Spatially inhomogeneous population dynamics: beyond the mean field approximation

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Received 11 December 2018, revised 10 May 2019
Accepted for publication 10 June 2019
Published 1 July 2019

Abstract

We propose a novel method for numerical modeling of spatially inhomogeneous moment dynamics of populations with nonlocal dispersal and competition in continuous space. It is based on analytically solvable decompositions of the time evolution operator for a coupled set of master equations. This has allowed us—for the first time in the literature—to perform moment dynamics simulations of spatially inhomogeneous birth-death systems beyond the mean-field approach and to calculate the inhomogeneous pair correlation function using the Kirkwood superposition ansatz. As a result, we revealed a number of new subtle effects, possible in real populations. Namely, for systems with short-range dispersal and mid-range competition, strong clustering of entities at small distances followed by their deep disaggregation at larger separations are observed in the wavefront of density propagation. For populations in which the competition range is much shorter than that of dispersal, the pair correlation function exhibits long-tail asymptotics. Remarkably, the latter effect takes place only due to the spatial inhomogeneity and thus was completely unknown before. Moreover, the both effects get stronger in the direction of propagation. All these types of behaviour are interpreted as a trade-off between the dispersal and competition in the coexistence of reproductive pair correlations and the inhomogeneity of the density of the system.

Keywords: population dynamics, birth-death systems, decomposition methods, numerical simulations, spatial inhomogeneity, moment closures, clustering

(Some figures may appear in colour only in the online journal)
1. Introduction

The description of the evolution of large systems of interacting entities is a paramount problem common to physics, chemistry, biology, ecology, life and social sciences, etc [1–5]. Perhaps, statistical physics was the first where this problem has been considered at a microscopic (individual-based) level and the relationship between the microscopic and more coarse-grained (meso- or macroscopic) approaches has been methodologically studied [1]. Because of the large (infinite) number of the constituents, micro-states of such systems are usually described in terms of probability distributions defined on the corresponding configuration spaces. This way, however, is mathematically very demanding and the results obtained herein are typically of existential nature, giving not too much for practical applications. On the other hand, numerical individual-based simulations—yielding the most detailed and practically valued data—appear to be usually computationally very expensive, especially in the case of population dynamics of large-size systems [3, 6–8].

The meso- and macroscopic approaches deal with aggregated parameters of a reduced description, the first of them is density of entities. It is the only such parameter in a mean-field (MF) approximation [1] invoked for most models of population dynamics to simplify consideration (see, e.g. [9]). However, the MF approximation totally neglects the second-, third- and higher-order spatial correlations, meaning that any information that was held in these correlations is lost. One of the key issues in understanding the dynamics of populations is how the whole information on spatial structure can be retrieved from the interactions between the constituents. In view of this, during the last two decades there has been developed an approach called spatial moment dynamics (SMD) [10–24]. In SMD, the populations are described by time-dependent spatial moments (aka correlation functions [22–25]). The first two of them are local density of entities and their pair distribution. It should be emphasized that contrary to MF, the SMD approach allows one to explicitly account the spatial correlations of arbitrary orders.

The SMD models were applied to ecological dynamics, spatial epidemics, surface chemistry reactions, herding behaviour, predator-prey metapopulations (see [3, 17] and the references therein). They are particularly useful in detecting patchiness and clustering [13, 26] in the spatial distribution of different organisms, such as trees in a beech forest [27] or breast cancer cells at an in vitro growth-to-confluence assay [28]. Strictly speaking, the SMD approach is able to predict subtle effects which are unreachable within the MF framework. The former can also be employed to improve or revisit some MF data, e.g. on the formation of patterns in evolution of bacterial colonies [29].

The set of spatial moments of all orders yields an exact description of the ensemble average of the stochastic dynamical processes in the system [18, 23, 30, 31]. As the density depends on the second-order correlation function, or more generally, the moment of order $p$ depends on the moment of order $p + 1$ for models with pairwise interactions, we come to an infinite hierarchy ($p = 1, 2, \ldots, \infty$) of coupled governing equations. For practical reasons, this hierarchy needs to be truncated (i.e. decoupled), since in computer simulations we cannot operate with the infinite number of functions. The aim is to attain a closed form of the infinite set by expressing higher-order moments in terms of lower-order ones. Usually the truncation is performed at the third-order level, so that solutions are found for the first two equations.

The moment truncation arises in myriad scientific disciplines when modelling complex systems. It can be derived in different contexts, including kinetic and stochastic differential equations as well as network dynamics, and applied to epidemiological, ecological, and socio-economic models, chemical reactions, cell motion, game theory, and others (see a brief review [32] and the references therein). Several closures of powers one, two, and three have been
introduced for the SMD approach \[12, 14, 19–21\]. It was realized that their precision increases with increasing the power number. Indubitably, the SMD description is superior to the MF approximation and can provide \[12, 19, 20\] a high accuracy (comparable to that of individual-based simulations) of calculating observables such as population density and pair correlation function.

Despite the mentioned achievements, all the previous SMD simulations of continuous-space models were restricted exclusively to the spatially homogeneous case \[10–14, 16, 19–21\]. Obviously, this presents a significant limitation as then most of the principal properties of population systems are inaccessible. For example, the account of spatial inhomogeneity is essential in the study of the wavefront and spread dynamics. Inhomogeneous processes are important in ecological invasions, in vitro cell invasion assays, embryogenesis and wound healing, malignant tumor proliferation, etc (see \[18\] and the references therein). All these processes involve colonisation of a region by a population of agents that is initially spatially confined. As was underlined in \[18\], very little is known about SMD for inhomogeneous systems (although some estimations of the inhomogeneous pair correlation function as a weighted sum of its homogeneous counterparts corresponding to different local constant densities were made \[27\]).

Until now, there have been no publications on continuous-space inhomogeneous SMD (ISMD) simulations of birth-death populations. This is explained by the fact (carefully inspected in this work) that the standard numerical methods are incapable for ISMD in the presence of reproductive pair correlations. Thus, the main goals of this work are: (i) development of an approach enabling to solve the problem with spatial inhomogeneity; (ii) carrying out first ISMD simulations of birth-death systems in continuous space; and (iii) discovering new population dynamics effects.

2. Model

Consider a population of point interacting entities dwelling in continuous space \(\mathbb{R}^d\) of dimensionality \(d \geq 1\). We will deal with a popular model \[10, 11, 13, 22–24, 30, 31\] according to which the entities stochastically reproduce themselves, disperse, and die on their own or due to competition. The (pure) microscopic state of the population system is configuration—a locally finite subset \(\eta \subset \mathbb{R}^d\). Locally finite means that each bounded subset of \(\mathbb{R}^d\) contains only finite number of the elements of \(\eta\), called particles or entities. However, the whole configuration \(\eta\) can be infinite. The evolution of the population can be described by the following Kolmogorov equation

\[
\frac{\partial}{\partial t} F_t(\eta) = (\mathcal{L} F_t)(\eta), \quad t > 0, \quad F_t|_{t=0} = F_0.
\]

where \(F_t(\eta)\) is an observable—a suitable function of \(\eta\). The operator \(\mathcal{L}\) determines the model. For the case considered, it is (see, e.g. \[24\]):

\[
(\mathcal{L} F_t)(\eta) = \int_{\mathbb{R}^d} \left( \sum_{x \in \eta} a(x, y) \right) \left[ F_t(\eta \cup y) - F_t(\eta) \right] dy + \sum_{x \in \eta} \left( m + \sum_{y \in \eta \setminus x} b(x, y) \right) \left[ F_t(\eta \setminus x) - F_t(\eta) \right].
\]

The first term in the rhs of equation (2) relates to the dispersal: the particle located at \(x \in \eta\) gives birth (sends a seed) to a new entity that instantly appears at distant point \(y \in \mathbb{R}^d\) with
the probability density function $a(x, y) = a(y, x) > 0$ and thus becomes a population member given by the whole configuration. The second term defines the death of an individual at $x \in \eta$ caused by: (i) intrinsic factors, with rate $m > 0$; (ii) interactions with the other population members located at $y \in \eta \setminus x$, by rate $b(x, y) = b(y, x) > 0$. The functions $a(x, y)$ and $b(x, y)$ are assumed to be non-negative and possess a number of properties [24].

In the ISMD approach, the Kolmogorov equation (1) for observable $F_t$ is replaced by the evolution equations for spatial moments. Let us denote the first three of them as $n_t(x)$, $u_t(x, y)$ and $w_t(x, y, z)$. They determine correspondingly the probability density of finding at time $t$ a single entity at $x \in \mathbb{R}^d$, a pair of entities at $x, y \in \mathbb{R}^d$, or a triplet at $x, y, z \in \mathbb{R}^d$. Then, taking into account equation (2), the first two coupled evolution equations of the ISMD hierarchy can be written in the following integro-differential form.

\[
\frac{\partial n_t(x)}{\partial t} = - mn_t(x) + \int a(x, y)n_t(y)dy - \int b(x, y)u_t(x, y)dy,
\]

\[
\frac{\partial u_t(x, y)}{\partial t} = - 2mu_t(x, y) + a(x, y)\left(n_t(x) + n_t(y)\right) - 2b(x, y)u_t(x, y)
+ \int \left(a(x, z)u_t(y, z) + a(y, z)u_t(x, z)\right)dz
- \int \left(b(x, z) + b(y, z)\right)w_t(x, y, z)dz.
\]

Note that equation (3) was already explicitly derived earlier in [22–24], while the second equation (4) coincides with that of [15, 18–20] in a particular case when the processes of movement and neighbour-dependent birth are excluded.

We mention that the functions $a(x, y)$ and $b(x, y)$ define the probabilities per unit time for dispersal to point $x$ of an entity born ($+$) at $y$ and its death ($-$) in $x$ caused by competition with a neighbour at $y$, while $m$ is the intrinsic mortality parameter. The dispersal $a$ and competition $b$ kernels are commonly modeled by the Gaussians $c_\pm/(2\pi \sigma_\pm^d)^{d/2} \exp[-(x-y)^2/(2\sigma_\pm^2)]$ or the top-hat functions $c_\pm/(2\sigma_\pm)^d$ for $|x-y| \leq \sigma_\pm$ with intensities $c_\pm$ and ranges $\sigma_\pm$ of dimensionality $d = 1$, 2, or 3. These kernels are normalized so that $\int a(x, y)dy = c_+$ and $\int b(x, y)dy = c_-$. The most general form of the ISMD equations (which includes motility and mutation of entities) is presented in [18]. The infinite chain of master equations for spatial moments of arbitrary orders is also given there. It is very similar to the Bogoliubov (or Bogolyubov–Born–Green–Kirkwood–Yvon) hierarchy [1, 33] used for correlation functions in the Hamiltonian dynamics of continuum systems of interacting particles.

The birth-dispersal-death-competition (BDDC) population model just considered was first introduced in spatial ecology by Bolker and Pacala [10, 11] as well as by Dieckmann, Murrell and Law [13] (aka BDLMP [15] or BDLP [31] model). It is known also as the spatial and stochastic logistic model [10, 13, 22–24, 30] (abbreviated as SLM [22] or SSLM [23]). A population here is represented by a configuration of motionless organisms (plants) located in an infinite habitat. Each plant (near $y$) produces at random seeds independently of others and then the former are distributed in space (to point $x$) accordingly to the dispersion kernel $a(x, y)$. This is a cumulative effect of the whole configuration (the integration over $y$ should be carried out). Also, the model includes a mortality mechanism. The mortality rate consists of an intrinsic part (any plant can die independently of others after a random time exponentially distributed with parameter $m$) and a density-dependent contribution which is accounted by the competition kernel $b(x, y)$ that describes additional mortality (at any given point $x$ of the configuration) coming from the rest of the population (by integrating over $y$). Versions of the
BDLMP model which take into account regular movement [12] or Brownian motion [15] of entities were derived as well.

It is worth pointing out that the BDDC equations (3) and (4) appear from the general ISMD form [18] as a particular case in which some of the parameters are equal to zero. Choosing another set of values for these parameters we can describe quite other systems, e.g. animal pray-predator populations. Then the assumption that an individual instantaneously travels to a new location immediately after birth made for the BDDC model should be avoided (by setting the dispersal range to zero). Instead, we should involve different species and add a new event concerning regular movement of entities. Therefore, the BDDC model (with nonzero dispersal range) is appropriate to describe dynamics of plant populations with seed dispersal as well as collections of such organisms as bugs or branching diffusion of the plankton (Brownian movement should be added), and others.

Note also that in the ISMD equations the infinite habitat is taken to be a continuous space as opposed to discrete spatial lattices used in most of mathematical models on population dynamics. The lattice representation, however, can modify to some extent real populations where entities take positions continuously in space instead to be located in predefined knots. In this context, continuous-space models can be considered as more preferable (see, e.g. a review [3] where continuum, lattice, network, spatial moment and other models are described and compared).

As far as we have two equations (3) and (4), and three unknown functions to be found, $n_t(x)$, $u_t(x, y)$ and $w_t(x, y, z)$, the infinite ISMD hierarchy should be decoupled. This can be done by complementing the master equations (3) and (4) by the power-3 closure [12, 14, 19, 20]:

$$\begin{align*}
    w_t(x, y, z) &= \frac{u_t(x, y)u_t(x, z)u_t(y, z)}{n_t(x)n_t(y)n_t(z)} 
    \end{align*}
$$

for the inhomogeneous third-order correlation function which is expressed in terms of the second- and one-order moments. This closure is well known in theoretical physics [34–37] as the Kirkwood superposition approximation (KSA). Its simplified version, $w_t(\xi, \xi') = u_t(\xi)u_t(\xi')u_t(\xi' - \xi)/n_t^3$, where $\xi = x - y$ and $\xi' = x - z$, is widely used for spatially homogeneous population systems [12, 14, 19, 20]. A high efficiency of the spatially inhomogeneous KSA (equation (5)) has been proven previously for lattice [38–42] and off-lattice models [43, 44]. Note also that in the absence of pairwise interactions (i.e. when $b(x, y) = 0$), the first two equations (3) and (4) of the ISMD hierarchy appear to be decoupled automatically without using any additional approximate closure, providing an exact description in this case (that corresponds to the so-called contact model [45]).

Although more complex ISMD models [18–21] can be introduced, too, equations (3) and (4) are quite complicated. In simplified limits, equation (3) transforms to the well-known equations of previous models of spatial population dynamics. For example, neglecting the pair correlations within the MF approximation by putting $u_t(x, y) \approx n_t(x)n_t(y)$, we come from equation (3) to the kinetic equation of [22–24]. Additionally, by letting $\sigma_+ \ll 1$ (local dispersal) we have $\int a(x, y)n_t(y)dy \approx c_+n_t(x) + D\partial^2 n_t(x)/\partial x^2$ that leads to the diffusion MF model [29], where $D = c_+\sigma_+^2/2$ is the diffusion coefficient. Finally, in the limit $\sigma_- \to +0$ of local competition when $b(x, y) \to c_-\delta(x - y)$, we reproduce from equation (3) the classical Fisher–Kolmogorov–Petrovsky–Piscunov [46–48] reaction-diffusion equation $\partial n_t(x)/\partial t = (c_+ - m)n_t(x) - c_-n_t^2(x) + D\partial^2 n_t(x)/\partial x^2$, exploited in early investigations.

Despite the importance of the ISMD equations (3) and (4), there were no successful attempts reported to find their solutions numerically (usually for the most of the integro-differential equations of this kind, the explicit analytic solution seems unrealistic, in general,
see section 5). As will be shown later, the reason is that the existing numerical methods are inappropriate to solve these equations in the case of inhomogeneous conditions. That is why the assumption of spatial homogeneity, i.e. that \( n_t(x) \) does not change on coordinate \( x \), was made [10–14, 19–21]. Then, the second-order function \( u(x,y) \) will depend only on the difference \( |x - y| \) and not on \( x \) and \( y \) separately, significantly simplifying the computations and enabling to obtaining spatially homogeneous results. It was mentioned in the Introduction that the homogeneous approach is very restrictive in comparison with ISMD. By ignoring density variations, similar simplifications were used when incorporating spatial correlations into lattice models [38–40].

First studies on improving the MF approach by including inhomogeneous correlations were carried out in [41]. The spatially inhomogeneous moment equations within the MF and KSA closure approximations were solved as well [42]. However, the consideration in [41, 42] was devoted solely to lattice models within a nearest-neighbour scheme in terms of the average site occupancy probability. Quite recently [43, 44], lattice-free spatially inhomogeneous models were studied, too, in one-dimensional space using the MF and KSA ansatzes. In these models, however, only migration and adhesion processes were included without taking into account the reproduction, so that they are not applicable for birth-and-death population systems.

3. Method

Our method is grounded on the theoretically rigorous framework developed for continuous-space ISMD models in the presence of spatial inhomogeneity and reproductive pair correlations, where homogeneous configurations appear as a particular case. This method is very general in the sense that it can be used for more complex models (consisting of different species, genotypes, sexes, and which may have marks to represent sizes of agents, age classes, etc, see, for instance, [18]). In order to simplify the introduction of the mathematical framework, we will restrict the discussion in the present paper to the specific BDDC model (equations (3) and (4)) which is considered as an illustrative example of efficiency of our new method.

The main concepts of our ISMD approach consist in the following. Firstly, in order to solve equations (3) and (4) we perform their discretization using the equalities

\[
\frac{d n_i}{dt} = -m n_i + h \sum_j (a_{ij} n_j - b_{ij} u_{ij}),
\]

\[
\frac{d u_{ij}}{dt} = -2(m + b_{ij}) u_{ij} + a_{ij}(n_i + n_j)
+ h \sum_k \left( a_{ik} u_{ik} + a_{jk} u_{jk} - (b_{ik} + b_{jk}) w_{ijk} \right).
\]

Here the sums represent the spatial integrals over \( y \) and \( z \), while \( n_i(t) = n_i(x_i) \), \( u_{ij}(t) = u_{ij}(x_i, x_j) \) and \( w_{ijk}(t) = w_{ijk}(x_i, x_j, x_k) \) are the values of the correlation functions in grid points \( x_{i,j,k} \) uniformly distributed inside the region \([-L/2, L/2]^d\) with spacing \( h = (L/N)^d \), and \( i,j,k = 1,2,\ldots, N^d \). The kernel values in the grid points are denoted by \( a_{ij} = a(x_i, x_j) \) and \( b_{ij} = b(x_i, x_j) \). Area \([-L/2, L/2]^d\) constitutes an interval, a square, or a cube in the cases \( d = 1, 2, \) or 3, respectively.

Note that the length \( L \) should be sufficiently long with respect to all characteristic coordinate scales of the population system in order to exclude boundary effects. The number \( N \) of grid points must be large enough to minimize the noise caused by the discretization. Then mesh \( h \) will be sufficiently small to provide a high accuracy of the spatial integration.
Obviously, in the limits $L, N \to \infty$ and $h \to 0$, the discretized equations (6) and (7) coincide with their original, continuous counterparts (equations (3) and (4)). The finite-size effects can be reduced by employing the corresponding boundary conditions when mapping our infinite range $x, y, z \in [-\infty, \infty]^d$ by the finite area $x_i, x_j, x_k \in [-L/2, L/2]^d$. If the entities initially ($t = 0$) exist only within a narrow region $[-l/2, l/2]$ with $l \ll L$ and they are absent outside of it, i.e. $\left. \{n_0(x), u_0(x, y)\right|_{|x|,|y|>|l/2}} = 0$, we can apply the Dirichlet boundary conditions $\lim_{x, y \to \pm \infty} \left. \{n_t(x), u_t(x, y)\right|_{|x|,|y|}| = 0$. This means that nonzero values of the spatial moments will not reach the area boundaries $\pm L/2$ in each direction during the simulations over the finite observation time $0 < t \leq T$. When $n_0(x)$ and $u_0(x, y)$ take nonzero values anywhere in the infinite space, it is necessary to use the periodic (or toroidal) boundary conditions and the minimum-image convention for the calculation of interparticle interactions.

Secondly, we complement equations (6) and (7) by the discretized duplicate

$$w_{ijk} = \frac{u_{ij}u_{ik}u_{jk}}{n_i n_j n_k}$$

of the power-3 KSA ansatz (equation (5)), where the moment $w_{ijk}$ of the highest (third) order is expressed in terms of the lower-order correlation functions $u_{ij}$ and $n_i$. As was shown earlier in the spatially homogeneous case, this ansatz provides much better accuracy when reproducing the second- and third-order correlations than the so-called power-2 and power-1 closures [12, 14, 19, 20]. This statement will be confirmed in our present studies of inhomogeneous systems (see section 5).

Thirdly, let us introduce the set $\Gamma = \{n_i, u_{ij}\}$ of dynamical variables. Then, taking into account equation (8), the complicated coupled system of $N^d + N^d \times N^d$ autonomous ordinary differential equations (6) and (7) with respect to the same number of unknown quantities $n_i$ and $u_{ij}$, where $i, j = 1, 2, \ldots, N^d$, can be cast in the compact Liouville-like form

$$\frac{d \Gamma}{dt} = \Psi \Gamma,$$

where

$$\Psi = \sum_{i=1}^{N^d} \Psi_i + \sum_{i \neq j=1}^{N^d} \Psi_{ij}$$

is the differential operator. Its components are $\Psi_{ij} = \Psi^I_{ij} + \Psi^II_{ij}$ and

$$\Psi_i = \left(\alpha_i - \beta_i n_i\right) \frac{\partial}{\partial n_i},$$

$$\Psi^I_{ij} = \left(\alpha_{ij} - \beta_{ij} u_{ij}\right) \frac{\partial}{\partial u_{ij}},$$

$$\Psi^II_{ij} = -\left((1-\delta_{ij})\gamma_{ij} u_{ij}^3 + \delta_{ij} \zeta_{ij} u_{ij}^3\right) \frac{\partial}{\partial u_{ij}}.$$  

The decomposition coefficients entering to equations (11)–(13) can be expressed using equations (6) and (7) as

$$\alpha_i = h \sum_{j \neq i} a_{ij} n_j - h \sum_j b_{ij} u_{ij}, \quad \beta_i = m - ha_{ii},$$

as well as
\[ \alpha_{ij} = a_{ij}(n_i + n_j) + h \sum_{k \neq i} a_{ik}u_{jk} + h \sum_{k \neq j} a_{jk}u_{ik}, \]
\[ \beta_{ij} = 2(\beta_i + b_{ij}) + h \sum_{k \neq i,j} (b_{ik} + b_{jk})(u_{ik}n_k/n_j + u_{jk}n_j/n_k), \]
\[ \gamma_{ij} = h \frac{b_{ij} + b_{ji}}{n_in_j}(u_{ii} + u_{jj})/n_j, \quad \zeta = \frac{2hb_{ij}}{n_j}. \] (15)

Fourthly, in view of equation (9), the solution to the ISMD equations is
\[ \Gamma(t) = \left[ e^{\Psi \Delta t} \right]^K \Gamma(0), \] (16)
where \( \Delta t \) and \( K = t/\Delta t \) denote the time increment and total number of steps, respectively. Since the time evolution operator \( e^{\Psi \Delta t} \) cannot be handled exactly, proceeding in the spirit of [49] and [50] we derive the multistage decomposition propagation (DP):
\[ e^{\Psi \Delta t} = \prod_{i,j=1}^{N^d} e^{\Psi ij \Delta t} \prod_{i=1}^{N^d} e^{\Psi i \Delta t} \prod_{i,j=1}^{N^d} e^{\Psi ij \Delta t} + O(\Delta t^3). \] (17)

Here the factorization is performed symmetrically with respect to \( i \) and \( j \), while \( i \leq j \) because of \( u_i(y,x) = u_i(x,y) \), i.e. \( u_{ij} = u_{ji} \). Due to the specially tailored decomposition (equations (10)–(15)) of \( \Psi \), each of the single exponentials appearing in equation (17) can be evaluated analytically. Indeed, the coefficients \( \alpha_i \) and \( \beta_i \) do not depend on \( n_i \) for every \( i \), as this follows from equation (14). Then according to equation (11), the operator \( e^{\Psi ij \Delta t/2} \) acting on the local density \( n_i \) results in the analytical solution
\[ e^{\Psi ij \Delta t/2} n_i = n_i e^{-\beta_i \Delta t/2} + (1 - e^{-\beta_i \Delta t/2}) \alpha_i / \beta_i. \] (18)

Moreover we perform further symmetrical decomposition,
\[ e^{\Psi ij \Delta t/2} u_{ij} = e^{\Psi ii \Delta t/2} e^{\Psi ij \Delta t/2} e^{\Psi jj \Delta t/2} u_{ij} + O(\Delta t^3), \] (19)
where the single exponential propagators acting on the local correlation density \( u_{ij} \) lead to the exact solutions
\[ e^{\Psi ii \Delta t/2} u_{ij} = u_{ij} e^{-\beta_i \Delta t/2} + (1 - e^{-\beta_i \Delta t/2}) \alpha_i / \beta_i, \]
\[ e^{\Psi ii \Delta t/2} u_{ij} = u_{ij} / \left( 1 + \gamma_{ij} u_{ij} \Delta t / 4 \right), \quad \text{for } i \neq j, \]
\[ e^{\Psi jj \Delta t/2} u_{ii} = u_{ii} / \left( 1 + \zeta_i u_{ii} \Delta t / 2 \right)^{1/2}. \] (20)

Identities (20) were obtained by using equations (12) and (13) as well as the independence of \( \{ \alpha, \beta, \gamma \}_i \) or \( \zeta_i \) on \( u_{ij} \) or \( u_{ji} \) at given \( i \) and \( j \) (see equation (15)).

It is worth underlining that the applied above combination of the analyticity with symmetry has allowed us to reach the maximal possible precision of the factorization equation (17) at a given number of exponential operators. This factorization can be related to a Verlet-like integration since it is symmetrical and accurate to the second-order in the time step \( \Delta t \). As is well known, the Verlet-type algorithms [49, 50] are the main workhorse for molecular dynamics simulations of classical and quantum systems [51] including complex biochemical liquids [52] as well as for hybrid Monte Carlo simulations in quantum chromodynamics [53]. The third-order \( O(\Delta t^3) \)-uncertainties appear because, in general, the operators \( \Psi_i \) and \( \Psi_j \) do not commute between themselves for different integers \( i \) and \( j \). An Euler-like
counterpart of equation (17) can be drawn from the decomposition method [49, 50] by using the unsymmetrical factorization

$$e^{\Psi \Delta t} = \prod_{i \leq j = 1}^{N^d} e^{\Psi_{ij} \Delta t} \prod_{i = 1}^{N^d} e^{\Psi_{i} \Delta t} + O(\Delta t^2). \tag{21}$$

The number of exponential operators in equation (21) is $N^d + N^d(N^d + 1)/2$, i.e. twice smaller than that of the Verlet-like integration (17), but now the precision of the computations decreases to the first order. For this reason, the Euler-like scheme (21) is not recommended and the preference should be given to the symmetrical second-order decomposition algorithm (17).

More accurate algorithms of higher orders can also be constructed. The straightforward way is to apply the composition approach [49, 50] to the second-order signature

$$\Theta_2(\Delta t) = \prod_{i \leq j = 1}^{N^d} e^{\Psi_{ij} \Delta t} \prod_{i = 1}^{N^d} e^{\Psi_{i} \Delta t} = \Theta_2(\lambda \Delta t) \Theta_2((1 - 2\lambda)\Delta t) \Theta_2(\lambda \Delta t) + O(\Delta t^5), \tag{22}$$

of equation (17). For example, the fourth-order algorithm can be derived with the help of the symmetrical triple product

$$e^{\Psi \Delta t} = \Theta_2(\lambda \Delta t) \Theta_2((1 - 2\lambda)\Delta t) \Theta_2(\lambda \Delta t) + O(\Delta t^5), \tag{23}$$

where $\lambda = 1/(2 - \sqrt{2})$. The computational efforts in equation (23) increase in three times with respect to those of equation (17), but the uncertainties decrease up to the fifth order. Similarly, the integrators of arbitrary higher order can be assembled. Their optimization can be performed, too. All these questions as well as a comprehensive analysis on building the best algorithms for ISMD in context of accuracy and efficiency will be considered in a separate study.

In view of the aforesaid, the numerical solutions $n_i(t)$ and $u_{ij}(t)$ are obtained for any time $0 < t \leq T$ by consecutively applying equations (16)–(20) and (23). Of course, the DP factorizations (equation (17) or (23)) are not exact, so that the $O(\Delta t^3)$- or $O(\Delta t^5)$-uncertainties arise. However, they can be reduced to an arbitrary small level by decreasing the size $\Delta t$ of the time step.

4. Results

The ISMD/KSA/DP simulations were carried out in $d = 1$ at $L = 80$ and $h = 0.0125$ with $N = 6400$. Time integration was done with a step of $\Delta t = 0.05$ by using the second-order decomposition algorithm (equation (17)). Further increasing space and time resolution does not affect the solutions. The initial ($t = 0$) density distribution $n_0(x)$ was the Gaussian centered at $x = 0$ with $c_0 = 1$ and $\sigma_0 = 1$. Then $n_i(-x) = n_i(x)$, and thus $n_i(x)$ will be presented only for $x \geq 0$. The Dirichlet boundary conditions were applied to exclude the finite-size effects. Since we have five parameters ($m, c_{\pm},$ and $\sigma_{\pm}$) of the BDDC model, equations (3) and (4) can describe various populations (see section 2). We consider two characteristic examples. The first one is a system (of type 1) with short-range dispersal, $\sigma_{+} = 0.1$, and mid-range competition, $\sigma_{-} = 1$, modeled by the top-hat kernels. The second example (type 2) concerns short-range competition, $\sigma_{-} = 0.1$, and mid-range dispersal, $\sigma_{+} = 1$, for the Gaussians. For both types, a small mortality, $m = 0.01$, and moderate intensities, $c_{\pm} = 1$, were supposed.
The ISMD/KSA/DP densities $n_\ell(x)$ are shown in figures 1(a) (type 1) and 2(a) (type 2). The MF data (type 1) are presented in figure 1(b). From figure 1 one can see that the MF approximation incorrectly predicts a periodic structure with deep amplitude modulation in a steady state at $t \gtrsim 160$. On the other hand, no such pattern arises within the accurate ISMD description. Here, with increasing $t$, the function $n_\ell(x)$ becomes flat in $x$ near $x = 0$, while a strong oscillating-like inhomogeneity is maintained at the wavefront of the propagation. This striking difference is a consequence of the MF assumption that spatial correlations are completely neglected altogether. The fact that the MF approach can fail dramatically in some cases was mentioned earlier for lattice models [38–40]. For type 2, the ISMD density profiles are more smooth (see figures 1(a) and 2(a)) and similar in shape with the MF ones (not shown) but noticeably larger than the latter in amplitude.

The total number $S(t) = \int n_\ell(x)\,dx$ of entities (population size) and their mean square displacement (msd) $\langle x^2 \rangle(t) = \int x^2 n_\ell(x)\,dx/S(t)$ are plotted in figure 2(b) versus $t$ with the help of curves labeled by ‘size’ and ‘msd’. We see that the MF model appreciably underestimates values of $S(t)$ for both the types. The ISMD function $\langle x^2 \rangle$ of type 1 begins to depend linearly on $t$ in a steady state after a relaxation time of $t \sim 32$. The linearity $\langle x^2 \rangle \sim t$ indicates about a diffusive-like behaviour inherent to local dispersal ($\sigma_+ \ll 1$). For type 2, we have $\langle x^2 \rangle \sim t^2$ in a steady state at $t \gtrsim 24$, meaning that a regular regime with $S \sim t$ takes place.

Once the steady states have been achieved at $t = T$, where $T \sim 32$ or 24 for systems of type 1 or 2, respectively, we come to a persistent wave-propagation regime. In this regime $\partial n_\ell(x)/\partial t = 0$ and the spreading speed $v_\ell(x) = dx/\partial t = -(\partial n_\ell(x)/\partial t)/(\partial n_\ell(x)/\partial x)$ does not depend on time, i.e. $\partial v_\ell(x)/\partial t = 0$. Moreover, this speed will be independent of coordinate at significantly large $x$, where $v_\ell(x) \approx v$. Then, having the numerical solution $n_\ell(x) \equiv n(x,t)$ for $0 < t \leq T$, further time behaviour of local density at $t > T$ can be non-simultaneously evaluated using the relation $n(x + vt, T + \tau) = n(x,T)$, where $\tau > 0$. In this context, $v$ could be associated with the velocity of travelling-like waves [54]. A separate numerical computation of $n_\ell(x)$ and $v_\ell(x)$ in steady states ($t > T$) applying the condition $\partial v_\ell(x)/\partial t = 0$ complemented by the stability analysis will be done in our next studies.

Note that the spatial moments $n_\ell(x)$ and $u_\ell(x,y)$ can be rigorously defined [15, 18] as the averages $n_\ell(x) = \frac{1}{K} \sum_{\kappa=1}^{K} \langle \hat{n}_\ell^{(\kappa)}(x) \rangle$ and $u_\ell(x,y) = \frac{1}{K} \sum_{\kappa=1}^{K} \langle \hat{u}_\ell^{(\kappa)}(x,y) \rangle$ of the microscopic
\(\sum_{x} = \). Moreover, contrary to the integer numbers \(x_Nx_u\equiv N=\sum_{x} \), as well as finite numbers \(\delta x_N\sum_{x}=\delta -x_{\kappa}x_{\kappa}\) densities at a given time \(t\) over the infinite number \(K\to\infty\) of identical realizations, the deterministic equations \(3\) and \(4\) for spatial moments depend continuously on coordinates and time.

It should be mentioned also that after the aforementioned averaging over the statistical ensembles (realizations) on the microscopic level, the stochastic dynamical processes can be described by the self-consistency relation

\[
\langle \rangle_s = \hat{\overline{n}}(0) = \frac{1}{N}\sum_{\kappa} \hat{\overline{n}}(\kappa) = n_0(x).
\]

where, \(\hat{\overline{n}}(\kappa)\) denotes the macroscopic (coarse-grained) averages followed by the ensemble (realization) averaging (designated by the overline), giving expectation values, while \(x_x(0)\) and \(x_x(\kappa)\) are the positions of entity \(x\) at times \(t = 0\) and \(t > 0\), respectively, related to the \(\kappa\) th realization. Then, in particular, \(\lim_{K\to\infty} \frac{1}{K}\sum_{\kappa=1}^K \hat{\overline{n}}_\kappa = \int n_x dx = N(t) = S(t)\), and \(\int \int u_x(x,y) dxdy = \frac{1}{N}[N-1] = \frac{N^2}{N}\). Moreover, contrary to the integer numbers \(N_x(\kappa)\) of entities, their mean value \(S(t)\) is a continuous function of time, while the spatial moments depend continuously on coordinates and time.

It should be mentioned also that after the aforesaid averaging over the statistical ensembles (realizations) on the microscopic level, the stochastic dynamical processes can be described by the (mesoscopic) deterministic equations \(3\) and \(4\) for spatial moments \(n(x)\) and \(u(x,y)\).

Such equations are able to describe populations with infinite \((N\to\infty)\) as well as finite number \(N(t)\) of entities. The first- and second-order moments are connected between themselves by the self-consistency relation \(\int u_x(x,y) dy = (N^2/N - 1)n_x(x)\). This relation was fulfilled in our numerical ISMD/KSA/DP simulations with a great precision, confirming a high efficiency of the proposed method.

The inhomogeneous pair correlation function (IPCF) \(g_0(x,y) = u_x(x,y)/\langle n_x(x)n_x(y)\rangle\) is depicted in figure 3 at \(t = 32\) (type 1) and \(t = 24\) (type 2) as dependent on \(y - x\) on \(x = 0\) and three wavefront points \(x = x_{\text{III}}\). The latter were chosen such that \(n_x(x_{\text{III}})\) decreases to levels 3/4, 1/2, and 1/4 with respect to the maximum of \(n_x\) (see circles connected by dashed curves in figures 1(a) and 2(a)). Figure 3 demonstrates that \(g_0(x,y)\) can deviate significantly from the MF value 1. Note that the initial condition \(g_0(x,y) = 1\) with no pair correlations was utilized at \(t = 0\). These correlations are quickly reproduced owing to the interactions, so that already at \(t \geq 32\) (type 1) or \(t \geq 24\) (type 2) we achieve the steady states.

For type 1, we observe a strong clustering, \(g_0(x,y) \gg 1\), of entities in the narrow interval \(|y - x| < \sigma_x\) at the wavefront \((x = x_{\text{III}})\) of density propagation, see figure 3(a). With
increasing distance $|y - x|$, the clustering suddenly transforms into a wide area of deep disaggregation, $g_t \approx 0$. In the homogeneous domain ($x = 0$) these effects are not so visible. Note also that $g_t(x, y) = g_t(y, x)$, whereas $g_t(x, y)$ is an asymmetric function in $y - x$ at $x \neq 0$. For type 2, the IPCF identifies an intense disaggregation at small separations $|y - x| \sim 0$, where $g_t(x, y) \ll 1$ (look at figure 3(b)). Near $|y - x| \gtrsim \sigma -$, the disaggregation changes to a moderate clustering ($1 < g_t < 2$). At the wavefront ($x = x_{I,II,III}$), the spatial correlations are maintained up to long distances $|y - x| \sim 10 - 20$, where $g_t(x, y)$ decreases to its asymptotic value 1 very slowly with increasing $|y - x|$. This effect becomes stronger in the direction of propagation. No such long tails are detected in the homogeneous region $x = 0$, where $g_t(x, y) \to 1$ already at $|y - x| \gtrsim 3$, just as in figure 3(a) for type 1 at any $x$.

5. Discussion and conclusions

The above effects can be explained by a subtle interplay between the dispersal and competition forces in the presence of reproductive pair correlations at inhomogeneous density distributions. Indeed, as the distance over which offspring disperse is made shorter (by reducing $\sigma_+$), individuals are increasingly clustered in space, $g_t \gg 1$, around points where they were born. That small portion of entities which has dispersed outside the narrow interval $|x - y| < \sigma_+$ is soon killed, $g_t \approx 0$, by the neighbouring agents owing to the competition with them in the wide domain $\sigma_+ < |x - y| < \sigma_-$. This leads to deep disaggregation, the pattern observed in figure 3(a), where $\sigma_+ \ll \sigma_-$. In the opposite regime $\sigma_- \ll \sigma_+$, the competition interactions acting over the narrow interval $|x - y| < \sigma_+$ are local and strong. As a result, a sizeable part of agents in this interval dies immediately after their birth, $0 < g_t \ll 1$, while survivors are overdispersed up to long distances $|x - y| \gtrsim \sigma_+$ with moderate correlations $1 < g_t < 2$. This picture is seen in figure 3(b), where $\sigma_+ \gg \sigma_-$. The two types of behaviour just described are visible to some extent even in the homogeneous zone (0-curves of figure 3). In the inhomogeneous region, they become much more evident (I,II,III-curves), especially in the direction of density propagation. This somewhat unexpected behaviour can be treated as follows. At the wavefront, the local density $n_t(x)$ rapidly decreases.
to zero with increasing $|x|$. Then the relative contribution of the term $a(x, y)\left(n_t(x) + n_t(y)\right)$ in the rhs of the first line of equation (4) grows. It describes dispersal of the daughter cell to $x$ from the parent at $y$ and vice versa, and thus is responsible for reproductive pair correlations (RPCs). This term is proportional to $n_t$, while all others are weighted by $n_t^2$ or $n_t^3$ since $u_t(x, y) = g_t(x, y)n_t(x)n_t(y)$ and $w_t \sim n_t^3$. At small $n_t$ this means that the RPC processes are dominant over the competition ones, leading to an increase of $g_t$. For the same reason, the asymmetric long tails appear at $\sigma_+ \gg \sigma_-$ in the inhomogeneous regions, as the correlations are strong enough ($1 < g_t < 2$) at $|x - y| \sim \sigma_+$ and cannot quickly disappear with increasing $|x - y|$ due to the RPCs. No long tails arise at $\sigma_+ \ll \sigma_-$ because of the wide-range deep disaggregation in this case. They are also absent in the homogeneous regions where the relative impact of the RPCs is small.

It should be emphasized that the RPCs are a uniquely biological complication with no analogue in the physical and chemical problems [26]. The most conspicuous example is from physics of liquids where $g_t$ tends to 1 in the limit $n_t \to +0$ of small densities [36]. In our case, this function can take arbitrary positive values at $n_t \to +0$ unless $|x - y| \to \infty$. The reproduction of entities is a compelling reason [15] for the failure of the MF (Poisson) assumption $g_t(x, y) = 1$ even at $n_t \to +0$. Remember that $g_t(x, y)$ is the probability of finding one entity at $x$ and another one at $y$ relative to the probability of having entities at $x$ and $y$ if they were independently distributed. Any real organisms are born next to their siblings. Therefore, reproduction ineluctably creates non-Poisson spatial correlations ($g_t \neq 1$) between individuals (daughter cells).

The wavefront dynamics is displayed in figure 4 using the continuous spatio-temporal representation for $n_t(x)$. Mention that having $n_t(x)$ in a wide region of varying $x$ and $t$, the spreading speed can be calculated as $v_t(x) = -(\partial n_t(x)/\partial t)/(\partial n_t(x)/\partial x)$. We see that the shape and curvature of the wavefront are quite different in the two cases. As for the inhomogeneous pair correlation functions, this is caused by the different types of the interference between the dispersal, competition, and RPCs at spatial inhomogeneity. Similar results to those presented in figures 1–4 for $d = 1$ were observed at $d = 2$. They will be presented and discussed in a separate paper elsewhere.

Our investigations have shown that the previously known standard methods working well at spatially homogeneous conditions are unsuitable for solving the ISMD equations at the presence of reproductive processes. As an illustration, in figure 2(b) we include the data obtained for $S(t)$ by the classical Runge–Kutta (RK4) scheme of the fourth order. This scheme is commonly exploited in spatial population dynamics of lattice [38–42] and off-lattice [43, 44] models. It can be seen that the RK4-values for $S(t)$ quickly become negative and unstable with huge deviations even though a very small time step of $\Delta t = 10^{-4}$ is employed. As was realized, the same drawback is inherent to all other standard numerical methods. The difficulty with these methods in the presence of the RPCs for spatially inhomogeneous systems can be explained by the existence of a singularity in the KSA (equation (5)) third-order correlation function $w_t(x, y, z) = u_t(x, y)u_t(x, z)u_t(y, z)/(n_t(x)n_t(y)n_t(z))$ for regions where $n_t$ is close to zero. The standard methods cannot handle this singularity because they are built on regular finite-difference schemes. In the ISMD/KSA/DP approach, the above singularity is removed since this part of the dynamics is integrated analytically by the product (17) of exponential transformations (18)–(20), guarantying the positiveness of the spatial moments. For instance, the rhs of the equalities in equation (20) always remains positive by construction for any $\beta$ owing to the fact that $\alpha, \gamma$, and $\zeta$ are greater than zero according to equation (15). As these equalities are exact, they can be applied at any values of $\alpha, \beta, \gamma, \zeta$, and $\Delta t > 0$. The RK4 method fails in the singular region, where $\gamma$ and $\zeta$ can be large due to the RPCs, because
then the conditions $\gamma u \Delta t / 4 \ll 1$ and $\zeta u^2 \Delta t / 2 \ll 1$ are violated at normal sizes of $\Delta t$. These conditions are mandatory for RK4 but not for DP in view of the analyticity of the latter.

Recently, an interesting approach has been proposed [55] for exploring the adaptive voter model dynamics. It combines heterogeneous expansions to approximate the network by an infinite system of ordinary differential equations, generating functions, and solution of the resulting partial differential equation. Taking into account that moment expansions are widely used in network models [32, 55–57] and the fact that the discretized version of the spatially inhomogeneous model considered is nothing but a particular network, a natural question arises: can the above triple jump trick [55] be used to solve the infinite system (when $N \to \infty$) of autonomous ordinary differential equations (6) and (7). Unfortunately, this is impossible because the adaptive voter model differs significantly from our spatially inhomogeneous BDDC model. For instance, the first two steps of the triple jump trick are not necessary in our case since we have already the partial integro-differential equations (equations (3) and (4)) at the very beginning. In general, these equations cannot be solved analytically because of the presence of spatial integrals. The latter are absent in the partial differential equations for the voter model dynamics [55]. Only in a particular case of the MF approximation $n_t = n_0^2$ and the spatially homogeneous initial distribution when $n_0(x) \equiv n_0$ does not depend on $x$, we obtain the unique exact solution of equation (3) in the analytical form $n_t = (c_+ - m)n_0/((c_+ - m - n_0c_-) \exp[-(c_+ - m)t] + n_0c_-)$.

The positiveness of $n_t(x)$ and $u_t(x,y)$ in our approach is also provided by the inhomogeneous third-order KSA ansatz (5). Closures of lower orders cannot ensure positive solutions and thus are not appropriate. In order to demonstrate this, the functions $S(t)$ obtained within the power-1 and -2 closures [12, 14] are included in figure 2(b) as well (curves marked by CL1 and CL2) for the system of type 1. We see that the CL2 scheme produces the results even worse than those of the MF approximation, while the CL1 curve falls at all into the negative region (the same behaviour was observed for type 2). It is worth mentioning that similar conclusions on inferiority of the lower-order closures were made earlier in the case of spatially homogeneous systems [12, 14, 19, 20].

The limitations of the ISMD/KSA/DP approach are caused by the approximate character of the KSA closure [36, 37]. As a consequence, it cannot be used at those values of the ISMD model parameters $(c_\pm, \sigma_\pm, m)$ which lead to critical regimes or to $(x, y)$-regions where $g_t(x,y)$ is extremely high. The exact closure can be represented as an infinite diagrammatic series in

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**Figure 4.** The ISMD wavefront dynamics for short-range dispersal (subset (a)) and short-range competition (subset (b)).
terms of multiple integrals of correlation functions [36]. However, these integrals are cumbersome and computationally intractable. Similar challenges, including effects of short loops in graph topologies, arise within adaptive network models [4, 56, 57]. A way to improve the ISMD/KSA/DP method consists in adding the third equation [18] for the fourth-order spatial moment to equations (3) and (4), complemented by the Fisher–Kopeliovich closure [58, 59]. The latter is more precise than KSA and thus should further increase accuracy of the ISMD description. All these questions will be the subject of our future researches.

The DP technique developed in this paper can be considered as the first extension of the powerful decomposition methodology [49, 50] widely exploited in molecular dynamics simulations of liquids to the field of population dynamics. Its powerfulness is provided by the preservation of characteristics features inherent in exact solutions, such as reversibility and symplecticity of flow in phase space for liquids or positiveness of spatial distribution functions for population systems. Other techniques such as the Liouville formalism, concepts of dynamical variables, infinite hierarchy for correlation functions, and moment closures, all taken from non-equilibrium statistical physics, were also used in our work.

6. Summary

We have derived the novel ISMD/KSA/DP approach to population dynamics simulations of spatially inhomogeneous birth-death systems with nonlocal dispersal and competition. It is based on the decomposition technique to solve numerically the master equations for spatial moments of entity distribution in continuous space by splitting the time evolution operator into analytically solvable parts. This has enabled us to perform the first spatial moment dynamics modeling of such systems as well as to find and explain new subtle effects which can take place in real populations. They include the possible presence of asymmetric long tails in inhomogeneous pair correlation functions, as well as the coexistence of strong clustering and deep disaggregation in the wavefront of spatial propagation.

The proposed approach can readily be adapted to more complex, multicomponent ISMD models [18–21] by including neighbour-dependent birth, motility, marked agents, mutation, directionally biased movement, etc. The ISMD/KSA/DP simulations can also be expanded to higher dimensions. The corresponding results on these topics will be presented in separate publications.

Acknowledgments

Part of this work was supported in 2017 by the European Commission under the project STREVCOMS PIRSES-2013-612669. YK acknowledges the support in 2018 of the National Science Centre, Poland, grant 2017/25/B/ST1/00051.

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