Reaction and Concentration Dependent Diffusion Model

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We study the formation of patterns in the genuinely nonlinear reaction diffusion model equation $u_t + 2a(u^2)_x = (u^2)_{xx} + F(x, u)$, where u may be viewed as an amplitude of a thermal wave in plasma or density of a biological species and F = u(1 - u) or $F = q(x)u^l$, l = 0, 2. We provide a transformation which maps the model into a purely diffusive process free of its interacting part and its intrinsic temporal and spatial scales. The well known attractors of the diffusive process enable us to completely characterize the emerging patterns which, depending on F and initialization, may be a semicompact, or a compact, traveling wave or a nontrivial equilibrium.

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The reaction-diffusion processes encompass a wide variety of phenomena ranging from chemical reactions, combustion fronts, thermal waves in plasma, to biological processes such as spread of favorite genes or population dynamics [1-3]. Though a realistic description of these processes is quite complex and, depending on the problem at hand, may involve a variety of state variables and external fields, on the level of a paradigm, the celebrated Kolmgoroff-Petrovski-Piskunoff (KPP) equation,

$$u_t = u_{xx} + u - u^2, (1)$$

in spite of its simplicity encapsulates the essence of these processes. Surprisingly enough, nonlinear diffusion, which is universally acknowledged as an important mechanism in these processes, is very rarely included in the studies of these problems [1,2]. In this Letter I address the impact of nonlinear diffusion on reaction-diffusion processes. The model problem studied is

$$u_t = (u^2)_{xx} + u - u^2.$$
 (2)

Depending on the interpretation of u, the nonlinear diffusion in Eq. (2) reflects the fact that the population (chemical concentration or plasma temperature) disperses to regions of lower density (concentration or temperature) more rapidly as it gets more crowded. Notably, unlike the conventional diffusive tails, nonlinear diffusion supports compact fronts. Other aspects of reaction-nonlineardiffusion interaction will be described shortly. In a biological context the colonial development of lubricating bacteria such as Paenibacillus dendritiformis (which extract fluid from the substrate for swimming) is described by diffusion which is proportional to the bacterial When grown on high nutrient substrate the density. bacterial density u(x, t) is given by Eq. (2) [3]. Though the nonlinear diffusion may take a variety of forms, on the level of a paradigm Eq. (2) seems to be not only the simplest relevant extension of the KPP, but it also has the most enticing property of a nonlinear model: it is solvable. Since, with a very few exceptions, each of which is celebrated in its own right, nonlinear spatiotemporal dynamics cannot be resolved analytically, any solvable case makes it into a very valuable bench mark from both theoretical and computational points of view. This is achieved via a transformation which maps Eq. (2) into a purely (nonlinear) diffusive process given by Eq. (18), completely free from the reactive part. Since the later stage of a diffusive process is governed by its well known global attractors, this provides us a complete description of later phases of the process with the memory of the initial setup encapsulated into one global invariant. We start with an extension of Eq. (2),

$$u_t = (u^n)_{xx} + u - u^n, \qquad n > 1.$$
 (3)

If *u* is a solution of Eq. (3) and new variables *V* and τ are defined as $[mk_m = \ln(1 + z_0), z_0 = \text{const}]$

$$u(x,t) = \phi(t)V(x,\tau), \qquad \tau = \ln[z_0 + e^{mt}]^{1/m} - k_m,$$
(4)

where $\phi = [1 + z_0 e^{-mt}]^{-1/m}$, then Eq. (3) is invariant under $u \to V$, $t \to \tau$; i.e., $V(x, \tau)$ satisfies Eq. (3). Indeed, if we use (4) in (3) we obtain (m = n - 1)

$$\phi^{-n}(\phi - \phi)V + \phi^{-m}V_t = \mathbf{L}_{\mathbf{x}}V^n, \qquad (5)$$

where $\mathbf{L}_{\mathbf{x}} = \partial^2 - 1$. Let $\phi^{-n}(\dot{\phi} - \phi) = -1$ define ϕ . If $\tau \equiv \int_0 \phi(t)^m dt$, V satisfies Eq. (3). The invariance property holds for a variety of linear operators. For instance,

$$u_t = \nabla^2(u^{m+1}) + u(1 - u^m), \qquad m = n - 1.$$
 (6)

Using (4) one generates a whole family from a given solution. Two special cases are of interest.

1. Traveling kink [1].—Let s = x - t, then

$$(\partial_s + 1)[(\partial_s - 1)u^n + u] = 0, \quad n > 1.$$
 (7)

The common factor simplifies the problem and yields

$$u^{n-1} = \begin{cases} 1 - \exp[\alpha(s - s_0)], & s \le s_0, \\ 0, & \text{otherwise,} \end{cases}$$
(8)

which, due to nonlinear diffusion, is a semicompact pulse. Here $\alpha = (n - 1)/n$. Taking s = x + t yields a kink moving to the left. Introducing *delta* into the reactive part, $u - u^2/\delta$, reveals that while in KPP the speed of the wave remains unchanged, in Eq. (2): $s \rightarrow (x - \delta t)/\delta$.

2. A compact expanding wave [1,2].—Let

$$u^{n-1} = A(t) [1 - D(t) \cosh(x/2)]_+;$$
 (9)

then A(t) and D(t) are given via $(B = D^2, \sigma = 1/A)$

$$n\sigma B' = -2B(1 - B)$$
 and $\sigma' + \sigma = 1 + B/n$.
(10)

It is easily seen that as $t \uparrow \infty$, $\sigma \to 1$, and $B \to 0 \Rightarrow [A(t), D(t)] \to (1, 0)$. Here $D(0) = \cosh^{-1}(a/2)$, where (-a, +a) is the initial spread of the pulse. Also, as $t \uparrow \infty$, each front approaches a steadily traveling wave.

Bounds: Using property (4) we rewrite solution (8) as

$$u^{m} = \frac{e^{mt}}{z_{0} + e^{mt}} V^{m} \bigg[x - \frac{1}{m} \ln \bigg(\frac{z_{0} + e^{mt}}{z_{0} + 1} \bigg) \bigg].$$
(11)

As $t \to \infty$, all solutions of Eq. (11) converge to the same state, but with a shift in phase:

$$u \to V[x - t + k_m]$$
 as $t \to \infty$.

Consider now Eq. (2), appended with

$$u(x,t=0) = \begin{cases} 0 < f(x) < \infty, & \text{if } x < 0, \\ 0, & \text{otherwise.} \end{cases}$$
(12)

We now use the freedom to choose z_0 to construct a sub <u>u</u> and a supersolution <u>u</u> such that at t = 0

$$\underline{u}(x,t=0,z_{01}) < f(x) < \overline{u}(x,t=0,z_{02}).$$
(13)

Then, by the maximum principle, $\underline{u}(x,t) \le u(x,t) \le \overline{u}(x,t)$ at all times. Now, since both $\underline{u}(x,t)$ and $\overline{u}(x,t)$ converge to the exactly same, albeit phase shifted kink, our solution is "trapped" in between. Thus, though lemma bounds the front and fixes its speed, it falls short of providing its exact location.

Compact initial datum: From Eqs. (9) and (4) we have

$$u^{m} = \frac{e^{mt}}{z_{0} + e^{mt}} A(\tau) [1 - D(\tau) \cosh(x/2)]_{+}.$$
 (14)

Family (14) is now used to construct a sub- and a supersolution such that if $at t = 0, \underline{u} < f(x) < \overline{u}$, where u(x, t = 0) = f(x), for -a < x < a and u = 0 elsewhere, then the solution is trapped for all times in between. Again, the velocity of each left(right) moving sub(super) front is the same and equals the speed of the actual front.

Attractors: Our goal is to eliminate the intrinsic temporal and spatial lengths. To this end let

$$\tau = [\exp(mt) - 1]/m, \qquad u = e^t v, \qquad (15)$$

and m = n - 1. Thus

$$\boldsymbol{v}_{\tau} = (\boldsymbol{v}^n)_{\boldsymbol{x}\boldsymbol{x}} - \boldsymbol{v}^n. \tag{16}$$

Equation (16) is now cast into $v_{\tau} = (\partial_x + 1)(\partial_x - 1)v^n$; thus

$$v_{\tau} = e^{-x} [e^{2x} (v^n e^{-x})_x]_x.$$
(17)

We now define $R = e^{2x} > 0$ and $Z = R^{1/2n}v$, to obtain

$$\rho(R)Z_{\tau} = D_0[Z^n]_{RR} \text{ and } Z(R=0,\tau) = 0.$$
 (18)

 $\rho(R) = R^{-\Omega}$ where $\Omega = (3n - 1)/2n$ and here $D_0 = 4$. Equations (17) and (18) have two invariants:

$$I_{\pm} = \int_0^\infty Z R^{-[2+(1/n)\mp 1]/2} \, dR = 2 \int_{-\infty}^\infty v \, e^{\pm x} \, dx \,. \tag{19}$$

Equation (18) is a key to what follows; we started with Eq. (2) and reduced it into a purely diffusive process. If *u* is understood as a plasma temperature in a heated homogeneous medium with radiative losses, then in mapped coordinates Eq. (18) describes a "pure" thermal diffusion in an inhomogeneous background with density distribution $\rho(R)$. The fact that the intrinsic lengths and times of Eq. (2) are removable gives to the process an obvious universality. For instance, in the biological context, the evolution of the bacterial colony is a scalable process which can exist on different scales. As a consequence, Eq. (18) admits a group of scalings $Z \sim R^{1/2n}/\tau^{1/(n-1)}$. Conservation of I_+ then implies $Z \sim R^{(1-n)/2n}$, which in turn yields a similarity solution which for n = 2 is

$$Z_s = \frac{1}{\sqrt{\tau_*}} \zeta (1 - a_0 \zeta)_+ \quad \text{where } \zeta = (R/\tau_*^2)^{1/4}, \quad (20)$$

and a similar response for any n > 1. In (20) it was convenient to set $\tau \to \tau_* \equiv \tau + 1$. Thus $\tau_* = 0 \Leftrightarrow t = -\infty$. Equation (20) is a response to a weighted dipole at the origin: $Z(R, \tau_* = 0) = I_+ R^{7/4} \delta'(R)$ which yields $a_0 = 1/\sqrt{6I_+}$. Now, if $s_0 = \ln 2I_+$, then in terms of u

$$u_s = [1 - e^{(s-s_0)/2}]_+, \qquad (21)$$

which is recognized at once as the kink solution (8). However, now we invoke the fact that the self-similar solutions of diffusive processes like (18) are well known to be their strong attractors. An example of a numerical solution of Eq. (18) is displayed in Fig. 1 and shows a typical initial datum $[Z(R, \tau = 0) = R^{1/4}u(x, 0)]$, converging into the self-similar regime. For an observer at a distance from the initial setup, the response after a while appears as though it was due to a concentrated source sharing the same global invariant I_+ with the actual process: $I_{+} = \int_{-\infty}^{0} e^{x} u(x,0) dx$. All other initial details are washed away. The proof of the convergence toward self-similarity given in [4] for $\rho \equiv 1$ was extended to certain inhomogeneous media [5]. In the present case the process converges to the self-similar regime, but the singularity of ρ necessitates the modification of the proof in [5] (see [6] for details).

In conclusion, the equivalence of processes (2) and (18) means that the convergence of solutions of Eq. (18) to the self-similar flow (20) implies the convergence of processes given via Eqs. (2) and (12) into the universal state (8).

Remarks.—(A) If in (16) the sink turns into a source, $+K^2v^2$, the characteristic length becomes essential and the system explodes in a finite time over a finite domain [7]:



FIG. 1. Evolution of initial datum toward the self-similar stage with the location of the front normalized to one.

$$v(x,\tau) = \frac{4\cos^2(Kx/4)}{3K^2(\tau_* - \tau)}, \qquad |x| < 2\pi/K, \qquad (22)$$

and vanishes elsewhere. (B) Solution (9) rewritten as $Z^{n-1} = A(t)r^{2n-3}(r_- - r)(r_+ - r)/2$, where $r^{2n} = R$ and $r_{\pm}(t) = (1 \pm \sqrt{1 - D^2})/D$, describes the motion of two fronts: one moving inward, the other outward. Since Eq. (18) is no longer spatially invariant, the location of initial distribution matters. The initial distribution over the [-a, +a] interval is mapped into $[r_0, r_1]$. Note that now it takes an infinite time for the left front to arrive at the center. We show in [6] that the *Z*-solution is also an attractor. Thus any initial patch of bacterial colony acquires a scale invariant, globally stable, universal pattern.

Advection: Adding advection to Eq. (2) we have

$$u_t + 2a(u^2)_x = (u^2)_{xx} + u - u^2.$$
 (23)

Two traveling waves are obtained from (8) for $\lambda_{\pm} = a \pm \sqrt{\Delta}$ where $\Delta = 1 + a^2$, with $\alpha = 2\lambda_{\pm}$. Now both kinks are different. We eliminate the source and let $R = \exp[\delta_+(1 + \delta_-^2)x]$ and $Z = R^{\eta}v$, where $\delta_{\pm} = a \pm \sqrt{\Delta}$, $\eta = \sigma/(4 + 2\sigma)$, and $\sigma = 2\delta_-^2$, to obtain Eq. (18) with

$$\Omega = (4 + 3\sigma/2)/(2 + \sigma) \text{ and}$$
$$D_0 = (2 + \sigma)^2 \delta_+^2/4.$$
(24)

Equation (23) is thus mapped into a purely diffusive process which turns its traveling kinks into global attractors. Without the reactive part Eq. (23) is a variant of the Burgers equation being mapped into (18) ($\Omega = 2$).

Initial boundary value problem (IBVP): If the bacterial colony is confined to a rigid domain with, say, $u(\pm L) = 0$, then we shall show that unlike the KPP case which has both stable and unstable states, here any domain and initial setup support a globally stable nontrivial equilibrium, y(x), given, for n = 2, via

$$12(y')^2 - 3y^2 + 4y - E_*y^{-2} = 0$$
 (25)

 $(0 < E_* < 1)$ with y'(0) = 0 and $E_* = 4y(0) - 3y^2(0)$. The linear stability of (25) with $L \uparrow \infty$ as $E_* \to 1$ is easy. To obtain global stability we turn to its mapped form, Eq. (18), with $u(\pm L) = 0 \Rightarrow Z(R^{\pm}) = 0$. The separable solution $Z_* = Z_1(R)Z_2(\tau)$ of Eq. (18) leads to

$$u_*(x,t) = \frac{y(x)}{1 + c_0 e^{-t}}, \qquad c_0 = \text{const.}$$
 (26)

Clearly, $u_* \rightarrow y(x)$. Since, however, $Z_*(R, \tau)$ is well known to be a strong attractor of the IBVP with homogeneous boundary conditions [5], this uplifts $u_*(x, t)$, the mirror picture of Z_* , into a universal, later time description of the process, with the final equilibrium shape attained during the later stages of the evolution.

Spatial inhomogeneity: We now consider how explicit spatial dependence of sinks and sources facilitates the emergence of localized states. In the present context the simplest such problem is perhaps

$$u_t = (u^2)_{xx} + (K^2 - x^2)u^l$$
 and $l = 0, 2.$ (27)

1. We start with l = 0 and assume a solution of the form

$$u(x,t) = [K^{2}A(t) - B(t)x^{2}]_{+}, \qquad K^{2}A(0) > B(0).$$
(28)

The evolution of A(t) and B(t) is easily determined. As $t \uparrow \infty$ the system settles into an equilibrium state

$$u = u_0[3K^2 - x^2]_+,$$
 where $u_0 = 1/2\sqrt{3}$, (29)

and u = 0 elsewhere. The original motivation in seeking such patterns was to find stable self-confined thermal states of plasma, *free of thermal flux on the boundary* [8]. This turns out to be impossible *unless some explicit spatial dependence* is introduced. In a biological context, spatial dependence represents a patch of a fully protected domain surrounded by a completely hostile environment. Using the freedom to choose K, A(0), and B(0), we construct sub- and supersolutions which "trap" the actual initial datum and "force" the pattern to settle into (29).

2. Let l = 2. *K* is now a *control parameter*. For K = 1Eq. (27) may be written $u_t = (\partial - x)(\partial + x)u^2$ and thus $u_t = e^{-x^2/2} [e^{-x^2}(e^{x^2/2}u^2)_x]_x.$ (30)

We now generalize the problem and consider

$$u_t = (u^n)_{xx} + q(x)u^n.$$
 (31)

Observe that if $\theta(x)$ is the ground state

$$\theta''(x) + q(x)\theta(x) = 0, \qquad \theta(x) > 0, \qquad (32)$$

then Eq. (31) may be rewritten as

$$u_t = \frac{1}{\theta} \left[\theta^2 \left(\frac{u^n}{\theta} \right)_x \right]_x.$$
(33)

We now define new variables via

$$v = u/\theta^{1/n}$$
 and $z = \int dx/\theta^2(x)$, (34)

and the problem takes the form $(\rho[z(x)] = \theta^{3+1/n})$

$$\rho(z)\boldsymbol{v}_t = (\boldsymbol{v}^n)_{zz}.$$
(35)

To understand the impact of $\rho(z)$ we define

$$M = \int \rho(z) dz = \int \theta^{1+1/n} dx.$$
 (36)

If $M < \infty$ then, as shown in [5], the diffusion process undergoes a fundamental change for now in 1D or 2D (but not in 3D) as $t \uparrow \infty, v \rightarrow v_0 = E(0)/M > 0$, where

$$E(0) \equiv \int \rho(z)v(z,0) dz = \int \theta(x)u(x,0) dx.$$

Note that we have implicitly assumed that for a given q(x) there is a unique $\theta(x) > 0$. When q(x) begets multiple θ solutions, the associated M [see (36)] are unbounded, so that the resulting equilibria of (35) are trivial. If $q(x) = K^2 - x^2$ then, for K = 1, $\theta(x) = \exp[-x^2/2]$ and $M < \infty$. Now $v = u/\sqrt{\theta} \rightarrow v_0$, i.e.,

$$u(x,t) \to v_0 \exp[-x^2/2n].$$
 (37)

For $K \neq 1$ the eigenstates $\theta_m(x)$ are possible for $K^2 = 2m + 1$ and $\theta_m(x) = H_m \exp[-x^2/2]$, where H_m are the Hermite polynomials which for m > 1 admit negative values and are thus unacceptable. Thus for $K \neq 1$ all initial data either decay or blow up. If q(x) decays algebraically things are more delicate for, say,

$$q(x) = 2\alpha \frac{[A - 2(1 + \alpha)x^2]}{(A + x^2)^2} \Rightarrow \theta = \frac{1}{(A + x^2)^{\alpha}},$$

unless $2\alpha \ge n < (n + 1)$, *M* is unbounded, and absorption is too weak to arrest the diffusive spread.

Radial symmetry: We consider

$$u_t = r^{-N} \frac{\partial}{\partial r} \left(r^N \frac{\partial u^2}{\partial r} \right) + q(r)u^2, \qquad N = 2, 3.$$
(38)

Let q(r) be given with $\theta(r)$ being the ground equilibrium solution of (38) and $v = u/\sqrt{\theta}$. Then in 2D

$$\theta^{3/2} \boldsymbol{v}_t = r^{-1} \frac{\partial}{\partial \tau} \left(r \theta^2 \frac{\partial \boldsymbol{v}^2}{\partial \tau} \right). \tag{39}$$

Using $z = \int_0^\tau dr/r\theta^2$ we remap Eq. (39) into Eq. (35), $z \in \mathbb{R}^1$, with the total mass now given as $M = \int_0^\infty r\theta^{3/2} dr$. Using our study case, we find planar equilibrium for $q(r) = 2 - r^2$ with the ground states being given, again, via $\theta(r) = \exp[-r^2/2]$. Numerical experiments, like the one in Fig. 2, confirm that for $K^2 < 2$ ($K^2 > 2$) all initial conditions decay (blow up). We also find that all *elliptic equilibria* for $q(x, y) = K^2 - (x^2 + by^2)$ with



FIG. 2. The equilibrium pulse which emerges for $q(r) = 2 - r^2$ from the initial datum: $u(x, y, t = 0) = \cos(\pi x/2) \cos(\pi y/2)$ given over the $(|x|, |y|) \le 1$ square. The maximal amplitude of the pulse is ~0.3 and its diameter ~10.

 $K^2 = 1 + b$ and $\theta(x, y) = \exp[-(x^2 + by^2)/2]$ as the ground state are numerically unstable unless b = 1.

In 3D diffusion undergoes a fundamental change, for now zero is not in the spectrum of the Laplace operator and $E(t) \downarrow 0$ even when *M* is finite. Thus v_0 vanishes [9] and all 3D stable equilibria of Eq. (38) are trivial.

In summary.—The reaction-diffusion process given by Eq. (2) was mapped into a well understood purely diffusive process which made it possible to unmask its universal features.

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