = \left(\begin{array}{c|c} 2\varepsilon\partial_{X^\perp}V^\perp - \varepsilon^{-1}Q & 2\left(\partial_{X^\perp}\overline{V} + \varepsilon^2\nabla_{\overline{X}}V^\perp\right)^T \\ \hline 2\left(\partial_{X^\perp}\overline{V} + \varepsilon^2\nabla_{\overline{X}}V^\perp\right) & 2\varepsilon\left(\nabla_{\overline{X}}\overline{V} + \nabla_{\overline{X}}\overline{V}^T\right) - \varepsilon^{-1}Q\,\mathrm{Id}_\mathrm{d} \end{array}\right)$$

where Id_d is the identity on the plane P. Finally, for the normal n and a tangent vector r on $\overline{\partial}D$ and their scaled counterparts $N = (N^\perp, \overline{N})$ and $R = (R^\perp, \overline{R})$ we get

$$n = \frac{(N^\perp, \varepsilon\overline{N})}{\|(N^\perp, \varepsilon\overline{N})\|}, \qquad r = \frac{(\varepsilon R^\perp, \overline{R})}{\|(\varepsilon R^\perp, \overline{R})\|}.$$

From $Sn \cdot n = -\sigma h$ and $Sn \cdot r = 0$ we deduce

$$Q = \Sigma H, \qquad \partial_{X^\perp}\overline{V} = 0.$$

Now we ask for a differential equation for U. Thus, we integrate the incompressibility condition and obtain

$$\int_0^U \mathrm{div}_X V = 0 \quad \Rightarrow$$

$$V^\perp(U, \cdot) - \underbrace{V^\perp(0, \cdot)}_{=0} + \int_0^U \mathrm{div}_{\overline{X}}\overline{V}(\xi, \cdot)\,\mathrm{d}\xi = 0 \quad \Rightarrow$$

$$\partial_T U + (\overline{V} \cdot \nabla_{\overline{X}})U + \int_0^U \mathrm{div}_{\overline{X}}\overline{V} = 0 \quad \Rightarrow$$

$$\partial_T U + \mathrm{div}_{\overline{X}}\left(\int_0^U \overline{V}\right) = 0.$$

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Furthermore, we observe that $P := Q + W'$ is constant in $X^\perp$ for fixed $\overline{X}$. Hence

$$\partial^2_{X^\perp}\overline{V} = \nabla_{\overline{X}}P = C(\overline{X}),$$
$$\overline{V}(0,\overline{X}) = \beta\partial_{X^\perp}\overline{V}(0,\overline{X}),$$
$$\partial_{X^\perp}\overline{V}(U,\overline{X}) = 0.$$

Finally, we see that for fixed $\overline{X}$ the velocity component $\overline{V}$ is a quadratic polynomial p in $s = X^\perp$ with $p''(s) = C$, $p(0) = \beta p'(0)$, and $p(U) = 0$. This results in $p(s) = C\left(\frac{1}{2}s^2 - U(s+\beta)\right)$. Hence,

$$\overline{V}(X^\perp,\overline{X}) = \nabla_{\overline{X}}P(X^\perp,\overline{X})\left(\frac{1}{2}(X^\perp)^2 - U(X^\perp + \beta)\right).$$

Inserting this in the above differential equation for U, and employing the usual expression for the mean curvature and the basic scaling argument we obtain an equation for P as well. Altogether we end up with the problem

$$\partial_T U = \operatorname{div}_{\overline{X}}\left(\left(\frac{U^3}{3} + \beta U^2\right)\nabla_{\overline{X}}P\right),$$
$$P = W' - \varepsilon^2\Sigma\operatorname{div}_{\overline{X}}\left(\frac{\nabla_{\overline{X}}U}{\sqrt{1+\varepsilon^2|\nabla_{\overline{X}}U|^2}}\right).$$

Transferring this back to the original variables and again confining ourselves to the highest order terms leads to the problem

$$\partial_t u = \operatorname{div}_{\overline{x}}(\mathcal{M}(u)\nabla_{\overline{x}}p),$$
$$p = -\operatorname{div}_{\overline{x}}\left(\frac{\nabla_{\overline{x}}u}{\sqrt{1+|\nabla_{\overline{x}}u|^2}}\right) + w',$$

where we have set $\sigma = 1$. If we linearize the mean curvature $h = -\operatorname{div}_{\overline{x}}\left(\frac{\nabla_{\overline{x}}u}{\sqrt{1+|\nabla_{\overline{x}}u|^2}}\right)$ by $-\Delta_{\overline{x}}u$ and assume $w \equiv 0$ we immediately end up with the thin film equation. The case of nontrivial w will be dealt with in Section 6.

3. Weak solutions and fundamental a priori estimates

Crucial for all these applications of thin film models is the fact that it is possible to construct solutions of (1) which preserve nonnegativity as has been proved for space dimension $d = 1$ by Bernis and Friedman [9] and for higher space dimensions by Grün [19] and by Elliott, Garcke [14]. This behaviour is in strong contrast to that of the classical solutions to linear parabolic equations of fourth order which in

general become negative even in the case of strictly positive initial values. Thus we consider solutions of equation (1) in the following weak sense:

$$\int_0^T \int_\Omega (u - u_0)\frac{\partial}{\partial t}\vartheta \, \mathrm{d}x \, \mathrm{d}t = \int_{[u>0]} \mathcal{M}(u)\nabla p \nabla \vartheta \, \mathrm{d}x \, \mathrm{d}t$$

$$\text{for all } \vartheta \in C^1([0,T]; H^{1,2}(\Omega)) \text{ satisfying } \vartheta(T) = 0,$$

$$\int_\Omega p(t,x)\psi(x) \, \mathrm{d}x = \int_\Omega \nabla u(t,x)\nabla \psi(x)$$

$$\text{for almost all } t \in (0,T) \text{ and every } \psi \in H^{1,2}(\Omega).$$

Moreover, the papers of Beretta, Bertsch, Dal Passo [5] and of Bertozzi, Pugh [10] who study this equation in space dimension $d = 1$ reveal a rich structure of qualitative behaviour of solutions depending on the mobility growth exponent n. To put it concisely, the larger n is, the stronger is the tendency of solutions to stay positive and the weaker is the regularity at the boundary of the set where u vanishes. In space dimension $d = 1$ for instance, solutions to strictly positive initial data remain strictly positive if $n > \frac{7}{2}$. On the contrary, if $n < \frac{1}{2}$ the theoretical results in [5] show that film rupture may occur.

This already indicates that for solutions to (1) maximum or comparison principles cannot be valid. Indeed, all the results about existence and qualitative behaviour mentioned above are consequences of two basic types of integral estimates, namely the so-called energy estimate

$$\int_\Omega |\nabla u(T,\cdot)|^2 + 2\int_0^T \int_\Omega \mathcal{M}(u)|\nabla p|^2 = \int_\Omega |\nabla u_0(\cdot)|^2$$

and the entropy or pressure estimate which reads in its simplest form as follows:

$$(2) \qquad \int_{[u(T,\cdot)>0]} G(u(T,\cdot)) + \int_0^T \int_\Omega p^2 \leqslant \int_\Omega G(u_0),$$

where $G(u) := \int_1^u \int_1^s 1/\mathcal{M}(r) \, \mathrm{d}r \, \mathrm{d}s$. Here, it is formulated in the version that has been found by Bernis and Friedman in [9] (for the multi-dimensional equivalent, see [19]). Although comparison principles do not hold, inequality (2) permits the construction of globally non-negativity-preserving solutions. Note that for a generic mobility like $\mathcal{M}(u) = u^n$ and for values of $n > 2$ the entropy $G(u)$ behaves like u^{2-n} to leading order. Hence, solutions are forced to stay positive almost everywhere provided the initial data are strictly positive. For different positive values of n, results on non-negativity can still be proven. However, the corresponding arguments are more involved, and therefore we refer to literature for details (see [13] and the references therein).

4. Finite element approximation

The numerical schemes which we are going to propose are inspired both by the analysis in the continuous setting and the physics to be modeled. Any algorithmical realization of the problem requires implementation of a discrete mobility appropriately representing $\mathcal{M}(\cdot)$ from the continuous setting. Choosing the discrete mobility via seemingly straightforward, simple interpolation turns out to be the wrong choice. It does not correspond to a proper discrete model for the flux $\mathcal{M}(u)\nabla p$, which will be significantly over- or underestimated, especially close to the free boundary. Let us recall from the numerical analysis of hyperbolic conservation laws that the proper— in fact entropy consistent—choice of the numerical flux is of great importance for the reliability of the numerical algorithm. Likewise, a proper choice of the mobility and thereby of the flux will lead to reliable numerical solutions, which especially fulfil a discrete entropy inequality.

Let us first present a finite element scheme. However, before stating the corresponding discrete problem we have to introduce some notation.

Let $\mathcal{T}_h$ be a regular and admissible triangulation of the domain Ω for $d = 1, 2$ (cf. Ciarlet's monograph [12]) with simplicial elements T. The maximal diameter over all cells is denoted by h and called the grid size. Let us suppose in addition that the discretization is *rectangular* in the sense that for each simplicial element $E \in \mathcal{T}_h$, there exists a vertex $x_0(E)$ such that the edges connecting $x_0(E)$ with vertices $x_i(E)$ and $x_j(E)$ are perpendicular to each other for $i, j \in \{1, \ldots, d\}$, $i \neq j$. This assumption is used mainly in the proof of the entropy estimate. Note that it does not exclude the applicability of standard strategies for local mesh refinement. Neither does it induce a severe restriction on the class of domains that can be considered. By V^h we denote the subspace of $H^{1,2}(\Omega)$ consisting of continuous functions which are linear on each element $E \in \mathcal{T}_h$. In the sequel, elements of V^h will be denoted by capitals, and functions contained in non-discrete function spaces will be denoted by lower-case characters. A function $V \in V^h$ is uniquely defined by its values on the set of nodes $\{x_j\}_{j \in J}$ of the triangulation $\mathcal{T}_h$, where J denotes the corresponding index set. A set of basis functions corresponding to the set of nodal points is given by the "hat"-type functions $\Phi_j \in V^h$ with $\Phi_j(x_i) = \delta_{ij}$, where δ_{ij} is the usual Kronecker symbol. Let us furthermore introduce the well-known lumped masses scalar product corresponding to the integration formula

$$(\Theta, \Psi)_h := \int_\Omega \mathcal{I}_h(\Theta\Psi)$$

where $\mathcal{I}_h \colon C^0(\Omega) \to V^h$ is the interpolation operator with $\mathcal{I}_h u = \sum\limits_{j \in J} u(x_j)\Phi_j$. By (u, v) we denote the usual L^2-scalar product on Ω. The diagonal, positive definite

lumped masses matrix is given by

$$(M_h)_{ij} = (\Phi_i, \Phi_j)_h, \tag{3}$$

and L_h stands for the standard stiffness matrix

$$(L_h)_{ij} = (\nabla\Phi_i, \nabla\Phi_j). \tag{4}$$

Then in matrix form the discrete Laplacian Δ_h takes the form $-M_h^{-1}L_h$. Let the time interval $I := [0, T]$ be subdivided into intervals $I_k = [t_k, t_{k+1})$ with $t_{k+1} = t_k + \tau_k$ for time increments $\tau_k > 0$ and $k = 0, \ldots, N - 1$. For simplicity, we assume $\tau_k \equiv \tau$ for $k = 0, \ldots, N - 1$. We will denote the backward difference quotients with respect to time by ∂_τ^-. Finally, we assume $M(U)$ to be an appropriate approximation of the true mobility $\mathcal{M}(\cdot)$ for a discrete height field U. At least $M(U)$ is a positive semidefinite and symmetric tensor on each simplex $T \in \mathcal{T}_h$.

Then, an implicit backward Euler discretization scheme for Equation (1) reads as follows [25]:

For given $U^0 \in V^h$ and $k = 0, \ldots, N - 1$, find functions $(U^{k+1}, P^{k+1}) \in V^h \times V^h$ such that

$$(\partial_\tau^- U^{k+1}, \Theta)_h + (M(U^{k+1})\nabla P^{k+1}, \nabla\Theta) = 0, \tag{5}$$
$$(\nabla U^{k+1}, \nabla\Psi) = (P^{k+1}, \Psi)_h$$

for all $\Theta, \Psi \in V^h$.

Obviously the second equation can be rewritten as $P^{k+1} = -\Delta_h U^{k+1}$. Choosing $\Psi \equiv 1$, we immediately observe that

$$\int_\Omega P^{k+1} = 0,$$

and the choice $\Theta \equiv 1$ enables us to verify a discrete conservation of mass:

$$\int_\Omega U^{k+1} = \int_\Omega U^k = \int_\Omega U^0.$$

The discrete initial values U^0 are assumed to be approximations of the continuous initial values u_0. Suppose $u_0 \in C^0$, then we can prescribe $U^0 := \mathcal{I}_h u_0$.

Furthermore, for the discrete solutions U^k, P^k corresponding to the sequence of timesteps $\{t_k\}_{k=1,\ldots,N}$, we define a piecewise constant extension $U_{\tau h}, P_{\tau h}$ in time by $U_{\tau h}(t) := U^k$ and $P_{\tau h}(t) := P^k$ for $t \in I_k$. Furthermore,

$$\tilde{U}_{\tau h}(t) := \frac{t_{k+1} - t}{\tau_k} U^k + \frac{t - t_k}{\tau_k} U^{k+1}$$

represents a linear and continuous interpolation of $U_{\tau h}$ in time. A discrete pressure $\tilde{P}_{\tau h}$ can be defined by analogy. In particular, $P_{\tau h} = -\Delta_h U_{\tau h}$ and $\tilde{P}_{\tau h} = -\Delta_h \tilde{U}_{\tau h}$. We will call a pair $(U_{\tau h}, P_{\tau h})$ a discrete solution if it solves the problem (5) with the initial condition $U^0 = \mathcal{I}_h u_0$. To simplify the writing, we will skip the indices whenever a misunderstanding is ruled out by the context.

Existence of discrete solutions.

Due to the nonlinearity of the problem the first question to be dealt with is that of the existence of discrete solutions. Hence let us consider a suitable fixed-point argument. For $W^k = U^k - \alpha$ with $\alpha := 1/|\Omega| \int_\Omega U^0$ we obtain weak equations

$$(6) \qquad (\partial_\tau^- W^{k+1}, \Theta)_h + (M(W^{k+1} + \alpha)\nabla P^{k+1}, \nabla \Theta) = 0$$
$$(P^{k+1}, \Psi)_h = (\nabla W^{k+1}, \nabla \Psi)$$

and the initial condition $W^0 = U^0 - \alpha$. First let us define the weighted stiffness matrix $L_h(U)$ for $W \in V^h$ by

$$(7) \qquad (L_h(U)_{ij})_{i,j \in J} := \int_\Omega M(U)\nabla \varphi_i \cdot \nabla \varphi_j.$$

Then a solution of (5) is obtained by solving the following nonlinear system of $q = \dim V^h$ equations for each time step. If we denote the nodal value vector for a function $V \in V^h$ by $\overline{V}$, and with a slight misuse of notation rewrite $L_h(\overline{U})$ for $L_h(U)$, then for given $\overline{W}^k \in \mathbb{R}^q$ we search $\overline{W}^{k+1} \in \mathbb{R}^q$ such that $F(\overline{W}^{k+1}) = 0$ for

$$F(\overline{W}) = (\mathrm{Id} + \tau_k M_h^{-1} L_h(\overline{W} + \alpha) M_h^{-1} L_h)\overline{W} - \overline{W}^k.$$

Let us now introduce a new bilinear form on $\mathbb{R}^q$ by

$$\langle \overline{W}, \overline{V} \rangle := L_h \overline{W} \cdot \overline{V},$$

where $\cdot$ indicates the Euclidean scalar product on $\mathbb{R}^q$. By definition this form is symmetric and hence represents a scalar product on $K^\perp := \{\overline{W} \mid M_h \overline{W} \cdot (1, \ldots, 1) = 0\}$. We easily verify that $\overline{W}^0 \in K^\perp$ and by induction that $F \colon K^\perp \to K^\perp$. Furthermore, considering especially the assumptions on $M(U)$ we estimate

$$\langle F(\overline{W}), \overline{W} \rangle = \langle \overline{W} - \overline{W}^k, \overline{W} \rangle + \tau_k L_h(\overline{W} + \alpha) M_h^{-1} L_h \overline{W} \cdot M_h^{-1} L_h \overline{W}$$
$$\geqslant \langle \overline{W} - \overline{W}^k, \overline{W} \rangle \geqslant 0$$

for $\langle \overline{W}, \overline{W} \rangle^{1/2} \geqslant R$ with $R := \langle \overline{W}^k, \overline{W}^k \rangle^{1/2}$. Therefore we can apply Brouwer's fixed-point theorem and prove existence of a root $\overline{W}^{k+1}$ for the mapping $F(\cdot)$. Finally, we

define by $U^{k+1} := (W^{k+1} + \alpha)$ a solution of the original problem. Let us remark that the restriction on $K^\perp$ reflects the mass conservation property. We follow this fixed-point argument also in the numerical implementation. Indeed, in each timestep, we set $\overline{U}_0^{k+1} = \overline{U}^k$ and find for $i = 0, 1, \dots$ vectors $\overline{U}_{i+1}^{k+1}$ satisfying

$$B(\overline{U}_{i+1}^{k+1}) = M_h(\overline{U}_{i+1}^{k+1} - \overline{U}^k) + \tau_k L_h(\overline{U}_i^{k+1}) M_h^{-1} L_h \overline{U}_{i+1}^{k+1} = 0.$$

We immediately observe that $F(\overline{W}) = M_h^{-1} B(\overline{W} + \alpha)$. In each iteration the non-symmetric linear system is solved by applying a preconditioned BiCG algorithm.

A priori estimates.

As announced in the introduction let us now state discrete counterparts of the fundamental a priori estimates known for the problem. First, we obtain the a priori energy identity

$$\frac{1}{2} \int_\Omega |\nabla U^N(x)|^2 \, dx + \frac{1}{2} \sum_{i=0}^{N-1} \int_\Omega |\nabla(U^{i+1}(x) - U^i(x))|^2 \, dx$$

$$+ \int_0^T \int_\Omega M(U)|\nabla P|^2 \, dx \, dt = \frac{1}{2} \int_\Omega |\nabla U^0(x)|^2 \, dx.$$

In particular, if $U_{\tau h}^0$ is uniformly bounded in $H^1(\Omega)$, then $U_{\tau h}$ and $M(U_{\tau h})|\nabla P_{\tau h}|^2$ are uniformly bounded in $L^\infty((0,T); H^1(\Omega))$ and $L^1((0,T) \times \Omega))$, respectively, independently of the discretization parameters τ and h.

To prove this, we choose $\Theta = P^{k+1}$ in Equation (5), sum over k and obtain for the parabolic part

$$\frac{1}{\tau} \sum_{k=0}^{N-1} (U^{k+1} - U^k, P^{k+1})_h = \frac{1}{\tau} \sum_{k=0}^{N-1} (\nabla U^{k+1} - \nabla U^k, \nabla U^{k+1})$$

$$= \frac{1}{2\tau} \sum_{k=0}^{N-1} \int_\Omega |\nabla U^{k+1}|^2 + |\nabla U^{k+1} - \nabla U^k|^2 - |\nabla U^k|^2 \, dx,$$

and for the elliptic term

$$\sum_{k=0}^{N-1} (M(U^{k+1})\nabla P^{k+1}, \nabla P^{k+1}) = \frac{1}{\tau} \int_0^T (M(U)\nabla P, \nabla P).$$

Hence, multiplying by τ, the stated estimate is established. If we furthermore consider the mass conservation $\int_\Omega U^k = \int_\Omega U^0$, we obtain as a straightforward consequence uniform bounds for the H^1 norm of $U_{\tau h}$ in time.

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Now we will prove a discrete counterpart of the continuous entropy estimate. Let us start with some notation. By $m\colon \mathbb{R} \to \mathbb{R}_0^+$ we denote an approximation of the continuous mobility $\mathcal{M}$ that will be specified later and will involve a constant $A \in \mathbb{R}^+$.

We call a pair of functions $G\colon \mathbb{R} \to \mathbb{R}_0^+$, $M\colon V^h \to \mathbb{R}^{d \times d}$ on $\mathcal{T}_h$ an *admissible entropy-mobility pair with respect to the triangulation* $\mathcal{T}_h$ if the following axioms are satisfied:

(i) $M(U) \in \mathbb{R}^{d \times d}$ is piecewise constant on every $E \in \mathcal{T}_h$, M is continuous, and $M(U)$ is symmetric and positive semidefinite.

(ii) $M(U)|_E = m(U)\mathrm{Id}$ if $U|_E$ is constant.

(iii) $M(U)\nabla \mathcal{I}_h G'(U) = \nabla U$, where $G(s) := \int_A^s g(r)\,\mathrm{d}r$ with $g(s) = \int_A^s m(r)^{-1}\,\mathrm{d}r$.

Let us remark that G is nonnegative and convex by construction.

Based on these assumptions we obtain the following discrete entropy estimate:

Let (U, P) be a solution to the system of Equations (5) and assume that (G, M) is an admissible entropy-mobility pair as described above. Then, for arbitrary $T = K\tau$, $K \in \mathbb{N}$, the following estimate holds:

$$(8) \qquad \int_\Omega \mathcal{I}_h G(U(T, x))\,\mathrm{d}x + \int_\tau^T (P(t, \cdot), P(t, \cdot))_h\,\mathrm{d}t \leqslant \int_\Omega \mathcal{I}_h G(U^0(x))\,\mathrm{d}x.$$

To prove this, we take the function $\mathcal{I}_h G'(U^{k+1})$ as test function in the discrete problem and obtain

$$(\partial_\tau^- U^{k+1}, \mathcal{I}_h G'(U^{k+1}))_h - \int_\Omega M(U^{k+1})\nabla P^{k+1}\nabla \mathcal{I}_h G'(U^{k+1})\,\mathrm{d}x = 0.$$

Using property (i) of admissible entropy-mobility pairs (G, M) as well as property (iii), we get

$$(\partial_\tau^- U^{k+1}, \mathcal{I}_h G'(U^{k+1}))_h + (P^{k+1}, P^{k+1})_h = 0.$$

The convexity of G implies

$$\frac{1}{\tau}\big(G(U^{k+1}(x)) - G(U^k(x))\big) \leqslant \partial_\tau^- U^{k+1}(x)G'(U^{k+1}(x)).$$

Hence, we can estimate

$$\big(\mathcal{I}_h(G(U^{k+1}(x)) - G(U^k(x))), 1\big)_h + \big(P^{k+1}, P^{k+1}\big)_h \leqslant 0.$$

Summing up from $k = 0$ to $K - 1$, multiplying by τ, and using the fact that $(\mathcal{I}_h \eta, 1)_h = \int_\Omega \mathcal{I}_h \eta(x)\,\mathrm{d}x$, we obtain the result.

Finally, we have to convert our abstract assumptions above into a constructive definition of $M(U)$. We restrict ourselves—as already discussed—to elements whose faces form right angles at one vertex. Without any restriction let us assume that T is a simplex in $\mathbb{R}^d$ with corners $x_0 = 0$, $x_i = \alpha_i e_i$ for $i = 1, \ldots, d$ and $\alpha_i \in \mathbb{R}$. Here e_i denotes the i-th unit vector. Applying the notation $U_i = U(x_i)$ and $g = G'$, we now look for a matrix M on T with $M \nabla \mathcal{I}_h g(U) = \nabla U$. Due to

$$g(U_i) - g(U_0) = \int_{U_0}^{U_i} \frac{1}{m(s)} \, \mathrm{d}s$$

we immediately verify that

$$\widehat{M} = (\widehat{M}_{ij})_{i,j=1,\ldots,d} \text{ with } \widehat{M}_{ij} = \left(\fint_{U_0}^{U_i} \frac{1}{m(s)} \, \mathrm{d}s \right)^{-1} \delta_{ij}$$

satisfies our axioms above. For $U_k = U_0$ the definition simplifies to $\widehat{M}_{kk} = m(U_0)$. For the case of translated and rotated simplices T we refer to [25]. Finally, it remains to choose a suitable approximation $m(u)$ of $\mathcal{M}(u)$. E.g., in the case $n \geqslant 1$ we consider $m(u) = m_\sigma(u) := \mathcal{M}(\max(\sigma, u))$, where σ is a small constant. The case $n < 1$ is discussed in [25].

Based on these fundamental discrete a priori estimates, results on non-negativity and convergence of solutions of problem (5) to a solution of the continuous problem (2) can be proved. For details we refer to [25], [26], [18].

5. FINITE VOLUME APPROXIMATION

In contrast to the finite element method presented above, we will now present a finite volume discretization for the complete problem. In particular, we find it instructive to compare them with respect to their qualitative properties.

To begin with, let us assume the computational domain Ω to be polygonally bounded and completely covered by non-degenerate, polygonal finite volume cells $T_i \in \mathcal{T}$ for $i \in \mathcal{I}$ (not necessarily simplices), where I is some index set. The cells are assumed to overlap only at faces and all interior cell faces are shared by exactly two cells. For neighboring cells T_i, T_j (written $j \in \mathcal{N}(i)$), there exists a common edge which we denote by e_{ij}, furthermore $|e_{ij}|$ is its length and $\mathcal{E}$ denotes the set of all edges. Let ν_{ij} be the normal on e_{ij} oriented from T_i to T_j, and let us assume that there is a family of points x_i, one for every cell, such that $\nu_{ij} = (x_j - x_i)/|x_j - x_i|$ for all faces e_{ij}. Finally, let $d_{ij} := |x_j - x_i|$.

In one space dimension, e_{ij} is the common point of two neighboring intervals T_i and T_j, and we set $|e_{ij}| := 1$. The normal $\nu_{ij} = \pm 1$ so that the restriction $\nu_{ij} = (x_j - x_i)/|x_j - x_i|$ holds true for arbitrary choices of the points x_i within T_i.

Let h be the maximum diameter of the cells and τ the time step applied for the discretization of the time interval $[0, T]$ (cf. Section 4). Finite volume functions that are constant on cells and time intervals are denoted again by capital letters $U, P, \ldots$. By writing U_i^k, we mean the constant values of U on the cell T_i in the k-th time step. By V^h we again denote the corresponding discrete function space.

Based on these notational preliminaries we are now able to discretize the thin film flow problem using finite volumes. Here we pick up ideas for the discretization of second order degenerate diffusion problems due to Hilhorst at al. [16] and used in a similar fashion by Mikula and Ramarosy [30] and transfer them to a mixed formulation for the actual fourth order degenerate diffusion problem. Again it will turn out to be essential to replace the continuous mobility $\mathcal{M}$ by a discrete mobility. We integrate both equations of problem (1) over a single cell of a mesh and obtain

$$\int_T \partial_t u = \int_T \operatorname{div}(\mathcal{M}(u)\nabla p) = \int_{\partial T} \mathcal{M}(u)\partial_\nu p,$$
$$\int_T p = -\int_T \Delta u = -\int_{\partial T} \partial_\nu u$$

where ν denotes the outer normal on ∂T and ∂_ν is the corresponding normal derivative. Now, the main question of a finite volume discretization turns out to be that of replacing for suitable discrete fluxes the continuous fluxes $\mathcal{M}(u)\partial_\nu p$ and $\partial_\nu u$ above. At least they should be conservative and again should satisfy a discrete entropy estimate. The discretization of the second equation is straightforward whereas the discrete version of the first equation has to be chosen carefully. On edges e_{ij} shared by two cells T_i, T_j there is no unique height value U. Indeed, on the two sides in general different values U_i and U_j respectively are given. Hence we assume a discrete mobility $M(U_i, U_j)$ to depend on both height values. For the proper choice of $M(\cdot, \cdot)$ see below. Finally, we obtain the following discrete problem:

For given $U^0 \in V^h$ and $k = 0, \ldots, N-1$, find piecewise constant functions $(U^{k+1}, P^{k+1}) \in V^h \times V^h$ such that

$$(9) \qquad \frac{U_i^{k+1} - U_i^k}{\tau} = \frac{1}{|T_i|} \sum_{j \in N(i)} M(U_i^{k+1}, U_j^{k+1}) |e_{ij}| \frac{P_j^{k+1} - P_i^{k+1}}{d_{ij}},$$

$$(10) \qquad P_i^{k+1} = -\frac{1}{|T_i|} \sum_{j \in N(i)} |e_{ij}| \frac{U_j^{k+1} - U_i^{k+1}}{d_{ij}}.$$

Existence of discrete solutions.

In each time step again a system of nonlinear equations has to be solved. The nonlinearity is given by the nonlinear mobility term $M(\cdot, \cdot)$. The problem can be

reformulated in terms of a mass matrix M_h and stiffness matrices L_h and $L_h(U)$ similar to (3), (4), and (7). Furthermore let us already assume $M(U_i, U_j) \geqslant 0$. Then the proof of existence of discrete solutions is fairly identical to the one for the finite element approximation. Thus we omit it here and refer to [24].

A priori estimates.

As in the finite element setting we are able to prove certain a priori estimates that especially allow to derive results on discrete non-negativity and on convergence. The discrete energy estimate now reads as follows: Let U and P be a solution of the finite volume scheme. Then

$$(11) \quad \sum_{e_{ij} \in \mathcal{E}} \frac{|e_{ij}|}{d_{ij}} (U_j^N - U_i^N)^2 + \sum_{k=0}^{N-1} \sum_{e_{ij} \in \mathcal{E}} \frac{|e_{ij}|}{d_{ij}} ((U_j^{k+1} - U_i^{k+1}) - (U_j^k - U_i^k))^2$$
$$+ 2\tau \sum_{k=0}^{N-1} \sum_{e_{ij} \in \mathcal{E}} M(U_i^{k+1}, U_j^{k+1}) \frac{|e_{ij}|}{d_{ij}} (P_j^{k+1} - P_i^{k+1})^2$$
$$= \sum_{e_{ij} \in \mathcal{E}} \frac{|e_{ij}|}{d_{ij}} (U_j^0 - U_i^0)^2.$$

The different terms of this equation correspond exactly to those in the finite element energy estimate. The proof is straightforward following the advice given above in Section 4 and in [16] and is thus left to the reader.

To formulate an entropy estimate, we need a suitable definition of entropy mobility pairs now in the case of a finite volume scheme:

Assume that m is a (continuous, non-negative) approximation of $\mathcal{M}$ and $A \in \mathbb{R}^+$ (cf. Section 4). Then functions $G \colon \mathbb{R} \to \mathbb{R}_0^+$ and $M \colon \mathbb{R}^2 \to \mathbb{R}_0^+$ are called an *admissible entropy-mobility pair* iff

(i) M is continuous and symmetric with respect to its two arguments;
(ii) $M(U, U) = m(U)$;
(iii) $M(U_i, U_j)(G'(U_j) - G'(U_i)) = U_j - U_i$, where $G(s) := \int_A^s g(r)$ and $g(s) = \int_A^s m(r)^{-1}$.

These assumptions are satisfied if we choose M as the harmonic integral mean of the continuous mobility $\mathcal{M}$ on the interval $[U_i, U_j]$ (which is in clear correspondence to the construction in the case of finite elements (cf. Section 4)):

$$M(U_i, U_j) = \begin{cases} \left(\fint_{U_i}^{U_j} \frac{1}{m(r)} \, \mathrm{d}r \right)^{-1} & \text{if } U_i \neq U_j \\ m(U_i) & \text{if } U_i = U_j. \end{cases}$$

We obtain a discrete entropy estimate. Let (G, M) be an admissible entropy-mobility pair. Then the following inequality holds:

$$(12) \qquad \int_\Omega G(U^N) + \tau \sum_{k=1}^N \int_\Omega (P^k)^2 \leqslant \int_\Omega G(U^0).$$

To prove this, we start with Equation (9) of our finite volume scheme and test with $G'(U^{k+1})$, i.e. we multiply by $G'(U_i^{k+1})$ and sum over i for all cells:

$$\sum_{i \in \mathcal{I}} |T_i|(U_i^{k+1} - U_i^k)G'(U_i^{k+1})$$

$$= \tau \sum_{i \in \mathcal{I}} \sum_{j \in N(i)} M(U_i^{k+1}, U_j^{k+1})\frac{|e_{ij}|}{d_{ij}}(P_j^{k+1} - P_i^{k+1})G'(U_i^{k+1}).$$

Let us emphasize that each face e_{ij} appears twice on the right-hand side. With the convention that $\mathcal{E}$ contains each side only once, we can write

$$\sum_{k=0}^{N-1} \sum_{i \in \mathcal{I}} |T_i|(U_i^{k+1} - U_i^k)G'(U_i^{k+1})$$

$$= \tau \sum_{k=0}^{N-1} \sum_{e_{ij} \in \mathcal{E}} M(U_i^{k+1}, U_j^{k+1})\frac{|e_{ij}|}{d_{ij}}(P_j^{k+1} - P_i^{k+1})(G'(U_i^{k+1}) - G'(U_j^{k+1})).$$

Applying the convexity of G (on the left-hand side) and the entropy-mobility property (iii) (on the right-hand side) we obtain

$$\sum_{k=0}^{N-1} \sum_{i \in \mathcal{I}} |T_i|(G(U_i^{k+1}) - G(U_i^k)) \leqslant \tau \sum_{k=0}^{N-1} \sum_{e_{ij} \in \mathcal{E}} \frac{|e_{ij}|}{d_{ij}}(P_j^{k+1} - P_i^{k+1})(U_i^{k+1} - U_j^{k+1}).$$

The left-hand side simplifies further by telescopic summation, while we transform the summation on the right-hand side to a summation over cells:

$$\sum_{i \in \mathcal{I}} |T_i|G(U_i^N) - \sum_{i \in \mathcal{I}} |T_i|G(U_i^0) \leqslant -\tau \sum_{k=0}^{N-1} \sum_{i \in \mathcal{I}} \sum_{j \in N(i)} \frac{|e_{ij}|}{d_{ij}}P_i^{k+1}(U_i^{k+1} - U_j^{k+1}).$$

Inserting Equation (10) into the right-hand side the statement is established.

As in the case of a finite element scheme, from these inequalities one can derive results on discrete non-negativity and on convergence (at least for $d = 1$). For details we refer to [29].

6. Additional potential terms

In physical applications the evolution of viscous thin films is not only influenced by surface tension as the main driving force but is governed by various physical effects such as gravity, intermolecular forces, thermocapillarity, evaporation and condensation. This leads to generalized models for the evolution of the film height u and a now generalized pressure p: Find a pair of functions $u, p \colon \Omega \times (0, T) \to \mathbb{R}$ where Ω is a domain in $\mathbb{R}^d$ $(d = 1, 2)$ such that

$$
\begin{aligned}
\partial_t u - \operatorname{div}(\mathcal{M}(u)\nabla p) &= f(u) && \text{in } \Omega \times (0, T), \\
p &= -\Delta u + w'(u) && \text{in } \Omega \times (0, T), \\
\frac{\partial}{\partial \nu} u = \frac{\partial}{\partial \nu} p &= 0 && \text{on } \partial\Omega \times (0, T), \\
u(0, \cdot) &= u_0(\cdot) && \text{in } \Omega.
\end{aligned} \tag{13}
$$

The generalized pressure $p := -\Delta u + w'(u)$ is given as the sum of a capillarity term and an additional nonlinearity $w'(u)$ which is to model various physical effects. In many cases of interest, it will be singular at $u = 0$. Via the source-term $f(u)$, effects of evaporation or condensation can be described.

Gravity.

Let us now simulate the evolution of a thin film below a horizontal plane and subject to gravity. We follow [31], and in dimensionless form, we consider the evolution equation for the film height

$$
\partial_t u + \operatorname{div}(u^2 \nabla(\Delta u + c_1 u)) = 0
$$

with a positive constant c_1 which refers to gravity. Choosing the domain $\Omega = [-1, 1]^2$ and $c_1 = 200$, we find with a resolution of 129^2 gridpoints, see Fig. 3. As initial data we take a slightly corrugated film of height 1, namely

$$
u_0(x_1, x_2) = \big(1 + 0.005\sin(50(x_1 - 0.4)^2)\big)\big(1 + 0.0005\sin(50(x_2 + 0.4)^2)\big).
$$

During the evolution, the film splits into various droplets of different magnitude.

Thermocapillarity.

The second example is devoted to film instabilities due to thermocapillarity. A. Oron, S. H. Davis and S. G. Bankoff suggested in [31] the additional potential term
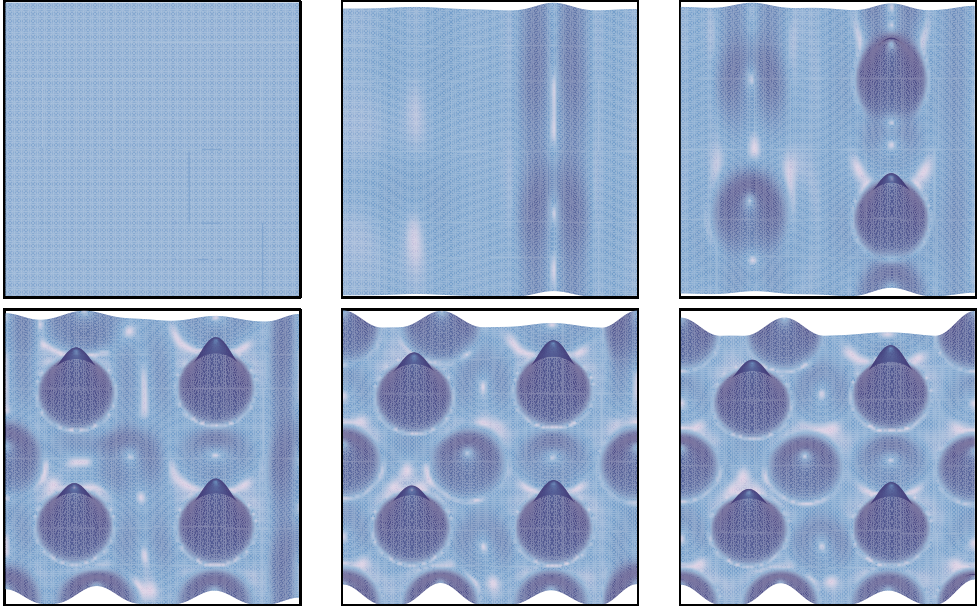
$$
w'(u) = -c_2 \log u.
$$

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Figure 3. Droplet formation due to gravity effects; snapshots at times $t = 0.0, 8.0, 12.0, 22.0, 32.0, 44.0$.

We use in the implementation a linear C^1-continuation for values $u < 10^{-6}$, set $c_2 = 1$, $\Omega = [0, 20]^2$ and start again with a slightly perturbed flat film of height 1. Fig. 4 shows snapshots of the beginning of droplet formation.

Evaporation and condensation.

If we intend to incorporate also effects of evaporation and condensation into our model, mass is no longer preserved. As a consequence, the right-hand side $Q(\cdot)$ cannot be chosen identically zero any longer. Instead, we obtain

$$f(u) = -\frac{1}{u + c} \, \chi_{[u > 0]}$$

in the case of an evaporating film, and

$$f(u) = \frac{1}{u + c}$$

in the case of condensation. Numerically we have to evaluate this right-hand side implicitly. Fig. 5 and 6 show evaporation and condensation of a thin film subject to van-der-Waals forces, which can be modelled by the term (cf. [31])

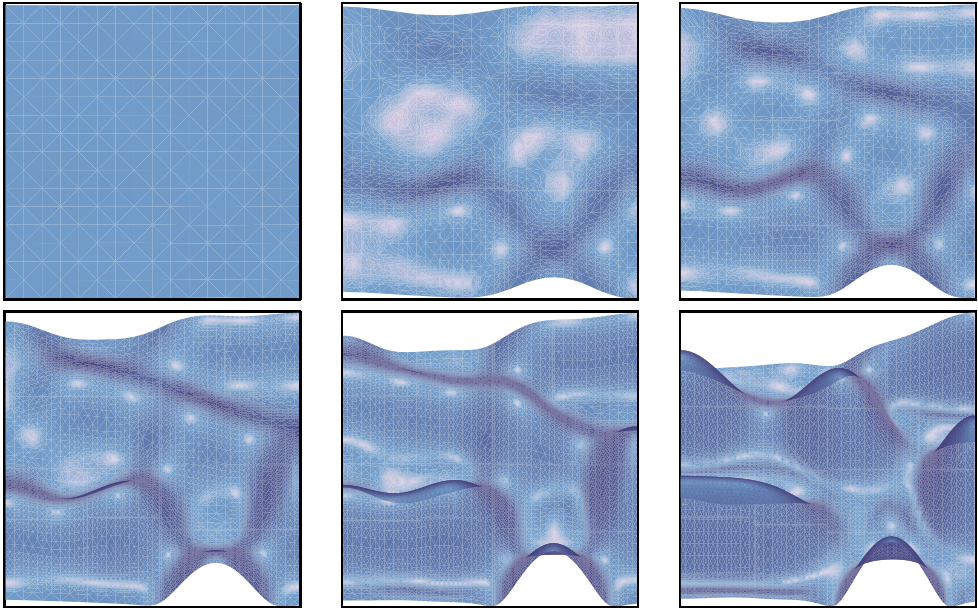$$w'(u) = c_3 u^{-3} - c_4 u^{-4}.$$

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Figure 4. Film instabilities due to thermocapillarity. The series shows timesteps $t = 12.3$, 29.3, 32.4, 35.1, 39.3 and 46.3.
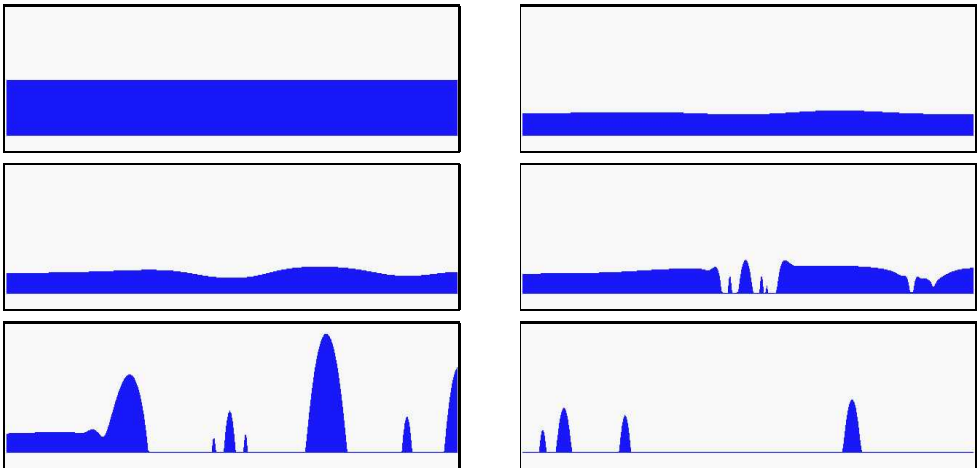

Figure 5. From left to right and from top to bottom: Evolution of a thin film and droplet formation due to evaporation ($t = 0.0$, 10.0, 10.35, 10.46, 10.52, 14.0).

In both cases this potential causes the initially flat, slightly disturbed film to rupture. In the case of evaporation the remaining droplets disappear with time, whereas in the case of condensation the remaining droplets grow larger and larger.
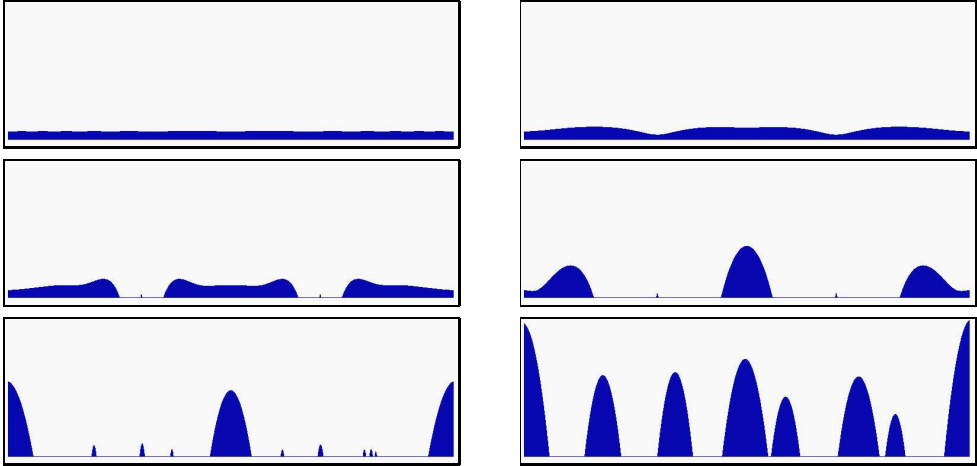
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Figure 6. From left to right and from top to bottom: Evolution of a thin film undergoing successive condensation ($t = 0.0, 0.54, 0.545, 0.55, 0.6, 3.2$).

Numerical approximation.

Let us assume that $w \in C^1(\mathbb{R}; \mathbb{R}_0^+)$ can be decomposed into a sum

$$w(u) = w_+(u) + w_-(u)$$

with $w_+ \in C^1(\mathbb{R}; \mathbb{R}_0^+)$ convex and $w_- \in C^1(\mathbb{R})$ concave.

Then an implicit backward Euler finite element discretization scheme for Equation (13) reads as follows (cf. Equation (5)):

For given $U^0 \in V^h$ and $k = 0, \ldots, N - 1$, find functions $(U^{k+1}, P^{k+1}) \in V^h \times V^h$ such that

(14)
$$(\partial_\tau^- U^{k+1}, \Theta)_h + (M(U^{k+1}) \nabla P^{k+1}, \nabla \Theta) = 0,$$
$$(\nabla U^{k+1}, \nabla \Psi) + (w_+'(U^{k+1}), \Psi)_h + (w_-'(U^k), \Psi)_h = (P^{k+1}, \Psi)_h$$

for all $\Theta, \Psi \in V^h$.

Here we refer to the notation introduced in Section 4. First, let us explain the implementation of the algorithm.

In each timestep, set $\overline{U}_0^{k+1} = \overline{U}^k$ and for $i = 0, 1, \ldots$ find vectors $\overline{U}_{i+1}^{k+1}$ satisfying

$$B(\overline{U}_{i+1}^{k+1}) = M_h(\overline{U}_{i+1}^{k+1} - \overline{U}^k) + \tau_k L_h(\overline{U}_i^{k+1})(M_h^{-1} L_h \overline{U}_{i+1}^{k+1} + w_+'(\overline{U}_{i+1}^{k+1}) + w_-'(\overline{U}^k)) = 0.$$

We apply Newton's method to solve this semi-implicit equation, and we obtain a sequence $(\overline{U}_i^{k+1})_{i=0,1,\ldots}$ of approximate solutions to the fully implicit problem. In each Newton step one has to solve a linear system similar to the one discussed in

Section 4 for Equation (5). Due to the monotonicity of $w'_+(\cdot)$ the existence proof in Section 4 can easily be generalized to prove existence for the generalized model presented here.

Furthermore, the following a priori estimate holds:

$$\frac{1}{2}\int_\Omega |\nabla U^N(x)|^2\,\mathrm{d}x + \int_\Omega \mathcal{I}_h w(U^N)\,\mathrm{d}x + \int_0^T \int_\Omega M(U)|\nabla P|^2\,\mathrm{d}x\,\mathrm{d}t$$

$$+ \frac{\tau}{2}\sum_{i=0}^{N-1}\int_\Omega |\nabla(U^{i+1}(x) - U^i(x))|^2\,\mathrm{d}x$$

$$\leqslant \frac{1}{2}\int_\Omega |\nabla U^0(x)|^2\,\mathrm{d}x + \int_\Omega \mathcal{I}_h w(U^0)\,\mathrm{d}x.$$

In particular, if for initial data U^0 the quantities $\|U^0\|_1^2 + \int_\Omega \mathcal{I}_h w(U^0)$ are uniformly bounded as h tends to zero, then U and $M(U)|\nabla P|^2$ are uniformly bounded in $L^\infty((0,T);H^1(\Omega))$ and $L^1((0,T)\times\Omega))$, respectively, by a constant C that is independent of the discretization parameters.

The proof follows the lines of the corresponding one for the simplified model. However, the decomposition of $w'(\cdot)$ into $w'_+(\cdot)$ and $w'_-(\cdot)$ is crucial to control the physical energy at later stages of the evolution by the initial energy.

Similarly, one succeeds in proving generalizations of the entropy estimate. For the derivation and the consequences of these estimates, we refer the reader to [18].

7. Nonlinear surface tension term

In Section 2 we have derived a model which takes into acount the curvature of the free boundary between gas and liquid described by the graph of u. Frequently this is being simplified via a linearization and we replace the curvature $-\operatorname{div}\bigl(\nabla u/\sqrt{1+|\nabla u|^2}\bigr)$ by $-\Delta u$. The results given above can be generalized to the case of surface tension proportional to the mean curvature on the interface. We consider the problem

$$\partial_t u - \operatorname{div}(m(u)\nabla p) = 0,$$

$$p = -\operatorname{div}\left(\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right)$$

with initial conditions $u = u_0$ as before.

Numerical Approximation.

A finite element algorithm then consists of a sequence of fully implicit timesteps, where in each step a nonlinear system of equations has to be considered. In the

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implementation we proceed similarly to the scheme discussed in Section 6. I.e., we have to find $U^{k+1}, P^{k+1} \in V^h$ such that

$$(\partial_\tau^- U^{k+1}, \Theta)_h + (M(U^{k+1})\nabla P^{k+1}, \nabla\Theta) = 0,$$

$$(P^{k+1}, \Psi)_h = \left(\frac{\nabla U^{k+1}}{\sqrt{1 + |\nabla U^{k+1}|^2}}, \nabla\Psi\right)$$

for all $\Theta, \Psi \in V^h$ and $k = 1, \ldots$. Again by a fixed-point argument one can prove existence of discrete solutions. For a discrete solution (U, P) the following energy estimate holds true:

$$\int_\Omega \sqrt{1 + |\nabla U^N|^2} + \int_\Omega \int_0^T M(U)|\nabla P|^2 \leqslant \int_\Omega \sqrt{1 + |\nabla U^0|^2}.$$

Furthermore, let (G, M) be an admissible entropy-mobility pair as in Section 4, then at least for $d = 1$ one can prove the following entropy estimate:

$$\int_\Omega \mathcal{I}_h G(U^N) \leqslant \int_\Omega \mathcal{I}_h G(U^0).$$

For details we refer to [3] and the forthcoming paper [4].

8. SURFACTANT DRIVEN FLOW

Finally, let us have a look at a certain PDE system extending Equation (1). Thus, we consider a surfactant (SURFace ACTive AgenNT), a chemical agent that accumulates as a mainly mono-molecular layer at the surface of a liquid and influences its surface tension and thereby its spreading behavior. Applications of surfactant-covered thin films range from medicine (the liquid lining of the human lung) to modern coating technology (e.g. aircraft anti-icing films). The evolution of a thin film which bears a surfactant monolayer at the liquid-gas interface can be described by a system of convection diffusion equations

$$\partial_t u + \frac{1}{3}\mathcal{S}\operatorname{div}(u^3\nabla\Delta u) - \frac{1}{2}\operatorname{div}(u^2\nabla w) = 0,$$

$$\partial_t w + \frac{1}{2}\mathcal{S}\operatorname{div}(u^2 w\nabla\Delta u) - \operatorname{div}(uw\nabla w) - \mathcal{D}\Delta w = 0.$$

Here u denotes the height of the film and w represents the concentration of the surfactant at the surface of the fluid.

The first equation results from a lubrication approximation similar to the one in Section 2, where the additional (first-order) term is generated by the inclusion of

tangential stresses at the gas-liquid interface that are due to surface tension gradients (*Marangoni effect*).

The mobility is assumed to be of the form $\mathcal{M}(u) = u^3$, i.e. we premise a *no-slip* boundary condition at the bottom of the film. We call $\mathcal{S}$ the (scaled) capillarity number that indicates the relative magnitude of the two effects governing the height of the film.

Simultaneously, the evolution of the surfactant concentration on the surface of the film is influenced by two effects: the transport by the fluid's horizontal velocity and the surface diffusion. Here $\mathcal{D}$ is the inverse Péclet number.

In literature (cf. [27]), the convective term usually has the form

$$+\frac{1}{2}\operatorname{div}(u^2\nabla\sigma(w)),$$

where σ is the surfactant concentration dependent on the surface tension. Here we assume that w as well as σ are scaled to the interval $[0, 1]$ and use the linearization $\sigma(w) = 1 - w$ that entails the equation given above.

Numerical approximation.

We will now extend the finite volume scheme from Section 5 to a method for this system of equations. Let us especially focus on the time discretization. Here we apply a natural operator splitting: We isolate the horizontal velocity v (cf. Section 2) from the second equation, and split each of the remaining equations as follows—indices $i + 0.5$ indicate in the usual way an intermediate time step of the splitting scheme:

(15) $$(u_{i+0.5} - u_i)/\tau_i = \frac{1}{2}\operatorname{div}(u_i^2\nabla w_i),$$

(16) $$(u_{i+1} - u_{i+0.5})/\tau_i = -\frac{1}{3}\mathcal{S}\operatorname{div}(u_{i+1}^3\nabla\Delta u_{i+1}),$$

(17) $$v_{i+1} = \frac{1}{2}\mathcal{S}u_{i+1}^2\nabla\Delta u_{i+1} - u_{i+1}\nabla w_i,$$

(18) $$(w_{i+0.5} - w_i)/\tau_i = -\operatorname{div}(v_{i+1}w_i),$$

(19) $$(w_{i+1} - w_{i+0.5})/\tau_i = \mathcal{D}\Delta w_{i+1}.$$

The terms involving higher order derivatives are all computed with an implicit method, while the first-order terms can be treated explicitly. Let us now inspect more closely the separate steps of the splitting scheme proposed and their physical meaning:

(15) Marangoni Flow: The flow of the film that is induced by surface tension gradients. Our method is especially designed for convection dominated problems, i.e. where $\mathcal{S}$ and $\mathcal{D}$ are very small. In order to reduce the numerical damping, which

might even artificially superpose the effects of the parabolic parts, it turns out to be indispensable to use a higher order scheme where possible. We consider the Engquist-Osher up-winding method from [15]. The values on cell faces from both sides (which are required for the evaluation of the numerical flux) are extrapolated linearly from the given (constant) values in the usual neighborhood. To avoid oscillations, a minmod limiter function is applied. For an overview on these methods in general we refer to [28].

(16) Thin Film Flow: The thin film flow (induced by surface tensions absolute values) is treated as described in Section 5 above, except that we take into account explicit terms on the right hand side of the equation.

(17) Velocity: The horizontal velocity is computed explicitly from values known so far.

(18) Surfactant Transport: The surfactant is transported linearly with the velocity computed in the previous step. This term is treated with the same up-winding scheme as used in step 15.

(19) Surface Diffusion: The surfactant diffusion step is computed by a plain finite volume scheme. For the discretization of the Laplacian, cf. the treatment of the pressure equation in Section 5.

Numerical results.

The scheme described above has been implemented so far for problems in one space dimension.
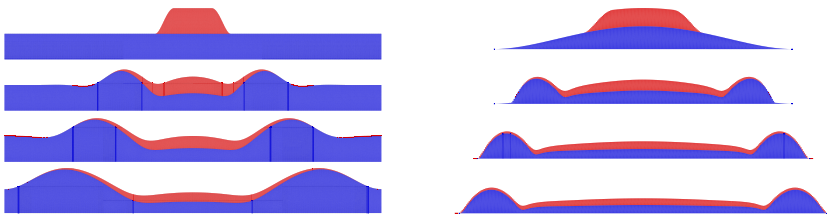

Figure 7. Numerical results for the surfactant driven thin film flow in one space dimension.

Fig. 7 depicts two characteristic simulations that have been computed with the described scheme. On the left-hand side, we see the evolution of a film of initially constant thickness after a drop of surfactant has been applied. The large surface tension gradients at the boundary of the surfactant droplet give rise to Marangoni forces which initiate the motion of the liquid and the spreading of the surfactant monolayer. To ensure better visibility we apply a scaling of the film height and especially of the surfactant concentration graph drawn on top of the thin film graph. On the right-hand side, we consider an initial configuration with a surfactant on

top of a compactly supported thin film. Note how, after the Marangoni flow has reached the boundary of the film, it causes the film's support to spread, which is remarkable because the film is expected not to spread in the absence of a surfactant. Furthermore, the method has been tested on the similarity solution given in [27] for $\mathcal{S} = \mathcal{D} = 0$.

References

[1] *J. W. Barrett, J. F. Blowey and H. Garcke*: Finite element approximation of a fourth order nonlinear degenerate parabolic equation. Numer. Math. *80* (1998), 525–556.

[2] *J. W. Barrett, J. F. Blowey and H. Garcke*: On fully practical finite element approximations of degenerate Cahn-Hilliard systems. Math. Model. Num. Anal. *35* (2001), 713–748.

[3] *J. Becker*: Finite-Elemente-Verfahren zur Dünne-Filme-Gleichung mit nichtlinearem Oberflächenspannungsterm. Diplomarbeit. Universität Bonn, 2000.

[4] *J. Becker, G. Grün*: Numerical schemes for the thin film equation with nonlinear surface tension term. In preparation.

[5] *E. Beretta, M. Bertsch and R. Dal Passo*: Nonnegative solutions of a fourth order nonlinear degenerate parabolic equation. Arch. Rational Mech. Anal. *129* (1995), 175–20.

[6] *F. Bernis*: Viscous flows, fourth order nonlinear degenerate parabolic equations and singular elliptic problems. Free Boundary Problems: Theory and Applications. Pitman Research Notes in Mathematics 323 (J. I. Diaz, M. A. Herrero, A. Linan and J. L. Vazquez, eds.). Longman, Harlow, 1995, pp. 40–56.

[7] *F. Bernis*: Finite speed of propagation and continuity of the interface for thin viscous flows. Adv. Differential Equations *1* (1996), 337–368.

[8] *F. Bernis*: Finite speed of propagation for thin viscous flows when $2 \leqslant n < 3$. C. R. Acad. Sci. Paris Sér. I Math. *322* (1996), 1169–1174.

[9] *F. Bernis, A. Friedman*: Higher order nonlinear degenerate parabolic equations. J. Differential Equations *83* (1990), 179–206.

[10] *A. L. Bertozzi, M. Pugh*: The lubrication approximation for thin viscous films: Regularity and long time behaviour of weak solutions. Nonlin. Anal. *18* (1992), 217–234.

[11] *M. Bertsch, R. Dal Passo, H. Garcke and G. Grün*: The thin viscous flow equation in higher space dimensions. Adv. Differential Equ. *3* (1998), 417–440.

[12] *Ph. G. Ciarlet*: The Finite Element Method for Elliptic Problems. North Holland, Amsterdam, 1978.

[13] *R. Dal Passo, H. Garcke and G. Grün*: On a fourth order degenerate parabolic equation: global entropy estimates and qualitative behaviour of solutions. SIAM J. Math. Anal. *29* (1998), 321–342.

[14] *C. M. Elliott, H. Garcke*: On the Cahn-Hilliard equation with degenerate mobility. SIAM J. Math. Anal. *27* (1996), 404–423.

[15] *B. Engquist, S. Osher*: One-sided difference approximations for nonlinear conservation laws. Math. Comp. *31* (1981), 321–351.

[16] *R. Eymard, M. Gutnic and D. Hilhorst*: The finite volume method for the Richards equation. Computational Geosciences *3* (1999).

[17] *L. Giacomelli, F. Otto*: Droplet spreading: intermediate scaling law by pde methods. Comm. Pure Appl. Math. *55* (2002), 217–254.

[18] *G. Grün*: On the convergence of entropy consistent schemes for lubrication type equations in multiple space dimensions. Math. Comp. To appear.

[19] *G. Grün*: Degenerate parabolic equations of fourth order and a plasticity model with nonlocal hardening. Z. Anal. Anwendungen *14* (1995), 541–573.

[20] *G. Grün*: On free boundary problems arising in thin film flow. Habilitationsschrift. Universität Bonn, 2001.

[21] *G. Grün*: Droplet spreading under weak slippage: the optimal asymptotic propagation rate in the multi-dimensional case. Interfaces and Free Boundaries *4* (2002), 309–323.

[22] *G. Grün*: Droplet spreading under weak slippage: a basic result on finite speed of propagation. Submitted.

[23] *G. Grün*: On the numerical simulation of wetting phenomena. In: Proceedings of the 15th GAMM-Seminar Kiel, Numerical Methods of Composite Materials (W. Hackbusch, S. Sauter, eds.). Vieweg-Verlag, Braunschweig. To appear.

[24] *G. Grün, M. Lenz, M. Rumpf*: A finite volume scheme for surfactant driven thin film flow. Finite volumes for complex applications III (R. Herbin, D. Kröner, eds.). Hermes Penton Sciences, 2002, pp. 567–574.

[25] *G. Grün, M. Rumpf*: Nonnegativity preserving convergent schemes for the thin film equation. Numer. Math. *87* (2000), 113–152.

[26] *G. Grün, M. Rumpf*: Simulation of singularities and instabilities arising in thin film flow. European J. Appl. Math. *12* (2001), 293–320.

[27] *O. E. Jensen, J. B. Grotberg*: Insoluble surfactant spreading on a thin viscous film: shock evolution and film rupture. J. Fluid Mech. *240* (1992), 259–288.

[28] *D. Kröner*: Numerical Schemes for Conservation Laws. Willey-Teubner Series Advances in Numerical Mathematics. Willey-Teubner, Chichester-Stuttgart, 1997.

[29] *M. Lenz*: Finite Volumen Methoden für degenerierte parabolische Systeme—Ausbreitung eines Surfactant auf einem dünnen Flüssigkeitsfilm. Diplomarbeit. Universität Bonn, 2002.

[30] *K. Mikula, N. Ramarosy*: Semi-implicit finite volume scheme for solving nonlinear diffusion equations in image processing. Numer. Math. *89* (2001), 561–590.

[31] *A. Oron, S. H. Davis and S. G. Bankoff*: Long-scale evolution of thin liquid films. Rev. of Mod. Phys. *69* (1997), 931–980.

[32] *L. Zhornitskaya, A. L. Bertozzi*: Positivity preserving numerical schemes for lubrication-type equations. SIAM J. Numer. Anal. *37* (2000), 523–555.

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