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A lattice-model representation of continuous-time random walks

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Abstract

We report some ideas for constructing lattice models (LMs) as a discrete approach to the reaction-dispersal (RD) or reaction-random walks (RRW) models. The analysis of a rather general class of Markovian and non-Markovian processes, from the point of view of their wavefront solutions, let us show that in some regimes their macroscopic dynamics (front speed) turns out to be different from that by classical reaction–diffusion equations, which are often used as a mean-field approximation to the problem. So, the convenience of a more general framework as that given by the continuous-time random walks (CTRW) is claimed. Here we use LMs as a numerical approach in order to support that idea, while in previous works our discussion was restricted to analytical models. For the two specific cases studied here, we derive and analyze the mean-field expressions for our LMs. As a result, we are able to provide some links between the numerical and analytical approaches studied.

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1. Introduction

Reaction-dispersal (RD) models have been a vastly explored field in the last decades and nowadays their applications cover practically all the areas of science. One of the most general ways to define such processes is the mesoscopic description supplied by the continuous-time random walks (CTRW) [1] with reactions, where the equation

$$P(x,t) = \int_0^t \mathrm{d}t'\,\varphi(t') \int_R \mathrm{d}x'\,\Phi(x')P(x-x',t-t') + \int_0^t \mathrm{d}t'\,\phi(t')\mathcal{R}[P(x,t-t')] \tag{1}$$

describes the evolution of the density of particles $P(x,t)$ at point x and at time t. $\varphi(t)$ and $\Phi(x)$ are the waiting-time and length distribution functions, respectively, and $\phi(t) \equiv 1 - \int_0^t \varphi(t')\,\mathrm{d}t'$

denotes the probability that individuals stay at least a time t at their position before a new jump. Finally, the operator $\mathcal{R}[\cdot]$ accounts for the creation and/or annihilation of individuals (it is, reaction kinetics). For Markovian random walks (Brownian motion) in the diffusive limit, one has $\varphi(t) = \tau^{-1}\,\mathrm{e}^{-\tau t}$ and $\mathcal{F}[\Phi(x)] = \int_{-\infty}^{\infty} \mathrm{e}^{px}\,\Phi(x)\,\mathrm{d}x \simeq 1 + p^2$ (where $\mathcal{F}(\cdot)$ is the bilateral Fourier transform, so $\Phi(x)$ can be seen as a first-order expansion of the Gaussian distribution for short jumps). It has been shown that in this case [2] the integro-difference equation (1) turns into

$$\partial_t P = \partial_x^2 P + \mathcal{R}[P], \tag{2}$$

the classical reaction–diffusion (Fisher) equation. This means that despite (2) is a widely known and commonly used equation which has given excellent results in the past, it just represents a limit of the more general process (1). Indeed, it is well known that the classical equation involves some fundamental problems from the microscopical point of view, as the fact that a small fraction of the individuals are supposed to move with an infinite speed [3, 4]. It also yields that the speed of the wavefront solutions derived from (2) cannot be realistic in the fast reaction limit where the process is diffusion-controlled [5].

A different scenario within this field arises when one has to deal with discrete RD. For many practical applications [6–8], it has been claimed that a discrete-in-space but continuous-in-time model (which is usually obtained by discretizing the diffusion term in the classical equation) is able to predict some results that continuous models cannot, and actually some interesting phenomena arise from those models (probably the best known is the propagation failure [9, 10]). Finally, models which are explicitly discrete in time and space have received less attention (as an exception, we cite the work in [11] and some references therein).

Our goal here is to focus on lattice models (LMs) implementing reaction-random walks (RRW) as a discrete individual-scale approach to RD models, and their connection to the mesoscopic continuous models mentioned above (by means of a mean-field description) in order to establish a connection between the numerical and analytical approaches. This may help us to understand the microscopic mechanisms behind the CTRW approach, since the results obtained from this analytical approach are often difficult to understand from a phenomenological point of view. This idea of linking the numerical and analytical approaches is not new, and has been explored before from many different points of view. We cite as an example the very recent work by Simpson *et al* [12]. In that paper, the authors claim that the comparison between the continuum models (population-scale) and LMs (individual-scale) may substantially increase our knowledge of invasion RD processes, and they provide some arguments to show the interest of that approach on the field of cellular invasions.

As far as we know, most of the previously proposed LMs (or, similarly, cellular automatas) for RD systems [13–16, 19] fit one of the two following schemes: (i) the rules which determine the individual behavior of the particles are taken from the direct discretization of equation (2) or some extended form of it, or (ii) these rules are determined from microscopical arguments, but they are chosen in such a way that equation (2) (or some extended form) is the mean-field description of the model. So, equation (2) is always the main basis for these microscopical models, despite we have mentioned above that this equation has some important limitations. In this paper, we claim that a more general expression as that in (1) is many times required in order to implement LM models and give a correct mean-field approximation for them.

In the following, we shall describe the general algorithm, and then the corresponding mean-field description, for our one-component LM's modeling RRW, which turns out to reproduce the macroscopic dynamics predicted analytically from the general framework in (1), but not that from (2).

We identify and compare the macroscopic dynamics of our systems by studying the wavefront solutions arising from each particular case, and comparing the corresponding propagation speeds found both numerically and analytically. The analytical derivation of those speeds can be achieved from the Hamilton–Jacobi approach, as has been shown in some of our recent works [2, 20].

2. General model

For convenience, we consider one-dimensional models and assume (i) that the transport process is not affected by interactions among individuals (so each individual moves freely and independently of the other ones) and (ii) multiparticle models as defined in [14–16], with an arbitrarily large number of individuals N allowed at each node to avoid undesirable noise (although this is not a very realistic assumption, it allows us to focus exclusively on the aspects we want to show here; other effects like finite occupancy at the nodes will be explored in further studies).

In some previous approaches, the procedure used was: the transport rules were applied to all of the individuals or nodes and after that reaction rules were applied to all of them. These could be called as 'diffusion-preceding-reaction' models and they obviously yield a process discrete in time and space, in the sense that all the individuals move or react together exactly at the same time. Nevertheless, real RRW systems where time can be considered as discrete are not very usual. A more appropriate choice (and commonly used too) to mimic a continuous-in-time process is to consider transport rules applied to a randomly-chosen individual and then reaction rules applied to another individual (again randomly chosen). That is what we call 'diffusion and reaction taking turns'. There still exists many other ways to implement diffusion and reaction, but those mentioned are probably the most common and simplest.

In our case, according to the assumption of multiparticle models made above, we express our model in terms of the density of individuals $P(x,t) = N(x,t)/N_{\max}$, where $N_{\max}$ is the maximum number of individuals allowed at each node (as mentioned above, we consider here $N_{\max} \to \infty$). Then, we propose the following evolution procedure: transport rules are applied to a fraction f of the density of individuals at every node, and then reaction rules are applied to a fraction f of the density of individuals resulting after the random walk process at every node. So, for $f = 1$ we recover the 'diffusion-preceding-reaction' case, and in the mesoscopic limit $f \to 0$ our model must be equivalent to the 'diffusion and reaction taking turns' case (we have proved this numerically and the agreement found was excellent, as shown below). We also stress that, in comparison with the latter, our approach is less time-consuming and allows us to identify easily the characteristic evolution time of the model as the time for which $1/f$ cycles have been carried out.

In general, our LM approach is not very different to many previous numerical models for RD systems based on the fractional-step method, as those in the works by Muzzio and Ottino [17, 18]. Let us first show for simplicity the case where memory effects are absent in our model. For that case, the evolution algorithm for our LM, with the combined effect of transport rules and the reaction process $\mathcal{R}[\cdot]$, can be written by the mean-field description

$$P(x,t+f\Delta t) = (1-f)P(x,t) + f\sum_{i\neq 0}\gamma_i P(x+i,t) + \mathcal{R}\left[f\left((1-f)P(x,t) + f\sum_{i\neq 0}\gamma_i P(x+i,t)\right)\right], \tag{3}$$

where the sum in i is over all the nodes of the system (excluding the node at position x), and the values of the coefficients γ_i determine the transport rules governing the RRW process (they can be understood as a discrete dispersal kernel).

The meaning of equation (3), which is the mathematical transcription of our LM algorithms, is the following: the migration term accounts for the contributions from every point in the lattice (which are weighted according to the probabilities γ_i) at the immediately previous time step, while the reaction term is just the $\mathcal{R}$ function applied to a fraction f of the density resulting from the migration term.

Now, if we also consider memory effects in the model a new sum (over all the previous times) appears in the evolution equation, and so the resulting expression has the form

$$P(x,t+f\Delta t) = (1-f)P(x,t) + f\sum_{j=0}^{t/f\Delta t}\theta_j\sum_{i\neq 0}\gamma_i P(x+i,t-jf\Delta t) + \mathcal{R}\left[f\left((1-f)P(x,t) + f\sum_{j=0}^{t/f\Delta t}\theta_j\sum_{i\neq 0}\gamma_i P(x+i,t-jf\Delta t)\right)\right], \tag{4}$$

where the coefficients θ_j measure the memory kernel, in analogy with the coefficients γ_i for the spatial coordinate. In this realization, and also in the whole discussion given below, we are considering implicitly that a whole simulation step in our LMs lasts a time Δt and involves $1/f$ cycles, according to the definition of f given above.

It is evident that (4) tries to reproduce approximately the form of (1) for a discrete time and space (this equivalence is studied in the appendix). As mentioned above, in our model we are assuming an infinite occupancy in the nodes of the system, and that is why we can write the corresponding expressions (3) and (4) in terms of the density function P. In case we wanted to consider a finite occupancy of the nodes, then our algorithm should be changed by introducing $\mathrm{nint}(\theta_j\gamma_i P(x+i,t-jf\Delta t))$ instead of the expression $\theta_j\gamma_i P(x+i,t-jf\Delta t)$, where nint( ) is a function that determines 'the nearest integer number'. So, we would ensure that the number of individuals migrating at any time is an integer number. Another important aspect of our LMs, which has not received much attention in previous works, is the fact that $\mathcal{R}[\cdot]$ is explicitly applied to the scenario resulting after transport rules, because it is impossible in practice to implement in the lattice both processes simultaneously.

3. Markovian RRW

Let us now explore a very simple case resulting from (3) in which a fraction f of the individuals perform an isotropic random walk (they can move to each one of the nearest neighbors with probability $1/2$) and a fraction f of the resulting density of individuals reacts with a reaction term of the Fisher–Kolmogorov–Petrovskii–Piskunov (FKPP) type, i.e., $\mathcal{R}_F[P] = aP(1-P)$. It is easy to see that the general mean-field equation for this specific case takes the form

$$P(x,t+f\Delta t) = (1-f)P(x,t) + f\xi + \mathcal{R}_F[f((1-f)P(x,t) + f\xi)], \tag{5}$$

with

$$\xi \equiv \tfrac{1}{2}P(x+1,t) + \tfrac{1}{2}P(x-1,t). \tag{6}$$

We now find the speed of the wavefront solutions that would arise from this expression using the Hamilton–Jacobi procedure. The starting point is to consider the hyperbolic scaling $x \to x/\varepsilon, t \to t/\varepsilon$ and to represent the rescaled density $P^\varepsilon(x,t) = P(x/\varepsilon, t/\varepsilon)$ in terms of the action functional $G^\varepsilon(x,t)$ as $P^\varepsilon(x,t) = \exp[-G^\varepsilon(x,t)/\varepsilon]$. Introducing the hyperbolic

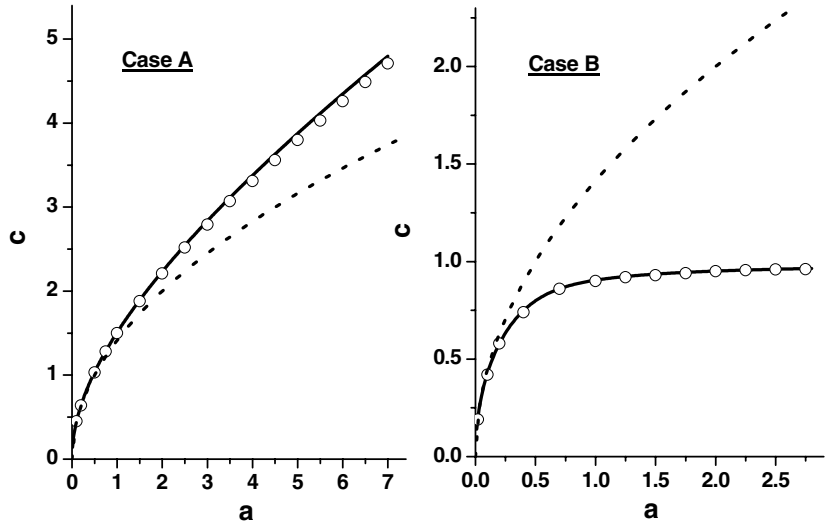

Figure 1. Wavefront speed values as a function of the FKPP reaction rate a for (A) the Markovian and (B) the non-Markovian RRWs analyzed in the text. In both cases, we compare the speed found from the numerical implementation of the CA models presented here (circles), the results obtained from the mean-field description together with the Hamilton–Jacobi techniques (solid lines) and the prediction from the classical RD $c = \sqrt{2a}$ (dotted lines). For CA implementation, we used $\Delta t = 1$ and $f = 0.01$ as a good approximation to the limit $f \to 0$ (see figure 2).

scaling and the action functional into (5) and taking the asymptotic limit $\varepsilon \to 0$ one finds that the front speed is given by

$$c = \min_H \frac{H}{p} = \min_H \frac{H}{\cosh^{-1}\left[\frac{1}{f}\left(\frac{e^{Hf\Delta t}}{1+af} - 1\right) + 1\right]}, \tag{7}$$

where $H = -\partial_t G$ and $p = \partial_x G$ are the Hamiltonian and the generalized momentum, respectively, and $G(x,t) = \lim_{\varepsilon\to 0} G^{\varepsilon}(x,t)$. Taking the mesoscopic limit $f \to 0$ up to first order, equation (7) becomes

$$c = \min_H \frac{H}{\cosh^{-1}(H\Delta t - a + 1)}. \tag{8}$$

The speed given in equation (8) can be compared with that from the CTRW framework computed directly from equation (1). For Markovian RRW, one considers $\Phi(x) = \frac{1}{2}[\delta(x+1) + \delta(x-1)]$ and $\varphi(t) = \tau^{-1} e^{-\tau t}$ (so, the remaining individuals at a certain position jump with a constant probability $\tau^{-1} e^{-\tau}$ at any time). Now, using the Hamilton–Jacobi techniques [5, 20] in equation (1), one finds exactly the form in (8) for the front speed (where the identity $\tau \equiv \Delta t$ holds). In figure 1(A), we compare this result (solid line) with the front speed obtained from our LM model governed by the rules given above (circles) with $f = 0.01$ and using step-like initial conditions. We observe that there exists a perfect agreement between these simulations and our analytical predictions given in equation (8). In figure 1(A) we also plot (dotted line) the front speed from the classical equation (2), i.e., Fisher's speed $c = \sqrt{2a}$, which always underestimates the results in the region $a > 1$ (it is, in the diffusion-controlled regime).

Likewise, we note that the expressions displayed could be easily generalized just by redefining ξ formally as

$$\xi \equiv \sum_i \gamma_i P(x+i,t). \tag{9}$$

Therefore, any jump length distribution function could be considered instead of isotropic random walk rules, and so the cases reported here can be in practice applied to a wide range of situations.

4. Non-Markovian RRW

Next, we examine the case in which any individual performs an isotropic random walk after a constant waiting-time Δt (so according to equation (4) we consider $\theta_j = 1$ for $j = 1/f$ and $\theta_j = 0$ for any other value of j), while the reaction term is again of FKPP type. In this case, every individual can only move after it has stayed at the same position for a fixed time, but we stress that it does not mean that all the individuals move together at discrete times $\Delta t, 2\Delta t, \ldots$. What we really have is a process where a fraction f of the individuals present at $t = 0$ jump at times $t = f\Delta t, \Delta t + f\Delta t, 2\Delta t + f\Delta t, \ldots$ another fraction f jump at times $t = 2f\Delta t, \Delta t + 2f\Delta t, \ldots$ and so on, while all the new individuals appeared from the reaction process jump for the first time at time Δt after they are created. So, we consider the effect of a latent time for the particles after moving or being created.

Now we define $\nu(x,t)$ as the fraction of individuals arrived or created at the node x at the nth cycle of a simulation step over the total number of individuals present at the same position after the whole simulation step has finished (i.e., after the $1/f$ cycles have been carried out or, equivalently, after a time Δt). This can be written as

$$\nu(x, t + nf\Delta t) = \frac{\phi + \mathcal{R}_F\{f\phi + fP[x, t + (n-1)f\Delta t] - \nu[x, t + (nf-1)\Delta t]P(x,t)\}}{P(x, t+\Delta t)}, \tag{10}$$

with

$$\phi \equiv \tfrac{1}{2}\nu[x+1, t + (nf-1)\Delta t]P(x+1,t) + \tfrac{1}{2}\nu[x-1, t + (nf-1)\Delta t]P(x-1,t). \tag{11}$$

In equation (10), ϕ represents the particles moving to x at the nth cycle of the simulation step (it is, a time $nf\Delta t$ after the simulation step began), and the function $\mathcal{R}_F$ is applied to a fraction f of those particles ϕ arriving at x, plus those who were there in the previous cycle ($P[x, t + (n-1)f\Delta t]$), less those particles that have left the position x at that cycle ($\nu[x, t + (nf-1)\Delta t]P(x,t)$).

Note that in this specific case is necessary to introduce the function $\nu(x,t)$ because the reaction process is density dependent. At any successive cycle n, the density of individuals at x increases and thus $\nu(x,t)$ is not a constant function, because the fraction of new individuals created increases as n does. However, as we are considering wavefront stationary solutions, we expect that after a transient regime the behavior of $\nu(x,t)$ is stationary too, and so we can assume that $\nu(x,t) \simeq \nu(x-\Delta x, t) \simeq \nu(x+\Delta x, t) \simeq \nu(x, t+\Delta t)$. Thus, we assume that the function ν only depends explicitly on n and so we can redefine it as $\nu_n \equiv \nu(x, t + nf\Delta t)$. This assumption is supported by the numerical simulations we have performed using our LMs (not shown here for the sake of simplicity). In those simulations, we have found that in the leading edge of the front (which is the region responsible for the front speed in the case of pulled wavefronts [21]) the function ν, for any fixed value of n, is approximately constant in x during a finite time (after that regime, the saturation effects due to the nonlinear part of the FKPP reaction term appear and the behavior becomes more complex).

As we are specially interested in the behavior near the leading edge of the front, we can use the assumption mentioned for ν and consider the linearized form of the FKPP reaction term $\mathcal{R}_F = aP$, as usual in the analysis of traveling fronts [21]. By doing so, we can write (10) for ν_n and ν_{n+1} to get the relation

$$\frac{\nu_n}{\nu_{n+1}} = \frac{P(t+\Delta t) - \xi + af(\xi + P(x,t))}{(1+af)(P(x,t+\Delta t) - \xi)}, \tag{12}$$

where ξ has the form defined before in (6).

On the other hand, we can now easily write a recursive relation for the density of particles P as

$$\begin{aligned} P(x,t+\Delta t) &= (1+af)(P[x,t+(n-1)f\Delta t] + \nu_n\xi - \nu_n P(x,t)) \\ &= \cdots = (\xi - P(x,t)) \sum_{n=1}^{1/f} [(1+af)^n \nu_n] + (1+af)^{1/f} P(x,t), \end{aligned} \tag{13}$$

where the recurrence has been applied over n up to the $1/f$ cycles of a whole simulation step. So, we get a relation between $P(x,t+\Delta t)$ and $P(x,t)$ that apparently depends on the parameter n, though this dependence will vanish in the limit $f \to 0$, as we show below.

Using the normalization condition $\sum_{n=1}^{1/f} \nu_n = 1$ (at time $t+\Delta t$ all of the particles present at time t must have already performed a new jump) in (12) we find an explicit expression for ν_n, and introducing it into (13) leads, in the mesoscopic limit $f \to 0$ up to first order, to the equation

$$\begin{aligned} P(x,t+\Delta t) = {} & \frac{1 - \exp\left(\frac{-a(\xi - P(x,t))}{P(t+\Delta t)}\right)}{1 - \exp\left(-a + \frac{-a(\xi - P(x,t))}{P(t+\Delta t)}\right)} (P(x,t+\Delta t) - P(x,t)) \\ & + \exp(a) P(x,t). \end{aligned} \tag{14}$$

After some algebra, we can write this expression as

$$P(x,t+\Delta t) = \xi + a \frac{P(x,t+\Delta t) - P(x,t)}{\ln\left[\frac{P(x,t+\Delta t)}{P(x,t)}\right]}, \tag{15}$$

which can be also inverted by the Lambert W-function $W(\cdot)$:

$$P(x,t+\Delta t) = \frac{-\xi}{1+a} W\left[\mathrm{e}^{\frac{aP(x,t)}{\xi}} P(x,t) \frac{1+a}{\xi} \right]. \tag{16}$$

The Hamilton–Jacobi procedure applied to (14) allows us to write the wavefront speed as

$$c = \min_H \frac{H}{\cosh^{-1}\left[\mathrm{e}^{H\Delta t}\left(1 - \frac{a}{H\Delta t}\right) + \frac{a}{H\Delta t}\right]}. \tag{17}$$

One can note that this expression is exactly the same as that predicted from (1) with

$$\begin{aligned} \Phi(x) &= \tfrac{1}{2}[\delta(x+1) + \delta(x-1)], \\ \varphi(t) &= \delta(t - \Delta t), \end{aligned} \tag{18}$$

as we found in [5]. In this case the jump speed of particles is $1/\Delta t$ and imposes an upper bound for the front speed, as it would be unrealistic that the front moves faster than the individuals. This fact may be seen in figure 1(*B*) where the solid curve saturates as the reaction rate increases in such a way that for an infinitely fast reaction ($a \to \infty$) one has $c \to 1$. This important physical property, which is absent for the Markovian RRW, was explored in deeper detail by us in [5].

The results in (17) agrees perfectly with the wavefront speed directly computed from our LM simulations (figure 1(*B*)) and, as expected, they are clearly different from the Fisher's

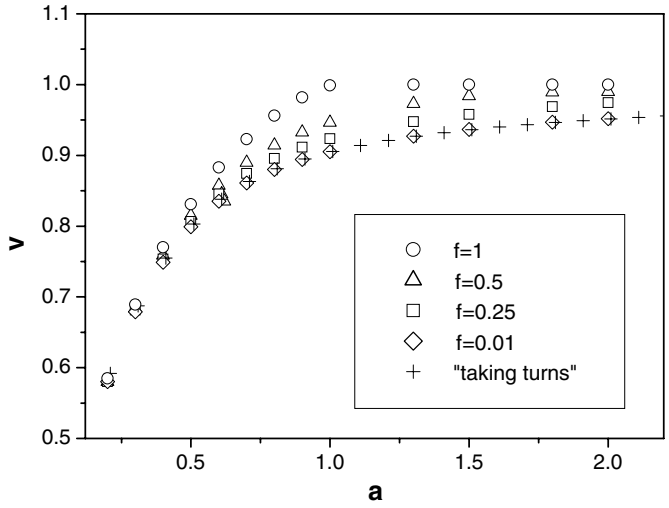

Figure 2. Front speed values for the non-Markovian RRW as a function of the reaction parameter a. Results are shown for the '*diffusion and reaction taking turns*' case in comparison with our CA approach for different values of f.

speed except in the limit $a \to 0$, where the transport rules play a minor role in the general dynamics of the system. So, it proves that the macroscopic dynamics of these RRW models can be properly described by the classical equation (2), but only within the slow reaction limit.

We have also performed for this non-Markovian case a comparison between our LMs and the 'diffusion and reaction taking turns' approach as defined above, since in the limit $f \to 0$ we expect that both models are equivalent. In figure 2, we show how the front speed found from our model changes as a function of the parameter f. We certainly observe that the agreement with the 'diffusion and reaction taking turns' case becomes excellent as f decreases, and there is no need to take f specially small (for $f = 0.01$, the deviation between both values is below 0.1% in all the range of a studied), so the running times of the simulations are still quite short.

4.1. On the meaning of expression (15)

In this subsection, we want to explore the meaning of equation (15), which is probably the most novel analytical result reported here.

First of all, let us note that if we expand $P(x, t + \Delta t)$ for $\Delta t \to 0$ (it is, $P(x, t + \Delta t) \simeq P(x, t) + \Delta t P_t(x, t) + \cdots$), then equation (15) up to zeroth order in Δt takes the form of a classical RRW

$$P(x, t + \Delta t) = \xi + aP(x, t), \tag{19}$$

which would become the classical reaction–diffusion equation by subtracting the term $-P(x, t)$ on every side of this expression and taking the space as continuous

$$P_t(x, t) = DP_{xx}(x, t) + rP(x, t), \tag{20}$$

where $D \equiv 1/(2\Delta t)$ and $r \equiv a/\Delta t$ would be defined as the diffusion coefficient and the reaction rate per unit time, respectively.

So, it is clear that when we remove from our non-Markovian case the role of the waiting time between jumps, the classical Markovian process is recovered. Now, let us compare equations (15) and (19), and observe that the general CTRW expression (1) together with (18) can be written in the very similar form

$$P(x, t + \Delta t) = \xi + r \int_0^{\Delta t} \mathrm{d}t' P(x, t + \Delta t - t'), \tag{21}$$

so now is easy to investigate (15) and (19) as particular cases of (21).

First, comparing (19) and (21) it is clear that the classical case assumes that $\int_0^{\Delta t} \mathrm{d}t' P(x, t + \Delta t - t') = \Delta t P(x, t)$. This means that $P(x, t)$ is assumed to remain constant during the integration interval. That integration interval represents the waiting time of the particles before a new jump, with $\Delta t \to 0$. So that the assumption $\int_0^{\Delta t} \mathrm{d}t' P(x, t + \Delta t - t') = \Delta t P(x, t)$ means that the density of particles remain constant (despite the growth process) during the waiting time, which can only be explained if we consider that the transport process is much faster (as a consequence that its characteristic time Δt tends to zero) than the reaction process.

In contrast with that, our non-Markovian case (15) compared to (21) leads to the identity

$$a \frac{P(x, t + \Delta t) - P(x, t)}{\ln\left[\frac{P(x,t+\Delta t)}{P(x,t)}\right]} = r \int_0^{\Delta t} \mathrm{d}t' P(x, t + \Delta t - t'). \tag{22}$$

If the classical case assumed that transport was very fast and so $P(x, t)$ remained constant in the integration interval from 0 to Δt, now we can think intuitively that for an arbitrary value of the waiting time Δt the reaction process could take place during that waiting interval. As a consequence, we could assume that $P(x, t)$ grows in that interval according to the given reaction function. Equation (15) was derived by assuming the linear form $\mathcal{R}_F = aP$, so we will consider that $P(x, t)$ grows exponentially with time while particles are waiting, i.e., $P(x, t) \sim C(x)\, \mathrm{e}^{C'(x)t}$ (where $C(x)$ and $C'(x)$ represent the dependences of $P(x, t)$ on x). It is straightforward to prove that if this exponential form is considered, then identity (22) holds.

All the previous discussion leads us to a clear understanding on the meaning of the mean-field expression (15), which may be seen as the generalization of the classical RRW expression to the case when the waiting time between jumps is non-vanishing. We remark that the results and the discussion given in this section are only valid for the case of linear reaction terms. Despite this limitation, our results are still of great interest for the study of pulled RD fronts with sufficiently steep initial conditions, where the leading edge of the fronts governs the dynamics of the system [21].

5. Conclusions

As a whole, we have shown that, despite equation (2) usually being taken as the starting-point for the formulation of LMs or other microscopical models of RRW, a more general RD process as that determined by (1) may be more adequate for many real situations. The main reason for this is that in the mesoscopic description the exact pattern of movement by the individuals is explicitly considered (by means of the probability functions $\Phi(x)$ and $\varphi(t)$) and so their microscopical properties are implemented with a higher accuracy. Moreover, one is allowed to consider a richer phenomenology, as memory effects or long-distance dispersal, which are necessary in the description of many biological and chemical processes.

In our previous works, we already supported this idea by means of continuous analytical models, but here we have faced the problem from the point of view of LM (individual-scale) approaches, and we have tried to link both perspectives by a mean-field description of the latter. These links may serve to give analytical support to LMs or they may be used to implement

numerical algorithms able to mimic the behavior of some given RRW or RD processes. We stress that our models are in general much faster than the numerical integration of the CTRW equations, so our approach can be also interesting from the point of view of optimization; actually, we used these LMs in order to provide numerical support to analytical results in some of our previous works.

Some mean-field expressions, which may be seen as a generalization of the classical RD and RRW equations, have been derived for rather general Markovian and non-Markovian processes. We consider that these new results, as expression (15) which has been explored in some detail here, are of general interest since they may describe a wide class of real RD processes. A good example of the experimental interest that our approaches may have is in the analysis of cellular invasions, as has been recently analyzed in [12]. Another important case we want to mention here is that of the viruses spreading through a media of host infective bacteria. In that case, when a virus adsorbs into a cell, then there is a waiting time it needs in order to reproduce itself, and after that the viruses generated get out of the bacteria and look for new hosts. As has been shown in previous works, the waiting time for viruses between successive infections can be well approximated as a constant waiting time Δt [22]. If the bacteria are homogeneously distributed, then every host can be seen as a node of a discrete lattice where the viruses spread. Thus, if experimental data on the dispersal pattern followed by viruses were available, it would be possible to apply our LM approach in order to know if it can fit the values of experimental front speeds better than the previous RD approaches used before [22, 23]. Equation (3) could also be generalized by incorporating a cutoff in the reaction function to deal with the effect of particle discreteness or finite number of particles [24]. The effect would be a shift on the front velocity.

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Appendix A

In this appendix, we will study analytically the regime where the equivalence between our general expression (4) and the CTRW formalism holds exactly.

First of all, let us note that the CTRW expression (1) admits an equivalent description in terms of a temporal derivative as [20]

$$\frac{\partial P(x,t)}{\partial t} = \int_0^t \mathrm{d}t' \alpha(t') \int_R \mathrm{d}x' \Phi(x')(P(x-x', t-t') - P(x,t)) + \mathcal{R}[P(x,t)], \tag{A.1}$$

with the function $\alpha(t)$ defined by its Laplace transform

$$\widehat{\alpha}(s) \equiv \int_0^\infty \mathrm{d}t \alpha(t)\, \mathrm{e}^{-st} = \frac{s\widehat{\varphi}(s)}{1-\widehat{\varphi}(s)}. \tag{A.2}$$

In the limit when the characteristic waiting time of the system is small, we can approximate $\widehat{\varphi}(s)$ by the Taylor expansion $\widehat{\varphi}(s) \approx 1 - \Delta t s$, so that $\alpha(t) \approx \varphi(t)/\tau$. As a result, equation (A.1) turns into

$$\tau \frac{\partial P(x,t)}{\partial t} = \int_0^t \mathrm{d}t' \varphi(t') \int_R \mathrm{d}x' \Phi(x') P(x-x', t-t') - P(x,t) + \tau \mathcal{R}[P(x,t)]. \tag{A.3}$$

On the other side, we take expression (4) and study the case $f \to 0$ required for the continuous-in-time limit, so we neglect the terms of order $\mathcal{O}(f^2)$ that appear in the reaction

term. In addition, we will consider a linear reaction term $aP(x,t)$; all this leads us to

$$P(x,t+f\Delta t)-P(x,t)=f\left(\sum_{j=0}^{t/f\Delta t}\upsilon_j\sum_{i\neq 0}\gamma_i P(x+i,t-jf\Delta t)-P(x,t)+aP(x,t)\right). \tag{A.4}$$

Remember that, as said above, we choose the probabilities υ_j and γ_i as the discrete equivalents to the probability density functions $\varphi(t)$ and $\Phi(x)$. So that, the sums appearing in (A.4) will become integrals in the continuous limit and (A.4) will become the CTRW expression (A.3) just by redefining $f \equiv \mathrm{d}t/\tau$ and introducing again the reaction rate per unit time by $r \equiv a\tau$.

In consequence, we have proved that our LM in the continuous limit becomes a CTRW process, provided that (i) the characteristic waiting time of the individuals is small and (ii) the reaction term is linear. However, we note that for the case of wavefront solutions we have found numerically also a really good concordance between our model and the results from the CTRW even when these assumptions are relaxed.

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