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Localization in Lattice and Continuum Models of Reinforced Random Walks

K. J. PAINTER
Department of Mathematics, Heriot-Watt University
Riccarton, Edinburgh EH14 4AS, Scotland, U.K.
painter@ma.hw.ac.uk

D. HORSTMANN
Mathematisches Institut der Universität zu Köln
Weyertal 86-90, D-50931 Köln, Germany
dhorst@mi.uni-koeln.de

H. G. OTHMER
School of Mathematics, University of Minnesota
Minneapolis, MN 55455, U.S.A.
othmer@math.umn.edu

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Abstract—We study the singular limit of a class of reinforced random walks on a lattice for which a complete analysis of the existence and stability of solutions is possible. We show that at a sufficiently high total density, the global minimizer of a lattice 'energy' or Lyapunov functional corresponds to aggregation at one site. At lower values of the density the stable localized solution coexists with a stable spatially-uniform solution. Similar results apply in the continuum limit, where the singular limit leads to a nonlinear diffusion equation. Numerical simulations of the lattice walk show a complicated coarsening process leading to the final aggregation.

Keywords—Aggregation, Lattice walks, Forward-backward parabolic, Coarsening process.

1. INTRODUCTION

Movement is a fundamental process for almost all biological organisms, ranging from the single cell level to the population level, and two major classes of models are widely used to describe movement. In space-jump processes, movement is via a sequence of position jumps at random time intervals, while in velocity-jump processes movement consists of straight-line motion punctuated by random changes in velocity at random times [1]. Space jump processes include the familiar

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lattice walks, and the simplest nearest-neighbor version in one space dimension leads to the master equation

$$\frac{dp_i}{dt} = \hat{\mathcal{T}}_{i-1}p_{i-1} - 2\hat{\mathcal{T}}_i p_i + \hat{\mathcal{T}}_{i+1}p_{i+1} \tag{1}$$

for the number density at site i. When the transition rates $\hat{\mathcal{T}}_i$ are constant this leads to the diffusion equation for the continuum density $p(x,t)$. A general theory of random walks with time- and space-independent waiting times and jump kernels leads to a renewal equation, and from this both the above master equation description and the continuum (PDE) limits can be derived by special choices of the kernels [1].

However, in many biological applications the transition rates depend on external fields or the number density, and the external fields may be altered by signals produced by the walkers. Here the theory is not as well developed and analysis proceeds from more specialized descriptions, because a general formulation that leads to either discrete or continuum limits is not available as yet.

One tractable generalization of walks with constant transition probabilities begins with a reinforced random walk, in which a walker on a one-dimensional lattice modifies the transition probability for succeeding passages [2]. One example of this arises in the motion of gliding bacteria such as *Myxococcus xanthus*, which glides along slime trails it produces [3]. We suppose that the transition rates depend on the density of a control substance w that evolves according to

$$\frac{dw_i}{dt} = \mathcal{F}(P, W), \tag{2}$$

where $P = (p_1, \dots, p_N)$ and $W = (w_1, \dots, w_N)$. Continuum limits of such walks were studied in [4], where it is shown that a variety of asymptotic states are possible, ranging from blowup in finite time to collapse to a uniform distribution. Here we assume that $\hat{\mathcal{T}}_i = \mathcal{T}_d(w_i)$, i.e., the sensing is strictly local, which corresponds to reinforcement at the lattice sites rather than the intervals between sites. Let h be the lattice spacing and assume there is a scaling $\mathcal{T}_d(W) = \lambda\mathcal{T}_c(W/h)$ such that $\lim_{h\to 0,\lambda\to\infty} \lambda h^2 = D$; then the diffusion limit of (1) is

$$\frac{\partial p}{\partial t} = D\frac{\partial^2}{\partial x^2}\left(\mathcal{T}_c(w)p\right). \tag{3}$$

Whether this limit is legitimate for solutions that are not smooth was not addressed in [4]. For $\mathcal{T}_d(u) = \nu K_d^2/(K_d^2 + u^2)$ and $\mathcal{F} = (p - w)/\epsilon$, numerical simulations indicate that there are only two possible asymptotic states, blowup in finite time (or more precisely, essentially complete localization at one lattice point, since mass conservation implies that no finite-dimensional approximation to (3) can blow up in finite time), or convergence to a spatially-uniform solution. An example of the former is shown in Figure 1a. It can be proven that the solution exists for a finite time for $\epsilon > 0$, and in Figure 1b we show how the computed numerical blowup time depends on ϵ. To understand why there appear to be at most two attractors for the evolution, we consider here the singular limit $\epsilon = 0$, and show that for any finite-dimensional approximation to (3) there are at most two stable steady states.

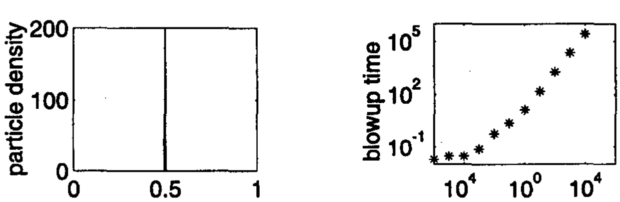

Figure 1. Left: The solution of (3) for $\epsilon = 1$, $K_d = 1$, and $\nu = 1$ on a lattice of 201 points. Right: The numerically-computed blowup time as a function of ϵ.

2. ANALYSIS OF THE SINGULAR MODEL

For the choice of $\mathcal{T}_d(p)$ used here, (1) becomes

$$\frac{dp_i}{dt} = \nu \frac{K_d^2\, p_{i-1}}{K_d^2 + p_{i-1}^2} - 2\nu \frac{K_d^2\, p_i}{K_d^2 + {p_i}^2} + \nu \frac{K_d^2\, p_{i+1}}{K_d^2 + p_{i+1}^2}. \tag{4}$$

By scaling p by K_d and t by ν we can assume that $K_d = 1$ and $\nu = 1$. Let Δ_d be the lattice Laplacian with zero Neumann boundary data; then (4) reads

$$\frac{dP}{dt} = \Delta_d(\mathcal{T}_d(P)P), \tag{5}$$

where $(\mathcal{T}_d(P)P)_i = \mathcal{T}_d(p_i)p_i$. The flows defined by (5) and by (3) (with homogeneous Neumann data) both conserve the total mass. We first focus on (5), and let Π be the simplex given by the intersection of the plane $\sum p_i = p_0$ with the nonnegative cone of R^N.

Steady states of (5) are such that $\mathcal{T}_d(P^s)P^s$ is proportional to the eigenfunction of Δ_d belonging to the zero eigenvalue, and therefore, $\mathcal{T}_d(p_i^s)p_i^s = \mu$ for $i = 1, \dots, N$ where μ is a constant. Since $\mathcal{T}_d(p)p$ is monotone increasing for $p \in [0, 1)$ and decreasing for $p \in (1, \infty)$, there are exactly two possible values for each p_i^s, p^*, and $p_* \equiv 1/p^*$, and $(\mathcal{T}_d(p)p)' < 0$ for one of these solutions. All admissible steady states can be characterized by the fractions ω_1 and $\omega_2 = 1 - \omega_1$ of sites at p^* and $1/p^*$. Admissible pairs (p, ω_1), $p \in [0, \infty)$, $\omega_1 = i/N$, $i = 1, \dots, N$ satisfy

$$\omega_1 p + \frac{\omega_2}{p} = \frac{p_0}{N} \equiv M_d \tag{6}$$

where M_d is the average number per site. The solutions are $p_1^+ = M_d$, which exists for all M_d, and at most $2(N-1)$ others given by

$$p_{\omega_1}^{\pm} = \frac{M_d \pm \sqrt{M_d^2 - 4\omega_1\omega_2}}{2\omega_1}. \tag{7}$$

Since $p_{\omega_1}^{\pm} = 1/p_{\omega_2}^{\mp}$, the admissible nonuniform solutions are obtained by pairing the branches as

$$\left(p_{\omega_1}^{\pm}, \frac{1}{p_{\omega_1}^{\pm}}\right) = \left(p_{\omega_1}^{\pm}, p_{\omega_2}^{\mp}\right). \tag{8}$$

The steady states are $P^s = (p_{\omega_1}^{\pm}, \dots, p_{\omega_1}^{\pm}, p_{\omega_2}^{\mp}, \dots, p_{\omega_2}^{\mp})$, to within a permutation. The steady states can be uniquely labeled as $(q^{\pm}, (N-q)^{\mp})$, where $q = \omega_1 N$ and $N - q = \omega_2 N$. $p_{\omega_1}^+ > 1$ for $q = 1, \dots, [N/2]$ and $p_{\omega_1}^- > p_{\omega_2}^+$ for $M_d \in (2\sqrt{\omega_1\omega_2}, 1)$. All branches of the type $(q^-, (N-q)^+)$ intersect the uniform solution $p_1^+ = M_d$ transversely at $M_d = 1$ as M_d varies.

The linearization of (5) leads to the equation

$$\frac{d\xi}{dt} = \Delta_d\left((\mathcal{T}_d(p^s)\,p^s)'\right)\xi, \tag{9}$$

and at the uniform steady state this reduces to

$$\frac{d\xi}{dt} = \left((\mathcal{T}_d(p^s)\,p^s)'\right)\Delta_d\xi. \tag{10}$$

It follows that the uniform steady state is stable as long as $(\mathcal{T}_d(p^s)p^s)' > 0$, i.e., for $M_d < 1$, and unstable to all modes otherwise. In the latter case, the shortest wavelengths grow most rapidly.

To illustrate how the existence and stability of solutions depends on the total density M_d, consider a three-site lattice; a complete analysis of stability is done later. In addition to the homogeneous solution, $p_i^s = M_d$, which is of type $(3^+, 0^-)$, we have the nonuniform steady states of type $(1^+, 2^-)$ and $(1^-, 2^+)$, as well as the permutations of these. The spatial variation in a type $(1^+, 2^-)$ solution is always of the form 'two low and one high', or LLH. The relative heights for $(1^-, 2^+)$ solutions interchange at $M_d = 1$, where the branches $p^-_{\omega_1}$ and $p^+_{\omega_2}$ intersect transversely. When $M_d \in (2\sqrt{2}/3, 1)$ the pattern is LLH, whereas when $M_d > 1$ it is HHL (cf. Figure 2). Similar remarks apply for more sites. For $N = 3$ the stability properties of the steady states can be established analytically by calculation of the eigenvalues of $\Delta_d((\mathcal{T}_d(P^s)P^s)')$ for each of steady states. The result is that the type $(1^+, 2^-)$ solution is linearly stable whenever it exists, whereas the type $(1^-, 2^+)$ is unstable wherever it exists. As noted, the homogeneous steady state is unstable for $M_d > 1$ and stable otherwise. Consequently, there is only one (to within permutations) stable nonuniform solution, and therefore, two locally-stable solutions whenever $M_d \in (2\sqrt{2}/3, 1)$.

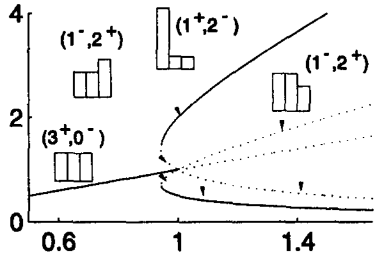

Figure 2. The complete steady-state bifurcation diagram showing p_i^s as a function of M_d for a three-site system.

For general N it is easier to determine stability by analyzing the critical points of the following 'energy' or Lyapunov functional. Let $\Phi(p) = \int \mathcal{T}_d(p)p\,dp$, define

$$\mathcal{E}_d(P(t)) = \alpha_d \sum_i \Phi(p_i(t)) = \frac{\alpha_d}{2} \sum_{i=1}^{N} \log\left(1 + p_i^2(t)\right), \tag{11}$$

and let $\bar{\mathcal{E}}_d$ be the restriction of $\mathcal{E}_d$ to Π. For a continuum domain $[0, L]$ the corresponding energy is

$$\mathcal{E}_c(p(t)) = \frac{\alpha_c}{2} \int_0^L \log\left(1 + p^2(x,t)\right)\,dx. \tag{12}$$

Both $\mathcal{E}_d$ and $\mathcal{E}_c$ are bounded below, and one can show that these energies are strictly nonincreasing along solutions of the corresponding evolution equation.

By construction, the critical points of $\bar{\mathcal{E}}_d$ in Π correspond to steady states on the lattice, and it is easy to see that there are no critical points of $\bar{\mathcal{E}}_d$ on $\partial\Pi$. Stability is determined by the eigenvalues of the Hessian of $\bar{\mathcal{E}}_d$ at P^s. Suppose that the solution has q sites with $p_i^s = p > 1$ and $N - q$ with $p_i^s = 1/p < 1$, and let $\alpha = \alpha_d\Phi''(p)$ and $\beta = \alpha_d\Phi''(1/p)$. Then the Hessian of $\bar{\mathcal{E}}_d$ is given by

$$\mathcal{H}_d = \begin{bmatrix} \alpha+\beta & \beta & \beta & \beta & \cdots & \beta \\ \beta & \alpha+\beta & \beta & & \cdots & \beta \\ \beta & \cdots & \cdots & & 2\beta & \beta \\ \beta & \beta & & \cdots & \beta & 2\beta \end{bmatrix}.$$

This is the same form as in a system of coupled springs with a nonconvex elastic energy function [5].

It follows that $q - 1$ eigenvalues of $\mathcal{E}$ are equal to α and $N - q - 1$ are equal to β: simply note that the corresponding eigenvectors can be chosen to have exactly one 1 and one -1 in the first $q - 1$ positions or in the last $N - q - 1$ positions. By hypothesis $p > 1$, therefore, $\alpha < 0$ and $\beta > 0$. Consequently, if $q > 1$ the corresponding critical point must either be a saddle point or a local maximum. The latter is precluded except at the uniform steady state.

One can show that $\alpha = (1 - p^2)/(1 + p^2)^2$, $\beta = -\alpha p^2$, and if we factor the characteristic equation as

$$P(\lambda) = (\lambda - \alpha)^{q-1}(\lambda - \beta)^{N-q-1}\left(\lambda^2 - a_1\lambda + a_2\right),$$

it follows that

$$a_1 = -\alpha\left(Np^2 - 1\right), \qquad a_2 = (N - q - 1) - (q - 1)p^2.$$

Since $p > 1$ we have that $a_1 > 0$, and $a_2 > 0$ for $q = 1$, and therefore there are no further negative eigenvalues. We summarize the results as follows.

1. For any M_d there are at most two asymptotically stable steady states, one of which is constant.
2. The uniform solution is a local minimum (maximum) of $\bar{\mathcal{E}}_d$ when $M_d < 1$ ($M_d > 1$).
3. When it exists, the single peak solution is a local minimizer of $\bar{\mathcal{E}}_d$. When $M_d > 1$ it is the only minimizer and hence attracts the flow for almost all initial data.

These results show that in any finite-dimensional lattice the only stable solutions are the single-peak solution and possibly the uniform solution, and they suggest why one expects either a blowup, as in Figure 1a, or convergence to a uniform solution for the PDE. They also suggest how to prove that the conclusions apply to (3) as well. It should be noted that none of the general conclusions depend on the specific form of $T(p)$, as long as the conditions on the sign of $(T(p)p)'$ are satisfied. The conditions for stability of the uniform solution are also given in [6], as well as a partial analysis of stability of nonuniform solutions by direct study of the spectrum of the Jacobian.

3. GLOBAL EVOLUTION ON THE LATTICE

When $M_d > 1$ the energy analysis shows that the single peak solution attracts almost all initial data. However, because there are many saddle points when the lattice has many sites, the evolution of general initial data may be complicated because the saddles all have at least one stable direction and solutions may be transiently attracted to them. This is demonstrated in Figure 3 for one simulation in which $M_d > 1$. Although many peaks develop initially, a period of coarsening ensues during which the number of peaks decreases, until only one peak remains. When there are two stable states, the outcome for general initial data is difficult to predict. If $p(x, 0) < 1$ for all x the diffusion coefficient is positive everywhere, the nonlinear diffusion equation behaves like a linear diffusion equation, and one expects evolution to the homogeneous solution: this is proven in [7]. However, when the initial particle density *locally* exceeds 1 at some points one expects that the density will grow at these points, at least initially, but the solution may still converge to the uniform state. A more complete analysis of this phenomenon is given in [7].

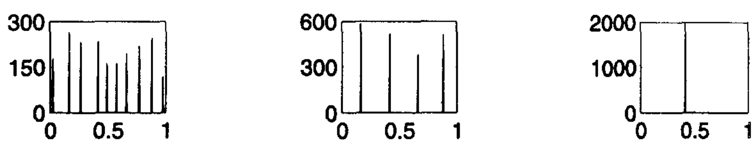

Figure 3. The coarsening process on a lattice with 201 sites at times 5, 50, and 5000. $u(x, 0) = 10.0 - 0.1\cos(\pi x)$ on $[0, 1]$.

4. THE CONTINUUM PROBLEM

In the foregoing, the solution is defined on the lattice, but the transition to the continuum problem requires the dual viewpoint, in which the particles are distributed on an interval of length $h = L/N$ centered at the lattice site. This leads to a new p_N that is the sum of a finite number of step functions of height $p^+_{\omega_1}/h$ and $1/hp^+_{\omega_1}$. The only stable nonconstant solution is a single-peak solution, and as $N \to \infty$, $\omega_1 = 1/N \to 0$, $p^+_{\omega_1} \to \infty$, and $1/p^+_{\omega_1} \to 0$, $\lim_{N\to\infty} p_N$ becomes concentrated at a point $a \in I$. More precisely, one can show that p_N defines a δ-sequence in $H^{-1}(I)$, the dual of the Sobolev space $H^1(I)$, and p_N converges weakly in $H^{-1}(I)$ to the Dirac functional defined by $\delta_a(u) = u(a)$ for all $u \in H^1(I)$. The precise sense in which the limiting distribution provides a solution of the continuum evolution equation is addressed in [7]. Here we will consider two continuum regularizations of (3). First, we add a term of Cahn-Hilliard type to $\mathcal{E}_c$ that increases the energy in proportion to the spatial variation of p. Define

$$\mathcal{E}_c^\gamma = \int_I \frac{\gamma}{2}|p'|^2 + \frac{\alpha_c}{2}\log\left(1+p^2\right)\, dx, \tag{13}$$

where $\gamma > 0$ and $p \in \mathcal{D}_0 \subset H^1(I)$, the set of functions of L^1-norm equal to $M|I|$. The existence of a minimizer of $\mathcal{E}_c^\gamma$ follows from the direct method of the calculus of variations, and by using arguments similar to those in [8], we can show that the global minimizer is either a single-peaked or a monotonic solution, depending on whether the solution is symmetric about the midpoint. Furthermore, as $\gamma \to 0$ we again obtain the Dirac distribution as the solution that minimizes $\mathcal{E}_c^0$ [7]. The evolution equation for this regularization is

$$\frac{\partial p}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\mathcal{T}_c(p)p - \gamma\frac{\partial^2 p}{\partial x^2}\right), \tag{14}$$

which is obtained by assuming that the driving potential for movement is the functional derivative of (13). This equation with zero flux conditions has global solutions in $H^1(I)$ for $\gamma > 0$ [9], and in Figure 4, we show an example of the evolution of initial data that would lead to a completely-localized solution when $\gamma = 0$. An alternate regularization is to add a small random component αp_{xx} to (3), both for $\epsilon = 0$ and $\epsilon > 0$. The first of these produces a van der Waals potential. Examples of the resulting time evolutions are shown in Figure 4. As the response time of the control species increases ($\epsilon \uparrow$), the individual peaks coalesce into a square wave.

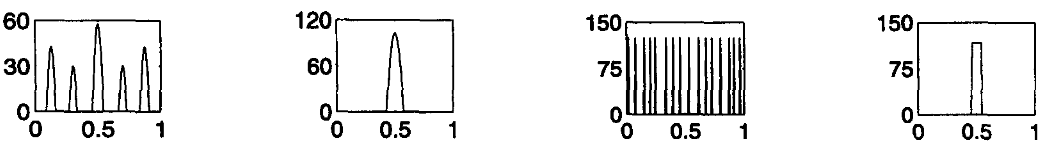

Figure 4. The evolution of solutions of (14) with $\gamma = 10^{-6}$ at times 10 (left) and 100 (centre-left). The steady-state solution of (3) for $(\alpha, \epsilon) = (10^{-4}, 0)$ (centre-right) and $(10^{-4}, 10)$ (right). We use an initial distribution $p(x, 0) = 10 - 0.1\cos(2\pi x)$, $w(x, 0) = 10.0$.

5. DISCUSSION

We have focused on the one-dimensional problem, but it is clear from the analysis that the lattice results are independent of the spatial dimension and do not require that the underlying connectivity of the sites correspond to a regular lattice; the only requirement is that the Laplacian for the graph have a simple zero eigenvalue, which is true if the graph is strongly-connected. The extension to higher space dimensions is not so direct in the continuum problem: for instance, the phase plane analysis that proves monotonicity of the minimizer cannot be carried over. In addition, the changes in the number and type of steady-state solutions as the parameter α, γ, and ϵ vary remains to be investigated.

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