

SPATIALLY DISCRETE NONLINEAR DIFFUSION EQUATIONS

JOHN W. CAHN, SHUI-NEE CHOW AND ERIK S. VAN VLECK

ABSTRACT. We consider spatially discrete nonlinear diffusion equations that are similar in form to the Cahn-Hilliard and Cahn-Allen equations. Since these equations are spatially discrete, solutions exist even for negative gradient energy coefficients. In order to study these equations analytically on finite subsets of one, two and three dimensional lattices, we propose a discrete variational calculus. It is shown that, under very general boundary conditions, these equations possess a gradient structure. We prove the existence of a global attractor and show that when all equilibria are hyperbolic the global attractor consists of the equilibria and the connecting orbits between the equilibria. The equilibria of specific one-, two- and three-dimensional equations are studied. We exhibit constant, two-periodic and three-periodic equilibrium solutions and study their stability properties. Numerical methods for solving the time dependent equations are proposed. We employ a fully implicit time integration scheme and solve the equations on a massively parallel SIMD machine. To take advantage of the structure of our problem and the data parallel computing equipment, we solve the linear systems using the iterative methods CGS and CGNR. Finally, we exhibit the results of our numerical simulations. The numerical results show the robust pattern formation that exists for different values of the parameters.

1. Introduction. In this paper we consider spatially discrete nonlinear diffusion equations that occur as models for binary alloys. These equations are truly spatially discrete and are not space discretized partial differential equations. In fact, for some of the parameter values that we consider there may not exist a well-posed PDE even in a weak sense. The differential equations we consider are analogous in form to the Cahn-Hilliard equation (see [4]) and the Cahn-Allen equation (see

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[1]). The Cahn-Hilliard equation with Neumann boundary conditions is given by

$$(1.1) \quad \begin{aligned} u_t &= \Delta(f(u) - \varepsilon \Delta u), & x \in \Omega \\ n \cdot \nabla u &= n \cdot \nabla \Delta u = 0, & x \in \partial\Omega \end{aligned}$$

for $\varepsilon > 0$ where $\Omega \subset \mathbf{R}^N$, $N = 1, 2, 3$ is a bounded domain and f is a “cubic” nonlinearity, typically $f(u) = u^3 - u$. The Cahn-Allen equation with Neumann boundary conditions is given by

$$(1.2) \quad \begin{aligned} u_t &= -f(u) + \varepsilon \Delta u, & x \in \Omega \\ n \cdot \nabla u &= 0, & x \in \partial\Omega \end{aligned}$$

The Cahn-Hilliard equation models the evolution of a binary alloy after it has been quenched to a constant temperature. The Cahn-Allen equation models the motion of the interface between two phases of a binary alloy.

Spatially discrete equations have long been considered in the material sciences (see [12, 5]). The model considered by Hilbert in [12] is a one-dimensional model and allows for order-disorder and spinodal decomposition. There is no restriction on the amplitude of the composition in Hilbert’s model. A three-dimensional model was considered in [5] on face-centered and body-centered cubic lattices and allows for spinodal decomposition and order-disorder, but with an analytic solution only for small amplitudes. Our models are for subsets of one-, two- and three-dimensional lattices. We have observed spinodal decomposition, order-disorder, twinning and the coexistence of up to three distinct phases. We will present high amplitude equilibrium solutions for certain model equations.

Our major contribution is to show that spatially discrete diffusion equations on a finite subset of a lattice can be analyzed in terms of a variational calculus and that the systems we consider possess a gradient structure and hence have a global attractor. Our initial task is to set up a discrete variational calculus for discrete nonlinear diffusion equations. Using the fact that these are gradient systems we are able to prove that there exists a compact, connected invariant set for a large range of parameter values that includes the case in which there is no continuum limit PDE. We show that for a negative coefficient in the gradient energy term of the Lyapunov function the period two solution

replaces the constant solution as the low energy equilibrium solution for a model spatially discrete Cahn-Allen type equation. We present a numerical method that we have implemented on a massively parallel SIMD machine. Using this efficient algorithm, we are able to exhibit the pattern formation that occurs for a wide range of parameter values.

This paper is outlined as follows. In Section 2 we consider spatially discrete diffusion equations of Cahn-Allen and Cahn-Hilliard type on finite subsets of lattices. We show that, for general nonlocal boundary conditions, the spatially discrete Cahn-Hilliard equation conserves mass. For specific forms of the spatially discrete Cahn-Hilliard equation on one-, two- and three-dimensional subsets of lattices for which the boundaries are a line, a rectangle and a cube, respectively, we show that the discrete analog of periodic and Neumann type boundary conditions imply the general boundary conditions. In Section 3 a definition of a gradient system is given for a spatially discrete nonlinear diffusion equation with an arbitrary gradient energy coefficient. It is shown that there exists a compact, connected invariant set, i.e., a global attractor. Furthermore, we show that if all the equilibrium solutions are hyperbolic, then the global attractor consists of the equilibrium solutions and the connecting orbits. In Section 4 we exhibit constant, period two and period three equilibrium solutions for the specific spatially discrete Cahn-Allen and Cahn-Hilliard equations with periodic boundary conditions that were introduced in Section 2. We study the stability properties of the nonzero constant solution and the period two solution and show that there exists a region in parameter space where both solutions are stable. Moreover, the portion of parameter space where both solutions are stable can be divided into a region where the constant solution has lower energy and a region where the period two solution has lower energy. For the one-dimensional equation the existence of a period three solution is shown to imply the existence of equilibrium solutions of all periods that divide the number of lattice points. In Section 5 we present a fourth order variable step method to solve spatially discrete nonlinear diffusion equations. The method is implemented using iterative linear system solvers to allow for efficient computation on SIMD machines. In Section 6 the results of our numerical simulations are exhibited. The simulations show the diverse pattern formation that is possible with these equations.

2. Nonlinear diffusion equations. In this section we consider a general class of spatially discrete nonlinear diffusion equations on integer valued subsets of lattices in one-, two- and three-dimensions. We then consider specific equations that occur as models for the evolution of binary alloys. We define what we mean by a subset of a lattice and its boundary with respect to discrete Laplacian type operators. In this way we are able to develop a variational calculus for spatially discrete diffusion equations using a discrete Green's formula that is easy to derive by considering one-dimensional summation by parts formulas. A general form for equations is given that, although spatially discrete, are of reaction diffusion and Cahn-Hilliard type. With a boundary-sum boundary condition, the spatially discrete Cahn-Hilliard equations conserve mass. For rectangular boundaries it is shown that these boundary-sum conditions are satisfied with the discrete analog of periodic and Neumann boundary conditions.

Given a \mathbf{Z}^N module for $N = 1, 2, 3$ we wish to construct a finite subset, L , of this lattice. For $N = 1, 2, 3$ we have that $\eta \in L$ is of the form $\eta = (i)$, $\eta = (i, j)$, $\eta = (i, j, k)$, respectively, where i, j, k are integers. First we construct a subgroup of \mathbf{Z}^N using a set $\{\eta_k\}_{k \in D}$ of translations (see [3]) where D is an indexing set and $\eta_k \in \mathbf{Z}^N$ act as generators. An example of such a subgroup of \mathbf{Z}^3 would be the face-centered cell where the η_k are all permutations of (1.1). Here the translations in the subgroup are those $\eta = (i, j, k)$ for which $i + j + k$ is even and the size of face-centered unit cell is double that of the unit cell for \mathbf{Z}^3 . This allows us to retain integer components for centered cells. We may also wish to consider the lattice complexes that are formed by the complement of a subgroup or the union of some of the cosets of the subgroup with respect to \mathbf{Z}^N (see [13]). We specify L to be the points in a finite subset of this lattice or lattice complex, i.e., a collection of N -tuples with integer components, a finite subset of \mathbf{Z}^N .

We now define the boundary and interior of L with respect to the set of translations $\{\eta_k\}_{k \in D}$. A point $\eta \in L$ is in the interior of L if $\eta \pm \eta_k \in L$ for all the translations η_k . A point $\eta \in \partial L_{\eta_k}^-$, the negative boundary with respect to the translation η_k , if $\eta \in L$ and $\eta - \eta_k \notin L$. Similarly, a point $\eta \in \partial L_{\eta_k}^+$, the positive boundary with respect to η_k , if $\eta \in L$ and $\eta + \eta_k \notin L$. We define the boundary of L to be those $\eta \in L$ such that either $\eta \in \partial L_{\eta_k}^-$ or $\eta \in \partial L_{\eta_k}^+$ for some translation η_k .

For a one-dimensional discrete Laplacian, we have the following

summation by parts formula.

Theorem 2.1 (Summation by parts). *Given a positive integer M and sequences $\{v(i)\}_0^{M+1}$ and $\{w(i)\}_0^{M+1}$, we have*

$$(2.1) \quad \sum_{i=1}^M \{\Delta v(i) \cdot w(i) + \nabla v(i) \cdot \nabla w(i)\} \\ = -\nabla v(0) \cdot w(1) + \nabla v(M) \cdot w(M+1)$$

where $\Delta v(i) = v(i+1) - 2v(i) + v(i-1)$ and $\nabla v(i) = v(i+1) - v(i)$.

We define higher dimensional discrete Laplacians as the sum of one-dimensional discrete Laplacians using the set of translations $\{\eta_k\}_{k \in D}$ as follows

$$(2.2) \quad \Delta_i u(\eta) = \sum_{k \in D_i} \{u(\eta - \eta_k) - 2u(\eta) + u(\eta + \eta_k)\}$$

where $\{\eta_k\}_{k \in D_i}$ is the set of crystallographically equivalent translations. For point groups with little symmetry, each D_i may contain only one element, while for point groups with a large degree of symmetry, the corresponding D_i will contain several elements.

Using the summation of parts formula (2.1) and the construction (2.2) of higher dimensional discrete Laplacian type operators Δ_i , we have the following discrete Green's formula

Theorem 2.2 (Green's Formula).

$$(2.3) \quad \sum_{\eta \in L} \Delta_i v(\eta) \cdot w(\eta) + \sum_{\eta \in L} \nabla_i v(\eta) \cdot \nabla_i w(\eta) \\ = \sum_{k \in D_i} \left\{ \sum_{\eta \in L} (v(\eta - \eta_k) - 2v(\eta) + v(\eta + \eta_k)) \right. \\ \left. \cdot w(\eta) + (v(\eta + \eta_k) - v(\eta)) \cdot (w(\eta + \eta_k) - w(\eta)) \right\}$$

$$= \sum_{k \in D_i} \left\{ \sum_{\eta \in \partial L_{\eta_k}^-} -(v(\eta) - v(\eta - \eta_k)) \cdot w(\eta) + \sum_{\eta \in \partial L_{\eta_k}^+} (v(\eta + \eta_k) - v(\eta)) \cdot w(\eta + \eta_k) \right\}.$$

Given L , we consider differential equations that take on a value at each point $\eta \in L$. The differential equations are similar in form to the Cahn-Hilliard equation and the corresponding Cahn-Allen equation. For $\eta \in L$, what we will call the Spatially Discrete Cahn-Hilliard equation (SDCH) has the form

$$(2.4) \quad \dot{u}(\eta, t) = \Delta_B(f(u(\eta, t)) - \Delta_A u(\eta, t))$$

where $\dot{u} = du/dt$, $f(u(\eta, t)) = \log((1 + u(\eta, t))/(1 - u(\eta, t))) + \sigma u(\eta, t)$ and $\Delta_A = \sum_{i \in I_A} \alpha_i \Delta_i$, $\Delta_B = \sum_{i \in I_B} \beta_i \Delta_i$ where I_A and I_B are indexing sets. Note that for $\sigma < -2$, $f(x)$ has three unique real roots. In what follows, we will assume that the α_i and β_i are real constants, but $\alpha_i \equiv \alpha_i(\eta)$ or $\beta_i \equiv \beta_i(\eta)$, the weights as functions of position, may also be useful in some applications. For $\eta \in L$, the Spatially Discrete Cahn-Allen equation (SDCA) has the form

$$(2.5) \quad \dot{u}(\eta, t) = \Delta_A u(\eta, t) - f(u(\eta, t)).$$

For both equations, we consider the following boundary conditions

$$(2.6) \quad \sum_{i \in I_A} \alpha_i \sum_{k \in D_i} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (u(\eta, t) - u(\eta - \eta_k, t)) + \sum_{\eta \in \partial L_{\eta_k}^+} (u(\eta + \eta_k, t) - u(\eta, t)) \right\} = 0.$$

Additionally, for the SDCH equation, we employ the boundary condition

$$(2.7a) \quad \sum_{i \in I_B} \beta_i \sum_{k \in D_i} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (h(u(\eta, t)) - h(u(\eta - \eta_k, t))) + \sum_{\eta \in \partial L_{\eta_k}^+} (h(u(\eta + \eta_k, t)) - h(u(\eta, t))) \right\} = 0.$$

$$(2.7b) \quad \sum_{i \in I_B} \beta_i \sum_{k \in D_i} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (h(u(\eta, t)) - h(u(\eta - \eta_k, t))) \cdot h(u(\eta, t)) \right. \\ \left. + \sum_{\eta \in \partial L_{\eta_k}^+} (h(u(\eta + \eta_k, t)) - h(u(\eta, t))) \cdot h(u(\eta + \eta_k, t)) \right\} = 0,$$

where h is given by

$$(2.8) \quad (h(u))_\eta = \Delta_A u(\eta) - f(u(\eta)).$$

Equation (2.7a) is necessary to maintain conservation of mass and equation (2.7b) is necessary to have a gradient system.

We now present explicit examples of SDCH equations and subsequently present local boundary conditions that imply the boundary conditions of (2.6) and (2.7).

Our model one-dimensional SDCH equation with parameters $\alpha_1 \in \mathbf{R}$ and $\beta_1 = 1$ is

$$(2.9) \quad \dot{u}(i, t) = \Delta_B (f(u(i, t)) - \Delta_A u(i, t))$$

where $\Delta_1 u(i) = u(i+1) - 2u(i) + u(i-1)$, $\Delta_A = \alpha_1 \Delta_1$ and $\Delta_B = \beta_1 \Delta_1$. Note that this corresponds to the standard central difference approximation to the Laplacian.

The model two-dimensional equation has parameters $\alpha_{10}, \alpha_{11} \in \mathbf{R}$ and $\beta_{10} = \beta_{11} = 1$ and is given by

$$(2.10) \quad \dot{u}(i, j, t) = \Delta_B (f(u(i, j, t)) - \Delta_A u(i, j, t))$$

where $\Delta_B = \Delta_{10} + \Delta_{11}$ and $\Delta_A = \alpha_{10} \Delta_{10} + \alpha_{11} \Delta_{11}$ and

$$(2.11) \quad \Delta_{10} u(i, j) = u(i+1, j) + u(i-1, j) \\ + u(i, j+1) + u(i, j-1) - 4u(i, j)$$

and

$$(2.12) \quad \Delta_{11} u(i, j) = u(i+1, j+1) + u(i+1, j-1) \\ + u(i-1, j+1) + u(i-1, j-1) - 4u(i, j).$$

Here Δ_{10} represents the standard five point star approximation to the Laplacian and Δ_{11} represents a scaled version of Δ_{10} rotated by $\pi/4$ radians.

Our model three-dimensional SDCH equation has parameters α_{100} , α_{110} , $\alpha_{111} \in \mathbf{R}$ and $\beta_{100} = \beta_{110} = \beta_{111} = 1$ and is of the form

$$(2.13) \quad \dot{u}(i, j, k, t) = \Delta_B(f(u(i, j, k, t))) - \Delta_A u(i, j, k, t)$$

where $\Delta_B = \Delta_{100} + \Delta_{110} + \Delta_{111}$ and $\Delta_A = \alpha_{100}\Delta_{100} + \alpha_{110}\Delta_{110} + \alpha_{111}\Delta_{111}$, where

$$(2.14) \quad \begin{aligned} \Delta_{100}u(i, j, k) &= u(i+1, j, k) + u(i-1, j, k) \\ &+ u(i, j+1, k) + u(i, j-1, k) \\ &+ u(i, j, k+1) + u(i, j, k-1) - 6u(i, j, k), \end{aligned}$$

$$(2.15) \quad \begin{aligned} \Delta_{110}u(i, j, k) &= u(i+1, j+1, k) + u(i+1, j-1, k) \\ &+ u(i+1, j, k+1) + u(i+1, j, k-1) \\ &+ u(i, j+1, k+1) + u(i, j+1, k-1) \\ &+ u(i, j-1, k+1) + u(i, j-1, k-1) \\ &+ u(i-1, j+1, k) + u(i-1, j-1, k) \\ &+ u(i-1, j, k+1) + u(i-1, j, k-1) \\ &- 12u(i, j, k) \end{aligned}$$

and

$$(2.16) \quad \begin{aligned} \Delta_{111}u(i, j, k) &= u(i+1, j+1, k+1) + u(i+1, j+1, k-1) \\ &+ u(i+1, j-1, k+1) \\ &+ u(i+1, j-1, k-1) + u(i-1, j+1, k+1) \\ &+ u(i-1, j+1, k-1) \\ &+ u(i-1, j-1, k+1) + u(i-1, j-1, k-1) \\ &- 8u(i, j, k). \end{aligned}$$

The operator Δ_{100} represents the standard central difference approximation to the Laplacian in three dimensions and corresponds to the neighbors of a primitive cubic lattice. The operators Δ_{110} and Δ_{111}

correspond to the neighbors in face centered and body centered cubic lattices by themselves, respectively.

For the one-, two- and three-dimensional SDCH equations, the boundary conditions (2.6) and (2.7) are satisfied for regular boundaries if we use the following “local” boundary conditions.

For the one-dimensional equation (2.9) and a lattice L of the form $\eta = (i) \in L$ if $1 \leq i \leq N_1$ for some positive integer N_1 , we consider both periodic boundary conditions

$$(2.17) \quad u(i) = u(i + N_1), \quad i = -1, \dots, 2$$

and reflected or Neumann type boundary conditions

$$(2.18) \quad u(i) = u(i + 1), \quad u(i - 1) = u(i + 2), \quad i = 0, N_1.$$

For the two-dimensional equation (2.10) and an L of the form $\eta \equiv (i, j) \in L$ provided $1 \leq i \leq N_1$ and $1 \leq j \leq N_2$ where N_1 and N_2 are positive integers, we consider periodic

$$(2.19) \quad \begin{aligned} u(i, k) &= u(i, N_2 + k), & i &= -1, \dots, N_1 + 2, & k &= -1, \dots, 2 \\ u(k, j) &= u(N_1 + k, j), & j &= -1, \dots, N_2 + 2, & k &= -1, \dots, 2 \end{aligned}$$

and Neumann type boundary conditions

$$(2.20) \quad \begin{aligned} u(i, k) &= u(i, k + 1), & u(i, k - 1) &= u(i, k + 2), \\ i &= -1, \dots, N_1 + 2, & k &= 0, N_2 \end{aligned}$$

$$\begin{aligned} u(k, j) &= u(k + 1, j), & u(k - 1, j) &= u(k + 2, j), \\ j &= -1, \dots, N_2 + 2, & k &= 0, N_1. \end{aligned}$$

For the three-dimensional equation (2.11) and $\eta \equiv (i, j, k) \in L$ when $1 \leq i \leq N_1$, $1 \leq j \leq N_2$ and $1 \leq k \leq N_3$ for positive integers N_1 , N_2 , N_3 , we consider periodic boundary conditions

$$(2.21) \quad \begin{aligned} u(i, j, l) &= u(i, j, N_3 + l), \\ i &= -1, \dots, N_1 + 2, & j &= -1, \dots, N_2 + 2, & l &= -1, \dots, 2 \\ u(i, l, k) &= u(i, N_2 + l, k), \\ i &= -1, \dots, N_1 + 2, & k &= -1, \dots, N_3 + 2, & l &= -1, \dots, 2 \\ u(l, j, k) &= u(N_1 + l, j, k), \\ j &= -1, \dots, N_2 + 2, & k &= -1, \dots, N_3 + 2, & l &= -1, \dots, 2 \end{aligned}$$

and Neumann or reflected boundary conditions

$$\begin{aligned}
(2.22) \quad & u(i, j, k) = u(i, j, k + 1), \quad u(i, j, k - 1) = u(i, j, k + 2), \\
& \quad i = -1, \dots, N_1 + 2, \quad j = -1, \dots, N_2 + 2, \quad k = 0, N_3 \\
& u(i, j, k) = u(i, j + 1, k), \quad u(i, j - 1, k) = u(i, j + 2, k), \\
& \quad i = -1, \dots, N_1 + 2, \quad k = -1, \dots, N_3 + 2, \quad k = 0, N_2 \\
& u(i, j, k) = u(i + 1, j, k), \quad u(i - 1, j, k) = u(i + 2, j, k), \\
& \quad j = -1, \dots, N_2 + 2, \quad k = -1, \dots, N_3 + 2, \quad i = 0, N_1.
\end{aligned}$$

Proposition 2.3. *Each of the local boundary conditions (2.17)–(2.22) imply the boundary conditions (2.6) and (2.7).*

Proof. The proof follows easily for the one-dimensional boundary conditions (2.17) and (2.18) since $f(-x) = -f(x)$. For the two-dimensional boundary conditions it is clear that the components of the global boundary conditions (2.6) and (2.7) in the directions defined by the discrete Laplacian Δ_{10} are zero. For the Laplacian Δ_{11} we set the η_k for $k \in D_{11}$ to be $(1, 1)$ and $(-1, 1)$ so that the terms in (2.6) corresponding to Δ_{11} become

$$\begin{aligned}
& \sum_{k \in D_{11}} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (u(\eta) - u(\eta - \eta_k)) + \sum_{\eta \in \partial L_{\eta_k}^+} (u(\eta + \eta_k) - u(\eta)) \right\} \\
& 2 \sum_{k \in D_{10}} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (u(\eta) - u(\eta - \eta_k)) + \sum_{\eta \in \partial L_{\eta_k}^+} (u(\eta + \eta_k) - u(\eta)) \right\} \\
& \quad + u(N_1 + 1, N_2 + 1) - u(N_1, N_2) + u(N_1, N_2) \\
& \quad - u(N_1, N_2 + 1) + u(N_1, N_2) - u(N_1 + 1, N_2) \\
& \quad + u(N_1 + 1, 0) - u(N_1, 1) + u(N_1, 1) - u(N_1, 0) + u(N_1, 1) \\
& \quad - u(N_1 + 1, 1) \\
& \quad + u(0, N_2 + 1) - u(1, N_2) + u(1, N_2) - u(1, N_2 + 1) + u(1, N_2) \\
& \quad - u(0, N_2) \\
& \quad + u(0, 0) - u(1, 1) + u(1, 1) - u(1, 0) + u(1, 1) - u(0, 1) \\
& = 0.
\end{aligned}$$

The boundary condition (2.7a) follows by applying this argument to $h(u)$ instead of u . To see that (2.7b) is true for periodic boundary

conditions, observe that for the boundary terms corresponding to Δ_{11} we have pairs of terms of the form

$$\begin{aligned} & (h(u(0, j-1)) - h(u(1, j)))h(u(1, j)) \\ & + (h(u(N_1 + 1, j)) - h(u(N_1, j-1)))h(u(N_1 + 1, j)) \end{aligned}$$

where $j = 2, \dots, N_2$. The periodic boundary conditions imply that these terms are all zero. Here we have exhibited the terms for the right and left sides of L that correspond to the directions $\pm(1, 1)$. The other three cases follow in the same way. The remaining corner terms also cancel with the periodic boundary conditions. For the Neumann type boundary conditions we apply an argument similar to that above after redefining the boundary terms in a consistent manner so that

$$\begin{aligned} u(1, j) &\in \partial_{\mp(1,1)}^{\pm} & \text{and} & & u(1, j-1) &\in \partial_{\pm(-1,1)}^{\mp}, & j=2, \dots, N_2 \\ u(N_1, j) &\in \partial_{\mp(-1,1)}^{\pm} & \text{and} & & u(N_1, j-1) &\in \partial_{\pm(1,1)}^{\mp}, & j=2, \dots, N_2 \\ u(j, 1) &\in \partial_{\mp(1,1)}^{\pm} & \text{and} & & u(j-1, 1) &\in \partial_{\pm(-1,1)}^{\mp}, & j=2, \dots, N_1 \\ u(j, N_2) &\in \partial_{\pm(-1,1)}^{\mp} & \text{and} & & u(j-1, N_2) &\in \partial_{\mp(1,1)}^{\pm}, & j=2, \dots, N_1 \end{aligned}$$

Then we consider pairs of terms, for instance for the left side, of the form

$$(h(u(0, j-1)) - h(u(1, j)))h(u(1, j)) + (h(u(0, j)) - h(u(1, j-1)))h(u(0, j))$$

where $j = 2, \dots, N_2$. The Neumann type boundary conditions imply that these terms are all zero.

The same type of argument shows that the statement of the theorem is true for the three-dimensional case as well. \square

Boundary conditions for the SDCH equation should imply that the concentration or mass of a solution is conserved, i.e.,

$$(2.23) \quad \sum_{\eta \in L} u(\eta, t) = c$$

for all $t \geq 0$ where c is a given constant.

Proposition 2.4. *The SDCH equation (2.4), (2.6), (2.7) conserves mass, while the SDCA equation (2.5), (2.6) conserves mass if and only if $\sum_{\eta \in L} f(u(\eta, t)) = 0$ for all $t \geq 0$.*

Proof. Upon differentiating (2.23), we have for the SDCH equation and using Green's formula that

$$\begin{aligned}
 \sum_{\eta \in L} \frac{du(\eta, t)}{dt} &= \sum_{\eta \in L} \Delta_B(f(u(\eta, t)) - \Delta_A(u(\eta, t))) \cdot 1 \\
 (2.24) \quad &= \sum_{i \in I_B} \beta_i \sum_{k \in D_i} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (h(u(\eta, t)) - h(u(\eta - \eta_k, t))) \right. \\
 &\quad \left. + \sum_{\eta \in \partial L_{\eta_k}^+} (h(u(\eta + \eta_k, t)) - h(u(\eta, t))) \right\} \\
 &= 0
 \end{aligned}$$

by (2.7a) where h is given by (2.8).

For the SDCA equation we have

$$\begin{aligned}
 \sum_{\eta \in L} \frac{du(\eta, t)}{dt} &= \sum_{\eta \in L} \{\Delta_A u(\eta, t) - f(u(\eta, t))\} \cdot 1 \\
 &= \sum_{i \in I_A} \alpha_i \sum_{k \in D_i} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (u(\eta, t) - u(\eta - \eta_k, t)) \right. \\
 (2.25) \quad &\quad \left. + \sum_{\eta \in \partial L_{\eta_k}^+} (u(\eta + \eta_k, t) - u(\eta, t)) \right\} \\
 &\quad - \sum_{\eta \in L} f(u(\eta, t)) \\
 &= - \sum_{\eta \in L} f(u(\eta, t))
 \end{aligned}$$

so that $\sum_{\eta \in L} du(\eta, t)/dt = 0$ if and only if $\sum_{\eta \in L} f(u(\eta, t)) = 0$. \square

3. Gradient systems. Nonlinear semigroups that occur as solution operators of gradient partial differential equations have been studied by

Hale [9], Ladyzhenskaya [14] and Temam [18], among others. They show that the compact, connected invariant set or global attractor consists of the equilibrium solutions and the unstable manifolds of the equilibrium solutions. Using methods most similar to those considered in [14] we show that the SDCH equations and SDCA equations possess an attracting set with a similar structure. Throughout this section we will assume that the values of the parameters associated with the discrete Laplacian type operator Δ_B satisfy $\beta_i > 0$ for all $i \in I_B$.

The SDCH and SDCA equations have the same Lyapunov or free energy function

$$(3.1) \quad V(u) = \sum_{\eta \in L} \left\{ F(u(\eta, t)) + \frac{1}{2} \sum_{i \in I_A} \alpha_i \nabla_i u(\eta, t) \cdot \nabla_i u(\eta, t) \right\}.$$

An example of a function $F(x)$ that confines x to $[-1, +1]$ is

$$(3.2) \quad F(x) = (1+x) \log(1+x) + (1-x) \log(1-x) + \frac{\sigma}{2} x^2$$

so that $F'(x) = f(x)$. The function F is a free energy with normalized temperature and corresponds to a zeroth order approximation to the entropy. Therefore, the parameters σ and α_i are roughly inversely proportional to temperature. For $\sigma < -2$ the function F is a double well potential function, while for $\sigma > -2$ it is a single well potential. The use of this function F ensures that during the time evolution the variables $u(\eta, t)$ satisfy $-1 \leq u(\eta, t) \leq +1$ for all $t \geq 0$.

Upon differentiating the Lyapunov function with respect to time and applying Green's formula, we find that

$$(3.3) \quad \begin{aligned} \frac{dV(u)}{dt} &= \sum_{\eta \in L} \left\{ F'(u(\eta, t)) \dot{u}(\eta, t) + \sum_{i \in I_A} \alpha_i \nabla_i u(\eta, t) \cdot \nabla \dot{u}(\eta, t) \right\} \\ &= \sum_{\eta \in L} \left\{ f(u(\eta, t)) - \sum_{i \in I_A} \alpha_i \Delta_i u(\eta, t) \right\} \dot{u}(\eta, t). \end{aligned}$$

For the SDCA equation (3.3) becomes

$$(3.4) \quad \frac{dV(u)}{dt} = - \sum_{\eta \in L} \dot{u}(\eta, t)^2.$$

For the SDCH equation (3.3) becomes, after an application of Green's formula and using (2.7b),

$$(3.5) \quad \frac{dV(u)}{dt} = - \sum_{\eta \in L} \left\{ \sum_{i \in I_B} \beta_i \nabla_i h(u(\eta, t)) \cdot \nabla_i h(u(\eta, t)) \right\}$$

where h is given in (2.8). Thus, for both the SDCA equation and the SDCH equation (since $\beta_i > 0$) V is nonincreasing in time.

Let Ω_L denote the sequences $u := \{u(\eta)\}_{\eta \in L}$ such that $-1 \leq u(\eta) \leq +1$ for $\eta \in L$.

Definition. We say that $T(t)$ is the *solution operator* for the differential equation SDCA or SDCH if

- (i) $T(t+s)u_0 = T(t)T(s)u_0$ for $s, t \geq 0$ and $u_0 \in \Omega_L$;
- (ii) $T(0)u_0 = u_0$ for $u_0 \in \Omega$;
- (iii) $T(t)u_0$ satisfies the differential equation SDCA or SDCH, respectively.

For any bounded set C , let $B_\varepsilon(C)$ denote the union of all open balls of radius ε centered at points in C . A compact set $A \subset \Omega_L$ is said to be a *global attractor* if \mathcal{A} is a connected set such that

- (i) $T(t)\mathcal{A} = \mathcal{A}$ for all $t \geq 0$ (invariance);
- (ii) For every $\varepsilon > 0$ and bounded set $C \subset \Omega_L$, there exists a time $t_1(\varepsilon, C)$ such that $T(t)C \subset B_\varepsilon(\mathcal{A})$ for all $t \geq t_1(\varepsilon, C)$ (attractivity).

Note that in our context this definition of a global attractor corresponds to the definition given in [9].

A sequence $u \in \Omega_L$ is said to be an *equilibrium solution* if u satisfies $(H(u))_\eta = 0$ for the SDCH equation where H is given by

$$(3.6) \quad (H(u))_\eta = -\Delta_B(h(u))_\eta$$

with boundary conditions given by (2.6) and (2.7) or $(h(u))_\eta = 0$ with the boundary conditions (2.6) where h is given by (2.8) for the SDCA equation for all $\eta \in L$.

Lemma 3.1. *We have that $u \in \Omega_L$ is an equilibrium solution of SDCA or SDCH if and only if $\dot{V}(u) = 0$.*

Proof. From (3.4) it is easy to see that the lemma is true for the SDCA equation. For the SDCH equation we have that if u is an equilibrium solution, then by (3.3), $\dot{V}(u) = 0$.

Conversely, if u is such that $\dot{V}(u) = 0$, then by (3.5), $\nabla_i h(u(\eta, t)) = 0$ for all i . Thus, $\Delta_i h(u(\eta, t)) = 0$ for all i , so that u is an equilibrium solution. \square

Lemma 3.2. *If $u_0 \in \Omega_L$, then for the SDCA equation, $T(t)u_0 \in \Omega_L$ for all $t \geq 0$.*

Proof. The lemma follows since $\dot{u}(\eta, t) \rightarrow -\infty$ as $u(\eta, t) \uparrow +1$ and $\dot{u}(\eta, t) \rightarrow +\infty$ as $u(\eta, t) \downarrow -1$. \square

To understand stability properties of equilibrium solutions, we consider the linearized operators $Dh(u)$ and $DH(u)$ given by

$$(3.7) \quad (Dh(u))_\eta = \Delta_A - f'(u(\eta))$$

with the linearization of the boundary conditions (2.6) and

$$(3.8) \quad (DH(u))_\eta = -\Delta_B(Dh(u))_\eta$$

with the linearization of the boundary conditions (2.6) and (2.7) for the SDCA and SDCH equations, respectively.

An equilibrium solution u is said to be *hyperbolic* if $\operatorname{Re}(\lambda_n) \neq 0$ where $\{\lambda_n\}_{n \in L}$ are the eigenvalues of $Dh(u)$ or $DH(u)$ for SDCA or SDCH, respectively. If, in addition, the equilibrium solution satisfies $\operatorname{Re}(\lambda_\eta) < 0$ for all λ_η , then the equilibrium is said to be stable. Otherwise, it is unstable. Note that this is linearized stability, so a stable equilibrium need not be the lowest energy equilibrium.

The *unstable manifold* of an equilibrium solution u is

$$(3.9) \quad W^u(u) = \{v \in \Omega_L : T(t)v \text{ is defined for } t \leq 0 \\ \text{and } T(t)v \rightarrow u \text{ as } t \rightarrow -\infty\}.$$

The dimension of the unstable manifold of an equilibrium solution u , $\dim(W^u(u))$, is equal to the number of eigenvalues of the linearized operator about the equilibrium solution with negative real part.

For $x \in \Omega_L$ the positive trajectory $\gamma^+(x)$ is defined to be the $\gamma^+(x) = \cup_{t \geq 0} T(t)x$. The ω -limit set is defined to be $\omega(x) = \cap_{\tau \geq 0} Cl \cup_{t \geq \tau} T(t)x$. The negative trajectory $\gamma^-(x)$ when it exists is defined similarly, as is the α -limit set $\alpha(x)$. If the negative orbit $\gamma^-(x)$ is defined, then there exists a complete trajectory $\gamma(x)$ so that $T(t)x$ is defined for $t \in \mathbf{R}$ with $T(0)x = x$.

Lemma 3.3. *If all equilibrium solutions are hyperbolic, then the number of equilibrium solutions is finite.*

Proof. For any hyperbolic equilibrium solution, u , there exists by the implicit function theorem an $\varepsilon > 0$ such that u is the unique equilibrium solution in $B_\varepsilon(z)$ (the ball of radius ε about z). Thus, since Ω_L is compact, the number of equilibrium solutions is finite. \square

Lemma 3.4. *If $\gamma^+(x)$ is precompact, then $\omega(x)$ is nonempty, compact, connected and invariant. If there is a precompact negative orbit through x , then $\alpha(x)$ is nonempty, compact, and invariant.*

Proof. See [10, p. 44]. \square

Let E denote the set of equilibrium solutions and consider the following hypotheses:

(H1) We have that u is an equilibrium solution if and only if $\dot{V}(u) = 0$;

(H2) If $u_0 \in \Omega_L$, then $T(t)u_0 \in \Omega_L$ for all $t \geq 0$;

(H3) The Lyapunov function $V(u)$ is bounded below for $u \in \Omega_L$;

(H4) If $u \in \Omega_L$ and u is not an equilibrium solution, then $\dot{V}(u) < 0$.

Lemma 3.5. *Suppose we have (H1)–(H4); then the ω -limit set $\omega(x)$ is an equilibrium solution for every $x \in \Omega_L$. Moreover, if $\gamma^-(x)$ is precompact, then the α -limit set $\alpha(x)$ is an equilibrium solution.*

Proof. Since $\{V(T(t)x), t \geq 0\}$ is bounded below and nonincreasing, $V(T(t)x) \rightarrow c$ a constant as $t \rightarrow \infty$. By (H2), $\gamma^+(x)$ is precompact, so $\omega(x)$ is nonempty, compact, connected and invariant by Lemma 3.4. The continuity of V implies that $V(T(t)y) = c$ for all $y \in \omega(x)$ and $t \in \mathbf{R}$. Thus, y is an equilibrium solution by (H1).

Suppose now that $\gamma^-(x)$ is precompact, $x \notin E$ and there exists a sequence $\{t_n\}$, $t_n \rightarrow \infty$ as $n \rightarrow \infty$ such that $T(t_n)x \rightarrow y$ as $n \rightarrow \infty$. Choose t_n such that $t_n - t_{n-1} \geq 1$ for all n . Then, for any $t \in (0, 1)$, (H1) and (H4) imply that $V(T(t_{n-1})x) \leq V(T(t_n + t)x) \leq V(T(t_n)x)$ for all n . Thus, $V(T(t + t_n)x) \rightarrow V(y)$ as $n \rightarrow \infty$. Since $V(T(t + t_n)x)$ also converges to $V(T(t)y)$ as $n \rightarrow \infty$, we have that $V(T(t)y) = V(y)$ for all $t \in (0, 1)$, hence for all $t \in \mathbf{R}$. Thus, (H1) implies that y is an equilibrium solution. \square

The following theorem provides conditions for the existence and gives the structure of the global attractor (see also [9, Theorem 3.8.5, 14, Theorem 2.3] and [18, Theorem VII.4.1 and VII.4.2]).

Theorem 3.6. *Suppose (H1)–(H4) are satisfied; then the ordinary differential (2.5), (2.6) and (2.4), (2.6), (2.7) has a global attractor \mathcal{A} such that $\mathcal{A} = W^u(E)$. Moreover, if all the equilibrium solutions are hyperbolic, then $\mathcal{A} = \cup_{y \in E} W^u(y)$.*

Proof. By Lemma 3.5, $T(t)x \rightarrow E$ as $t \rightarrow \infty$ for all $x \in \Omega_L$. Let B be any bounded neighborhood of E . Then there exists a time $t_0 = t_0(x, B)$ such that $T(t)x \in B$ for all $t \geq t_0$. For some $\varepsilon_0 > 0$, let $C = B_{\varepsilon_0}(B)$. We wish to show that $\mathcal{A} = \omega(C)$.

Now there exists $\varepsilon(x) > 0$ such that $T(t_0)B_{\varepsilon(x)}(x) \subset C$. Hence, $T(t + t_0)B_{\varepsilon(x)}(x) \subset T(t)C \subset \gamma^+(C)$ for all $t \geq 0$. Thus, for every compact set K there exists $\varepsilon_1 = \varepsilon_1(K)$ and a time $t_1 = t_1(K)$ such that

$$(3.10) \quad T(t)B_{\varepsilon_1}(K) \subset \gamma^+(C)$$

for all $t \geq t_1$. For any bounded set D , $\omega(D)$ attracts D since $\omega(D) = \cap_{t \geq 0} Cl \gamma^+(T(t)D)$. Hence, for $\varepsilon_2 > 0$,

$$(3.11) \quad T(t)D \subset B_{\varepsilon_2}(\omega(D))$$

for all $t \geq t_2 = t_2(\varepsilon_2, D)$. Since $\omega(D)$ is compact, $T(t + t_2)D \subset \gamma^+(C)$ for all $t \geq t_1$. Thus, $T(t)D \subset \gamma^+(C)$ for all $t \geq t_1 + t_2$. In particular, $T(t)\gamma^+(C) \in \gamma^+(C)$ for $t \geq t_1 + t_2$ and so $\gamma^+(T(t_1 + t_2)\gamma^+(C)) \subset \gamma^+(C)$. So we have that $\omega(\gamma^+(C))$ is nonempty, compact, connected and invariant and $\omega(\gamma^+(C))$ attracts $\gamma^+(C)$. Now, for every $\varepsilon > 0$, there exists a time $t_3 = t_3(\varepsilon) \geq 0$ such that $T(t)\gamma^+(C) \subset B_\varepsilon(\omega(\gamma^+(C)))$ for all $t \geq t_3$. Therefore, given any bounded set D , we have

$$(3.12) \quad T(t)D \subset B_\varepsilon(\omega(\gamma^+(C)))$$

for all $t \geq t_1 + t_2 + t_3$. Note that $T(t)\gamma^+(C) = \gamma^+(T(t)C)$ and $\gamma^+(T(t)C) \rightarrow \omega(C)$ as $t \rightarrow \infty$ so that $\omega(C) = \omega(\gamma^+(C))$. Since Ω_L is connected, $\omega(C)$ is connected.

Since every element $x \in \mathcal{A}$ has a complete trajectory $\gamma(x)$, Lemma 3.5 implies that $\alpha(x) \in E$ for all $x \in \mathcal{A}$. Thus, $\mathcal{A} = W^u(E)$. If all equilibrium solutions are hyperbolic, then by Lemma 3.3 there exists a finite number of equilibria so that $\mathcal{A} = \cup_{y \in E} W^u(y)$. \square

4. Equilibrium solutions. Lemmas 3.1 and 3.2 and the fact that we consider an L with a finite number of points imply that the hypotheses (H1)–(H4) are satisfied for the SDCH and SDCA equations. In view of Theorem 3.6, it is natural to study the equilibrium solutions and their stability properties in order to determine the structure of the global attractor. In this section we give conditions for the existence of constant, two periodic and three periodic equilibrium solutions on one-, two- and three-dimensional rectangular boundaries with periodic boundary conditions. In particular, we exhibit equilibrium solutions for the specific SDCA equations that correspond to the SDCH equations given in (2.9), (2.10) and (2.13). Note that an equilibrium solution of the SDCA equation is an equilibrium solution of the SDCH equation. For the one-dimensional equation (2.9) with the periodic boundary conditions (2.17), we exhibit regions in (σ, α_1) -parameter space where the constant solution is stable and the regions in parameter space where the period two solution is stable. In the region where both the constant solution and the period two solution are stable, we compare these solutions through the value of the Lyapunov function.

For the nonlinearity $f(x) = \log((1+x)/(1-x)) + \sigma x$ it is easy to see that, for $\sigma \geq -2$, the value $x = 0$ is the only solution to $f(x) = 0$. For

$\sigma < -2$ there exist the additional solutions $x = \pm a$ where $0 < a < 1$. The constant solutions $u(i) = 0$ or $u(i) = \pm a$ for all i are therefore equilibrium solutions for the SDCA equations for $\sigma < -2$ independent of any other parameters. These constant solutions are also equilibrium solution of the SDCH equation provided they correspond to the mass of the system. Indeed, independent of all parameter values the trivial solution $u(i) = 0$ for all i is always an equilibrium solution for the case in which the mass is zero.

We now turn our attention to the case of one-, two- and three-dimensional boundaries that are straight lines, rectangular, and rectangular cubes, respectively. We consider the case of periodic boundary conditions and give conditions for the existence of two-periodic and three-periodic solutions. In the one-dimensional case for an L of the form $i \in L$ if $1 \leq i \leq N_1 \equiv 2M_1$ there is a period two solution of the form $u(i) = b$ for i odd and $u(i) = -b$ for i even provided $\sigma + 4\alpha_1 < -2$ where b satisfies $f(b) + 4\alpha_1 b = 0$.

We now consider the regions of stability for the nonzero constant solution and the period two solution in (σ, α_1) parameter space. Let $c \equiv c(\sigma)$ denote the value of the nonzero positive constant solution, and let $b \equiv b(\sigma, \alpha_1)$ denote the positive value of the period two solution. By Gershgorin's theorem (see [8, p. 200]), the nonzero constant solution is stable provided $(f'(c) + 2\alpha_1) \pm 2\alpha_1 > 0$. Since c satisfies $f(c) = 0$ we find that, upon differentiating with respect to the parameter σ for $\sigma < -2$, $f'(c) \equiv (2/(1 - c^2)) + \sigma = -c(\sigma)/c'(\sigma) > 0$. Thus, $(f'(c) + 2\alpha_1) - 2\alpha_1 > 0$. The other inequality is satisfied, provided $\alpha_1 > -(1/4)f'(c)$. Therefore, the nonzero constant solution is stable for the region in parameter space defined by $\sigma < -2$ and $\alpha_1 > -(1/4)f'(c)$.

Provided it exists, the period two solution is stable when $(f'(b) + 2\alpha_1) \pm 2\alpha_1 > 0$ using Gershgorin's theorem. Since b satisfies $f(b) + 4\alpha_1 b = 0$, we have upon differentiation with respect to the parameter σ that $f'(b) + 4\alpha_1 \equiv (2/(1 - b^2)) + \sigma + 4\alpha_1 = -b(\sigma)/b'(\sigma) > 0$ so $(f'(b) + 2\alpha_1) + 2\alpha_1 > 0$. The other inequality is satisfied provided $f'(b) > 0$. Thus, the period 2 solution is stable for the region in parameter space defined by $\sigma + 4\alpha_1 < -2$ and $f'(b) > 0$.

It is easy to see that there is a region where both the nonzero constant solution and the period two solution are stable. Let u denote the nonzero constant solution and v the period two solution for some fixed

$\sigma < -2$ and all α_1 such that $f'(b) > 0$. We will show that the constant solution has lower energy for $\alpha_1 > 0$ and the period 2 solution has lower energy for $\alpha_1 < 0$ in regions where both solutions exist. We have that $(\partial/\partial\alpha_1)[F(b) + 2\alpha_1 b^2] = 2b^2 > 0$ for $b \neq 0$ and since $F(b) + 2\alpha_1 b^2 = F(c)$ for $\alpha_1 = 0$, we conclude that $F(b) + 2\alpha_1 b^2 > F(c)$ for $\alpha_1 > 0$ and $F(b) + 2\alpha_1 b^2 < F(c)$ for $\alpha_1 < 0$. Thus, $V(v) > V(u)$ for $\alpha_1 > 0$ and $V(u) > V(v)$ for $\alpha_1 < 0$.

In the two-dimensional case for an L of the form $(i, j) \in L$ if $1 \leq i \leq M_1 = 2N_1$ and $1 \leq j \leq M_2 = 2N_2$ there is an equilibrium solution of the form $u(i, j) = b$ for $i + j$ odd and $u(i, j) = -b$ for $i + j$ even provided $\alpha_{11} = 0$ and $\sigma + 8\alpha_{10} < -2$ where b satisfies $f(b) + 8\alpha_{10}b = 0$, i.e., there exists a solution that is period two in both directions simultaneously. It can be shown using Gershgorin's theorem that this equilibrium solution is stable provided $f'(b) > 0$. Similarly, there exists an equilibrium solution of the form $u(i, j) = b$ for i odd and $u(i, j) = -b$ for i even provided $\alpha_{10} = 0$ and $\sigma + 8\alpha_{11} < -2$. This equilibrium solution is stable when $f'(b) > 0$. In the case of an average concentration of $c_0 = 0.5$ there exists an equilibrium solution of the form $u(i, j) = b$ for i or j even and $u(i, j) = -b$ for i and j odd provided $\alpha_{10} = 2\alpha_{11}$ and $\sigma + 24\alpha_{11} < -2$.

For a three-dimensional L of the form $(i, j, k) \in L$ if $1 \leq i \leq N_1 = 2M_1$, $1 \leq j \leq N_2 = 2M_2$ and $1 \leq k \leq N_3 = 2M_3$ there exist period two equilibrium solutions similar to those that occur for the two-dimensional equation. For $\alpha_{110} = \alpha_{111} = 0$ there exists an equilibrium solution with unit cell that is period two in each coordinate direction of the form

$$\begin{array}{ccccccccc} +b & -b & +b & -b & +b & -b & +b & -b & +b \\ -b & +b & -b & +b & -b & +b & -b & +b & -b \\ +b & -b & +b & -b & +b & -b & +b & -b & +b \end{array}$$

provided that $\sigma + 12\alpha_{100} < -2$. As is conventional in crystallography, the periodicity is shown by repeating the boundary of the unit cell. This is known to crystallographers as the sodium chloride structure with space group $Fm\bar{3}m$ (see [13]). In fact, this equilibrium solution is stable when $f'(b) > 0$. For $\alpha_{100} = \alpha_{110} = 0$ there exists an equilibrium solution that is period two in one of the coordinate directions of the

form

$$\begin{array}{cccccc} +b & +b & -b & -b & +b & +b \\ +b & +b & -b & -b & +b & +b \end{array}$$

when $\sigma + 16\alpha_{111} < -2$. This is a tetragonal layer structure with space group $P4/mmm$. This equilibrium solution is stable when $f'(b) > 0$.

For a one-dimensional L there exists a period three equilibrium solution provided the number of lattice points is a multiple of three and $\sigma + 3\alpha_1 < -2$. The equilibrium solution is of the form $(b \ 0 \ -b)$. Any equilibrium solution of a one-dimensional lattice equation is equivalent to a trajectory of a map $F : \mathbf{R}^n \rightarrow \mathbf{R}^n$. If $n = 1$ and F has a periodic point of period 3, then by Sarkovskii's theorem (see [6]) this implies that there exist equilibrium solutions of all periods that divide the number of lattice points. For higher space dimension lattice equations, we know of no analogous results.

For a two-dimensional L with the number of lattice points a multiple of three in both directions, there exists a solution that is period three in both directions with centered rectangular unit cell of the form

$$\begin{array}{ccccc} & & & & 0 \\ & & & -b & +b & 0 \\ +b & & 0 & -b & & \\ 0 & -b & +b & & & \\ & & & & & 0 \end{array}$$

provided $\sigma + 6\alpha_{10} < -2$ and $\alpha_{11} = 0$. The space group is cm .

For a three-dimensional L where the period in each of the cube directions is a multiple of three, there exists an equilibrium solution on the cube plane of the form

$$\begin{array}{cccc} 0 & -b & +b & 0 \\ +b & 0 & -b & +b \\ -b & +b & 0 & -b \\ 0 & -b & +b & 0 \end{array}$$

In this structure, closed packed (111) sheets attain constant values alternating $0, -b, +b, 0, -b$, etc. This forms a polar rhombohedral unit cell with cell constants equal to (300), (030) and (003) and a space group $R3m$. This equilibrium solution exists for $\sigma + 9\alpha_{100} < -2$ and $\alpha_{110} = \alpha_{111} = 0$.

Stability properties may be derived for the SDCH equation using the norm that we develop below. We use a construction similar to that proposed in [2]. Consider the collection \mathbf{R}^L of real-valued sequences $w := \{w(\eta)\}_{\eta \in L}$ and \mathbf{R}_0^L the real-valued sequences with the property that $\sum_{\eta \in L} w(\eta) = 0$, i.e., the real-valued sequences with mean zero. Note that \mathbf{R}_0^L is a subspace of \mathbf{R}^L of dimension $\text{card}(L) - 1$. Consider the operator $-\Delta_B$ together with the boundary conditions

$$(4.1) \quad \sum_{i \in I_B} \beta_i \sum_{k=1}^{d_i} \left\{ - \sum_{\eta \in \partial L_{\eta_k}^-} (u(\eta) - u(\eta - \eta_k)) + \sum_{\eta \in \partial L_{\eta_k}^+} (u(\eta + \eta_k) - u(\eta)) \right\} = 0.$$

Let $\{\lambda_n\}_{n \in L}$ and $\{\phi^{(\eta)}\}_{\eta \in L}$ denote the eigenvalues and corresponding eigenvectors of the operator $-\Delta_B$ together with the boundary conditions (4.1). Then there exists an eigenvalue λ_{η^*} with corresponding eigenvector of the form $\phi^{(\eta^*)} = c$ for some nonzero constant c . All other eigenvalues are positive. Thus, $\phi^{(\eta^*)} \notin \mathbf{R}_0^L$, so that for each $v \in \mathbf{R}_0^L$ there exists a unique $w \in \mathbf{R}_0^L$ such that $v = -\Delta_B w$ with the boundary conditions (4.1).

We now define a norm on \mathbf{R}_0^L . Given $v \in \mathbf{R}_0^L$, let $w \in \mathbf{R}_0^L$ be the unique element such that $v = -\Delta_B w$. Define

$$\begin{aligned} \|v\|_{-1}^2 &= \sum_{\eta \in L} -\Delta_B w(\eta) \cdot w(\eta) \\ &= \sum_{\eta \in L} \left\{ \sum_{i \in I_B} \beta_i \nabla_i w(\eta) \cdot \nabla_i w(\eta) \right\} \end{aligned}$$

using Green's formula.

Note that with this norm we have, for the CDCH equation, $\|\dot{u}\|_{-1}^2 = -dE(u)/dt$ since $\dot{u} \in \mathbf{R}_0^L$.

5. Numerical methods. In this section we present the methods that we use to solve the SDCH equations numerically. Because we are most interested in the two- and three-dimensional case we develop methods for a massively parallel architecture so that we may solve the SDCH equation when the cardinality of L is large. These equations are highly nonlinear and, like the continuous Cahn-Hilliard equation,

require stiff solvers to integrate effectively. We use the A -stable implicit trapezoidal method which is a second order method (see [7]). We halve the given step size and perform two half steps and a single full step so that we may obtain an estimate of the local error. If the error is sufficiently small, then Richardson extrapolation (see [17]) is used to obtain a solution with a fourth order local error. A finite difference approximation or further extrapolation can be used to obtain a posteriori estimates of the fourth order local error.

When solving a nonlinear problem using implicit numerical integration methods, a nonlinear system of equations must be solved. We solve the nonlinear system of equations using Newton's method. Each Newton step results in a linear system of equations to be solved. Because we typically consider L with many points, indirect methods will be used to solve the linear systems. In particular, we employ the conjugate gradient type iterative methods (see [15]) that exist for nonsymmetric systems. We apply both the method CGNR (see [11]) and the more recent CGS method (see [16]).

We solve the differential system numerically on a Connection machine which is a data parallel (SIMD) machine with up to 64K processors. This allows us to take advantage of the neighborhood structure that exists for the SDCH equations. In general, we employ the following algorithm applied to the general equation $\dot{u} = g(u)$ combined with the given boundary conditions.

Algorithm. 1. Given a step size Δt discretize using implicit trapezoid to obtain the nonlinear system of equations

$$u_{n+1} = u_n + \frac{\Delta t}{2}(g(u_n) + g(u_{n+1})).$$

2. Take two steps of size $\Delta t/2$ and one step of size Δt and compare to obtain a local error estimate.

3. If the local error is less than or equal to the specified tolerance, then extrapolate to obtain a fourth order accurate solution.

4. If the local error is greater than the tolerance, then reduce the step size and goto 1.

5. If the local error is too small and the fourth order error is small enough, then increase the step size and goto 1 for the next step.

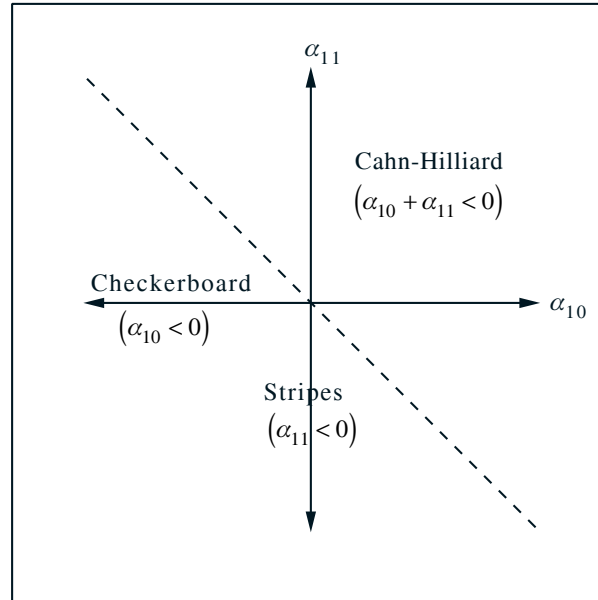


FIGURE 1. Patterns in different regions of parameter space for model 2D problem.

When using iterative methods it is necessary that we are able to multiply the Jacobian by an arbitrary vector. With the CGNR method it is also necessary that we are able to multiply the transpose of the Jacobian by an arbitrary vector. The cost of a Jacobian times vector multiply is the same as the cost of a function evaluation in our implementation on the Connection machine.

6. Numerical results. In this section we exhibit the results of our numerical simulations. We consider the spatially discrete Cahn-Hilliard type equation given by (2.10) together with both the Neumann type boundary conditions (2.20) and the periodic type boundary conditions (2.19). Figures 2–5 were obtained using the Neumann conditions with a 60×60 square grid of variables, while Figures 6 and 7 were obtained using periodic type boundary conditions on a 63×63 square grid.

(a) $T = 5.93$.(b) $T = 10.93$.(c) $T = 21.93$.(d) $T = 47.93$.

FIGURE 2. Cahn-Hilliard PDE type behavior using the spatially discrete model. Neumann BCs, $\sigma = -2.5$, $\alpha_{10} = -0.5$, $\alpha_{11} = 0.25$, $c_0 = 0.0$.

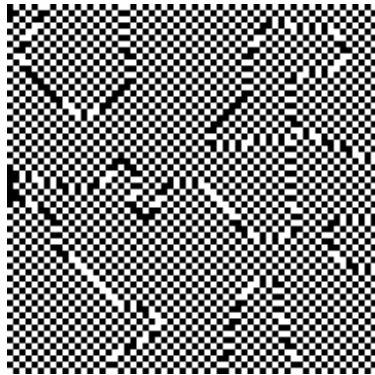
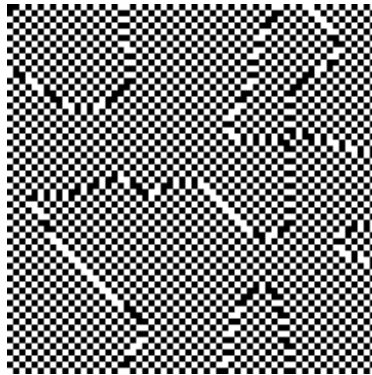
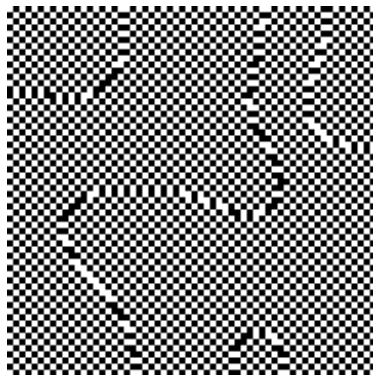
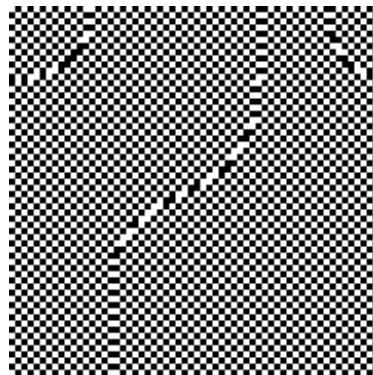
(a) $T = 0.96$.(b) $T = 1.35$.(c) $T = 2.76$.(d) $T = 10.82$.

FIGURE 3. Checkerboard patterns that are not found in Cahn-Hilliard PDE. Neumann BCs, $\sigma = -1.0$, $\alpha_{10} = -0.25$, $\alpha_{11} = 0.5$, $c_0 = 0.0$.

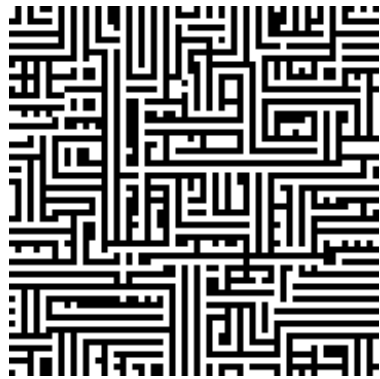
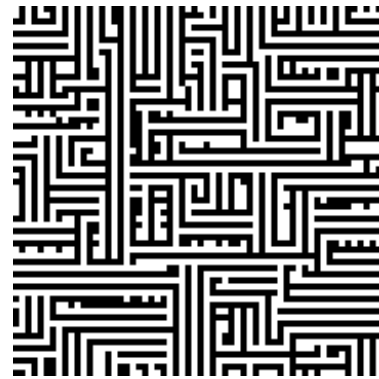
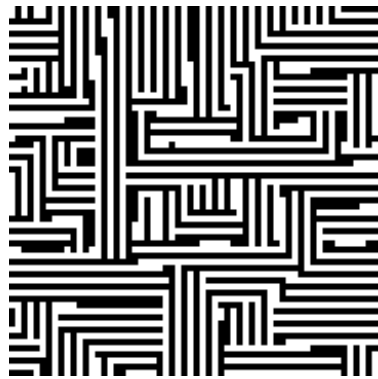
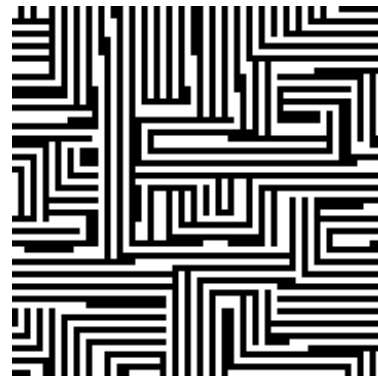
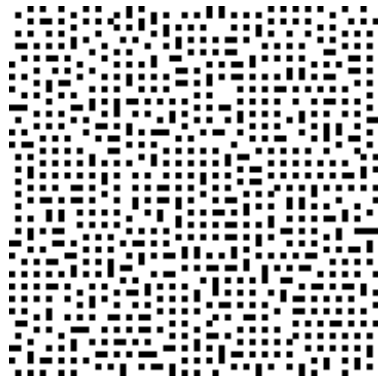
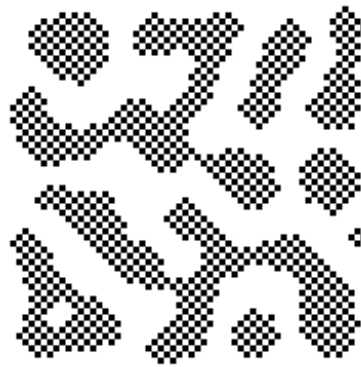
(a) $T = 0.28$.(b) $T = 0.36$.(c) $T = 0.68$.(d) $T = 1.78$.

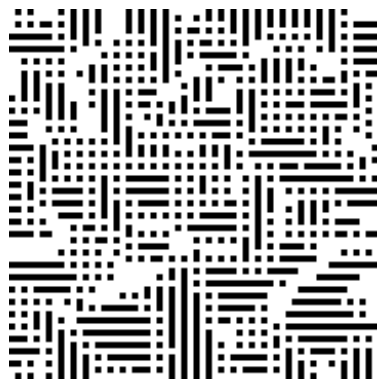
FIGURE 4. Striped patterns that are not found in Cahn-Hilliard PDE. Neumann BCs, $\sigma = -4.0$, $\alpha_{10} = 2.0$, $\alpha_{11} = -1.0$, $c_0 = 0.0$.



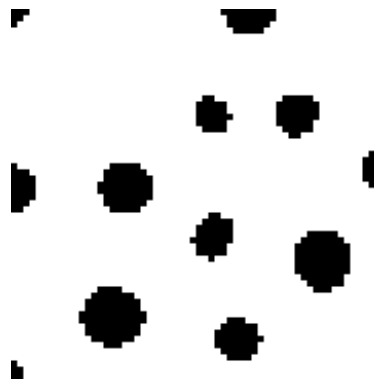
(a) $\sigma = -2.1$, $\alpha_{10} = -0.25$,
 $\alpha_{11} = -0.5$, $T = 0.20$.



(b) $\sigma = -2.1$, $\alpha_{10} = -0.25$,
 $\alpha_{11} = 0.5$, $T = 5.65$.



(c) $\sigma = 4.0$, $\alpha_{10} = 1.0$,
 $\alpha_{11} = -2.0$, $T = 0.15$.



(d) $\sigma = -3.0$, $\alpha_{10} = 0.25$,
 $\alpha_{11} = 0.5$, $T = 77.63$.

FIGURE 5. Neumann BCs, $c_0 = 0.5$.

All computations were performed on a Connection machine using 8K processors.

The iterative method CGS was used as the primary iterative solver, but CGNR was invoked if CGS failed to converge within the specified tolerance in \sqrt{N} iterates where N is the number of lattice points. The initial data was generated randomly to obtain a small perturbation about the constant solution corresponding to the given concentration, c_0 . The computations were performed with average concentration $c_0 = 0.0$ (a 50/50% distribution) or $c_0 = 0.5$ (a 25/75% distribution).

We will usually consider only the case in which there is a double well potential, i.e., when $\sigma < -2$, but when either $\alpha_{10} < 0$ or $\alpha_{11} < 0$ we may consider $\sigma > -2$ since with a negative gradient energy coefficient the constant solution is not a minimizer. Since we typically obtain high amplitude solutions, “snapshots” of the time evolution are displayed using a white square to indicate a value greater than zero and a black square to indicate a value less than zero.

Figure 1 shows the different patterns that are expected in different regions of parameter space for the 2D model problem given by (2.10) and either the periodic boundary condition (2.19) or the Neumann boundary conditions (2.20). For $\alpha_{10} + \alpha_{11} > 0$ the continuum limit of our discrete model gives a well-posed PDE, the Cahn-Hilliard equation.

In Figure 2 we display “snapshots” of the time evolution in the range of parameters that corresponds to a well-posed PDE, i.e., the Cahn-Hilliard equation. Note that the solution undergoes coarsening like the continuous equation. Figure 2 shows what is known as a spinodal decomposition.

Figure 3 shows the ordering that occurs for $\alpha_{10} < 0$ and $\alpha_{11} > 0$. The bulk phases here are “checkerboard” patterns, one with even parity and one with odd parity. The bulk phases are separated by an interface.

We have $\alpha_{10} > 0$ and $\alpha_{11} < 0$ in Figure 4. For these parameter values the bulk phases are even and odd parity horizontal stripes and even and odd parity vertical stripes.

All the snapshots in Figure 5 are for a 25/75% concentration. In Figure 5(a) we see another of the bulk phases which we were able to identify as an equilibrium solution. Figure 5(b) shows the coexistence

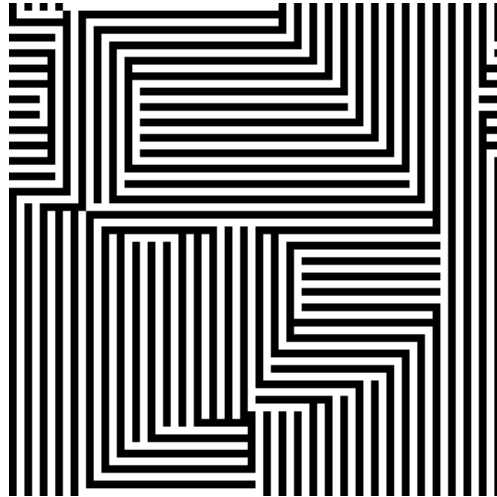


FIGURE 6. Striped patterns and quad junctions. Periodic BCs, $\sigma = 4.0$, $\alpha_{10} = 1.0$, $\alpha_{11} = -2.0$, $c_0 = 0.0$, $T = 2.7786$.

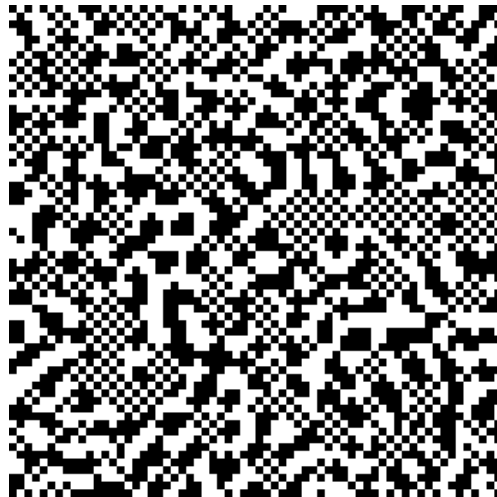


FIGURE 7. Transient behavior unlike that found in C-H PDE in parameter region where continuum limit PDE is well-posed. Periodic BCs, $\sigma = -12.0$, $\alpha_{10} = 1.0$, $\alpha_{11} = 2.0$, $c_0 = 0.0$, $T = 0.1089$.

of a single solid phase and a checkerboard phase. We see the coexistence of three bulk phases in Figure 5(c). Note that here we have a single well potential. What appears to be the result of coarsening and curvature dependent behavior is depicted in Figure 5(d).

Figures 6 and 7 were obtained using periodic boundary conditions. We see quad junctions in Figure 6, i.e., the meeting of even and odd parity horizontal striped phases and even and odd parity vertical phases at a single point. In Figure 7 we see the coexistence of two solid phases and two checkerboard phases.

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MATERIAL SCIENCE AND ENGINEERING LABORATORY, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, GAITHERSBURG, MD 20899

SCHOOL OF MATHEMATICS, GEORGIA INSTITUTE OF TECHNOLOGY, ATLANTA, GA 30332

DEPARTMENT OF MATHEMATICS AND STATISTICS, SIMON FRASER UNIVERSITY, BURNABY, B.C. V5A 1S6 CANADA

Current address: DEPARTMENT OF MATHEMATICAL AND COMPUTER SCIENCES, COLORADO SCHOOL OF MINES, GOLDEN, CO 80401