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Lubrication Approximations for Surface Tension Driven Interfaces: Some Open Problems

This paper discusses some interesting open problems concerning the equations of motion for a lubrication approximation of fluid interfaces driven by surface tension. A number of different physical examples are considered.

Free surface flow in which surface tension plays a role in the dynamics of an interface is an extremely complex phenomenon which can produce a myriad of different dynamics and patterns. Typically one must simultaneously solve equations of motion for the fluid coupled with a dynamically evolving fluid/vapor or fluid/fluid interface on which surface tension plays an important role. Examples range from a drop of liquid spreading on a surface to a jet of fluid being ejected from a nozzle. Such problems have important industrial and engineering applications ranging from de-icing of airplane wings to coating of microchips and the design of inkjet printers.

Solving the full system of equations is often an extremely difficult task both for rigorous analysis and for numerical computation. However, in many instances, the particular geometry of the problem allows for a simplification of the dynamics via a “lubrication approximation”. The end result is a more tractable mathematical formulation of the free boundary (often as a local PDE for some thickness associated with the fluid).

Here we discuss a number of different physical problems and some interesting mathematical questions associated with the equations resulting from a lubrication-type approximation of the dynamics. In each problem we address at least one of the following three topics: singularity formation (describing some kind of topological transition), weak solution theory, and pattern formation.

1. Droplet breakup

Consider a jet of liquid falling from a nozzle. This system exhibits singularities (e.g. when a droplet breaks off) which are often accompanied by complex pattern formation involving the interaction between multiple droplets, the recoiling of fluid necks, etc. The full system can be studied by coupling the 3D NAVIER-STOKES equations to the free surface condition. This is a difficult set of equations to understand even in the case of axisymmetry. To analyze the specific problem of the droplet pinch off, EGGERS and DUPONT [19] derived an approximate equation for an axisymmetric jet of fluid forced by gravity along the axis of the jet. Denoting the outer surface radius by h and expanding the pressure and velocities as a series in the radius coordinate r , they approximated the full NAVIER-STOKES/surface tension equations by the following coupled system:

$$\begin{aligned}\rho(\partial_t v + vv_x) &= \gamma(h_x/h^2 + h_{xxx}) + 3\eta(h^2 v_x)_x/h^2 - \rho g \\ \partial_t h + vh_x &= -v_x h/2.\end{aligned}\tag{1}$$

Here x denotes the position along the axis of the jet and v is a leading order fluid velocity depending only on x . The constants γ , ρ , and η denote respectively the surface tension, density of the fluid, and viscosity of the fluid. EGGERS [20] showed that close to singularity higher order terms become arbitrarily small so that the above equations are an *exact* representation of the asymptotic behavior of the full system. He went on to show that this system has a universal self similar solution describing the breaking of the jet. In [21] he analyzed the drop formation after breakup. Further work by BRENNER et. al. [12, 13] showed EGGERS’ similarity solution describing breakup to be unstable to small perturbations. They showed that this instability ultimately results in a cascade of necks seen in droplet breakoff experiments [31]. A somewhat related phenomenon occurs in the breakup of a long thin fluid filament in a viscous background fluid [33]. In low viscosity ratio systems, the break up mechanism is ‘self-repeating’ in that as a neck forms it tries to pinch in two points forming yet more necks. The outcome is a self-similar like pattern of repeating satellite drops.

All of the numerical evidence to date indicates that finite time singularities (describing a droplet break up) occur in the system (1). However, no proof of this fact exists. Another interesting question concerns the consistency of the approximation. A conjecture due to CONSTANTIN states ¹ that before breakup solutions to (1) retain bounded

¹see [19] for conjecture on equations with full curvature term

first derivative in h . This is a necessary condition to insure that the approximation remains valid up to the pinch off time. Such behavior has also been observed in numerical simulations of the droplet break up.

2. The Hele Shaw cell

A less violent, but equal complex system is the behavior of a thin neck in a HELE SHAW cell. Consider a body of liquid trapped between two glass plates (referred to as a HELE SHAW cell). When the plates are very close together, the problem can be treated as a two dimensional fluid/free boundary problem. Inside the fluid the velocity satisfies DARCY'S law $v = -\nabla p$ and is incompressible $\nabla \cdot v = 0$. On the boundary of the fluid, surface tension controls the dynamics, $p = -\sigma\kappa$ where σ is the surface tension, and κ is the local curvature of the interface. The fluid is then dynamically evolved by its velocity (recovered from DARCY'S law). Near circular patches of fluid are known to relax back to a circle [15] however little analysis has been done on the problem when the patch is far from equilibrium.

Despite the apparent simplicity of the problem, there are many unanswered questions. For example, can finite time singularities occur, in which a connected region of fluid separates into two disconnected regions? This question has not been solved analytically, although there is numerical evidence for such behavior [1]. In particular, when the fluid tries to break, near the 'pinch off point' it exhibits a rather flat 'neck like' structure. This motivated analysis [14, 16] which a lubrication approximation reduced the nonlocal 2-D HELE SHAW problem into a 1-D local PDE for the thickness of the neck, $h(x, t)$:

$$h_t + (hh_{xxx})_x = 0. \quad (2)$$

Here x denotes position along the axis of the neck and t is time. In particular [16] considered special forcing boundary conditions and showed numerical evidence for a locally asymmetric finite time singularity in which the solution could be described by scaling and matched asymptotics. In [8] a second symmetric singularity was shown and in the work [2] a new third type of singularity is described along with the dynamical interactions of the three types in an unforced thin neck geometry. Related work described similar dynamics under the influence of gravity is described in [23, 24].

As in the droplet break up equations (1) solutions to (2) also seem to preserve the validity of the approximation up to the break up time. In particular, singularities are always observed to occur with bounded second derivative in h . To respect the approximation, we require the solution to have at least a bounded first derivative as a singularity forms. However, to date the best we can prove is a bounded $C^{1/2}$ HÖLDER norm [5].

3. Thin films, moving contact lines, and fourth order degenerate diffusion equations

Another physics problem which can be described by a fourth order PDE similar to (2) is that of a thin film on a solid surface. The subtlety in thin film dynamics is the modeling of the contact line, the triple juncture where the liquid/gas interface meets the solid boundary.

In the 1970's several studies of this problem [18, 28] made the following key observations: Given a Navier-Stokes fluid with a no slip boundary condition on the liquid/solid interface, the movement of a contact line necessarily produces an infinite energy dissipation in the bulk of the fluid. One can remove this singularity by enforcing a 'slip' condition on the liquid/solid interface. Other researchers have suggested including mesoscopic forces such as long range VAN DER WAALS interactions to describe ways to dissipate energy at the contact line.

A popular model for thin films is the weakening of the no-slip boundary condition on the liquid/solid interface by replacing it with a slip condition, usually of the form $v(z) = \lambda(h)v_z$. Here z is the direction perpendicular to the surface. The slip coefficient, λ , may in general depend on the local film height. It is simplest to assume power law dependence of λ on h , $\lambda \sim h^{p-2}$. A lubrication approximation, involves depth averaging the fluid velocity in the z direction. By approximating the curvature by Δh and assuming the pressure gradient is due to surface tension, one obtains for the highly viscous case, (see GREENSPAN [25]) a fourth order degenerate diffusion equation

$$h_t + \nabla \cdot ((h^3 + \beta h^p)\nabla \Delta h) = 0 \quad (3)$$

as an evolution equation for a film height h . Here the no-slip boundary condition gives $\beta = 0$ while the slip boundary condition introduces the additional term, βh^p , in the diffusion coefficient. Since (3) is degenerate as $h \rightarrow 0$ it is unclear what boundary conditions are required at the edge of the support. GREENSPAN proposed the need for two boundary conditions at the edge of the drop (contact line) due to the order of the equation. The first boundary condition is simply $h(x_0(t), t) = 0$ where x_0 is the 'contact line'. The second is a 'constitutive law' which determines the motion of x_0 as a function of the local properties of the solution at the edge, e.g. the local 'contact angle'. Several authors have studied this equation with such boundary conditions via numerical simulations [22, 26] and asymptotics [17, 27].

In the past few years, mathematicians have become interested in these lubrication equations and in particular the nature of the solution at the edge of its support. The simplest model equation assumes a power law in the diffusion coefficient,

$$h_t + \nabla \cdot (|h|^n \nabla \Delta h) = 0 \quad (4)$$

One obvious technical difficulty in understanding fourth order degenerate diffusion equations lies in the fact that there is no inherent maximum principle associated with the spatial operator, as in the case of the well-known ‘porous media equation’, the second order analogue of (4). This can pose problems when a physical solution to (4) demands that $h(x, t)$ remain nonnegative. It also naturally leads to two related mathematics problems: (a) the well-posedness of the initial value problem with nonnegative initial data and (b) the existence of finite time singularities in which an initially positive solution will extinguish at a point. These topics have the corresponding physical applications (a) a self-consistent model for the dynamics of thin films and (b) an understanding of the dynamics of thin film rupture or in the case of the HELE SHAW cell thin neck rupture. BERNIS and FRIEDMAN [5] considered (4) in one space dimension on a bounded domain and showed that the equation possesses a weak maximum principle for sufficiently large values of n ($n \geq 4$). This fact is proved by showing continuity of the solution from an a priori H^1 bound and a priori boundedness of an ‘entropy’ which takes the form of an integral of a power of h . They proved several existence results for nonnegative weak solutions. The two recent papers [3, 10] proved sharper results for the existence theory on bounded domains in one space dimension. In particular they showed that for $0 < n < 3$ a weak solution exists which has precisely the same regularity as a special ‘source type solution’ [6] for the equation. Moreover, [10] showed that for $3/8 < n < 3$, the weak solution satisfies the equation in a ‘sense of distributions’ with either two or three spatial derivatives on the test function. Both papers showed that as $t \rightarrow \infty$ the support of this particular weak solution increases to fill the entire domain. In contrast, for $n \geq 4$, any weak solution obtained by an approximation scheme has nonincreasing support [3]. It is interesting to note that $n = 3$ corresponds precisely to the case of the paradoxical no-slip boundary condition. The analysis to date strongly suggests that $n = 3$ is a critical exponent for the PDE (4) in 1D. In a recent announcement, BERNIS [4] shows that for $0 < n < 2$, the weak solutions constructed in [10, 3] have support with finite speed of propagation. This provides useful existence theory for the Cauchy problem on the line with compactly supported initial data. Numerical results [11] show that this solution tends to the source type solution from [6] as t increases. An important feature of these “strong” [4] solutions for the full equation (3) is that they model the phenomenon of complete wetting without imposing a ‘constitutive law’ at the contact line. We note however that such solutions have a ‘zero contact angle’ which could be thought of as an extra boundary condition.

Regarding finite time pinch off, the only proofs to date are for special situations with forcing boundary conditions (see e.g. [3]). For the HELE SHAW thin neck, ($n = 1$) the first papers to exhibit numerical evidence of both finite and infinite time singularities for a ‘pressure forced’ neck were [14, 16]. More recent numerical work has been done on this problem for the unforced neck [2] and for the gravity driven neck [23, 24]. The paper [8] is the most comprehensive account of numerical observations of finite time singularities in 1D for equation (4) for general n . Here the authors show that such singularities typically exhibit second type scaling. Another work analyzing the case of symmetric singularities in (4) and related equations is [7]. This paper reinforces the observation that second type scaling predominates in these singularities.

There are numerous open problems including (in 1D) a proof of singularity formation for an unforced system, well-posedness of the initial value problem with nonnegative data, and convergence onto the source type solution for the CAUCHY problem on the line. In 2D, very little is known about these equations. Some related problems include models with VAN DER WAALS attractions (see [9] and references therein) the interaction of surfactants [29, 32, 34] and the thin film and HELE SHAW problems with inertia (resp. [30, 16]). We expect to see a lot of exciting work on all of these problems over the course of the next decade.

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Convergence of Relaxation Schemes for Conservation Laws

We study a class of relaxing numerical schemes for conservation laws. Following the approach recently proposed by S. Jin and Z. Xin, we use a semilinear local relaxation approximation, with a stiff lower order term, and we construct some numerical first and second order accurate algorithms, which are uniformly bounded in the L^∞ and BV norms with respect to the relaxation parameter. The relaxation limit is also investigated

1. Introduction

In this contribution we shall present a new class of numerical schemes, which are based on the local relaxation approximation of conservation laws. Consider the equation

$$\partial_t u + \partial_x f(u) = 0, \quad (1)$$

for $(x, t) \in \mathbb{R} \times (0, \infty)$. Here f is a given (say C^1) smooth function.

We want to approximate this equation by a sequence of semilinear hyperbolic systems with a stiff relaxation term of the following type

$$\begin{cases} \partial_t u + \partial_x v = 0, \\ \partial_t v + a \partial_x u = -\frac{1}{\epsilon} (v - f(u)), \quad (\epsilon > 0) \end{cases} \quad (2)$$

when $\epsilon \rightarrow 0$ and for some $a > 0$ to be fixed later. This system is supplemented by the following initial data:

$$u(x, 0) = u_0(x), \quad v(x, 0) = f(u_0)$$

This kind of approximation was recently proposed in [9] in the general setting of the quasilinear systems of, possibly multidimensional, hyperbolic conservation laws. It possesses some very interesting features: finite speed of propagation, great generality (in particular it is possible to avoid the use of Riemann problems), strong physical motivations. In fact it is possible to trace back the origin of this approximation on one side from the investigations concerning hyperbolic conservation laws with relaxing source [15], [10], [3], [4]. In these papers the authors considered some relaxing models arising in applications and derived some stability conditions for convergence (see also the references therein).

On the other hand this approximation is strongly connected with the study of fluid-dynamical limits [2] and in particular for the discrete Boltzmann equations [14]. In fact the main idea here is to replace the physically underlying non-equilibrium Boltzmann kinetic, with an artificial “minimalist” model, which recovers in the limit the same equilibrium hydrodynamic configuration.

The analytical study of the stability and convergence to equilibrium of the solutions of 2 has been done in [11] (see also [12]). However, here we investigate some numerical questions arising by this approximation. Recall that, from a numerical point of view, hyperbolic conservation laws with stiff (relaxing) source were extensively studied in [7], [8], [13]. The main emphasis in these essentially computational investigations was on numerical schemes which can work in the unresolved domain, i.e.: when the relaxation parameter ϵ is small with respect to the time and space mesh-length.

Here we take advantage on the monotonicity properties of system 2, [11], [12], to prove some rigorous stability and convergence results. Let us write 2 in its Riemann (diagonal) coordinates:

$$\begin{cases} \partial_t w^\epsilon + \sqrt{a} \partial_x w^\epsilon = -\frac{1}{\epsilon} G(w^\epsilon, z^\epsilon) \\ \partial_t z^\epsilon - \sqrt{a} \partial_x z^\epsilon = \frac{1}{\epsilon} \tilde{G}(w^\epsilon, z^\epsilon), \end{cases} \quad (3)$$

where

$$G(w, z) = \frac{-w + z}{2} - f\left(-\frac{w + z}{2\sqrt{a}}\right), \quad (4)$$

and (w^ϵ, z^ϵ) are given by

$$w^\epsilon = -v^\epsilon - \sqrt{a} u^\epsilon, \quad z^\epsilon = v^\epsilon - \sqrt{a} u^\epsilon. \quad (5)$$

The main argument used in this paper is the following: under the subcharacteristic conditions [15], [10]:

$$|f'(u^\epsilon(x, t))| < \sqrt{a}, \quad (6)$$

the system 3 is a quasimonotone weakly coupled system (see [6]). Recall that the quasimonotonicity is a necessary and sufficient condition for a flow generated by a weakly coupled (diagonal) $N \times N$ system of semilinear hyperbolic equations to preserve the partial ordering in \mathbb{R}^N . So it is possible to use comparison arguments to establish uniform bounds.

Here we present first and second order numerical schemes preserving this property. This is done by considering a fractional-step scheme, where the homogeneous (linear) part is treated by some monotone or even higher order scheme (as the Goodman–LeVeque one) and then the source term is solved exactly.

In both cases we are able to prove the uniform stability with respect to ϵ of the schemes in the L^∞ , L^1 , BV norms and the convergence for fixed ϵ . Then we can prove that, for a fixed time step, the approximated solutions converge, as $\epsilon \rightarrow 0$, to the numerical approximations given by a TVD, L^∞ -stable discretization of the limit conservation law 1.

More details, complete statements, proofs and numerical tests can be found in [1].

2. The Scheme

For simplicity in this section we shall drop the superscript ϵ in our notations. Let us consider the Cauchy problem for the diagonal system 3 with initial data

$$w^\epsilon(x, 0) = w_0(x), \quad z^\epsilon(x, 0) = z_0(x). \quad (7)$$

Set $Z = (w, z)$ and $Z_0 = (w_0, z_0)$. For any given $\Delta t, \Delta x$ we fix $\lambda = \frac{\sqrt{a}\Delta t}{\Delta x}$ and construct the numerical approximation Z_Δ on a strip $\mathbb{R} \times [0, T]$ for 3–7, which is equal to Z_j^n on each interval $]x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}[\times [t_n, t_{n+1}[$, where $x_{j-\frac{1}{2}} = x_j - \frac{h}{2} \Delta x$, $x_j = j \Delta x$ and, setting $N\Delta t = [T] - 1$, $t_n = n \Delta t$, $n \in \{0, \dots, N\}$.

System 3 is splitted into a linear hyperbolic part and an ordinary differential system. For any given Z , $Z^{n+\frac{1}{2\epsilon}}$ is an approximate solution at time t_{n+1} of the system

$$\begin{cases} \partial_t w^\epsilon + \sqrt{a} \partial_x w^\epsilon = 0, \\ \partial_t z^\epsilon - \sqrt{a} \partial_x z^\epsilon = 0, \end{cases} \quad (8)$$

with initial condition at time $t = t_n$:

$$Z(t_n, x) = Z_\Delta^n(x).$$

The approximation $Z^{n+\frac{1}{2\epsilon}}$ is then obtained by discretizing each equation by two alternative ways. The first is a consistent monotone scheme written in the conservative form:

$$Z_j^{n+\frac{1}{2\epsilon}} = Z_j^n - \lambda(\phi_{j+\frac{1}{2}}^n - \phi_{j-\frac{1}{2}}^n) \quad (9)$$

where $\phi_{j+\frac{1}{2}}^n = (\varphi(w_{j-k+1}^n, \dots, w_{j+k}^n), -\psi(z_{j-k+1}^n, \dots, z_{j+k}^n))$, and φ, ψ are Lipschitz continuous fluxes. Generally we take the same scheme for each equation so that $\varphi = \psi$. Of course such a scheme is only first order accurate.

We also study the case of a second order Goodman–Leveque scheme [5]. Using standard notation we denote:

$$\begin{cases} \sigma_j^n = \frac{1}{\Delta x} \min\text{mod}(w_{j+1}^n - w_j^n, w_j^n - w_{j-1}^n) \\ \tau_j^n = \frac{1}{\Delta x} \min\text{mod}(z_{j+1}^n - z_j^n, z_j^n - z_{j-1}^n), \end{cases} \quad (10)$$

where the minmod function is defined by $\min\text{mod}(a, b) = \frac{1}{2}[\text{sgn}(a) + \text{sgn}(b)] \min(|a|, |b|)$.

Then the scheme may be written as:

$$\begin{cases} w_j^{n+\frac{1}{2}} = w_j^n - \lambda(w_j^n - w_{j-1}^n) - \frac{1}{2}\lambda(1-\lambda)\Delta x(\sigma_j^n - \sigma_{j-1}^n) \\ z_j^{n+\frac{1}{2}} = z_j^n - \lambda(z_{j+1}^n - z_j^n) - \frac{1}{2}\lambda(1+\lambda)\Delta x(\tau_{j+1}^n - \tau_j^n). \end{cases} \quad (11)$$

Note that the linear system is diagonal, so that the Riemann problem for a piecewise linear function can be solved exactly. The right-end side is treated in both cases by solving exactly on $[t_n, t_{n+1}]$ the problem:

$$\begin{cases} \omega' = \frac{1}{\epsilon}G_a(\omega, \zeta) \\ \zeta' = -\frac{1}{\epsilon}G_a(\omega, \zeta), \end{cases} \quad (12)$$

with the initial data at $t = t_n$:

$$\omega(t_n) = w_j^{n+1/2}, \quad \zeta(t_n) = z_j^{n+1/2}.$$

If we denote $S_t^a(\theta_0, (\omega_a, \zeta_0))$ the solution at time t of 12 with $(\omega(\theta_0), \zeta(\theta_0)) = (\omega_0, \zeta_0)$, Z_j^{n+1} is given by:

$$Z^{n+1} := S_{t_{n+1}}^a(t_n, Z_j^{n+1/2}). \quad (13)$$

It is possible to solve 12 exactly, which gives:

$$\begin{cases} w_j^{n+1} = w_j^{n+\frac{1}{2}} + (1 - e^{-\frac{\Delta t}{\epsilon}})G_a(w_j^{n+\frac{1}{2}}, z_j^{n+\frac{1}{2}}) \\ z_j^{n+1} = z_j^{n+\frac{1}{2}} - (1 - e^{-\frac{\Delta t}{\epsilon}})G_a(w_j^{n+\frac{1}{2}}, z_j^{n+\frac{1}{2}}). \end{cases} \quad (14)$$

3. Uniform Bounds

For the above schemes we are able to establish, thanks to our special monotonicity properties, the uniform bounds for the approximating solutions. Let us set

$$A = \sup_j |w_j^0|, \quad B = \sup_j |z_j^0|$$

and

$$C = \sup_{|\xi| \leq \frac{A+B}{2\sqrt{a_0}}} |f(\xi)| + \frac{A+B}{2}.$$

Theorem 1. *There exists a positive constant a_0 , which depends only on the initial data, such that if $a \geq a_0$, for all $n \in \{0, \dots, N\}$, it holds*

$$\|Z_\Delta^n\|_{L^\infty} \leq A + B + 2C. \quad (15)$$

Moreover

$$TV(Z_\Delta^{n+1}) \leq TV(Z_\Delta^n) \leq TV(Z_{(0)}). \quad (16)$$

Now, by coupling standard arguments with the particular properties of our schemes, we are able to give the following stability result in L^1 .

Theorem 2. *Let $Z_\Delta^\epsilon, \tilde{Z}_\Delta^\epsilon$ be two numerical approximations given by one of our schemes with respect to the initial data Z_0 and \tilde{Z}_0 respectively, with $\|\tilde{Z}_0\|_\infty \leq \|Z_0\|_\infty$. Then we have*

$$\|Z_\Delta^\epsilon(t) - \tilde{Z}_\Delta^\epsilon(t)\|_{L^1} \leq \|Z_0 - \tilde{Z}_0\|_{L^1};$$

$$\|Z_\Delta^\epsilon(t) - Z_\Delta^\epsilon(t')\|_{L^1} \leq C\sqrt{a}(\Delta t + |t - t'|)TV(Z_0).$$

4. Convergence Results

The above estimates allow us to prove the convergence of our numerical scheme. For this we reintroduce superscript ϵ in the notations.

Theorem 3. Let $\epsilon > 0$, $Z_0 \in L^1(\mathbb{R})^2 \cap L^\infty(\mathbb{R})^2 \cap BV(\mathbb{R})^2$, $a > a_0$. For any $T > 0$, $\lambda = \frac{\sqrt{a}\Delta t}{\Delta x}$ constant and $\Delta t \rightarrow 0$, $Z_\Delta^{(\epsilon)}$ converges to the unique solution $Z^{(\epsilon)}$ of 3-7 in $L^\infty(0, T; L^1(\mathbb{R})^2)$, $Z^{(\epsilon)} \in C^0([0, T], L^1(\mathbb{R})^2) \cap L^\infty(0, T; L^\infty(\mathbb{R})^2)$ and:

$$\begin{aligned} \sup_{t \in (0, T)} \|Z^{(\epsilon)}(t)\|_{L^1} &\leq \|Z_0\|_{L^1}; \\ \|Z^{(\epsilon)}(t) - Z^{(\epsilon)}(t')\|_{L^1} &\leq \left[C\sqrt{a} TV(Z_0) + \frac{1}{\epsilon \ln 2} \|v_0 - f(u_0)\|_{L^1} \right] |t - t'|; \\ \sup_{t \in [0, T]} \|v^\epsilon(t) - f(u^\epsilon(t))\|_{L^1} &\leq e^{-t/\epsilon} \|v_0 - f(u_0)\|_{L^1} + \epsilon TV(Z_0)(1 - e^{-T/\epsilon}). \end{aligned}$$

Next we are interested in the behaviour of the above numerical schemes as the relaxation parameter ϵ tends to zero. A good criteria to appreciate the quality of the numerical solution in the undersolved domain is that the relaxed scheme obtained by letting $\epsilon \rightarrow 0$ should be a stable and consistent discretization of the limit conservation law 1, [9].

Proposition 4. Let $\Delta t > 0$, $Z_0 \in L^1(\mathbb{R})^2 \cap BV(\mathbb{R})^2 \cap L^\infty(\mathbb{R})^2$, $T > 0$, $a > a_0$.

Then the approximating solution Z_Δ^ϵ converges in $L^\infty(0, T; L^1_{loc}(\mathbb{R})^2)$ to a limit Z_Δ which satisfies:

$$\|Z_\Delta(t)\|_{L^\infty(\mathbb{R})^2} \leq A + B + 2C \quad \forall t \in [0, T].$$

Moreover

$$\|Z_\Delta(t)\|_{L^1(\mathbb{R})^2} \leq \|Z_0\|_{L^1(\mathbb{R})^2};$$

and

$$\|Z_\Delta(t)\|_{L^1(\mathbb{R})^2} \leq CT.TV(Z_0) + \|Z_0\|_{L^1}.$$

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CHEN, G.-Q.

Relaxation Limit for Conservation Laws

We are concerned with the limit behavior of hyperbolic systems of conservation laws with stiff relaxation terms to the local systems of conservation laws as the relaxation time tends to zero. The connections of this limit problem with many important challenging problems in related areas are discussed. Some recent developments in this direction are reviewed and analyzed.

1. Introduction

There are two basic theories to describe the nonequilibrium phenomena in mechanics: kinetic theory from microscopic level and continuum theory from macroscopic level. Since the pioneering work of Hilbert [16] and Chapman-Enskog (cf. [5]), there have been many activities in studying the kinetic limits from the kinetic nonequilibrium processes to the continuum (equilibrium or nonequilibrium) processes with the aid of the moment closure techniques from kinetic theory and the kinetic formulation techniques from continuum theory (cf. [1,3,4,20,21,26,27,29,40,41]).

we are concerned with the relaxation limit of hyperbolic systems of conservation laws with stiff relaxation terms to the local systems, which models dynamic limit from the continuum and kinetic nonequilibrium processes to the equilibrium processes, as the relaxation time tends to zero. Typical examples for the limit include gas flow near thermo-equilibrium, viscoelasticity with vanishing memory, kinetic theory with small Knudsen number, and phase transition with small transition time. An important case is that the relaxation depends only on the local values of the basic dependent variables and can be modeled by the following hyperbolic system in the form:

$$\partial_t U + \nabla_x \cdot F(U) + \frac{1}{\epsilon} R(U) = 0, \quad x \in \mathbf{R}^D, \quad (1)$$

where $U = U(x, t) \in \mathbf{R}^N$ represents the density vector of basic physical variables. The relaxation term is endowed with an $n \times N$ constant matrix Q with rank $n < N$ such that $QR(U) = 0$. There are two basic types of relaxation terms: (I) the manifold of local equilibria is uniquely determined by n independent conserved quantities $u = QU$: $U = \mathcal{E}(u)$; (II) the dimension of the manifold of local equilibria equals the number, N , of equations in (1). The local equilibrium limit turns out to be highly singular because of shock and initial layers and to involve many challenging problems in nonlinear analysis and applied sciences. Roughly speaking, the relaxation time measures how far the nonequilibrium states are away from the corresponding equilibrium states; understanding its limit behavior is equivalent to understanding the stability of the equilibrium states. It connects nonlinear integral partial differential equations with nonlinear partial differential equations. This limit also involves the singular limit problem from nonlinear strictly hyperbolic systems to mixed hyperbolic-elliptic ones, even purely elliptic ones in some cases (see [8]). The basic issue for such a limit problem is the stability theory. In this article we focus on Type (I) relaxation terms in Sections 2-4. We remark Type (II) and related topics in Section 5.

2. Stability of Zero Relaxation Limit

In general, the zero relaxation limit is not stable even for the linear case: the characteristic speeds of the local system must be interlaced with the characteristic speeds of the relaxing system to ensure the stability of the limit. The same condition is true (see [28]) for the 2×2 quasilinear case to ensure that the local relaxation approximation is dissipative. This condition is referred to as the subcharacteristic condition by Liu [28]. This can be understood by improving upon the local relaxation approximation with the aid of the idea of Chapman-Enskog expansion for the kinetic theory. For $N \times N$ system (1), the use of the same spirit of Chapman-Enskog expansion leads to the following first order correction to the local relaxation approximation, which is the analogue of the compressible Navier-Stokes approximation in the kinetic theory:

$$\partial_t u + \nabla_x \cdot QF(\mathcal{E}(u)) = \epsilon \nabla_x \cdot [D(u) \nabla_x u], \quad (2)$$

where $D(u)$ is nonlinear 4-tensor in $\mathbf{R}^{N \times N} \otimes \mathbf{R}^{D \times D}$, which is very complicated. It is not generally clear that this first-order correction will be dissipative. It can be shown that this will be the case whenever the linear constant

coefficient problem obtained by linearizing the original problem about any absolute equilibrium $\mathcal{E}(\bar{u})$ is stable as $\varepsilon \rightarrow 0$. However, this is a cumbersome criterion to check.

In Chen-Levermore-Liu [8] we introduced a simple alternative criterion, namely, the existence of a strictly convex entropy Φ with corresponding entropy flux Ψ : For the case $R(U) = 0$, (Φ, Ψ) is consistent with the classical entropy-entropy flux (see Lax [25]); in order to be consistent with the relaxation terms, the entropy Φ is required to be locally dissipated and to characterize completely the local equilibria $\mathcal{E} = \mathcal{E}(u)$ in terms of Φ and \mathcal{Q} . This is a refinement of the notion of entropy introduced by Boltzmann into his kinetic theory to describe kinetic relaxation to fluid dynamics. His key observation was that his entropy characterizes the local equilibria of the kinetic equation, the celebrated H theorem (cf. [4]). We adopt the notion of entropy that shares all of above properties in the level of nonlinear hyperbolic systems of balance laws. In Chen-Levermore-Liu [8], we establish the following stability theory: The existence of strictly convex entropy Φ implies the followings: (a) The local equilibrium system is hyperbolic with a strictly convex entropy pair $(\phi(u), \psi(u)) = (\Phi, \Psi)|_{U=\mathcal{E}(u)}$; (b) The characteristic speeds of the local system are interlaced with the characteristic speeds of the original system (1); (c) The first-order correction is locally dissipative with nonnegative diffusion $D(u)$. For the 2×2 case, the pure dissipativity $D(u) > 0$ with the coupling condition (see [28]) is equivalent to the strict stability condition on the equilibrium curve. This leads to the converse of (a)-(c) as follows: Let (ϕ, ψ) be a strictly convex entropy pair for the local equilibrium equation. Assume that the subcharacteristic condition holds. Then there exists a strictly convex entropy pair (Φ, Ψ) for the 2×2 system (1) over an open set containing the local equilibrium curve, along which it takes $(\phi(u), \psi(u))$. For the converse, the strict stability criterion and the coupling condition imply that the local equilibrium curve is a noncharacteristic curve for the entropy equation, which is a second-order hyperbolic equation for which we pose the Cauchy data in the form $\Phi = \phi(u)$, $\partial_\nu \Phi = 0$ along the local equilibrium curve. The classical local existence theory ensures that there is a solution Φ of this Cauchy problem over an open domain containing the local equilibrium curve. Since the strict stability condition is satisfied along the local equilibrium curve, then it will also be satisfied in some open domain containing the local equilibria curve by continuity. In the stability theory, the convexity of entropy Φ is essential. The most physical systems with stiff relaxation term are endowed with a convex entropy. In the context, we refer to Levermore [26], where such systems are systematically derived via the moment closures from kinetic theory.

3. Convergence of Relaxation Limit

This limit is the compressible Euler type one and the solutions of the relaxation systems tend to those of the local relaxation approximation, which are inviscid conservation laws. This limit is highly singular because of shock and initial layers. The main difficulty is that the solutions of the full systems are only the measurable functions with certain boundedness. The most basic class of the systems is the 2×2 one. Consider uniformly bounded solutions $U^\varepsilon = (u^\varepsilon, v^\varepsilon) \in L^\infty$ of the 2×2 systems satisfying the entropy inequality in the sense of distributions. Assume that the strict stability condition holds and the subcharacteristic speed is monotone almost everywhere for the local variable $u \in \mathbf{R}$. The stability theory ensures the existence of such a strictly convex entropy. Then it is proved in [7,8] that U^ε strongly converging to (u, v) and the limit functions $(u(x, t), v(x, t))$ are on the equilibrium curve for almost all (x, t) , $t > 0$, where $u(x, t)$ is the entropy solution of the Cauchy problem for scalar conservation law with the Cauchy data $w^* - \lim u_0^\varepsilon(x)$ in L^∞ . We remark: (a) Notice that the initial data may even be far from equilibrium. The convergence result indicates that the limit functions (u, v) indeed come into local equilibrium as soon as $t > 0$. This shows that the limit is highly singular. In fact, this limit consists of two processes simultaneously: one is the initial layer limit, and the other is the shock layer limit. (b) The compactness of the zero relaxation limit indicates that the sequence U^ε is compact no matter how oscillatory the initial data are. Note that the relaxation systems are allowed to be linearly degenerate; the initial oscillations can propagate along the linearly degenerate fields for the homogeneous systems (cf. [6]). This fact shows that the relaxation mechanism coupling with the nonlinearity of the equilibrium equations can kill the initial oscillations, just as the nonlinearity for the homogeneous system can kill the initial oscillations. (c) The above discussions are based on the L^∞ a priori estimate. In many physical systems, the estimate can be achieved. Such examples include the p -system and models in viscoelasticity, chromatography, and combustion (see [7,8,37,41,33,39,22,31]), which have natural invariant regions. For some special models, even uniform BV bound of relaxation solutions $(u^\varepsilon, v^\varepsilon)$ can be achieved [39], which ensures the convergence of zero relaxation limit via the Helly principle.

4. Convergence of Weakly Nonlinear Relaxation Limit

The weakly nonlinear relaxation limit is the incompressible Navier-Stokes type one just as the limit from the Boltzmann equations to the incompressible Navier-Stokes equations [1]. The main observation is that the linearization of the local relaxation approximation about an equilibrium gives a simple advection dynamics with the equilibrium

characteristic speed. This can be understood in a formal fashion (see [8]). If one applies the same asymptotic scaling to the first correction to the local equilibrium approximation, one again arrives at the weakly nonlinear approximation. This shows that the latter is a distinguished limit of the former and makes clear why it inherits the good features of the former. Its advantage is that the solutions of the Burgers equation are smooth even for the case that the initial data are not smooth. Thus the solutions remain globally consistent with all the assumptions that were used to derive the weakly nonlinear approximation. In Chen-Levermore-Liu [8], this approximation is justified by using the stability theory and the energy estimate techniques. Linearized version of the limit is well understood which relates the "random walk" in Brownian motion (cf. [12,35,24]).

5. Relaxation Limit for the Systems with Type (II) Relaxation Terms

When the dimension of local equilibrium manifold is equal to the number of equations of the relaxation systems, the situation is different and our stability theory established in [8] can not be directly applied. Such systems arise from many physical areas including elastoplasticity and combustion. In [9] we established a similar stability theory and applied this theory to study the limit behavior of the zero relaxation limit for such systems. A notion of admissible weak solutions for the rate-independent systems as the limit functions of the zero relaxation limit is formulated. More details can be found in [9].

Remark 1. For the systems violating the strict stability criterion, the equilibrium speed may equal one of the frozen speeds. It is shown in Chen-Liu [7] for a model in phase transitions that no oscillation arises when the dissipation is present and goes to zero more slowly than the relaxation. It would be interesting to further investigate relaxation systems arising from various physical areas to understand how the feature of the failure of the strictly stability criterion affects the limiting behavior of zero relaxation and dissipation limits.

Remark 2. The relaxation systems with more than one local equilibrium manifold in the level of reaction-diffusion equations have been studied for the typical models (See [13,14,38] and references cited therein). It would be interesting to investigate the zero relaxation limit behavior of such relaxation systems in the level of reaction-convection equations, which are modeled by the hyperbolic conservation laws with stiff relaxation terms.

Remark 3. For the systems with stiff relaxation terms such that the corresponding dynamic systems $\partial_t U + \frac{1}{\epsilon} R(U) = 0$ are of limit circles, the situation is much more complicated. Such systems in the level of reaction-diffusion equations have been studied for some models (see [23,32] and references cited therein). One of interesting connections of such a limit with physics is the characterization of the Ginzburg-Landau vortices. Such a limit problem for stationary Ginzburg-Landau equations has been systematically studied in Bethuel-Brezis-Hélein [2]. It would be interesting to study the zero relaxation limit behavior for the hyperbolic systems with such stiff relaxation terms.

Remark 4. It is natural to use the relaxation methods to construct shock capturing schemes to calculate the numerical solutions to the local systems. Some efforts have been made in this direction with the aid of the stability theory of local relaxation limit (See [17,18,19,33,42]). Such ideas closely relate to those of the kinetic schemes.

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Uniform Convergence to Equilibrium for Conservation Laws with Relaxation

We study the solutions to the Cauchy problem for 2×2 semilinear and quasilinear hyperbolic systems with a singular relaxation term. A special comparison principle is established, by assuming the subcharacteristic condition, which yields uniform bounds and compactness properties of the sequence of the solutions. Therefore we can prove the convergence to equilibrium of these solutions as the singular perturbation parameter tends to zero.

1. Introduction

In this talk we present some new results concerning the relaxation behaviour of the following system of hyperbolic conservation laws with a singular perturbation source

$$\begin{cases} \partial_t u + \partial_x v = 0, \\ \partial_t v + \partial_x \sigma(u) = -\frac{1}{\epsilon} (v - f(u)) \quad (\epsilon > 0) \end{cases} \quad (1)$$

for $(x, t) \in \mathbb{R} \times (0, \infty)$. Here σ, f are some given smooth functions such that $\sigma'(u) \geq \nu$ ($\nu > 0$).

The sequence of solutions is expected to converge, as the relaxation parameter ϵ tends to zero, to some solution of the equilibrium (or reduced) equation

$$\partial_t u + \partial_x f(u) = 0, \quad v = f(u). \quad (2)$$

This model was proposed, in the semilinear case $\sigma(u) = \alpha u$, in [8] for numerical purposes. It supplies a new and powerful framework for the approximation of equilibrium conservation laws, which possesses some important properties: simplicity and generality, finite speed of propagation, regularity of the approximating solutions. It was shown in [8], by providing some very interesting numerical tests, that, for computational purposes, general systems of higher dimensions can be treated in the same way as the scalar one-dimensional equation. The main advantage of the linear hyperbolic structure of the relaxing systems lies in fact in the possibility to avoid the resolution of the Riemann problems in the approximation of conservation laws.

The relaxation limit for 2×2 systems of conservation laws was first analyzed by Liu [12], who justified some non linear stability criteria for diffusion waves, expansion waves and traveling waves. The main stability criterium (or *subcharacteristic condition*) can be (formally) derived by using the Chapman-Enskog expansion and reads as follows:

$$|f'(u)| \leq \sigma'(u). \quad (3)$$

This condition was first recognized by Whitham [19], and largely justified as long as the solutions of the equilibrium equation 2 are smooth see for example [16], [18] and references therein. Unfortunately, in the general case, these solutions may become discontinuous in a finite time. The rigorous justification of the relaxation approximation to equilibrium solutions containing shock waves was started in [2] and [3], where the authors considered some special models, including the system 1, by using the methods of compensated compactness [17], [5]. They proved that uniformly bounded sequences of perturbed solutions converge strongly to some weak equilibrium solutions as the relaxation parameter tends to zero, when the subcharacteristic condition 3 is verified, for initial data close to the equilibrium. Observe that, for system 1, the uniform boundedness of relaxing solutions was recovered only by truncating the function f out of a bounded set. On the contrary one of the main results of this paper is to show that uniform estimates are just a consequence of the stability condition 3.

Here we shall present some rigorous results on this problem in the semilinear case. Nevertheless, let us observe that the uniform boundedness of the solutions, with respect to the relaxation parameter ϵ , can be recovered by using similar arguments also in the quasilinear case. First we show that there exists a constant $\alpha_0 > 0$, only depending on the L^∞ norm of the initial data and on the flux function f , such that for any $\alpha \geq \alpha_0$ the solutions of the relaxing problems are uniformly bounded (independently on ϵ). This follows by using some comparison tools developed in [7]. In fact it is possible to show that the stability condition 3 is actually equivalent to the quasimonotonicity condition

(see below), which yields the monotone properties of the problem. Observe also that, for this problem, it is not possible to apply the standard theory of the invariant regions of [4], usually employed to establish L^∞ estimates.

Next we can show that the same stability condition implies also the compactness properties of the approximating sequence: uniform estimates on the L^1 modulus of continuity in space and equicontinuity in time with values in L^1 . This yields the strong convergence to the equilibrium.

Finally we investigate the *entropy* properties of the equilibrium limit [9], [10]. The checking of these conditions is found to be quite delicate for the presence of the singular perturbation term on the right-hand side. It turns out that in general some slight supplementary assumptions on the flux function f are needed to establish entropy inequalities for the limit function.

Let us note that our approach shares some ideas with the kinetic approximations and the related fluid dynamical limits. In particular we found some analogies with the artificial kinetic approximations to conservation laws given in [6], [15] and [11].

Finally let us point out that related first and second order numerical schemes, which incorporate the monotonicity properties of the approximation 1, are studied in [1]. More details and proofs about the results presented here can be found in [14].

2. Main Results

Let us restrict to the following Cauchy problem

$$\begin{cases} \partial_t u + \partial_x v = 0, \\ \partial_t v + \alpha \partial_x u = -\frac{1}{\epsilon} (v - f(u)), \quad (\epsilon > 0), \end{cases} \quad (4)$$

with the initial conditions

$$u^\epsilon(x, 0) = u_0^\epsilon(x) \quad , \quad v^\epsilon(x, 0) = v_0^\epsilon(x). \quad (5)$$

Assume

(H₁) f is a locally Lipschitz continuous function (for simplicity let us assume $f(0) = f'(0) = 0$);

(H₂) the functions $(u_0^\epsilon, v_0^\epsilon)$ verify $v_0^\epsilon = f(u_0^\epsilon)$, for all $\epsilon > 0$, and are uniformly bounded in $L^\infty(\mathbb{R})^2$ by

$$N_0 = \max \left(\sup_{\epsilon > 0} \|u_0^\epsilon\|_\infty, \sup_{\epsilon > 0} \|v_0^\epsilon\|_\infty \right)$$

Moreover the sequence $(u_0^\epsilon, v_0^\epsilon)$ converges in $L^1_{loc}(\mathbb{R})^2$ to some limit $(\bar{u}_0, f(\bar{u}_0)) \in L^\infty(\mathbb{R})^2$, as $\epsilon \rightarrow 0^+$.

It is obviously also possible to deal with initial data not verifying the assumption (H₂), with a suitable treatment of the initial boundary layer.

Finally let us denote, for any $N > 0$,

$$F(N) := \sup_{|\xi| \leq N} |f(\xi)|,$$

$$B(N) := 2N + F(2N),$$

and

$$M(N) := \sup_{|\xi| \leq B(N)} |f'(\xi)|.$$

First we give our main global existence and boundedness result for the Cauchy problem 4–5. A similar result, but using very different arguments, can be found in [13].

Theorem 1. Assume (H₁) and (H₂). For any $N_0 > 0$ and $\epsilon > 0$, if

$$\sqrt{\alpha} > M(N_0), \quad (6)$$

then there exists a unique globally bounded solution (u^ϵ, v^ϵ) to 4-5 in $C([0, \infty); L^1_{loc}(\mathbb{R})^2)$ and we have

$$\|v^\epsilon \pm \sqrt{\alpha} u^\epsilon\|_{L^\infty(\mathbb{R} \times (0, \infty))} \leq \sqrt{\alpha} B(N_0). \quad (7)$$

Moreover there holds the subcharacteristic inequality

$$|f'(u^\epsilon(x, t))| < \sqrt{\alpha} \quad (8)$$

for all $\epsilon > 0$ and for almost every $(x, t) \in \mathbb{R} \times (0, \infty)$.

The key point in the above result is the monotonicity properties of the system under the subcharacteristic condition 8. Let us recall that, if Ω is a convex subset of \mathbb{R}^N , a function $G : \Omega \rightarrow \mathbb{R}^N$ is quasimonotone (non decreasing) if each component g_i of G is non decreasing in u_j for $i \neq j$. The quasimonotonicity is a necessary and sufficient condition for a flow generated by a weakly coupled (diagonal) systems of semilinear hyperbolic equations to preserve the partial ordering in \mathbb{R}^n (see [7] and references therein for more details in the general quasilinear weakly coupled case). In particular consider the general $N \times N$ system

$$\partial_t U + A \partial_x U = G(U). \quad (9)$$

Here U is a vector-valued function and A is a $N \times N$ diagonal matrix. Let U and \tilde{U} be two weak solutions in $(x, t) \in \mathbb{R} \times (0, T)$ of the Cauchy problem for the initial data U^0 and \tilde{U}^0 respectively and let G be quasimonotone. If $U^0 \leq \tilde{U}^0$ for almost every $x \in \mathbb{R}$, then $U \leq \tilde{U}$ for almost every $(x, t) \in \mathbb{R} \times (0, T)$. Now the main step in the proof of the above result is the fact that the right-hand side in 4 (in the Riemann coordinates) is quasimonotone if and only if the subcharacteristic condition 8 is verified.

Next let us state some stability results for the solutions of 4-5.

Theorem 2. *Under the assumptions of Theorem 1, let $\sqrt{\alpha} > M(N_0)$ and $\epsilon > 0$. Let (u^ϵ, v^ϵ) and $(\tilde{u}^\epsilon, \tilde{v}^\epsilon)$ be the solutions of 4-5 for the initial data $(u_0^\epsilon, v_0^\epsilon)$ and $(\tilde{u}_0^\epsilon, \tilde{v}_0^\epsilon)$ respectively. Then, for any interval $(a, b) \subseteq \mathbb{R}$ and for every $t \geq 0$ we have*

$$\begin{aligned} & \int_a^b |u^\epsilon(x, t) - \tilde{u}^\epsilon(x, t)| + |v^\epsilon(x, t) - \tilde{v}^\epsilon(x, t)| dx \\ & \leq \frac{(1+\sqrt{\alpha})^2}{\sqrt{\alpha}} \int_{a-\sqrt{\alpha}t}^{b+\sqrt{\alpha}t} |u_0^\epsilon(x) - \tilde{u}_0^\epsilon(x)| + |v_0^\epsilon(x) - \tilde{v}_0^\epsilon(x)| dx. \end{aligned}$$

Again the key point in the proof is the condition 8. Moreover, as a consequence of the above results, it is possible to obtain some compactness properties of the sequence $\{(u^\epsilon, v^\epsilon)\}$: uniform estimates on the L^1_{loc} modulus of continuity in space and equicontinuity in time with values in L^1_{loc} , see [14] for more details and proofs.

Also it turns out that, as $\epsilon \rightarrow 0^+$, the sequence $\{(u^\epsilon)\}$ converges towards the entropy solution $w = w(x, t)$, in the sense of Kruzkov [9], of the scalar problem

$$\partial_t w + \partial_x f(w) = 0, \quad (10)$$

for $(x, t) \in \mathbb{R} \times (0, \infty)$, with the initial condition

$$w(x, 0) = w_0(x), \quad (11)$$

for $x \in \mathbb{R}$. More precisely we have the following statement.

Theorem 3. *Assume (H_1) , (H_2) and 6 and let (u^ϵ, v^ϵ) be the global solution to problem 4-5 given by Theorem 1. Then there exists a weak solution w to 10-11 and a subsequence, still denoted (u^ϵ, v^ϵ) , such that*

$$u^\epsilon \rightharpoonup w \quad \text{in } C([0, \infty); L^1_{loc}(\mathbb{R})), \quad (12)$$

$$v^\epsilon \rightharpoonup f(w) \quad \text{in } C([0, \infty); L^1_{loc}(\mathbb{R})), \quad (13)$$

as $\epsilon \rightarrow 0^+$.

Assume moreover that one of the following hypothesis holds true:

1. $\sup_{u \in \mathbb{R}} |f'(u)| < \infty$;

2. $f \in C^2$ and there is $M > 0$ such that if $|u| \geq M$, then $|f''(u)| > 0$.

Then, for every $N_0 > 0$ there exists $\alpha_0 > 0$, with $\sqrt{\alpha_0} > M(N_0)$, such that, for any $\alpha \geq \alpha_0$ the weak solution w of 10–11, given by the first part of the statement, is actually an entropy solution.

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Local minimizers and phase transformations

We discuss a metastability problem arising in martensitic phase transformations, for which it can be proved that hysteresis occurs as a consequence of the geometric incompatibility between the parent and nucleating phases. This result does not follow from the existing general theory of local minimisers in the calculus of variations.

1. A metastability problem arising in martensitic phase transformations

We consider the following apparently simple problem of the calculus of variations. Let $\Omega \subset \mathbb{R}^n$ be a bounded domain, and let

$$I(y) = \int_{\Omega} f(Dy(x)) dx$$

for mappings $y : \Omega \rightarrow \mathbb{R}^m$. Here $Dy(x) = \left(\frac{\partial y_i}{\partial x_j}(x) \right)$ denotes the gradient of $y = (y_1, \dots, y_m)$ at $x = (x_1, \dots, x_n)$, and $f : M^{m \times n} \rightarrow \mathbb{R}$ is continuous, where $M^{m \times n}$ denotes the space of real $m \times n$ matrices. We suppose that f has two unequal energy wells; that is, there exist distinct matrices A, B which are strict local minimizers of f with $f(B) < f(A)$.

For $1 \leq p \leq \infty$ we consider the Lebesgue space $L^p = L^p(\Omega; \mathbb{R}^m)$ of mappings $y : \Omega \rightarrow \mathbb{R}^m$ with norm $\|\cdot\|_{L^p}$, and the usual Sobolev space of such mappings $W^{1,p} = W^{1,p}(\Omega; \mathbb{R}^m)$ with norm $\|\cdot\|_{W^{1,p}}$.

Question

Is $\bar{y}(x) := Ax$ a local minimizer of I in X , where $X = W^{1,p}$ or L^p ?

That is, does there exist $\varepsilon > 0$ such that $I(y) \geq I(\bar{y})$ if $\|y - \bar{y}\|_X < \varepsilon$? Note that we impose no boundary conditions; in particular, if \bar{y} is a local minimizer so is $\bar{y} + c$ for any constant vector c .

If $X = W^{1,\infty}$ then the answer to the question is clearly yes, since if $\|y - \bar{y}\|_{W^{1,\infty}}$ is sufficiently small $Dy(x)$ is uniformly close to A , hence $f(Dy(x)) \geq f(A)$ a.e. in Ω , from which $I(y) \geq I(\bar{y})$ follows by integration. However, if $X = W^{1,p}$ with $1 \leq p < \infty$, or if $X = L^p$ with $1 \leq p \leq \infty$ the answer is not immediately obvious, since however small $\|y - \bar{y}\|_X$ is there can be a (small) subset of Ω where $Dy(x)$ is close to B , and in this subset $f(Dy(x)) < f(A)$.

The above problem arises in the mathematical modelling of the bi-axial loading experiments of Chu & James [1, 9, 10] on single CuAlNi crystals. In this case $m = n = 3$, $y(x)$ denotes the deformed position of the material point $x \in \Omega$ of the crystal in its reference configuration, and $f = f_{\lambda}$, where

$$f_{\lambda}(F) = \varphi(F) - T(\lambda) \cdot F. \quad (1)$$

In (1) φ denotes the free-energy function of the crystal (at the temperature at which the experiments were conducted, this being less than the critical temperature at which CuAlNi undergoes a cubic to orthorhombic phase transformation) and $T(\lambda)$ is a 3×3 matrix depending on a real loading parameter λ . Thus

$$I(y) = \int_{\Omega} [\varphi(Dy(x)) - T(\lambda) \cdot Dy(x)] dx,$$

the second term representing the potential energy of the loading device.

For appropriate loading paths f_{λ} has local minimizers $A(\lambda), B(\lambda)$ which respectively lie very close to two different components $SO(3)U_1$ and $SO(3)U_2$ of the set of matrices $\cup_{i=1}^6 SO(3)U_i$ minimizing φ (different components $SO(3)U_i$ representing different variants of the martensite). At a critical value λ_c there is an exchange of stability, so that

$$\begin{aligned} f_{\lambda}(A(\lambda)) &< f_{\lambda}(B(\lambda)) \text{ for } \lambda < \lambda_c \\ f_{\lambda}(A(\lambda)) &> f_{\lambda}(B(\lambda)) \text{ for } \lambda > \lambda_c. \end{aligned}$$

In the experiments it is, however, observed that the homogeneous deformation

$$\bar{y}_\lambda(x) = A(\lambda)x$$

remains stable in some interval $\lambda_c \leq \lambda \leq \lambda_c + \delta$, $\delta > 0$, suggesting that \bar{y}_λ is a local minimizer in this interval. As λ increases further the specimen transforms to the new variant having gradient $B(\lambda)$. This metastability implies that the transformation between variants occurs with *hysteresis*. For details of this and the mathematical model see Ball, Chu & James [3, 4].

2. The general problem of local minimizers in the calculus of variations

What can general theory tell us about the problem described in §1? Suppose we are given the more general integral

$$I(y) = \int_{\Omega} f(x, y(x), Dy(x)) dx$$

where $\Omega \subset \mathbb{R}^n$ is a bounded domain with boundary $\partial\Omega$ and where we assume for simplicity that f is smooth. We suppose that the admissible mappings $y : \Omega \rightarrow \mathbb{R}^m$ are subjected to the boundary condition

$$y|_{\partial\Omega_1} = g, \tag{2}$$

where g is a given mapping and where $\partial\Omega_1 \subset \partial\Omega$. No boundary condition is imposed on $\partial\Omega_2 = \partial\Omega \setminus \partial\Omega_1$. We ask the

Question

What are necessary, and what are sufficient, conditions for a given (sufficiently smooth) \bar{y} to be a local minimizer of I subject to (2) in X , where $X = W^{1,p}$ or L^p ?

Clearly, we want the sufficient conditions to be as close to the necessary ones as possible. *If $m > 1, n > 1$ this is a completely open question.* Even for $m = n = 1$ there remain unresolved issues, especially if \bar{y} is not smooth (even $\bar{y} \in W^{1,\infty}$ is outside standard theory).

To illustrate the difficulties, consider the case of $X = W^{1,p}$ with $1 \leq p < \infty$. Here four necessary conditions for $\bar{y} \in C^1$ to be a local minimizer in $W^{1,p}$ are known. They are the *weak form of the Euler–Lagrange equation*

$$\frac{d}{dt} I(\bar{y} + t\varphi) |_{t=0} = 0$$

for all smooth φ with $\varphi|_{\partial\Omega_1} = 0$, the *positivity of the second variation*

$$\frac{d^2}{dt^2} I(\bar{y} + t\varphi) |_{t=0} \geq 0$$

for the same φ , and the conditions of *quasiconvexity* at $Dy(x)$ for $x \in \Omega$ (see [13, 2, 7]) and *quasiconvexity at the boundary* for points $x \in \partial\Omega_2$ (see [7]). It is not known whether these conditions (suitably strengthened) are sufficient for \bar{y} to be a local minimizer in $W^{1,p}$.

If $m = 1$ or $n = 1$ the quasiconvexity conditions turn into convexity conditions and with suitable strengthenings the above four conditions become sufficient. In the case $m \geq 1, n = 1$ this is the classical *fundamental sufficiency theorem* of the calculus of variations, usually proved via the field theory of the calculus of variations (see, for example, [8]). There is also the ‘indirect sufficiency proof’ of Hestenes [11], recently made ‘direct’ in Ball & James [5]. The conclusion of the fundamental sufficiency theorem is in fact the stronger one that \bar{y} is a local minimizer in L^∞ . The case $m = 1, n \geq 1$ is discussed by Morrey [14] for the case when $\partial\Omega_1 = \partial\Omega$; the case of general mixed boundary conditions perhaps has not been treated explicitly in the literature but would seem not to pose essential difficulties.

The lack of a satisfactory answer for the case $m > 1, n > 1$ means that we cannot hope to apply general theory to the problem posed in §1. Even if appropriate strengthening of the above four necessary conditions into a set of sufficient conditions were achieved, it might in practice not be of much use due to our lack of understanding of how to verify the quasiconvexity conditions, a difficulty reinforced by the counterexample of Šverák [15].

3. Incompatibility-induced local minimizers

We return to the question posed in §1. A necessary condition (which in fact follows from quasiconvexity of f at A) for $\bar{y} = Ax + c$ to be a local minimizer in $W^{1,p}$ for $1 \leq p < \infty$ or in L^p for $1 \leq p \leq \infty$ is that there does not exist

C with $\text{rank}(A - C) = 1$ and $f(C) < f(A)$. In particular, $\text{rank}(A - B) > 1$. To see this, suppose $A - C = a \otimes N$ for nonzero vectors $a \in \mathbb{R}^m$, $N \in \mathbb{R}^n$, with $f(C) < f(A)$. Introduce a thin layer with normal N in which $Dy = C$ and outside which $Dy = A$. This reduces the energy and y can be made arbitrarily close to \bar{y} by choosing the layer thickness sufficiently small.

So suppose A and B are incompatible, i.e. $\text{rank}(A - B) > 1$. Then we have the following

Theorem 1. *Let $\text{rank}(A - B) > 1$, and let Ω satisfy the cone condition. Suppose we have a family of integrands $f(\tau, F)$ depending on a real parameter τ , defined and continuous for $|\tau| \leq \tau_0$, $F \in M^{m \times n}$, and satisfying*

$$f(0, A) = f(0, B) = 0,$$

$$f(0, C) > 0 \text{ if } C \neq A \text{ or } B$$

together with the growth condition

$$f(\tau, F) \geq c_0 |F|^p - c_1, \quad \text{for } |\tau| \leq \tau_0, F \in M^{m \times n}$$

for constants $p > 1, c_0 > 0$ and c_1 . For a fixed $\delta > 0$ sufficiently small ($\delta = \frac{1}{2}|A - B|$ will do) let $F = A(\tau)$ minimize $f(\tau, F)$ subject to $|F - A| \leq \delta$. Then there exist $\varepsilon > 0, \sigma > 0$ such that if $|\tau| \leq \varepsilon, c \in \mathbb{R}^m$ and

$$\|y - A(\tau)x - c\|_{L^1} \leq \sigma$$

then

$$\int_{\Omega} f(\tau, Dy) dx \geq \int_{\Omega} f(\tau, A(\tau)) dx.$$

The intuition behind the theorem is that in order to reduce the energy and stay close to $\bar{y}_\tau(x) = A(\tau)x + c$ in L^1 we need to nucleate a small amount of the new phase represented by matrices near B . But B is incompatible with $A(\tau)$ and so there must be a transition layer where Dy takes values far away from A, B , and the increase of energy in this layer will exceed the reduction of energy due to the introduction of the new phase. For a related but weaker result see Kohn & Sternberg [12]. The proof of the theorem uses results on Young measures of gradients and a covering lemma. Some condition on the regularity of $\partial\Omega$ is essential. A more general version of the theorem, in which the matrices A, B are replaced by Young measure disjoint sets, in which f can take infinite values, and in which the competing deformations can possess microstructure, can be found in [6]. In fact the last two of these more general hypotheses are important for making clear the connection with the experiments of Chu & James (see [4]).

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MICHEL CHIPOT AND DAVID KINDERLEHRER

Analysis and Computation in Non-convex Well Problems

We study minimization problems associated with non-convex energy densities with multiple potential wells, and, in particular, we investigate the question the numerical analysis of the minimizing sequences.

1. Introduction

Let us denote by φ an energy density

$$\varphi : M^{m \times n} \rightarrow \mathbb{R}^+ \quad (1)$$

($M^{m \times n}$ denotes the space of $m \times n$ matrices, $m=n=2$ or 3 in the applications). We assume, for instance to describe some natural states of an ordered material, that

$$\varphi(W_1) = \varphi(W_2) = \dots = \varphi(W_k) = 0 \quad (2)$$

i.e. φ has some wells. For Ω a polyedral domain of \mathbb{R}^n with boundary Γ , $A \in M^{m \times n}$ let us consider

$$W_A^{1,\infty}(\Omega) = \{v = (v^1, \dots, v^m)^T : v^i \in W^{1,\infty}(\Omega) \ \forall i = 1, \dots, m, v(x) = Ax \text{ on } \Gamma\}.$$

It is well known (see [11]) that

$$\inf_{W_A^{1,\infty}(\Omega)} \int_{\Omega} \varphi(\nabla v(x)) \, dx = |\Omega| Q\varphi(A) \quad (3)$$

where $|\Omega|$ denotes the Lebesgue measure of Ω , $Q\varphi$ the quasiconvex envelope of φ .

If one is interested in computing $Q\varphi$ numerically one can consider a regular triangulation τ_h of Ω with simplices of diameters less than h . If K is a simplex of τ_h we denote by $P_1(K)$ the space of polynomials of degree 1 on K and set

$$V^h = \{v = (v^1, \dots, v^m)^T : \Omega \rightarrow \mathbb{R}^m, \text{ continuous, } v^i|_K \in P_1(K) \ \forall K \in \tau_h, \ \forall i = 1, \dots, m\},$$

$$V_A^h = \{v \in V^h \mid v = Ax \text{ on } \Gamma\}$$

($v|_K$ denotes the restriction of v to K). Then the discrete analogue of (3) is given by

$$\inf_{V_A^h} \int_{\Omega} \varphi(\nabla v(x)) \, dx = |\Omega| Q_h \varphi(A). \quad (4)$$

So, one way to compute $Q\varphi(A)$ would be to compute the right hand side of (4) since it can be shown (see [2]) that for every A

$$\lim_{h \rightarrow 0} Q_h \varphi(A) = Q\varphi(A).$$

We will not pursue this question here (cf. also [12]). A more delicate issue is to get estimates of $Q_h \varphi(A) - Q\varphi(A) \geq 0$ in terms of the mesh size h . Except in the scalar case, i.e. when $m = 1$ (see [2]) very little is known. In order to attack the problem one has to consider first the case

$$A \in Co(W_i)$$

where $Co(W_i)$ denotes the convex hull of the W_i 's. Somehow, in this case, the study of

$$\inf_{W_A^{1,\infty}(\Omega)} \int_{\Omega} \varphi(\nabla v(x)) \, dx$$

is of independent interest (see for instance [1], [6] for physical motivations).

2. Energy estimate

The best result available up to now in the direction mentioned above is the following (see [5])

Theorem 1. *Assume that (1), (2) hold and that φ is a Borel function bounded on bounded subset of $M^{m \times n}$. Moreover, assume that*

$$\text{the wells } W_i \text{ are pairwise rank one compatible,} \quad (5)$$

then there exists a constant C such that

$$\inf_{v \in V_A^h} \int_{\Omega} \varphi(\nabla v(x)) \, dx \leq C \cdot h^{\frac{1}{2}}. \quad (6)$$

For a proof we refer the interested reader to [5]. To give some insight on the role of the assumption (5), let us just recall that due to the Hadamard compatibility condition one can build piecewise affine functions having their gradients on the wells W_i on some domain relatively large with respect to the mesh size of our grid (see for instance the next section for a similar construction).

In the case where one drops the rank one compatibility condition, there is no general estimate. To see the difficulties involved let us consider the so called four-well problem.

If

$$M = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}$$

denotes a generic element of $M^{2 \times 2}$, let us consider in the x_{11}, x_{22} -plane the wells

$$W_1 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad W_2 = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}, \quad W_3 = \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix}, \quad W_4 = \begin{pmatrix} -2 & 0 \\ 0 & 1 \end{pmatrix}.$$

This arrangement of "wells" has been first introduced by L. Tartar for separately convex functions and then found independently by R. James and R. Kohn. One sees immediately that they are rank-one incompatible i.e.

$$Rk(W_i - W_j) > 1 \quad \forall i \neq j.$$

Let us denote by $\varphi : M^{2 \times 2} \rightarrow \mathbb{R}^+$ a continuous function vanishing at these wells and such that

$$\varphi(W) > 0 \quad \forall W \neq W_i.$$

For $\Omega \subset \mathbb{R}^2$ a bounded polygonal domain with boundary Γ . Consider the problem

$$\inf_{W_0^{1, \infty}(\Omega)} \int_{\Omega} \varphi(\nabla v(x)) \, dx. \quad (7)$$

First if one computes the above infimum one sees that it is 0 and it is not achieved. So, we can turn to the study of the uniformly bounded minimizing sequences. We can show that they all share the following properties:

-they all converge toward 0 uniformly in Ω ,

-they all define the same Young measure $= \frac{1}{4} \sum_{i=1}^4 \delta_{W_i}$.

The first point could be expressed by saying that the limit deformation in (7) is 0, the second that the microstructure associated with (7) is unique (see [6]). If now we consider the approximated problem

$$\inf_{V_0^h} \int_{\Omega} \varphi(\nabla v(x)) \, dx$$

we see that in order to obtain estimates in term of h we need to construct a sequence v_h such that $v_h \rightarrow 0$, ∇v_h uses at the limit each of the wells with the same probability. This is not an easy task. Even a computer is reluctant to

seek numerically the appropriate minimizing sequence (cf. [7]) and it is a challenging question to determine what kind of information it needs in order to find its way and not get stuck at some local minima. To conclude this note we would like to mimic this four-well problem by a simpler one having some of its features and present a simple way to build minimizing sequences.

3. Constructing minimizing sequences

Let us assume that Ω is a bounded polygonal domain of \mathbb{R}^2 . Then let us show that

$$\inf_{V_0^h} \int_{\Omega} v_x^2 + (v_y^2 - 1)^2 \, dx dy \leq Ch^{\frac{1}{2}}$$

which is in this case (6). Our functional

$$\varphi(\xi_1, \xi_2) = \xi_1^2 + (\xi_2^2 - 1)^2$$

has two wells on $M^{2 \times 1}$

$$W_1 = -W_2 = (0, 1)^T.$$

First, note that there is no loss of generality in assuming $h < 1$. Let \hat{u}_h be the function periodic of period $2h^\alpha$ in the y direction and defined by

$$\hat{u}_h(x, y) = \begin{cases} y & \text{for } 0 \leq y \leq h^\alpha \\ -y + 2h^\alpha & \text{for } h^\alpha \leq y \leq 2h^\alpha. \end{cases} \tag{8}$$

One has clearly

$$\int_{\Omega} (\hat{u}_h)_x^2 + ((\hat{u}_h)_y^2 - 1)^2 \, dx dy = 0.$$

However, $\hat{u}_h \notin V_0^h$ since the boundary conditions are not matched and also they are some triangles where \hat{u}_h fails to be affine. In order to correct this, one introduces

$$\hat{u}'_h = \hat{u}_h \wedge \text{dist}(\cdot, \Gamma) \tag{9}$$

where \wedge denotes the minimum of two numbers, and $\text{dist}(\cdot, \Gamma)$ the distance to the boundary Γ of Ω . Finally one sets

$$u_h = \text{the interpolate of } \hat{u}'_h \tag{10}$$

i.e. the unique function of V_0^h that agrees with \hat{u}'_h at the nodes of the triangulation. It is easy to check that

$$0 \leq u_h, \hat{u}'_h, \hat{u}_h \leq h^\alpha.$$

Moreover,

$$\nabla u_h = W_1 \text{ or } W_2$$

(see (8)-(10)) except in a neighbourhood N_1 of Γ where u_h could be equal to $\text{dist}(\cdot, \Gamma)$ and in a neighbourhood N_2 of thickness $2h$ around the lines $y = k.h^\alpha$, $k \in \mathbb{Z}$ where interpolation takes place. If $|\Gamma|$ denotes the measure of Γ , i.e. its length, and $|\cdot|$ the area of domains in \mathbb{R}^2 one has by (9)

$$|N_1| \leq C|\Gamma|h^\alpha.$$

Moreover,

$$|N_2| \leq 2Nh$$

where N is the number of horizontal lines $y = k.h^\alpha$ cutting the domain Ω . If D denotes the diameter of Ω one has

$$(N - 1)h^\alpha \leq D$$

so that for $h < 1$,

$$N \leq Ch^{-\alpha}$$

for some constant C so, for maybe an other constant C ,

$$|N_2| \leq Ch^{1-\alpha}.$$

Since the triangulation τ_h has been assumed to be regular the gradient of u_h remains uniformly bounded as well as the one of \hat{u}'_h and \hat{u}_h . So, for some constant C one has

$$\int_{\Omega} (u_h)_x^2 + ((u_h)_y^2 - 1)^2 dx dy \leq C\{|N_1| + |N_2|\} \leq C(h^\alpha + h^{1-\alpha}) \leq Ch^{\alpha \wedge 1 - \alpha}.$$

Now, $\alpha \wedge 1 - \alpha$ is minimum when $\alpha = 1/2$ which gives (6).

Thus, in this case we have been able to construct a minimizing sequence that converges uniformly toward 0 and uses each of the wells W_1, W_2 with the same probability. Constructions of this type are the key point in order to understand more complex microstructures for instance in material science. Further advances in this direction is one of our goal for the future.

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DESIMONE, A.

Characterization of the macroscopic response of magnetostrictive materials via microstructural analysis

This paper discusses recent progress on the prediction of magnetization and magnetostriction curves for magnetoelastic solids. Our approach hinges on the characterization of energetically optimal microscopic domain patterns based on the use of Young measures and H -measures.

1. Introduction

Magnetostrictive materials are solids which undergo reversible deformations when subjected to the action of an applied magnetic field. The recent discovery of Terfenol-D, an alloy of terbium, iron, and dysprosium that exhibits magnetostrictive strains of the order of 10^{-3} at room temperature [2] and has considerable potential as an actuator material [8], has fostered a renewal of interest in the subject of magnetoelasticity, from the point of view of both experiment and theory.

The use of a microscope reveals that a specimen of magnetostrictive material is typically subdivided into fine regions in each of which the material is approximately uniformly magnetized and deformed (magneto-elastic domains). The application of an external field, which favors magnetization directions aligned with it, causes a rearrangement of the domain patterns, and macroscopic deformations result from the cooperative evolution of microscopic domains. The macroscopic response of magnetostrictive materials to applied magnetic fields and loads bears a deep imprint of these microscopic processes: a change of slope in a magnetostriction curve (i.e., a plot of, say, the elongation of a magnetostrictive rod vs. the strength of the applied field) corresponds to the transition from one to another microstructure evolution mode. Since larger slopes imply that larger strains are achieved with the same field strength increment, predicting the location of the “knees” of the curves, and how they are affected by applied mechanical loads is of great interest for applications. Thus, appraising the behavior of fine domain patterns under given environmental conditions is a fundamental step in the modelling of magnetoelasticity.

2. Formulation of the problem

Within the framework of continuum theories, the most widely accepted mathematical model of the behavior of magnetostrictive solids is variational, and is known as Micromagnetics [1]. We restrict our attention to a simplified version of the theory (see [2], [6], and [3]) and we are interested in minimizing a free-energy functional, whose summands enforce the following competing features of the experimentally observed behavior:

1. the magnetization tends to be aligned with preferred crystallographic directions (*easy axes*);
2. the magnetization tends to be aligned with the applied magnetic field \mathbf{h} ;
3. configurations such that the energy stored in the induced magnetic field $\mathbf{h}_m = -\nabla(\Delta^{-1}(\operatorname{div}(\mathbf{m}\chi_\Omega)))$ (i.e., the magnetic self-field generated by the magnetized body) are preferred;
4. stress-free configurations are preferred.

Precisely, we are interested in minimizing over the space $L^2(\Omega, S^2) \times \frac{1}{2}(\nabla + \nabla^T)(W^{1,2}(\Omega, \mathbb{R}^3))$ the following energy functional

$$E_{\mathbf{h}}(\mathbf{m}, \mathbf{E}) = \int_{\Omega} \varphi(\mathbf{m}) - \int_{\Omega} \mathbf{h} \cdot \mathbf{m} + \frac{1}{2} \int_{\mathbb{R}^3} |\mathbf{h}_m|^2 + \frac{1}{2} \int_{\Omega} (\mathbf{E} - \mathbf{E}_0(\mathbf{m})) \cdot \mathbf{C}(\mathbf{E} - \mathbf{E}_0(\mathbf{m})). \quad (1)$$

Here, the unknown functions \mathbf{m} (the magnetization: a unit vector field) and \mathbf{E} (the linear strain, namely, the symmetric part of the gradient of the displacement vector field $\mathbf{u} \in W^{1,2}(\Omega, \mathbb{R}^3)$: $\mathbf{E}(x) = \frac{1}{2}(\nabla + \nabla^T)(\mathbf{u}(x))$, with values on symmetric 3×3 matrices) describe the state of magnetization and distortion of the material at each point of the “body” Ω , assumed of unit volume without loss of generality. We also assume \mathbf{h} to be constant and,

for brevity, we restrict our attention to the case of no applied mechanical loads. Finally, the (symmetric, positive definite) fourth order elasticity tensor \mathbf{C} and the functions φ and \mathbf{E}_0 contain the constitutive information peculiar to a given material. Both of these even, continuous functions are defined on the unit sphere S^2 . The former is non-negative, and its zeroes identify the easy axes; the latter takes values in the space of symmetric 3×3 matrices, and $\mathbf{E}_0(\mathbf{m})$ represents the stress-free deformation corresponding to the magnetization state \mathbf{m} . In order to simplify the exposition of our results, we will also set $\mathbf{C} = \beta \mathbb{I}$, with β a positive constant, and \mathbb{I} the identity.

Following a suggestion of Tartar [10], we minimize over \mathbf{E} first, with \mathbf{m} fixed. We are thus led to minimizing over $L^2(\Omega, S^2)$ the functional

$$I_{\mathbf{h}}^{\beta}(\mathbf{m}) = \int_{\Omega} \varphi(\mathbf{m}) - \int_{\Omega} \mathbf{h} \cdot \mathbf{m} + \frac{1}{2} \int_{\mathbb{R}^3} |\mathbf{h}_{\mathbf{m}}|^2 + \frac{1}{2} \int_{\Omega} \beta |\mathbf{E}_{\mathbf{m}} - \mathbf{E}_0(\mathbf{m})|^2, \quad (2)$$

where, for given \mathbf{m} , $\mathbf{E}_{\mathbf{m}}$ denotes the unique minimizer of the last summand in (1), obtained as the solution of the associated Euler-Lagrange equation $\operatorname{div} \mathbf{E} = \operatorname{div} \mathbf{E}_0(\mathbf{m})$. (Note that the last summand in (1) is convex in \mathbf{E} , and that $\mathbf{E}_{\mathbf{m}}(x) = \mathbf{E}_0(\mathbf{m}(x))$ only if the matrix valued field $\mathbf{E}_0(\mathbf{m})$ satisfies the conditions of kinematic compatibility of linear elasticity). In particular, we are interested in characterizing the energetics of minimizing sequences of $I_{\mathbf{h}}^{\beta}$. This is expedient in either proving existence of minimizers using the direct methods of the Calculus of Variations or, when the infimum of $I_{\mathbf{h}}^{\beta}$ is not attained, to guide the search for well-posed (relaxed) formulations of the given variational problem.

Since an arbitrary sequence of magnetizations is bounded in L^2 , from every sequence with bounded energy we can extract weakly converging subsequences, and we can pose the question of computing the corresponding limiting energy. We observe that, for a given sequence $\{\mathbf{m}_k\}$, the limit of the first summand in (2) can be thought of as the value on the function φ of a continuous linear functional over $C^0(\Omega, S^2)$. Indeed, the given sequence generates a one-parameter family of probability measures (a *Young measure*) ν_x , $x \in \Omega$, and the desired limit is obtained by testing ν_x against the function φ (see [7]). In view of their definition, Young measures can capture only some of the asymptotic features of the sequence $\{\mathbf{m}_k\}$, namely, the limiting distribution of the values taken by the sequence in a neighborhood of each point of Ω . In particular, since the weak limit of $\{\mathbf{m}_k\}$ is the center of mass of ν_x , the limit of weakly continuous functionals of the magnetization, such as the second summand in (2), are trivially computed with the aid of Young measures. However, more information is needed to compute the limit of the last two summands in (2), since these contain the solutions $\mathbf{h}_{\mathbf{m}}$ and $\mathbf{E}_{\mathbf{m}}$ to systems of PDE's in which the given sequence appears on the right hand side. In this case, in fact, it is to be expected that the geometric arrangement of domain patterns should play a role while, as shown in the next section, this information is not recorded by Young measures. For each of the two terms at hand, a further measure, introduced in [9] with the name of *H-measure*, suffices. Focussing, e.g., on the energy stored in the induced magnetic field, we again have that the given sequence $\{\mathbf{m}_k\}$ (or, more precisely, the sequence minus its weak limit) generates a measure. The desired limit is computed by testing the measure against the symbol of the pseudo-differential operator defining $\mathbf{h}_{\mathbf{m}}$ in terms of \mathbf{m} (we recall that the symbol σ_L of the pseudo-differential operator L is defined by the identity $(L\hat{\mathbf{m}})(\xi) = \sigma_L(\xi)\hat{\mathbf{m}}(\xi)$, where the hat denotes Fourier transform, and that for $L = \nabla \Delta^{-1} \operatorname{div}$, $\sigma_L(\xi) = \frac{\xi \otimes \xi}{|\xi|^2}$, see [11]). Similarly, to compute the limit of the fourth summand in (2), the H-measure of $\{\mathbf{E}_0(\mathbf{m}_k)\}$ (minus its weak limit) can be exploited.

Summarizing, for a sequence $\{\mathbf{m}_k\}$ with finite energy, the calculation of the limit of $I_{\mathbf{h}}^{\beta}(\mathbf{m}_k)$ amounts to computing three measures: the Young measure of $\{\mathbf{m}_k\}$, an H-measure associated with $\{\mathbf{m}_k\}$, and an H-measure associated with $\{\mathbf{E}_0(\mathbf{m}_k)\}$. The problem of characterizing minimizing sequences and their asymptotic properties is then reduced to an abstract minimization problem over triples of measures. In principle, this approach would enable us to select energetically optimal domain patterns, and to compute the average quantities needed for the prediction of macroscopic response curves, by using the minimal amount of information on the underlying microscopic picture. In practice, however, an outstanding problem needs to be solved in order to make this program feasible. Indeed, the set of all admissible triples of measures generated by the same sequence of magnetizations is unknown. In spite of the lack of a complete characterization of the set of compatible Young measures and H-measures, some encouraging partial results are available, demonstrating the possibility of predicting magnetization and magnetostriction curves with the methods described in this paper. In the next section we briefly discuss a simple example, with the aim of illustrating the abstract notions introduced above in a concrete setting.

3. Simple laminates

We restrict our attention to a special class of sequences of magnetizations, that we call *simple laminates*, which are constructed as follows. Let f be the 1-periodic function obtained as the periodic extension to the whole real line of

a function taking the value one in the interval $(0, \theta)$ and the value zero in the interval $(\theta, 1)$. For a given unit vector \mathbf{n} , let $\chi_a^k(x) = \chi_\Omega f(\frac{x \cdot \mathbf{n}}{k})$ and consider the sequence of magnetizations defined by

$$\mathbf{m}_k = \mathbf{a}\chi_a^k + \mathbf{b}(1 - \chi_a^k), \quad k \in \mathbb{N}, \quad (3)$$

where \mathbf{a} and \mathbf{b} are given unit vectors. For each value of k , (3) represents a piecewise constant magnetization field, with values \mathbf{a} and \mathbf{b} taken on layers with interface normal \mathbf{n} , with volume fractions θ and $1 - \theta$, and width tending to zero as k tends to ∞ .

The simplicity of the geometry of these layered domain patterns enables us to give a detailed physical interpretation of the quantities introduced in the previous section. First, we observe that the weak limit of (3) is $\mathbf{m}_\infty = \theta\mathbf{a} + (1 - \theta)\mathbf{b}$, its Young measure is independent of x , and it is given by the convex combination of two Dirac masses $\nu = \theta\delta_{\mathbf{a}} + (1 - \theta)\delta_{\mathbf{b}}$. Moreover, since both \mathbf{m}_k and $\mathbf{E}_0(\mathbf{m}_k)$ depend on x only through χ_a^k , the associated H-measures are proportional to the H-measure of $\chi_a^k - \theta$, which captures the only microgeometric feature of the domain patterns of interest through the layering direction \mathbf{n} . These observations should explain the following result, whose proof will be found in [5]:

$$\begin{aligned} \lim_{k \rightarrow \infty} I_h^\beta(\mathbf{m}_k) &= \theta(\varphi(\mathbf{a}) - \mathbf{h} \cdot \mathbf{a}) + (1 - \theta)(\varphi(\mathbf{b}) - \mathbf{h} \cdot \mathbf{b}) + \frac{1}{2} \int_{\mathbb{R}^3} |\mathbf{h}_{(\theta\mathbf{a} + (1 - \theta)\mathbf{b})}|^2 \\ &+ \frac{1}{2}\theta(1 - \theta)|(\mathbf{b} - \mathbf{a}) \cdot \mathbf{n}|^2 + \frac{1}{2}\beta\theta(1 - \theta)|(\mathbf{B} - \mathbf{A}) - \Pi_{\mathbf{d}, \mathbf{n}}(\mathbf{B} - \mathbf{A})|^2, \end{aligned} \quad (4)$$

where $\mathbf{A} = \mathbf{E}_0(\mathbf{a})$, $\mathbf{B} = \mathbf{E}_0(\mathbf{b})$, $\mathbf{d} = (2\mathbf{I} - \mathbf{n} \otimes \mathbf{n})(\mathbf{B} - \mathbf{A})\mathbf{n}$, with \mathbf{I} the identity, and finally

$$\Pi_{\mathbf{d}, \mathbf{n}}(\mathbf{B} - \mathbf{A}) = \begin{cases} 0 & \text{if } \mathbf{d} = 0 \\ ((\mathbf{B} - \mathbf{A}) \cdot \frac{\mathbf{d} \odot \mathbf{n}}{\mathbf{d} \odot \mathbf{n}}) \frac{\mathbf{d} \odot \mathbf{n}}{\mathbf{d} \odot \mathbf{n}} & \text{otherwise,} \end{cases}$$

where $\mathbf{d} \odot \mathbf{n}$ stands for $\frac{1}{2}(\mathbf{d} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{d})$. As an interesting corollary of (4) we recover the following classical result. For $\mathbf{d} \neq 0$, the layered domain pattern (3) can give rise to zero stored elastic energy, i.e., to a stress-free configuration, if and only if the Hadamard compatibility condition $\mathbf{B} - \mathbf{A} = \mathbf{c} \odot \mathbf{n}$ holds for some vector \mathbf{c} .

As a first application of (4), we compute a trivial solution of the minimization problem for (2), which is valid for an arbitrary magnetoelastic body under no applied magnetic field ($\mathbf{h} = 0$). We notice that I_0^β is non negative, and we construct a simple laminate $\{\mathbf{m}_k\}$ such that $I_0^\beta(\mathbf{m}_k) \rightarrow 0$ (hence $\{\mathbf{m}_k\}$ is a minimizing sequence for (2)) in the following fashion. Let \mathbf{a} be a zero of φ , and set $\mathbf{b} = -\mathbf{a}$ and $\theta = \frac{1}{2}$, so that $\mathbf{m}_\infty = 0$. Moreover, choose the layering direction \mathbf{n} so that $(\mathbf{b} - \mathbf{a}) \cdot \mathbf{n} = 0$, and observe finally that $\mathbf{B} - \mathbf{A} = \mathbf{E}_0(-\mathbf{a}) - \mathbf{E}_0(\mathbf{a}) = 0$ since \mathbf{E}_0 is even.

As a further application of (4) we extend to the magnetoelastic setting a result of [7], which establishes that for a uniaxial material (i.e., a material such that $\varphi(\mathbf{m}) = 0 \Rightarrow \mathbf{m} = \pm \mathbf{e}$, with \mathbf{e} a given unit vector), the infimum of I_0^β is not attained. (Indeed in this case every minimizing sequences of I_0^β generates the Young measure $\frac{1}{2}\delta_{\mathbf{e}} + \frac{1}{2}\delta_{-\mathbf{e}}$, failing to converge strongly to a function in $L^2(\Omega, S^2)$, hence showing that energy minimization drives the system to fine domain patterns: this is experimentally observed for uniaxial materials under no applied magnetic field). To this extent, we simply observe that, for $I_0^\beta(\mathbf{m})$ to vanish for some magnetization field \mathbf{m} , it is necessary that all of its non-negative summands vanish. In particular, it is simultaneously required that \mathbf{m} take only the values $\pm \mathbf{e}$ and satisfy $\text{div}(\mathbf{m}\chi_\Omega) = 0$, which is impossible [7].

Finally, we consider the case of a spherical specimen of uniaxial material under an arbitrary (constant) magnetic field. The solutions for the minimization problem for I_h^0 (i.e., the functional obtained from (2) by setting $\beta = 0$) are computed in [3], and they consist of simple laminates for small field strengths, and of uniform states for strong enough applied fields. Obviously, uniform states give rise to kinematically compatible stress-free deformations, hence they provide also solutions for the case $\beta \neq 0$. The same is true, however, for the configurations consisting of simple laminates, as a consequence of the symmetry properties of the constitutive functions φ and \mathbf{E}_0 . Defining

$$\mathcal{P} = \{\mathbf{Q} \in O(3) : \varphi(\mathbf{Q}\mathbf{m}) = \varphi(\mathbf{m}) \text{ and } \mathbf{E}_0(\mathbf{Q}\mathbf{m}) = \mathbf{Q}\mathbf{E}_0(\mathbf{m})\mathbf{Q}^T \text{ for every } \mathbf{m} \in S^2\} \quad (5)$$

as the group of the material symmetries for the material at hand, we observe that for a uniaxial material with easy axis \mathbf{e} , \mathcal{P} is the group generated by $-\mathbf{I}$ and the proper rotations about \mathbf{e} . The simple laminates which minimize I_h^0 are such that $\mathbf{b} = -\mathbf{R}\mathbf{a}$, with \mathbf{R} a rotation of π about \mathbf{e} , and \mathbf{a} in the plane P generated by \mathbf{h} and \mathbf{e} . Moreover,

they consist of layers with interface normal $\mathbf{n} = \mathbf{e}_\perp$, where \mathbf{e}_\perp is a unit vector in \mathcal{P} orthogonal to \mathbf{e} . Thus, a simple calculation based on (5) shows that

$$(\mathbf{b} - \mathbf{a}) \cdot \mathbf{n} = (\mathbf{R}\mathbf{a} + \mathbf{a}) \cdot \mathbf{n} = 0, \quad (6)$$

and

$$\mathbf{B} - \mathbf{A} = \mathbf{R}\mathbf{A}\mathbf{R}^T - \mathbf{A} = \alpha \mathbf{e} \odot \mathbf{e}_\perp = \mathbf{c} \odot \mathbf{n}, \quad (7)$$

with α a scalar, hold simultaneously. We conclude that, for minimizing sequences, the energy contribution due to the H-measures vanishes (i.e., the energy of the “minimizers” is independent of the microgeometry), and that energetically optimal domain patterns correspond to stress-free states. These results are enough to compute magnetization and magnetostriction curves, as discussed in [4].

4. Discussion

The examples discussed in the previous section suggest a natural question: is it always true that, for minimizing sequences, the energy contribution due to the H-measures vanishes?

Interestingly, the answer is positive (with no restrictions on the geometry of the specimen, or on the type of material, or on the applied field) in the case $\beta = 0$ (see, e.g., [3]). Even for $\beta \neq 0$, the same result holds true for a surprisingly large class of materials, at least for spherical specimens. The relevance of results of this nature is in that they allow to explicitly compute the relaxation of the given energy functional (i.e., in more physical terms, the effective energy of the system governing its macroscopic response), and to identify which are the relevant parameters (e.g., values and local volume fractions of the magnetization field, microgeometric parameters such as the normals to domain interfaces) needed to characterize energetically optimal configurations without resolving them in their finest details. In contrast with models based on the introduction of internal variables, within the approach discussed in this paper these effective energies, and the variables on which they depend, arise as properties of the solutions of a definite mathematical problem.

The answer to the question posed above is however negative in general (in fact, even for simple laminates, the constraints posed on the microgeometry in order to satisfy simultaneously the two conditions (6) and (7) may be incompatible, see [5]), and no relaxation result seems yet available in this case.

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Magnetoelastic Interactions

To understand the role played by the complex microstructural arrangements in a giant magnetostrictive material, we developed a micromagnetic theory where equilibria are described by the oscillatory statistics of approximating or minimizing sequences of a variational principle. Predictions based on the theory may be used to seek optimal microstructures and to offer specific recommendation for improvement of actuator and sensor materials.

1. Introduction

Current interest in magnetostrictive materials owes to the discovery of high magnetostriction $TbFe_2$ by A. E. Clark in 1971 and the subsequent discovery by him that the pseudobinary alloy of $Tb_xDy_{1-x}Fe_2$, $x \approx 0.3$, had both high magnetostriction and low anisotropy [4,5]. This material, called Terfenol-D, has a relative elongation of up to 2000 parts per million and is called a giant magnetostrictive material. Terfenol-D condenses with a dendritic structure consisting of growth twins remaining fixed relative to the material under deformation and separating what appear to be domains of simpler lamellar structures. Understanding the nature of the magnetoelastic response requires identifying this microstructure and elucidating its role. The presence of several stable variants suggests that the material has a free energy with a multiple potential well structure, and thus is highly non convex. The spatially oscillatory fine structure indicates a competition between the free energy and other effects, leading to a certain frustration in the material. A classical description of configurations may not be available even in unloaded equilibrium.

In the constitutive theory [9], the location of the potential wells has a prominent role while surface energies, magnetic domain wall energies, and similar effects are neglected. This large body approximation is particularly appropriate owing to the highly mobile character of the lamellar structure, [6]. From the viewpoint of analysis, information about equilibrium configurations arises from oscillatory statistics of approximating or minimizing sequences of a variational principle, namely, the Young measures.

An interesting feature revealed by the analysis is that two kinds of laminated microstructures may occur. In the first, coherence across the growth twin interface is achieved only in the fine phase limit, they are *fine phase coherent*, and thus in the material the laminates are separated by a transition layer, which, of course gives some energetic contribution. The second kind of laminate is *exactly coherent* and has no transition layer. With exchange energy present, it is reasonable to think that exactly coherent laminates are preferred.

For a review of the status of the simulation efforts, we refer to [12].

2. The energy of a magnetostrictive configuration

The stored energy density $W(F, m)$ for the "single crystal", a portion of the material that derives from a single lattice, depends on the deformation gradient $F \in \mathcal{M}$, 3×3 matrices and magnetization $m \in \mathcal{S}^2$ and is subject to the conditions of frame indifference and material symmetry

$$W(QFP, mQ^T) = W(F, m), Q \in SO(3) \text{ and } P \in \mathcal{P}.$$

For us, \mathcal{P} is the proper cubic group (of order 24.) In Terfenol-D, the onset of ferromagnetism is associated with a stretch of the high temperature cubic unit cell along a main diagonal parallel to the magnetization. Thus W achieves its minimum on the eight pairs $(U_i, \pm m_i)$,

$$U_i = \eta_1 \mathbf{1} + (\eta_2 - \eta_1) m_i \otimes m_i, i = 1, 2, 3, 4, \text{ and}$$

$$m_1 = \frac{1}{\sqrt{3}}(1, 1, 1), m_2 = \frac{1}{\sqrt{3}}(1, -1, -1), m_3 = \frac{1}{\sqrt{3}}(-1, 1, -1), m_4 = \frac{1}{\sqrt{3}}(-1, -1, 1)$$

and the potential wells $\Sigma = \bigcup \{(QU_i, \pm m_i Q^T) : Q \in SO(3)\}$ they determine. Here we have relied on [3], [8].

The typical rod configuration consists of parallel growth twins. To describe these, we assume the rod is a composite for which we must introduce an inhomogeneous energy $W(F, m, x)$. For example, we may view a lower

lamellar structure as arising from a 180° rotation R_o about the m_1 axis of an upper lamellar structure. Assuming coordinates to have been arranged so that the two regimes are separated by $x \cdot m_1 = 0$, we have that

$$W(F, m, x) = \begin{cases} W(F, m), & x \cdot m_1 > 0, \\ W(FR_o, m), & x \cdot m_1 < 0. \end{cases}$$

Note that R_o is not a symmetry operation although holding invariant the wells about $(U_1, \pm m_1)$.

The total energy of the configuration $y = y(x), m = m(y(x))$ occupying reference domain Ω is given, in mixed spatial/reference form, by

$$E(y, m) = \int_{\Omega} W(\nabla y, m, x) dx + \frac{1}{2} \int_{\mathbb{R}^3} |\nabla_y v|^2 dy,$$

where the potential v of the magnetic field satisfies

$$\operatorname{div}_y(-\nabla_y v + \frac{1}{\det \nabla y} m) = 0 \text{ in } \mathbb{R}^3 \text{ and } |m| = 1 \text{ in } y(\Omega).$$

We have a criterion to characterize minimum energy:

$$\inf E(y, m) = (\min W)|\Omega|.$$

This minimum is not achieved, however, but offers a goal for Young measure minima, for example, with $\nu = (\nu_x(A, \mu))_{x \in \Omega}$ denoting the measure, $\operatorname{supp} \nu_x \subset \Sigma$ and the average magnetization

$$\bar{m}(x) = \int_{\Sigma} \mu d\nu_x(A, \mu) = 0.$$

3. Equilibrium microstructures and the mechanism of magnetostriction

The problem of determining the equilibrium microstructures is divided into two parts, finding the structure within the lamella and assembling this information to find the structure of the growth twins. Given two wells with transformation strains and magnetizations (U_i, m_i) and (U_j, m_j) , there are two solutions (R^\pm, a^\pm, n^\pm) of

$$R^\pm U_j = U_i(1 + a^\pm \otimes n^\pm), i, j = 1, \dots, 4, i \neq j,$$

corresponding to "twins" and "reciprocal twins". The resulting twin planes are (100) and (110) planes, in agreement with DIC experiments [1]. There are corresponding magnetic substructures in each lamella with average magnetization 0. A typical Young measure is of the form

$$\nu = \frac{1}{2}(1 - \lambda)(\delta_{(U_i, m_i)} + \delta_{(U_i, -m_i)}) + \frac{1}{2}\lambda(\delta_{(RU_j, m_j R^T)} + \delta_{(RU_j, -m_j R^T)}),$$

$$0 \leq \lambda \leq 1, x \cdot m_1 > 0$$

and has average deformation and magnetization

$$F = (1 - \lambda)U_i + \lambda RU_j = U_i(1 + \lambda a \otimes n), \bar{m} = 0 \text{ in } x \cdot m_1 > 0.$$

It is possible that λ depends on $x \in \Omega$. Analogously, we find a Young measure ν' and average deformation and magnetization

$$F' = (1 - \lambda')PU'_i + \lambda'PR'U'_j = PU'_i(1 + \lambda'a' \otimes n'), \bar{m} = 0 \text{ in } x \cdot m_1 < 0, P \in SO(3),$$

determined by the R_o -rotated well structure $(U'_k, m'_k), U'_k = R_o U_k R_o, m'_k = m_k R_o$ in $x \cdot m_1 < 0$.

The composite structure is found by solving for $P \in SO(3)$ in F' in

$$F' - F = b \otimes m_1, b \in \mathbb{R}^3. \quad (*)$$

Note that m_1 is a fixed direction. There are 144 possible combinations $(ij, k'l')$. Applying conditions of kinematic compatibility, we find that only 12 combinations can be realized and they are the ones of the form

$(ij, i'j')$, either twins or reciprocal twins, and $\lambda = \lambda'$ on $x \cdot m_1 = 0$. All of these have been observed, [1],[7]. The fine phase coherence condition determined by (*) implies that there is a transition layer across $x \cdot m_1 = 0$ and a minimizing sequence (y^k, m^k) satisfies

$$\int_{\Omega} W(\nabla y^k, m^k, x) dx = |\Omega| \min W + O\left(\frac{1}{k}\right).$$

The condition for exact coherence is that $a \cdot m_1 = 0$, where a is either of the two (referential) twinning shears of the four gradient structure, [11]. This means that

$$PU'_i = U_i = b_1 \otimes m_1, \text{ and } PR'U'_j - RU_j = b_2 \otimes m_1 \quad (**)$$

which is stronger than (*). This is satisfied for the combinations (23, 2'3'), (34, 3'4'), and (24, 2'4'), (twins only). For exact coherence, no transition layer is necessary and a minimizing sequence (y^k, m^k) may be chosen so that

$$\int_{\Omega} W(\nabla y^k, m^k, x) dx = |\Omega| \min W.$$

The mechanism of giant magnetostriction may now be explained by analogy with twinning in martensitic materials. When a magnetic field H is applied parallel to the (-211) direction, the magnetization vectors in the lamella rotate towards H . The system decreases its energy by choosing the mechanical variant most agreeable to the magnetization. Thus the applied field induces an exchange of stability among elastic domains creating a much larger elongation than would be available by mere stretching of the material lattice.

4. Optimal microstructures

The issue which now arises is whether or not all the possible dendritic lamellar systems have the same magnetostrictive properties. We may calculate the minimum and maximum macroscopic lengths in the longitudinal $[211]$ rod direction. The maximum is achieved by the (12, 1'2'), (23, 2'3'), and (24, 2'4') systems but the minimum only by the (12, 1'2') system, which is fine phase coherent. This suggests that a compressive stress will provide a preference for the (12, 1'2') system. In addition, fine phase coherent structures prefer extremely planar interfaces, [10]. As mentioned in the introduction, exactly coherent configurations are likely chosen by the unloaded material in equilibrium, however, by attempting to grow the sample with as planar as possible growth twin boundary and applying a compressive stress along the $[211]$ axis, the special properties of the (12, 1'2') variant structure can be exploited.

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Numerical analysis of a microstructure for a rotationally invariant, double well energy

The laminated microstructure observed in martensitic crystals can be modeled by energy minimizing sequences of deformations for a rotationally invariant (or frame-indifferent), double well energy density [1, 2, 10]. The deformation gradients of energy minimizing sequences oscillate between energy wells across layers (with width converging to zero) so that the effective energy density becomes the relaxed energy density [2, 12]. We present error estimates for the minimization of the energy $\int_{\Omega} \phi(\nabla v(x)) dx$ where the energy density $\phi(A)$ is a rotationally invariant, double well energy density by a general class of approximation methods for the deformation in L^2 , the weak convergence of the deformation gradient, the convergence of the microstructure (or Young measure) of the deformation gradient, and the convergence of nonlinear integrals of the deformation gradient.

1. The Laminated Microstructure

We denote the reference domain for the crystal by the polygonal domain $\Omega \subset \mathbb{R}^3$, and we consider deformations $v : \Omega \rightarrow \mathbb{R}^3$ and corresponding deformation gradients $\nabla v(x) : \Omega \rightarrow \mathbb{R}^{3 \times 3}$ where $\mathbb{R}^{3 \times 3}$ denotes the space of 3×3 matrices. To model the microstructure in a martensitic crystal, we consider an energy density $\phi : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ that is a continuous, nonnegative function which attains its minimum value only on the rotationally invariant set

$$\mathcal{U} \equiv SO(3)F^+ \cup SO(3)F^-$$

for energy minimizing deformation gradients $F^+ \in \mathbb{R}^{3 \times 3}$ and $F^- \in \mathbb{R}^{3 \times 3}$, where $SO(3)$ denotes the space of proper rotations. Since F^+ and F^- represent symmetry-related states [1, 2], we assume that they satisfy the condition

$$\det F^+ = \det F^- > 0$$

and the Hadamard condition that there exist $a, n \in \mathbb{R}^3$ with $a, n \neq 0$ such that

$$F^+ = F^- + a \otimes n \tag{1}$$

where $a \otimes n \in \mathbb{R}^{3 \times 3}$ is the tensor product of a and n defined by $(a \otimes n)_{ij} = a_i n_j$. The Hadamard condition (1) allows the existence of a continuous deformation with planar interfaces with normal n separating layers in which the deformation gradient alternates between F^+ or F^- .

We shall assume that ϕ grows quadratically away from the energy wells, so for $\nu > 0$ we have that

$$\begin{aligned} \phi(A) &\geq \nu \|A - \pi(A)\|^2 & \forall A \in \mathbb{R}^{3 \times 3}, \\ \phi(A) &= 0 & \text{if and only if } A \in \mathcal{U}, \end{aligned}$$

where $\pi : \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U}$ is a Borel measurable projection onto the energy wells defined by

$$\|A - \pi(A)\| = \min_{B \in \mathcal{U}} \|A - B\| \quad \text{with matrix norm} \quad \|A\|^2 \equiv \sum_{i,j=1}^3 A_{ij}^2 \quad \text{for } A \in \mathbb{R}^{3 \times 3}.$$

The projection π exists since \mathcal{U} is compact, although the projection is not uniquely defined at $A \in \mathbb{R}^{3 \times 3}$ where the minimum above is attained at more than one $B \in \mathcal{U}$.

We can construct a simple laminate by the continuous deformation

$$w_{\delta}(x) = F^- x + \left[\int_0^{x \cdot n} \chi\left(\frac{s}{\delta}\right) ds \right] a$$

for $\delta > 0$ where $\chi(s) : \mathbb{R} \rightarrow \mathbb{R}$ is a characteristic function with period 1 such that for $0 < \lambda^+ < 1$

$$\chi(s) = 1 \text{ for } 0 \leq s \leq \lambda^+ \quad \text{and} \quad \chi(s) = 0 \text{ for } \lambda^+ < s < 1.$$

Now

$$\nabla w_\delta(x) = F^- + \chi \left(\frac{x \cdot n}{\delta} \right) a \otimes n, \quad x \in \Omega,$$

so

$$\nabla w_\delta(x) \in \mathcal{U} \quad \text{or equivalently} \quad \phi(\nabla w_\delta(x)) = 0 \quad \text{for } x \in \Omega.$$

We have for $F = \lambda^+ F^+ + \lambda^- F^-$ where $\lambda^- = 1 - \lambda^+$ that

$$|w_\delta(x) - Fx| \leq C\delta, \quad \forall x \in \Omega.$$

So, boundary conditions that are compatible for an energy minimizing simple laminate are given by [2, 13]

$$v(x) = [\lambda^+ F^+ + \lambda^- F^-] x = Fx \quad \forall x \in \partial\Omega.$$

We present results for the approximation of the problem

$$\inf \{ \mathcal{E}(v) : v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3) \} \quad (2)$$

where the bulk energy of the crystal is defined by

$$\mathcal{E}(v) = \int_{\Omega} \phi(\nabla v(x)) \, dx, \quad (3)$$

and where the subspace of continuous functions, $C^F(\Omega; \mathbb{R}^3)$, is defined by

$$C^F(\Omega; \mathbb{R}^3) = \{ v(x) \in C(\Omega; \mathbb{R}^3) : v(x) = Fx \text{ for } x \in \partial\Omega \}.$$

It has been proven by Ball and James [2] that the microstructure (or Young measure) for minimizing sequences for the problem (2) with energy density (3) is unique.

The problem (2) with energy density (3) is the most basic and widely used test problem for the computation of microstructure [7, 9]. We have given an analysis for the approximation of this problem in [13], and the results are summarized in the following section. A two-dimensional, rotationally invariant, double well model with bulk energy

$$\hat{\mathcal{E}}(v) = \int_{\Omega} \phi(\nabla v(x)) + |v(x) - Fx|^q \, dx \quad (4)$$

for $1 < q < \infty$ was analyzed in [5, 11]. However, the term $|v(x) - Fx|^q$ in the integrand of (4) is not part of the physical elastic energy density, but has been added as a "penalty term" for mathematical convenience to force the convergence of $v(x) \rightarrow Fx$ in $L^q(\Omega; \mathbb{R}^2)$ for energy minimizing sequences of deformations. The results proved in [13] and described here do not utilize a term $|v(x) - Fx|^q$ in the energy density, but rather show that the convergence of the microstructure depends only on minimizing the elastic energy (3).

Our analysis is based on the theory for the numerical analysis of microstructure that we developed and applied to one-dimensional problems in [6, 8]. We have also used this theory to analyze the three-dimensional microstructure in micromagnetics [14]. Extensions to some multi-dimensional problems with point wells (so the energy density is not rotationally invariant) have been given in [3, 4].

2. The Approximation of Microstructure

Our first theorem demonstrates that the directional derivatives orthogonal to n (called "twin planes" in the physical theory) of sequences of energy minimizing deformations converge strongly. Thus, the oscillations in the deformation gradient are essentially one-dimensional. We give the proofs of this result and of the following results in [13].

Theorem 1. For all $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3)$ and all $w \in \mathbb{R}^3$ such that $w \cdot n = 0$, we have

$$\int_{\Omega} |(\nabla v(x) - F)w|^2 \, dx \leq C\mathcal{E}(v)^{1/2}.$$

The next theorem follows from Theorem 1 and the Poincaré inequality. An important consequence of Theorem 2 is that it is not necessary to include the "penalty term" $|v(x) - Fx|^2$ in the energy density to be able to conclude that $v(x) \rightarrow Fx$ in $L^2(\Omega; \mathbb{R}^3)$ for energy minimizing sequences.

Theorem 2. For all $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3)$ we have the estimate

$$\int_{\Omega} |v(x) - Fx|^2 dx \leq C\mathcal{E}(v)^{1/2}.$$

The following theorem shows that deformation gradients of energy minimizing sequences converge weakly to F .

Theorem 3. For any open set $\omega \subset \Omega$ with smooth boundary $\partial\omega$, we have that

$$\left\| \int_{\omega} (\nabla v(x) - F) dx \right\| \leq C\mathcal{E}(v)^{1/8}$$

for all $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3)$ such that $\mathcal{E}(v) \leq 1$.

The next theorem shows that the deformation gradients of energy minimizing sequences converge to the set $\{F^+, F^-\}$. We utilize the operators $R: \mathbb{R}^{3 \times 3} \rightarrow SO(3)$ and $\Pi: \mathbb{R}^{3 \times 3} \rightarrow \{F^+, F^-\}$ which are uniquely defined by the relation

$$\pi(A) = R(A)\Pi(A), \quad \forall A \in \mathbb{R}^{3 \times 3}.$$

Theorem 4. For all $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3)$ such that $\mathcal{E}(v) \leq 1$ we have

$$\int_{\Omega} \|\nabla v(x) - \Pi(\nabla v(x))\|^2 dx \leq C\mathcal{E}(v)^{1/2}$$

To study the approximation of microstructure, we define for $\rho > 0$ and $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3)$ the sets

$$\omega_{\rho}^{\pm} = \omega_{\rho}^{\pm}(v) = \{x \in \omega : \Pi(\nabla v(x)) = F^{\pm} \text{ and } \|\Pi(\nabla v(x)) - \nabla v(x)\| < \rho\}.$$

We can then use the above theorems to prove the following estimate which describes the convergence of the microstructure (or Young measure) of the deformation gradients of energy-minimizing sequences.

Theorem 5. We have for all $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3)$ such that $\mathcal{E}(v) \leq 1$:

$$\left| \frac{\text{meas}(\omega_{\rho}^{\pm}(v))}{\text{meas}(\omega)} - \lambda^{\pm} \right| \leq C\mathcal{E}(v)^{1/8}.$$

We next show that nonlinear integrals of the deformation gradient can be estimated in terms of the bulk energy.

Theorem 6. For any measurable function $f: \Omega \times \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$, we have the bound:

$$\left| \int_{\Omega} f(x, \nabla v(x)) - [\lambda^+ f(x, F^+) + \lambda^- f(x, F^-)] dx \right| \leq C \left\{ \int_{\Omega} \left[\left\| \frac{\partial f}{\partial A}(x, \cdot) \right\|_{L^{\infty}}^2 + |\nabla [f(x, F^+) - f(x, F^-)] n|^2 + [f(x, F^+) - f(x, F^-)]^2 \right] dx \right\}^{1/2} \mathcal{E}(v)^{1/4}$$

for all $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\Omega; \mathbb{R}^3)$ such that $\mathcal{E}(v) \leq 1$.

3. Estimates for Finite Element Approximations

The results in § 2 can be applied to any approximation method which gives a deformation with small energy. We let

$$\mathcal{M}_h^F \subset C^F(\Omega; \mathbb{R}^3) \cap W^{1,\infty}(\Omega; \mathbb{R}^3), \quad \text{for } 0 < h < h_0,$$

be a family of finite element spaces defined on quasi-regular meshes with maximal diameter h . For a class of families of finite element methods which includes all of the classical finite element methods we have that [5, 13]

$$\min_{v_h \in \mathcal{M}_h^F} \mathcal{E}(v_h) \leq Ch^{1/2}. \quad (5)$$

Each of the preceding theorems implies a corresponding lemma for finite element approximations $u_h \in \mathcal{M}_h^F$ which satisfy the bound (5). We give here the corresponding lemmas for Theorems 1, 2, 5, and 6.

Lemma 1. For $u_h \in \mathcal{M}_h^F$ which minimizes the energy $\mathcal{E}(v)$ in \mathcal{M}_h^F and all $w \in \mathbb{R}^3$ such that $w \cdot n = 0$

$$\int_{\Omega} |(\nabla u_h(x) - F)w|^2 dx \leq Ch^{1/4}.$$

Lemma 2. If the deformation $u_h(x)$ minimizes the energy $\mathcal{E}(v)$ in \mathcal{M}_h^F , then

$$\int_{\Omega} |u_h(x) - Fx|^2 dx \leq Ch^{1/4}.$$

Lemma 3. For any deformation $u_h(x)$ which minimizes the energy $\mathcal{E}(v)$ in \mathcal{M}_h^F , we have that

$$\left| \frac{\text{meas}(\omega_{\rho}^{\pm}(u_h))}{\text{meas}(\omega)} - \lambda^{\pm} \right| \leq Ch^{\frac{1}{16}}.$$

Lemma 4. If $u_h(x)$ minimizes the energy $\mathcal{E}(v)$ in \mathcal{M}_h^F , then for any measurable function $f : \Omega \times \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$

$$\left| \int_{\Omega} f(x, \nabla u_h(x)) - [\lambda^+ f(x, F^+) + \lambda^- f(x, F^-)] dx \right| \leq C \left\{ \int_{\Omega} \left[\left\| \frac{\partial f}{\partial A}(x, \cdot) \right\|_{L^{\infty}}^2 + |[f(x, F^+) - f(x, F^-)] n|^2 + [f(x, F^+) - f(x, F^-)]^2 \right] dx \right\}^{1/2} h^{1/8}.$$

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Error estimates for nonlinear Stefan problems obtained as asymptotic limits of a Penrose–Fife model

In this note I review some results achieved from a collaboration with Jürgen Sprekels and concerning the asymptotic behaviour of initial–boundary value problems for the Penrose–Fife phase–field model as the coefficients of the differential terms for the order parameter tend to zero. In the limit procedure one gets either standard or relaxed Stefan problems, still with heat flux proportional to the gradient of the inverse absolute temperature. After focusing on the problems relaxed in time and recalling the convergence results, we add a small new contribution by proving an error estimate.

1. Introduction

In a recent issue [9] Penrose and Fife proposed a model for diffusive phase transitions with non–conserved order parameter which, contrary to previous phase field models [10], has the advantage to be thermodynamically consistent. Moreover, their approach allows to describe non–isothermal phase changes (see also [1]) and to take the heat flux as a function of the gradient of the inverse absolute temperature (what it is quite usual in thermodynamics) instead of the gradient of temperature (think of the Fourier law).

The Cauchy problem for corresponding sets of equations and boundary conditions has been studied by several authors (see [4–8,11–12] and references therein) under different conditions. In particular, here we are interested to the following system

$$\frac{\partial}{\partial t}(c_0\vartheta + \lambda(\chi)) + k\Delta\left(\frac{1}{\vartheta}\right) = g \quad \text{in } Q := \Omega \times (0, T), \quad (1)$$

$$\delta\chi_t - \varepsilon\Delta\chi + \beta(\chi) \ni \sigma'(\chi) - \frac{\lambda'(\chi)}{\vartheta} \quad \text{in } Q, \quad (2)$$

$$k\frac{\partial}{\partial n}\left(\frac{1}{\vartheta}\right) = \gamma\left(\frac{1}{\vartheta_\Gamma} - \frac{1}{\vartheta}\right), \quad \frac{\partial\chi}{\partial n} = 0 \quad \text{in } \Sigma := \Gamma \times (0, T), \quad (3)$$

for the absolute temperature $\vartheta : Q \rightarrow \mathbb{R}$ and the phase variable $\chi : Q \rightarrow [0, 1]$ (for instance, volume density of one of the phases), where $\Omega \subset \mathbb{R}^3$ denotes a bounded domain with smooth boundary Γ , $T > 0$ is some final time, c_0 and k represent positive physical constants as well as the *small* quantities δ and ε (intended to approach 0 in the asymptotic analysis of [2,3,11]). The known right hand side $g : Q \rightarrow \mathbb{R}$ gives account of the heat supply in the energy balance equation (1), while $\gamma : \Sigma \rightarrow \mathbb{R}$ and $\vartheta_\Gamma : \Sigma \rightarrow \mathbb{R}$ are positive data involved in the first boundary condition of (3), the outer heat flux being thus proportional to the difference of inverse absolute temperatures between exterior and interior of the body. Finally, the functions λ and σ are smooth, with the further assumption for λ to be convex, and β denotes the maximal monotone graph

$$\beta(\chi) = \begin{cases} (-\infty, 0] & \text{if } \chi = 0 \\ \{0\} & \text{if } 0 < \chi < 1 \\ [0, +\infty) & \text{if } \chi = 1 \end{cases},$$

subdifferential of the indicator function of the interval $[0, 1]$.

By supplying (1–3) with the initial conditions

$$\vartheta(\cdot, 0) = \vartheta_{0\delta\varepsilon}, \quad \chi(\cdot, 0) = \chi_{0\delta\varepsilon} \quad \text{in } \Omega \quad (4)$$

and admitting linear expressions for σ and λ , the paper [3] deals with the behaviour of the resulting problem first as $\varepsilon \searrow 0$ and δ is fixed, then as $\delta \searrow 0$ and ε is fixed, and finally as both ε and δ (without any order relation between the two parameters) go to zero. Clearly, in each of the three cases the initial values $\vartheta_{0\delta\varepsilon}$ and $\chi_{0\delta\varepsilon}$ are supposed to converge, in a suitable sense, to the respective initial values for the limit problems, the requirements on these last data being stronger for the relaxed problems (where one of δ , ε remains positive) than for the pure Stefan problem (where $\delta = \varepsilon = 0$).

More precisely, the asymptotic investigation of [3] is based on the following outline. Letting g , γ , ϑ_Γ be

sufficiently smooth, for any $\delta > 0$, $\varepsilon > 0$ the initial-boundary value problem (1-4) possesses one and only one variational solution (this statement comes as a consequence of the work developed in [6-8]). The next step of the procedure is the derivation of global estimates independent of δ and ε . Such *a priori* bounds are those enabling us to pass to the limit in (1-4), by compactness and monotonicity arguments. Hence, we find that all the weak star limits of subsequences of solutions must solve (in a weak sense) the corresponding limit Stefan problem. By showing the uniqueness property for the limit problems, we can so conclude for the convergence of the whole sequences of solutions.

In this paper we concentrate on the case in which $\delta > 0$ is fixed and ε goes to 0, allowing nonlinearities for σ and λ , and exploit additional regularity properties of the solutions inferred within the analysis of [2]. Other remarks on this class of asymptotic processes have been pointed out by Shirohzu, Sato, and Kenmochi in [11]. However, we follow the approach of [2] and in the next section we collect the convergence and the existence and uniqueness results stated there. The concluding section is devoted to estimate the difference between the Penrose-Fife and Stefan solutions with respect to ε .

2. Convergences

Keeping δ constant, for any $\varepsilon \in (0, 1]$ we deal with the problem (1-4), where henceforth the initial data $\vartheta_{0\delta\varepsilon}$, $\chi_{0\delta\varepsilon}$ are simply and properly denoted by $\vartheta_{0\varepsilon}$, $\chi_{0\varepsilon}$, and look at its asymptotic behaviour as $\varepsilon \searrow 0$. For our convenience, we make use of the auxiliary variable $u = 1/\vartheta$, representing the inverse temperature. Setting also $u_\Gamma := 1/\vartheta_\Gamma$, note that the variational equality

$$\int_{\Omega} (c_0\vartheta + \lambda(\chi))_t v = k \int_{\Omega} \nabla u \cdot \nabla v + \int_{\Gamma} \gamma(u - u_\Gamma) v + \int_{\Omega} g v \quad \forall v \in H^1(\Omega), \text{ a.e. in } (0, T). \tag{5}$$

can be easily obtained from multiplication of (1) by the test function v and formal integration by parts with the help of (3). Actually, (5) gives a weak formulation of the equation (1) coupled with the boundary condition in (3).

It is worth now providing precise hypotheses. We require that $\lambda, \sigma \in C^2([0, 1])$, λ is convex, g and its time derivative (in the sense of distributions) g_t both lie in $L^\infty(Q)$, as well as $\gamma, 1/\gamma, \vartheta_\Gamma, u_\Gamma$ and $\gamma_t, (\vartheta_\Gamma)_t$ all are in $L^\infty(\Sigma)$. Concerning the sequences $\{\vartheta_{0\varepsilon}\}$ and $\{\chi_{0\varepsilon}\}$, we assume that $\vartheta_{0\varepsilon} \in H^1(\Omega) \cap L^\infty(\Omega)$, $\chi_{0\varepsilon} \in H^2(\Omega)$, $\frac{\partial}{\partial n} \chi_{0\varepsilon} = 0$ a.e. in Γ ,

$$0 < a \leq \vartheta_{0\varepsilon} \leq b \quad \text{and} \quad 0 \leq \chi_{0\varepsilon} \leq 1 \quad \text{a.e. in } \Omega, \tag{6}$$

$$\|\vartheta_{0\varepsilon}\|_{H^1(\Omega)} + \|\chi_{0\varepsilon}\|_{H^1(\Omega)} \leq C, \quad \|\vartheta_{0\varepsilon} - \vartheta_0\|_{L^2(\Omega)} + \|\chi_{0\varepsilon} - \chi_0\|_{L^2(\Omega)} \leq C\varepsilon^{1/2} \tag{7}$$

for any $\varepsilon \in (0, 1]$, where a, b, C stand for uniform constants and ϑ_0, χ_0 are functions in $H^1(\Omega)$ representing the initial values for the limit problem. Let us remark that, if one starts from prescribing $\vartheta_0, \chi_0 \in H^1(\Omega)$ obeying (6), it is not difficult to construct sequences $\{\vartheta_{0\varepsilon}\}$ and $\{\chi_{0\varepsilon}\}$ in the same conditions as above. For instance, we can choose $\vartheta_{0\varepsilon} = \vartheta_0$ and let $\chi_{0\varepsilon}$ be the solution of the elliptic problem

$$\int_{\Omega} \chi_{0\varepsilon} v + \varepsilon \int_{\Omega} \nabla \chi_{0\varepsilon} \cdot \nabla v = \int_{\Omega} \chi_0 v \quad \forall v \in V$$

(further details can be found in [2]). However, neglecting (7) for the moment, the remaining assumptions enable us to conclude that (see [6-8]) for any $\varepsilon \in (0, 1]$ there exists one and only one triple $(\vartheta_\varepsilon, u_\varepsilon, \chi_\varepsilon)$, with $\vartheta_\varepsilon \in H^1(0, T; L^2(\Omega)) \cap L^\infty(0, T; H^1(\Omega)) \cap L^\infty(Q)$, $u_\varepsilon \in H^1(0, T; L^2(\Omega)) \cap L^2(0, T; H^2(\Omega)) \cap L^\infty(Q)$, and $\chi_\varepsilon \in H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^2(\Omega))$, satisfying the equality (5) (obviously in the place of (ϑ, χ, u)), $u_\varepsilon = 1/\vartheta_\varepsilon$ a.e. in Q , $\frac{\partial}{\partial n} \chi_\varepsilon = 0$ a.e. in Σ ,

$$\delta \frac{\partial}{\partial t} \chi_\varepsilon - \varepsilon \Delta \chi_\varepsilon + \beta(\chi_\varepsilon) \ni \sigma'(\chi_\varepsilon) - \lambda'(\chi_\varepsilon) u_\varepsilon \quad \text{a.e. in } Q, \tag{8}$$

$$\vartheta(\cdot, 0) = \vartheta_{0\varepsilon}, \quad \chi(\cdot, 0) = \chi_{0\varepsilon} \quad \text{a.e. in } \Omega, \tag{9}$$

that is, the pair $(\vartheta_\varepsilon, \chi_\varepsilon)$ yields the unique solution to the initial-boundary value problem (1-3), (9).

Using also the first bound in (7), the following two statements are proved in [2]. The former contains the basic estimates for $\vartheta_\varepsilon, u_\varepsilon, \chi_\varepsilon$, while the latter is related to the limit procedure for the corresponding sequences.

Proposition 1. *A constant C_1 can be determined in order that for any $\varepsilon \in (0, 1]$ there holds*

$$\begin{aligned} & \|\vartheta_\varepsilon\|_{W^{1,\infty}(0,T;(H^1(\Omega))' \cap L^\infty(0,T;L^2(\Omega)))} + \|u_\varepsilon\|_{H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^\infty(Q)} \\ & + \|\chi_\varepsilon\|_{W^{1,\infty}(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^\infty(Q)} + \varepsilon^{1/2} \|\chi_\varepsilon\|_{H^1(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega))} \leq C_1. \end{aligned} \tag{10}$$

Proposition 2. *There exist $\vartheta \in W^{1,\infty}(0, T; (H^1(\Omega))') \cap L^\infty(0, T; L^2(\Omega))$, $u \in H^1(0, T; L^2(\Omega)) \cap L^\infty(0, T; H^1(\Omega)) \cap L^\infty(Q)$, and $\chi \in W^{1,\infty}(0, T; L^2(\Omega)) \cap L^\infty(0, T; H^1(\Omega)) \cap L^\infty(Q)$ such that*

$$\begin{aligned} \vartheta_\varepsilon &\rightarrow \vartheta \text{ strongly in } C^0([0, T]; (H^1(\Omega))'), \quad u_\varepsilon \rightarrow u \text{ and } \chi_\varepsilon \rightarrow \chi \\ &\text{strongly in } C^0([0, T]; L^2(\Omega)) \cap L^2(0, T; H^{3/4}(\Omega)) \text{ as } \varepsilon \searrow 0 \end{aligned} \tag{11}$$

and the triple (ϑ, u, χ) uniquely solves the relaxed Stefan problem specified by (5), $u = 1/\vartheta$ a.e. in Q ,

$$\delta\chi_t + \beta(\chi) \ni \sigma'(\chi) - \lambda'(\chi)u \quad \text{a.e. in } Q, \tag{12}$$

$$\vartheta(\cdot, 0) = \vartheta_0, \quad \chi(\cdot, 0) = \chi_0 \quad \text{a.e. in } \Omega. \tag{13}$$

We point out that uniqueness can be deduced by arguing as in the subsequent analysis of the differences $\vartheta_\varepsilon - \vartheta$, $u_\varepsilon - u$, and $\chi_\varepsilon - \chi$.

3. Error estimate

Let $\vartheta_\varepsilon, u_\varepsilon, \chi_\varepsilon$ and ϑ, u, χ be the above defined solutions and let $\Theta_\varepsilon := \vartheta_\varepsilon - \vartheta, U_\varepsilon := u_\varepsilon - u, \mathcal{X}_\varepsilon := \chi_\varepsilon - \chi$. We also set $\mathcal{X}_{0\varepsilon} := \chi_{0\varepsilon} - \chi_0$ and $E_{0\varepsilon} := c_0(\vartheta_{0\varepsilon} - \vartheta_0) + \lambda(\chi_{0\varepsilon}) - \lambda(\chi_0)$, observing that $c_0\vartheta_{0\varepsilon} + \lambda(\chi_{0\varepsilon})$ and $c_0\vartheta_0 + \lambda(\chi_0)$ play as initial internal energies. Then we can establish and show the main result of this note.

Theorem 3. *There is a constant C_2 such that*

$$\|\Theta_\varepsilon\|_{C^0([0, T]; (H^1(\Omega))')} + \|U_\varepsilon\|_{L^2(Q)} + \|\mathcal{X}_\varepsilon\|_{C^0([0, T]; L^2(\Omega))} \leq C_2 \varepsilon^{1/2} \quad \forall \varepsilon \in (0, 1]. \tag{14}$$

Proof. Integrate (5) from 0 to $t \in [0, T]$ and subtract it from the corresponding equality for $\vartheta_\varepsilon, u_\varepsilon, \chi_\varepsilon$. With the help of (9), (13), and of the Lipschitz continuity of λ we deduce that

$$\begin{aligned} &\int_\Omega c_0\Theta_\varepsilon(\cdot, t)v - k \int_\Omega \nabla \int_0^t U_\varepsilon(\cdot, \tau)d\tau \cdot \nabla v - \int_\Gamma \int_0^t (\gamma U_\varepsilon)(\cdot, \tau)d\tau v \\ &\leq \int_\Omega \left(\|\lambda'\|_{L^\infty(0, 1)} |\mathcal{X}_\varepsilon(\cdot, t)| + |E_{0\varepsilon}| \right) |v| \quad \forall v \in H^1(\Omega), \quad \forall t \in [0, T]. \end{aligned} \tag{15}$$

Here we take $v = -U_\varepsilon(\cdot, t)$. Since $\vartheta_\varepsilon = 1/u_\varepsilon, \vartheta = 1/u$ and (cf. (10–11)) $\max\{\|u_\varepsilon\|_{L^\infty(Q)}, \|u\|_{L^\infty(Q)}\} \leq C_1$, we have that

$$-c_0\Theta_\varepsilon U_\varepsilon = c_0|U_\varepsilon|^2/(u_\varepsilon u) \geq C_3|U_\varepsilon|^2 \quad \text{a.e. in } Q,$$

where $C_3 = c_0/C_1^2$. Noting that

$$\|E_{0\varepsilon}\|_{L^2(\Omega)} \leq C \max\{c_0, \|\lambda'\|_{L^\infty(0, 1)}\} \varepsilon^{1/2} \tag{16}$$

because of (7), by applying the elementary Young inequality in the right hand side of (15) it is straightforward to find a constant C_4 such that

$$\begin{aligned} &\frac{C_3}{2} \|U_\varepsilon(\cdot, t)\|_{L^2(\Omega)}^2 + \frac{k}{2} \int_\Omega \frac{\partial}{\partial t} \left| \nabla \int_0^t U_\varepsilon(\cdot, \tau)d\tau \right|^2 \\ &+ \int_\Gamma \frac{1}{2\gamma(\cdot, t)} \frac{\partial}{\partial t} \left| \int_0^t (\gamma U_\varepsilon)(\cdot, \tau)d\tau \right|^2 \leq C_4 \left(\|\mathcal{X}_\varepsilon(\cdot, t)\|_{L^2(\Omega)}^2 + \varepsilon \right) \quad \forall t \in [0, T]. \end{aligned} \tag{17}$$

Next, consider the two inclusions (8) and (12), take the difference, and multiply by \mathcal{X}_ε . The monotonicity of the graph β and the smoothness of σ entail

$$\begin{aligned} \frac{\delta}{2} \frac{\partial}{\partial t} |\mathcal{X}_\varepsilon|^2 &\leq (\varepsilon \Delta \chi_\varepsilon) \mathcal{X}_\varepsilon + \|\sigma''\|_{L^\infty(0, 1)} |\mathcal{X}_\varepsilon|^2 \\ &\quad - u_\varepsilon (\lambda'(\chi_\varepsilon) - \lambda'(\chi)) (\chi_\varepsilon - \chi) + \|\lambda'\|_{L^\infty(0, 1)} |U_\varepsilon| |\mathcal{X}_\varepsilon| \end{aligned} \tag{18}$$

a.e. in Q . As λ is convex and $u_\varepsilon > 0$, it turns out that

$$u_\varepsilon (\lambda'(\chi_\varepsilon) - \lambda'(\chi)) (\chi_\varepsilon - \chi) \geq 0$$

a.e. in Q . Therefore, on account of (17), from (18) we can recover the inequality

$$\begin{aligned} \frac{\delta}{2} \frac{\partial}{\partial t} \|\mathcal{X}_\varepsilon(\cdot, t)\|_{L^2(\Omega)}^2 &\leq \frac{\varepsilon^2}{4} \|\Delta \mathcal{X}_\varepsilon(\cdot, t)\|_{L^2(\Omega)}^2 + \frac{C_3}{4} \|U_\varepsilon(\cdot, t)\|_{L^2(\Omega)}^2 \\ &+ \left(1 + \|\sigma''\|_{L^\infty(0,1)} + \|\lambda'\|_{L^\infty(0,1)}^2 C_3^{-1}\right) \|\mathcal{X}_\varepsilon(\cdot, t)\|_{L^2(\Omega)}^2 \quad \text{for a.e. } t \in (0, T). \end{aligned} \quad (19)$$

Remark that $\varepsilon^2 \|\Delta \mathcal{X}_\varepsilon\|_{L^2(Q)}^2 \leq C_1^2 \varepsilon$ because of (10). Hence, adding (19) to (17), integrating by parts with respect to t , and making use of (7) we obtain

$$\begin{aligned} \frac{C_3}{4} \|U_\varepsilon\|_{L^2(0,t;L^2(\Omega))}^2 + \frac{k}{2} \int_\Omega \left| \nabla \int_0^t U_\varepsilon(\cdot, \tau) d\tau \right|^2 + \int_\Gamma \frac{1}{2\gamma(\cdot, t)} \left| \int_0^t (\gamma U_\varepsilon)(\cdot, \tau) d\tau \right|^2 \\ + \frac{\delta}{2} \|\mathcal{X}_\varepsilon(\cdot, t)\|_{L^2(\Omega)}^2 \leq \|\gamma_t/\gamma\|_{L^\infty(\Sigma)} \int_0^t \int_\Gamma \frac{1}{2\gamma(\cdot, \tau)} \left| \int_0^\tau (\gamma U_\varepsilon)(\cdot, s) ds \right|^2 \\ + C_5 \int_0^t \|\mathcal{X}_\varepsilon(\cdot, \tau)\|_{L^2(\Omega)}^2 d\tau + \frac{4C_4 T + 2\delta C^2 + C_1^2}{4} \varepsilon \quad \forall t \in [0, T], \end{aligned} \quad (20)$$

with $C_5 = C_4 + 1 + \|\sigma''\|_{L^\infty(0,1)} + \|\lambda'\|_{L^\infty(0,1)}^2 C_3^{-1}$. Now it suffices to apply the Gronwall lemma and recall that $1/\gamma \geq c$ for some constant $c > 0$. Indeed, this procedure leads to the estimate

$$\begin{aligned} \|U_\varepsilon\|_{L^2(Q)}^2 + \max_{0 \leq t \leq T} \int_\Omega \left| \nabla \int_0^t U_\varepsilon(\cdot, \tau) d\tau \right|^2 \\ + \max_{0 \leq t \leq T} \int_\Gamma \left| \int_0^t (\gamma U_\varepsilon)(\cdot, \tau) d\tau \right|^2 + \|\mathcal{X}_\varepsilon\|_{C^0([0,T];L^2(\Omega))}^2 \leq C_6 \varepsilon \end{aligned} \quad (21)$$

(where C_6 depends only on $C_3, k, c, \delta, \|\gamma_t/\gamma\|_{L^\infty(\Sigma)}, C_5, C_4, C, C_1$, and T) and (14) is then a consequence of (21) and (16), via comparison of the terms in (15).

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Remarks on the existence for the one-dimensional Frémond model of shape memory alloys

In this paper we outline a rigorous proof of the existence of solutions to one-dimensional initial-boundary value problems for the general and complete version of the Frémond thermo-mechanical model applying to shape memory alloys.

1. Introduction

This note is concerned with the following system of partial differential equations

$$c_0 \vartheta_t - h \vartheta_{xx} = F + \partial_t (L \chi_1 - (\alpha(\vartheta) - \vartheta \alpha'(\vartheta)) \chi_2 u_x) + \alpha(\vartheta) \chi_2 u_{xt}, \quad (1)$$

$$u_{tt} - \partial_x (-\nu u_{xxx} + \omega u_x + \alpha(\vartheta) \chi_2) = G, \quad (2)$$

$$k \partial_t \begin{bmatrix} \chi_1 \\ \chi_2 \end{bmatrix} + \begin{bmatrix} \ell(\vartheta - \vartheta^*) \\ \alpha(\vartheta) u_x \end{bmatrix} + \partial I_{\mathcal{K}}(\chi_1, \chi_2) \ni \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad (3)$$

holding in $Q = (0, 1) \times (0, T)$, where $T > 0$ is some final time, x and t denote space and time variables, respectively, and $\partial_t = \partial/\partial t$, $\partial_x = \partial/\partial x$. Such a system comes out from the derivation of a macroscopic model proposed by Frémond [10,11] to describe the thermo-mechanical phase transitions in shape memory materials. The equation (1) reflects the universal balance law of energy, ϑ standing for the absolute temperature, while (2) yields the equilibrium equation for the longitudinal displacement u . The relationship (3) governs the evolution of the phase proportions χ_1, χ_2 (related to the volumetric fractions of austenite and martensites phases) and it complies with the second principle of thermodynamics. As the Frémond model assumes a non differentiable free energy (weighted sum of smooth free energies associated with the individual phases and of the mixture free energy $\vartheta I_{\mathcal{K}}$), in (3) we find the maximal monotone graph $\partial I_{\mathcal{K}}$, representing exactly the subdifferential of the indicator function $I_{\mathcal{K}}$ of the plane triangle

$$\mathcal{K} := \{(\chi_1, \chi_2) \in \mathbb{R}^2 : |\chi_2| \leq \chi_1 \leq 1\}$$

(convex set containing the admissible phase proportions), that is, $I_{\mathcal{K}}(\chi_1, \chi_2) = 0$ if $(\chi_1, \chi_2) \in \mathcal{K}$, $= +\infty$ otherwise. A more detailed presentation of (1–3), extending to the multidimensional case as well, is provided in [6,7] to which we refer for the physical meaning of the positive constants $c_0, h, L, \nu, \omega, k, \ell$, and ϑ^* . Let us just point out here that the data F, G are proportional to the distributed heat source and body force, respectively, and that the function α (giving account of the thermal expansion) is non negative, non increasing, and vanishing above a critical temperature (the so-called Curie point) $\vartheta_c > \vartheta^*$.

Initial and boundary value problems have been investigated for various simplified versions of the field equations, in one or three dimensions of space (see [2,13,9], addressed to the one-dimensional case, and [6,1,12,3,7,4,5] quoted in chronological order), obtaining existence and, in some framework, also uniqueness and continuous dependence. Simplifications regard the removal of (part of) the nonlinearities from the energy balance equation (1) (actually, in the right hand side of (1) there are three highly nonlinear terms, namely $(\vartheta \alpha'(\vartheta) - \alpha(\vartheta)) u_x \partial_t \chi_2$, $\vartheta \alpha'(\vartheta) \chi_2 \partial_t u_x$, $\vartheta \alpha''(\vartheta) \chi_2 u_x \vartheta_t$, including the time derivative of phase variable or strain or temperature) and the quasi-stationary form (in which the inertial term u_{tt} is neglected) for the momentum balance equation (2). On the other hand, some effort has been done to treat the situation where $\nu = 0$, thus avoiding the regularizing fourth-order term in (2) (the use of a second gradient theory, to account for mechanical actions exerted on surfaces, is rather disputed by physicists). In addition, a possible line of future intriguing research could be the study of (1–3) with the coefficient k reduced to 0, so that no dissipation or phase relaxation enters into the dynamics of phase transition (compare with the standard multiphase Stefan problem).

However, concerning the general set of equations, in the paper [8] we have proved that, under weak and reasonable assumptions on the data, any sufficiently smooth solution has the property the absolute temperature component ϑ attains non negative values almost everywhere. This positivity result, independent of the particular form of the momentum balance equation, plays a crucial role in the argumentation of the present paper, to show

the existence of solutions to (1–3) satisfying the following boundary and initial conditions

$$h\vartheta_x(0,t) = h_0(\vartheta(0,t) - f_0(t)), \quad -h\vartheta_x(1,t) = h_1(\vartheta(1,t) - f_1(t)), \quad (4)$$

$$u(0,t) = u(1,t) = 0, \quad u_{xx}(0,t) = u_{xx}(1,t) = 0, \quad (5)$$

$$\vartheta(x,0) = \vartheta^0(x), \quad u(x,0) = u^0(x), \quad u_t(x,0) = w^0(x), \quad (6)$$

$$\chi_1(x,0) = \chi_1^0(x), \quad \chi_2(x,0) = \chi_2^0(x), \quad (7)$$

for $t \in (0, T)$ and $x \in (0, 1)$, where h_0, h_1 are positive heat exchange coefficients, the functions f_0, f_1 give the outside temperature distributions, and $\vartheta^0, u^0, w^0, \chi_1^0, \chi_2^0$ denote the initial data.

In fact, our contribution is devoted to sketch the proof of the next statement. For the sake of brevity, in the notation of Sobolev spaces like $L^2(0, 1)$ or $H^1(0, 1)$ we omit the indication of the interval $(0, 1)$. Besides, let (\cdot, \cdot) represent both the scalar product in L^2 and the duality pairing between H^{-1} and H_0^1 .

Theorem 1. Assume that $\vartheta^0 \in H^1$, $\vartheta^0 \geq 0$ in $[0, 1]$, $u^0, (u^0)_{xx}, w^0 \in H_0^1$, $\chi_1^0, \chi_2^0 \in L^\infty$, $(\chi_1^0, \chi_2^0) \in \mathcal{K}$ a.e. in $(0, 1)$, $f_0, f_1 \in W^{1,1}(0, T)$, $f_0 \geq 0$ and $f_1 \geq 0$ in $[0, T]$, $F \in L^2(0, T; L^2) \equiv L^2(Q)$, $F \geq 0$ a.e. in Q , $G \in W^{1,1}(0, T; L^2)$, $\alpha \in C^2(\mathbb{R})$, $\alpha'(\xi) = 0$ if $\xi \leq 0$ and $\xi \geq \vartheta_c$, and that the constant $c_\alpha = \|\alpha''\|_{L^\infty(\mathbb{R})}$ is small enough (this last requirement is nothing but a compatibility condition among some data, as it will become clear in the sequel). Then the problem (1–7) has at least one solution $(\vartheta, u, \chi_1, \chi_2)$ with

$$\begin{aligned} \vartheta &\in H^1(0, T; L^2) \cap C^0([0, T]; H^1) \cap L^2(0, T; H^2), \quad \vartheta \geq 0 \text{ a.e. in } Q, \\ u &\in W^{2,\infty}(0, T; H^{-1}) \cap C^1([0, T]; L^2) \cap W^{1,\infty}(0, T; H_0^1) \cap C^0([0, T]; H^2) \cap L^\infty(0, T; H^3), \\ \chi_1, \chi_2 &\in H^1(0, T; L^2) \cap L^\infty(Q), \quad (\chi_1, \chi_2) \in \mathcal{K} \text{ a.e. in } Q, \end{aligned}$$

fulfilling (1) and (3) a.e. in Q , (2) in the sense of $L^2(0, T; H^{-1})$, (4–5) a.e. in $(0, T)$, and (6–7) a.e. in $(0, 1)$.

This theorem is inferred by using a sort of elliptic regularization, deriving uniform bounds for the approximating solutions, and finally passing to the limit with the help of compactness techniques. We notice that an independent proof is proposed in [14].

2. A priori estimates

First thing, we prefer to deduce the formal a priori estimates allowing us, basically, to get the existence result. Letting the comments on approximation and limit procedure for the last section, we start by recalling that an alternative expression for (1) is

$$(c_0 - \vartheta\alpha''(\vartheta)\chi_2 u_x)\vartheta_t - h\vartheta_{xx} = F + L\partial_t\chi_1 + (\vartheta\alpha'(\vartheta) - \alpha(\vartheta))u_x\partial_t\chi_2 + \vartheta\alpha'(\vartheta)\chi_2 u_{xt} \quad \text{a.e. in } Q. \quad (8)$$

Moreover, a weak formulation of (2), which accounts for the boundary conditions in (5), reads

$$(u_{tt}, v) + \nu(u_{xx}, v_{xx}) + (\omega u_x + \alpha(\vartheta)\chi_2, v_x) = (G, v) \quad \forall v \in H_0^1 \cap H^2, \text{ a.e. in } (0, T), \quad (9)$$

and the inclusion (3) can be equivalently rewritten as the pointwise variational inequality

$$\begin{aligned} (\chi_1(x, t), \chi_2(x, t)) \in \mathcal{K}, \quad \sum_{j=1}^2 k(\partial_t\chi_j)(x, t)(\chi_j(x, t) - \gamma_j) + \ell(\vartheta(x, t) - \vartheta^*)(\chi_1(x, t) - \gamma_1) \\ + (\alpha(\vartheta)u_x)(x, t)(\chi_2(x, t) - \gamma_2) \leq 0 \quad \forall (\gamma_1, \gamma_2) \in \mathcal{K}, \end{aligned} \quad (10)$$

to be satisfied for a.e. $(x, t) \in Q$. By using essentially (10), the special form of the convex \mathcal{K} , the fact that α is constant on negative values, the sign hypotheses on F, f_0, f_1 , and ϑ^0 , one obtains $\vartheta \geq 0$ a.e. in Q (see [8] for the details).

The second step consists in an estimate already performed in [15] (for a different shape memory model) and involving just the energy and momentum balance equations. Indeed, we integrate (1) over $(0, 1) \times (0, t)$, taking advantage of (4) and (6), and choose $v = u_t$ in (9), integrating then from 0 to $t \in [0, T]$. Summing the two identities, the terms containing $\alpha(\vartheta)\chi_2 u_{xt}$ cancel each other out. Also, owing to the properties of α and the boundedness of \mathcal{K} , we have that $\int_0^t \int_0^1 \partial_t(L\chi_1 - (\alpha(\vartheta) - \vartheta\alpha'(\vartheta))\chi_2 u_x) \leq 2L + 2\vartheta_c^2 c_\alpha (\|u_x(\cdot, t)\|_{L^2} + \|\partial_x u^0\|_{L^2})$. Hence, in view of the positivity of ϑ , by the elementary Young inequality one can easily find two constants C_1, C_2 , depending only on $c_0, \|\vartheta^0\|_{L^1}, \|F\|_{L^1(Q)}, h_0, h_1, \|f_0\|_{L^1(0, T)}, \|f_1\|_{L^1(0, T)}, L, \vartheta_c, \omega, \nu, \|\partial_x u^0\|_{H^1}$, and $\|G\|_{L^1(0, T; L^2)}$, such that

$$\|\vartheta(\cdot, t)\|_{L^1} + \|u_t(\cdot, t)\|_{L^2}^2 + \|u_x(\cdot, t)\|_{H^1}^2 \leq C_1 + C_2 c_\alpha^2 \quad \forall t \in [0, T]. \quad (11)$$

Since H^1 is continuously embedded into L^∞ (here the space dimension 1 is crucial), (11) ensures that $\|u_x\|_{L^\infty(Q)} \leq C_3 + C_4 c_\alpha$ for some constants C_3, C_4 related to C_1, C_2 . Now, the assumption of smallness for c_α can be made precise: in order that the coefficient of ϑ_t in (8) (such coefficient represents the specific heat which ought to) be positive everywhere, it is demanded that $C_5 := c_0 - \vartheta_c c_\alpha (C_3 + C_4 c_\alpha) > 0$.

The subsequent estimate gives further information about the regularity of ϑ and u as well as it deals with the phase variables χ_1, χ_2 too. Multiply formally (8) by ϑ_t , (2) by $-u_{xxt}$ (or take $v = -u_{xxt}$ in (9)), and (3) both by the vector of components $\partial_t \chi_1, \partial_t \chi_2$ and by the scaling constant (to be specified later) $C > 0$. Adding and integrating by parts in space and time, on account of (4–7) and of the previous bounds it is not difficult to verify that (see [5] for analogous calculations)

$$\begin{aligned} C_5 \int_0^t \int_0^1 |\vartheta_t|^2 + \frac{h}{2} \|\vartheta_x(\cdot, t)\|_{L^2}^2 + \sum_{i=0}^1 \frac{h_i}{4} |\vartheta(i, t)|^2 + \frac{1}{2} \|u_{xt}(\cdot, t)\|_{L^2}^2 + \frac{\nu}{4} \|u_{xxx}(\cdot, t)\|_{L^2}^2 \\ + C \sum_{j=1}^2 \frac{k}{2} \int_0^t \int_0^1 |\partial_t \chi_j|^2 \leq C_6 + C_7 \int_0^t \int_0^1 \left(|F| + \sum_{j=1}^2 |\partial_t \chi_j| + |u_{xt}| \right) |\vartheta_t| \\ + \sum_{i=0}^1 h_i \int_0^t |(f_i)_t(s)| |\vartheta(i, s)| ds + C_8 \int_0^t \int_0^1 (|\vartheta_t| + |\partial_t \chi_2|) |u_{xxx}| + \frac{\ell C}{2} \int_0^t \|\vartheta(\cdot, s)\|_{L^2}^2 ds \end{aligned} \quad (12)$$

for a.e. $t \in (0, T)$, where C_6, C_7, C_8 depend on the data (T included) and C_6 depends also on C . By applying the Young inequality in the right hand side of (12), we can control the integrals of $|\vartheta_t|^2$ in a way that the sum of them be less than $(C_5/2) \int_0^t \int_0^1 |\vartheta_t|^2$. Then we choose C sufficiently large so that the terms containing $|\partial_t \chi_1|^2, |\partial_t \chi_2|^2$ are dominated by the corresponding ones in the left hand side. Finally, exploiting an extended version of the Gronwall lemma we come to the conclusion that

$$\|\vartheta\|_{H^1(0,t;L^2) \cap L^\infty(0,t;H^1)} + \|u\|_{W^{1,\infty}(0,t;H^1) \cap L^\infty(0,t;H^3)} + \sum_{j=1}^2 \|\chi_j\|_{H^1(0,t;L^2) \cap L^\infty((0,1) \times (0,t))} \leq C_9 \quad (13)$$

for all $t \in (0, T]$, C_9 being a constant with the most of dependences, according to the framework of Theorem 1.

3. Approximation

Letting $\varepsilon > 0$, we substitute (2) with the regularized equation

$$\partial_{tt} (u + \varepsilon u_{xxxx} - \varepsilon u_{xx}) - \partial_x (-\nu u_{xxx} + \omega u_x + \alpha(\vartheta)\chi_2) = G \quad (14)$$

and we prescribe the initial datum w_ε^0 instead of w^0 (while u^0 remains unchanged), where $w_\varepsilon^0 \in H_0^1 \cap H^4$ solves the variational equality $(w_\varepsilon^0, v) + \varepsilon (\partial_{xx} w_\varepsilon^0, v_{xx}) + \varepsilon (\partial_x w_\varepsilon^0, v_x) = (w^0, v)$ for any $v \in H_0^1 \cap H^2$. Thanks to the property $w^0 \in H_0^1$, it turns out that the quantity $\|w_\varepsilon^0\|_{H^1}^2 + \sqrt{\varepsilon} \|\partial_{xx} w_\varepsilon^0\|_{L^2}^2 + \varepsilon \|\partial_{xxx} w_\varepsilon^0\|_{L^2}^2$ is bounded independently of ε , and that $w_\varepsilon^0 \rightarrow w^0$ strongly in L^∞ as $\varepsilon \searrow 0$.

Consider now the problem (1), (14), (3–7) in which w^0 is replaced by w_ε^0 . For simplicity we denote this approximating problem by (P_ε) . First one shows a local existence and uniqueness result for (P_ε) . Namely, by applying the Contraction Mapping Principle we can find a value $\tau \in (0, T]$ (possibly depending on ε) such that, for ε sufficiently small, there exists one and only one solution of (P_ε) in the time interval $[0, \tau]$. Our fixed point argument works as follows. Take a pair (Θ, \mathcal{X}_2) with $\Theta, \mathcal{X}_2 \in L^2(0, \tau; L^2)$ and $|\mathcal{X}_2| \leq 1$ almost everywhere (see the definition of \mathcal{K}). Put Θ (in place of ϑ) and \mathcal{X}_2 (in place of χ_2) in (14). Hence the initial–boundary value problem in (14), (5–6) admits a unique solution $u \in W^{2,\infty}(0, T; H^3)$. Moreover, multiplying (14) by u_t , integrating by parts in $(0, 1) \times (0, t)$ ($t \leq \tau$), and observing that

$$\frac{\varepsilon}{2} \|\partial_{xx} w_\varepsilon^0\|_{L^2}^2 + \frac{\varepsilon}{2} \|\partial_x w_\varepsilon^0\|_{L^2}^2 - \int_0^t \int_0^1 \alpha(\Theta) \mathcal{X}_2 u_{xt} \leq C_{10} \left(\varepsilon^{1/2} + \varepsilon^{-1/2} \int_0^t \sqrt{\varepsilon} \|u_{xt}(\cdot, s)\|_{L^2} ds \right)$$

(C_{10} independent of ε and τ), one infers that (cf. (11))

$$\|u_t(\cdot, t)\|_{L^2}^2 + \varepsilon \|u_{xt}(\cdot, t)\|_{H^1}^2 + \|u_x(\cdot, t)\|_{H^1}^2 \leq C_1 + C_2 c_\alpha^2 \quad \forall t \in [0, \tau], \quad (15)$$

provided ε and τ^2/ε are small enough. Therefore, $\|u_x\|_{L^\infty((0,1) \times (0,\tau))} \leq C_3 + C_4 c_\alpha$ (the constants are the same as in Section 2) and also $\|u_{xt}\|_{L^\infty((0,1) \times (0,\tau))}$ is bounded, by a constant proportional to $\varepsilon^{-1/2}$ (but this is not so important). Next, use the already found u_x and u_{xt} in the system coupling (1) and (3). Here you can prove the well-posedness of the corresponding initial–boundary value problem arguing as in [9], determining thus the solution $(\vartheta, \chi_1, \chi_2)$ and, in

particular, a new pair (ϑ, χ_2) . At this point, by means of suitable contracting estimates (similar to those developed in [9]), setting other restrictions on ε and τ if necessary, we arrange for the mapping $(\Theta, \mathcal{X}_2) \mapsto (\vartheta, \chi_2)$ to be a contraction.

Then we can proceed exactly as in the previous section, starting from the positivity of ϑ (we stress again that the result of [8] does not rely on the form of the momentum balance equation) and ending with an estimate like (13), where $\sqrt{\varepsilon} \|u_\varepsilon\|_{L^\infty(0,t;H^3)}$ has to be added in the left hand side and where the respective constant C_9 is independent of τ and ε . Thus the solution $(\vartheta_\varepsilon, u_\varepsilon, \chi_{1\varepsilon}, \chi_{2\varepsilon})$ of the problem (P_ε) actually exists in the whole interval $[0, T]$. From comparisons in (8), (4) and in (14) we recover bounds also for $\|\vartheta_\varepsilon\|_{L^2(0,T;H^2)}$ and $\|u_\varepsilon + \varepsilon \partial_{xx}(\partial_{xx}u_\varepsilon - u_\varepsilon)\|_{W^{2,\infty}(0,T;H^{-1})}$. Consequently, we are able to pass to the limit as $\varepsilon \searrow 0$ by weak and weak star compactness and to show that any limit $(\vartheta, u, \chi_1, \chi_2)$ of subsequences of $(\vartheta_\varepsilon, u_\varepsilon, \chi_{1\varepsilon}, \chi_{2\varepsilon})$ must yield one of the solutions defined by Theorem 1. In fact (see [5] for similar arguments), compact injections along with direct verifications allow us to deduce strong convergences for (subsequences of) $\vartheta_\varepsilon, \partial_x u_\varepsilon, \chi_{1\varepsilon}, \chi_{2\varepsilon}$ helping to take the limit in the nonlinearities. Moreover, since $\partial_{tt}(u_\varepsilon + \varepsilon \partial_{xxxx}u_\varepsilon - \varepsilon \partial_{xx}u_\varepsilon)$ weakly star converges to some η in $L^\infty(0, T; H^{-1})$ and $(\varepsilon \partial_{xxxx}u_\varepsilon - \varepsilon \partial_{xx}u_\varepsilon) \rightarrow 0$ in $W^{1,\infty}(0, T; H^{-1})$, it turns out that $\eta = u_{tt}$ and (9) holds.

Remark 2. In regard of experimental situations, it would be more interesting to treat the problem (1–7) with non-zero Dirichlet boundary conditions for u , assuming for instance a prescribed displacement $u(1, t) = g(t)$ on one end. In this case it suffices to let $g \in W^{3,1}(0, T)$ and use the new unknown $\hat{u}(x, t) = u(x, t) - xg(t)$, $(x, t) \in Q$, instead of u , with obvious modifications in (1–3). What it seems more difficult to handle is a Neumann boundary condition for the conormal derivative, e.g. $(-\nu u_{xxx} + \omega u_x + \alpha(\vartheta)\chi_2)(1, t) = g_n(t)$ (where g_n would represent an external traction), as it was instead done in [9] and [5], for instance. Thus, the study of (1–7) with other boundary conditions for u remains an open question as well as the extension of the above existence result to the three-dimensional case.

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Non-local Effects in Phase Separation Dynamics

We consider two non-local effects in phase separation dynamics. One is a non-local self-stress effect for a binary substitutional solid solution and the other is a non-local constraint arising in block copolymers. The origins of the above two non-localities are different, namely, for the first case, it comes from the fact that the characteristic time for stress change is much smaller than that for atomic diffusion ([8]). On the other hand, for the second case, the binding between two different monomers causes a spacial non-local connectivity ([11], [3], [9]). The coarsening process is usually very slow without stress effects, however it is accelerated drastically by adding the stress effect. The non-local effect for copolymer case makes a sharp contrast with the stress case, namely, the spacial connectivity stops the coarsening process at mesoscopic level and very fine micro-structures are formed spontaneously.

1. Rapid coarsening by non-local self-stress effects

The following model was presented by [8] and was studied numerically by [4].

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 M}{\partial x^2} & \text{for } -\frac{1}{2} < x < \frac{1}{2}, \\ \frac{\partial M}{\partial x} &= 0 & \text{at } x = \pm \frac{1}{2}, \\ \frac{\partial u}{\partial x} &= 0 & \text{at } x = \pm \frac{1}{2}, \end{aligned} \quad (1)$$

where

$$M := (u^2 - 1)u + \alpha(u - \bar{u}) - \varepsilon^2 \frac{\partial^2 u}{\partial x^2} - 12\alpha \left(\int_{-\frac{1}{2}}^{\frac{1}{2}} xu \, dx \right) x,$$

α is a (positive) stress parameter, and \bar{u} ($0 < \bar{u} < 1$) is the average concentration $\bar{u} := \int_{-\frac{1}{2}}^{\frac{1}{2}} u \, dx$. The associated Lyapunov functional is given by

$$F^{\varepsilon, \alpha}(u) := \int_{-\frac{1}{2}}^{\frac{1}{2}} \left\{ \frac{\varepsilon^2}{2} \left(\frac{\partial u}{\partial x} \right)^2 + \frac{1}{4} (u^2 - 1)^2 + \frac{\alpha}{2} u^2 \right\} dx - 6\alpha \left\{ \int_{-\frac{1}{2}}^{\frac{1}{2}} xu \, dx \right\}^2. \quad (2)$$

Apparently (1) is reduced to the Cahn-Hilliard equation when $\alpha = 0$, which is known to have very slow motion at the late stage of coarsening process.

Theorem 1. ([10]) $F^{\varepsilon, \alpha}$ has a unique non-constant monotone global minimizer in $H^1(-\frac{1}{2}, \frac{1}{2})$ with the constraint $\int_{-\frac{1}{2}}^{\frac{1}{2}} u \, dx = \varsigma$ for small α and ε and for $\varsigma \in (-\sqrt{(1-\alpha)/3}, \sqrt{(1-\alpha)/3})$. In the coarsening process toward the global minimizer, the largest (real) eigenvalue at any layered stationary solution of (1), which is not symmetric at $x = 0$, is at least of order $\alpha\varepsilon$.

This implies that the layer motion is NOT very slow even when $\alpha = O(\varepsilon)$, which is consistent with the numerics in [4]. One of the key ingredients to show Theorem 1 is the next comparison result for spectra between the linearized problem of (1) and that of the following auxiliary second order equation of conservative type:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \varepsilon^2 \frac{\partial^2 u}{\partial x^2} - (u^2 - 1)u - \alpha(u - \bar{u}) + \int_{-\frac{1}{2}}^{\frac{1}{2}} (u^2 - 1)u \, dx + (12\alpha \int_{-\frac{1}{2}}^{\frac{1}{2}} x u \, dx) x & \text{for } -\frac{1}{2} < x < \frac{1}{2}, \\ \frac{\partial u}{\partial x} &= 0 & \text{at } x = \pm \frac{1}{2}. \end{aligned} \quad (3)$$

The corresponding linearized eigenvalue problems at a stationary solution v to (1) and (3) (note that the set of stationary solutions of (1) coincides with that of (3)) are the following, respectively,

$$\begin{aligned} \lambda\psi &= -\frac{\partial^2 L}{\partial x^2} \quad \text{for } -\frac{1}{2} < x < \frac{1}{2}, \\ \frac{\partial L}{\partial x} &= 0 \quad \text{at } x = \pm\frac{1}{2}, \\ \frac{\partial \psi}{\partial x} &= 0 \quad \text{at } x = \pm\frac{1}{2}, \end{aligned} \quad (4)$$

where

$$L := -f'(v)\psi + \alpha\psi - \varepsilon^2 \frac{\partial^2 \psi}{\partial x^2} - 12\alpha \left(\int_{-\frac{1}{2}}^{\frac{1}{2}} x\psi \, dx \right) x,$$

$f(u)$ stands for the nonlinear term $u - u^3$, and

$$\begin{aligned} \mu\phi &= -\left[\varepsilon^2 \frac{\partial^2 \phi}{\partial x^2} + f'(v)\phi - \alpha\phi - \int_{-\frac{1}{2}}^{\frac{1}{2}} f'(v)\phi \, dx + (12\alpha \int_{-\frac{1}{2}}^{\frac{1}{2}} x\phi \, dx)x \right] \quad \text{for } -\frac{1}{2} < x < \frac{1}{2}, \\ \frac{\partial \phi}{\partial x} &= 0 \quad \text{at } x = \pm\frac{1}{2}. \end{aligned} \quad (5)$$

Note that the average of ψ and ϕ are equal to 0. The n -th eigenvalues of (4) and (5) are denoted by λ_n and μ_n , respectively. It can be shown that both $\{\lambda_n\}_{n=0}^{\infty}$ and $\{\mu_n\}_{n=0}^{\infty}$ tend to infinity. Moreover the following spectral comparison result holds;

L e m m a 2. For any $n = 0, 1, 2, 3, \dots$,

$$\begin{aligned} \mu_n \leq 0 & \quad \text{implies that} \quad \lambda_n \leq \pi^2 \mu_n, \\ \mu_n \geq 0 & \quad \text{implies that} \quad \lambda_n \geq \pi^2 \mu_n, \end{aligned}$$

and, especially, $\lambda_n = 0$ if and only if $\mu_n = 0$.

It should be remarked that stability and instability properties of (1) can be determined by those of (3). This is sharper than the similar result in [2], however the second order equation (3) becomes more difficult due to non-local term.

2. Micro-phase separation and scaling law for diblock copolymers

The following model was proposed by [11], [3] and [9] to describe the phase separation dynamics for diblock copolymers.

$$\begin{aligned} u_t &= \Delta \{ -\varepsilon^2 \Delta u - f(u) + \sigma (-\Delta_N)^{-1} (u - \bar{u}_0) \} & \text{in } \Omega, \\ &= \Delta \{ -\varepsilon^2 \Delta u - f(u) \} - \sigma (u - \bar{u}_0) & \text{in } \Omega, \\ u(x, 0) &= u_0(x) \\ \frac{\partial u}{\partial n} &= \frac{\partial \Delta u}{\partial n} = 0 & \text{on } \partial\Omega, \\ \frac{1}{|\Omega|} \int_{\Omega} u_0(x) dx &= \bar{u}_0 : & \text{a given constant,} \end{aligned} \quad (6)$$

where $f(u) := u - u^3$, $(-\Delta_N)^{-1}$ is the inverse of the Laplacian with zero flux boundary condition (defined on the space orthogonal to constant functions), ε is a positive constant related to interfacial thickness, and σ is a positive constant inversely proportional to the square of total length of polymer chain. Note that the non-local term represents the connection of two different monomers, and \bar{u}_0 determines the ratio of those composition. It was confirmed experimentally and numerically that coarsening stops at certain stage and the solution of (6) settles down to a very fine steady state (see [3], [5], [6] and [7]), and the morphology of final state changes according to the composition ratio \bar{u}_0 . One of the most important problems is that how the domain size of the final state depends on ε and σ .

Theorem 3. ([9]) *The characteristic domain size of stationary patterns of (6) is proportional to $(\frac{\varepsilon}{\sigma})^{\frac{1}{3}}$.*

The above scaling law can be derived in order for (6) to have a well-defined singular limiting equations independent of parameters ε and σ by using the method of [1]. See [9] for more details of the above result and the free boundary problem which determines the morphology of steady states.

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