Letter to the Editor

On positive solutions in a phytoplankton–nutrient model[☆]

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Abstract

On the basis of an application from aquatic ecology, we discuss the behaviour of the widely used time integration package VODE by Brown et al. (SIAM J. Sci. Statist. Comput. 10 (1989) 1038). When used in a default setting this code smoothly produces a negative steady state solution, which is not realistic in this application.
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1. Introduction

Phytoplankton, the generic name of microorganisms living in lakes, seas and oceans [8], are at the basis of the aquatic foodweb. Their role for a proper functioning of the aquatic ecosystem has been recognized for a long time and has been widely studied both empirically [17] as well as theoretically [9,5].

For their primary production of biomass, phytoplankton use photosynthesis [12], a process where solar energy (light) and carbon dioxide are utilized. Due to the sequestration of carbon dioxide, phytoplankton have a significant impact on the reduction of the greenhouse effect on a global scale (see e.g. [6]).

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In many regions (and some seasons) light availability is the major factor limiting phytoplankton growth [18]. In other regions, and seasons, phytoplankton growth is largely influenced by the availability of nutrients, such as nitrogen, phosphorous, and iron (see [16,1,3]).

In this note we consider a model in which both limiting factors, light and nutrient, are taken into account. These two factors give rise to contrasting gradients since light is coming from above, whereas nutrients are supplied at the sediment (see e.g. [13,19,4]). As a result, the vertical distribution of the phytoplankton population can be quite heterogeneous in the sense that a large aggregation of phytoplankton is formed at a subsurface depth, where both light and nutrient are just sufficiently available to sustain a population.

2. The mathematical model

Here, we describe the phytoplankton–nutrient model for one single species (a multi-species extension of the model can be found in [15]). The mono-species formulation is sufficient for the purpose of this note: showing the peculiar behaviour of the time integrator VODE [2].

We consider a water column in which the depth co-ordinate z runs from $z = 0$ (the surface) to $z = z_B$ (the bottom). Furthermore, let $\omega(z, t)$ denote the population density of a phytoplankton species at vertical position z at time $t \geqslant 0$. The distribution of phytoplankton is determined by the combined effect of growth (the main biological factor) and local transport processes (the main physical factor) through the partial differential equation

$$\frac{\partial \omega}{\partial t} = g\omega - \frac{\partial J}{\partial z},\tag{1}$$

where g and J are, respectively, the growth rate and the flux at depth z at time t.

The flux J is determined by the convective transport, due to the settling speed v and the diffusive transport, due to mixing,

$$J(z, t) = v\omega(z, t) - D(z)\frac{\partial \omega}{\partial z}(z, t),\tag{2}$$

where $D(z)$ is the space-dependent mixing rate.

In our model, the growth rate g is assumed to depend on the light intensity $\mathscr{L}$ and the nutrient concentration $\mathscr{N}$. In fact, it depends on the balance between the production rate p and the specific loss rate ℓ as given by

$$g(\mathscr{L}, \mathscr{N}) = p(\mathscr{L}, \mathscr{N}) - \ell.\tag{3}$$

Here, the loss rate is assumed constant and represents grazing by zooplankton, mortality, excretion, etc. The production rate p determines the growth of phytoplankton and is defined by the two limiting environmental resources (i.e., light and nutrient) in the following way (see e.g. [13,19]),

$$p(\mathscr{L}, \mathscr{N}) = \mu \min\left(\frac{\mathscr{L}}{L_H + \mathscr{L}}, \frac{\mathscr{N}}{N_H + \mathscr{N}}\right),\tag{4}$$

where μ, L_H and N_H, respectively, denote the maximum specific production rate and the half-saturation constants of light and nutrient.

Owing to shading and absorption, light intensity (the energy source) decreases with depth. At a particular depth, light intensity depends on the incident light intensity L_{in}, the light absorption coefficient of the water in the absence of phytoplankton K_{bg} and on the total light attenuation of the phytoplankton species above that particular depth (see e.g. [10]),

$$\mathcal{L}(z, t) = L_{in}e^{-K_{bg}z}e^{-r\int_0^z \omega(\sigma,t)\,d\sigma}, \tag{5}$$

where r denotes the specific light attenuation coefficient.

The change in the nutrient concentration $\mathcal{N}$ — the second environmental source that drives the growth rate g — is governed by the total amount of nutrient converted by the phytoplankton species and by the turbulent diffusion

$$\frac{\partial \mathcal{N}}{\partial t}(z, t) = -\alpha p(\mathcal{L}, \mathcal{N})\omega(z, t) + \frac{\partial}{\partial z}\left(D(z)\frac{\partial \mathcal{N}}{\partial z}(z, t)\right), \tag{6}$$

where α denotes the conversion factor.

In summary, the phytoplankton–nutrient dynamics are studied through the following *system of integro-partial differential equations* (integro-PDEs):

$$\frac{\partial \omega}{\partial t} = (p(\mathcal{L}, \mathcal{N}) - \ell)\omega - \left[v\frac{\partial \omega}{\partial z} - \frac{\partial}{\partial z}\left(D(z)\frac{\partial \omega}{\partial z}\right)\right],$$
$$\frac{\partial \mathcal{N}}{\partial t} = -\alpha p(\mathcal{L}, \mathcal{N})\omega + \frac{\partial}{\partial z}\left(D(z)\frac{\partial \mathcal{N}}{\partial z}\right). \tag{7}$$

To complete the model, we prescribe the following boundary conditions:

- Phytoplankton remains between two system boundaries: $J(z, t) = 0$ at $z = 0$ and $z = z_B$.
- There is no nutrient entering or leaving the surface: $\partial \mathcal{N}/\partial z = 0$ at $z = 0$.
- Nutrient is supplied from the sediment: $\mathcal{N}(z_B, t) = N_B$.

Remark. In this note we are interested in the long term behaviour of the solution. Therefore, we derive an explicit expression for the biomass of phytoplankton (i.e., the depth integral over the concentrations) in steady state. Dividing the second equation in (7) by α, adding to the first equation in (7) and integrating over space, results in

$$\frac{\partial}{\partial t}\int_0^{z_B}\left(\omega + \frac{1}{\alpha}\mathcal{N}\right)dz = -\ell\int_0^{z_B}\omega\,dz + \frac{D}{\alpha}\frac{\partial \mathcal{N}}{\partial z}(z_B, t),$$

where we have used the boundary conditions. Hence in steady state we obtain for the biomass of phytoplankton

$$\int_0^{z_B}\omega\,dz = \frac{D}{\ell\alpha}\frac{\partial \mathcal{N}}{\partial z}(z_B, t). \tag{8}$$

3. Numerical approach

For the numerical solution of the model (7) we follow the so-called Method of Lines approach. That is, we first discretize the spatial differential operators as well as the integral term in the light function. Subsequently, the resulting large system of ordinary differential equations (ODEs), which is still continuous in time, will be integrated numerically.

For the spatial discretization we use the same method as described in [10,14]: symmetric second-order discretizations for the diffusion terms (both in the equations for the phytoplankton species and for the nutrient) and third-order upwind-biased formulae for the advection term. For the integral term the repeated trapezoidal rule has been used. For a detailed discussion on these aspects, the interested reader is referred to [11].

The resulting stiff ODE system has been integrated in time by means of an implicit method, because an explicit time integrator has to obey an extremely severe time step restriction to avoid numerical instabilities. For the concept of stiffness, as well as other technical details about the time integration process, we refer to [7,11]. For our simulations, we have selected the code VODE of Brown et al. [2]. This widely used code is based on a family of implicit backward differentiation formulas and proved to be efficient in many cases. VODE includes all kinds of strategies, necessary for automatic integration. It is available both in C and Fortran and is freely downloadable from the internet site http://www.netlib.org/ode/.

4. Application

We will discuss the simulation results of the phytoplankton–nutrient model for a sinking species (i.e., $v > 0$), the parameters of which have been specified in Table 1. The environmental parameters are given the values $D = 1\,\text{cm}^2/\text{s}$, $K_{\text{bg}} = 2 \cdot 10^{-3}\,\text{cm}^{-1}$, $z_{\text{B}} = 100\,\text{m}$, $N_{\text{B}} = 10\,\mu\text{mol nutrient/cm}^3$, and $L_{\text{in}} = 6 \cdot 10^{-2}\,\mu\text{mol photons/(cm}^2\,\text{s)}$. For the initial condition we assume that nutrient is uniformly distributed over depth (i.e., equal to 10, $\forall z$), whereas phytoplankton is initialized according to a Gaussian profile with a maximum of 50 cells/cm^3 at 50 m (halfway down). Based on the experience that we obtained with the simulations described in [15], we use an equidistant spatial grid with 500 points. Such a grid is sufficiently fine to adequately capture the spatial variation in the solution.

To first obtain insight in the exact ODE solution, VODE was applied with an extremely stringent value for the tolerance parameter. This solution is shown in Fig. 1a. We see that initially the phytoplankton biomass strongly increases (the peak near $t = 0$). This is due to a bloom of plankton near the water surface, since light and nutrient are amply available. This bloom causes a substantial consumption of nutrient, which starts to decrease in the upper water level. As a consequence, also the phytoplankton concentration reduces over there (because of lack of food) and its maximum shifts downward to a position where light and nutrient are just sufficiently available to sustain a phytoplankton population. Already after about 400

Table 1
Species parameters

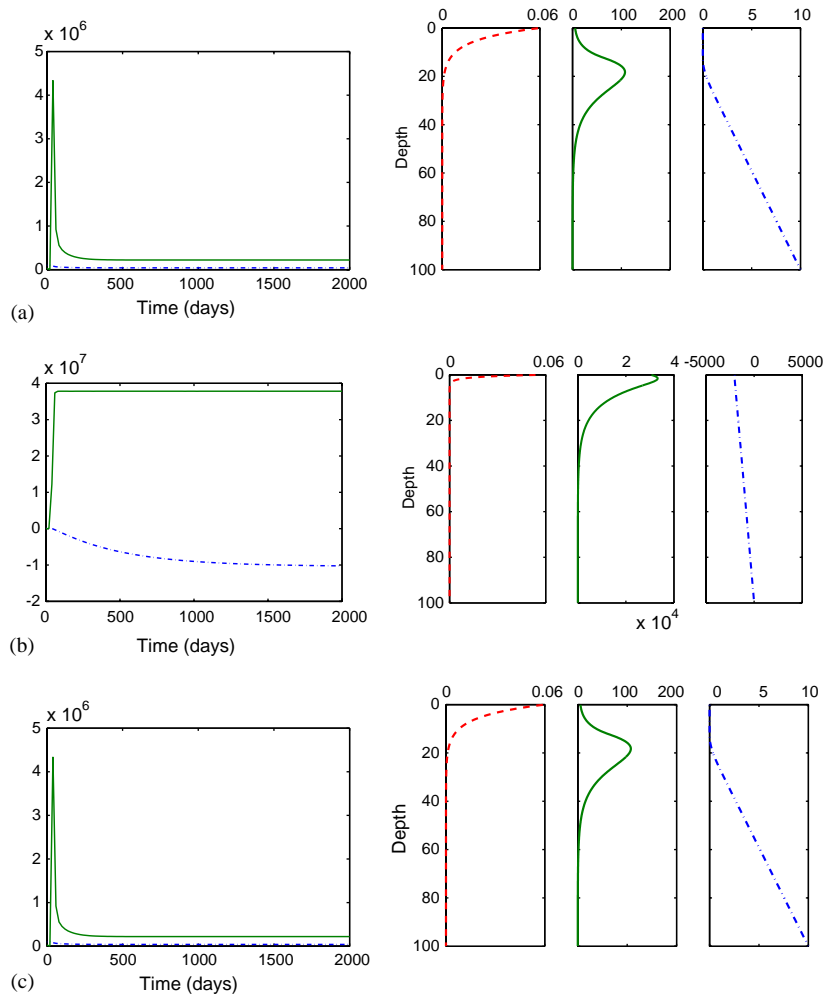| v (cm/h)	r (cm^2/cells)	μ (h^{-1})	L_{H} (μmol photons/(cm^2 s))	N_{H} (μmol nutrient/cm^3)	ℓ (h^{-1})	α (const)
+4.2	$3 \cdot 10^{-7}$	0.04	$2 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.01	$2 \cdot 10^{-3}$

Fig. 1. Left: phytoplankton biomass (solid line) and total amount of nutrient (dash–dotted line) as functions of time. Right: distributions over depth (vertical axis, in m) of light intensity (dashed line), phytoplankton density (solid line) and nutrient concentration (dash–dotted line) at steady state. (a) The exact solution; (b) solution without positivity control; (c) solution with positivity control.

days a stable stationary profile has been established, which is shown in the right panel of Fig. 1a. In passing we remark that, using a numerical approximation for $\partial \mathcal{N}/\partial z$ at the bottom, it is easily verified that relation (8) is indeed satisfied by the stationary solution.

Next we solve the problem with a coarser resolution in time: setting the tolerance parameter to 10^{-4} is more realistic in the present context of PDEs. However, using this value, we observe an unacceptable behaviour of VODE: it produces a *fundamentally wrong solution* (even negative components occur), which is shown in Fig. 1b. Although the integration statistics (such as number of time steps, number of rejected steps, number of Newton iterations to solve the nonlinear implicit relations, etc.) did not give rise to any suspicion, VODE returned a steady state with a completely wrong phytoplankton biomass and

a negative value for the total amount of nutrient. This is of course not feasible (and hence unacceptable) and we did not observe such a behaviour before with this time integrator. Here we remark that it is known (see e.g. [11, p. 187]) that linear multistep methods of order larger than 1 (which are used in VODE) have to obey a time step restriction for positivity reasons. However, in all previous simulations, the local error control in VODE prevented the code to converge to an unrealistic (i.e., negative) steady state solution. As an additional experiment, we applied VODE with the maximum order set to 1 (viz. the Backward Euler method, which has no step size restriction w.r.t. positivity). This test indeed yielded the correct solution, however, at a high price, since in this test the time steps were kept very small to meet the accuracy requirements.

To prevent the unwanted situation corresponding to Fig. 1b and to avoid the excessive costs when using an extremely small tolerance (or first-order method), we implemented a provisional remedy by adapting the control strategy in VODE: after each time step, all solution components are checked for positivity. If one or more negative components occur, the step will be rejected and the time step is drastically reduced for a new try. Fig. 1c shows the results. Due to this 'brute force' strategy, the solution remains positive and is in fact quite close to the exact solution, shown in Fig. 1a. From this example, it is obvious that positivity-control is of utmost importance for this application.

5. Discussion

We have shown the behaviour of VODE when applied to a model from microbiology. In a default setting, VODE's behaviour is not satisfactory, since it yields negative solutions.

Hence, the lesson to learn is that using VODE as a 'black box' solver needs precaution in case of an application where the positivity of the solution is a prerequisite.

We have implemented an 'ad hoc' strategy to enforce positivity but this approach is far from optimal. Therefore, in a forthcoming paper, we will concentrate on efficient time integration methods that guarantee positivity of the solution.

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