Novel approach to Design and Analysis of Water Resources Development Model in Terms of Phytoplankton Population Dynamics

M Polyak\(^1\), S Kolesnikova\(^1\)

\(^1\)Computer Technologies and Software Engineering department, Saint-Petersburg State University of Aerospace Instrumentation, Bolshaya Morskaya str. 67, Saint-Petersburg 190000, Russia

E-mail: markpolyak@gmail.com

Abstract. Phytoplankton is one of the key markers of ecosystem health. In this article we explore a phytoplankton model described by a system of differential equations. The analytical design of aggregate regulators method is applied to the model in order to investigate its behaviour. The development of algal blooms and their diminution to the normal state of a water body are simulated. The results of simulations align well with the expected ecosystem behaviour.

1. Introduction
Mathematical models are used to formalize and generalize notion on different properties and characteristics of a complex dynamic system. One of the widely used mathematical tools for that purpose is differential calculus [1]. Models based on differential (and difference) equations are used in physics, economy, biology and many other fields of science. For example, in biology and ecology differential equations allow to explicitly express mechanics of a biological system [2, 3, 4].

One of possible approaches to model development of an aquatic ecosystem is to divide the model into several components. Those components could be phytoplankton, zooplankton, benthos, fish, etc. Each component in this case is described by an individual set of equations (i.e. a submodel). Interaction between components is managed by variables which are common among several components of the model [5].

Phytoplankton is one of the key components of any aquatic ecosystem. It absorbs solar radiation that penetrates water and uses it to produce new organic matter. Process of photosynthesis is accompanied by release of oxygen into the water and absorption assimilation of dissolved of nitrogen and phosphorus.

Part of phytoplankton biomass adds to organic substance present in the water due to natural mortality of phytoplankton and mortality caused by unfavorable conditions. Also, a significant part of phytoplankton biomass is grazed by zooplankton.

Photosynthetic activity of phytoplankton and its mortality rate heavily depend on nutrients and toxic substances accumulated in cells, which in turn depends on their concentration in the water. Photosynthetic activity of phytoplankton also depends on intensity of solar radiation, water
transparency, water temperature and intensity of water mixing processes as it controls phytoplankton sedimentation rate.

In this work, we explore a component of an ecosystem model that deals with phytoplankton. Similar results can be achieved for other components of the model as well.

The model under study was developed by A.A. Umnov in his work [5] and applied to the Neva Bay, the Gulf of Finland [6, 7] and several lakes in Russia [5]. The model reveals flow of carbon (or corresponding energy flow) as well as biotic flow of nitrogen and phosphorus. It is described by the following equations:

\[
\begin{align*}
\frac{dx_1}{dt} &= a_{11}x_1 - a_{12}x_1 - a_{13} \\
\frac{dx_2}{dt} &= a_{21}x_2 - a_{22}x_2 - a_{23}, \\
\frac{dx_3}{dt} &= a_{31}x_1 - a_{32}x_3 - a_{33}
\end{align*}
\]  

(1)

where \( x_1, x_2, x_3 \) – is the biomass of phytoplankton expressed in carbon, nitrogen and phosphorus respectively; \( a_{11}, a_{21}, a_{31} \) – assimilation of carbon, nitrogen and phosphorus respectively per unit biomass expressed in carbon; \( a_{12}, a_{22}, a_{32} \) – total expenses on metabolism, mortality and sedimentation rate expressed in carbon, nitrogen and phosphorus respectively; \( a_{13}, a_{23}, a_{33} \) – total grazing of phytoplankton by zooplankton and benthos expressed in carbon, nitrogen and phosphorus respectively.

System of equations (1) could be written in a compact form using matrix notation as follows:

\[
\frac{dX}{dt} = AX + B,
\]

(2)

where

\[
A = \text{diag}(a_{11} - a_{12}, a_{21} - a_{22}, a_{31} - a_{32}),
\]

\[
X = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T,
\]

\[
B = \begin{bmatrix} -a_{13} & -a_{23} & -a_{33} \end{bmatrix}^T.
\]

Main source of biogenic matter in water bodies is the waste water [8]. Increase in nitrogen and phosphorus concentrations in water reported in many countries is caused by human population growth, urban development, industry growth and incomplete waste water treatment [9]. Water body pollution with nutrients facilitates algal blooms. Blooms caused by phytoplankton species like toxic cyanobacteria poses a serious environmental concern [10, 11, 12]. The important role of nitrogen and phosphorus in development of algae blooms is confirmed by many researchers [13, 14].

The goal of this research is to simulate phytoplankton dynamics described by equation (2) when the ecosystem transitions between two states.

For the sake of simulation, we investigate two different states of a water body: an algal bloom with high concentrations of phytoplankton and a state with low or moderate concentrations of phytoplankton. By applying the analytical design of aggregate regulators method to the model (2) we explore the process of transition between those two states.

2. ADAR method

The main method of synergetic control theory is the analytical design of aggregate regulators (ADAR) method [15, 16, 17, 18]. Classical ADAR method has the following features and applicability conditions for solving vector control problems of poorly formalized objects.

Condition 1. The initial object is presented as a system of ordinary (nonlinear) differential or difference equations. For example, such an object would have a continuous description of the form
\[
\frac{dx_i(t)}{dt} = f_i(x_1, \ldots, x_n) + u_j, i = 1, n, j = 1, m, m \leq n,
\]

where \( x \in \mathbb{R}^n, u \in \mathbb{R}^m \) are the vector variables of state and control, respectively.

\textbf{Remark.} Solutions of the system of equations (3) must exist and be bounded for any admissible input action \( u \in \mathbb{R}^m \).

\textbf{Condition 2.} Analytical (expert) description of the desired states \( x(t) \) of the control object must be provided. Those states are treated as a set of target states with an attractive property (hereinafter, the target set of states): \( \psi(t) = \psi(x(t)) = 0 \), where \( \psi(t) \) - is a well known function-macrovariable. Here we have the stabilization problem, therefore

\[
\psi_j(t) = \psi_j(x_1, \ldots, x_n), j = 1, m
\]

where \( \psi_j(t) \) are the target values of variables \( x_j, j = 1, 3 \).

\textbf{Condition 3.} A special type of quality criterion for the synthesized control system should be postulated. It reflects certain requirements on the target system, here

\[
\Phi(\psi_j(t), \dot{\psi}_j(t)) = \int_0^\infty \sum_{j=1}^m (\psi_j^2(t) + \omega_j^2 \dot{\psi}_j^2(t)) dt,
\]

where weighting factors \( \omega_j, j = 1, m \) are the parameters of the control system settings that have the meaning of time regulators for reaching the target set. Here \( \dot{\psi}_j(t) \) denotes the time derivative \( \frac{\psi_j(t)}{dt} \).

\textbf{Condition 4.} The global minimum of function \( \Phi(\cdot) \) is ensured by a special form of the Euler-Lagrange equations having a linear form with respect to the macro variable \( \psi \):

\[
\omega_j \ddot{\psi}_j(t) + \dot{\psi}_j(t) = 0,
\]

\[
\omega_j > 0, t \geq 0, \psi_j, \omega_j \in \mathbb{R}, j = 1, m.
\]

\textbf{Condition 5.} There is theoretical proof of the vector control action, determined from the solutions of the Euler-Lagrange problem. It is based on transferring the object to the prescribed manifold and supporting it in this manifold, thereby ensuring the asymptotic stability of the control system on the whole.

Classical optimal control problem statement according to ADAR method can be described as follows.

It is required to perform control in the state space of an object by transferring object (3) from its given initial state \( x_{0,j}, j = 1, 3 \) into the neighborhood of the target manifold \( \psi(x) = 0 \) and minimizing the quality functional (5).

\section{Results and discussion}

Let us investigate a way to analytically model behavior of system (2) when it is transitioning between two different states. In biological sense those two states of water body would be an algal bloom and normal conditions without a bloom. According to (4) we can describe those states as

\[
\psi_j(t) = \psi_j(x_1, x_2, x_3), \psi_j = 0, j = 1, 3,
\]

where \( \psi = (\psi_1, \psi_2, \psi_3) \) is the target vector macrovariable or some aggregated function of the state of the object.

Let us assume that behavior of the system (2) is complicated by deterministic fluctuations of variables \( x_1, x_2, x_3 \). It is necessary to trace the representation point of the system (2) on its way to manifold (7) in order to investigate those fluctuations.
Problem description. Let us assume that system (2) is complicated by deterministic fluctuations \( z_i(t), z_2(t), z_3(t) \) of variables \( x_1(t), x_2(t), x_3(t) \) respectively:

\[
\frac{dX}{dt} = A(X + Z) + B = AX + AZ + B, \tag{8}
\]

where \( Z = [z_1, z_2, z_3]^T \).

Let \( u_j(t) = \sum_{i=1}^{3} a_{ij} z_j, j = 1,3 \). Then (8) can be written as

\[
\frac{dX}{dt} = AX + B + U. \tag{9}
\]

where \( U = [u_1, u_2, u_3]^T = AZ \).

Problem setting. Determine phase trajectories \( x_1(t), x_2(t), x_3(t) \) that bring representation point of system (9) to the targeted state (7) by numerical simulation.

Solution Let us choose the following macrovariables in the form of deviation of current value of \( x_j(t) \) from the target values \( x_j^* = \text{const}, j = 1,3 \):

\[
\psi_j(t) = x_j(t) - x_j^*, j = 1,3. \tag{10}
\]

Here \( x_j^*, j = 1,3 \) are constants that can be interpreted as target values of variables \( x_j, j = 1,3 \). These target values represent a special state of an object described by system of equations (9). We will reference it as a target state as it is a state we target system (9) at.

Representation point of system (9) arrives at special (target) state (7) at a minimum of functional (5). Coefficients \( \omega_j, j = 1,3 \) determine moving speed of representation point on its way to state (7) here (10).

The following assumption is made about equation (5). If current state of system (9) is moving towards a special state (7) (or (10)) then self-organization of natural environment will be described by equation (5). It means that nature will not search through all possible trajectories that lead an object described by system (9) to state (7). It will rather choose most cost effective trajectories available for that object.

Step 1. Euler-Lagrange equation with extremals for equation (5) can be written as:

\[
\omega_j \frac{\psi_j(t)}{dt} + \psi_j(t) = 0, j = 1,3. \tag{11}
\]

Step 2. Let us substitute (10) for (11):

\[
\omega_j (x_j(t) - x_j^*) + \psi_j(t) = \omega_j x_j'(t) + \psi_j(t) = 0, j = 1,3. \tag{12}
\]

We convert (12) to vector form and substitute (9) for derivatives of \( x_j, j = 1,3 \):

\[
\omega \frac{dX}{dt} + \psi = \omega (AX + B + U) + \psi = 0, \tag{13}
\]

where \( \omega = \text{diag}(\omega_1, \omega_2, \omega_3) \). It is possible to use Hadamard product instead of matrix product if \( \omega \) is defined as a vector \( \omega = [\omega_1, \omega_2, \omega_3]^T \).

Step 3. Now we can find \( U \), i.e. determine the form of fluctuations \( z_1(t), z_2(t), z_3(t) \):

\[
U = -\omega^{-1} \psi - AX - B. \tag{14}
\]

Step 4. Equations (9) and (14) allow us to solve the inverse problem, i.e. determine the behavior of trajectories of variables \( x_j, j = 1,3 \).
Numerical simulation. Matrix $A$ was prepared in a following way. Coefficients $a_{11}, a_{21}, a_{31}$ where chosen according to well-known Redfield ratio [19] which describes atomic ratio of carbon, nitrogen and phosphorus in phytoplankton. Use of Redfield ratio guaranties that individual independent equations from system (1) (here (9)) are bound together and produce meaningful results. According to [5] coefficient $a_{12}$ was calculated as follows

$$a_{12} = R + D + Y,$$

where $R = 5\%$ – specific cost on phytoplankton metabolism, $D = 10\%$ – specific cost on phytoplankton mortality and $Y = 10\%$ – specific cost on phytoplankton sedimentation rate. Coefficients $a_{22}$ and $a_{32}$ are proportional to $a_{12}$.

Simulations were performed by solving equations (9) and (14) with different initial conditions and target values. Accuracy difference between results of Euler method and Runge-Kutta formula [20] for this task were found to be small, so a simpler Euler method was used to solve a system of differential equations.

Test case 1. The initial condition $X_0 = [x_{10}, x_{20}, x_{30}]^T$ corresponds to the normal state of the water body. Target values $x_j^*, j = 1, 3$ are set to be 100 times larger than the initial condition. Here target values correspond to an algal bloom. The results of simulation are shown on figure 1.

It can be seen from figure 1 that during the initial phase of algal bloom large amounts of carbon, nitrogen and phosphorus are utilized. The consumption of carbon decreases after the phytoplankton biomass becomes stable.

![Figure 1](image1.png)

**Figure 1.** Trajectories of $x_j, j = 1, 3$ (left) and fluctuations $(a_{j1} - a_{j2})z_j(t), j = 1, 3$ (right) for a case of an algae bloom development, $a_j = 1, j = 1, 3$.

Test case 2. The initial condition $X_0$ corresponds to an algal bloom with high phytoplankton biomass. Target values $x_j^*, j = 1, 3$ are set to be 100 times lower than the initial condition and indicate an average abundance of phytoplankton in the water body.

The results of simulation on figure 2 show that during termination of an algal bloom large amounts of carbon and nutrients are discharged, see negative values of $U$ on the chart to the right. It can be seen that nutrients consumption rises to normal values when phytoplankton concentration decrease and the bloom stops.
Figure 2. Trajectories of $x_j, j = 1,3$ (left) and fluctuations $(a_{j_1} - a_{j_2})z_j(t), j = 1,3$ (right) for a case of an algae bloom decline, $\omega_j = 1, j = 1,3$.

4. Conclusions
ADAR method and its modification (non-linear adaptation to a target manifold) allow designing optimal control for complex multidimensional multiply-connected and even non-linear objects. Primary result of this research suggests that it can be also successfully applied to solve the inverse problems discussed in this work.

We have used this method to synthesize new states and ways of reaching them for a phytoplankton model, which itself is a submodel inside a large ecosystem model. The results of simulations align well with the expected ecosystem behaviour.

Application of synergetic control theory for prediction of ecological situations in water bodies will be based on decision rules of the form “what will happen, if …”. Those rules will form the basis of mathematical tools for the environmental decision support system.

References
[1] Fursova P and Levich A 2002 Mathematical modelling of synecology: review Environmental problems (VINITI reviews) 9
[2] Rosenberg G, Shitikov V and Brusilovskiy P 1994 Ecological Forecasting (Functional Predictors of Time-Series) (Togliatti: RAS)
[3] Polyak M 2012 Aspects of data analysis and principles of building mathematical models in hydroecology Proc. of Scientific Session of SUAI: Technical Sciences (Saint-Petersburg: SUAI) p 137
[4] Polyak M 2013 Evolutionary predator-prey model with stochastic disturbance Forum proc. (Saint-Petersburg: SUAI) pp 59-63
[5] Umnov A 1997 Mathematical Modelling of Flow of Biological substance and Energy in Water Ecosystems (Saint-Petersburg: Nauka)
[6] The Neva Bay: Modelling Record 1997 ed V V Menshutkin (Saint-Petersburg: RC RAS)
[7] Integrated Control of Water Resources in Saint-Petersburg and Leningrad Region. Track Record in Development of Decision Support System 2001 ed A F Alimov, V F Buderina et al (Saint-Petersburg: RC RAS)
[8] Paerl H and Fulton R 2006 Ecology of harmful cyanobacteria Ecology of Harmful Algae (Berlin: Springer-Verlag GmbH) pp 95-109
[9] Van Drech G, Bouwman A, Harrison J and Knoop J 2009 Global nitrogen and 1651 phosphate in urban wastewater for the period 1970 to 2050 Global Biogeochem. Cycles. 23(4) 1-19
Acknowledgements
This work was supported by grant 17-08-00920 from the Russian Foundation for Basic Research.