Population Formulation of Adaptative Meso-evolution: Theory and Numerics

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Abstract. The population formalism of "adaptive evolution" has been developed in the last twenty years along ideas presented in other chapters in this volume. This mathematical formalism addresses the question of explaining how selection of a favorable phenotypical trait in a population occurs. In the language of Metz's Chapter, it refers to meso-evolution. It uses models based, usually, on integro-differential equations for the population structured by a phenotypical trait. A self-contained mathematical formulation of adaptive evolution also contains the description of mutations and leads to partial differential equations. Then the complete evolution picture follows from the model ingredients mostly driven by the changing adaptive landscape.

It is possible to introduce scaling parameters and perform asymptotic analysis. Then highly concentrated population densities (well-separated Dirac masses) arise that can undergo branching patterns. This phenomenon is interpreted as the speciation process.

The process in which concentrated solutions occur and a continuous set of traits cannot be present is subtle and numerical methods can induce artifacts if not correctly shaped. Simulations on Monte-Carlo methods can be compared to deterministic numerical methods as finite differences.

Mathematics Subject Classification (2000). 35K57, 47G20, 49L25, 65C05, 65M06, 92D15.

Keywords. Adaptive evolution, Lotka-Volterra equation, Darwinian evolution, Hamilton-Jacobi equation, Viscosity solutions, Dirac concentrations, Monte-Carlo simulations, Finite differences.

1. Introduction

Since the 1980's the word "adaptive evolution" has been coined to describe the mathematical formalisms addressing the selection of a favorable trait in a population structured by a continuous phenotypical trait. In the language of [1] it refers to meso-evolution. Closely related to the concept of "Evolutionary game theory"

[2, 3, 4], the models ingredient are the three principles underlying Darwin's explanation of Evolution:

- multiplication of the population,
- selection by competition for resources,
- variability (mutations).

Simple models based on these ingredients explain how the fittest traits can emerge and populations characterized by several well-separated traits (also called strategies) can possibly coexist. The theory and numerical simulations show the appearance of clusters and speciation that can be explained simply: the limited resources lead to competition and individuals with close traits use similar resources, therefore competition between them is higher. The question of understanding how, in such a population, a mutant can invade or not a population has been initiated in [5, 6, 7] and a recent survey can be found in [8], see also [1]. In a self-contained population model, the mutations are part of the dynamics and take into account that the newborn may inherit a slightly different trait than its parent.

The formalism for describing selection, in an asexual population, uses integro-differential equations for the population density $n(x,t)$ where x denotes the phenotypical trait and several models have been derived or postulated for mutations, leading to parabolic partial differential equations (PDEs) [9, 10, 11]. In this Chapter, we aim at explaining how speciation occurs in such PDE models. This corresponds to highly concentrated population densities, which means that $n(x,t)$ is close to well-separated Dirac masses. Because of their regularizing effects, parabolic PDEs cannot sustain such singular solutions and this phenomenon can only happen asymptotically. With this respect, two typical asymptotic regimes are possible. The first one consists in introducing a small parameter for mutations frequency or size and considers the limiting behavior when this parameter vanishes [12, 13, 14, 15]. The second asymptotic is to consider long times and this leads to singular steady state solutions, very similar to the pure selection case [16, 17]. We present these models in Sections 2 and 3 on two different type of competition kernels that we have chosen for their simplicity.

The appearance of these singular solutions is related to an instability mechanism of Turing type. Numerical methods may produce artificially this Turing mechanism in particular because artificial boundary conditions are needed. We discuss this fact in Section 4 based on finite differences or Monte-Carlo simulations.

2. A model with a single nutrient

2.1. The chemostat

Following [8, 12], the simplest example to build up a self-contained mathematical model for adaptive evolution is the *chemostat*. Micro-organisms characterized by a parameter $x \in \mathbb{R}$ (it can be thought of as the logarithm of their size) live in a bath containing a nutrient which is continuously renewed with a rate $d > 0$. The

nutrient concentration is denoted by $S(t) \geq 0$ (for substrate) and the fresh nutrient $S_{\text{in}} > 0$, the population density of the micro-organism is denoted by $n(x,t)$ and the uptake rate for individuals of trait x is $\eta(x) > 0$.

In such a simple situation, the standard equations for the chemostat is written

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}S(t) = d\left(S_{\text{in}} - S(t)\right) - S(t)\displaystyle\int_{-\infty}^{\infty} \eta(x)n(x,t)\mathrm{d}x, \\ \dfrac{\partial}{\partial t}n(x,t) = -dn(x,t) + (1-\mu)S(t)\eta(x)n(x,t) \\ \qquad\qquad + \mu S(t)\displaystyle\int_{-\infty}^{\infty} M(y,x)\eta(y)n(y,t)\mathrm{d}y. \end{cases}$$

The first two principles mentioned earlier from Darwin theory are directly included in the model: the population growth comes from the equation on $n(x,t)$ and the competition comes from the limited amount of nutrients. We assume that initially $S(0) \leq S_{\text{in}}$, then all along the dynamics we have $S(t) \leq S_{\text{in}}$ because $S(t)$ decreases if it attains S_{in}. The term $(1-\mu)\eta(x)n(x,t)$ represents the birth rate without mutations. The parameter $0 < \mu < 1$ represents the proportion of birth undergoing mutations.

Mutations are represented by the probability $M(y,x)$ that a newborn has the trait x when its parent has the trait y. We therefore assume $M(y,x) \geq 0$, $\int\int_{-\infty}^{\infty} M(y,x)\mathrm{d}x = 1$.

We may simplify the model in various ways to make it more amenable to analysis. One can suppose that the nutrients reach quickly an equilibrium compared to the evolution time scale for the population. Then one can replace the differential equation on $S(t)$ by the relation

$$S(t) = \frac{dS_{\text{in}}}{d + \int_{-\infty}^{\infty} \eta(x)n(x,t)\mathrm{d}x}.$$

One can also replace the mutation term by a mere diffusion leading to

$$\frac{\partial}{\partial t}n(x,t) = -dn(x,t) + S(t)\eta(x)n(x,t) + \lambda\Delta n(x,t).$$

Note however that both representations of mutations by integral terms or by a Laplace term $\lambda\Delta$ can be derived from stochastic individual based models (IBM) depending on the scaling of microscopic mutations, [18, 19, 20]. See also [21].

We can write a general form of the resulting model, that we will keep for the end of this section

$$\begin{cases} \dfrac{\partial}{\partial t}n(x,t) = n(x,t)R\left(x, I(t)\right) + \lambda\Delta n(x,t), \quad x \in \mathbb{R},\ t > 0, \\ I(t) = \displaystyle\int_{-\infty}^{\infty} \eta(x)n(x,t)\mathrm{d}x. \end{cases} \tag{2.1}$$

With these notations, the neat growth rate $R(x, I)$ contains both birth and death terms. In the case at hand, it is given by

$$R(x, I) = -d + \frac{dS_{\text{in}}}{d + I}\eta(x).$$

It is natural to handle more general models and then we need some general hypothesis. We assume that R is smooth enough and there are $I_{\text{M}} > I_{\text{m}} > 0$ such that

$$\begin{cases} \sup\limits_{x \in R} R_I(x, I) < 0, & \forall I \geq 0, \\ \max\limits_{x \in \mathbb{R}} R(x, I_{\text{M}}) = 0, \\ \min\limits_{x \in \mathbb{R}} R(x, I_{\text{m}}) = 0. \end{cases} \tag{2.2}$$

We also assume that there are positive constants η_{m}, η_{M} such that

$$0 < \eta_{\text{m}} \leq \eta(x) \leq \eta_{\text{M}} < \infty, \quad \text{with} \quad \eta \in W^{2,\infty}(\mathbb{R}). \tag{2.3}$$

2.2. Rescaling

As mentioned earlier, such parabolic models cannot exhibit high concentrations as long as the diffusion coefficient $\mu > 0$ is fixed. This is the reason why we rescale the problem and set $\lambda = \varepsilon^2$. Having in mind that the mutation rate is small we consider the limit $\varepsilon \to 0$. Such a limit only leads to the same equation with $\lambda = 0$, the selection model. This is because the effect of rare mutations on the population can be observed only on a very long time. This leads us naturally to change time and replace t by t/ε so as to consider the evolution on a long time rather than a generation time scale. Then equation (2.1) is changed to

$$\begin{cases} \varepsilon \dfrac{\partial}{\partial t} n_\varepsilon(x, t) = n_\varepsilon(x, t) R\left(x, I_\varepsilon(t)\right) + \varepsilon^2 \Delta n_\varepsilon(x, t), \quad x \in \mathbb{R},\ t > 0, \\ I_\varepsilon(t) = \displaystyle\int_{-\infty}^{\infty} \eta(x) n_\varepsilon(x, t) \mathrm{d}x. \end{cases} \tag{2.4}$$

But we can point out that other scales are also interesting [10].

We are now ready for a possible interpretation of the speciation phenomena

Theorem 2.1 ([14, 15]). *We assume* (2.2)–(2.3)*, that R is monotonic in x and the initial data is "well prepared" (see below). Then, there are two constants $\rho_m > 0$, $\rho_M > 0$ such that*

$$\rho_{\text{m}} \leq \int_{-\infty}^{\infty} n_\varepsilon(x, t) \mathrm{d}x \leq \rho_{\text{M}} \tag{2.5}$$

and $I_\varepsilon(t) \to \bar{I}(t)$ almost everywhere and in the weak sense of measures

$$n_\varepsilon(x, t) \rightharpoonup \bar{\rho}(t) \delta\big(x - \bar{x}(t)\big).$$

The above assumptions, and in particular monotonicity on R in x, can be replaced by strong concavity on R with quadratic behavior at infinity [22].

This theorem is a mathematical version of the famous *competitive exclusion principle* in ecology. With a single nutrient, a single species will be selected. With N nutrients, we expect in general that N species will coexist.

It is not easy to characterize the fittest trait $\bar{x}(t)$ and the total population size $\bar{\rho}(t)$. In the situations covered by Theorem 2.1, it is proved (see [14, 22]) that

$$R\big(\bar{x}(t), \bar{I}(t)\big) = 0, \qquad \bar{I}(t) = \bar{\rho}(t)\eta\big(\bar{x}(t)\big).$$

Such points appear naturally in the language of evolutionary game theory and are called "singular points'. Of course this identity only relates $\bar{x}(t)$ and $\bar{I}(t)$. It is possible to go further and establish an analogue of the so-called *canonical equation* [23]

$$\dot{\bar{x}}(t) = \big(-D^2 u\big(\bar{x}(t), t\big)\big)^{-1} \cdot \nabla_x R\big(\bar{x}(t), \bar{I}(t)\big),$$

where $u(x,t)$ is introduced below. Such a differential equation was formally introduced in [12] and it can be established rigorously in a multidimensional framework, see [22].

2.3. The constrained Hamilton-Jacobi equation

The proof of Theorem 2.1 relies on a WKB approach, as in front propagation [24, 25, 26]. In the context of adaptive dynamics the method was introduced in [12] and yields a new type of Hamilton-Jacobi equation because an algebraic constraint appears. It is based on the real phase defined by the Hopf-Cole transform

$$u_\varepsilon = \varepsilon \ln(n_\varepsilon).$$

This requires that the initial data itself is "well prepared', that is "exponentially" concentrated as $u_\varepsilon^0 = \varepsilon \ln(n_\varepsilon^0)$ with u_ε^0 a function that behaves nicely as $\varepsilon \to 0$ (even though this can be somehow relaxed, see [15]).

The equation on u_ε is written

$$\frac{\partial}{\partial t} u_\varepsilon(x,t) = R\big(x, I_\varepsilon(t)\big) + \varepsilon \Delta u_\varepsilon(x,t) + \big|\nabla u_\varepsilon(x,t)\big|^2.$$

One can prove that u_ε is uniformly Lipschitzian (this requires that u_ε^0 is so) and that I_ε is uniformly with bounded variations. This allows us to pass to the limit $\varepsilon \to 0$ and obtain the *constrained Hamilton-Jacobi* equation

$$\begin{cases} \dfrac{\partial}{\partial t} u(x,t) = R\big(x, I(t)\big) + |\nabla u(x,t)|^2. \\ \max\limits_{x \in \mathbb{R}} u(x,t) = 0, \qquad \forall t > 0. \end{cases} \tag{2.6}$$

The algebraic constraint $\max_{x\in\mathbb{R}} u(x,t) = 0$ comes from the uniform a priori bound on the total mass stated in (2.5) together with the definition of u_ε by the Hopf-Cole transform.

Being a parabolic limit, the solution $u(x,t)$ should be understood as a viscosity solution to (2.6), see [27].

As mentioned earlier, the originality of this problem stems from the two unknowns $u(x,t)$ et $I(t)$ which should be solved together. The latter is a Lagrange

multiplier associated with the algebraic constraint. This makes the main difference with the standard eikonal equation arising in geometrical optics. A uniqueness result is proved in [14], however under restrictive assumptions. The method of Hopf-Cole transform is very general and, in the present context, it has been extended to systems in [28] (for fronts see [25]).

3. Competition models

In a chemostat, the competition between species is global because it arises through the substrate described by $S(t)$. All individuals are equally competing for the resource. This is not always the case and, in many situations, it is more realistic to assume that there is higher competition between individuals with closer traits. This is the reason why other models have been proposed that implement a trait dependent competition. A class of such models (see [16, 29, 30, 31, 32]) are given by the population dynamics of Lotka-Volterra type

$$\frac{\partial n(x,t)}{\partial t} - \lambda \frac{\partial^2 n(x,t)}{\partial x^2} = n(x,t)\big(R(x) - (K * n)(x,t)\big), \qquad t \geq 0,\ x \in \mathbb{R}. \quad (3.1)$$

The model is completed by an initial data $n(x, t = 0) = n^0(x)$ which we take highly concentrated for the numerical simulations presented below in Section 4.

The interpretation of the quantities arising in this model are

- $n(x,t)$ still denotes the population density at position x and time t,
- $R(x) > 0$ is the intrinsic growth rate of individuals with trait x (if isolated without competition)
- $K \in L^\infty(\mathbb{R})$ is called the competition kernel. It is a probability density: $K \geq 0$, $\int_{-\infty}^{\infty} K(z)dz = 1$. The convolution $(K*n)(x) = \int_{-\infty}^{\infty} K(x-y)n(y,t)\mathrm{d}y$ represents the competition for resource,
- λ is the mutation rate that is supposed to be a constant.

When derived from stochastic IBM, as in [9, 19, 20] such models are called *mean field* equations [33, 34]. They arise not only in evolution theory but also in ecology for non-local resources (and x denotes the location then) [35, 36, 37, 38].

The large variety of regimes that can appear in such models can be seen in special cases. Below, we use simple examples to describe two of them, regularly distributed traits, or concentration as a Dirac mass. The main interest of the model (3.1) is mostly from the branching patterns that correspond to multiple concentration points which can either die out or branch again and create new structures (see [39]).

3.1. The Gaussian case without mutations

Firstly we consider the case

$$\lambda = 0, \qquad R(x) = \frac{1}{\sqrt{2\pi\sigma_1}} \mathrm{e}^{-\frac{|x|^2}{2\sigma_1}}, \qquad K(z) = \frac{1}{\sqrt{2\pi\sigma_2}} \mathrm{e}^{-\frac{|x|^2}{2\sigma_2}}. \quad (3.2)$$

This corresponds to widely used standard forms of the input parameters because of their statistical meaning.

As usual for pure selection models, $\lambda = 0$, there are Dirac mass stationary solutions $N(x) = \bar{\rho}\delta(x - \bar{x})$ with $R(\bar{x}) = \bar{\rho}K(0)$. But this can be obtained in a long time asymptotic only when

$$R(x) < \bar{\rho}K(x - \bar{x}) \ , \qquad \forall x \neq \bar{x},$$

or, replacing $\bar{\rho}$ from the first condition

$$\frac{R(x)}{R(\bar{x})} < \frac{K(x - \bar{x})}{K(0)} \ , \qquad \forall x \neq \bar{x}.$$

One can deduce from this calculation the

Proposition 3.1. *For $\sigma_1 > \sigma_2$ there is a smooth steady state to* (3.1) *given by*

$$N(x) = \frac{1}{\sqrt{2\pi\sigma}} \mathrm{e}^{-\frac{|x|^2}{2\sigma}}, \qquad \sigma = \sigma_1 - \sigma_2,$$

and Dirac masses are not stable steady states.

For $\sigma_1 < \sigma_2$ the Dirac mass $\bar{\rho}\delta(x)$ is a stable steady state (*and only the Dirac mass at* 0 *is stable*).

The authors in [17] prove that the corresponding stable states are also the long time limits of the dynamics described by equation (3.1). They use a relative entropy method built on the corresponding steady state. The construction of this entropy is rather easy when the positive steady state exists. It is much more difficult in the case where the Dirac masses have to be handled.

3.2. The Nonlocal-Fisher equation

We now consider the case

$$R \equiv 1. \tag{3.3}$$

Then, the equation (3.1) is called the *Nonlocal-Fisher* (NLF) equation. It also arises in mathematical ecology, as an extension of the Fisher/KPP equation. As mentioned earlier, the nonlocal aspect induced by the convolution represents long range access to resources, see [32, 36, 38] and the references therein.

The positive steady state is simply given by $N \equiv 1$ but a result from [30] states that it can be Turing unstable (i.e., only a bounded set of linearly unstable modes occur). In order to explain this, we may use the Fourier transform of the competition kernel K defined as

$$\widehat{K}(\xi) = \int_{-\infty}^{\infty} K(x)\mathrm{e}^{-ix\xi}\mathrm{d}x.$$

Then one has

Proposition 3.2 ([30]). *Assume there is a ξ_0 such that*

$$\widehat{K}(\xi_0) < 0, \tag{3.4}$$

then for λ small enough the steady state $N \equiv 1$ is linearly unstable.

The result of this statement corresponds qualitatively to the case $\sigma_1 < \sigma_2$ in Proposition 3.1 (with mutations neglected).

The Fourier transform also characterizes a nonlinear stability result; this is the case in the

Theorem 3.3 ([32]). *Take $R \equiv 1$ and assume*

$$\widehat{K}(\xi) > 0 \qquad \forall \xi \in \mathbb{R}. \tag{3.5}$$

Then $n \equiv 0$ and $n \equiv 1$ are the only two nonnegative and bounded steady states of (3.1).

Furthermore, there are traveling waves connecting the states $n = 0$ and $n = 1$.

The result of this theorem corresponds to the situation $\sigma_1 > \sigma_2$ in Proposition 3.1.

In the Turing unstable case it is possible to rescale the problem as we did it in Section 2.2 and it is observed numerically that, in general, the asymptotic limit leads to Dirac concentrations characterized again by a constrained Hamilton-Jacobi equation [31].

4. Numerical methods and branching patterns

In general it is very difficult, in the direct competition model (3.1), to distinguish between the two behaviors: convergence towards a continuous state or speciation. Numerical methods are useful to get an intuition but they can create artifacts and we explain this now.

We present two numerical approaches that allow to simulate solutions to equation (3.1). The first is a standard finite difference scheme, the second one is a Monte-Carlo simulations related to IBM that solves the same equation.

For the sake of simplicity we concentrate on the Nonlocal Fisher equation as in Section 3.2 with a Gaussian competition kernel

$$R \equiv 1, \qquad K(x) = \frac{1}{\sqrt{2\pi\sigma}} \mathrm{e}^{-\frac{|x|^2}{2\sigma}}. \tag{4.1}$$

Because the Fourier transform of K is positive (a Gaussian), we do not expect appearance of concentrations (speciation).

At this stage we insist that the Monte Carlo algorithms are only seen here as an approximation to (3.1). From this point of view, the closer it is from the PDE, the better it is because one looks only for possible computational cost reduction. Monte-Carlo methods are also used as a modeling tool and allow to include further stochastic effects. One of them is "demographic stochasticity" which makes that too small populations can die out by statistical effects [40, 41]. These effects are not included in the models under consideration here and give quantitatively different answers (in terms of evolution speed, branching patterns). It is shown in [39] that the notion of "survival threshold" in the equations as (3.1) is able to reproduce these effects in great details.

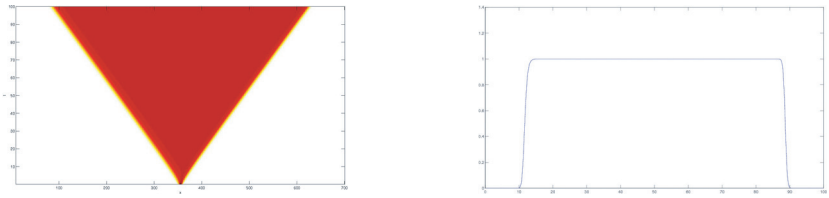

FIGURE 4.1. Left: Numerical population density dynamics obtained for model (3.1)–(4.1) when the initial population is concentrated in the center of the computational domain. Horizontally is x and vertically is t, in gray zone $n \equiv 1$ and the white zone corresponds to $n \equiv 0$. Right: The population density $n(x,T)$ at final time. The deterministic finite difference scheme (4.2)–(4.4) has been used with parameters in (4.5). We observe convergence toward the constant solution in accordance with Theorem 3.3.

4.1. Finite differences

We consider the solution on interval $\left[-\frac{L}{2}, \frac{L}{2}\right]$. We use a uniform grid with N points on the segment, with $\Delta x = \frac{L}{N}$ the space step. We denote by $n_i^k \geq 0$ the numerical solution at grid point $x_i = i\triangle x$, $1 \leq i \leq N$, and time $t^k = k\triangle t$ where $\triangle t$ is the time step

$$n(x_i, k\triangle t) \approx n_i^k.$$

We use a time splitting algorithm between the growth term and the diffusion that is we solve alternatively the two equations

$$\frac{\mathrm{d}}{\mathrm{d}t} n(x,t) = n(x,t)\left[1 - (K * n)(t)\right],$$

and

$$\frac{\partial n(x,t)}{\partial t} - \lambda \frac{\partial^2 n(x,t)}{\partial x^2} = 0.$$

1. First compute, with a semi-implicit method, the solution to the discrete reaction term

$$\frac{\mathrm{d}}{\mathrm{d}t} n_i(t) = n_i(t)\left[1 - K_d * n_i^k\right].$$

The exact solution is

$$n_i^{k+\frac{1}{2}} = n_i^k \exp\left(\frac{\Delta t}{\lambda}\left(1 - K_d * n_i^k\right)\right), \qquad 1 \leq i \leq N. \tag{4.2}$$

The discrete convolution is computed according to

$$\begin{cases} K_d * n_i^k = \Delta x \cdot \displaystyle\sum_{j=-N}^{N} K_d(j\triangle x) n_{i-j}^k, \\ n_{i-j}^k = 0 \ \text{ for } i - j \notin [1, N]. \end{cases} \tag{4.3}$$

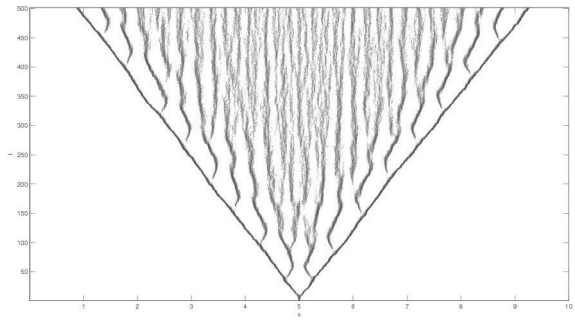

FIGURE 4.2. Numerical solution with the Monte-Carlo algorithm in section 4.2. Horizontally is the trait x and vertically is time t. Initially the population is concentrated in one Dirac mass at the center of the domain. We observe that the population distribution converges weakly towards the constant solution as expected (see also Fig. 4.1).

Indeed, as a consequence of the domain truncation, only those terms satisfying $1 \leq i - j \leq N$ are well defined and the extension by zero amounts to extend n by 0 outside $\left[-\frac{L}{2}, \frac{L}{2}\right]$. This is some kind of Dirichlet boundary condition.

2. As for the Laplace term, we use a three points explicit scheme

$$n_i^{k+1} = n_i^{k+\frac{1}{2}} + \frac{\lambda \Delta t}{2\Delta x^2}\left(n_{i+1}^{k+\frac{1}{2}} + n_{i-1}^{k+\frac{1}{2}} - 2n_i^{k+\frac{1}{2}}\right), \qquad 1 \leq i \leq N. \tag{4.4}$$

Because we choose λ small, the explicit scheme is not penalizing in terms of computational time. We use Neumann boundary condition, $n_0^{k+1} = n_1^{k+1}$ and $n_N^{k+1} = n_{N-1}^{k+1}$, but as far as the wave does not reach the boundary, the Dirichlet boundary condition $n_1^{k+1} = n_N^{k+1} = 0$ gives equivalent results.

The stability of the scheme is ensured by the CFL condition $\frac{\lambda \Delta t}{2\Delta x^2} \leq 1$, which is verified for

$$\begin{aligned} &\lambda = 0.004, \qquad &&\sigma = 0.04, \qquad &&\Delta t = 0.025, \\ &\Delta x = 0.1, \qquad &&L = 100, \qquad &&N = 1000. \end{aligned} \tag{4.5}$$

We have implemented this method. We choose the initial data concentrated in the center of the domain. The numerical results are depicted in Fig. 4.1. We can observe that the population propagates as a traveling wave. For L large enough, for $0 \leq t \leq T$ the front does not reach the numerical boundary and there is almost no mass on the boundary of the interval $[-\frac{L}{2}, \frac{L}{2}]$. This is in accordance to the theory in [32] and the statement in Theorem 3.3.

4.2. The stochastic individual-based method

We also compare the finite volume simulation with a Monte Carlo algorithm. Then, the solution is approximated by a sum of Dirac masses

$$n(t) \approx \omega \sum_{j=1}^{N(t)} \delta\big(x - y_j(t)\big).$$

Here the weight ω is taken constant. The simulation starts with a number $N(0)$ of "individuals located" distributed on an interval of length L. Then $N(0)$ and ω are related by the approximation $n(0) \approx \omega \sum_{j=1}^{N(0)} \delta\big(x - y_j(0)\big)$ in the weak sense of measures.

Several Monte Carlo algorithms are possible. See for instance [35, 38] for another algorithm motivated by models from ecology.

Here we use the method proposed in [33, 34]. The number of individuals is denoted by $N(k)$ at iteration k. The algorithm uses also a time splitting but not with the same operators as in Section 4.1. We solve alternatively the two equations

$$\frac{d}{dt} n(x,t) = -n(x,t)(K * n)(t),$$

and

$$\frac{\partial n(x,t)}{\partial t} - \lambda \frac{\partial^2 n(x,t)}{\partial x^2} = n(x,t).$$

Finally, in the rationale of small mutations and long times, as in section 2.2, we choose $\triangle t = 1$. Then the algorithm [33, 34] reads as follows.

1. The competition term is now computed as (this makes a difference with [33, 34])

$$C(x) = \frac{\omega}{\sqrt{2\pi\sigma}} \sum_{j=1}^{N(k)} \exp\left(-\frac{|x - y_j|^2}{2\sigma}\right). \tag{4.6}$$

   Because the value of $C(x)$ is small, it defines the probability that an individual located at x dies. For a given j, we compute this probability and set $N(k+1) = N(k) - 1$ if this individual dies.
2. If the individual survives, it reproduces. The newborn undergoes a mutation from its parent trait to a new trait given by a Gaussian distribution with variance $\lambda' = 2\lambda$. Then $N(k+1) = N(k) + 1$.

   We notice that for n the solution of

$$\partial_t n = \lambda' \triangle n, \qquad n(x, t^k) = n^k(x),$$

   we have $n(t^{k+1}) = n^k * \frac{1}{\sqrt{4\pi\lambda'}} \mathrm{e}^{\frac{-x^2}{4\lambda'}}$. Hence the choice $\lambda' = 2\lambda$ in the second step of the Monte Carlo method. We act a Gaussian mutation to the new-born only but with twice stronger intensity.

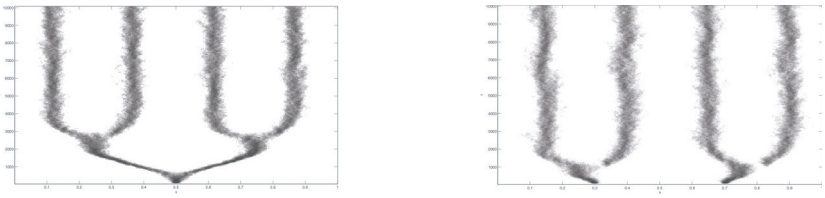

FIGURE 4.3. Dynamics of the concentration points with the Monte-Carlo algorithm in section 4.3 based on periodizing the convolution. Horizontally is the trait x and vertically is time t. Initially the population is concentrated in one Dirac mass on the left and two Dirac masses on the right.

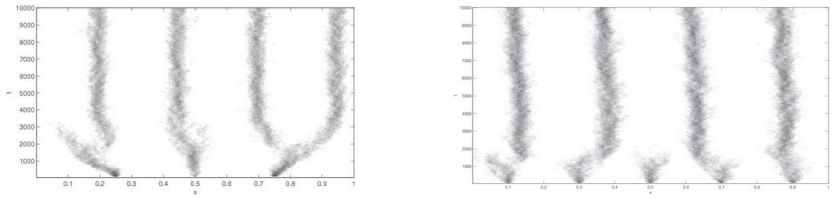

FIGURE 4.4. Dynamics of the concentration points. Same as above but with different initial data. A new phenomena occurs with extinction of branches.

We have used the following parameters values which take into account the small time step in the deterministic algorithm

$$\lambda' = 10^{-6}, \quad \sigma = 0.04, \quad L = 10, \quad N = 3000, \quad \frac{\omega}{\sqrt{2\pi\sigma}} = \frac{1}{18000}.$$

These values are such that the mutations are very weak compared to intraspecific competition, again in accordance with the parameters used in the finite difference method. The numerical results are depicted in Fig. 4.2. We can observe that the population propagates as a traveling wave as in Fig. 4.1 and according to the theoretical prediction in Theorem 3.3.

4.3. The convolution formula

Surprisingly, in [33, 34] the authors observed that simulations based on this Monte-Carlo method may yield concentration patterns too (clusters). The main difference is that, rather than with equation (4.6), the convolution kernel is computed assuming the y_j are on the circle

$$C(x) = \frac{\omega}{\sqrt{2\pi\sigma}} \sum_{j=1}^{N(k)} \exp\left(-\frac{d(x, y_j)^2}{2\sigma}\right), \tag{4.7}$$

where d is the shortest distance on the circle.

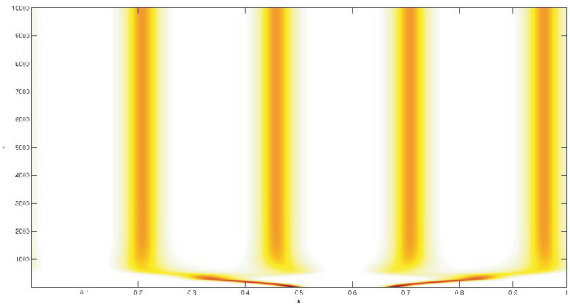

FIGURE 4.5. Numerical population density dynamics obtained by deterministic simulations for model (3.1)–(4.1) with periodic boundary conditions. We have used the following parameter values: $\lambda = 0.001$, $\sigma = 0.04$, $\Delta t = 0.0001$, $\Delta x = 0.001$, $L = 1$, $N = 1000$.

This can be interpreted as periodic boundary conditions rather than extension by zero or as a periodic convolution kernel

$$K_s(x) \propto \exp\left(-\frac{(x\,[L])^2}{2\sigma}\right), \qquad x[L] = x \mod L, \;\; x \in \mathbb{R}.$$

In opposition with the Gaussian kernel because it has some Fourier coefficients with a negative real part. In this case the Fourier condition (3.4) is not fulfilled. Therefore according to the linear analysis in [30], and Proposition 3.2, the constant state is unstable for problem (3.1)–(4.1) and we expect to observe pattern formation.

We have run both the Monte Carlo and finite difference approximations with this periodic kernel. The numerical results are in accordance with those obtained in different contexts in [30, 31, 33, 34]. They can be found in Fig. 4.3 and Fig. 4.4 for Monte Carlo simulations and Fig. 4.5 for finite differences.

5. Conclusion

Mathematical models explaining how speciation occurs in biological population have been developed since the 1980s. They involve a population dynamics under local competition and with mutations. A self-contained formalism can be established. It allows to represent the speciation phenomena as the convergence of the solution to a sum of Dirac masses, either in the large time limit or the small mutation rate limit. However, competition models not always yield speciation and a population with a continuous set of traits can occur. It is difficult to predict between these two alternatives.

Numerical methods are therefore useful tools to observe the model prediction. We presented two numerical methods: finite differences and the individual based

approach. These methods give compatible numerical results either in the case when a uniform trait distribution is produced by the model and when patterns are obtained.

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