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Development of a specialized software complex for modeling the biogeochemical cycles in the Azov sea, including calculation modules of transformation of phosphorus, nitrogen, silicon, sulfur and dissolved oxygen forms, as well as the dynamics of phyto-and zooplatonkton

Alla Nikitina [1,2,3], *Alyona* Filina[2], *Vladimir* Litvinov[1], and *Asya* Atayan[1*]

[1] Don State Technical University, Rostov-on-Don, 344000, Russia
[2] Supercomputers and Neurocomputers Research Center, Taganrog, Russia
[3] Southern Federal University, Taganrog, Russia

Abstract. The paper is devoted to the development of a software complex for predictive modeling of biogeochemical cycles in the Azov Sea on high-performance computer systems in a limited time. The complex development includes the creation of software modules of the computational structure to calculate the concentrations of phosphorus, nitrogen, silicon, sulfur, dissolved oxygen forms and describe in detail phyto- and zooplankton dynamics in the Azov Sea; the integration of various environmental databases, satellite monitoring. The complex is adapted to solve a wide class of predictive problems of water ecology and water resources management. It includes the implementation of developed 3D mathematical model of hydrophysics and biological kinetics on computational grids, consistent with the complex shape of the water coastline. Parallel algorithms have been developed for numerical implementation of water ecology problems, oriented to high-performance computer systems. To increase the calculation efficiency of computational grid fragments assigned to graphics accelerators, an algorithm and its software implementation were developed in the CUDA C language. Based on the developed specialized software tools focused on supercomputers, scenarios for the development of the environmental situation and sustainable development management at biological rehabilitation of the Azov Sea were developed, including forecasts of changes in harmful algae concentration; dynamics of spatial interaction processes between phyto- and zooplankton populations; evolution of biological kinetics processes on the example of plankton interaction.

[*] Corresponding author: atayan24@mail.ru

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1 Introduction

One of the most important aquatic ecology problems is to maintain the sustainable water development, performed by researching the parameters and ways of pollutants of various etiologies entering the aquatic environment. A detailed research of biological communities' dynamics, the identification of cause-and-effect relationships and mechanisms of individual processes in ecological systems, the circulation of matter and energy balance are among the fundamental problems of ecology and hydrobiology. The relevance of performed research is due to the excessive deterioration of ecological situation in shallow waters due to an increase in anthropogenic influence (intensification of industrial and agricultural production, etc.), changes in natural and climatic conditions on the planet. To solve these problems, it is necessary to develop tools for predictive modeling of interrelated hydrophysical and biogeochemical processes in shallow waters, like the Azov Sea, which are still quite fish-producing waters [1], in accelerated time. The recently increasing anthropogenic impact (intensification of industrial and agricultural production, etc.) leads to eutrophication of the Azov Sea waters and the rapid phytoplankton growth. According to experts, along with anthropogenic causes, negative impacts on aquatic ecosystems are also caused by the evolution of natural and climatic conditions (changes in salinity and temperature regimes) [2]. In recent decades, there has been a negative trend in the reduction of valuable and commercial fish populations (sturgeon, pike perch, bream, sterlet, beluga, carp, etc.), as well as the introduction of alien species. It is known that various biogenic substances enter waters with river runoff, causing the dangerous phenomenon – eutrophication, as well as a burst of algae growth ("blooming"). The main concentration of biogenic substances is located in the upper water layers, contributing to the active microflora development (phytoplankton, fouling algae) in this area and, thereby, to increase the zooplankton biomass. One of the problems is the presence of potentially dangerous microalgae species, which cause "water bloom" and "red tides", and some produce phytotoxins.

Shallow waters, like the Azov Sea, are characterized by hypoxia phenomena, the causes of which are a decrease of dissolved oxygen concentration at increasing water temperature, which, in turn, contributes to the active zooplankton reproduction; prolonged calm; discharge of industrial effluents or the influx of marsh water containing a large amount of organic matter and decay products that take oxygen from the water during oxidation, etc.

Thus, the creation of mathematical and software and algorithmic tools for predictive modeling of significant spatial hydrobiological processes using data from relatively inexpensive experiments that do not adversely affect the ecosystem is relevant.

To ensure the efficiency of simulation calculations, it is necessary to use high-performance computer systems for operational prediction calculations of ecological situation in water, especially in emergency [3].

The priority measures aimed at eliminating the pollution consequences and other negative impacts on the environment as a result of natural and/or technogenic challenges was approved by the Decree of the Russian Federation Government dated December 4, 2014, No.2462-r. According to the Federal Law No.7-FL on January 10, 2002 (as amended on January 1, 2017) "About Environmental Protection"; Water Code of the Russian Federation (as amended on October 31, 2016 No. 384-FZ); Decree of the Russian Federation Government on December 30, 2003 No.794 (as amended on January 26, 2017) "On the unified state system for preventing emergencies", the time for making decisions and eliminating emergencies should be from several hours to 2 – 3 days [7, 8]. According to the Decree of the Russian Federation Government No.240 dated April 15, 2002 "When a message is received about oil and oil product spill, the spill localization time should not exceed 4 hours in case of a spill in water, and 6 hours – in case of a spill on the soil from the moment the oil and oil product spill is detected or from the moment information about the spill is received". In other words, the prediction time of water ecosystem situation in the event of the occurrence of natural and technogenic phenomena should be tens to hundreds of times less than the standard time. It requires predictive modeling of hydrobiological processes on high-performance computer systems in the accelerated time.

In this paper, a specialized software complex (SSC) was designed. It focused on high-performance computer systems. The SSC is intended to solve computational labor problems of water ecology, perform experiments and forecasting (both short-term and long-term) at various hydrological and meteorological situations. The SSC implements interconnected mathematical models of hydrodynamic and biogeochemical processes in shallow waters, due to which, in comparison with known models, we can more accurately simulate hydrophysics and biological kinetics processes, including sediment transport, primary and secondary pollution by impurities at rising it from the water bottom under the wave processes, eutrophication, predict the distribution of pollution concentrations, biogenic substances (nitrogen, phosphorus, silicon compounds), dissolved oxygen, the phyto- and zooplankton dynamics in shallow waters with complex spatial current structures, obtain the accurate assessment of ecological situation in shallow water and operational forecast of it development, especially at emergency.

The following regulatory documents were used at development algorithms for predictive modeling [4-8]: Federal Law No.7-FL on January 10, 2002 "On Environmental Protection"; Federal Law No.174-FZ on November 23, 1995 "On Environmental Expertise"; Decree of the Russian Federation Government No.420 on May 3, 1994 “On protecting the life and health of the population of the Russian Federation in the event of the occurrence and elimination of the consequences of emergency situations caused by natural disasters, accidents and catastrophes"; Decree of the Russian Federation Government on July 24, 1995, No.738 "On the procedure for preparing the population in the field of protection against emergency situations"; Decree of the Russian Federation Government on August 3, 1996, No.924 "On the forces and means of the unified state system for the prevention and elimination of emergency situations"; Art. 67 Requirements for the prevention of emergencies at POO and life support facilities, introduced by the order of the Ministry of Emergency Situations of the Russian Federation dated February 26, 2003 No.105 "On approval of requirements for the prevention of emergencies at potentially dangerous objects and life support facilities"; Decree of the Russian Federation Government on December 30, 2003 No.794 "On the Unified State Emergency Prevention System".

2 Model of the biotic cycle in shallow water

The primary cycle, which is a closed cycle of a substance in the system "phyto-plankton-bacterioplankton-mineral compounds of biogenic elements", occupies a central place in the biotic cycle. The high water productivity, changes in climatic conditions (temperature rise, low wind, increased water salinity, etc.), the presence of organic suspension in the summer months lead to oxygen deficiency, the formation of anoxia and hypoxia zones, where zoobenthos dies over an area of several tens and often hundreds of square kilometers.

The distribution and transformation of biogenic substances are influenced by such physical factors as the spatial three-dimensional movement of water environment taking into account advective transport and microturbulent diffusion, and the spatially inhomogeneous distribution of temperature, salinity and oxygen. Nutrients, as a rule, enter the water basin with river runoff. They are associated with the weather and climatic features of the geographical region, and are the result of uncontrolled discharges of insufficiently treated domestic and industrial effluents and other types of anthropogenic impact. That, in turn, contributes to the disruption of the water biological cycle, the active growth of algae, reducing the light flow into the lower water layers, slowing down the photosynthesis processes, reducing the oxygen concentration, etc.

The fishery significance of shallow waters and rivers flowing into them is determined not only by the reproduction conditions for valuable fish species, but also to a large extent by the presence of feeding grounds for fish species under consideration. The actual assessment of the impact on the food supply of fish is impossible without the use of the most modern and optimized mathematical models that make it possible to predict both the spread of suspended plumes in water environment and changes in the bottom topography due to the precipitation of suspended soil particles. Note that one of the reasons of fish and bottom organisms' death is the active development of blue-green and peridinium algae, which release toxic substances at dying.

A mathematical model of self-purification processes in shallow water was developed for simulation biogeochemical cycles in shallow waters on the example of the Azov Sea. It based on papers of Matishov G.G., Ilyichev V.G. [9], Tyutyunov Yu.V. [10], Sukhinov A.I. [11], Chetverushkin B.N. [12], Yakushev E.V. [13], Weiner E.R. [14], devoted to the simulation of hydrochemical processes. At developing a mathematical model, it was taken into account that the oxygen-deficient conditions arise in the bottom layers of the Azov Sea during calm and wind situations close to them. The model is a set of equations for each q_i concentration values of the *i*-th substance:

$$\frac{\partial q_i}{\partial t}+u\frac{\partial q_i}{\partial x}+v\frac{\partial q_i}{\partial y}+\left(w-w_{gi}\right)\frac{\partial q_i}{\partial z}=\mu_i\Delta q_i+\frac{\partial}{\partial z}\left(\nu_i\frac{\partial q_i}{\partial z}\right)+\psi_i, \quad (1)$$

$$\psi_1=g_1\left(q_1,q_3,q_8,q_9\right)-\lambda_1\left(q_{11}\right)q_1,\ \psi_2=g_2\left(q_2,q_4,q_{10}\right)-\lambda_2q_2,$$

$$\psi_3=\gamma_3\alpha_2\left(q_4\right)q_2q_3-g_3\left(q_1,q_3\right)-\lambda_3q_3+B\left(\tilde{q}_3-q_3\right)+f,$$

$$\psi_4=\lambda_1q_1+\lambda_2q_2+\lambda_5q_5-g_4\left(q_2,q_4,q_5\right),\ \psi_5=g_5\left(q_4,q_5,q_8\right)-\lambda_5q_5,$$

$$\psi_6=\left(g_6\left(q_4,q_8\right)-\lambda_6\right)q_6,\ \psi_7=g_7\left(q_6\right)-\lambda_7q_7,\ \psi_8=\left(g_8\left(q_2,q_7\right)-\lambda_8\right)q_8-\gamma_8\alpha_1\left(q_8\right)q_1,$$

$$\psi_9=g_9\left(q_1\right)-\lambda_9q_9,\ \psi_{10}=g_{10}\left(q_1,q_{10}\right)+\gamma_2\alpha_2\left(q_{10}\right)q_2-\left(\sigma_1q_1+\gamma_7q_7\right)q_{10},$$

$$\psi_{11}=g_{11}\left(q_1,q_{11}\right)-\lambda_{11}q_1,$$

where $\mathbf{U}=(u,v,w)$ is the water flow velocity vector; w_{g_i} is the rate of gravitational settling of the *i*-th component, if it is in suspension; Δ is the two-dimensional Laplace operator; μ_i, ν_i are the turbulent exchange coefficients in the horizontal and vertical directions, respectively; ψ_i is a chemical-biological source (sink) or a term describing aggregation (sticking-spreading), if the corresponding component is a suspension, index *i* indicates the substance type, $i=\overline{1,11}$: 1 is the phytoplankton concentration (P); 2 is the aerobic thionic bacteria *Thiobacillus* (*BT*); 3 are mineral nutrition (biogenic substances: compounds of nitrogen, phosphorus, silicon) (M); 4 is the detritus (*D*); 5 is the anaerobic bacteria of the *Desulfovibrio* genus (*BD*); 6 is the hydrogen sulfide (H_2S); 7 is the elemental sulfur (S); 8 are sulfates (SO_4); 9 is the phytoplankton metabolite (*MP*); 10 is the dissolved oxygen (O_2); 11 is the zooplankton concentration (*Z*).

The biogeochemical cycle's processes of chemical elements under oxygen-deficient conditions were parameterized.

Let's get $\alpha_m\left(q_j\right)=\alpha_{mj}^{\max}q_j/\left(K_m^j+q_j\right)$, $m=\{1,2,5,10\}$, $j=\{3,4,8\}$, $\alpha_m\left(q_j\right)$ is the absorption rate by the *m*-th hydrobiont of the *j*-th substance; $\alpha_{mj}^{\max}$ is the maximum possible absorption rate for the *m*-th hydrobiont (at high concentration of the *j*-th nutrient); K_m^j is the half-saturation constant of the *m*-th hydrobiont with the *j*-th substance; $g_1\left(q_1,q_3,q_8,q_9\right)=\left(\gamma_1\alpha_1\left(q_3\right)+\gamma_8\alpha_1\left(q_8\right)+\gamma_9q_9\right)\phi_1q_1$, $g_2\left(q_2,q_4,q_{10}\right)=\left(\gamma_2\alpha_2\left(q_4\right)+\gamma_{10}\alpha_2\left(q_{10}\right)\right)\phi_2q_2$, $g_3\left(q_1,q_3\right)=\alpha_1\left(q_3\right)q_1$, $g_4\left(q_2,q_4,q_5\right)=\alpha_2\left(q_4\right)q_2+\alpha_4\left(q_5\right)q_4$, $g_5\left(q_4,q_5,q_8\right)=\phi_5\left(\alpha_5\left(q_4\right)+\sigma_5q_8\right)q_5$, $g_6\left(q_4,q_8\right)=\left(\gamma_4q_4+\gamma_8q_8\right)q_6$, $g_7\left(q_6\right)=\gamma_6q_6q_7$, $g_8\left(q_2,q_5,q_7\right)=\left(\gamma_2q_2-\sigma_5q_5+\gamma_7q_7\right)q_8$, $g_9\left(q_1\right)=\gamma_9q_1$, $g_{10}\left(q_1,q_{10}\right)=\gamma_{10}q_1q_{10}$, $g_{11}\left(q_1,q_{11}\right)=\gamma_{11}\phi_{11}q_1q_{11}$, $\tilde{q}_3$ is the maximum possible entry rate of pollution biogenic substance; B is a specific rate of pollutant intake; $f(x,y,z)$ is pollutant source function; $\lambda_i,\ i\in\overline{1,11},\ (i\neq4)$ are coefficients that take into account the phytoplankton, bacteria and substances loss due to the elimination (mortality), grazing by representatives of higher trophic levels and decomposition; $\gamma_i,\ i\in\overline{1,11},\ i\notin\{3,6,10\}$ are transfer coefficients of trophic functions; γ_{10} is the oxygen release coefficient by phytoplankton during photosynthesis; σ_1 is the oxygen consumption coefficient for phytoplankton respiration; σ_5 is the reduction factor of sulfate to hydrogen sulfide by bacteria (*BD*) as a result of anaerobic respiration.

The dependence functions of phytoplankton and bacteria growth rate on temperature (T), salinity (S) (according to Lehman) and illumination (I) (according to Steele):

$$\phi_m\left(T,S,I\right)=\frac{I}{I_{opt}}\exp\left\{1-\alpha_m\left(\left(T-T_{opt}\right)/T_{opt}\right)^2-\beta_m\left(\left(S-S_{opt}\right)/S_{opt}\right)^2-I/I_{opt}\right\},\ m=\{1,2,5,11\},$$

where $I\left(h\right)=I_0\exp\left(-\theta h\right)$, h is the water depth; I_0 is the total solar radiation on the water surface; θ is the attenuation coefficient proportional to the concentration of substances suspended in water (phytoplankton and detritus); where T_{opt}, S_{opt} are temperature and salinity, optimal for this type of water organisms; $\alpha_m>0$, $\beta_m>0$ are width coefficients of the tolerance interval of plankton and bacteria to temperature and salinity, respectively.

The computational domain G is a closed area bounded by a cylindrical side surface σ, unperturbed by the water surface Σ_0, bottom $\Sigma_H=\Sigma_H(x,y)$. Σ is a piecewise-smooth boundary of the domain G, $\Sigma=\Sigma_0\cup\Sigma_H\cup\sigma$, $0<t\le T_0$.

Let us add boundary conditions:

$$q_i=0\ \ on\ \sigma,\ if\ U_n<0;\ \ \frac{\partial q_i}{\partial n}=0\ \ on\ \sigma,\ if\ U_n\ge0;$$

$$\frac{\partial q_i}{\partial z}=-\varepsilon_iq_i\ \ on\ \Sigma_H,\ \frac{\partial q_i}{\partial z}=\varphi\left(q_i\right)\ \ on\ \Sigma_0,\ \varphi\left(q_i\right)=\begin{cases}\xi_i\left(q_i\right),\ i\in\{3,4,6,7\};\\ \dfrac{a_0}{v_i}\left(K_i-q_i\right),\ i=10;\\ 0,\ i\in\{1,2,5,8,9,11\},\end{cases}\qquad(2)$$

where a_0 is the aeration coefficient; K_{10} is the oxygen concentration, dissolved in water at saturation; ε_i is the absorption coefficient of the i -th substance by bottom sediments; ξ_i are given functions; $i=\overline{1,11}$.

Let us add initial conditions:

$$q_i\big|_{t=0} = q_{i0}(x,y,z),\ i=\overline{1,11}. \tag{3}$$

The scheme of biotic cycle in shallow water is presented in Fig.1.

The developed mathematical model of biological kinetics (1) – (3), which is part of the SSC, is based on a system of non-stationary convection-diffusion-reaction equations with nonlinear terms, takes into account the water flow movement, gravitational sedimentation of impurities, microturbulent diffusion, detritus decomposition as a result of the activity of aerobic and anaerobic bacteria. The introduction of a non-linear dependence of the growth rate of phytoplankton and bacteria makes it possible to describe the production-destruction processes in water, to control their dynamics at excessive intake of biogenic substances (nitrogen, phosphorus and silicon compounds), sulfur compounds, including hydrogen sulfide and sulfates, various oxygen distribution modes, detritus, spatial and temporal variability of illumination, salinity and temperature.

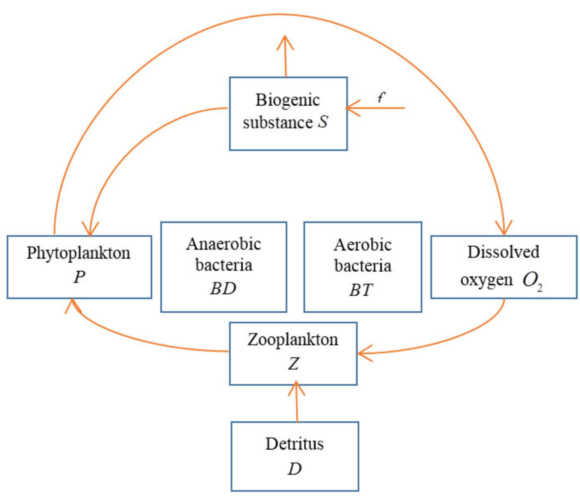

Fig. 1. Biotic cycle in shallow water.

A specialized software complex has been developed to monitor and predict changes in ecological situation of shallow waters at natural or anthropogenic hazards in them, including storm surges, coastal abrasion, accidental oil spills, eutrophication and "water blooming" processes that cause fish kills. The software includes the developed mathematical models of hydrophysics and biological kinetics in shallow waters and numerical methods for their solution [15]. The advantage of the SSC is its focus on high-performance computer systems that allow quickly obtain the calculation results in limited time. It is especially important in the case of natural or technogenic emergencies.

The SSC features:

– assessment and forecast of ecosystem regime situation in shallow waters, like the Azov Sea, food supply and stocks of commercial objects; calculation the risk factor associated with pollution of water area; determination of type and concentration of pollutants and microparticles, biogenic substances (compounds of nitrogen, phosphorus, silicon), heavy metals, oil and oil products, with exceeding the maximum permissible concentration (MPC); assessment of the probability of ingress and accumulation of microdispersed (including oil) and other pollution microparticles into the organisms of the main commercial fish, depending on their spawning and feeding places;

– development of new, approbation and application of promising methods for researching the water ecosystems conditions and individual components for hydrobionts, including early and differential diagnostics of eutrophication and mortality phenomena, as well as the search for antidote protection of aquatic ecosystems, including assimilation methods of measurement data, diagnostics of the quality of developed models, restoration of the state function, research of the models' sensitivity to variations input data, integration of models of various scales;

– development of proposals and measures to ensure the optimal regime, conservation of the fishery resources biodiversity, ecosystems of shallow waters, including planning of observations and assessment of the information content of monitoring systems, detection, assessment of the power of sources of pollutants and their management, assessment of the impact on the food base of fish using the developed mathematical models and it numerical implementation to predict both the distribution of suspended plumes in water environment and the change of bottom topography due to the precipitation of suspended soil particles during the operation of various types of dredging equipment;

– organization and research to identify trends and patterns of changes in water ecosystem conditions under the influence of anthropogenic factors, including assessment risks and vulnerability to anthropogenic impacts, the observability of areas, zoning the shallow water in accordance with the levels of anthropogenic loads;

– development of a number of proposals and measures for the prevention, implementation of environmental design from the standpoint of sustainable development, elimination of the negative consequences of climatic and industrial challenges.

The SSC includes the implementation of 2D and 3D mathematical models on computational grids consistent with the complex coastline shape of research domain. The SSC is intended to perform calculations for substance transfer problem in shallow water on various computational grids. During the implementation of the project, a number of computational experiments and researches of obtained simulation results were performed.

3 Development of software tools for predictive modeling of biogeochemical processes in shallow water

Algorithms for numerical implementation of mathematical models of hydrodynamics and biogeochemistry of shallow water were developed in this research. They are implemented in the C++ programming language. A software module (library) of iterative solvers for systems of linear algebraic equations (SLAE) was developed by the modified alternating-triangular iterative method (MATM) (for the self-adjoint and non-self-adjoint cases) for the convection-diffusion problem based on decomposition in two spatial directions [16].

Parallel algorithms have been developed for numerical implementation of discrete models of pollution transport in a shallow water, oriented towards high-performance computer systems. Due to it, the computation time was significantly reduced by dozens of times at large amount of input data and, depending on the used refining grid along the coastal part of computational domain and the problem being solved, compared with sequential algorithms that implement methods of variational type.

A numerical implementation of fast-converging parallel iterative algorithms for grid equations obtained by approximating the original problem by schemes of a higher order of accuracy, which have high efficiency coefficients for systems with distributed memory, is proposed.

With the parallel implementation of hydrophysics and biological kinetics problems posed in this work, methods for decomposition of grid domains were developed for solving computationally laborious diffusion-convection problems taking into account the architecture and parameters of the computer system. The analysis of the effectiveness of the developed parallel algorithms was performed, and researches of the obtained solutions of water ecology problems were conducted. For acceleration calculations, the Message Passing Interface (MPI) was used to solve the pollutant transport problems on systems with distributed memory.

The numerical implementation of the MPTM for solving high-dimensional SLAE is based on the developed parallel algorithms that implement the pipelined computation process. Due to these algorithms, all available computing resources are involved, including high-performance graphics accelerators. It is assumed that each computing node of the system can contain from 1 to 2 central processing units (CPUs) containing from 1 to 32 cores, and from 1 to 12 NVIDIA video accelerators with support for CUDA technology (GPUs) with at least 192 (NVIDIA GeForce GT 710) up to 5120 (NVIDIA Tesla V100) CUDA cores. An algorithm that controls all available threads of the CPU (Central Processing Unit) and GPU (Graphics Processing Unit) (computers) performs the organization of calculations on each node. Each calculator performs calculations only for its own fragment of the computational domain. To do this, the computational domain is divided into subdomains assigned to individual computing nodes. Further, each subdomain is divided into fragments assigned to each CPU core and each GPU computational unit [17].

To increase the calculation efficiency of computational grid fragments assigned to graphics accelerators, an algorithm and its software implementation in the CUDA C language were developed. NVIDIA Tesla K80 graphics accelerator has high computing performance and supports all modern both closed (CUDA) and open (OpenCL, DirectCompute) technologies [18]. The use of graphics accelerator with CUDA technology is necessary to solve the problem of efficient resource allocation at SLAE solution with high dimension.

The NVIDIA Tesla K80 specifications: the GPU frequency of 560 MHz, the GDDR5 video memory of 24 GB, the video memory frequency of 5000 MHz, the video memory bus digit capacity is equaled to 768 bits. The NVIDIA CUDA platform characteristics: Windows 10 (x64) operating system, CUDA Toolkit v10.0.130, Intel Core i5-6600 3.3 GHz pro cess or, DDR4 of RAM 32 GB, the NVIDIA Ge Force GTX 750 Ti video card of 2GB, 640 CUDA cores. The distinctive feature of the software implementation is the use of a more compact data structure for storing sparse matrix.

For software implementation of the corresponding algorithm based on NVIDIA CUDA technology, the dependence of the SLAE solution time by the alternating-triangular method on matrix dimension and the number of non-zero diagonals was obtained. The paper proposes a modification of the CSR (Compressed Sparse Rows) matrix storage format to increase the efficiency of data storage with a repeating sequence of CSR1S elements (Fig. 2). The proposed format is effectively used for simulation continuous hydrobiological processes using the finite difference method. In additionally, to change a differential operator instead of repeatedly searching and replacing values in an array of nonzero elements, it is enough to just change them in an array that preserves a repeating sequence.

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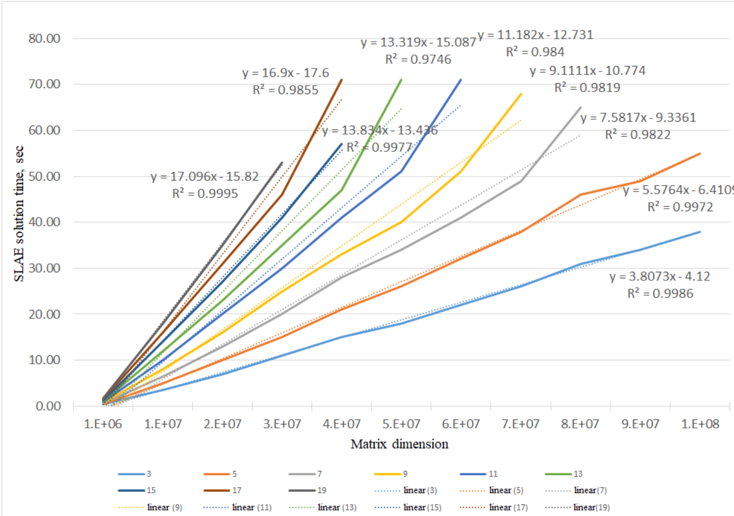

Fig. 2. Graph of SLAE solution time dependence on the order of a square matrix with a given number of nonzero diagonals.

Due to the developed efficient parallel algorithms for numerical implementation of the of biological kinetics problem on NVIDIA Tesla K80 graphics accelerator, it possible to researched both intra- and interspecies chemical communications between plankton populations of the coastal system – the Azov Sea in limited time. It is relevant in the event of catastrophic ecological situations, which include eutrophication and exogenous hypoxia processes.

A three-dimensional mathematical model of the transformation of phosphorus, nitrogen and silicon forms of plankton dynamics problem for shallow waters has been developed and researched taking into account the convective and diffusion transports, absorption and release of nutrients by phytoplankton, cycles of transformations of phosphorus, nitrogen and silicon forms, as well as numerical methods for solving it. The finite-difference schemes with weights of high-order of accuracy taking into account the degree of filling of the control cells of the computational domain were implemented on high-performance computer system. Due to it, the error of numerical solution of the problem and the calculation time were reduced by several times. Based on the numerical implementation of the developed models, the reconstruction of hazardous phenomena of the coastal system associated with the spread of harmful pollutants was performed [19].

To solve the water ecology problems, the high-performance computing cluster K-60 was used, launched at the M.V. Keldysh Institute of Applied Mathematics in 2017. The K-60 cluster has a modular structure that includes computing nodes, routing and remote access nodes, a backup node, switching nodes, management and monitoring nodes. The additional module contains emergency power batteries. Each computing node is based on two Intel Xeon E5-2690 v4 processors and is equipped with 256 GB of RAM. The computing modules are interconnected using several networks. Two different networks are used to connect the branches of a parallel program and to access the servers of a distributed file system. The Infiniband network provides low latency when transmitting messages between nodes and has a data transfer rate of up to 56 Gbit/s. The cluster is managed via 1 Gbit/s network. The management server performs the functions of an access server, and is used for preparing and storing the source texts of user programs, data, calculation results, as well as for compiling and preparing tasks. Through this server, users get access to the calculator. All the main elements of the computing system are located in six server blocks of the 47U form factor. The results of parallel algorithms based on MPI technology and hybrid MPI+OpenMP technology (splitting scheme into two-dimensional and one-dimensional problems) are shown in Fig. 3. The simulation was performed on a rectangular grid of 1000 x 1000 x 60 even nodes.

Parallel algorithms based on hybrid MPI+OpenMP technology were used to solve three-dimensional diffusion-convection problems and have shown higher efficiency compared to parallel algorithms based on MPI technology.

During the implementation of the project, testing and optimization of parallel algorithms and programs were performed taking into account the architectural features of the high-performance systems. The verification and validation of the developed models and programs that implement them were performed on the basis of various environmental databases, available field data, including space sensing data [20]. The developed parallel algorithms for solving the problems of hydrodynamics and biological kinetics set in this project make it possible to shorten the calculation time by tens to hundreds of times. The performance evaluation of the developed software components of the computational structure was conducted for predictive modeling of biological kinetics processes in comparison with sequential algorithms, including the velocity and efficiency of the developed parallel algorithms and programs for high-performance computer systems, the expected accuracy (sinfulness) of predictive modeling and the development of recommendations and suggestions for their further improvement.

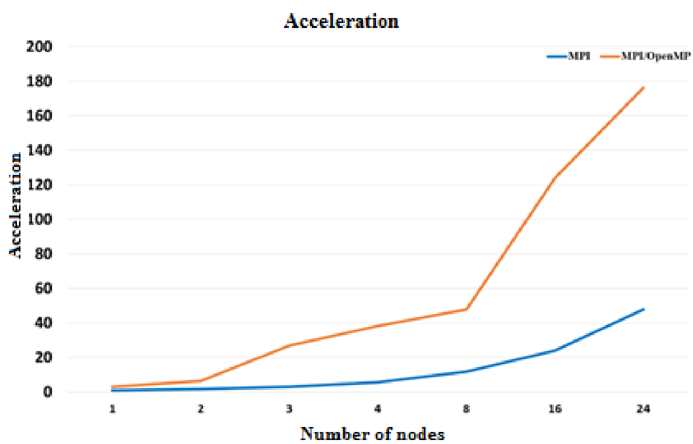

Fig. 3. The dependence of the acceleration of parallel algorithms based on MPI and MPI+OpenMP technologies on the number of calculators (the splitting scheme into one-dimensional and two-dimensional problems).

The developed SSC combines a wide database of environmental data and the library of application programs focused on high-performance systems, implements the developed hydrobiological models. The SSC specificity are: to assess the current conditions of the Azov Sea and predict the environmental situation development in the event of hazardous situations; predict the pollutant dynamic, including compounds of nitrogen, phosphorus and silicon, oil and oil products, sediment transport, distribution of nutrient concentrations, oxygen, plankton populations; indicate the parameters for managing the eutrophication processes and "water blooming", the hydrogen sulfide volume and hypoxic zones. The SSC is planned to be replicated in the future to other shallow water systems in the South of Russia. The developed software and algorithmic tools will increase the predictive accuracy for simulation of shallow ecosystem conditions by 20 – 30%.

To control the simulation quality of processes of hydrodynamics and biological kinetics, we used data from satellite monitoring of the Earth obtained by NOAA (National Oceanic and Atmospheric Administration), the system of the Analytical GIS portal developed by the Institute for Information Transmission Problems of the Russian Academy of Sciences (IITP RAS, Moscow), data portal of the Unified State System of Information on the situation in the World Ocean "ESIMO", data from the Federal State Budgetary Institution "Scientific Research Center for Space Hydrometeorology" Planeta" Siberian Center. The use of satellite data makes it possible to identify areas of coastal zone that are most susceptible to climatic and industrial impacts [21].

4 SSC structure and operation

The SSC was designed to create information support for the prevention and elimination of the consequences of adverse catastrophic natural and technogenic phenomena in shallow water, including the pollution of water environment with harmful impurities, oil and oil products, increased concentration of harmful and toxic algae, freezing phenomena, flooding, etc. Due to it, we can develop preventive measures to ensure environmental safety and reduce possible damage. The block diagram of the SSC operation is given in Fig. 3.

The SSC components (program modules): the input-output and visualization system; the interface system; the control block; various ecological (oceanological, meteorological) databases; the geographic information systems (GIS); the library of applied programs for solving grid problems of shallow water hydrobiology; satellite monitoring data; global database of resources for geotagging and access to satellite data acquisition systems; NCEP/NCAR reanalysis database.

– SPC input data:

– satellite monitoring data (LANDSAT, NOAA, AQUA, TERRA, SPOT, etc.), results of data processing obtained by hyperspectral (Hyperion) and multispectral (ALI) spectroradiometers of the EO-1 satellite; SAR radar images (Envisat ASAR, ERS) NOAA GFS data (website: dvs.net.ua/mp) were used to analyze wind velocity fields and other meteorological conditions. Satellite images (combinations of optical channels of the MODIS AQUA scanner with NASA LANCE Web Mapping Service) were used for the analysis of threats and anomalies;

– aerial photography images (presence of coastline places with dead fish; oil slick shapes and oil film thickness, assessment of areas with increased plankton concentrations, natural and anthropogenic changes, etc.);

– land and water measurements (hydrophysical, chemical, biological indicators), obtained at expeditions and field measurements;

– additional data from the scene (pollution type, source capacity, spill nature, etc.).

Distinctive SSC features, compared to the existing developments in this problem area, are reliability, high performance, and high accuracy of simulation results, due to the following factors:

– implementation of improved interconnected mathematical models of hydrophysics and biological kinetics in shallow water, which differ from the known ones by taking into account a number of determining factors (biotic and abiotic) that affect the pollution transport dynamics by various etiologies;

– the integration of additional software modules, which, in turn, does not affect the SPC performance;

– possibility of SSC replication to other shallow waters;

– availability of extensive databases and satellite information to high-quality calibrate and validate of obtained results.

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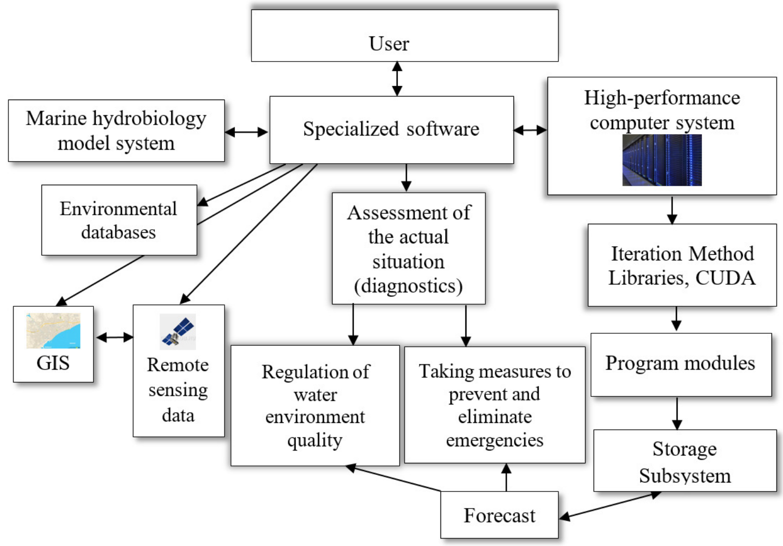

Fig. 4. Structural diagram of SC operation.

Due to the numerous GIS information, satellite data, SSC-simulation provides additional opportunities for better and more complex spatial analysis, and decisions based on it are more accurate [12]. Processing, analysis and visualization of various spatially distributed information (natural resource, environmental, legal and socio-economic, statistical, etc.) about the territory are provided. This ensures to use of electronic cartographic funds of the region, to systematize and improve the accounting and evaluation of natural resources, to organize the complex environmental monitoring, to provide the necessary information for managing the entire natural complex [13].

For a comprehensive interpretation of satellite data and establishment of a causal relationship between hydrodynamic and biotic processes, the calculation data based on the developed interconnected mathematical 3D were used. As a result, approaches have been developed to assess the sharing remote and model data.

The developed SSC and GIS make it possible not only to assess the extent of the development of a natural catastrophe. Due to it, we also can simulate the development conditions on accelerated time in order to prevent negative consequences associated with material damage and a threat to human health and life. The catastrophe forecast without the use of modern methods of mathematical modeling in accelerated time and GIS is difficult to predict due to the influence of many rapidly developing factors (climatic, hydrometeorological, and other conditions) on their development.

Early methods, taking into account the Earth remote sensing data, are used simplified models of environmental events development. Often, the model equations take into account only the diffusion component, use the Gaussian approximation, which is fundamentally wrong at model development for real water. At construction the predictive models of ecological situation development (spread of pollution biogenic substances, oil slicks on water surface, phyto- and zooplankton), the developed SSC uses not only satellite information, but also additional ground-based measurement data, a priori information on pollution parameters with an accuracy sufficient for environmental modeling and presenting the results in the form of a digital map as part of a GIS.

To calculate the impurity concentrations (chlorophyll-a, DOM, small and large particles) from optical data, standard algorithms for satellite data processing by leading

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space agencies (NASA, ESA) were used for the Azov Sea areas that are not optically complex.

The number of computational experiments and researches were performed using the developed software complex to predict possible scenarios of the pollutant transport by various etiologies, biogenic substances (phosphorus, nitrogen, sulfur, silicon), dissolved oxygen, the dynamics of phyto- and zooplankton, in shallow water.

At analyzing the SSC efficiency, which implements the constructed scenarios for ecological situation development in the Azov Sea using numerical implementation of model problems of biological kinetics, with similar work in the field of mathematical modeling of hydrobiological processes, it was found that the obtained simulation results are qualitatively and quantitatively consistent with satellite monitoring data.

5 Conclusion

The designed software is adapted for solving predictive problems of waer ecology and water resources management. The research results can be used by institutions, fisheries to develop schemes for optimal nature management, protection of unique natural waters, as well as assess the anthropogenic influence on the environment during work in waters, including dredging.

The number of computational experiments and researches of the obtained simulation results were performed. The developed SSC can be effectively used to research the transport processes in natural and technological systems.

Parallel algorithms for solving the biological kinetics problem on the sequence of condensing grids were developed, and their efficiency was analyzed in the case of the different number of involved flows. Results of numerical experiments on the NVIDIA Tesla K80 graphics accelerator showed the advantage of the parallel algorithm with a large number of computational nodes. As a research result, an algorithm and a software module that implements it were developed for SLAE solution (the self-adjoint and non-self-adjoint cases) arising at discretization of hydrodynamics problem of shallow water, MPTM using NVIDIA CUDA technology. The decomposition of computational grid method to heterogeneous computing systems was described. The graph model was proposed to organize the parallel pipelined computational process on the GPU, designed to solve systems of large-scale grid equations. For each of two video adapters with different characteristics, experimental researches were performed to determine the optimal two-dimensional configuration of threads in the computational unit, implemented on a single streaming multiprocessor, in which the implementation time on the GPU of one MPTM step is minimal. The conducted researches have shown that the choice of the decomposition method of computational domain in the form of parallelepipeds must be performed taking into account the architecture of the video adapter.

The developed software tools allow more efficient use of GPU computing resources to solve the computational labor three-dimensional hydrophysical problems.

The developed complex of interconnected spatial-three-dimensional non-stationary models of hydrobiology can be used to assess hydrophysical changes in geosystem monitoring of coastal systems in the South of Russia, which are most susceptible to anthropogenic impacts, to form scenarios for water purification, to strengthen the coastline, and to justify new observations.

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