A PARTICLE–MESH NUMERICAL METHOD FOR ADVECTION–REACTION–DIFFUSION EQUATIONS WITH APPLICATIONS TO PLANKTON MODELLING

F. PAPARELLA[1], F. OLIVERI[2]

[1] *Department of Mathematics "E. De Giorgi", University of Salento*
Via per Arnesano, 73100 Lecce, Italy
[2] *Department of Mathematics, University of Messina*
Salita Sperone 31, 98166 Messina, Italy
E-mail: francesco.paparella@unile.it; oliveri@mat520.unime.it

We present a new method for the numerical solution of advection-reaction-diffusion equations. The method is lagrangian for the advection-reaction part, and uses an auxiliary eulerian grid for the diffusive operator. We discuss the application of the method to the modelling of planktonic populations.

Keywords: Advection–reaction–diffusion equations; plankton modelling; numerical methods

1. Introduction

Any believable model of plankton dynamics should involve at least the three following key factors. *Population dynamics*: planktonic communities are complex ecosystems where tens or hundreds of different species interact through non–trivial food networks; a minimalistic model should at least include the predator–prey dynamics between zooplankton and phytoplankton; more realistic models also explicitly track the concentration of nutrients.[1,2] *Large–scale transport*: on large scales (from a few kilometers to planetary scale) plankton acts as a tracer carried by vortices and ocean currents; communities colonizing nearby water patches may be separated by large distances at later times, and, conversely, initially distant populations may be brought into contact by the oceanic transport. *Small–scale mixing*: plankton is subject to the mixing effects of small–scale turbulence and wave–induced drift; swimming patterns of individual animals, such as nictemeral migrations across the water column, also induce mixing.

Then, the mathematical form of a N–species plankton model is that of

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a set of advection–reaction–diffusion equations:

$$\frac{\partial c_i}{\partial t} = -\underbrace{J(\psi, c_i)}_{advection} + \underbrace{f_i(c_1, \ldots, c_i, \ldots, c_N)}_{reaction} + \underbrace{D_i \Delta c_i}_{diffusion} , \qquad (1)$$

where c_i is the concentration of the i–th plankton species, ψ is a known streamfunction, the jacobian operator J is defined by $J(A, B) = \partial_x A \partial_y B - \partial_x B \partial_y A$, and the numbers D_i are given diffusion coefficients.

Although equations (1) are a rather general formulation of the problem, several assumptions and approximations have already been made. The large–scale flow is assumed to be two–dimensional and incompressible. This is a reasonable approximation for mesoscale and basin–scale dynamics in most areas of the ocean.[3] The small–scale mixing processes are modeled by a Laplacian operator with a constant diffusion coefficient. In some cases a nonlinear diffusion operator might be more realistic, for example in the presence of swimming of the individuals,[4] or slumping of density fronts;[5] however, at the exploratory level of this paper, we prefer to limit ourselves to laplacian diffusion.

2. The Numerical Method

In the absence of diffusion, equations (1) are easily solved by the method of characteristics. A simple and effective numerical scheme, already used in plankton studies,[6] is the following. The initial positions $\{(x_p, y_p)\}_{p=1,\cdots,N_p}$ are assigned to a set of N_p particles with uniformly random distribution within the computational domain. Each particle represents a fluid parcel, which moves according to the law

$$\dot{x}_p = -\frac{\partial \psi}{\partial y}(x_p, y_p, t); \qquad \dot{y}_p = \frac{\partial \psi}{\partial x}(x_p, y_p, t). \qquad (2)$$

The concentration fields are sampled at the particle positions: $c_{p,i}(t)$ is the concentration of the i–th field at the position (x_p, y_p) at time t. They obey to the set of equations

$$\dot{c}_{p,i} = f_i(c_{p,1}, \ldots, c_{p,i}, \ldots, c_{p,N}). \qquad (3)$$

Finally, equations (2,3) may be discretized in time with one of the several well–known schemes for ODEs (for example, we use the second–order Runge–Kutta scheme). We recall that incompressible flows conserve the Lebesgue measure. This implies that an initially uniform distribution of particles moving according to (2) will remain uniform at any later time. As

a consequence there will be no undersampled or oversampled regions of the domain.

Adding a diffusion operator while maintaining the purely lagrangian nature of this scheme is not straightforward. Although particle–based methods for reaction–diffusion equations do exist,[7,8] their application to plankton modelling and a comparison with the method presented here is the topic for a future work.

In this paper we prefer to abandon a purely lagrangian approach. We introduce an auxiliary eulerian grid with meshes of fixed size $\Delta \times \Delta$ to approximate the diffusion operator. The p–th particle contributes to the value of the concentration fields on the k–th grid node, located at (x_k, y_k), with a weight

$$w_p(x_k, y_k) = \int_{x_k-\Delta/2}^{x_k+\Delta/2} \int_{y_k-\Delta/2}^{y_k+\Delta/2} \mathcal{P}(x - x_p, y - y_p) \, dx \, dy.$$

where the *cloud* $\mathcal{P}$ is a function having the following properties: $\mathcal{P}(x,y) \geq 0$; $\mathcal{P}(-x,y) = \mathcal{P}(x,-y) = \mathcal{P}(x,y)$; $\max_{x,y} \mathcal{P} = \mathcal{P}(0,0)$; $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{P}(x,y) \, dx \, dy = 1$.

We compute interpolated concentration fields $\tilde{c}_i$ on the eulerian grid nodes with the following weighted averages

$$\tilde{c}_i(x_k, y_k) = \frac{\sum_p w_p(x_k, y_k) \, c_{p,i}}{\sum_p w_p(x_k, y_k)}.$$

This is a *cloud–in–cell* interpolation scheme.[9] If P has a compact support (not larger than a few meshes), most of the terms in the above sums are zero, and this makes the algorithm $O(N_p)$ in execution time. If we define $\mathcal{P}(x,y) = \{(x,y) \in [-\Delta/2, \Delta/2]^2 : 1/\Delta^2; \text{ otherwise}: 0\}$ then each particle generates only four non–zero weights. Taking $x_k \leq x_p \leq x_k + \Delta$ and $y_k \leq y_p \leq y_k + \Delta$, their explicit expression are

$$w_p(x_k, y_k) = \Delta^{-2}(x_k + \Delta - x_p)(y_k + \Delta - y_p),$$
$$w_p(x_k + \Delta, y_k) = \Delta^{-2}(x_p - x_k)(y_k + \Delta - y_p),$$
$$w_p(x_k, y_k + \Delta) = \Delta^{-2}(x_k + \Delta - x_p)(y_p - y_k),$$
$$w_p(x_k + \Delta, y_k + \Delta) = \Delta^{-2}(x_p - x_k)(y_p - y_k).$$

The concentration fields interpolated on the grid are subject to a Jacobi sweep:

$$\tilde{c}_i(x_k, y_k) =$$
$$= \frac{\tilde{c}_i(x_k - \Delta, y_k) + \tilde{c}_i(x_k, y_k - \Delta) + \tilde{c}_i(x_k + \Delta, y_k) + \tilde{c}_i(x_k, y_k + \Delta)}{4},$$

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which is a second–order, finite–difference discretization of the heat equation.

Finally, after each time step in the numerical solution of (2)–(3), the concentration fields carried by the particles are relaxed toward their diffused counterparts known on the eulerian grid:

$$\dot{c}_{p,i} = \frac{4D_i}{\Delta^2} \left(\tilde{c}_i(x_p, y_p) - c_p \right), \tag{4}$$

where $\tilde{c}_i(x_p, y_p)$ is the value of the i–th gridded concentration field interpolated at the position of the p–th particle. We use bilinear interpolation:

$$\tilde{c}_i(x_p, y_p) = w_p(x_k, y_k)\tilde{c}_i(x_k, y_k) + w_p(x_k + \Delta, y_k)\tilde{c}_i(x_k + \Delta, y_k) +$$
$$w_p(x_k, y_k + \Delta)\tilde{c}_i(x_k, y_k + \Delta) + w_p(x_k + \Delta, y_k + \Delta)\tilde{c}_i(x_k + \Delta, y_k + \Delta)$$

and an Euler integration step for the temporal part of (4).

A remarkable feature of the numerical method embodied by (2)–(4) is the possibility of taking arbitrarily small values for the diffusivities D_i without destabilizing the scheme and to recover the non–diffusive case in the limit $D_i \to 0$.

3. Biological applications

A simple example of predator–prey model was given by May:[10]

$$\dot{P} = P(1 - P) - aZ(1 - \exp(-\lambda_1 P)),$$
$$\dot{Z} = -\gamma Z + bZ(1 - \exp(-\lambda_2 P)). \tag{5}$$

Here P is the concentration of preys and Z is the concentration of predators. Unlike the classical Lotka–Volterra model, these equations admit a structurally stable limit cycle in a wide range of parameters. In the following we use the values $a = 1$, $b = 2.5$, $\gamma = 1.5$, $\lambda_1 = \lambda_2 = 4$, which make the limit cycle about 10 non–dimensional time–units long.

To illustrate the importance of a small amount of diffusion in this class of problems, we solve the equations (1) with the reaction terms given by (5), and the streamfunction

$$\psi = \psi_0 \sin(kx) \sin(ky), \tag{6}$$

with $\psi_0 = 0.1$ and $k = 1.5$. This is a cellular flow of 3×3 steady vortices on the domain $[0, 2\pi]^2$. The initial conditions are $P(x, y) = 1$ and $Z(x, y) = \{(x, y) \in [7/10\pi, 13/10\pi] \times [5/6\pi, 7/6\pi] : 0.1;$ otherwise $: 0\}$; that is, the preys are initially uniformly distributed with a concentration equal to the carrying capacity of the system, and the predators are confined in a rectangular patch all contained inside the central vortex. Figure 1 shows
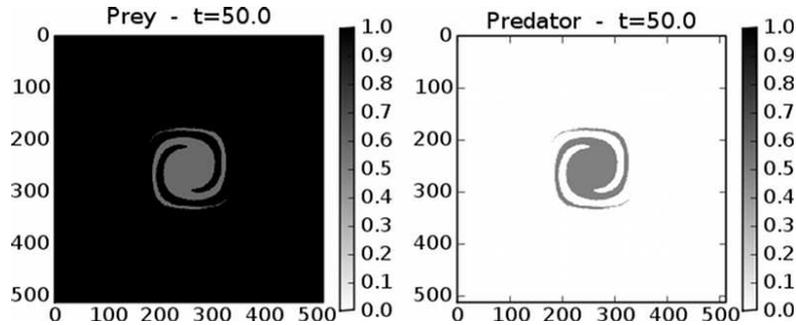
Fig. 1.   Predator–prey model with a cellular flow and no diffusion: the predators are unable to escape the central vortex. The prey in the other 8 vortices is unaffected.
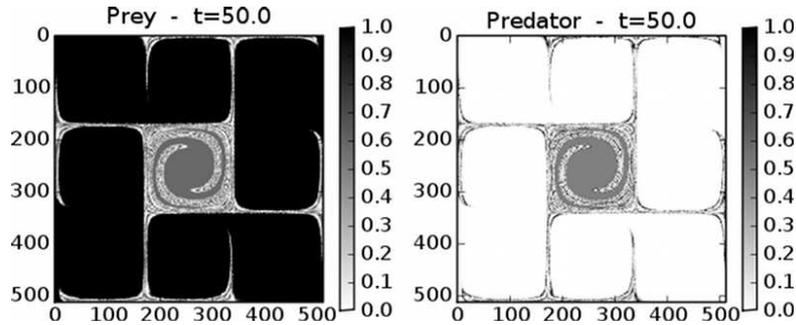

Fig. 2.   Predator–prey model with a cellular flow and small diffusivity ($D = 10^{-7}$ for both species): the predators escape the central vortex from each of its four stagnation points and invade the other vortices.

the situation after 50 non–dimensional time units in a simulation with no diffusion: because fluid parcels in this case follow the streamlines, which are closed, the predators are unable to leave the central vortex. With the addition of a very small diffusivity ($D = 10^{-7}$ for both species in the simulations of figure 2) the predators, within a few turnover times, are able to escape the central vortex from each of its four stagnation points and invade the other vortices.

An outstanding open problem in the study of plankton is the absence of a limit–cycle behavior in the available observations: while the relevant population models exhibit a limit cycle (or even a chaotic attractor) in a wide range of parameters, satellite images of clorophyll concentration do not show such oscillations.[12] A possible explanation is that, because of the mixing effect of ocean currents, nearby water patches oscillate with very

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different phases; coarse–grained satellite observations average them out, disguising the oscillations.

We performed several simulations with the renovating random wave streamfunction, a well–known homogeneously stirring flow which induces chaotic lagrangian trajectories.[11] In the absence of diffusion the coarse–graining explanation is upheld. However, when diffusion is not zero, we observe the sinchronization of phases among nearby particles: eventually, we reach a spatially uniform state which follows the limit cycle in time. The synchronization time increases steeply as diffusivity decreases. For low diffusivities, there is a large interval of times where synchronization is not evident, but stirring has already created enough fine structure that coarse graining observations would disguise the limit cycle (for further details on these simulations see `http://smaug.unile.it/plankton`).

At this stage it is not clear whether there is a small, but non–zero, diffusivity threshold below which complete synchronization is never attained. Furthermore, we have to stress that our simulations used the same diffusivities for both species. With different diffusivities, Turing–like instabilities might destabilize a spatially homogeneous situation. These lines of research will be pursued in future works.

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