A velocity–diffusion method for a Lotka–Volterra system with nonlinear cross and self–diffusion

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Abstract

The aim of this paper is to introduce a deterministic particle method for the solution of two strongly coupled reaction–diffusion equations. In these equations the diffusion is nonlinear because we consider the cross and self–diffusion effects. The reaction terms on which we focus are of the Lotka–Volterra type.

Our treatment of the diffusion terms is a generalization of the idea, introduced in [8] for the linear diffusion, of interpreting Fick’s law in a deterministic way as a prescription on the particle velocity. Time discretization is based on the Peaceman-Rachford operator splitting scheme.

Numerical experiments show good agreement with the previously appeared results. We also observe travelling front solutions, the phenomenon of pattern formation and the possibility of survival for a dominated species due to a segregation effect.

Key words: Particle Methods, Nonlinear Diffusion, Reaction–Diffusion, ADI Schemes, Pattern Formation, Travelling Fronts


1 Introduction

In this paper we shall be concerned with the following coupled equations for the two scalar quantities $u(x,t)$ and $v(x,t)$:

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\[ \partial_t u + \nabla \cdot J_u = f(u, v) , \tag{1.1} \]
\[ \partial_t v + \nabla \cdot J_v = g(u, v) , \tag{1.2} \]

where \((x, t) \in \Omega \times [0, T]\) with \(\Omega \subset \mathbb{R}^n\), and the fluxes of \(u\) and \(v\) are respectively:

\[ J_u = -\nabla (c_1 u + a_1 u^2 + b_1 uv) + d_1 u \nabla \phi , \tag{1.3} \]
\[ J_v = -\nabla (c_2 v + a_2 v^2 + b_2 uv) + d_2 v \nabla \phi . \tag{1.4} \]

In the expressions of the fluxes the quantities \(a_i, b_i, c_i\) and \(d_i\) are constants while \(\phi(x, t)\) is a scalar functions that, in agreement with the population dynamics literature, we shall call ecological potential. The system (1.1)-(1.2) must be supplemented with the initial conditions:

\[ u(x, 0) = u_0(x) , \quad v(x, 0) = v_0(x) , \tag{1.5} \]

and with boundary conditions. We shall impose Neumann boundary conditions assuming a zero net flux through the boundary:

\[ J_u \cdot n = J_v \cdot n = 0 \quad \text{for} \quad x \in \partial \Omega , \tag{1.6} \]

where \(n\) is the outgoing normal to the boundary.

The reaction terms \(f(u, v)\) and \(g(u, v)\) describe the kinetics of the interaction between \(u\) and \(v\). In this paper we shall consider Eqs.(1.1)-(1.2) as a population dynamics model and therefore we shall assume the kinetic to be of the Lotka–Volterra type, i.e.:

\[ f(u, v) = K (\mu_1 - \gamma_{11} u - \gamma_{12} v) u , \tag{1.7} \]
\[ g(u, v) = K (\mu_2 - \gamma_{21} u - \gamma_{22} v) v . \tag{1.8} \]

We shall assume all \(K, \mu_i\) and \(\gamma_{ij}\) as positive constants, meaning that we shall focus on the competitive interaction case. The role of the constant \(K\) is to tune the strength of the interaction or, alternatively, to regulate the size of the spatial domain and the time scale, see [19].

The nonlinear expression (1.3)-(1.4) for the fluxes was proposed in the context of population dynamics modelling (for the first time, to the best of our knowledge) by Shigesada, Kawasaki and Teramoto in [24] (see also [18]) as a model describing the tendency of two competing species to diffuse faster (than predicted by the usual linear diffusion) toward lower densities areas. This diffusion is driven by the local density; the coefficients \(a_i\) and \(b_i\) are called self–diffusion coefficients and cross–diffusion coefficients respectively. In the case of competing species, clearly, all the coefficients \(a_i, b_i\) and \(c_i\) are greater or equal.
to zero. For a derivation of nonlinear diffusion population models based on a microscopic approach see [25].

Equations (1.1)-(1.2) have been extensively studied in the literature. Regarding the time independent case and the asymptotic in time behavior of the solutions we refer to the papers [16,20,17,23,22] and to references therein. Basically these papers analyze the possibility of the existence of non constant steady state solutions. Regarding the evolutive problem we refer to [3,4]. In these papers the authors are able to show the existence of nonnegative weak solutions. Roughly speaking they assume that the initial data are nonnegative, and that either the classical diffusion coefficients $c_i$ or the self–diffusion coefficients $a_i$ are positive.

The problem of the numerical solution of Eqs.(1.1)-(1.2) has been tackled in [12] (see also [13]) and [1]. In [12] the authors consider the 1D case and used a numerical scheme based on finite–differences; nonlinearities in the equations are treated implicitly through iteration, while the nonlinear boundary conditions are treated explicitly. The scheme in [12] seems not able to handle the convection dominated case, for example when the coefficients $d_i$ are large and the diffusion coefficients are small. In [1] the authors solve the equations using a finite–element approximation. They can handle the case when the transport coefficients $d_i$ are large; in their numerical tests it seems they get a first order convergence in time and convergence in space of order somewhere in between first and second order. In all these papers the rigorous convergence of the schemes is proved.

The aim of the present paper is to introduce a different numerical method. Spatial discretization is achieved through a particle approximation of the solution. Time evolution is treated through operator splitting (convection–diffusion terms and reaction terms are treated separately) and an ADI scheme.

The plan of the paper is the following. In Section 2 we neglect the role of the reaction terms, and explain how the velocity–diffusion method can be implemented to deal with the purely convective–diffusive part of the model equations. In the numerical experiments first we reproduce some of the previously appeared results, then show how the system admits travelling wave solutions, a phenomenon that had already been analyzed from the theoretical point of view, see [27] and references therein. In Section 3 we solve the full reaction diffusion system through the Peaceman–Rachford operator splitting. In the numerical experiments we show, first that segregation effects allows to a dominated (in the sense that the reaction terms predict its extinction) species to survive in a spatial niche, second that for sufficiently large spatial domain a delicate interplay between nonlinear diffusion and kinetics leads to pattern formation. In Section 4 we draw some conclusions and suggest some possible future work.
2 The numerical method: no reaction terms

In this section we shall explain the method we have used to deal with the diffusive part of Eqs. (1.1)-(1.2). We shall therefore set the reactive part $f(u, v) = g(u, v) = 0$.

2.1 The diffusion–velocity method

During the last two decades, particle methods have become one of the most popular tools for the numerical solution of partial differential equations. There are many reasons for this increasing popularity and we mention only those who motivated us: the fact that they adapt quite well to the cases when the geometry of spatial domain is not a standard one; the fact that they are relatively easy (at least in principle) to implement; the capability, because of their intrinsic lagrangian nature, to resolve small scale phenomena (see e.g. the recent [5]) and to handle convection-dominated regimes.

Although particle methods have been originally introduced to deal with hydrodynamics equations, it has been shown that the method can effectively deal also with diffusive equations. In these case the method has been named diffusion–velocity method, and was introduced, for the scalar linear diffusion equation, by Degond and Mustieles in [8] (see also references therein and [7]). Lions and Mas–Gallic, in [15], gave a rigorous justification to the method with a generalization to nonlinear diffusion. In [6] the method was also used to solve equations with a dispersive character, while in [2] it was used to deal with anisotropic diffusion.

Suppose to have an equation for the scalar quantity $u(x, t)$ in the convective form:

$$\partial_t u + \nabla \cdot (V(x, t)u) = 0.$$  (2.1)

Then one can seek a particle approximation of the solution in the form:

$$u_N(x, t) = \sum_{i=1}^{N} w_i \delta(x - x_i(t)),$$  (2.2)

where $w_i$ is the mass of the $i$-th particle, $\delta$ is the Dirac distribution, and the $x_i(t)$ evolve according to:

$$\dot{x}_i = V(x_i, t).$$  (2.3)

The above characteristic equation is initialized by a particle approximation of the initial datum. If one wants to use the method to deal with the diffusion
equation $\partial_t u = \nabla^2 u$ one has to recast the equation in the form:

$$\partial_t u - \nabla \cdot \left( u \left( \frac{\nabla u}{u} \right) \right) = 0.$$  

In this case the convective velocity depends on the solution $u$ and on the gradient of $u$, and one has to use a smoothed approximation of the $\delta$ distribution. This approximation is done through a smooth positive kernel $\zeta_\epsilon$, depending on the parameter $\epsilon$ that, when $\epsilon \to 0$ converges to the $\delta$ distribution. Therefore instead of (2.2) one seeks a solution of the form:

$$u_N^\epsilon(x, t) = \sum_{i=1}^N w_i \zeta_\epsilon \left( x - x_i(t) \right), \quad (2.4)$$

with:

$$\zeta_\epsilon(x) = \epsilon^{-n} \zeta(x/\epsilon) \quad \text{and} \quad \int_{\mathbb{R}^n} \zeta(x) dx = 1.$$  

A widely used choice for the kernel $\zeta_\epsilon(x)$ is the gaussian kernel:

$$\zeta_\epsilon(x) = \frac{1}{\epsilon \sqrt{2\pi}} \exp \left( -\frac{x^2}{2\epsilon^2} \right) \quad \text{in 1D}, \quad (2.5)$$

but other choices are certainly possible, and in many cases more convenient, the main drawbacks of the gaussian kernel being the fact that the support is not compact and the fact that it gives only second order accuracy, for a discussion see e.g. [11] and [21].

Therefore, if one seeks a solution of the heat equation in the smoothed form (2.4), one is led to solve the characteristic equation in the form:

$$\dot{x}_i = -\nabla u_N^\epsilon(x_i, t) \frac{u_N^\epsilon(x_i, t)}{u_N^\epsilon(x_i, t)} = -\frac{\sum_{j=1}^N w_j \nabla \zeta_\epsilon \left( x_i - x_j \right)}{\sum_{j=1}^N w_j \zeta_\epsilon \left( x_i - x_j \right)}. \quad (2.6)$$

It is now straightforward the generalization of these ideas to the case of Eqs.(1.1)-(1.2) with the fluxes given by (1.3)-(1.4) (recall that here we are neglecting the role of the reaction terms $f$ and $g$). In fact, looking for an approximation of $u$ and $v$ of the form:

$$u_N^\epsilon(x, t) = \sum_{i=1}^N W_i^u \zeta_\epsilon \left( x - x_i^u(t) \right), \quad (2.7)$$

$$v_N^\epsilon(x, t) = \sum_{i=1}^N W_i^v \zeta_\epsilon \left( x - x_i^v(t) \right), \quad (2.8)$$

one is led to solve the following set of ODE’s for the particle positions $x_i^u, x_i^v$:  

5
\begin{align}
\dot{x}_i^u &= - \left[ 2a_1 \nabla u_N^u(x_i^u, t) + b_1 \nabla v_N^v(x_i^u, t) + \frac{c_1 + b_1 v_N^v(x_i^u, t)}{u_N^u(x_i^u, t)} \nabla u_N^u(x_i^u, t) + d_1 \nabla \phi(x_i^u, t) \right], \\
\dot{x}_i^v &= - \left[ 2a_2 \nabla v_N^v(x_i^v, t) + b_2 \nabla u_N^u(x_i^v, t) + \frac{c_2 + b_2 u_N^u(x_i^v, t)}{v_N^v(x_i^v, t)} \nabla v_N^v(x_i^v, t) + d_2 \nabla \phi(x_i^v, t) \right],
\end{align}

where the gradients \( \nabla u_N^u(x, t) \) and \( \nabla v_N^v(x, t) \) are given by:

\[ \nabla u_N^u(x, t) = \sum_{j=1}^{N} W_j^u \nabla \zeta_j \left( x - x_j^u(t) \right), \quad \nabla v_N^v(x, t) = \sum_{j=1}^{N} W_j^v \nabla \zeta_j \left( x - x_j^v(t) \right). \]

### 2.2 Time discretization

To simplify the notation we denote by \( U = (u, v)^T \) and write the equation (1.1)–(1.2) (with no reaction terms) in symbolic form as:

\[ \frac{dU(t)}{dt} = F(U(t)), \]

where \( F(U) \equiv - (\nabla J_u, \nabla J_v)^T \), with \( J_u, J_v \) defined by (1.3)–(1.4).

To solve (2.11) in \([0, T]\) we divide the interval in sub-intervals of size \( \Delta t \), \([t_m, t_{m+1}]\), for \( m = 0, \ldots, M \), with \( \Delta t = T/M \). We advance in time from \( t_m \) to \( t_{m+1} \) with an implicit time step of size \( \Delta t/2 \), followed by an explicit time step of size \( \Delta t/2 \), i.e.:

\begin{align}
U_{m+\frac{1}{2}} &= U_m + \frac{\Delta t}{2} F(U_{m+\frac{1}{2}}) \quad \text{(2.12)} \\
U_{m+1} &= \left( I + \frac{\Delta t}{2} F \right) U_{m+\frac{1}{2}}, \quad \text{(2.13)}
\end{align}

where \( I \) is the 2 \times 2 identity matrix. To solve (2.12) we use the iterative procedure:

\begin{align}
U_{m}^1 &= U_m \quad \text{(2.14)} \\
U_{m}^{k+1} &= U_m + \frac{\Delta t}{2} F(U_m^k) \quad \text{(2.15)}
\end{align}

until convergence. In our numerical experiments we have used the following
convergence criterion:

\[ U_{m+\frac{1}{2}} = U_m^k \text{ when } \|U_m^k - U_m^{k-1}\|_\infty < \Delta t \cdot 10^{-7}. \]  

(2.16)

2.3 Implementation details

In our numerical scheme it remains to be explained how we have computed the terms of the form \( U^{(1)} + hF(U^{(2)}) \), where \( h \) is a small time step (for example in (2.15) \( h = \Delta t/2 \), \( U^{(1)} = U_m \) and \( U^{(2)} = U_m^k \)).

Let \( U_{N}^{(1),\epsilon} = (u_N^{(1),\epsilon}, v_N^{(1),\epsilon})^T \) a particle approximation of \( U^{(1)} \), with \( u_N^{(1),\epsilon} \) and \( v_N^{(1),\epsilon} \) given by (2.7)–(2.8). Then move the particles from the positions \((x_i^u, x_i^v)\) solving the ODE system (2.9)–(2.10) for a time of size \( h \). The forcing terms of this ODE system are computed using the particle approximation of \( U^{(2)} \). The particles at the new location \((x_i^u(t+h), x_i^v(t+h))\) (and with the same weights \( W_i^u, W_i^v \)) define the particle approximation of \( U^{(1)} + hF(U^{(2)}) \).

To advance the system (2.9)–(2.10) from \( t \) to \( t+h \) we have used the following two–steps Runge–Kutta method:

\[
\begin{align*}
y_{m+\frac{1}{2}} &= y_{m} + \frac{h}{2} f(y_{m}, t_{m}) \\
y_{m+1} &= y_{m} + h f(y_{m+\frac{1}{2}}, t_{m+\frac{1}{2}})
\end{align*}
\]

As a mollifier we have always used the gaussian kernel (2.5). A crucial parameter in the particle approximation is the width \( \epsilon \). We have used \( \epsilon = k(\Delta x)^\alpha \) where \( \Delta x \equiv (b - a)/N \), \( b \) and \( a \) being the extremes of the 1D interval where we solve the equations, and \( 0 < \alpha < 1 \). For \( \alpha \) we have used \( \alpha = 1/2 \) or, to get better accuracy, \( \alpha = 3/4 \). For the constant \( k \) we have used values ranging from 0.2 up to 1.25. Higher values of \( k \), while usually giving poorer spatial accuracy (for example by causing an excessive smoothing of the solution), allows to take bigger time steps. As typical in most particle simulations, we found it necessary to redistribute occasionally the particles. This is necessary to avoid that a concentration of the particles in some places would lead to an excessive spacing between the particles in other places causing instabilities.

The boundary conditions (1.6) are imposed through a specular reflection rule for particles hitting the boundary. Our algorithm, when there is no reaction term, thus ensures an exact conservation of mass.
We have tested our code in all cases presented in [1] and [12]. In these papers the authors computed (using finite elements in [1] and finite differences in [12]) the equilibrium configurations reached by the two species densities under the influence of the ecological potential $\phi(x) = -3(x - 0.5)^2/2$ and for different choices of the parameters; the 1D spatial domain is $[0,3]$. Case I-IV below reproduce, with good qualitative agreement, the results reported in [1] and [12]. In our numerical tests we used $N = 300$ particles (which give the same numerical resolution of [1,12]). We found it necessary to have a smaller time step size (at least for the particle width we have used) in order to get a reasonably fast ($10^{-15}$ iterations at the most critical stages of the computations) convergence of the iterative procedure (2.14)-(2.15); notice however that our convergence criterion is much more restrictive than the criterion adopted e.g. in [1].

I: Large and small cross diffusion terms.
Picking $b_i = c_i = d_i = 1$ and imposing the initial conditions $u_0 = 10, v_0 = 20$, for different values of the self-diffusion coefficient ($a_i = 0, 0.1, 10$), we have obtained the results reported to the left of Fig.1. We have used a particle width of $\epsilon = 0.75\sqrt{\Delta x}$ and a time step of $\Delta t = 10^{-4}$.

II: Segregation effects due to a large ratio of transport coefficients.
Let $a_i = 0.1 b_i = c_i = 1 d_2 = 1, d_1 = 4, 8, 20, 40$ with initial $u_0 = 10, v_0 = 10$. One gets the results shown to the right of Fig.1. In the simulation we took a small particle width, $\epsilon = 0.25\sqrt{\Delta x}$, which needed a relatively small time step size; for example when $d_1 = 40$ we had to chose $\Delta t = 5.0 \times 10^{-5}$.

III: Discontinuous initial data.
Let $a_i = b_i = c_i = d_2 = 1, d_1 = 8, 40$ with initial data $v_0 = 10$ and $u_0(x) = 12$ when $x \in [0, 1.5]$ and $u_0(x) = 8$ when $x \in [1.5, 3]$. In this case we picked $\epsilon = 0.5\sqrt{\Delta x}$ which required a time step $\Delta t = 4 \times 10^{-4}$. The results are shown to the left of Fig.2.

IV: Segregation of the two species.
To the right of Fig.2 we show a different case of segregation when $a_1 = b_i = c_i = d_2 = 1$ and $d_1 = 40$ and $a_2 = 0.01$. The initial data are the same as in Case II.

V: Travelling fronts driven by the potential for small diffusion.
Differently from all other cases, we took a linear potential $\phi(x) = -3x$. Moreover for species $u$ we choose $a_1 = b_1 = 10^{-5}, c_1 = 10^{-4}, d_1 = 1$ with an initial datum of the form $u_0(x) = 0$ when $x \in [0, 1.5]$ and $u_0(x) = 15$.
when $x \in [1.5, 3]$. For species $v$ we took $a_2 = c_2 = d_2 = 1$, $b_2 = 10^{-5}$, and initial datum $v_0 = 10$. In this case, given that the cross diffusion is very small, the two species move independently. While species $v$ reaches the configuration where diffusion and self–diffusion compensate the effect of the potential, the wave front for species $u$ moves at speed $\phi'(x) = -3$.

**VI: Interacting travelling fronts.**

The coefficients are the same of the previous case, except $b_2 = 1$. In Fig. 4 one can therefore see a travelling front for the $v$ species caused by the interaction with the travelling front of the $u$ species.

![Fig. 1. Left: Case I. The equilibrium distribution of the two species $u$ (solid line) and $v$ (dashed line) labeled with different values of the cross–diffusion coefficients $a_i = 0, 0.1, 10$ when $b_i = c_i = d_i = 1$. Right: Case II. When the effect of the ecological potential is much stronger on species $u$, a segregation effect occurs. This effect is particularly evident given that the self–diffusion effect is small, $a_i = 0.1$ and would be mitigated in the presence of stronger self–diffusion.](image)

![Fig. 2. Left: Case III. A discontinuous initial datum for $u$ when all coefficients are 1 except $d_1 = 8, 40$ Right: Case IV. Another case when the two species segregate due to the different values of influence of the ecological potential. In this case given that self–diffusion for species $v$ is small a concentration effect is observed also for $v$. All coefficients are 1 except $d_1 = 40$ and $a_2 = 0.01.](image)
3 The numerical method in presence of reaction terms

We now solve Eqs.(1.1)–(1.2) written in symbolic form as:

\[
\frac{d U(t)}{dt} = F(U(t)) + G(U(t)) ,
\]  

(3.17)
where $G(U) = (f(u, v), g(u, v))^T$, with $f(u, v)$ and $g(u, v)$ defined in (1.7) and (1.8).

We shall solve the above equation using an operator splitting in the form of a Peaceman–Rachford ADI scheme (see e.g. [9,10,14,26] and references therein). The solution at $m + 1$-th time step, $U^{m+1}$, is given in terms of the solution at $m$-th time step, $U^m$, by:

$$U^{m+1} = \left( I - \frac{\Delta t}{2} G \right)^{-1} \left( I + \frac{\Delta t}{2} F \right) \left( I - \frac{\Delta t}{2} F \right)^{-1} \left( I + \frac{\Delta t}{2} G \right) U^m.$$

Said differently, we perform an explicit reactive time step, followed by an implicit diffusive time step, followed by an explicit diffusive time step, finally followed by an implicit reactive time step. The implicit steps (both reactive and diffusive) are done through iteration, as in (2.14)–(2.15), with the same convergence criterion (2.16). This method ensures second order convergence in time and should be able to deal with stiff reactive terms.

Reaction terms change the mass of the particles. We kept into account this effect through the following formula:

$$W_{i, \text{new}}^u = W_{i, \text{old}}^u \left( 1 + \frac{u_{\text{new}}(x_i) - u_{\text{old}}(x_i)}{u_{\text{old}}(x_i)} \right),$$

meaning that the mass of the $i$-th particle relative to species $u$ is changed proportionally to the change of $u$ at the particle location.

### 3.1 Numerical experiments I

Our first experiments deal with the data already studied in [1]. The diffusion coefficients are $a_1 = 0.1$, $a_2 = 0.05$, $b_i = c_i = d_i = 1$, with the parabolic potential of the previous section. The scale coefficient is $K = 1$, the reproduction coefficients are $\mu_i = 1$, while for the competition coefficients matrix $\Gamma = (\gamma_{ij})$ we study four cases:

$$\Gamma_1 = \begin{pmatrix} 0.1 & 0.1 \\ 0.1 & 0.1 \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0.5 & 0.1 \\ 0.5 & 0.1 \end{pmatrix}, \quad \Gamma_3 = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}, \quad \Gamma_4 = \begin{pmatrix} 0.5 & 0.5 \\ 0.1 & 0.1 \end{pmatrix}.$$

The results of the equilibrium solutions are shown in Fig.5, and compare qualitatively quite well with the results of [1]. The numerical solutions have been computed using $M = 300$ particles, with a time step $\Delta t = 10^{-4}$ and using a particle size $\epsilon = 0.5\sqrt{\Delta x}$.

In Table 1 we report some results showing the numerical convergence properties of our scheme. The test is performed in case $\Gamma_4$ above, with the same
diffusion coefficients except $c_i = 0$. To be consistent with [1] we have considered the solution at time $t = 0.2$, and compared the solution at different resolutions with the solution computed using an ultra–fine resolution. The resolutions adopted are $M = 2^i \cdot 10^3$ time steps and $N = 2^i \cdot 32$ particles for $i = 0, \ldots, 4$, while the ultra–fine solution is computed using $M = 2 \cdot 10^5$ time steps and $N = 2048$ particles. It is important to notice that in this experiment the particle size is $\epsilon = 0.5 \cdot (\Delta x)^{3/4}$.

The scheme shows a convergence of order $3/2$ which is consistent with the fact that we are using a second order blob, the Gaussian (2.5), and a particle size that goes like $(\Delta x)^{3/4}$.

### 3.2 Numerical experiments: the creation of a spatial niche

An interesting effect that seems to be shown by the model, is the capability of a species, which the kinetics predicts to go extinct, to survive by creating an ecological niche.

We have imposed the following coefficients for the kinetics: the scale factor is $K = 2$, the reproduction coefficients are $\mu_1 = 0.7$ and $\mu_2 = 0.75$, while the
competition matrix is:

$$\Gamma = \begin{pmatrix} 0.05 & 0.2 \\ 0.05 & 0.05 \end{pmatrix}.$$ 

With this coefficients the species $u$ is dominated by the species $v$ and it should go extinct. However, in some instances, segregation effects allows the survival of the species $u$.

I: **Repulsive potential.**
We have supposed, in the spatial domain $x \in [-\pi, \pi]$ the ecological potential to be of the form:

$$\phi = -\exp (-2x^2),$$

meaning that both species have the tendency to escape from places nearby the origin. Moreover the diffusion and transport coefficients are $a_i = 10^{-4}$, $b_1 = 4.1$, $b_2 = 0.3$, $c_i = 0.2$ and $d_i = 2$. The meaning of the above coefficients is that cross-diffusion is much stronger than self-diffusion, while the effect of linear diffusion is moderate. Starting from the initial conditions, $u_0(x) = v_0(x) = 3$ we have seen that the solution stabilizes in the configuration shown to the left of Fig.6.

The simulation was performed, with spatial resolution $N = 256$, $M = 8 \cdot 10^4$ time steps, and particle width of $\epsilon = 0.5\sqrt{\Delta x}$. Notice how, in places where $v$ dominates, the $v$ density gets closer to the value 15, which is the value $\mu_2/\gamma_{22}$ predicted by the logistic equation (in absence of species $u$).

II: **Attractive potential.**
In the same spatial domain as before we have supposed the ecological potential to be of the form:

$$\phi = \exp (-0.15x^4).$$

Both species are attracted by a spot close to the origin, and the constants in the above potential regulate the size of the spot. The diffusion and transport coefficients are: $a_1 = c_1 = 0.1$, $b_1 = 2$, $d_1 = 10$, $a_2 = c_2 = 0.04$, $b_2 = 10$, $d_2 = 0.4$. In this case the high transport coefficient $d_1$ allows species $u$ to build up enough density close to the origin; the high cross-diffusion $b_2$ prevents species $v$ from invading the niche created by $u$.

3.3 **Numerical experiments: pattern formation for stiff reaction terms**

Another effect shown by the model equations is pattern formation. The spatial domain we have considered is $[-\pi, \pi]$, with no ecological potential. We have picked $a_i = 10^{-4}$, $c_i = 0.2$, $b_1 = 4.1$, $b_2 = 0.3$, $\mu_1 = 1.2$, $\mu_2 = 1.0$; the
Fig. 6. The survival of a dominated species: the species \( u \) (solid line) creates a spatial niche where it can avoid extinction, even when dominated by species \( v \) (dashed line). Left: The equilibrium configuration when the ecological potential pushes both species away from origin and when self-diffusion is dominated by cross-diffusion. Right: The equilibrium configuration when the ecological potential attracts both species toward the origin and species \( v \) does not invade the niche occupied by \( u \) because the cross-diffusion dominates all other effects, \( b_2 >> a_2, c_2, d_2 \).

The competition matrix is:

\[
\Gamma = \begin{pmatrix}
0.5 & 0.4 \\
0.4 & 0.4
\end{pmatrix}.
\]

while the scale factor is \( K = 49.75 \). As initial data we have chosen a periodic perturbation of the stable equilibrium \((u, v) = (2, 0.5)\) predicted by the kinetics:

\[
u_0(x) = 2 + 0.1 \cos(x) + 0.27 \cos(3x/2), \quad v_0(x) = 0.5.
\]

In Fig. 7 one can see how, after a transient that seems to lead the solution toward the constant equilibrium, instabilities develop which finally evolve into a stationary periodic pattern.

We have tested for convergence considering the solution at time \( t = 2.75 \), when the growth of the unstable modes is apparent. We have used \( N = 2^i \cdot 64 \) particles and \( M = 2^{i-1} \cdot 10^4 \) time steps with \( i = 0, \ldots, 4 \). The particle size is \( \epsilon = 0.35 \cdot (\Delta x)^{3/4} \). The test has been performed by comparison with the solution computed at the resolution \( N = 2048 \) particles and \( M = 2^4 \cdot 10^4 \) time steps. The convergence results, which are shown in Table 2, suggest again a convergence of order \((\Delta x)^{3/2}\).

In the case under consideration, given the absence of the ecological potential, it is easy to show that the boundary conditions to be imposed are the homogeneous Neumann boundary conditions. We have therefore compared the results of the particle method with the results of a spectral method. The comparison are shown in Fig. 8, where one can see that at the resolution \( N = 256 \) particles the two solutions are almost indistinguishable.
Fig. 7. Pattern formation starting from a perturbation of the equilibrium predicted by the kinetics. The $u$ (solid line) and the $v$ (dashed line) represented are computed using a resolution of $N = 256$ particles.

Fig. 8. The solutions computed using a spectral method (solid line) compared with the solutions computed using a particle method with resolution $N = 256$ (dashed line) and resolution $N = 128$ (dotted line). When the number of particles is $N = 256$ the particle solution is almost undistinguishable from the spectral solution.

4 Conclusions

In this paper we have shown how particle methods can effectively tackle the problem of solving a coupled set of reaction–diffusion equations with nonlinear diffusion. In the literature [12,1], the system that we have considered had already been analyzed from the numerical point of view and with other methods. We have been able to reproduce, with good qualitative agreement, all the previously reported results. Moreover we have shown how the model equations lead to pattern formation for stiff reaction terms, to travelling wave solutions.
Table 2
Convergence of the numerical scheme in the case when the stiffness of the reaction terms, $K = 49.75$, leads to pattern formation. The solution is considered at time $t = 2.75$ when instabilities have already grown up, see Fig. 8. The figures are derived by comparison with the solution computed at the resolution $N = 2048$. A comparison with the spectral method solution would lead to slightly larger figures but to the same convergence rate of $(\Delta x)^{3/2}$.

<table>
<thead>
<tr>
<th>Grid $(M \times N)$</th>
<th>$L^1$ $\varepsilon_u$</th>
<th>$\varepsilon_v$</th>
<th>$L^2$ $\varepsilon_u$</th>
<th>$\varepsilon_v$</th>
<th>$L^\infty$ $\varepsilon_u$</th>
<th>$\varepsilon_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-1} \cdot 10^4 \times 64$</td>
<td>0.0357</td>
<td>0.0211</td>
<td>0.0183</td>
<td>0.0106</td>
<td>0.0164</td>
<td>0.0115</td>
</tr>
<tr>
<td>$10^4 \times 128$</td>
<td>0.0105</td>
<td>0.0060</td>
<td>0.0054</td>
<td>0.0031</td>
<td>0.0057</td>
<td>0.0034</td>
</tr>
<tr>
<td>$2 \cdot 10^4 \times 256$</td>
<td>0.0038</td>
<td>0.0021</td>
<td>0.0020</td>
<td>0.0011</td>
<td>0.0021</td>
<td>0.0012</td>
</tr>
<tr>
<td>$4 \cdot 10^4 \times 512$</td>
<td>0.0014</td>
<td>7.6 \cdot 10^{-4}</td>
<td>7.0 \cdot 10^{-4}</td>
<td>3.9 \cdot 10^{-4}</td>
<td>7.4 \cdot 10^{-4}</td>
<td>4.4 \cdot 10^{-4}</td>
</tr>
<tr>
<td>$8 \cdot 10^3 \times 1024$</td>
<td>3.9 \cdot 10^{-4}</td>
<td>2.2 \cdot 10^{-4}</td>
<td>2.0 \cdot 10^{-4}</td>
<td>1.1 \cdot 10^{-4}</td>
<td>2.2 \cdot 10^{-4}</td>
<td>1.3 \cdot 10^{-4}</td>
</tr>
</tbody>
</table>

when the diffusion coefficients ruling the behavior of one species are small, and to the creation of a spatial niche that allows the survival of a species that would otherwise be depleted.

Here we have focused on the case when reaction terms is of the competitive Lotka–Volterra type, but a generalization to different kinetics should be straightforward. Moreover the method, in principle, should be equally applicable to the case when the cross–diffusion, instead of being repulsive, is attractive, as e.g. in chemotaxis. However we believe this a more delicate case and the capability of our particle method to deal with phenomena like concentration is still to be tested.

In this paper we have used second order blobs (i.e. the Gaussian), and the rate of convergence we have been able to get is $\epsilon^2$, where $\epsilon$ is the particle size. The possibility of using higher order blobs is under current investigation, and a successful implementation of these would probably need the use of the particle strength exchange method.

Few words about computational costs. Particle methods are usually more demanding that other methods. For example a simulation with $N = 1048$ particle with $N \approx 10^6$ time steps required several hours of computation on a single processor Pentium Xeon 5160. Although code optimization was not our goal, we believe that under this point of view the finite–elements method of [1] is probably more convenient. However, among the other advantages of particle methods, there is the fact that parallelization is really simple. Therefore we believe that 2D and 3D simulations are a perfectly feasible task.
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References


