Mathematical modeling of hydrophysical processes for water with complex bottom geometry

A I Sukhinov¹, A E Chistyakov¹,², A L Leontyev²,³, ⁴, A V Nikitina²,³, ⁴ and A A Filina², ⁴
¹ Don State Technical University, Gagarin square 1, 344000 Rostov-on-Don, Russia
² Educational Center “Sirius”, Olumpiyskyi prospect 40, 354349 Sochi, Russia
³ Southern Federal University, 105/42 Bolshaya Sadovaya Str., 344006 Rostov-on-Don, Russia
⁴ Supercomputers and Neurocomputers Research Center, Co. Ltd., Italyansky lane 106, 347900 Taganrog, Russia

E-mail: Leontyev_Anton@mail.ru

Abstract. The paper covers the development and research of computational structure for mathematical modelling of hydrobiological processes for water with complex bottom geometry, based on the modern information technologies and computational methods. The models used in modelling take into account following: microturbulent diffusion; gravitational settling of pollutants; plankton populations nonlinear interaction; the salinity impact, temperature. The scheme with weights was proposed for discretization of the developed model, that allowed significantly reduce the error and the computational time. Practical significance of the work is that the proposed model was software implemented; the limits and prospects of its use were defined. The experimental software was designed on the basis of a graphics accelerator for mathematical modelling of possible development scenarios of the waters with complex bottom geometry, taking into account the environment influence. Parallel implementation was performed using the decomposition methods for computationally labours diffusion-convection problems taking into account the CUDA architecture characteristics.

1. Introduction

Many scientists have been engaged at mathematical modeling of hydrophysics and biological kinetics processes that have a significant impact on ecological situation and reproduction processes in waters. It should be noted fundamental works in the field of designing the mathematical models, development of methods of diagnostics and forecasting of changes of water ecosystems by such authors as Lotka A.Ya., Volterra V., Logofet D.O., Hutchinson G.E., Mono J., Mitcherlich E.A., Odum H.T., Gauz G.F., Vinberg G.G., Abakumov A.I., Menshutkin V.V., Rukhovets L.A., Vorovich I.I., Khodorevskaya R.P., Zhilkin A.A., Guliyev I.S., Naderi Beni A., Lahjani H., Gorstko A.B., Marchuk G.I., Bulion V., Imberger A., Jorgensen S.E., Vollenweider R.A. They developed principles, mathematical models and approaches widely used at solving scientific and practical problems for aquatic ecosystems. Fleishman B.S. developed and researched stochastic models of potential efficiency of ecosystems.

Hydrostatic models including advective-diffusion equations for temperature and salinity to determine the density field and closure for calculation the coefficients of turbulent exchange were described by Marchuk G.I., Volzinger N.E. and Kagan B.A., in which the successful construction of models of large-
scale long-wave processes was carried out [1, 2]. The nonhydrostatic models developed by Oliger J., Sundstrom A., Marchesiello P., Williams J.C., Shchepetkin A. proved to be correct in the region with an open boundary, in contrast to the hydrostatic models [3,4].

Androsov A.A. and Wolzinger N.E. described a hydrodynamic model in curvilinear boundary-consistent coordinates, describing the problem for vertically averaged equations for calculating the baroclinic pressure component and advective-diffusion equations of temperature and salinity for calculation the baroclinic pressure component [5].

Models of interaction of biota with separate factors, including solar radiation, temperature, then models of interaction of organisms with abstract ‘resources’ of Abrosova N.S. and Bogolyubova A.G. Detailed results and development of the formalized representations on examples of modeling of the mouth of Neva and some lakes of the Northwest of Russia are presented by authors in publications Umnov A.A., Alimov A.F.

Matishov G.G., Ilyichev V.G. [6], Yakushev E.V. [7] research the optimum use of water resources, development of pollution transport models in water. Tyutyunov Yu. [8], Tran J.K. [9], Roux B. [10] studied the interaction of populations, including taxis, interspecies competition and the delay effect. Perevarukha A.Y. was responsible for development and research the graph model of anthropogenic interaction and productivity of biotic factors of the Caspian Sea [11].

Despite a significant number of publications, many effects that have a significant impact on the spatial change of hydrophysical processes and storm phenomena of seas with variable bathymetry are not taken into account in the development of mathematical models, which leads to a deterioration in the quality of forecasts of changes in the ecological and hydrophysical situation of the studied waters.

In this regard, it’s necessary to develop a computational structure that implements parallel algorithms for modeling hydrological processes to predict changes in the ecological and hydrophysical situation of seas with complex bathymetry, including: storm surges, movement of pollutants and sediments, organic sediments, implemented on high-performance computer systems to provide a predictive basis for sustainable development of aquatic ecosystems.

Data, obtained from the database of the interdepartmental information system for access to the resources of marine information systems and integrated information support of marine activities (‘ESIMO’), as well as from the Atlas of climate change in Large marine ecosystems of the Northern hemisphere, were used to model hydrophysical processes [12].

2. Problem statements

The development of computer systems for modeling hydrophysical processes of waters with complex bottom geometry was based on a set of interrelated mathematical models, including a complete model of sea hydrodynamics, taking into account the distribution of pollutants.

The model of sea dynamics is described by the motion equations (the Navier-Stokes equation):

\[
\begin{align*}
\frac{\partial u'}{\partial t} + uu'_x + vu'_y + wu'_z &= -\frac{p_x'}{\rho} + (\mu u')_x + (\mu u')_y + (\nu u')_z + 2\Omega (\nu \sin \theta - \nu \cos \theta), \\
\frac{\partial v'}{\partial t} + uv'_x + vv'_y + wv'_z &= -\frac{p_y'}{\rho} + (\mu v')_x + (\mu v')_y + (\nu v')_z + 2\Omega \nu \sin \theta, \\
\frac{\partial w'}{\partial t} + uw'_x + vw'_y + ww'_z &= -\frac{p_z'}{\rho} + (\mu w')_x + (\mu w')_y + (\nu w')_z + 2\Omega \nu \cos \theta + g (\frac{\rho_p}{\rho} - 1), \\
\rho' + (\mu u')_x + (\nu u')_y + (\nu w')_z &= 0,
\end{align*}
\]

where \(u = \{u, v, w\}\) is the velocity vector of water flow movement; \(p\) is the overpressure on the hydrostatic pressure of the unperturbed liquid; \(\rho\) is a density; \(\Omega\) is the angular velocity of the Earth's rotation; \(\theta\) is the angle between the vertical and angular velocity; \(\mu, \nu\) are horizontal and vertical components of the turbulent exchange coefficient.
Depth maps were used for simulation the water flow fields with variable bathymetry such as the Azov Sea (figure 1), and the bottom surface restoration method was used to obtain smoothed relief images of the bottom of the reservoir.

Boundary conditions:

- the entrance (the mouth of rivers): \( \mathbf{u} = \mathbf{u}_0, p'_n = 0 \),
- the lateral boundary (the bank and the bottom): \( \rho \mu (\mathbf{u}_n)' = -\mathbf{t}, \mathbf{u}_n = 0, p'_n = 0 \),
- the upper boundary: \( \rho \mu (\mathbf{u}_i)' = -\mathbf{t}, w = -\omega - p'_t/\rho g, p'_n = 0 \),
- the output: \( p'_n = 0, \mathbf{u}_n = 0 \),

where \( \omega \) is the liquid evaporation rate; \( \mathbf{t} \) is the tangential stress vector, \( \mathbf{u}_n, \mathbf{u}_t \) are normal and tangential components of the water flow velocity vector; \( \rho_i \) is the density suspension.

The tangential stress vector for the free surface has the form: \( \mathbf{t} = \rho_a C_{d_s} |\mathbf{w}| \mathbf{w} \), \( \mathbf{w} \) is the vector of the wind speed relative to the water, \( \rho_a \) is the density of the atmosphere, \( C_{d_s} \) is dimensionless surface drag coefficient, which depends on the wind speed.

For the bottom: \( \mathbf{t} = \rho C_{d_b} |\mathbf{u}| \mathbf{u} \), \( C_{d_b} = \frac{g k^2}{h^{1/3}} \), where \( k \) is the group coefficient of roughness in Manning's formula; \( h = H + \eta \) is the total depth of the water area, [m]; \( H \) is the depth to undisturbed surface, [m]; \( \eta \) is the height of the free surface relative to the geoid (sea level), [m].

The tangential stress v

\[ \mathbf{t} = \rho \mu (\mathbf{u}_n)' = -\mathbf{t}, w = -\omega - \frac{p'_t}{\rho g}, p'_n = 0, \]

\[ \mathbf{u}_n = 0, \]

\[ p'_n = 0. \]

where \( \omega \) is the liquid evaporation rate; \( \mathbf{t} \) is the tangential stress vector, \( \mathbf{u}_n, \mathbf{u}_t \) are normal and tangential components of the water flow velocity vector; \( \rho_i \) is the density suspension.

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**Figure 1.** Depths map of the Azov Sea.

The approximation, considered below, makes it possible to creation the coefficient of vertical turbulent exchange on the basis of the measured velocity pulsations, inhomogeneous in depth:

\[ \nu = C^2 \Delta^2 \frac{1}{2} \left( \frac{\partial \bar{u}}{\partial z} \right)^2 + \left( \frac{\partial \bar{v}}{\partial z} \right)^2, \]

where \( \bar{u}, \bar{v} \) are the time-averaged pulsations of the horizontal velocity components; \( \Delta \) is the characteristic scale of the grid; \( C_s \) is the Smagorinsky dimensionless empirical constant, whose value is usually determined on the basis of calculation the decay process of homogeneous isotropic turbulence.

The described model takes into account the movement of water flow, micrometeorological diffusion, Coriolis force, spatial distribution of salinity and temperature, while it also takes into account the density of seawater.
Calculation of the sea water density can be carried out by two main methods: using a linear equation:

\[ \rho = 1028(1 - \beta T) \]

and state equation of seawater 1980:

\[ \rho = \rho_0 + 800.969062 \cdot 10^{-4} + 588.194023 \cdot 10^{-4}T + 797.018644 \cdot 10^{-3}S - \\
-811.465413 \cdot 10^{-5}T^2 - 325.310441 \cdot 10^{-5}TS + 131.710842 \cdot 10^{-6}S^2 + \\
+476.600414 \cdot 10^{-7}T^3 + 389.187483 \cdot 10^{-7}T^2S + 287.971530 \cdot 10^{-8}TS^2 - \\
-611.831499 \cdot 10^{-10}S^3, \quad (5) \]

where \( \beta \) is a coefficient given in the specialized Oceanographic tables, reflecting the dependence of the density change from temperature change; \( k(T, S, p) \) is an average modulus of elasticity; \( T \) is water temperature; \( S \) is water salinity; \( p \) is hydrostatic pressure; \( \rho \) is the water density.

Due to the fact that the linear equation of seawater density gives extremely rough results and can significantly reduce the accuracy of the developed model, the model described earlier used the state equation of seawater 1980 [13].

This model can be adapted to the problem of pollution transport by including in the system (1) – (5) a modified equation of the distribution of pollutants in coastal systems, which differs from others in the presence of a coefficient describing the change in the concentration of harmful substances in the coastal system, taking into account the process of biodegradation [14].

To adapt this model for simulation the phytoplankton and zooplankton interaction processes, it is necessary to take into account interspecific competition, spatially inhomogeneous distribution of nutrient, as well as temperature and oxygen regimes.

3. Solution method of model problems

The pressure correction method was used at solving a problem of the form (1) – (5). The case of variable density for this method is described in [15-17]. The transition to a system of grid equations for solving model problems of hydrodynamics was performed taking into account the ‘fullness’ of control cells of the computational domain. It possible to improve the accuracy of solving problems for dynamically change geometry of the computational domain due to a more accurate approximation of its boundary. Under the ‘fullness’ of control cell of the computational domain, we understand the coefficient, which is the ratio of the volume of the cell filled with the medium to the total volume of the cell [15, 18]. To solve the discrete analogs [19-20] of the system (1) – (5), the algorithm of the modified alternately triangular method (MATM) of variation type was used. Each hydrophysical equation after linearization in the two-dimensional case can be represent as a diffusion-convection problem in the form:

\[ \frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} + v \frac{\partial q}{\partial y} = \frac{\partial}{\partial x} \left( \mu \frac{\partial q}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial q}{\partial y} \right) + f \quad (6) \]

with boundary conditions:

\[ \frac{\partial q}{\partial n}(x, y, t) = \alpha_n q + \beta_n \quad (7) \]

where \( u, v \) are water velocity components; \( \mu \) is the turbulent exchange coefficient; \( f \) is the function, describing the intensity and distribution of sources; \( \alpha_n, \beta_n \) are given coefficients.

We introduced a uniform rectangular grid:

\[ \omega_h = \{ t^n = nt, x_i = ih_x, y_j = jh_y; \ n = 0, N_t, i = 0, N_x, j = 0, N_y, N_t \tau = T, N_x h_x = l_x, N_y h_y = l_y \}, \quad (8) \]

where \( \tau \) is a time step; \( h_x, h_y \) are spatial steps; \( N_t \) is an upper time boundary; \( N_x, N_y \) are spatial boundaries; \( l_x, l_y \) are maximum dimensions of computational domain.
For discretization of hydrophysical model we used the space splitting scheme, taking into account the partial filling of cells. The discrete analogue of the diffusion-convection problem (6), (7) has the form:

\[
\begin{align*}
\frac{q_{i,j}^{n+1/2} - q_{i,j}^n}{\tau} + \psi_{XL} \frac{q_{i-1,j}^n - q_{i,j}^n}{2\tau} + \psi_{XR} \frac{q_{i+1,j}^n - q_{i,j}^n}{2\tau} + u \frac{q_{i,j}^n - q_{i-1,j}^n}{4h_x} + \\
\frac{q_{i+1,j}^n - q_{i,j}^{n+1/2}}{\tau} + \psi_{XR} \frac{q_{i-1,j}^n - q_{i,j}^{n+1/2}}{2\tau} + u \frac{q_{i,j}^n - q_{i+1,j}^n}{4h_x} + \\
\frac{q_{i,j}^{n+1/2} - q_{i,j}^n}{h_y} + \psi_{YL} \frac{q_{i,j-1}^n - q_{i,j}^n}{2\tau} + \psi_{YR} \frac{q_{i,j+1}^n - q_{i,j}^n}{2\tau} + v \frac{q_{i,j}^n - q_{i,j+1}^n}{4h_y} + \\
\frac{q_{i,j+1}^n - q_{i,j}^{n+1/2}}{\tau} + \psi_{YR} \frac{q_{i,j-1}^n - q_{i,j}^{n+1/2}}{2\tau} + v \frac{q_{i,j}^n - q_{i,j+1}^n}{4h_y} +
\end{align*}
\]

where \(\psi_{XL} = 1, \psi_{XR} = 0\) at \(u > 0\), and \(\psi_{XL} = 0, \psi_{XR} = 1\) at \(u < 0\); \(\psi_{YL} = 1, \psi_{YR} = 0\) at \(v > 0\), and \(\psi_{YL} = 0, \psi_{YR} = 1\) at \(v < 0\).

The research of the scheme (9) showed that it is stable at the Courant numbers in the interval \([0; 0.75]\) and large Peclet numbers. In the limiting case (the diffusion coefficient is equal to zero) at large Peclet numbers, the maximum value of the numerical solution error of this problem (6), (7) on the basis of the proposed difference scheme (9) was equaled to the 0.125. The numerical solution error resulting at using the scheme (9) was less than the solution error of the problem (6), (7) with using the discretization of standard difference ‘cabaret’ schemes.

The grid equations, obtained in the result of discretization of the mathematical models of hydrophysics and biological kinetics, have been solved by the modified adaptive alternating-triangular method (MATM) [21, 22].

4. Program complex and results of experimental researches

For numerical implementation of proposed interrelated mathematical water hydrobiologicals models, we developed parallel algorithms which will be adapted for hybrid computer systems using the NVIDIA CUDA architecture and used for mathematical modeling of phytoplankton production and destruction process (figure 2).

**Figure 2.** The NVIDIA Tesla K80.

The NVIDIA Tesla K80 computing accelerator has the high computing performance and supports all modern both the closed (CUDA) and open technologies (OpenCL, DirectCompute). 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 processor, DDR4 10 of RAM 32 GB, the NVIDIA GeForce GTX 750 Ti video card of 2GB, 640 CUDA cores. Using the GPU with the CUDA technology is required to address the effective resource distribution at solving the system of linear algebraic equations (SLAE).

The dependence of the SLAE solution time on the matrix dimension and the number of nonzero diagonals was obtained for implementation the corresponding algorithm (see figure 3). Due to it, in particular, we can choose the grid size and to determine the time of solving systems of linear equations based on the amount of nonzero matrix diagonals.

Analysis of the CUDA architecture characteristics showed the applicability of algorithms for numerical implementation of the developed mathematical models of biological kinetics to design high-performance information systems.

The software complex (SC) was developed for the multiprocessor computer system (MCS) of the Southern Federal University for solving the problem (1) – (5). The SC is intended for mathematical modeling of possible development scenarios of hydrophysical conditions in coastal systems (we considered in this regard the Azov-Black Sea basin). The SC includes computational units allowing: to take into account factors influencing pollutant distribution in coastal systems (weather conditions, and bottom relief); to research the dependence of pollutant concentrations, the degree and size of the affected water zone on the intensity of water flows, hydrophysical parameters, climatic and meteorological factors. The features of SC are high performance, reliability, and high accuracy of simulation results.

Sequentially condensed rectangular grids by dimensions $251 \times 351 \times 15$, $502 \times 702 \times 30$, $1004 \times 1404 \times 60$, etc, were used for mathematical modeling of hydrodynamic and hydrobiological processes in a three-dimensional domain of complex shape, namely the Azov Sea.

The SC includes the following units: the control unit; the oceanological and meteorological databases; the application program library for solving the hydrobiology grid problems; the integration with various geoinformation system (GIS), Global Resource Database (GRID) for binding to the geographic coordinates and access to the satellite data collection systems, the NCEP/NCAR Reanalysis database. The use of satellite GIS information provides the additional possibilities for performing more qualitative and complex spatial analysis; the solutions, based on it, are more accurate. The high-
performance computer system was used for solving such problems, which allows performing a large amount of complex calculations, a huge amount of data processing in limited time mode.

The advantages of SC are the following:

- increased efficiency of implementation of the developed mathematical models;
- development the effective methods for numerical implementation of problems;
- the ability of dynamically change the input data in real time;
- GIS, databases sharing in a user-friendly interface;
- the use of integrated monitoring tools for precision the ecological situation of coastal systems;
- promising approaches of the parallel implementation.

The high-level language C++ was used for development the SC. Message Passing Interface technology (MPI) was employed for clusters.

Numerical experiments were performed for modeling hydrophysical conditions of coastal systems in summer taking into account the influence of the environment. The simulation results of the flow intensity are shown in figure 4. Calculation results of the flow directions and the level elevation function (initial distribution of water flow fields for the northern wind) are given in figure 5.

![Figure 4. Dynamics of the flow intensity at the Western wind velocity of 5 m/s.](image)

![Figure 5. Calculation results: a) the flow directions; b) the level elevation function.](image)
In addition, we obtained the results of water level elevation in the Azov Sea at the catastrophic storm surge in September 2014. The calculation of the flooding of the coastal areas of the Azov Sea due to the storm surge, occurred in 24 – 25 September 2014, was performed on the basis of the developed three-dimensional model. This problem is essentially nonlinear, because wind stresses on the free water surface was of critical value – there was intensive spray formation and destruction of waves; the difference in levels at modeling the process depending on the distance from the coast was 2 – 5 m.

The graph of the level elevation function from the time in the region of the Taganrog port is given in figure 10 (the dotted line – values, calculated on the grid with steps at the horizontal direction 1003 m and 1013 m; the thin line – values, calculated on the grid with steps at the horizontal direction 503 m и 510 m; the grid step at the vertical direction – 0.1 m; the polyline – the field data).

Actual data from the Unified State Information System on the Situation in the World Ocean (‘ESIMO’) portal were used for verification of the model and validation of the adequacy of SC.
Figure 11 shows numerical simulation of bioremediation process of petroleum hydrocarbons with the introduction of oil-degrading bacteria in coastal system (the Azov Sea) (N is the number of iteration). The initial distribution of light oil fraction is shown in figure 11a; the distribution of light oil fraction (two oil slicks) is shown in figure 11b (N = 121). The initial distribution of heavy oil fraction is shown in figure 11c; the distribution of heavy oil fraction concentration (a single localized spill with the subsidence of oil hydrocarbons to the water bottom) is shown in figure 11d (N = 148). Also for test we considered the case if measures are not taken to localize oil spills. According to the results of natural experiments, the calculated time must be equal to 20 – 30 days. The wind velocity of 3 – 8 m/s is an ideal for localization the oil pollution. In this case the slicks appear as dark spots on the bright (rough) water surface. The highest wind velocity was fixed in November 11, 2007 in Kerch Strait and amounted to 24 m/s according to the Gismeteo data. Results of numerical experiments of light oil transport simulation in the Kerch Strait on November 16, 2007 was performed on the basis of the developed SC and used to test the efficiency of this complex.

The SC, developed by our scientific team, implements possible scenarios of ecological conditions in the Azov Sea using numerical algorithms for model problems of biological kinetics. The Earth satellite data were used for checking the adequacy of mathematical model (1) – (5). Results of SC are shown in figure 12 (the variation of phytoplankton concentration).
An analysis of similar SC was carried out. The overall result is that the prediction accuracy of changes in pollutants and plankton concentrations in shallow waters increased by 10 to 20%, depending on the model problem of biological kinetics.

As criteria for checking the adequacy of the developed models was the error estimation with simultaneous consideration of the field data from the available $n$ measurements:

$$\delta = \frac{\sqrt{\sum_{k=1}^{n} q_{k,nat}^2 - q_k^2}}{\sqrt{\sum_{k=1}^{n} q_{k,nat}^2}}$$

(10)

where $q_{k,nat}$ is the value of the calculated function obtained using field measurements; $q_k$ is the value of the grid function, calculated by simulation. Concentrations of pollution and plankton, calculated for various wind conditions, were taken into account if the relative error did not exceed 30%.

### 5. Conclusion

The influence of physical characteristics such as temperature and salinity on changes in reservoir hydrodynamics and storm surges has been researched. A complete three-dimensional mathematical model of hydrodynamics for water of variable depth and density was developed and researched for predictive modeling of storm surges. This model takes into account the transport of minerals, the influence of water ionic composition on density and diffusion, transport, absorption and release of nutrients by phytoplankton, as well as phosphorus, nitrogen and silicon cycles.

Due to the analytical research of the developed continuous model, we can obtain the inequalities ensuring the existence and uniqueness of the problem solution. The numerical implementation of the model was performed on the MCS with distributed memory. We obtained theoretical estimates for the acceleration and efficiency of parallel algorithms. Experimental software was designed for mathematical modeling of possible development scenarios for water with complex bottom geometry. In this regard, the Azov Sea was considered as the example of water basin. Decomposition methods of grid domains for computationally labors diffusion-convection problems were employed for the parallel implementation, taking into account the architecture and parameters of the MCS. The parallel algorithm was developed for data distribution among processors.

Due to the application of MCS and NVIDIA Tesla K80 computing accelerator, the calculation time for the solution of the model problem was decreased at preservation the required accuracy for modeling of hydrophysical processes in seas with complex bathymetry. Note that this fact is one of primary importance in hydrophysical problems.

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