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Pattern formation in nonlinear reaction–diffusion systems

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Abstract. Reaction–diffusion equations are ubiquitous in population dynamics, laser physics, bacterial growth, domain wall kinetics, order parameter relaxation and a host of other problems, cutting across disciplines. The occurrence of nonlinearity adds further complexity in terms of bifurcation-solutions, phase transitions, fractal growth, etc. In most cases the non-transient, asymptotic solutions of these equations lead to patterns, the nature of which depends on certain symmetry properties of the underlying variable(s). In this paper we discuss a few such equations with applications to domain motion of different kinds in ferroelectrics, multiferroics and their switching characteristics because of the underlying nonlinearities, and glucose-induced fractal colony growth of *Bacillus thuringiensis*.

Keywords. Reaction–diffusion; ferroelectricity; time-dependent Ginzburg–Landau; domain pattern; fractal.

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1. Introduction

The existence of patterns in living organisms as well as in non-living structures has led scientists across disciplines to theorize both spontaneous and field-induced pattern formations. When two or more than two prey and predator orders react among themselves nonlinearly and diffuse either isotropically or anisotropically, complex spatio-temporal patterns arise. In 1952, Allan Turing in his pathbreaking work entitled 'The chemical basis of morphogenesis' [1] explained how two chemically interacting substances, diffusing at different rates can yield complex periodic patterns. He called them chemical morphogens and suggested that the spatio-temporal morphogenesis generated by the underlying reaction–diffusion (RD) equations can lead to embryo development. Meinhardt [2, 3], Murray *et al.* [4–6] and Mimura *et al.* [7] further extended Turing's work by modifying reaction and diffusion terms. Kessler and Levine [8] showed how fluctuation can induce front instability in RD systems. Here we present a set of RD systems of interest in materials and biological sciences. Our first examples pertain to 180° and 90°, vortex and antivortex domains, in ferroelectric and multiferroic thin films, endowed with fractal characteristics. Our last study concerns nutrient dependency in the fractal colony pattern for *Bacillus thuringiensis*. The generic RD equations that form the basis of our discussion can be written as

$$\frac{\partial u_1(r,t)}{\partial t} = D_1\nabla^2 u_1 + \phi_1(u_1,u_2), \quad (1)$$

$$\frac{\partial u_2(r,t)}{\partial t} = D_2\nabla^2 u_2 + \phi_2(u_1,u_2), \quad (2)$$

where ϕ's and D's are the respective reaction and diffusion coefficients.

2. Landau–Devonshire–Ginzburg theory of ferroelectricity

Pattern formation via Hopf bifurcation of a stationary state is widely studied in complex Ginzburg–Landau equations [9–11]. When it comes to displacive ferroelectrics these equations are based on Landau–Devonshire free energy [12–14].

$$g(T,P) = g_0(T) + \frac{1}{2}a(T)P^2 + \frac{1}{4}b(T)P^4 + \frac{\delta}{2}\{\nabla P\}^2 - EP, \quad (3)$$

where $a(T) = a_0(T - T_c)$. $a_0, b(T)$ and δ are positive constants and T_c is the phase transition temperature. The free energy expansion in eq. (3), retained up to a quartic order in the polarization P, reflects symmetry under $P \rightarrow -P$, in the absence of the external electric field E. The gradient term, which takes cognizance of inhomogeneity in P, has important consequences for domain formation, especially in combination with boundary conditions. The first term g_0 is dependent only on temperature T, and is therefore innocuous as far as phase transitions are concerned. Taking the derivative of g with respect to P, the spatio-temporal

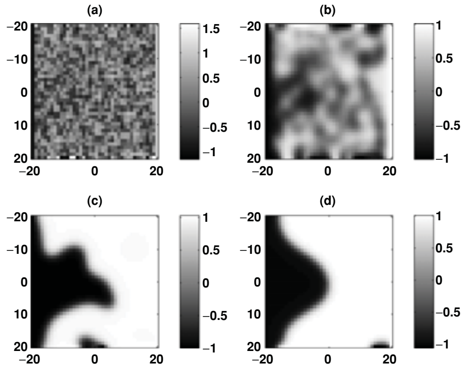

Figure 1. Evolution of 180° domains from the paraelectric phase under boundary conditions $P(x=-L,y)=-P_s=-1$ and $P(x=L,y)=P_s=1$ in different time steps [15].

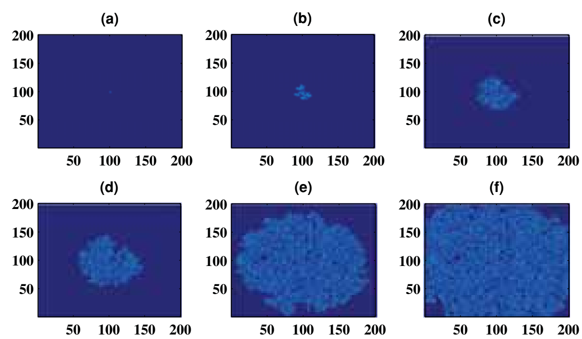

Figure 2. Growth of fractal 180° domain in different time steps is shown when the electric field is applied at the center of the film [16].

dynamics is governed by the time-dependent Ginzburg–Landau (TDGL) equation:

$$\frac{\partial P}{\partial t} = \delta\nabla^2 P + (aP - bP^3 + E). \tag{4}$$

Here $\pm P$ corresponding to $\pm E$ may be interpreted as prey and predator in population dynamics.

2.1 *Formation of* 180° *and fractal ferroelectric domain patterns*

Our first example is the formation of 180° domains which ensue from eq. (4) with the following boundary conditions $P(x=-L,y)=-P_s=-1$ and $P(x=L,y)=P_s=1$ and the initial condition as one of the random dipole orientations. Here $x=\pm L$ are left (right) boundaries and P_s is the saturation polarization (see figure 1 [15]). In figure 1 [15], 180° domain development at times (a) 0, (b) 2, (c) 10, and (d) 40 steps with initial condition $P_z(x,y,t=0)=\eta(x,y)$ where $\eta(x,y)$ is a random variable valued: $1 \leq \eta \geq 1$. In the presence of disorder the domains are pinned. The external field E causes depinning and hence it is useful to consider an effective field $E_{\text{eff}}=E-E_{\text{pin}}(r)$. The resulting fractal domains, caught in timeframes, (a) 1, (b) 5, (c) 10, (d) 15, (e) 30, and (f) 40 time steps, are shown in figure 2 [16].

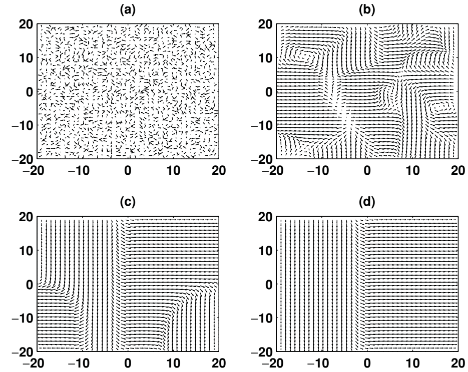

Figure 3. Formation of the 90° domain [15].

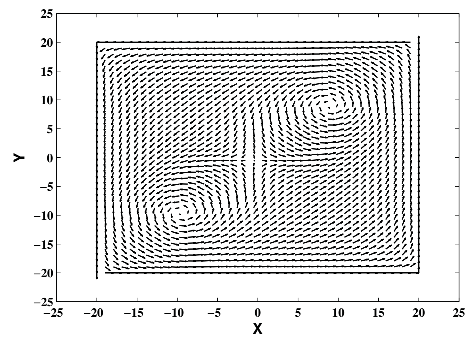

Figure 4. A vortex and antivortex pair of domains [17].

2.2 *Formation of* 90° *and vortex–antivortex ferroelectric domain patterns*

We consider a toroidal (vortex) moment [15, 17–19] of polarization as

$$\vec{G} = (2N)^{-1}\sum_i \vec{R}_i \times \vec{P}_i, \tag{5}$$

where $\vec{P}$ is a two-dimensional vector $\vec{P}(x,y)=P_x(x,y)\hat{i} + P_y(x,y)\hat{j}$. The corresponding TDGL equations are

$$\frac{\partial P_x}{\partial t} = \left[(AP_x - BP_x^3 - CP_xP_y^2) + \delta\nabla^2 P_x\right], \tag{6}$$

$$\frac{\partial P_y}{\partial t} = \left[(AP_y - BP_y^3 - CP_yP_x^2) + \delta\nabla^2 P_y\right]. \tag{7}$$

Figures 3 and 4 show the formation of 90° and vortex–antivortex [15, 17] domains by solving eqs (6) and (7). In figure 3, head-to-tail 90° formation at (a) $t=0$, (b) $t=4$, (c) $t=10$, and (d) $t=80$th time steps are shown. These domains can be mapped via the model described in [20] where we have theoretically mimicked the mechanism of piezoforce microscopy.

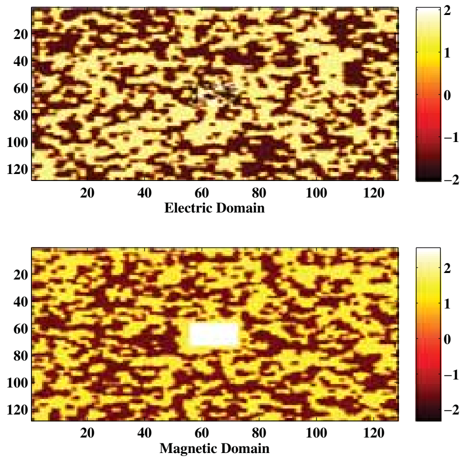

Figure 5. Ferroelectric and ferromagnetic domains under the influence of magnetic field alone.

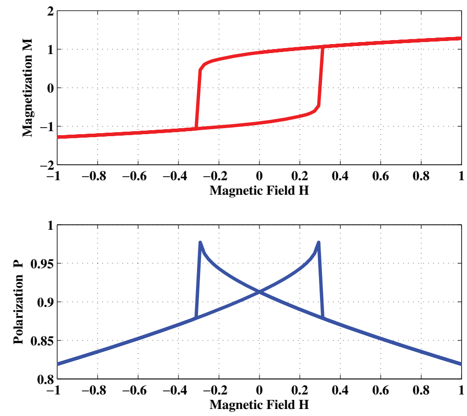

Figure 6. Magnetic and electric hysteresis under magnetic field variation in a multiferroic 2D film. Butterfly hysteresis is seen in ferroelectric hysteresis.

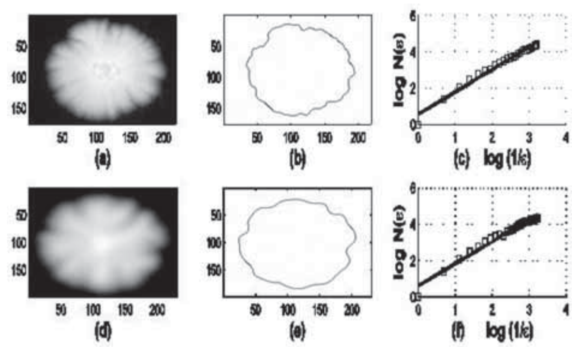

Figure 7. (**a**) and (**d**) are experimental and simulated images, respectively. (**b**) and (**e**) are edges of the colonies. (**c**) and (**f**) are plots for log $N(\epsilon)$ vs. log $(1/\epsilon)$ to calculate Hausdorff dimension ($D_{\mathrm{H.Expt}} = 1.1969$ and $D_{\mathrm{H.RD}} = 1.1965$) for length scale ϵ [25].

2.3 *Domain patterns in multiferroics*

Magnetoelectric positive biquadratic coupling supplies a reaction term to induce the multiferroic RD system in Ginzberg–Landau free energy [21–23]. RD equations for multiferroics [24] become

$$\frac{\partial P}{\partial t} = D_P \nabla^2 P + a_1 P - b_1 P^3 + cPM^2 + E, \tag{8}$$

$$\frac{\partial M}{\partial t} = D_M \nabla^2 M + a_2 M - b_2 M^3 + cP^2 M + H, \tag{9}$$

where P and M are the respective ferroelectric and ferromagnetic order parameters and E and H are the conjugate fields. Depending on the coupling, one or other order occurs at a lower temperature. Figure 5 shows ferroelectric and ferromagnetic domain switching by applying only the field $H(E=0)$. In figure 6 a butterfly loop is seen in the polarization hysteresis while the ferromagnet exhibits normal hysteresis.

3. Fractal colony pattern of *B. thuringiensis*

In this section we turn our attention to the experimental study of biological morphogenesis in glucose-induced fractal growth of bacteria [25]. The data are analyzed on the basis of the RD model [25], similar to earlier studies [6, 7, 26–35] and can be described by

$$\frac{\partial b(x,y;t)}{\partial t} = D_b \nabla^2 b(x,y;t) + f(n,b), \tag{10}$$

$$\frac{\partial n(x,y;t)}{\partial t} = D_n \nabla^2 n(x,y;t) - f(n,b), \tag{11}$$

where D_b and D_n are diffusion coefficients for the bacteria and the nutrients respectively and $f(n,b)$ is a reaction term. The latter is taken to be proportional to the nutrient concentration n but nonlinearly dependent on the bacterium concentration b, as in

$$f(n,b) = nb(1 - e^{(-b/b_0)}). \tag{12}$$

In figure 7 we present experimental (figure 7a) and numerical (eqs (10) and (11)) results (figure 7d) where glucose induces and controls colony behavior. Using the Canny algorithm, we detected edges (figures 7b and e) of the corresponding images to evaluate Hausdorff dimension (D_{H}) by the box counting method (figures 7c and f). We obtained $D_{\mathrm{H.Expt}} = 1.1969$ and $D_{\mathrm{H.RD}} = 1.1965$, in close agreement [25].

4. Concluding remarks

In this paper we present an overview of RD equations as applied to examples drawn from materials and biological sciences. In the first set of examples ferroelectric thin films are shown to exhibit different domain patterns depending on the spatial dimension, boundary conditions and disorder. Competing order parameter systems such as multiferroics show novel features, hitherto unexplored. The versatility of RD equations is further illustrated by considering a completely different application of fractal colony growth of bacteria. We conclude by remarking that the efficacy of RD models in generating experimentally observed patterns lies in judicious choice of numerical algorithm.

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