

A low-order approximation for viscous-capillary phase transition dynamics

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Abstract. The dynamics of an elastic bar that appears in two phases can be described by viscosity-capillarity models. They contain numerically complicated third-order or fully nonlocal terms to account for surface energies. Based on work of Solci&Vitali [20] we analyze an alternative modelling approach that does not involve third-order differential operators. It is proven that solutions of the new model tend to solutions of the classical viscosity-capillarity model provided a so-called coupling parameter tends to infinity.

Numerical experiments illustrate our findings. In fact it is shown that the new model provides a reliable and efficient approach to compute approximate solutions for the classical viscosity-capillarity model.

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1. Introduction

We consider the longitudinal dynamics of an elastic bar that can appear in two phases, i.e. a high-strain and a low strain phase. The reference configuration is supposed to be the interval $\Omega = [0, l]$, $l > 0$. Let us denote by $w : \Omega \times (0, \infty) \rightarrow \mathbb{R}$ the strain and by $v : \Omega \times (0, \infty) \rightarrow \mathbb{R}$ the velocity. Let $W \in C^2(\mathbb{R})$ be a double-well function. Without (too much) loss of generality we simply choose for some $\beta > 0$ the form

$$W(w) = \frac{1}{4}(w^2 - \beta^2)^2, \quad (1.1)$$

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such that W has two minima in $\pm\beta$. The strain values in the intervals $(-\infty, -\beta/\sqrt{3}]$ and $[\beta/\sqrt{3}, \infty)$ correspond to convex branches of W , and are called the *low strain phase* and *high strain phase*, respectively. The interval $(-\beta/\sqrt{3}, \beta/\sqrt{3})$ where W is concave, is called *elliptic*.

For an isothermal setting the classical Ericksen model describing two-phase materials is given through

$$\begin{aligned} w_t - v_x &= 0, \\ v_t - \sigma(w)_x &= 0. \end{aligned} \tag{1.2}$$

Here $\sigma = W'$ is the stress-strain relation. Note that (1.2) is a mixed type hyperbolic-elliptic system of conservation laws. The eigenvalues of the Jacobian $(-v, -\sigma(w))^T$ of the flux are

$$\lambda_1(w, v) = -\sqrt{\sigma'(w)}, \quad \lambda_2(w, v) = \sqrt{\sigma'(w)}, \tag{1.3}$$

which are real numbers if and only if $w \notin (-\beta/\sqrt{3}, \beta/\sqrt{3})$.

Dynamic phase boundaries can be interpreted as shock waves. However, it is well-known that standard entropy criteria cannot ensure the uniqueness of weak solutions for initial-boundary value problems for (1.2) if subsonic phase boundaries are involved. We refer to [1], [7], [13], [21] and references therein for details and the solution concept of kinetic relations. This approach will not be followed here further.

Rather we detect unique solutions of (1.2) as limits of regularizations for (1.2). A classical approach in this framework is the classical viscosity-capillarity regularization [12], [18] given through

$$\begin{aligned} w_t - v_x &= 0, \\ v_t - \sigma(w)_x &= \mu v_{xx} - \lambda w_{xxx}. \end{aligned} \tag{1.4}$$

By μ and $\lambda > 0$ we denote the given positive viscosity parameter and the capillarity parameter, respectively. The model has been analyzed in [2]. In particular Slemrod shows in [19] that (1.4) allows for moving travelling wave solutions that connect states in different phases. If we scale $\mu = \varepsilon$ and $\lambda = \varepsilon^2 \bar{\lambda}$ for some $\bar{\lambda} > 0$ solutions of (1.4) are expected to converge for $\varepsilon \rightarrow 0$ to weak solutions of (1.2) (see [12] for a rigorous result). The limit weak solution depends crucially on $\bar{\lambda}$ and contains subsonic phase boundaries.

Smooth solutions of appropriate initial-boundary value problems for (1.4) dissipate the energy

$$E^\infty[w(\cdot, t), v(\cdot, t)] = \int_\Omega \frac{(v(x, t))^2}{2} + W(w(x, t)) + \frac{\lambda}{2} (w_x(x, t))^2 \, dx. \tag{1.5}$$

In the static case E^∞ reduces to the Van-der-Waals like functional

$$F^\infty[w] = \int_{\Omega} W(w(x)) + \frac{\lambda}{2} (w_x(x))^2 dx. \tag{1.6}$$

The associated minimization problem under the constant volume constraint has been studied in [4] where in particular the existence of two-phase minimizers is verified for appropriate choice of total mass.

The Van-der-Waals functional has been criticized as it introduces a non-physical derivative on the strain. To avoid derivatives the following static minimization problem for the functional

$$F^\alpha[w^\alpha, p^\alpha] = \int_{\Omega} W(w^\alpha(x)) + \frac{\alpha}{2} (w^\alpha(x) - p^\alpha(x))^2 + \frac{\lambda}{2} (p_x^\alpha(x))^2 dx \tag{1.7}$$

has been analyzed in [3], [20]. Here $\alpha > 0$ is a positive *coupling parameter* and an additional unknown p^α has been introduced. Note that in (1.7) no strain derivative appears.

In this paper we study a dynamical model that is associated with the static energy F^α in (1.7) as the viscosity-capillarity model is connected to the Van-der-Waals functional F^∞ . Precisely, we introduce the system

$$\begin{aligned} w_t^\alpha - v_x^\alpha &= 0, \\ v_t^\alpha - \sigma(w^\alpha)_x &= \mu w_{xx}^\alpha - \alpha(p^\alpha - w^\alpha)_x, \\ \lambda p_{xx}^\alpha &= \alpha(p^\alpha - w^\alpha). \end{aligned} \tag{1.8}$$

The system (1.8) contains in addition to the strain w^α and the velocity v^α the unknown function $p^\alpha : \Omega \times (0, \infty) \rightarrow \mathbb{R}$, which satisfies an elliptic equation.

As will be proven below in Section 3 smooth solutions of appropriate initial-boundary value problems for (1.8) lead to the dissipation of the energy functional

$$\begin{aligned} E^\alpha[w^\alpha(\cdot, t), v^\alpha(\cdot, t), p^\alpha(\cdot, t)] &= \int_{\Omega} \frac{(v^\alpha(x, t))^2}{2} + W(w^\alpha(x, t)) \\ &\quad + \frac{\alpha}{2} (w^\alpha(x, t) - p^\alpha(x, t))^2 + \frac{\lambda}{2} (p_x^\alpha(x, t))^2 dx. \end{aligned} \tag{1.9}$$

We point out that (a variant of) the model (1.8) has been suggested in [15] in the framework of modelling the evolution of microstructure. It can also be seen as a nonlocal viscosity-capillarity model with specific kernel (cf. [16]).

Let us give an outline of this paper’s contributions. In Section 2 we derive the model (1.8) using the theory of internal variables [6], [22]. In passing let us

note that the derivation shows that the inverse of the coupling parameter α can be understood also as a measure for the amount of long-range interaction in the bar.

In the next step we will show in Section 3 by semigroup theory that appropriate initial-boundary value problems for (1.8) have unique strong solutions on the time interval $[0, T]$ for any $T > 0$. The result is proven in Theorem 3.2 and relies crucially on the energy inequality for E^α in (1.9).

Then we study as the main analytical contribution for a sequence of solutions for the low order approximation (1.8) the *capillarity limit* $\alpha \rightarrow \infty$. It is found out that the limit exists and corresponds to a weak solution of the viscosity-capillarity problem (1.4) (see Theorem 4). A similar capillarity limit has been analyzed in [8] for a scalar model problem. Moreover, we note that our study of the limit regime $\alpha \rightarrow \infty$ is motivated by the analysis of Solci&Vitali [20] for a sequence of minimizers of (1.7). Solci&Vitali have shown that this sequence converges in the sense of Γ -limits to a minimizer of the Van-der-Waals functional in (1.6) if α tends to infinity.

While the model (1.8) might have its own physical meaning, we see it also as a tool in numerics. The numerical solution of (1.4) and even more its multidimensional generalizations are quite intricate and computationally expensive. Realistic parameters μ and λ are extremely small such that the hyperbolic-elliptic operator as in (1.2) dominates. As a consequence fully explicit schemes are used, which give severe restrictions on the time step in view of the third-order term w_{xxx} . A second problem of (1.4) is the fact that the mixed hyperbolic-elliptic nature of (1.4) excludes any modern flux discretization as e.g. approximate Riemann solvers. The latter ones require hyperbolicity in the complete state space. Based on our convergence result for $\alpha \rightarrow \infty$ it makes sense to view solutions of (1.8) as approximations of solutions for (1.4). We will present in Section 5 that the solution of (1.7) for large α can be a more efficient way to solve (1.4) numerically as discretizing (1.4) directly. Finally, we show by one numerical example that the low-order approximation (1.8) can be easily generalised to multiple space dimensions.

2. Thermodynamical derivation and an internal length scale

Our motivation to consider the system (1.4) is mainly a numerical one: numerical methods based on (1.8) can lead to a more efficient computation of approximate solutions of (1.4). Nevertheless it is possible to derive (1.8) in the framework of rational thermodynamics such that the use of p can be interpreted as introducing a new length scale into viscosity-capillarity models.

As a guideline for our derivation we use the work of Tzavaras in [22] and that of Polizzotto [14] for nonlocal evolution.

We skip the index α in this section, e.g. $w = w^\alpha$, $v = v^\alpha$, and $p = p^\alpha$.

Let ρ_0 be the mass density of our bar in the reference domain $[0, l]$ with $l = 1$, for the sake of simplicity. If we ignore external body forces and radiative heat production the dynamics of an elastic bar are described through the evolution laws

$$\begin{aligned} w_t - v_x &= 0, \\ \rho_0 v_t - \tau_x &= 0. \end{aligned} \tag{2.1}$$

It remains to determine the total stress τ as a function of the unknowns.

Following Tzavaras in [22] let us assume that the free energy ψ is given as a function

$$\psi = \psi(w, p, p_x, \theta),$$

where $\theta = \theta(x, t) > 0$ is the temperature, and $p = p(x, t) \in \mathbb{R}$ is an additional internal variable. It is connected to the strain through the following boundary value problem

$$\begin{aligned} \lambda p_{xx} &= \alpha(p - w), \\ p_x(0) = p_x(l) &= 0, \end{aligned} \tag{2.2}$$

α, λ being a positive constants.

We remark that under sufficient regularity assumptions for w , there is a unique solution of (2.2) which admits the integral representation

$$p(x) = \int_{\Omega} G^\alpha(x, y)w(y) \, dy, \tag{2.3a}$$

$$G^\alpha(x, y) = \frac{\sqrt{\alpha}}{(e^{\sqrt{\alpha}} - e^{-\sqrt{\alpha}})} \left(\cosh\left(\frac{x+y-1}{1/\sqrt{\alpha}}\right) + \cosh\left(\frac{|x-y|-1}{1/\sqrt{\alpha}}\right) \right). \tag{2.3b}$$

This choice leads to a *nonlocal* dependence of the free energy (and later the stress) on the strain w . The representation (2.3) shows that the parameter α controls the strength of the attenuation function G^α . In this way a second length scale for long-range interaction is introduced into the model. Note that we could have used other attenuation functions but use of a Green's function implies that p is governed by the simple differential equation (2.2) (see also [15]).

The thermodynamic consistency of (2.1) together with (2.2) will be assessed in the remainder of this section via an approach similar to that used in classical constitutive theories, but accounting for the nonlocal character of the model.

Due to the nonlocal character of the model, conservation of energy, the first principle of thermodynamics, cannot hold pointwise, but only for the whole body (cf. [14])

$$\int_{\Omega} e_t \, dx = \int_{\Omega} (\tau w_t - q_x) \, dx. \quad (2.4)$$

Here e is the specific internal energy and q denotes the heat flux.

Following the seminal idea of Edelen and Lawes [9], the pointwise version of (2.4)

$$e_t = \tau w_t + q_x + R,$$

must contain an additional term R , called localization residual, which satisfies the constraint

$$\int_{\Omega} R \, dx = 0.$$

The second principle of thermodynamics, expressed by the Clausius-Duhem inequality

$$\rho_0 \eta_t \geq \left(\frac{q}{\theta} \right)_x \quad (2.5)$$

with η representing the specific entropy, has to be satisfied pointwise, see [14]. After introducing the Helmholtz relation

$$\psi = e - \eta\theta,$$

(2.5) can be rewritten in the equivalent form

$$\psi_t - \tau w_t + \eta\theta_t + \frac{q\theta_x}{\theta} - R \leq 0. \quad (2.6)$$

As the free energy is prescribed we derive the remaining constitutive functions such that they are consistent with the second law of thermodynamics. An alternative that we don't pursue here would be to postulate the stress τ and ask whether there is a compatible free-energy function ψ .

So, let ψ be given now for some functions $W = W(w)$ and $\Theta = \Theta(\theta)$ by the special choice

$$\begin{aligned} \psi &= \psi(w, p, p_x, \theta) \\ &= W(w) + \frac{\alpha}{2}(w - p)^2 + \frac{\lambda}{2}p_x^2 + \Theta(\theta). \end{aligned}$$

Then, developing the time derivative of ψ we have

$$\sigma(w)w_t + \alpha(w - p)(w - p)_t + \lambda p_x p_{xt} - \tau w_t + (\psi_\theta + \eta)\theta_t - \frac{q\theta_x}{\theta} - R \leq 0,$$

where $\sigma(w) = W'(w)$.

The above inequality must be satisfied by all thermo-mechanical processes. If we now employ Fourier’s law for the heat flux we get

$$\sigma(w)w_t + \alpha(w - p)(w - p)_t + \lambda p_x p_{xt} - \tau w_t + (\psi_\theta + \eta)\theta_t - R \leq 0. \quad (2.7)$$

We integrate (2.7) over the whole domain and use $\int_\Omega R \, dx = 0$ together with the fact that

$$\int_\Omega \alpha(w - p)p_t \, dx + \int_\Omega \lambda p_x p_{xt} \, dx = \int_\Omega (\alpha(w - p) - \lambda p_{xx})p_t \, dx = 0,$$

to obtain

$$\int_\Omega (\sigma(w) + \alpha(w - p) - \tau)w_t \, dx + \int_\Omega (\psi_\theta + \eta)\theta_t \, dx \leq 0.$$

This inequality must hold for arbitrary choices of w_t and θ_t , i.e., for arbitrary thermo-elastic processes, so one has

$$\begin{aligned} \tau &= \sigma(w) + \alpha(w - p), \\ \eta &= -\psi_\theta, \end{aligned} \quad (2.8)$$

as necessary and sufficient conditions. With this result and assuming isothermality the equations (2.1) become the reversible part of the desired state equations (1.8).

3. Global existence of solutions

In this section we discuss the existence, uniqueness, and regularity of solutions to an initial boundary value problem associated to

$$\begin{aligned} u_t - v &= 0, \\ v_t - \sigma(u_x)_x &= v_{xx} - \alpha(p - u_x)_x, \quad \text{in } (0, T) \times \Omega. \\ \frac{1}{\alpha} p_{xx} &= p - u_x \end{aligned} \quad (3.1)$$

The above system is a reformulation of (1.8) in terms of displacement-velocity state variables ($w = u_x$). Note that we have again dropped the index α , which is a positive fixed number for this section. For the sake of simplicity we have set

$$\mu = 1, \quad \lambda = 1, \quad l = 1,$$

and we will take $\beta = 1$, i.e.

$$\sigma(w) = w^3 - w. \quad (3.2)$$

To (3.1) we add Dirichlet boundary conditions for u and v , respectively Neumann conditions for p

$$\begin{aligned} u(t, 0) = u(t, 1) &= 0, \\ v(t, 0) = v(t, 1) &= 0, \\ p_x(t, 0) = p_x(t, 1) &= 0, \end{aligned} \quad (3.3)$$

for $t \in (0, T)$ and the initial conditions

$$\begin{aligned} u(0, x) &= u_0(x), \\ u_t(0, x) &= v_0(x) \end{aligned} \quad (3.4)$$

for $x \in \Omega$.

In the sequel the following notations will be used: L^2 , H^2 , etc. for $L^2(\Omega)$, $H^2(\Omega)$, and other Sobolev or L^p spaces on Ω . The standard norm and inner product of L^2 will be denoted simply by $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$, while, by contrast, all other norms will be specified explicitly.

The third equation in (3.1) gives the coupling between the internal variable p and the strain u_x . Rewritten in a more familiar form, one can see that, it is a *resolvent equation* for the Laplacian with Neumann boundary conditions. Some characteristic properties of this equation are recalled below.

Remark 3.1. For any fixed $w \in L^2$ and $\alpha > 0$ the elliptic boundary value problem

$$\begin{aligned} -\frac{1}{\alpha} p_{xx} + p &= w, \\ p_x(0) = p_x(1) &= 0 \end{aligned} \quad (3.5)$$

has a unique solution $p \in H^2$. Moreover, if $w \in H^1$ then $p \in H^3$. Thus we can derive (3.5) once with respect to x , and obtain from testing with p_x and w_x the inequalities

$$\|p_x\|^2 \leq \langle p_x, w_x \rangle \leq \|w_x\|^2. \quad (3.6)$$

We can also represent p in terms of w using Green’s function for the elliptic problem (3.5) given in (2.3).

The main result of this section is the following existence theorem.

Theorem 3.2 (Global existence). *Let $\alpha > 0$ be fixed and suppose that*

$$u_0 \in H^2 \cap H_0^1 \quad \text{and} \quad v_0 \in H^2 \cap H_0^1.$$

Then, given any $T > 0$, there is a unique weak solution (u, v, p) of the initial boundary value problem (3.1), (3.3), (3.4) in the sense that

$$\begin{aligned} v &= u_t \in H^1(0, T; L^2) \cap L^\infty(0, T; H_0^1) \cap L^2(0, T; H^2), \\ u &\in C^1([0, T], L^2) \cap C([0, T], H^2 \cap H_0^1), \\ p &\in C^1([0, T], H^1) \cap C([0, T], H^3). \end{aligned} \tag{3.7}$$

We will start by deriving standard energy estimates for the nonlocal model (3.1). For this, we need the following lemma which can be found in e.g. [11].

Lemma 3.3. *Let X be a Hilbert space and $A : D(A) \subseteq X \rightarrow X$ a densely defined, self-adjoint operator that generates a C_0 -semigroup of contractions. Let $u \in H^1(0, T; X)$ with $u(t) \in D(A)$ a.e. $t \in [0, T]$, and $Au \in L^2(0, T; X)$. Then the function $t \mapsto \langle Au(t), u(t) \rangle_X$ is absolutely continuous on $[0, T]$ and*

$$\frac{1}{2} \frac{d}{dt} \langle Au(t), u(t) \rangle_X = \left\langle Au(t), \frac{d}{dt} u(t) \right\rangle_X.$$

Lemma 3.4 (Energy estimates). *Let $(u, v, p)^T$ be a weak solution of (3.1) in the sense of (3.7) then for all $t \in [0, T]$*

$$E^\alpha[u, v, p] \leq E^\alpha[u_0, v_0, p_0], \tag{3.8}$$

$$\int_0^t \|v_x(\tau)\|^2 \, d\tau \leq E^\alpha[u_0, v_0, p_0], \tag{3.9}$$

where

$$E^\alpha[u, v, p] = \frac{1}{2} \|v\|^2 + \frac{1}{2} \langle p_x, u_{xx} \rangle + \int_\Omega W(u_x) \, dx. \tag{3.10}$$

Furthermore, $p_0 \in H^3$ is the unique solution of (3.5) for $w(0) = u_{0,x}$ and $W(w) = \frac{1}{4}(w^2 - 1)^2$.

Moreover, there exists a positive constant $C = C(T)$ (independent of α) such that

$$\|u_{xx}(t)\|^2 \leq C \quad \text{for all } t < T. \tag{3.11}$$

Remark 3.5. Note that (3.5) implies

$$\frac{1}{2}\langle p_x, u_{xx} \rangle = \frac{1}{2}\langle p_x, w_x \rangle = \frac{\alpha}{2}\langle p - w, p - w \rangle + \frac{1}{2}\langle p_x, p_x \rangle \geq 0.$$

Thus, the energy E^α in (3.10) is a nonnegative quantity and corresponds to the formulation in (1.9), which is given in terms of w .

Proof of Lemma 3.4.

$$\frac{d}{dt} \left(\frac{1}{2} \|v(t)\|^2 + \frac{1}{2} \langle p_x(t), u_{xx}(t) \rangle + \int_{\Omega} W(u_x(t)) \, dx \right) = - \|v_x(t)\|^2.$$

This means that the total energy

$$E^\alpha[u, v, p] = \frac{1}{2} \|v\|^2 + \frac{1}{2} \langle p_x, u_{xx} \rangle + \int_{\Omega} W(u_x) \, dx$$

is decreasing along solutions and bounded by the energy of the initial state

$$E^\alpha[u(t), v(t), p(t)] \leq E^\alpha[u_0, v_0, p_0].$$

Also, the energy dissipated in the time interval $[0, T]$ cannot exceed the initial energy

$$\int_0^T \|v_x(t)\|^2 \, dt \leq E^\alpha[u_0, v_0, p_0].$$

To prove the estimate (3.11) we take the inner product of the second equation in (3.1) with $u_{xx}(t)$, use Lemma 3.3, and get

$$\begin{aligned} & \frac{d}{dt} \langle v(t), u_{xx}(t) \rangle - \|v_x(t)\|^2 \\ &= \alpha \langle u_{xx}(t) - p_x(t), u_{xx}(t) \rangle + \frac{1}{2} \frac{d}{dt} \|u_{xx}(t)\|^2 + \langle \sigma(u_x(t))_x, u_{xx}(t) \rangle. \end{aligned}$$

Integration with respect to time yields

$$\begin{aligned} & \langle v(t), u_{xx}(t) \rangle - \int_0^t \|v_x(s)\|^2 \, ds + c_0 \\ &= \alpha \int_0^t \langle u_{xx}(s) - p_x(s), u_{xx}(s) \rangle \, ds + \frac{1}{2} \|u_{xx}(t)\|^2 + \int_0^t \langle \sigma(u_x(s))_x, u_{xx}(s) \rangle \, ds, \end{aligned}$$

where $c_0 := \frac{1}{2} \|u_{0xx}\|^2 - \langle v_0, u_{0xx} \rangle$.

Due to (3.6)

$$\langle u_{xx}(t) - p_x(t), u_{xx}(t) \rangle \geq 0$$

holds for any $t \in [0, T]$. This and Young’s inequality applied to $\langle v(t), u_{xx}(t) \rangle$ gives

$$\begin{aligned} 2\|v(t)\|^2 + \frac{1}{8}\|u_{xx}(t)\|^2 + \int_0^t \|v_x(s)\|^2 \, ds + c_0 \\ \geq \frac{1}{2}\|u_{xx}(t)\|^2 + \int_0^t \langle \sigma(u_x(s))_x, u_{xx}(s) \rangle \, ds. \end{aligned}$$

By taking into account the explicit form of the stress $\sigma(u_x)_x = 3u_x^2 u_{xx} - u_{xx}$ we finally obtain

$$2\|v(t)\|^2 + \int_0^t \|v_x(s)\|^2 \, ds + c_0 + \int_0^t \|u_{xx}(s)\|^2 \, ds \geq \frac{3}{8}\|u_{xx}(t)\|^2.$$

The first two terms on the left hand side of this inequality are either bounded by the initial energy, as we have seen in the first part of the proof, or constant, such that by Gronwall’s Inequality

$$\|u_{xx}(t)\|^2 \leq \left(\frac{40}{3} E^z[u_0, v_0, p_0] + c_0 \right) e^{(8/3)t}$$

and (3.11) has been proved. □

Proof of Theorem 3.2. Our proof relies on semigroup theory and will be carried out in four successive steps. We start with the linear part of the problem (Step 1 and 2), and show that the linear operator defined by the right hand side of (3.1) generates a semigroup. In Step 3 and 4 we study local and global existence for the full semilinear problem.

Step 1. If we consider only the u_{xx} and v_{xx} terms on the right hand side of (3.1) what we are left with is the linear viscoelastic system

$$\begin{aligned} u_t &= v, \\ v_t &= \alpha u_{xx} + v_{xx}. \end{aligned}$$

For this model existence results obtained by semigroup methods are known (see for example [10] and references therein). The system can be written in abstract form

$$\frac{d}{dt} z(t) = Az(t), \tag{3.12}$$

where $z(t) := (u(t), v(t))^T$ and the operator matrix

$$A = \begin{pmatrix} 0 & I \\ \alpha \partial_{xx} & \partial_{xx} \end{pmatrix},$$

with domain

$$D(A) = (H^2 \cap H_0^1) \times (H^2 \cap H_0^1)$$

generate a strongly continuous semigroup $S(t)$ on the Hilbert space

$$X = (H^2 \cap H_0^1) \times L^2.$$

Step 2. In this step we also take into account the p -term of (3.1). We deal with

$$\begin{aligned} u_t &= v, \\ v_t &= \alpha u_{xx} + v_{xx} - \alpha p_x. \end{aligned}$$

The additional p -term can be treated as a perturbation and (3.12) becomes

$$\frac{d}{dt} z(t) = Az(t) + Bz(t),$$

with A as before and

$$B = \begin{pmatrix} 0 & 0 \\ -\alpha \partial_x (-\frac{1}{\alpha} \partial_{xx} - I)^{-1} \partial_x & 0 \end{pmatrix}.$$

As a consequence of the regularity of p , which is defined via an integral operator (2.3), B is a bounded operator on X . This means that the Bounded Perturbation Theorem (Theorem III.1.3 in [10]) applies and the operator $C = A + B$ with domain $D(C) = D(A)$ generates a strongly continuous semigroup $\{S(t)\}_{t \geq 0}$ on X .

Step 3. We proceed to prove the existence of a unique local solution for the full semilinear problem

$$\frac{d}{dt} z(t) = (A + B)z(t) + F(z(t)),$$

where

$$F(z(t)) = \begin{pmatrix} 0 \\ \sigma(u_x(t))_x \end{pmatrix}.$$

This is the abstract form of (3.1).

Notice that $F : X \rightarrow X$ is locally Lipschitz continuous (cf. [2]), and hence, by Banach’s fixed point principle, there is a unique local solution $z \in C([0, T_0], X)$ of the integral equation

$$z(t) = S(t)z_0 + \int_0^t S(t - \tau)F(z(\tau)) \, d\tau,$$

for T_0 small enough. Furthermore, since $z_0 = (u_0, v_0)^T \in D(A)$, by [23] Theorem 2.4.5, $z(t)$ is a classical solution.

Step 4. Our aim is to extend the local solution of Step 3 to arbitrary time intervals. We can achieve this by using the energy estimates.

Obviously, the local classical solution obtained in Step 3 is also a solution in the sense of (3.7). We show that this solution cannot explode, or in other words, that regularity is not lost in finite time.

The estimates (3.8) and (3.11) assure that the velocity v and the strain gradient u_{xx} remain bounded independently of t . Furthermore, the second equation in (3.1) can be viewed as a heat equation

$$v_t - v_{xx} = g(t), \tag{3.13}$$

with a source term

$$g(t) = \sigma(u_x(t))_x - \alpha(p(t) - u_x(t))_x,$$

which is controlled by the strain gradient (its highest order term)

$$\|g(t)\| \leq C\|u_{xx}(t)\|.$$

Standard parabolic estimates applied to (3.13) yield

$$\int_0^T \|v_t(t)\|^2 \, dt + \operatorname{ess\,sup}_{t \in [0, T]} \|v_x(t)\|^2 + \int_0^T \|v_{xx}(t)\| \leq \|v_{0x}\|^2 + C\|u_{xx}\|_{L^2(0, T, L^2)}^2.$$

Finally, due to the fact that $u_{xx}(t)$ is bounded (3.11), we have

$$\int_0^T \|v_t(t)\|^2 \, dt + \operatorname{ess\,sup}_{t \in [0, T]} \|v_x(t)\|^2 + \int_0^T \|v_{xx}(t)\|^2 \, dt \leq C(T, E^\alpha[u_0, v_0]). \tag{3.14}$$

This shows that v has the regularity stated in (3.7). □

Remark 3.6. Starting from the solution of (3.1) one obtains a solution of (1.8) by taking $w = u_x$.

4. The capillarity limit

As mentioned in the introduction, energy arguments suggest that the appropriate limit problem for (3.1) as $\alpha \rightarrow \infty$ is the classical viscosity-capillarity model (1.4)

$$\begin{aligned} u_t - v &= 0, \\ v_t - \sigma(u_x)_x &= v_{xx} - u_{xxxx}, \end{aligned} \tag{4.1}$$

written here in displacement-velocity state variables (with $\mu = \lambda = 1$).

This model has been studied by Andrews and Ball [2] who prove that for any initial state

$$u_0 \in H^2 \cap H_0^1 \quad \text{and} \quad v_0 \in L^2$$

there exists a unique solution

$$\begin{aligned} u &\in C^1((0, T], H^2 \cap H_0^1), \\ v &\in C^1((0, T], L^2), \end{aligned}$$

defined on any time interval with $T > 0$ and with regularity given by

$$u(t) \in H^4 \cap H_0^1, \quad v(t) \in H^2 \cap H_0^1 \quad \text{for } t > 0.$$

The corresponding energy equation for (4.1) is

$$\frac{d}{dt} E^\infty[u(t), v(t)] = -\|v_x(t)\|^2$$

where

$$E^\infty[u, v] = \frac{1}{2}\|v\|^2 + \frac{1}{2}\|u_{xx}\|^2 + \int_{\Omega} W(u_x) \, dx. \tag{4.2}$$

In order to prove a convergence result for the family of solutions to (3.1) with $\alpha > 0$, α -independent estimates, especially for the strain, are needed. A key observation which leads to such estimates is that the initial energy for any of the problems (3.1) with $\alpha > 0$ is bounded by the initial energy

$$E_0^\infty := E^\infty[u_0, v_0] = \frac{1}{2}\|v_0\|^2 + \frac{1}{2}\|u_{0xx}\|^2 + \int_{\Omega} W(u_{0x}) \, dx.$$

The precise statement is given in the next lemma.

Note that for the rest of this section we use the α -index for solutions of (3.1). The energy E^∞ in (4.2) equals obviously E^∞ in (1.5) with $u = w_x$ and we use the same notation.

Lemma 4.1 (α -independent estimates). *Let $(u^\alpha, v^\alpha, p^\alpha)_{\alpha>0}^T$ be the family of solutions, in the sense of (3.7), to the initial boundary value problem (3.1)–(3.4) with the same initial conditions*

$$u_0 \in H^2 \cap H_0^1 \quad \text{and} \quad v_0 \in H^2 \cap H_0^1.$$

Then there exists a α -independent constant E_0^∞ (defined above) such that for all $t \in [0, T]$

$$E^\alpha[u^\alpha(t), v^\alpha(t), p^\alpha(t)] \leq E_0^\infty, \tag{4.3}$$

$$\int_0^t \|v_x^\alpha(\tau)\|^2 \, d\tau \leq E_0^\infty. \tag{4.4}$$

Furthermore, for any $\alpha > 0$ and any $t \in [0, T]$

$$\|u_{xx}^\alpha(t)\| \leq C(T, E_0^\infty) \tag{4.5}$$

and due to the embedding of H^1 in L^∞

$$\|u_x^\alpha(t)\|_{L^\infty} \leq C(T, E_0^\infty), \tag{4.6}$$

and

$$\int_0^T \|v_t^\alpha(t)\|^2 \, dt \leq C(T, E_0^\infty). \tag{4.7}$$

Proof. From the energy estimates (3.8) and (3.9) we know that for each $\alpha > 0$

$$E^\alpha[u^\alpha(t), v^\alpha(t), p^\alpha(t)] \leq E^\alpha[u_0, v_0, p_0^\alpha],$$

$$\int_0^t \|v_x^\alpha(\tau)\|^2 \, d\tau \leq E^\alpha[u_0, v_0, p_0^\alpha],$$

where

$$E^\alpha[u_0, v_0, p_0^\alpha] = \frac{1}{2} \|v_0\|^2 + \frac{1}{2} \langle p_{0x}^\alpha, u_{0xx} \rangle + \int_\Omega W(u_{0x}) \, dx. \tag{4.8}$$

One can see that in (4.8) the only α -dependent term, and the only difference to E_0^∞ is $\langle p_{0x}^\alpha, u_{0xx} \rangle$, but from the inequality (3.6) we know that

$$\langle p_{0x}^\alpha, u_{0xx} \rangle \leq \|u_{0xx}\|^2,$$

and hence

$$E^\alpha[u_0, v_0, p_0^\alpha] \leq E_0^\infty.$$

By combining the α -independent energy estimate (4.3) with (3.11) one obtains a uniform estimate for the strain gradient (4.5), which obviously implies the L^∞ estimate (4.6) for the strain.

Furthermore, (4.5) together with (3.14), which is an estimate for v_t , yield (4.7). □

The proof of the main result in this section relies on the well-known Lemma of Aubin (see [17]).

Lemma 4.2 (Aubin). *Let V, H, V' be reflexive Banach spaces such that the following embeddings hold $V \hookrightarrow$ (compactly) $H \hookrightarrow$ (continuously) V' . If the sequence (f_n) is bounded in $L^2(0, T; V)$ and the sequence of time derivatives $(\partial_t f_n)$ is bounded in $L^2(0, T; V')$ then (f_n) has a subsequence (f_{n_s}) which converges in $L^2(0, T; H)$.*

Theorem 4.3. *There exists a subsequence $(u^{\alpha_k}, v^{\alpha_k}, p^{\alpha_k})_{k \in \mathbb{N}}^T$ of the family of classical solutions of (3.1), (and a pair $(\bar{w}, \bar{v})^T \in L^2(0, T; L^2 \times H_0^1)$) such that*

(i) *we have*

$$\begin{aligned} u_x^{\alpha_k}, p^{\alpha_k} &\rightarrow \bar{w} && \text{in } L^2(0, T; L^2), \\ v^{\alpha_k} &\rightarrow \bar{v} && \text{in } L^2(0, T; L^2), \\ \sigma(u_x^{\alpha_k}) &\rightarrow \sigma(\bar{w}) && \text{in } L^2(0, T; L^2) \end{aligned}$$

as $k \rightarrow \infty$, and

$$\bar{w} \in L^\infty(\Omega \times (0, T)). \tag{4.9}$$

(ii) $(\bar{w}, \bar{v})^T$ *is a weak solution of the problem (4.1) in conservation form, i.e.,*

$$\int_0^T \int_\Omega \bar{w} \psi_t - \bar{v} \psi_x \, dx \, dt = 0, \tag{4.10}$$

$$\int_0^T \int_\Omega \bar{v} \psi_t - \bar{v} \psi_{xx} - \bar{w} \psi_{xxx} + \sigma(\bar{w}) \psi_x \, dx \, dt = 0, \tag{4.11}$$

for all $\psi \in C_0^\infty(\Omega \times (0, T))$.

Proof. We begin by showing that for a subsequence

$$p^{\alpha_k} \rightarrow \bar{w} \quad \text{in } L^2(0, T; L^2). \tag{4.12}$$

To this end we use Aubin’s Lemma. First, $(p^\alpha)_{\alpha>0}$ is uniformly bounded in $L^2(0, T; H^1)$ due to the inequality (3.6) and the first energy inequality (4.3)

$$\|p_x^\alpha(t)\|^2 \leq \langle p_x^\alpha(t), u_{xx}^\alpha(t) \rangle \leq E_0^\infty \tag{4.13}$$

a.e. $t \in [0, T]$ and any α .

To show that the sequence of time derivatives $(p_t^\alpha)_{\alpha>0}$ is also uniformly bounded, we differentiate the equation

$$-\frac{1}{\alpha} p_{xx}^\alpha(t) + p^\alpha(t) = u_x^\alpha(t)$$

with respect to time. Since $v^\alpha \in L^\infty(0, T; H_0^1)$, the resulting equation

$$-\frac{1}{\alpha} (p_t^\alpha)_{xx}(t) + p_t^\alpha(t) = v_x^\alpha(t)$$

holds in L^2 for a.e. $t \in [0, T]$ and the following inequality is analogous to (3.6)

$$\|p_t^\alpha(t)\| \leq \|v_x^\alpha(t)\|.$$

Based on the last inequality and on (4.4)

$$\int_0^T \|p_t^\alpha(t)\|^2 dt \leq \int_0^T \|v_x^\alpha(t)\|^2 dt \leq E_0^\infty.$$

Hence, according to the Lemma of Aubin, there exists $\bar{w} \in L^2(0, T; L^2)$ such that (4.12) holds some subsequence denoted by $(p^{\alpha_k})_{k \in \mathbb{N}}$.

Next, we prove that the corresponding subsequence $(u_x^{\alpha_k})_{k \in \mathbb{N}}$ also converges to \bar{w} . Indeed, turning once again to the elliptic equation

$$-\frac{1}{\alpha} p_{xx}^\alpha(t) + p^\alpha(t) = u_x^\alpha(t),$$

as $u_x^\alpha \in C([0, T], H^2)$, using (4.3) one has that for any $t \in [0, T]$

$$\begin{aligned} \|u_x^\alpha(t) - p^\alpha(t)\|^2 &= -\frac{1}{\alpha} \langle p_{xx}^\alpha(t), u_x^\alpha(t) - p^\alpha(t) \rangle \\ &= \frac{1}{\alpha} \langle p_x^\alpha(t), u_{xx}^\alpha(t) \rangle - \frac{1}{\alpha} \|p_x^\alpha(t)\|^2 \\ &\leq \frac{1}{\alpha} \langle p_x^\alpha(t), u_{xx}^\alpha(t) \rangle \\ &\leq \frac{1}{\alpha} E_0^\infty. \end{aligned}$$

This leads to

$$\|u_x^{\alpha_k}(t) - p^{\alpha_k}(t)\| \rightarrow 0 \tag{4.14}$$

for any $t \in [0, T]$ and, finally when $k \rightarrow \infty$, to

$$u_x^{\alpha_k} \rightarrow \bar{w} \quad \text{in } L^2(0, T; L^2). \tag{4.15}$$

Since the sequence $(u_x^{\alpha_k})_{k \in \mathbb{N}}$ is uniformly bounded in the L^∞ -norm (see (4.6)), from (4.15) we conclude from (4.15) that

$$\bar{w} \in L^\infty(\Omega \times (0, T)),$$

and \bar{w} satisfies the same bound as all u_x^α ,

$$\|\bar{w}(t)\|_{L^\infty} \leq C(T, E_0).$$

Consequently $\sigma(\bar{w})$ is well-defined.

Considering the specific form of σ we have that

$$\sigma(w) - \sigma(\bar{w}) = (w - \bar{w})(w^2 + w\bar{w} + \bar{w}^2 - 1). \tag{4.16}$$

If we take $w = u_x^{\alpha_k}$, then $w^2 + w\bar{w} + \bar{w}^2 - 1$ is bounded by a (α -independent) constant $M \geq 0$, due to the L^∞ -estimates for both $u_x^{\alpha_k}$ and \bar{w} . Thus the relation (4.16) gives

$$\begin{aligned} \|\sigma(u_x^{\alpha_k}) - \sigma(\bar{w})\|_{L^2(0, T; L^2)}^2 &\leq \int_0^T \int_\Omega (u_x^{\alpha_k}(t, x) - \bar{w}(t, x))^2 M^2 \, dx \, dt \\ &= M^2 \|u_x^{\alpha_k} - \bar{w}\|_{L^2(0, T; L^2)}^2. \end{aligned}$$

And by the convergence of $u_x^{\alpha_k}$ to \bar{w}

$$\sigma(u_x^{\alpha_k}) \rightarrow \sigma(\bar{w}) \quad \text{in } L^2(0, T; L^2)$$

for $k \rightarrow \infty$.

The strong convergence of a subsequence $(v^{\alpha_k})_{\alpha_k \in \mathbb{N}}$ is achieved by using Aubin’s lemma once again. The required uniform estimates are given in (4.4) and (4.7).

Finally, we can pass to the limit in the following weak formulation of (3.1)

$$\begin{aligned} \int_0^T \int_\Omega w^{\alpha_k} \psi_t - v^{\alpha_k} \psi_x \, dx \, dt &= 0, \\ \int_0^T \int_\Omega v^{\alpha_k} \psi_t - v^{\alpha_k} \psi_{xx} - p^{\alpha_k} \psi_{xxx} + \sigma(w^{\alpha_k}) \psi_x \, dx \, dt &= 0 \end{aligned}$$

which is satisfied by the solutions $(u^{\alpha_k}, v^{\alpha_k})^T$ for any $\psi \in C_0^\infty(\Omega \times (0, T))$. Since all the sequences involved converge, we can pass to the limit to obtain exactly (4.10) and (4.11). \square

5. Numerical experiments

In this section we numerically compare model (1.8) with (1.4). We study the capillarity limit $\alpha \rightarrow \infty$ and one sharp-interface limit given by the scaling $\mu = \epsilon$, $\lambda = \epsilon^2$, and $\epsilon \rightarrow 0$. Furthermore, we compare the computational time for the different approaches.

All computations are done using an explicit discontinuous Galerkin (DG) scheme of order 1 on an uniform grid with $N \in \mathbb{N}$ cells. The space discretisation is done using the local DG method introduced in [5] and the explicit Euler scheme is used as time discretisation. As a numerical flux for the first-order part we use the Lax-Friedrichs flux. The elliptic equation for p^α is solved by a finite difference scheme.

5.1. Numerical Tests for the Capillarity and the Sharp Interface Limit. In the following experiments we present numerical experiments for (1.8) and (1.4). In all cases we choose the parameters as

$$\Omega = [0, 1], \quad \mu = \epsilon, \quad \lambda = \epsilon^2,$$

with $\epsilon > 0$ given below. We take the free energy from (1.1) with $\beta = 1$. The initial conditions are given by

$$(v_0(x), w_0(x)) = \begin{cases} (v_L, w_L) : x \in (0, \frac{1}{4}) \cup (\frac{1}{2}, \frac{5}{8}) \cup (\frac{3}{4}, 1) \\ (v_R, w_R) : x \in (\frac{1}{4}, \frac{1}{2}) \cup (\frac{5}{8}, \frac{3}{4}) \end{cases}$$

with

$$v_L = 0.5, \quad w_L = -0.8, \quad v_R = 0.0 \quad \text{and} \quad w_R = 1.1,$$

and we choose periodic boundary conditions.

5.1.1. The Capillarity Limit $\alpha \rightarrow \infty$. In this section we numerically investigate the convergence shown in Theorem 4.3. In Figure 1 we plot numerical solutions at different time levels $t = 0.2, 0.4, 0.8$. All the experiments are done with $\epsilon = 0.03$ and $N = 480$ cells.

We observe that all discrete solutions tend to eliminate the isolated small strain phase which is initially associated with the interval $(1/2, 5/8]$. With increasing

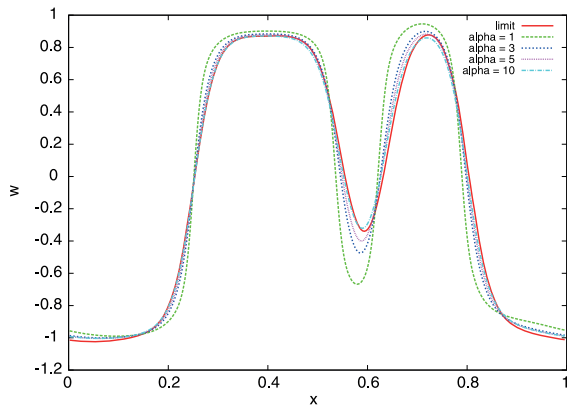
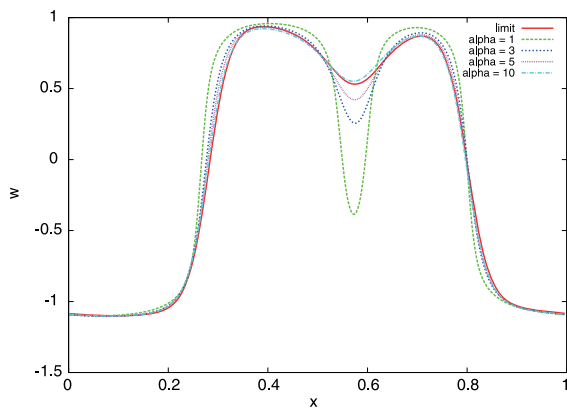
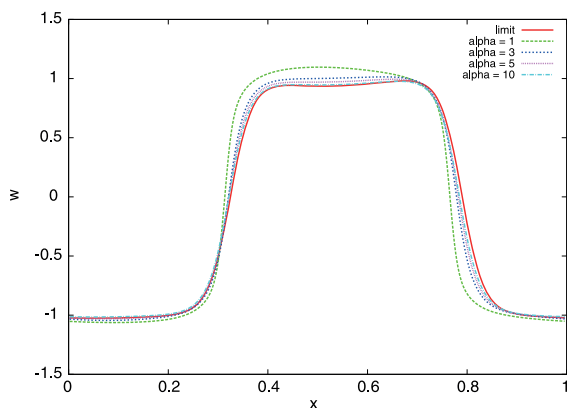
(a) $t = 0.2$ (b) $t = 0.4$ (c) $t = 0.8$

Figure 1. Convergence of the strain w for $\alpha \rightarrow \infty$, results for $\alpha = 1, 3, 5, 10$ are displayed. The graph denoted with the label “limit” corresponds to the numerical solution of (1.4). At any time we observe convergence for increasing α .

values of α we see convergence towards the solution of the viscosity capillarity model (1.4) as predicted by Theorem 4.3.

5.1.2. The Sharp-Interface Limit $\epsilon \rightarrow 0$. Now we fix $\alpha = 1$, but vary $\epsilon = 0.1, 0.01, 0.001$. In Figure 2 we plot the solutions at the time levels $t = 0.2, 0.4, 0.8$ on a grid with $N = 480$ cells.

We observe for $\epsilon \rightarrow 0$ a good approximation of (1.8) by (1.4). For $\epsilon = 0.1$ we have still a strong smoothing of the solution: two phase transitions combine here much faster than in the solution for $\epsilon \rightarrow 0$. This is the reason, why the solutions for different ϵ differ so much.

5.1.3. Runtime Comparison. In this section we compare the runtime of the DG method for the models (1.8) and (1.4) for different numbers of grid cells N . The runtimes are listed in Table 1.

We observe, that solving (1.8) is much faster than solving (1.4). This comes from the fact, that the time step restriction is weaker for (1.8). The computational complexity of an explicit numerical solution to (1.4) scales (formally) with $\mathcal{O}(\Delta x^{-3})$ time steps, $\Delta x > 0$ denoting the spatial mesh width. For the new model (1.8) we require only $\mathcal{O}(\Delta x^{-2})$ time steps.

5.2. An Experiment in 2D. We study the behavior of a generalization of (1.4) to two dimensions given by

$$\begin{aligned} w_t - \nabla v &= 0, \\ v_t - \operatorname{div} \sigma(w) &= \mu \Delta v - \lambda \operatorname{div} \Delta w. \end{aligned} \tag{5.1}$$

The unknowns are $w : \Omega \times (0, T) \rightarrow \mathbb{R}^{2 \times 2}$ and $v : \Omega \times (0, T) \rightarrow \mathbb{R}^2$. In the calculation we will use $\Omega = [0, 1]^2$. The stress-strain relation $\sigma : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}^{2 \times 2}$ is defined as the derivative of the free energy function $\Psi : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ given by

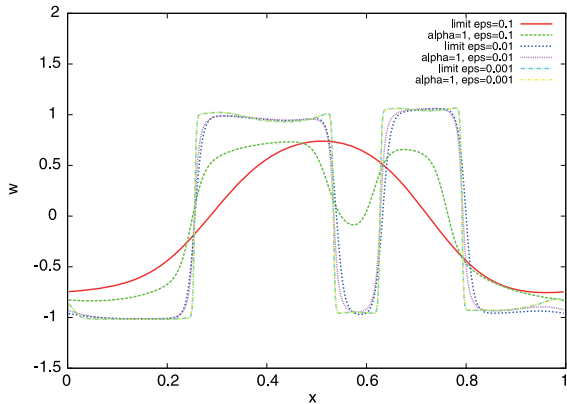
$$\begin{aligned} \Psi(w) &= \Psi(C = w^T w) \\ &= (C_{11} - 1 - \delta)^2 (C_{22} - 1 + \delta)^2 + (C_{11} - 1 + \delta)^2 (C_{22} - 1 - \delta)^2 + C_{12}^2. \end{aligned}$$

The free energy function Ψ has two minima at

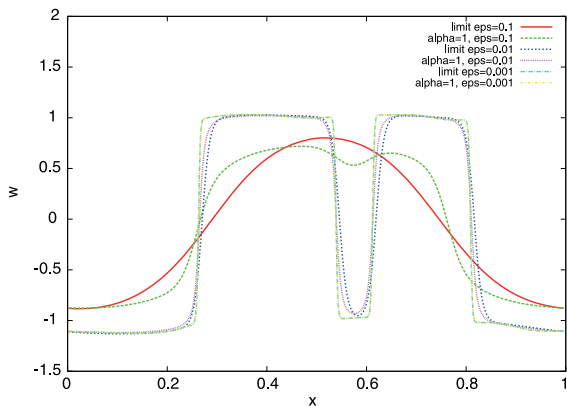
$$w_1 = \begin{pmatrix} \sqrt{1-\delta} & 0 \\ 0 & \sqrt{1+\delta} \end{pmatrix} \quad \text{and} \quad w_2 = \begin{pmatrix} \sqrt{1+\delta} & 0 \\ 0 & \sqrt{1-\delta} \end{pmatrix}, \quad \delta > 0.$$

The convex regions of Ψ around the minima are interpreted as the two phases of the described material. For the calculation we use the initial conditions

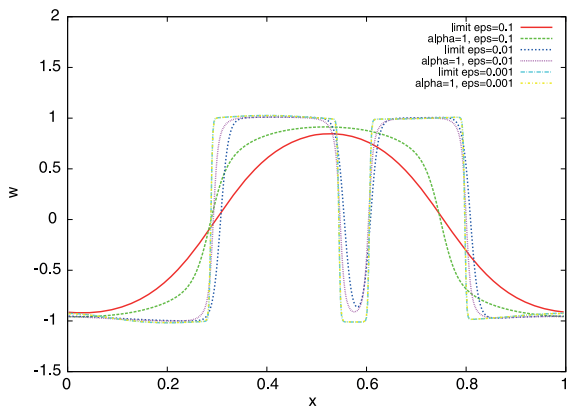
$$w(\cdot, 0) = w_1 \quad \text{and} \quad v(\cdot, 0) = 0.$$



(a) $t = 0.2$



(b) $t = 0.4$



(c) $t = 0.8$

Figure 2. Convergence of the strain w for $\epsilon \rightarrow 0$, results for $\epsilon = 0.1, 0.01, 0.001$ are displayed. The graph denoted with the label “limit” corresponds to the numerical solution of (1.4).

Table 1. This table lists the runtime (in seconds) for solving (1.4) and (1.8) with different α on different grids. The runtime is always given in milliseconds. By error we denote the L^2 -difference to the numerical solution of (1.4) on the same grid.

N	ϵ	(1.4)	(1.8) with $\alpha = 1$		(1.8) with $\alpha = 3$		(1.8) with $\alpha = 10$	
		runtime	runtime	error	runtime	error	runtime	error
40	1/4	1469	190	0.379	190	0.205	189	0.101
80	1/8	3099	424	0.227	424	0.094	424	0.057
120	1/12	4862	706	0.230	704	0.079	703	0.043
160	1/16	6991	1049	0.248	1049	0.088	1049	0.041
200	1/20	9172	1426	0.250	1435	0.090	1435	0.036
240	1/24	11470	1863	0.233	1854	0.086	1864	0.036
280	1/28	14013	2340	0.207	2342	0.079	2345	0.040
320	1/32	16670	2849	0.182	2851	0.073	2856	0.044
360	1/36	19447	3436	0.163	3441	0.067	3443	0.047
400	1/40	22428	4091	0.153	4076	0.064	4079	0.047

The boundary conditions are

$$\text{left: } v \cdot \vec{n} = 0.$$

$$\text{right: } v \cdot \vec{n} = 0.1.$$

$$\text{top: } \sigma(w) \cdot \vec{n} = 0.$$

$$\text{bottom: } \sigma(w) \cdot \vec{n} = 0.$$

In other words the plate is fixed at the left and pulled with constant velocity at the right. At the top and the bottom no forces act.

It is straight forward to extend the equation (1.8) to multiple space dimensions. We approximate (5.1) by

$$\begin{aligned} w_t^\alpha - \nabla v^\alpha &= 0, \\ v_t^\alpha - \operatorname{div} \sigma(w^\alpha) &= \mu \Delta v^\alpha - \alpha \operatorname{div}(p^\alpha - w^\alpha), \\ \lambda \Delta p^\alpha &= \alpha(p^\alpha - w^\alpha). \end{aligned} \tag{5.2}$$

For the calculation in Figure 3 the parameters

$$\mu = \epsilon, \quad \lambda = \epsilon^2, \quad \epsilon = 0.02 \quad \text{and} \quad \delta = 0.3$$

are chosen. Only the position of the phase transition is plotted: a material point with stress w belongs to phase 1, if and only if $\|w - w_1\| < \|w - w_2\|$. In other words we draw the line given by $\|w - w_1\| = \|w - w_2\|$. The figures are plotted in physical space and not in the reference domain Ω .

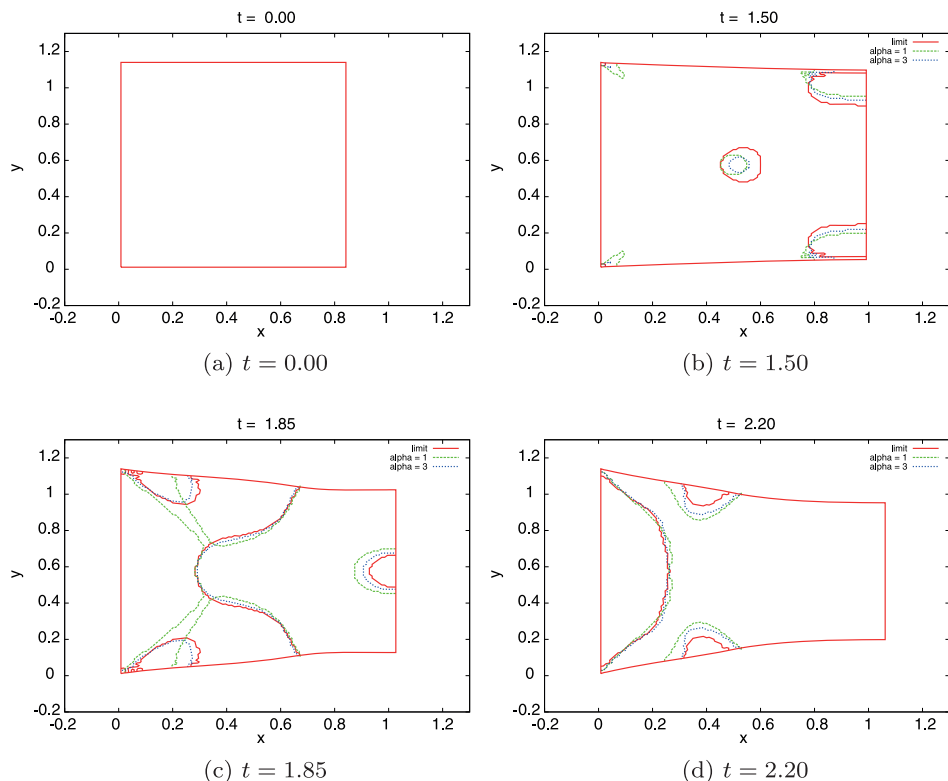


Figure 3. Elastic plane during deformation. Only the phase boundaries are plotted.

As in the one-dimensional case, we observe that model (5.1) is well approximated by model (5.2) for $\alpha \rightarrow \infty$.

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