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A dissipative discretization scheme for a nonlocal phase segregation model

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Abstract. We are interested in finite volume discretization schemes and numerical solutions for a nonlocal phase segregation model, suitable for large times and interacting forces. Our main result is a scheme with definite discrete dissipation rate proportional to the square of the driving force for the evolution, i. e., the discrete antigradient of the chemical potential v. Steady states are characterized by constant v and satisfy a nonlocal stationary equation. A numerical bifurcation analysis of that stationary equation explains the observed global behavior of numerically computed trajectories of the evolution equation.
For strong interaction forces the model shows steady states distinguished by small deformations of the 'mushy region' or 'interface states'. One essential open question in the discrete case is the global boundedness of v.

1 Introduction

In [5] a nonlocal phase segregation model [7] was applied to image reconstruction. Here we are interested in a numerical study of the phase segregation problem itself. The phase segregation model reads

$$\frac{\partial u}{\partial t} - \nabla \cdot \left(f(|\nabla v|) \, \left(\nabla u + \frac{\nabla w}{\phi''(u)} \right) \right) = 0, \quad u(0,\cdot) = u_0(\cdot), \text{ in } \Omega, \tag{1}$$

$$v = \phi'(u) + w, \quad w(t,x) = \int_\Omega \mathcal{K}(|x-y|)(1 - 2\,u(t,y))\,dy. \tag{2}$$

Here $\Omega \subset I\!R^N$, $1 \leq N \leq 3$ is a bounded Lipschitzian domain, ϕ is a convex function, the kernel $\mathcal{K}$ represents nonlocal attracting forces, w is the interaction potential and v may be interpreted as chemical potential. The system (1), (2) was rigorously derived in [8] in the case of constant f and can be seen as a nonlocal variant of the Cahn-Hilliard [1] equation which is associated with the local Ginzburg-Landau free energy

$$F_{gl}(u) = \int_\Omega \left\{ \phi(u) + \kappa u\,(1 - u) + \frac{\lambda}{2}\,|\nabla u|^2 \right\} dx. \tag{3}$$

The system (1), (2) was studied in [7]. For the non-isothermal case, we refer to [3], and to [9] for the multiple species case. A descent method has been established in [6].

It turns out that (1), (2) has the Lyapunov functional

$$F(u) = \int_\Omega \left\{ \phi(u) + u \int_\Omega \mathcal{K}(|x-y|)(1 - u(y))\,dy \right\} dx. \tag{4}$$

In the following we consider the specialized model: constant f, $\phi(u) = u \ln u + (1-u)\ln(1-u)$, and $\mathcal{K}$ is Green's function of the elliptic boundary value problem

$$-\sigma^2 \nabla \cdot \nabla w + w = m(1 - 2u), \quad \nu \cdot \nabla w = 0 \text{ on } \partial\Omega \tag{5}$$

with positive constants σ, m. We suppose the initial value to satisfy $0 < u_0 < 1$ and complete (1) by homogeneous Neumann boundary conditions, too.

In the next section we formulate the discrete version of the system (1), (5) and derive some bounds for w, u, v. The third section presents results of a numerical bifurcation analysis. These are corresponding to the typical structures observed during evolution processes.

2 Discretization

We apply a finite volume scheme. The notation follows [4] and is summarized as short introduction.

2.1 Notation

Definition 2.1 A partitioning of Ω by simplices $\mathbf{E}^N$ such that

$$\Omega = \cup_i \mathbf{E}_i^N$$

is called a *Delaunay grid* if the balls defined by the $N+1$ vertices of $\mathbf{E}_i^N$ $\forall$ i do not contain any vertex $\mathbf{x}_k$, $\mathbf{x}_k \in \mathbf{E}_j^N$, $\mathbf{x}_k \notin \mathbf{E}_i^N$. A Delaunay grid is called *conforming*, if the circum center of any simplex is in Ω (if $\Omega := \cup_i \Omega_i$, the circum center of any simplex in Ω_i has to be in $\bar{\Omega}_i$).

We suppose that Ω admits a conforming Delaunay decomposition with simplices of positive volume in a right–handed coordinate system. The $N \times (N+1)$ matrix of the vertex coordinates represents the simplex: $\mathbf{x}_i^T = (x_{1,i}, x_{2,i}, \ldots, x_{N,i})$ is the vector of the space coordinates of the vertex i of the simplex.
Edges (simplices with $N = 1$) are denoted by $\mathbf{e}_{ij} = \mathbf{x}_j - \mathbf{x}_i$. The simplex $\mathbf{E}_i^{N-1}$ is the 'surface' opposite to vertex i of the simplex $\mathbf{E}^N$.

Definition 2.2 Let $V_i = \{\mathbf{x} \in I\!R^N : \|\mathbf{x} - \mathbf{x}_i\| < \|\mathbf{x} - \mathbf{x}_j\|, \forall \text{ vertices } \mathbf{x}_j \in \Omega\}$ and $\partial V_i = \bar{V}_i \setminus V_i$. V_i is the *Voronoi volume* of vertex i and ∂V_i is the corresponding *Voronoi surface*.
The Voronoi volume element V_{ij} of the vertex i with respect to the simplex $\mathbf{E}_j^N$ is the intersection of the simplex $\mathbf{E}_j^N$ and the Voronoi volume V_i of vertex i. Accordingly $\partial V_{i,j} := \partial V_i \cap \mathbf{E}_j^N$ denotes the Voronoi surface of vertex i in simplex $\mathbf{E}_j^N$. The part of $\partial V_{i,j}$ related to the edge $\mathbf{e}_{ik}$ is denoted by $\partial V_{i,k(i,j)}$ ($\partial V_{i,k(i,j)} \perp \mathbf{e}_{ik}$). $k(i,j)$ denotes a vertex k (neighboring vertex of i), such that $k \in \mathbf{E}_j^N$ and $i \in \mathbf{E}_j^N$, $i \neq k$.

A function g defined at $\mathbf{E}^N$ is approximated by a discrete vector $\mathbf{g} = (g(\mathbf{x}_1), \ldots, g(\mathbf{x}_{N+1}))^T$ on the vertices. Hence its volume integral on $\mathbf{E}^N$ is

$$\int_{\mathbf{E}_j^N} g \, d\Omega \approx \sum_{i \in \mathbf{E}_j^N} g_i |V_{ij}|, \qquad \sum_{i,j} |V_{ij}| = |\Omega|.$$

$[\cdot]$ denotes diagonal matrices, i. e. $[V]$ is the diagonal matrix of the Voronoi volumes V_i defined above.

Differential operators like $-\nabla \cdot \epsilon \nabla$ are discretized by means of Gauss's theorem

$$\int_{V_{ij}} -\nabla \cdot \epsilon \nabla u dV = -\epsilon \sum_k \int_{\partial V_{i,k(i,j)}} \nabla u \cdot d\mathbf{S_k} + \sum_k \psi_{ik} \approx [\gamma_{k(i)}] \tilde{G}_N \mathbf{u}|_{E_j^N} + \sum_k \psi_{ik}.$$

The $\psi_{ik} := -\epsilon \int_{\mathbf{E}_{k(i,j)}^{N-1} \cap V_i} \nabla u \cdot d\mathbf{S_k}$ are either compensated by the neighboring simplex or represent boundary integrals. The latter vanish due to the homogenous Neumann boundary conditions. In the following nonnegative Voronoi surfaces $\partial V_{i,k(i,j)}$ between vertices i and next neighbors $k(i,j)$

$$\gamma_{k(i,j)} = \frac{|\partial V_{i,k(i,j)}|}{|\mathbf{e}_{i,k(i,j)}|} \geq 0$$

are assumed for simplicity. (A strong restriction with respect to grids, the general conforming Delaunay case can be handled but would require to discuss the compensation rules regarding next neighbors). One verifies on the simplex E_j^N

$$\sum_{i, V_i \in \mathbf{E}_j^N} \int_{V_{ij}} -\nabla \cdot \epsilon \nabla u dV \approx \epsilon \tilde{G}_N^T [\gamma] \tilde{G}_N \mathbf{u}|_{E_j^N},$$

where

$$\tilde{G}_2 = \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix}, \quad \tilde{G}_3 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix}, \quad \cdots,$$

is the difference matrix along all edges, hence a mapping from nodes to edges. Finally we define

$$G = [\sqrt{\gamma}]\tilde{G}_N.$$

If ϵ is not constant, but $\epsilon = \epsilon(u)$, its evaluation at the Voronoi surface requires approximations. A proper approximation for the phase segregation model is discussed next.

2.2 A dissipative discretization scheme

In the following we derive a dissipative discretization scheme. The starting point is the symmetry observation of

$$\int_\Omega (u_t w - u w_t) dx = 0. \tag{6}$$

Indeed, testing (5) with w_t yields

$$\begin{aligned} \int_\Omega u w_t dx &= -\int_\Omega \frac{1}{4m}\frac{d}{dt}(\sigma^2|\nabla w|^2 + w^2)dx \\ &= \int_\Omega u_t w dx. \end{aligned}$$

The free energy functional can be written as

$$F(u) = \int_\Omega \left(\Phi(u) + \frac{1}{2}uw\right) dx + c.$$

Using time differentiation and (6) we get

$$\begin{aligned} \frac{d}{dt}F(u(t)) &= \int_\Omega \left(\Phi'(u)u_t + \frac{1}{2}(u_t w + u w_t)\right) dx \\ &= \int_\Omega \left(\Phi'(u)u_t + w u_t\right) dx \\ &= -\int_\Omega f(|\nabla v|)\left(\nabla u + \frac{1}{\Phi''(u)}\nabla w\right)\cdot\left(\Phi''(u)\nabla u + \nabla w\right) dx \\ &= -\int_\Omega f(|\nabla v|)\Phi''(u)\left|\nabla u + \frac{1}{\Phi''(u)}\nabla w\right|^2 dx \le 0. \end{aligned}$$

Proposition 2.3 *The following time discretization preserves the descent property $F(u(t)) \ge F(u(t+\tau))$:*

$$\frac{u(t+\tau)-u(t)}{\tau} - \nabla\cdot f(|\nabla v|)\left(\nabla u(t+\tau) + \frac{\nabla(w(t+\tau)+w(t))}{2\Phi''(u(t+\tau))}\right) = 0,$$

$$-\nabla\cdot\sigma^2\nabla w(t+\tau) + w(t+\tau) = m(1-2u(t+\tau)).$$

P r o o f. A computation similar to the continuous case shows that

$$\begin{aligned}
\frac{1}{\tau}(F(u(t)) - F(u(t+\tau))) \geq \frac{1}{\tau}\int_\Omega \Big(& \Phi'(u(t+\tau))(u(t) - u(t+\tau)) + \\
&+\frac{1}{4}\{(u(t) - u(t+\tau))(w(t) + w(t+\tau)) + \\
&+(u(t) + u(t+\tau))(w(t) - w(t+\tau))\}\Big) dx \\
= \;& -\int_\Omega \left(\Phi'(u(t+\tau)) + \frac{1}{2}(w(t) + w(t+\tau))\right) \frac{u(t+\tau) - u(t)}{\tau} dx \\
= \;& \int_\Omega f(|\nabla v|)\left(\nabla(u(t+\tau) + \frac{\nabla(w(t+\tau) + w(t))}{2\Phi''(u(t+\tau))}\right) \times \\
& \times \left(\Phi''(u(t+\tau))\nabla u(t+\tau) + \frac{\nabla(w(t+\tau) + w(t))}{2}\right) dx \\
= \;& \int_\Omega f(|\nabla v|)\Phi''(u(t+\tau))\left|\nabla u(t+\tau) + \frac{\nabla(w(t+\tau) + w(t))}{2\Phi''(u(t+\tau))}\right|^2 dx \geq 0.
\end{aligned}$$

□

Remark 2.4 The symmetry in the time differentiation (6) is preserved by the standard space discretization of equation (5). Hence it can be used in the spatially discretized case, too.

Proposition 2.5 *Suppose that the average* $\left[\frac{1}{\Phi''_a}\right]$ *of* $\frac{1}{\Phi''(\mathbf{u})}$ *is defined by*

$$G\mathbf{\Phi}' =: \left[\frac{1}{\Phi''_a}\right]^{-1} G\mathbf{u}.$$

Then the discrete version of $-\nabla \cdot (f\nabla v)$ *is a positive semidefinite form.*

P r o o f. For $\mathbf{v} = \mathbf{\Phi}' + \mathbf{w}$ we have

$$\begin{aligned}
\mathbf{\Phi}'^{\mathbf{T}} G^T f(G\mathbf{u} + \left[\frac{1}{\Phi''_a}\right] G\mathbf{w}) + \mathbf{w}^{\mathbf{T}} G^T f(G\mathbf{u} + \left[\frac{1}{\Phi''_a}\right] G\mathbf{w}) &= \\
(\mathbf{\Phi}' + \mathbf{w})^T G^T f \left[\frac{1}{\Phi''_a}\right] (\left[\frac{1}{\Phi''_a}\right]^{-1} G\mathbf{u} + G\mathbf{w}) &= \\
(\left[\frac{1}{\Phi''_a}\right]^{-1} G\mathbf{u} + G\mathbf{w})^T f \left[\frac{1}{\Phi''_a}\right] (\left[\frac{1}{\Phi''_a}\right]^{-1} G\mathbf{u} + G\mathbf{w}) &\geq 0.
\end{aligned}$$

□

Remark 2.6 With $\Phi'(s) = \log(s/(1-s))$, $0 < s < 1$, this is indeed an averaging diagonal matrix function of $\frac{1}{\Phi''(\mathbf{u})} = u(1-u)$ with the following properties.

i) $$\left[\frac{1}{\Phi''_a}\right]\Bigg|_{\mathbf{e}_{ij}} = \frac{u_j - u_i}{\log(u_j/(1-u_j)) - \log(u_i/(1-u_i))} > 0, \text{if } u_i \neq u_j,$$

ii) $$\lim_{u_k \to 0,1} \left[\frac{1}{\Phi''_a}\right]\Bigg|_{\mathbf{e}_{ij}} = 0,\; k = i \text{ or } k = j,$$

iii) $$\lim_{u_i \to u_j} \left[\frac{1}{\Phi''_a}\right]\Bigg|_{\mathbf{e}_{ij}} = \frac{1}{\Phi''(u)} = u_j(1-u_j).$$

Here
i) holds w.l.o.g. due to $1 > u_{i+1} > u_{i+2} > 0$ and $\frac{u_{i+1}}{1-u_{i+1}} > \frac{u_{i+2}}{1-u_{i+2}}$ and the monotonicity

of Φ';
ii) the logarithmic singularity for one fixed argument guarantees the continuation by 0 to establish $1 \geq u \geq 0$ by the discrete weak maximum principle [5] and hence $-m \leq w \leq m$; finally *iii)* is just the definition of the derivative.

Now we are ready to state our main result.

Theorem 2.7 *The following discrete version of the system* (1), (5) *is dissipative* ($z(t) := z$, $z(t+\tau) := z^+$, $\left[\frac{1}{\Phi''_a}\right]$ *depends on* $\mathbf{u}^+$*):*

$$(G^T f G + [V])\mathbf{w}^+ = [V]m(\mathbf{1} - 2\mathbf{u}^+),$$

$$[V]\frac{\mathbf{u} - \mathbf{u}^+}{\tau} = G^T f(G\mathbf{u}^+ + \left[\frac{1}{\Phi''_a}\right]\frac{1}{2}G(\mathbf{w}^+ + \mathbf{w})).$$

P r o o f. Using the arguments for the time discretization again yields

$$V^T(\mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{u}^+)) \;\geq\; \tau(\left[\frac{1}{\Phi''_a}\right]^{-1} G\mathbf{u}^+ + \frac{1}{2}G(\mathbf{w}^+ + \mathbf{w}))^T f \times$$
$$\times \left[\frac{1}{\Phi''_a}\right](\left[\frac{1}{\Phi''_a}\right]^{-1} G\mathbf{u}^+ + \frac{1}{2}G(\mathbf{w}^+ + \mathbf{w})) \geq 0.$$

□

Using the averaging relation and $\Phi'(u) = v - w$ yields the discrete equation in v:

$$\left[\frac{V}{\tau}\right](u - u^+) = G^T f \left[\frac{1}{\Phi''_a}\right]\left(G\mathbf{v}^+ - G\frac{\mathbf{w}^+ - \mathbf{w}}{2}\right).$$

Remark 2.8 The second term (including $\mathbf{w}^+ - \mathbf{w}$) is due to the Crank-Nicholson like time discretization. Clearly, supposed $0 < u < 1$, $\mathbf{v} = c$, is a necessary condition for steady states. Hence the averaging relation is compatible with the analytic steady state condition. Its form is not surprising, it is just the analogy to an equation of the form $-\nabla\phi'(v)\nabla v$ (see [2]).

Proposition 2.9 *Suppose* $\mathbf{v}^+ \neq \mathbf{c}$, $0 < u < 1$. *Then the implicit Euler scheme preserves* $0 < u^+ < 1$.

P r o o f. *i)* Let x_0 be the node where $\hat{v}^+ = \max_x(\mathbf{v}^+(x))$ holds. Assume $u^+(x_0) > 1/2$ to be a local maximum of $\mathbf{u}^+$ at x_0, too. Suppose $\hat{v}^+ < v(x_0) + 3m$, hence $\Phi'(u^+)$ is bounded for all x_l with $u^+(x_l) > 1/2$. Let $\mathcal{E}_0$ be the set of elements containing x_0, n_0 the set of nodes in $\mathcal{E}_0$, and $u_1^+ := \max_{i, i\neq 0, i\in n_0} u^+(x_i)$. Testing the equation with

$$h(\Phi'(u^+(x_i))) = \begin{cases} \max(\Phi'(u^+) - \Phi'(u_1^+), 0) \text{ if } i \in n_0, \\ 0 \text{ else,} \end{cases}$$

yields ($c > 0$)

$$\frac{V_0 c}{\tau}(u(x_0) - u^+(x_0)) = \mathbf{h}(\mathbf{\Phi}'(\mathbf{u}^+))^{\mathrm{T}} G^T f \frac{[G\mathbf{u}^+]}{[G\mathbf{\Phi}'(\mathbf{u}^+)]} G\mathbf{v}^+,$$

$$\frac{V_0 c}{\tau}(u(x_0) - u^+(x_0)) = \mathbf{u}^{+\mathrm{T}} G^T f[\zeta] G\mathbf{v}^+,$$

where ζ_r denotes the 'radial' edges with respect to x_0 of

$$[\zeta] := \frac{[G\mathbf{h}(\mathbf{\Phi}'(\mathbf{u}^+))]}{[G\mathbf{\Phi}'(\mathbf{u}^+)]}.$$

All ζ_{r_i} fulfill $0 \leq \zeta_{r_i} \leq 1$ and at least $\zeta_{r_1} = 1$ holds. For all other (non'radial' with respect to x_0) edges holds $\zeta_i = 0$, due to $h(\Phi'(u^+(x_j))) = 0$ and $j \neq 0$. For all edges $\zeta_r > 0$

holds $\mathbf{u}^{+\mathbf{T}}G^TG\mathbf{v}^+|_r \geq 0$ and at least at one edge j $\mathbf{u}^{+\mathbf{T}}G^TG\mathbf{v}^+|_{j\in r} > 0$. That implies $u_0 - u^+ > 0$ (maxima of u coinciding with maxima in v decay) and $\hat{v}^+ \leq v(x_0) + 2m$.
ii) Let $\hat{v}^+$ be the maximum of $\mathbf{v}^+$ as before, but $\hat{u}^+ := u^+(x_u) := \max_x(u^+) > u^+(x_0)$. Hence $1 \geq \max(u^+) > u^+(x_0)$ holds as global bound, and $\hat{v}^+ = v^+(x_0) \leq \Phi'(u^+(x_0)) + m \leq c$ and $v^+(x_u) < \hat{v}^+$.

(That argument applies in case of $u^+ = const$ within the node set n_0 (defined by $\max_x(\mathbf{v}^+) = v^+(x_0)$ and the next neighbor nodes of x_0), too. One selects $x_1 = \min_{x_k\in n_0}(\mathbf{v}^+)$. $u^+(x_1) < 1$, hence $v^+(x_1)$ bounded and $v^+(x_0) \leq v^+(x_1) + 2m$ because $u^+(x_0) = u^+(x_1) = const$ and $-m \leq w^+(x) \leq m$.)
The same arguments apply to show $u > 0$. □

This rather weak result (v is known to be bounded in the analytic case, comp. [7]) ensures $0 < u^+ < 1$ for a next time step and sufficiently small τ. Finally v may decay in sufficiently large structures where the variation of w is small.

3 Numerical example

Steady states are defined by the interaction and conservation of mass:

$$G^T\sigma^2G\mathbf{w} + [V]\mathbf{w} = [V]m(1 - 2\phi'^{-1}(\bar{v} - \mathbf{w})),$$

$$2m\mathbf{V}^{\mathbf{T}}\phi'^{-1}(\bar{v} - \mathbf{w}) = 2m|\Omega|\bar{u} = c,$$

where the variable $\bar{v}$ denotes the constant chemical potential compatible with mass conservation and m is now a parameter representing the strength of the interaction forces. The Jacobian matrix of that problem is symmetric. The numerical bifurcation problem is solved by starting for sufficiently small $m \leq 2$ from the trivial solution $u = \bar{u}$, applying Newtons method, tracing the eigenvalues close to zero, and using the discrete bifurcation equations directly as described in books like [10].

The following figures show results for $\bar{u} = 1/2$ and a rectangular domain Ω. The naming convention used in the following figures is explained best by an example. 2aA stands for: 2 $\sim$ second branch from the trivial one, a $\sim$ first branch from 2, A $\sim$ first branch from 2a.The branches departing from the trivial solution reflect the symmetry of the domain directly, the other ones reflect the radial symmetry of the Green function of the operator $-\sigma^2\nabla\cdot\nabla + I$. The computed bifurcation diagram includes all zero eigenvalues of the Jacobian along a branch as markers.

For large m (here $m > 3$) 'interface deformations' are typical (the markers at the end of the branches). The related eigenvectors oscillate in regions with small modulus of the interaction potential and decay to zero inside regions with large modulus of w. Two eigenvectors of the Jacobian for different m corresponding to 'interface states' on the first nontrivial branch are shown in Figure 1.

A typical evolution process is shown in the following Figures 7, 6. The symmetric initial condition $u_0(x,y) = \epsilon + x/(128(1+2\epsilon))$ on the square $0 \leq x \leq 128$, $0 \leq y \leq 128$ is used ($m = 8$, $\epsilon = 10^{-7}$, $\sigma = \sqrt{f} = 2$).
The skinny strips decay into circles with a typical diameter related to the width of the strip. The symmetry is broken due to rounding (or any small perturbation in the initial data) and the fact, that the domain size is large compared to σ and not compatible with thickness of an arbitrary strip. The free energy is decreasing and $\max(|v(t_i,x,y)|)$ shows fluctuations during the pattern formation and finally decays to $2.43\cdot 10^{-7}$. The remaining variation is in the order of 100 times the machine precision times the initial value of v. The mass is preserved better than $10^{-8}\bar{u}$.

The presented scheme can be adapted to more general situations (integral equation for w, $f = f(|\nabla v|)$ for instance). Non-dissipative discretizations introduce the problem, that the free energy may increase and especially the computed 'steady state' may be far from that of true minimal energy.

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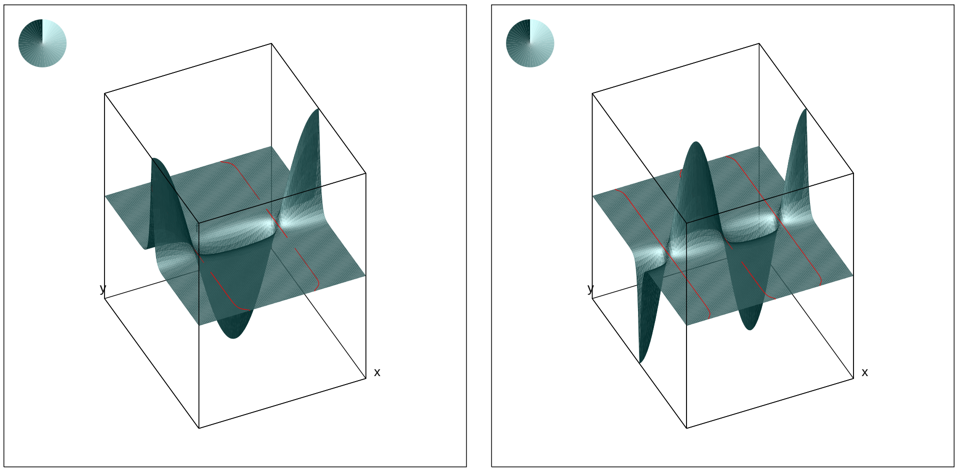

Fig. 1: Eigenvectors corresponding to 'interface states'

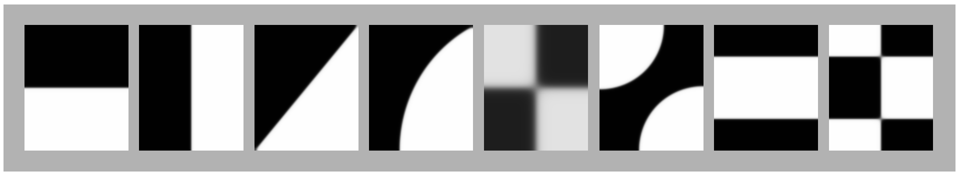

Fig. 2: Steady states: u at the end of a computed branch, cases
1, 2, 2a, 2aA, 3, 3a, 4, 5

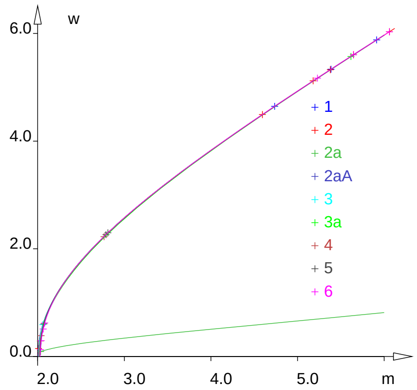

Fig. 3: w at the lower left corner of Ω, the markers for large m correspond to 'interface states'

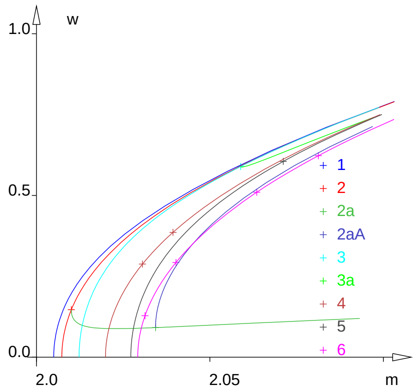

Fig. 4: w at the lower left corner of Ω, detail for small m

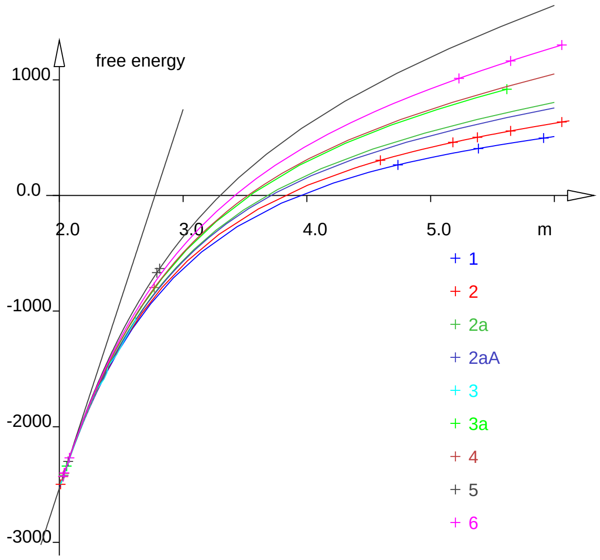

Fig. 5: Free energy as function of m for the different branches, the trivial solution corresponds to the straight (black) line

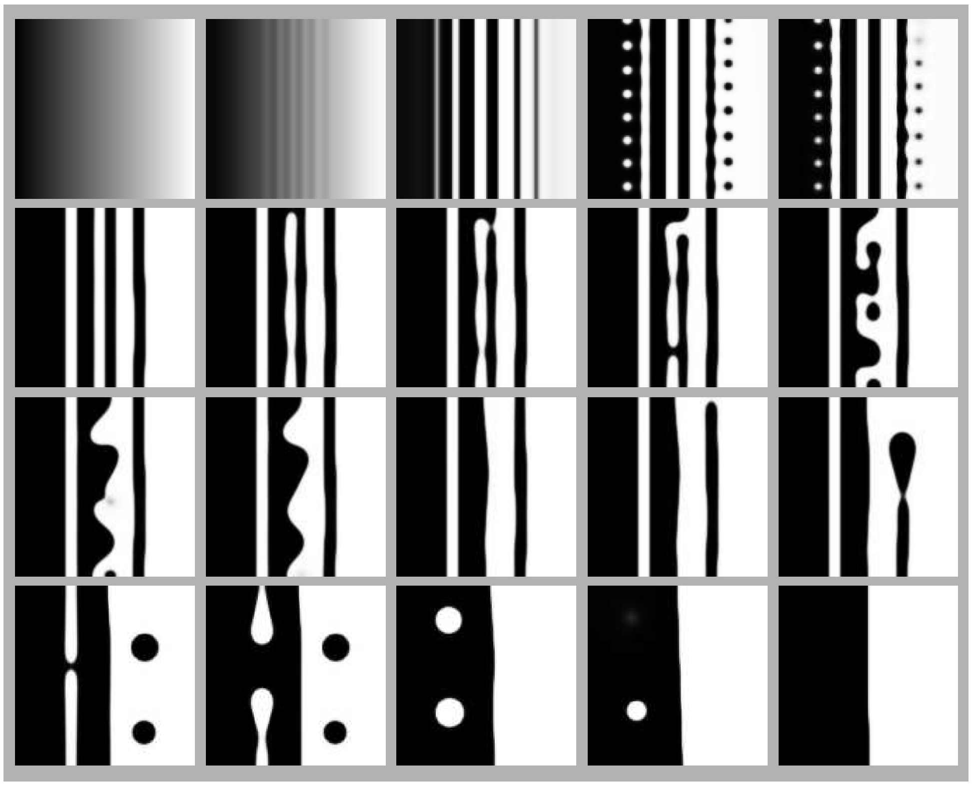

Fig. 6: Evolution: u at times labeled by markers in Figure 7.

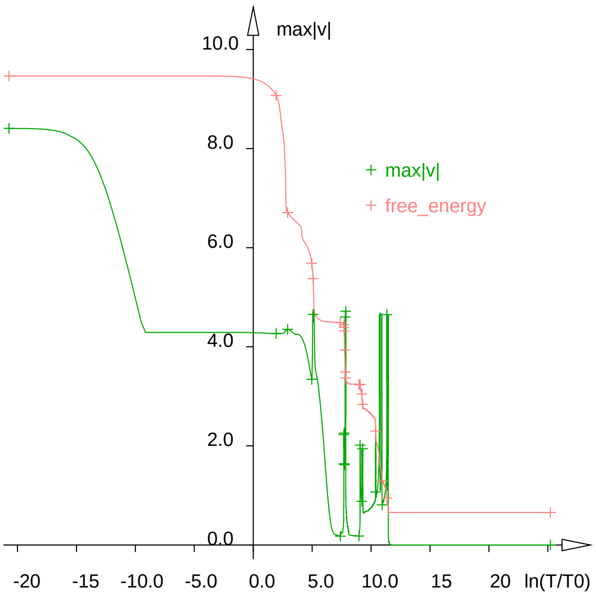

Fig. 7: Fluctuations in $||v||_\infty$ are correlated with the pattern formation, decreasing free energy (scaled).