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NUMERICAL MODELING OF HYDRODYNAMIC PROCESSES IN THE TAGANROG BAY OF THE AZOV SEA*

V. N. Litvinov [1,2], A. A. Filina[3], A. E. Chistyakov[1]

✉ litvinovvn@rambler.ru, j.a.s.s.y@mail.ru, cheese_05@mail.ru

[1] Don State Technical University, Rostov-on-Don, Russia
[2] Azov-Black Sea Engineering Institute of Don State Agrarian University, Zernograd, Russia
[3] Supercomputers and Neurocomputers Research Center, Taganrog, Russia

This paper covers the creation and numerical realization of proposed mathematical model of hydrodynamical processes in shallow water based on contemporary information technology and new computational methods that allow improve the prediction accuracy of the environmental situation using the example of the Taganrog Bay in the Azov Sea basin. The proposed mathematical hydrodynamics model takes into account surges, dynamically reconstructed geometry, elevation of the level and coastline, wind currents and friction against the bottom, Coriolis force, turbulent exchange, evaporation, river flow, deviation of the pressure field value from the hydrostatic approximation, the salinity and temperature impact. The discretization of the mathematical model of hydrodynamics was performed using the splitting schemes for physical processes. The constructed discrete analogs possess the properties of conservatism, stability, and convergence. Numerical algorithms are also proposed for solving the arising SLAEs that improve the accuracy of predictive modeling. The practical significance of this research is software implementation of the developed model and the determination of limits and prospects of its application. The experimental software development was based on a graphics accelerator for mathematical simulation the possible scenarios of shallow water ecosystems in consideration the environmental factors influence. The decomposition methods taking into account the CUDA architecture specifications were used at parallel implementation for computationally labors diffusion-convection problems.

Keywords: mathematical modeling, shallow water, splitting schemes, filtering methods, parallel algorithm, software.

Introduction. The seawater salinity is one of the most important abiotic factors and has a significant effect on the sea ecosystem conditions. The Azov Sea basin is an extensive mixing zone of fresh river waters from the Don River and the salty waters from the western part of the Azov Sea; the features of the Taganrog Bay waters are high spatial and temporal variability of salinity. A significant contribution to its dynamics is made by the effects of mixing of the aquatic environment caused by surges arising from the westerly wind.

Much work on the research of the hydrological mode of the Azov Sea, in particular the salinity and temperature, was done by Matishov G.G., Gargopa Yu. M. and others [1]. In work [2], it is noted that the salinity dynamics of the Azov Sea significantly depends on the inflow of salt water from the Black Sea, river flows and air processes that affect the balance of moisture evaporation from the sea surface and precipitation. Therefore, the periods of relative desalination and salinization are typical for the Azov Sea basin. Since 2007, there has been a modern period of salinization of the Azov Sea

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[3, 4], which is associated with a decrease in the Don River flow by 35.6% compared to the period from 1998 to 2006.

It is widely known that in spite of numerous publications, many effects have a great effect on the spatial change in hydrodynamic processes of shallow water, but it not taken into account at creation of mathematical models. This contributes to the deterioration of prediction quality of ecological situation change at researched water zones.

At this point, it is necessary to design a computational methods and tools for implementation the parallel algorithms to predict the hydrodynamic processes and changes of environmental conditions in shallow waters and coastal zones, among them the pollution transport and sedimentation, organic deposits. The implementation on high-performance computer systems allows provide the prediction of sustainable development of coastal systems.

The expedition researches in the Azov Sea basin were performed by the staff members of the Don State Technical University, the Southern Federal University, and the Southern Scientific Center of the Russian Academy of Sciences aboard the Scientific Research Vessel «Deneb» in July 2017 (Fig. 1).

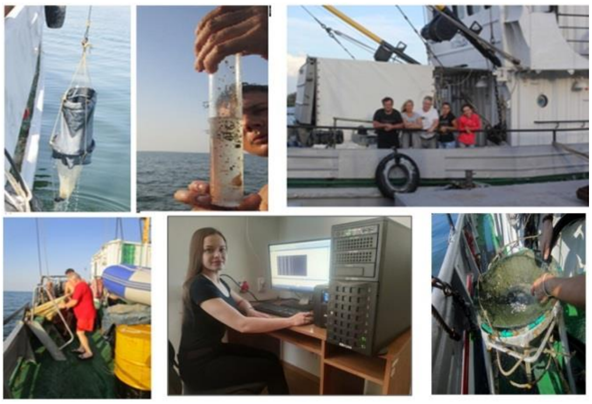

Fig. 1. Expedition researches on the «Deneb», 2017

The expedition data, the «USIWO» portal data on the situation in the World Ocean were used for complex geoinformation analysis of spatial-temporal processes and phenomena at simulation of hydrobiological shallow water processes.

Problem statement. For calculation three-dimensional fields of water velocity vector, salinity and temperature we developed the mathematical model which is based on the mathematical hydrodynamic model of shallow waters, considering the heat and salts transport [5, 6]:

– the Navier-Stokes motion equation

$$u'_t + uu'_x + vu'_y + wu'_z = -\frac{1}{\rho}P'_x + \left(\mu u'_x\right)'_x + \left(\mu u'_y\right)'_y + \left(\nu u'_z\right)'_z + 2\Omega(v\sin\theta - w\cos\theta), \qquad (1)$$

$$v'_t + uv'_x + vv'_y + wv'_z = -\frac{1}{\rho}P'_y + \left(\mu v'_x\right)'_x + \left(\mu v'_y\right)'_y + \left(\nu v'_z\right)'_z - 2\Omega u\sin\theta, \qquad (2)$$

$$w'_t + uw'_x + vw'_y + ww'_z = -\frac{1}{\rho}P'_z + \left(\mu w'_x\right)'_x + \left(\mu w'_y\right)'_y + \left(\nu w'_z\right)'_z + 2\Omega u\cos\theta + g\left(\rho_0/\rho - 1\right), \qquad (3)$$

– the continuity equation (the case of variable density)

$$\rho'_t + (\rho u)'_x + (\rho v)'_y + (\rho w)'_z = 0, \qquad (4)$$

– the heat transport equation

$$T_t' + uT_x' + vT_y' + wT_z' = \left(\mu T_x'\right)_x' + \left(\mu T_y'\right)_y' + \left(\nu T_z'\right)_z' + f_T, \quad (5)$$

– the salt transport equation

$$S_t' + uS_x' + vS_y' + wS_z' = \left(\mu S_x'\right)_x' + \left(\mu S_y'\right)_y' + \left(\nu S_z'\right)_z' + f_S, \quad (6)$$

where $\mathbf{V} = \{u, v, w\}$ are the velocity vector components; μ, ν are horizontal and vertical components of the turbulent exchange coefficient; ρ is the density of water; S is the water salinity; $\mathbf{\Omega} = \Omega \cdot \left(\cos\theta \cdot \mathbf{j} + \sin\theta \cdot \mathbf{k}\right)$ is the angular velocity of the Earth rotation; θ is the latitude of the region; g is the gravity acceleration; P is the full hydrodynamic pressure; f_T, f_S are sources of heat and salt (located on the border of water zone); T is the water temperature.

The pressure of the liquid column and the hydrodynamic part are components that are conditionally distinguished from the total hydrodynamic pressure [6, 7] in the form:

$$P(x, y, z, t) = p(x, y, z, t) + \rho_0 gz, \quad (7)$$

where p is the hydrostatic pressure of the unperturbed fluid; ρ_0 is the fresh water density under normal conditions.

The state equation for density has the form:

$$\rho = \rho + \rho_0, \quad (8)$$

where ρ_0 is the fresh water density under normal conditions; ρ is determined using the equation, recommended by UNESCO:

$$\rho = \rho_w + (8.24493 \cdot 10^{-1} - 4.0899 \cdot 10^{-3} T + 7.6438 \cdot 10^{-5} T^2 - 8.2467 \cdot 10^{-7} T^3 + 5.3875 \cdot 10^{-9} T^4) S +$$
$$+ (-5.72466 \cdot 10^{-3} + 1.0227 \cdot 10^{-4} T - 1.6546 \cdot 10^{-6} T^2) S^{3/2} + 4.8314 \cdot 10^{-4} S^2, \quad (9)$$

where ρ_w is the density of fresh water, specified by the polynomial in the form [8]:

$$\rho_w = 999.842594 + 6.793952 \cdot 10^{-2} T - 9.095290 \cdot 10^{-3} T^2 +$$
$$+ 1.001685 \cdot 10^{-4} T^3 - 1.120083 \cdot 10^{-6} T^4 + 6.536332 \cdot 10^{-9} T^5. \quad (10)$$

The equation (9) is applicable for the salinity values within the range 0 – 42‰ and the temperature values within the range -2 – 40°C.

The following boundary conditions are used for the system of equations (1–6) [9–11]:

– at the input:

$$\mathbf{V} = \mathbf{V}_0,\ P_{\mathbf{n}}' = 0,\ T = T_1,\ S = S_1 \quad (11)$$

– the bottom boundary:

$$\rho_v \mu \left(\mathbf{V}_\tau\right)_{\mathbf{n}}' = -\boldsymbol{\tau},\ \mathbf{V}_{\mathbf{n}} = 0,\ P_{\mathbf{n}}' = 0,\ T_{\mathbf{n}}' = 0,\ S_{\mathbf{n}}' = 0,\ f_T = 0,\ f_S = 0, \quad (12)$$

– the lateral boundary:

$$\left(\mathbf{V}_\tau\right)_{\mathbf{n}}' = 0,\ \mathbf{V}_{\mathbf{n}}' = 0,\ P_{\mathbf{n}}' = 0,\ T_{\mathbf{n}}' = 0,\ S_{\mathbf{n}}' = 0,\ f_T = 0,\ f_S = 0, \quad (13)$$

– the upper boundary:

$$\rho_v \mu \left(\mathbf{V}_\tau\right)_{\mathbf{n}}' = -\boldsymbol{\tau},\ w(x, y, t) = -\omega - P_t' / \rho g,\ P_{\mathbf{n}}' = 0,\ T_{\mathbf{n}}' = 0,\ S_{\mathbf{n}}' = 0,\ f_T = k\left(T_a - T\right),\ f_S = \frac{h_\omega}{h_z - h_\omega} S, \quad (14)$$

– at the output (the Kerch Strait):

$$P'_{\mathbf{n}} = 0, \mathbf{V}'_{\mathbf{n}} = 0, T'_{\mathbf{n}} = 0,\ S'_{\mathbf{n}} = 0,\ f_T = 0,\ f_S = 0, \qquad (15)$$

where ω is the liquid evaporation rate; $\mathbf{V}_{\mathbf{n}}$, $\mathbf{V}_{\boldsymbol{\tau}}$ are normal and tangential components of the velocity vector; $\mathbf{n}$ is the outer normal vector to the boundary of computational domain; T_a is the atmospheric temperature; $\boldsymbol{\tau} = \{\tau_x, \tau_y, \tau_z\}$ is the tangential stress vector; ρ is the density of water; ρ_v is the sediment density; k is the heat transport coefficient between the atmosphere and water environment.

The tangential stress components for free surface are the following: $\boldsymbol{\tau} = \rho_a Cd_s |\mathbf{w}|\mathbf{w}$, where ρ_a is the atmosphere density; $\mathbf{w}$ is the wind velocity vector relative to the water; $Cd_s = 0.0026$ is the dimensionless coefficient of the surface resistance that depends on the wind velocity, and considered within the range 0.0016–0.0032 [12].

The tangential stress for the bottom are the following: $\boldsymbol{\tau} = \rho Cd_b |\mathbf{V}|\mathbf{V}$, where $k = 0.025$ is a group roughness coefficient in the Manning formula and considered within the range 0.025–0.2; $Cd_b = gk^2 / h^{1/3}$; $h = H + \eta$ is the water depth; η is the height of free surface relative to the geoid (sea level); H is the depth of undisturbed surface.

The following initial conditions were used for the system of equations (1–6):

$$\mathbf{V} = \mathbf{V}_0, T = T_0, S = S_0, \qquad (16)$$

where $\mathbf{V}_0$, T_0 and S_0 are predefined functions.

Model discretization. According to the pressure correction method, the original model of hydrodynamics is subdivided into three problems [13–15]. For calculation of velocity vector field components on the intermediate layer in time the diffusion-convection-reaction equation is used; it's the first subproblem:

$$\frac{\tilde{u} - u}{\tau} + u\bar{u}'_x + v\bar{u}'_y + w\bar{u}'_z = \left(\mu\bar{u}'_x\right)'_x + \left(\mu\bar{u}'_y\right)'_y + \left(\nu\bar{u}'_z\right)'_z + 2\Omega(v\sin\theta - w\cos\theta),$$

$$\frac{\tilde{v} - v}{\tau} + u\bar{v}'_x + v\bar{v}'_y + w\bar{v}'_z = \left(\mu\bar{v}'_x\right)'_x + \left(\mu\bar{v}'_y\right)'_y + \left(\nu\bar{v}'_z\right)'_z - 2\Omega u\sin\theta,$$

$$\frac{\tilde{w} - w}{\tau} + u\bar{w}'_x + v\bar{w}'_y + w\bar{w}'_z = \left(\mu\bar{w}'_x\right)'_x + \left(\mu\bar{w}'_y\right)'_y + \left(\nu\bar{w}'_z\right)'_z + 2\Omega u\cos\theta + g\left(\frac{\rho_0}{\rho} - 1\right). \qquad (17)$$

Note that the term $g(\rho_0 / \rho - 1)$ describes the buoyancy (the Archimedes' Power). Numerical experiments for simulation the transport of water environment in shallow waters such as the Azov Sea have shown that this term makes a minor contribution to the problem solution and can be ignored. To approximate the diffusion-convection-reaction equation in time we used the schemes with weights. Here $\bar{u} = \sigma\tilde{u} + (1 - \sigma)u$, $\sigma \in [0,1]$ is the weight of the scheme.

The second subproblem is represented by the calculation of the pressure distribution which is based on the Poisson equation:

$$p''_{xx} + p''_{yy} + p''_{zz} = \frac{\hat{\rho} - \rho}{\tau^2} + \frac{\left(\hat{\rho}\tilde{u}\right)'_x}{\tau} + \frac{\left(\hat{\rho}\tilde{v}\right)'_y}{\tau} + \frac{\left(\hat{\rho}\tilde{w}\right)'_z}{\tau}. \qquad (18)$$

The velocity field value at the upper boundary (water surface) is calculated by the formula $w = -\omega - p'_t / \rho g$. A simplified hydrostatic model of the transport of water environment was used as an initial approximation for this problem. It significantly reduces the calculation time. At the third subproblem, we use the explicit formulas to determine the velocity distribution on the next time layer:

$$\frac{\hat{u}-\tilde{u}}{\tau}=-\frac{1}{\hat{\rho}}p'_x,\ \frac{\hat{v}-\tilde{v}}{\tau}=-\frac{1}{\hat{\rho}}p'_y,\ \frac{\hat{w}-\tilde{w}}{\tau}=-\frac{1}{\rho}p'_z, \tag{19}$$

where τ is the step along the time coordinate; $\tilde{u}$ is the value of the velocity field on the intermediate time layer; $\hat{u}$ is the value of the velocity field on the current time layer; u is the value of the velocity vector field on the previous time layer;.

The computational domain is inscribed in a parallelepiped. For software implementation of the three-dimensional mathematical model of hydrodynamics we introduced an uniform grid. $o_{i,j,k}$ is defined the "fullness" of the cell (i,j,k). The degree of cell occupancy is defined by the water column pressure at the bottom of the cell. In general, the degree of cell occupancy is calculated using the following expression [8]:

$$o_{i,j,k}=\frac{P_{i,j,k}+P_{i-1,j,k}+P_{i,j-1,k}+P_{i-1,j-1,k}}{4\rho g h_z}. \tag{20}$$

The approximation of problem the calculation of the velocity field of water environment by spatial variables is based on the balance method taking into account the "fullness" coefficients of control domains.

The grid equations were calculated using the scheme with weights as a result of finite-difference approximations of the problem (1) – (16) [16]. For solution of the problem (1) – (16) we used a modified alternating triangular method (MATM) [17 – 19] and the domain decomposition by the *k*-means algorithm [20, 21].

Features of software implementation. Parallel algorithms were designed for numerical implementation of the proposed mathematical model. It will be adapted for hybrid computer systems using the NVIDIA CUDA architecture that will be used to mathematically predict of described problems and to design the high-performance information systems.

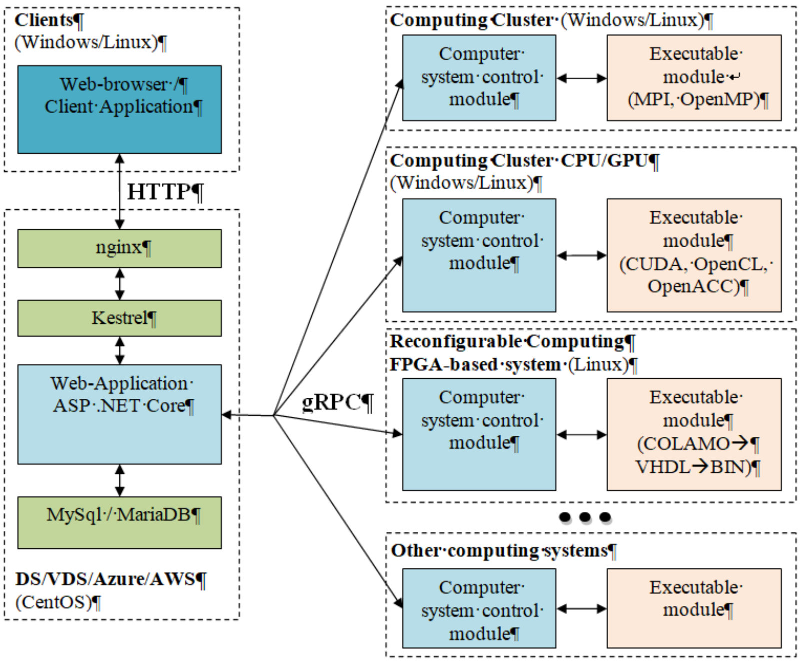

Fig. 2. Generalized system diagram

One of the most important tasks of the stable functioning of such systems is to ensure automatic adjustment of the threshold parameters of the simulation, such as the dimension of the SLAE, since the lack of RAM or video memory leads to a significant decrease of performance or an abnormal termination of the application. In order to implement the algorithm that solves the described problem, a software module for collecting information on the performance of a hybrid computing system has been developed (Fig. 2).

Computer modeling of the set tasks, while meeting the requirements for the accuracy and speed of calculation, requires large computing resources that are not always available in production conditions and in the event of emergencies that require immediate organizational and managerial decisions in order to eliminate them. To increase the efficiency of using available technical means, the architecture of an information system for supporting scientific research is proposed, which can function under conditions of using heterogeneous computing environments.

The system is based on the requirement to use free software as much as possible in order to minimize capital and operating costs. It is proposed to use CentOS 7 as the main operating system with the nginx http-server installed, MariaDB database management system and .NET Core 3.1 platform installed. The application software of the system is developed in the form of a server part, implemented in the form of an ASP .NET Core MVC / Blazor web application, and a client part, which is a set of services installed on all involved computers. The interaction between these system components is provided through the use of gRPC.

The server part provides the solution to the following tasks:

– management of system user accounts, including the assignment of roles;
– configuration management of available computing resources;
– managing the process of uploading modeling tasks to the server in the form of rpm packages;
– management of the monitoring service for performed tasks.
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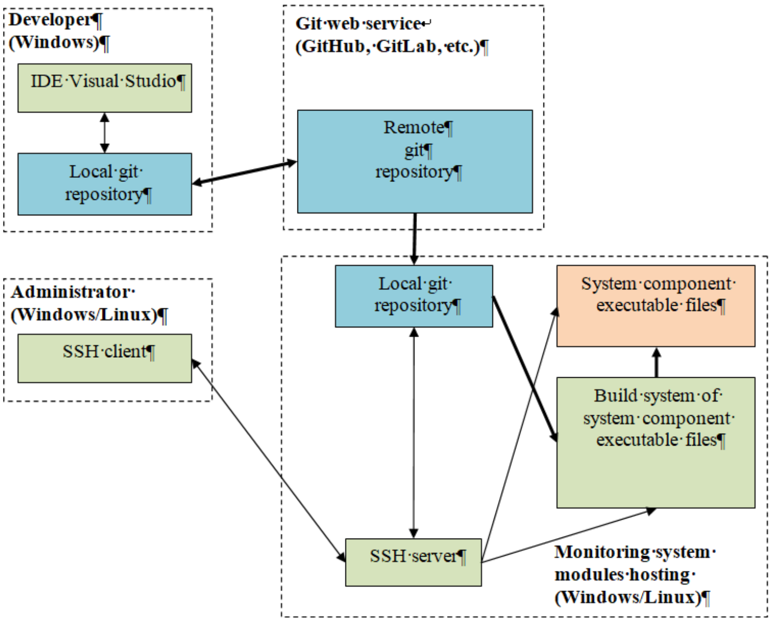

Fig. 3. System development process control diagram

Management of the development process of system and application software is performed using the *Git* version control system. Developers are working with the system code, based on their workstations, where local repositories of system components projects are deployed, synchronized with a remote repository accessible through a web service based on the *Git* version control system.

Management of the processes of deployment, configuration and operation of the system is performed by the administrator using any available SSH client, for example, *ssh* for the Linux console terminal or Bitvise SSH Client for Windows (Fig. 3).

The distinctive feature of the development is the usage of an algorithm for preliminary estimation of the time spent on executing the task based on the data of preliminary testing of the performance of the hardware platform. When the computer control module is launched, it checks for the presence of the performance.xml file. In the absence of a file, performance tests are performed, which are a number of problems for solving SLAEs with different parameters, and their results are written to a file. Results were obtained for the test system with following specifications: Windows 10 (x64), Intel Core i5-6600 3.3 GHz processor, CUDA Toolkit v10.0.130, NVIDIA GeForce GTX 750 Ti 2GB video adapter (640 CUDA cores), 32 GB DDR4 RAM, using NVIDIA CUDA technology (Fig. 4, 5).

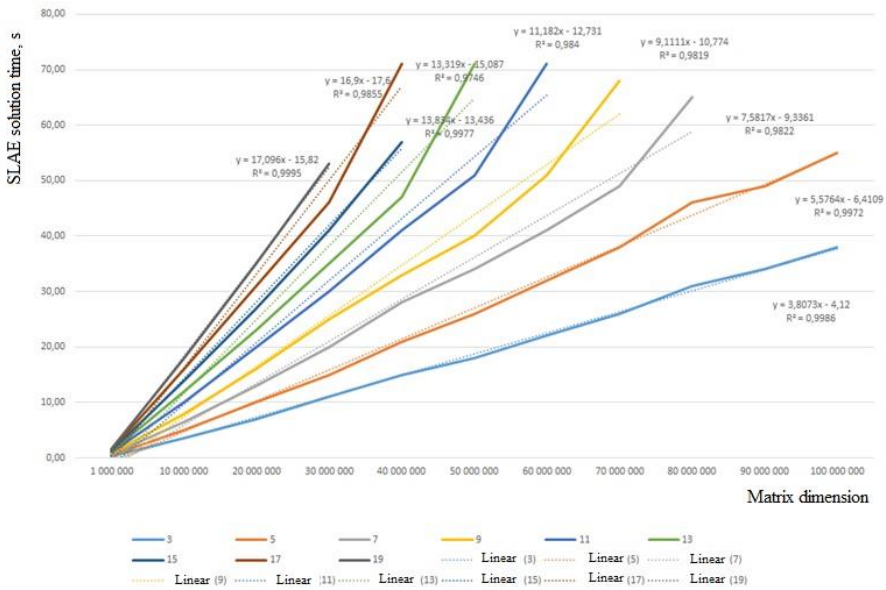

Fig. 4. Graph of time dependence of SLAE solution on the order of a square matrix

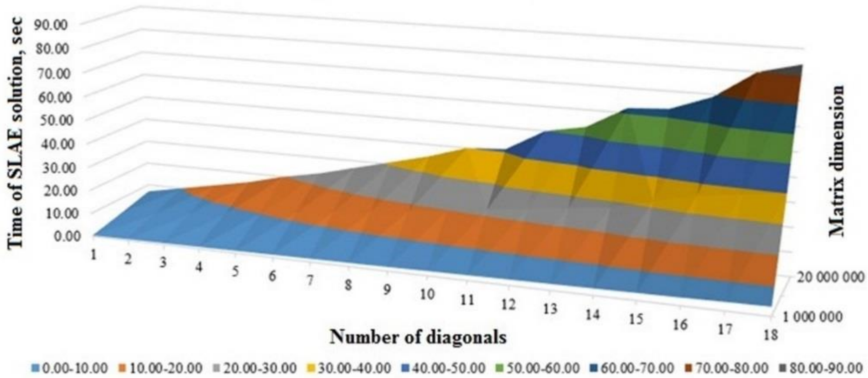

Fig. 5. Test system performance study results

The obtained data on the performance parameters are used then by the control modules of the computing system in the process of controlling the process of placing the computational problem in the queue based on the algorithm shown in Fig. 6.

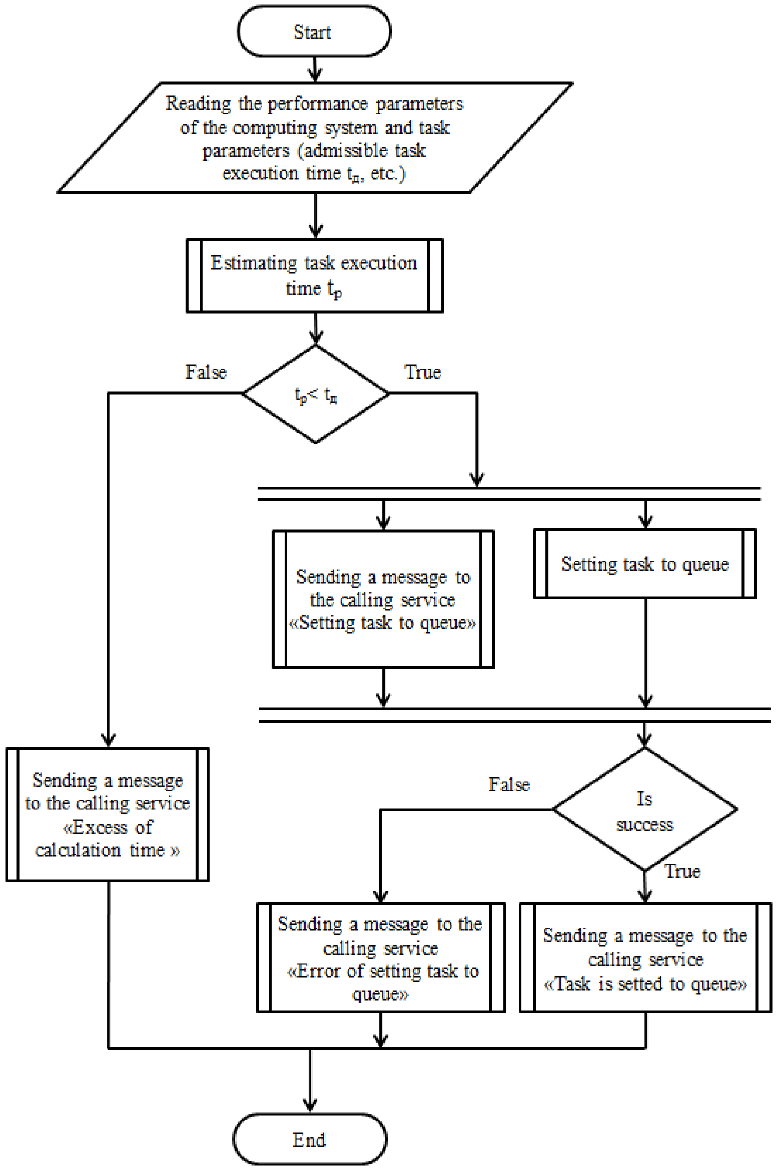

Fig. 6. Algorithm for managing the process of placing a computational problem in the queue

Experimental researches. For numerical solution of the developed mathematical model (1) – (16), we designed the adapted for hybrid computer systems parallel algorithms which use the NVIDIA CUDA architecture.

The program was designed to perform the turbulent flows of an incompressible velocity field of water environment on grids with high resolution. This program is used to calculate transport of heat and salts and takes into account the velocity field of the aquatic environment. Physical parameters are taken into account in the developed program such as: surges, dynamically reconstructed geometry, elevation of the level and coastline, wind currents and friction against the bottom, Coriolis force, turbulent exchange, evaporation, river flow, deviation of the pressure field value from the hydrostatic approximation. The program provides the following functions:

– calculation of the velocity field without taking into account pressure based on (17);
– calculation of hydrodynamic pressure based on (18);
– calculation of a three-dimensional velocity field taking into account pressure based on (19);
– calculation of transport of heat and salts.

The error estimation that are simultaneous considerate the field data from the available n measurements was used as a criterion to check the adequacy of the developed models: $\delta = \sqrt{\left(\sum_{k=1}^{n} q_{k\,nat} - q_k\right)^2} / \sqrt{\sum_{k=1}^{n} q^2{}_{k\,nat}}$, where $q_{k\,nat}$ is the value of the function, calculated with using field measurements; q_k is the value of the grid function, calculated by simulation.

The salinity and temperature fields reconstructed from cartographic information were used as input data for the developed hydrodynamical model at calculation the transport of heat and salts. The data of long-term observations and satellite images were taken in the form of images, from which, after applying the recognition algorithm, the salinity and temperature isolines were defined. The reconstructed temperature and salinity fields were obtained with using an interpolation algorithm based on high-order approximation schemes (Fig. 7). These fields are smoother functions for approximating functional dependencies describing the temperature and salinity fields, and can increase the accuracy of hydrodynamic calculations [5, 22].

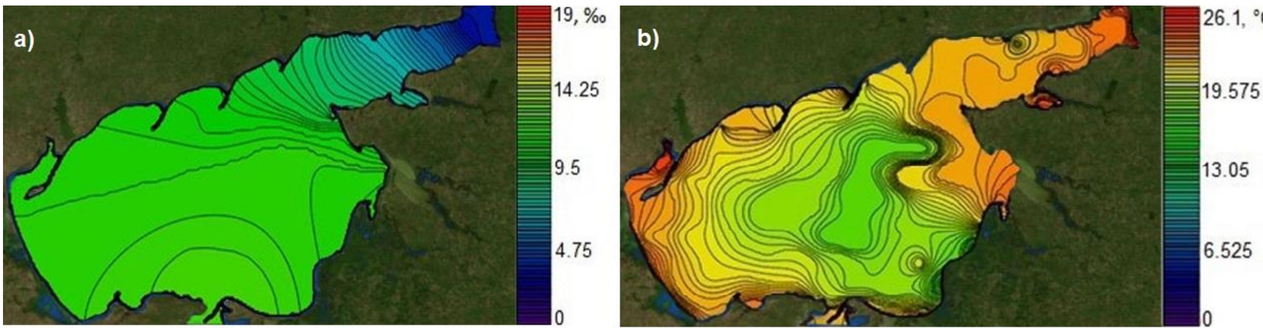

Fig. 7. Images of reconstructed salinity and temperature fields

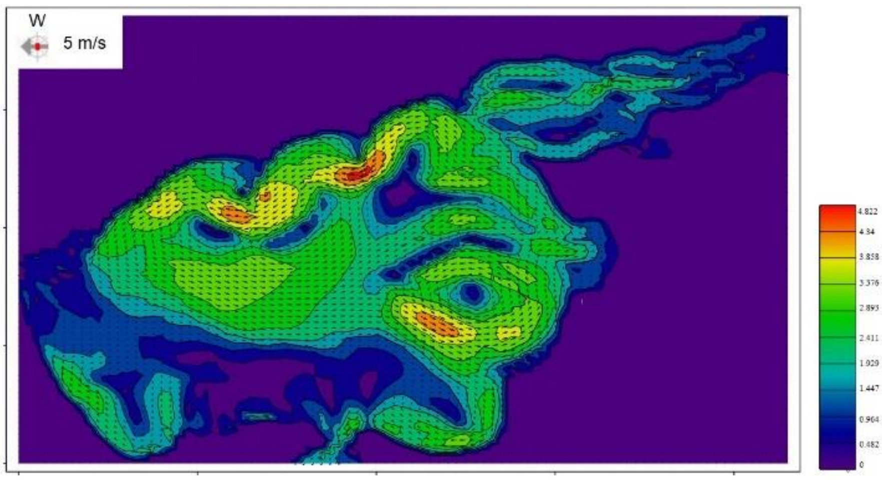

Fig. 8. Simulation results of water environment transport (barotropic flows)

As a result of this research, we designed a software which allow us to more accurately describe the hydrodynamical processes, heat and salts transport in shallow waters, such as the Azov Sea, with complex spatial structures of currents in the conditions of reducing the freshwater flow of the Don river, increasing the flow of highly saline waters of Sivash lake and filtering the waters of salt lakes in the North-East of Crimea. Software implementation of mathematical models takes into account wind currents and bottom friction, river flows, evaporation, the Coriolis force, turbulent exchange, as well as the complex geometry of water bottom and coastline. The computational domain corresponds to the physical dimensions of the Azov Sea: the horizontal step is 1000 m; the length is 355 km; the width is 233 km. The time interval is 30 days. Results of numerical simulation of water environment transport in the Azov Sea basin based on the developed software are given in Fig. 8.

Discussion and conclusions. Due to the proposed 3D hydrodynamical model of shallow waters we can calculate the three-dimensional fields of the water flow velocity vector, sea water density, pressure, salinity and temperature. The water bottom geometry has a great influence on the flow fields in hydrodynamical models of shallow water. Measurements of water flow velocities were performed; it based on the ADCP probe, which measures instantaneous values of the vertical profile of the velocity vector. Data results of expedition measurements were used at creation the hydrodynamical models of shallow waters. Parameters, specified at device setting, are the number of vertical measurements is 128; the vertical step is 10 cm; the measurement frequency is 1 s. The Kalman filter algorithm was used to filter the field data. We compared the simulation results and field measurements of the vertical turbulent exchange coefficient at various water horizons. Based on it, we concluded that the results of calculation the turbulent processes in shallow waters based on the Smagorinsky subgrid turbulence model are best consistent with the field data.

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Authors:

Vladimir N. Litvinov, PhD, associate Professor of the Department of Design and technical service of transport and technical systems, Don State Technical University (DSTU) (Gagarin sq., 1, Rostov-on-Don, Russian Federation); head of the Department of Mathematics and bioinformatics, Azov-Black Sea Engineering Institute of Don State Agrarian University (Lenin str. 21, Zernograd, Russian Federation), 8(918)517 21 38, litvinovvn@rambler.ru

Alena A. Filina, PhD, Scientific Researcher, Supercomputers and Neurocomputers Research Center (Italyansky lane, 106, Taganrog, Russian Federation), 8(951)539 15 94, j.a.s.s.y@mail.ru

Alexander E. Chistyakov, Dr.Sci., Professor, Don State Technical University (DSTU) (Gagarin sq., 1, Rostov-on-Don, Russian Federation), 8(950)859 38 72, cheese_05@mail.ru

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ГИДРОДИНАМИЧЕСКИХ ПРОЦЕССОВ В ТАГАНРОГСКОМ ЗАЛИВЕ АЗОВСКОГО МОРЯ *

В. Н. Литвинов[1,2], А. А. Филина[3], А. Е. Чистяков[1]

✉ litvinovvn@rambler.ru, j.a.s.s.y@mail.ru, cheese_05@mail.ru

[1] Донской государственный технический университет, г. Ростов-на-Дону, Россия
[2] Азово-Черноморский инженерный институт ФГБОУ ВО Донской ГАУ, г. Зерноград, Россия
[3] Общество с ограниченной ответственностью «Научно-исследовательский центр супер-ЭВМ и нейрокомпьютеров», г. Таганрог, Россия

Работа посвящена построению и численной реализации предложенной математической модели гидродинамических процессов в мелководных водоемах на основе современных информационных технологий и новых вычислительных методов, позволяющих повысить точность прогнозирования экологической обстановки на примере Таганрогского залива бассейна Азовского моря. Предложенная математическая модель гидродинамики учитывает пульсации, динамически перестраиваемую геометрию, подъем уровня и береговой линии, ветровые течения и трение о дно, силу Кориолиса, турбулентный обмен, испарение, речной поток, отклонение величины поля давления от гидростатического приближения, влияние солености и температуры. Дискретизация математической модели гидродинамики выполнена на основе схем расщепления по физическим процессам. Разработанные дискретные аналоги обладают свойствами консервативности, устойчивости и сходимости. Также предложены численные алгоритмы решения возникающих СЛАУ, позволяющие повысить точность прогнозного моделирования. Практическая значимость данной работы заключается в программной реализации разработанной модели и определении пределов и перспектив ее применения. Для математического моделирования возможных сценариев развития мелководных экосистем с учетом влияния факторов окружающей среды разработано экспериментальное программное обеспечение на базе графического ускорителя. При параллельной реализации вычислительно трудоемких диффузионно-конвективных задач использовались методы декомпозиции с учетом спецификаций архитектуры CUDA.

Keywords: математическое моделирование, мелководье, схемы расщепления, методы фильтрации, параллельный алгоритм, программное обеспечение.

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Авторы:

Литвинов Владимир Николаевич, кандидат технических наук, доцент кафедры «Проектирование и технический сервис транспортно-технических систем», Донской государственный технический университет (ДГТУ) (РФ, г. Ростов-на-Дону, пл. Гагарина, 1); заведующий кафедрой «Математика и биоинформатика», Азово-Черноморский инженерный институт ФГБОУ ВО Донской ГАУ (РФ, г. Зерноград, ул. Ленина, 21), 8(918)517 21 38, litvinovvn@rambler.ru

Филина Алёна Александровна, кандидат технических наук, научный сотрудник, Общество с ограниченной ответственностью «Научно-исследовательский центр супер-ЭВМ и нейрокомпьютеров» (РФ, г. Таганрог, пер. Итальянский, 106), 8(951)539 15 94, j.a.s.s.y@mail.ru

Чистяков Александр Евгеньевич, доктор физико-математических наук, профессор, Донской государственный технический университет (ДГТУ) (РФ, г. Ростов-на-Дону, пл. Гагарина, 1), 8(950)859 38 72, cheese_05@mail.ru