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Mathematical modeling of phytoplankton populations and biogeochemical processes in shallow water ecosystem

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Relevance





- The Azov Sea is the great shallow water in stretch. Such waters are suffered the significant anthropogenic influence. But most of them is the unique for fish productivity ecological systems. The biogenic matters are entered in the shallow waters with the river flows which causing the growth of the algae – «water bloom». The suffocation periodically occur in the shallow waters in summer. Because there is a significant decrease of dissolved oxygen in them, consumed in the decomposition of organic matter, due to the high temperature. The fish is suffering the oxygen starvation and the mass dying due to suffocation.
- The most important technogenic factors that have a significant impact on the water ecosystem are: metallurgical and chemical wastes of industrial activity and municipal polluted wastewater; oil and oil products pollution; sheep channel deepening. which are decreasing significantly water medium transparency and destroying bottom biocenoses; no regulated fishing; new costal engineering constructions (for example, Bagaevskaya dam on Don river - will be built in 2020); saturated chemicals. soil and water salinization; pollution, increasing uncontrolled discharge of pesticides into the reservoir and etc.



Relevance







- The development of interrelated models of hydrodynamics and biological kinetics will allow to designed a model of a complete ecosystem of shallow water in the future.
- Few works in the field of mathematical modeling of processes of hydrophysics and biological kinetics are devoted to the parallel numerical implementation of problems of this class. Although under the conditions for the development of catastrophic and adverse events in shallow waters, it's necessary to forecast the development of such phenomena and make decisions within tens of minutes units of hours, which, in turn, requires modeling of hydrobiological processes on multiprocessor computer systems at accelerated time.
- According to the Federal Law No.7 from 10.01.2002 (as amended 3.07.2016) «On environmental protection»; Water code of the Russian Federation; order of the Russian Government No.2462-p from 4.12.2014; Resolution of the Government of the Russian Federation No.794 from 30.12.2003 (as amended 19.10.2016) «On the unified state system of emergency prevention» time for decision and elimination of technogenic or natural disasters should be from a few hours to 2 3 days.



Analysis of existing models of hydrobiological processes and software complexes

SMASE (Simulation model of the Azov Sea ecosystem, 1976, 1987); DEMLL (Dynamic ecosystem models of Lake Ladoga, 1987); ЭКОМОД (1994); ECOPATH (1996); POM (Princeton Ocean Models, 1996); EFDC (The Environmental Fluid Dynamics Code, 1996); DEMLO (Dynamic Ecosystem Model of Lake Onego, 1997); AOOC WASP7; GLOBIO3 (Global Biodiversity Model, 2000); LakeMab (2000); PROTECH (Phytoplankton Responces To Environment Changes, 2001r.); PISCATOR (2002r.); LakeWeb (2002); DYRESM – CAEDUM (The computational aquatic ecosystem dynamics model, 2005); SALMO (Simulation of an Analytical Lake Model, 2006); ERSEM (the European Regional Seas Ecosystem Model, 2007); CAEDYM – ELKOM (2008); CE-QUAL-W2 (2008); DELFT 3D-ECO (2009); IPH-PCLake (2009); CHARISMA (2009); «Mars3d» (2009); NEMO-OPA; SYMPHONIE; GETM; PCLake (2010); ECOPATH with ECOSIM (2010); MyLake (Multi Year Lake, 2010); CHTDM (Climatic Hydro Termo Dynamic Model, 2011); NEMO (Nucleus for European Modelling of the Ocean, 2012), Aztec (2008, 2015). Applications that received the support of GPU-acceleration, as released to the market and still under development: AMBER, CHARMM, FastROCS, GROMACS, GTC, WL- LSMS, MILC, NAMD, QUDA, VASP, VMD, COSMO, GEOS-5, HOMME, HYCOM, WRF, NIM (2016-2019).

Disadvantages of existing software and research complexes

- Universal packages of hydrodynamic process modeling (FlowVision, FLUENT, GAS DYNAMICS TOOL, PHOENICS, Star-CD, etc.) are focused on multiprocessor systems, but it universality consists in the usage of fairly limited models, algorithms and methods to a variety of different cases. Programs specially focused on solving a particular class of problems are potentially applicable for solution these problems more effectively.
- Most well-known special software (ADAM, CAL3QHC, Chensi, TASCflow, ISC-3, PANACHE, REMSAD, UAM-IV, ЭКОЛОГ, ПРИЗМА, VITECON), designed for calculation the pollution spread, are focused on single-processor systems. In specialpurpose software systems (ECOSIM and MAQSIP), adapted for multiprocessor systems, only separate modules are parallelized, which in some cases does not allow to achieve the high parallelization efficiency.
- Simplified models of hydrobiological processes are used for water with little-changing salinity and, in most cases, depth.
- Existing complexes do not allow to obtain operational forecasts of environmental situation in shallow water after an emergency.

Model of Sceletonema costatum harmful algae dynamics

$$\begin{aligned} \frac{\partial X}{\partial t} + div(\mathbf{U}X) &= \mu_X \Delta X + \frac{\partial}{\partial z} \left(\mathbf{v}_X \frac{\partial X}{\partial z} \right) + \left(\alpha_0 + \gamma M \right) \psi X - \delta X, \\ \frac{\partial S}{\partial t} + div(\mathbf{U}S) &= \mu_S \Delta S + \frac{\partial}{\partial z} \left(\mathbf{v}_S \frac{\partial S}{\partial z} \right) - \left(\alpha_0 + \gamma M \right) \psi X + B \left(S_p - S \right) + f, \\ \frac{\partial M}{\partial t} + div(\mathbf{U}M) &= \mu_M \Delta M + \frac{\partial}{\partial z} \left(\mathbf{v}_M \frac{\partial M}{\partial z} \right) + k_M X - \varepsilon M. \end{aligned}$$

where X, S, M are concentrations of phytoplankton (Sceletonema costatum diatom), biogenic matter (silicon) and metabolite, respectively; $\mathbf{U} = (U, V, W)$ is the velocity vector of water flow; $\mu_X, \mu_S, \mu_M, v_X, v_S, v_M$ are diffusion coefficients in the horizontal and vertical directions of X, S, M substances, respectively; Δ is the two-dimensional Laplace operator; $\alpha = (\alpha_0 + \gamma M)$ is the growth dependency of X by M; α_0 is the growth velocity X in the absence of M; γ is the exposure parameter; C is the salinity concentration; \tilde{T} is the temperature; $\delta = \delta(C)$ is phytoplankton loss rate due to death (specific mortality), taking into account the influence of C; B is the specific pollution rate; f(x, y, z) is a source pollution function; S_p is a maximum possible concentration of pollution; k_M is the excretion rate; ε is the expansion coefficient of M; $\psi(I, \tilde{T}, S, C)$ is the coefficient taking into account the influence of light, temperature, concentration S and C on the growth of X. Let us supposed that $\psi = S$.

Model of Sceletonema costatum harmful algae dynamics

The computational domain *G* is a closed basin, limited by the undisturbed water surface Σ_0 , the bottom $\Sigma_H = \Sigma_H(x, y)$ and the cylindrical surface σ for $0 < t \le T_0$. $\Sigma = \Sigma_0 \cup \Sigma_H \cup \sigma$ is the sectionally smooth boundary of the *G* domain; **n** is the vector of the external normal to the surface Σ .



Computational domain G

n is the vector of the external normal to the surface Σ ; U_n is the normal component of the velocity water flow vector to the Σ .

 $\begin{array}{l} \mbox{Initial conditions: } \varphi(x,y,z,0) = \varphi_0(x,y,z), \ \varphi \in \left\{X,S,M\right\}, \ (x,y,z) \in \overline{G}, \ t = 0, \\ \mbox{Boundary conditions: } \varphi = 0 \ \ ha \ \sigma, \ if \ U_{\bf n} < 0; \ \frac{\partial \varphi}{\partial n} = 0 \ \ on \ the \ \sigma, \ if \ U_{\bf n} \geq 0; \ \frac{\partial \varphi}{\partial z} = 0 \ \ on \ the \ \Sigma_0; \\ \ \frac{\partial \varphi}{\partial z} = -\varepsilon_i \varphi \ \ on \ the \ \Sigma_H, \ i \in \{1,2,3\}, \ \varphi \in \{X,S,M\}, \end{array}$

where the coefficient ε_1 takes into account the lowering of algae to the bottom and their flooding; $\varepsilon_2, \varepsilon_3$ take into account the absorption of nutrients and metabolites bottom sediments.

Functional dependencies for models



A)
$$\mu(T) = \mu_0 \exp\left[-\left\{\left(T - T_{opt}\right)/\sigma_T\right\}^2 - \mu_1 T + \mu_2\right], T_{opt} = 25, \sigma_T = 12, \mu_0 = 0.12, \mu_1 = 0.06, \mu_2 = 0.43;$$

B) $\mu(C) = \mu_0 \exp\left[-\left\{\left(C - C_{opt}\right)/\sigma_c\right\}^2 - \mu_1 C + \mu_2\right], C_{opt} = 12, \sigma_C = 10, \mu_0 = 0.001, \mu_1 = 0.1, \mu_2 = 0.01;$
C) $\mu(I, T, C) = \alpha_0 \exp(aT)\left(I/I_{opt}\right)\exp\left(1 - I/I_{opt}\right)\eta_0 \exp\left[-\left\{\left(C - C_{opt}\right)/\sigma_c\right\}^2 - \eta_1 C + \eta_2\right], \alpha_0 = 0.8,$
 $a = 0.063, I = I_{opt} = 86, C_{opt} = 12, \sigma_C = 15, \eta_0 = 0.001, \eta_1 = 0.1, \eta_2 = 0.1;$ D) $I = 10, I_{opt} = 86.$

C, T, I are values of salinity, temperature and illumination

RESTORATION OF SALINITY AND TEMPERATURE FIELDS

It is necessary to take into account salinity and temperature, which are usually set on maps at separate points or level contours for modeling the dynamics of the development of phytoplankton populations. It is undesirable to use such cards due to a calculation error. Thus, the problem of processing hydrological information arises. The use of smoother functions to approximate the functional dependences describing salinity and temperature fields makes it possible to increase the accuracy of hydrodynamic calculations.

To obtain the salinity function, one can use the solution of the diffusion equation, which for long time intervals reduces to solving the Laplace equation. However, the salinity function obtained in this way may not have a sufficient degree of smoothness at the points of setting the field values. Therefore, use the equation used to obtain schemes of higher order of accuracy for the Laplace equation:

$$\Delta H - \frac{h^2}{12} \Delta^2 H = 0 \, .$$

where H- water salinity.

Isolines of salinity and temperature were obtained for solving the problem of processing hydrological information, for which a recognition algorithm was applied. Using the interpolation algorithm described above and by superimposing the boundaries of the region, maps of salinity and temperature of the Azov Sea were obtained.



a) the initial image of the isolines of the salinity level (isogaline) of the Azov Sea;

b) the restored salinity field of the Azov Sea.

RESTORATION OF SALINITY AND TEMPERATURE FIELDS



a) the initial image of temperature isolines (isotherms) of the Azov Sea (July 2019);
 b) the restored temperature field of the Azov Sea

Results of numerical simulation of harmful phytoplankton dynamics



Dynamics of harmful algae concentration at different times (T=2, 27, 39, 70, 85, 122 days, from March to September). Initial distribution of water flow velocities in the Azov Sea at the west wind

$$\begin{split} \tau_{X} &= 0,1; \ \mu_{X} = 5 \cdot 10^{-9}; \ \nu_{X} = 10^{-9}; \ \alpha_{0} = 0,0833; \ \gamma = 0,0416; \ \delta = 0,5; \ \varepsilon_{1} = 1; \\ \mu_{M} &= 5 \cdot 10^{-11}; \ \nu_{M} = 10^{-11}; \ k_{M} = 0,006; \ \tau_{\varphi} = 0,1; \ \varphi \in \left\{X,S,M\right\}; \ \varepsilon = 0,5; \ \varepsilon_{3} = 0,7 \end{split}$$

Model of biological rehabilitation of shallow waters based on basis of algolization of the *Chlorella Vulgaris BIN* green algae

The competition principle was used at constructing the interaction model of green algae (*Chlorella Vulgaris BIN*), blue-green phytoplankton (*Aphanizomenon flos-aquae*) and zooplankton (*Bosmina longirostris*).

$$\begin{split} &\frac{\partial X_{1}}{\partial t} + div \left(\mathbf{U}X_{1}\right) = \mu_{1} \Delta X_{1} + \frac{\partial}{\partial z} \left(v_{1} \frac{\partial X_{1}}{\partial z}\right) + \alpha_{1} \psi_{1}(S) X_{1} - g_{1}(X_{1}, Z) - \theta_{1} X_{1} X_{2} - \varepsilon_{1} X_{1}, \\ &\frac{\partial X_{2}}{\partial t} + div \left(\mathbf{U}X_{2}\right) = \mu_{2} \Delta X_{2} + \frac{\partial}{\partial z} \left(v_{2} \frac{\partial X_{2}}{\partial z}\right) + \alpha_{2} \psi_{2}(S) X_{2} - g_{2}(X_{2}, Z) - \theta_{2} X_{1} X_{2} - \varepsilon_{2} X_{2}, \\ &\frac{\partial Z}{\partial t} + div \left(\mathbf{U}Z\right) = \mu_{Z} \Delta Z + \frac{\partial}{\partial z} \left(v_{Z} \frac{\partial Z}{\partial z}\right) + \psi_{z}(X_{1}, X_{2}) Z - \lambda(M_{2}) Z, \\ &\frac{\partial S}{\partial t} + div \left(\mathbf{U}S\right) = \mu_{S} \Delta S + \frac{\partial}{\partial z} \left(v_{S} \frac{\partial S}{\partial z}\right) - \psi_{S}(X_{1}, X_{2}) S + \varepsilon_{1} X_{1} + \varepsilon_{2} X_{2} + \lambda(M_{2}) Z + B\left(S_{p} - S\right) + f, \\ &\frac{\partial M_{i}}{\partial t} + div \left(\mathbf{U}M_{i}\right) = \mu_{m} \Delta M_{i} + \frac{\partial}{\partial z} \left(v_{m} \frac{\partial M_{i}}{\partial z}\right) + k_{i} X_{i} - \varepsilon_{m} M_{i}, \end{split}$$

Model of biological rehabilitation of shallow waters (continuation)

where X_i are concentrations of green (*Chlorella Vulgaris BIN*) and blue-green algae (*Aphanizomenon flos-aquae*), respectively, $i \in \{1,2\}$; Z is the concentration of zooplankton (*Bosmina Longirostris*); S is the concentration of nutrient (nitrogen or phosphorus); M_i is the concentration of metabolite of *i*-th species; $\mu_r, \mu_z, \mu_s, v_r, v_z, v_s$ are diffusion coefficients in horizontal and vertical directions of substances X_i , Z, S, M_i , $r \in \{1,2,3,4\}$; α_{0i} , γ_i are the growth rate in the absence of the metabolite and the impact parameter of *i*-th species; α_z is the growth rate of zooplankton; $\alpha_i = (\alpha_{0i} + \gamma_i M_i)$ is the function of growth rate of *i*-th species due to M_i ; $g_i(X_i, Z)$ is the function of zooplankton absorption of phytoplankton *i*-th species; $\psi_z(X_1, X_2)$ is the function of nutrient consumption by algae; S_p is the maximum possible concentration of nutrients; *f* is the source function of zooplankton, including the risk of elimination due to the metabolite of blue-green algae; k_i are excretion rates of *i*-th species; ε_m are coefficients of metabolite decomposition, $m = \overline{3}, \overline{4}$; θ_i is the inter-species competition ratio of *i*-th species; \mathbf{u}_{0k} is the deposition rate of *k*-th substance; \mathbf{u} is the velocity field of water flow; $\mathbf{U} = \mathbf{u} + \mathbf{u}_{0k}$ is the velocity of substance convective transport; $k \in \{X_1, X_2, S, Z, M_1, M_2\}$.

Let us supposed that $\psi_i(S) = S$; $\psi_Z(X_1, X_2) = p_1 X_1 - p_2 X_2$; $g_i(X_i, Z) = \delta_i X_i Z$; $\lambda(M_2) = \varepsilon_Z M_2$; $\psi_S(X_1, X_2) = \beta_1 X_1 + \beta_2 X_2$, where $\beta_i = \beta_{0i} + \gamma_i M_i$ are the absorption coefficients of nutrients by phytoplankton of *i*-th species; p_i are coefficients of the processed algae biomass of *i*-th species to zooplankton biomass; δ_i are loss factors of algae biomass of *i*-th species due to the grazing by zooplankton.

Scheme for model of biological rehabilitation of shallow waters



Results of numerical simulation for the problem of biological rehabilitation (for the Azov sea)



Dynamics of green algae concentration changes for time intervals T=2, 27, 39, 70, 85, 122 days (after the beginning of phytoplankton vegetation period (March – September)). Initial distribution of flow fields in the Azov Sea at the north wind

 $\tau_1 = 0,3; \quad \mu_1 = 5 \cdot 10^{-7}; \quad \nu_1 = 10^{-7}; \quad \alpha_{01} = 0,1; \quad \delta_1 = 0,5; \quad \gamma_1 = 0,0416; \quad \varepsilon_1 = 0,0116; \quad \delta_1 = 0,5; \quad \theta_1 = 0,3; \quad \xi_1 = 0,5; \quad \theta_2 = 0,5; \quad \theta_3 = 0,5; \quad \theta_4 = 0,5; \quad \theta_5 = 0,5; \quad \theta_{11} = 0,5; \quad \theta_{12} = 0,5; \quad \theta_{13} = 0,5; \quad \theta_{14} = 0,5; \quad \theta_{15} = 0,5; \quad \theta$

Results of numerical simulation for the problem of biological rehabilitation (for the Azov sea)



Joint distribution of blue-green and green algae concentrations for time intervals T=2, 27, 39, 70, 85, 122 days. Initial distribution of flow fields in the Azov Sea at the north wind

 $\tau_{\varphi} = 0,3; \ \mu_{i} = 5 \cdot 10^{-7}; \ \nu_{i} = 10^{-7}; \ \mu_{S} = 5 \cdot 10^{-10}; \ \nu_{S} = 10^{-10}; \ \mu_{Z} = 1,6 \cdot 10^{-3}; \ \nu_{Z} = 1,5 \cdot 10^{-3}; \ \mu_{m} = 5 \cdot 10^{-11}; \ \nu_{m} = 10^{-11}; \ B = 0,001; \ S_{p} = 1; \ \delta_{1} = 0,5; \ \delta_{2} = 0,3; \ \delta_{1} = 0,3; \ \delta_{2} = 0,116; \ \varepsilon_{Z} = 0,116; \ \varepsilon_{Z} = 0,115; \ \varepsilon_{3} = 0,5; \ \varepsilon_{4} = 0,5; \ \delta_{1} = 0,5; \ \delta_{2} = 0,3; \ \beta_{0i} = 1,5; \ \theta_{1} = 0,3; \ \theta_{2} = 0,1; \ p_{1} = 0,95; \ \rho_{2} = 0,085; \ f = 3; \ \varphi \in \{X_{i},S,Z,M_{i}\}, \ i \in \{1,2\}, \ m \in \{3,4\}$

Model of interaction between ctenophores and plankton populations

$$\begin{split} & \left(P_{i}\right)_{i}' + div\left(\mathbf{U}P_{i}\right) = \mu_{i}\Delta P_{i} + \frac{\partial}{\partial z} \left(\nu_{i}\frac{\partial P_{i}}{\partial z}\right) + \psi_{i}, \, i \in \overline{1,9}. \\ & \psi_{1}\left(P_{1}, P_{2}, P_{3}\right) = \left\{\alpha_{1}P_{3} - \delta_{1}P_{2} - \varepsilon_{1}\right\}P_{1}, \, \psi_{2}\left(P_{1}, P_{2}\right) = \left\{\alpha_{2}P_{1} - \varepsilon_{2}\right\}P_{2}, \\ & \psi_{3}\left(P_{1}, P_{3}, P_{4}\right) = \left\{\alpha_{3}P_{4} - \delta_{3}P_{1} - \varepsilon_{3}\right\}P_{3}, \, \psi_{4}\left(P_{3}, P_{4}, P_{5}\right) = \left\{\alpha_{4}P_{5} - \delta_{4}P - \varepsilon_{4}\right\}P_{4}, \\ & \psi_{5}\left(P_{1}, P_{2}, ..., P_{9}\right) = \sum_{i=4}^{2} \varepsilon_{i}P_{i} - \delta_{5}P_{4}P_{5} + B\left(\overline{P}_{5} - P_{5}\right) + f, \\ & \psi_{m}\left(P_{1}, P_{2}, ..., P_{9}\right) = \sum_{l=1}^{i=4} k_{l}P_{l} - \varepsilon_{m}P_{m}; \, m \in \overline{6,9}, \quad \alpha_{4} = \left(\alpha_{04} + \gamma_{4}M_{4}\right), \end{split}$$



Mnemiopsis leidyi ctenophore

 P_i are concentration values, $i \in \overline{1,9}: 1$, 2 are ctenophores *M. leidyi* and *B. ovata*; 3 is zooplankton; 4 is phytoplankton; 5 is the biogenic matter; 6, 7, 8, 9 are metabolites of ctenophores (6, 7) and plankton (zoo- (8) and phyto- (9)); ψ_i are functions of trophic interactions; α_i is the function of ctenophores and plankton growth, $l = \overline{1,4}$; α_{04} , γ_4 are the growth rate of phytoplankton in the absence of metabolite and the effect parameter; *B* is the rate of arrival of nutrients P_5 ; $\overline{P_5}$ is the maximum possible concentration of nutrients; ε_i is a coefficient taking into account mortality of the *l*-th species; ε_m are the coefficients of metabolite decomposition, $m = \overline{6,9}$; k_i are the excretion coefficients of *l*-th species ($l = \overline{1,2}$), zooplankton (l = 3), phytoplankton (l = 4)); $\delta_1, \delta_3, \delta_4$ are coefficients of wastage due to grazing f = f(x, y, z, t) is the source function P_5 (pollution); $\mathbf{u} = (u, v, w)$ is the velocity field of water flow; $\mathbf{U} = \mathbf{u} + \mathbf{u}_{0l}$, $\mathbf{U} = (U, V, W)$ is the rate of convective mass transfer; \mathbf{u}_{0l} is the deposition rate of the *i*-th substance; $\mu_i v_i$ are the diffusion coefficients in the horizontal and vertical directions of the *i*-th substance.

Boundary conditions

 $P_i = 0 \text{ on } \sigma, \text{ if } \mathbf{U}_n < 0; (P_i)_n = \varphi_i \text{ on } \sigma, \text{ if } \mathbf{U}_n \ge 0; \quad (P_i)_z' = 0 \text{ on } \Sigma_0; (P_i)_z' = -\beta_i P_i \text{ on } \Sigma_H, i \in \overline{1,9}, \beta_i \text{ is the i-th bottom material absorption coefficient.}$ Initial conditions

$$P_i\Big|_{t=0} = P_{i0}(x, y, z), i = \overline{1,9}.$$

United mathematical model of eutrophication of shallow water system

The model of biochemical transformation of biogenic nutrients (forms of phosphorus, nitrogen and silicon) entering into the Azov Sea with river flows, includes three species of phytoplankton algae: the green – *Chlorella vulgaris*, the blue-green – *Aphanizomenon flos-aquae*, the diatomaceous – *Sceletonema costatum*. The model is based on the system of transport equations of biogenic substances for each model block q_i :

$$\frac{\partial q_i}{\partial t} + div(\mathbf{U}, q_i) = div(\mathbf{k}_i \operatorname{grad} q_i) + R_i, \mathbf{k}_i = \{\mu_i, \mu_i, \nu_i\}, \ i = \overline{1, 10}\}$$

where q_i is a concentration of the *i*-th component, u, v, w are velocity vector components of water flow, $\mathbf{u} = \{u, v, w\}$, $\mathbf{U} = \mathbf{u} + \mathbf{u}_{0i}$, $\mathbf{U} = \{U, V, W\}$ is the convective transport of matter velocity; \mathbf{u}_{0i} is the velocity of *i*-th component sedimentation; R_i is the chemical-biological source, the index *i* indicates the type of: 1–3 are substance the algae *Chlorella vulgaris, Aphanizomenon flos-aquae* and *Sceletonema costatum* concentrations; 4 is PO₄, 5 is POP, 6 is DOP, 7 is NO₃, 8 is NO₂, 9 is NH₄, 10 is Si}; PO₄ are phosphates; POP is the suspended organic phosphorus; DOP is the dissolved organic phosphorus; NH₄ is the ammonium; NO₂ are nitrites; NO₃ are nitrates; Si is the dissolved inorganic silicon; μ_i, v_i are diffusion coefficients in horizontal and vertical directions.

Mathematical model of eutrophication of shallow water system

Let the boundary Σ of a cylindrical domain G is the sectionally smooth, and $\Sigma = \Sigma_H \cup \Sigma_o \cup \sigma$, where Σ_H is the water bottom surface, Σ_o is the unperturbed surface of the aquatic environment, σ is the lateral (cylindrical) surface. Let \mathbf{u}_n is the normal to Σ component of the water flow velocity vector, \mathbf{n} is the outer normal vector to Σ .

Initial conditions: $q_i(x, y, z, 0) = q_i^0(x, y, z)$, $(x, y, z) \in \overline{G}$, $i = \overline{1, 10}$. Boundary conditions: at the lateral boundary $q_i = 0$, if $\mathbf{u}_n < 0$;

$$\frac{\partial q_i}{\partial \mathbf{n}} = 0, \text{ if } \mathbf{u}_n \ge 0, i = \overline{1,10};$$

at $\Sigma_o: \frac{\partial q_i}{\partial z} = \varphi_i, i = \overline{1,10};$
at the bottom: $\frac{\partial q_i}{\partial z} = \varepsilon_{1,i}q_i, i = \overline{1,3}, \frac{\partial q_i}{\partial z} = \varepsilon_{2,i}q_i; i = \overline{4,10},$

where φ_i are the given functions; $\varepsilon_{1,i}$, $\varepsilon_{2,i}$ are nonnegative constants: $\varepsilon_{1,i}$, $i = \overline{1,3}$ take into account the lowering of algae to the bottom and their flooding; $\varepsilon_{2,i}$, $i = \overline{4,10}$ take into account absorption the nutrient by bottom sediments.

Mathematical model of eutrophication of shallow water

Prediction of qualitative changes in primary production depending on the combined effect of external factors: resource (biogenic elements, light, etc.), physiological (temperature, salinity, medium reaction) on the basis of the principle of the cumulative effect of the Mitchell factors.

$$\begin{split} R_{i} &= C_{i} (1 - K_{R,i}) q_{i} - K_{D,i} q_{i} - K_{E,i} q_{i}, \ i = \overline{1,3}; \ R_{4} = \sum_{i=1}^{3} s_{P} C_{i} \Big(K_{R,i} - 1 \Big) q_{i} + K_{PN} q_{5} + K_{DN} q_{6} \\ R_{5} &= \sum_{i=1}^{3} s_{P} K_{D,i} q_{i} - K_{PD} q_{5} - K_{PN} q_{5}; R_{6} = \sum_{i=1}^{3} s_{P} K_{E,i} q_{i} + K_{PD} q_{5} - K_{DN} q_{6}; \\ R_{7} &= \sum_{i=1}^{3} s_{N} C_{i} \Big(K_{R,i} - 1 \Big) \frac{f_{N}^{(1)}(q_{7}, q_{8})}{f_{N}(q_{7}, q_{8}, q_{9})} \cdot \frac{q_{8}}{q_{7} + q_{8}} q_{i} + K_{23} q_{8}; \\ R_{8} &= \sum_{i=1}^{3} s_{N} C_{i} \Big(K_{R,i} - 1 \Big) \frac{f_{N}^{(1)}(q_{7}, q_{8})}{f_{N}(q_{7}, q_{8}, q_{9})} \cdot \frac{q_{7}}{q_{7} + q_{8}} q_{i} + K_{42} q_{9} - K_{23} q_{8}; \\ R_{9} &= \sum_{i=1}^{3} s_{N} C_{i} \Big(K_{R,i} - 1 \Big) \frac{f_{N}^{(2)}(q_{9})}{f_{N}(q_{7}, q_{8}, q_{9})} q_{i} - K_{42} q_{9}, R_{10} = s_{Si} K_{D,3} q_{3}, \end{split}$$

where $K_{R,i}$ is the specific rate of phytoplankton respiratory; $K_{D,i}$ is the specific rate of phytoplankton mortality; $K_{E,i}$ is the specific rate of phytoplankton excretion; K_{PD} is the specific rate of *POP* autolysis; K_{PN} is the ratio of *POP* phosphatification; K_{DN} is the ratio of *DOP* phosphatification; K_{42} is the specific rate of ammonium oxidation to nitrites in the process of nitrification; K_{23} is the specific rate of oxidation of nitrites to nitrates in the process of nitrification, s_P , s_N , s_{Si} are the normalization coefficients between *N*, *P*, *Si* content in organic matter.

Mathematical model of eutrophication of shallow water system

The phytoplankton algae growth rate:

 $C_i = K_{N_i} f_T(T) f_S(S) min \{ f_P(q_A), f_N(q_7, q_8, q_9) \}, i = \overline{1, 2}$

where $K_{N,i}$ is the maximum specific growth rate of phytoplankton.

The dependence of the nutrient content:

- for phosphorus $f_P(q_4) = \frac{q_4}{q_4 + K_4}$, where K_4 is the phosphate half-saturation constant;
- for silicon $f_{Si}(q_{10}) = \frac{q_{10}}{q_{10} + K_{10}}$, where K_{10} is the silicon half-saturation constant;
- for nitrogen

$$f_N(q_7, q_8, q_9) = f_N^{(1)}(q_7, q_8) + f_N^{(2)}(q_9) = \frac{(q_7 + q_8)\exp(-K_{psi}q_9)}{K_7 + (q_7 + q_8)} + \frac{q_9}{K_9 + q_9}$$

where K_{γ} is the nitrate half-saturation constant, K_{\circ} is the ammonium half-saturation constant, K_{psi} is the ammonium inhibition ratio.

- temperature dependent function
 salinity dependent function

$$f_T(T) = \exp\left(-\alpha \left(\frac{T - T_{opt}}{T_{opt}}\right)^2\right) \qquad \qquad f_S(S) = \exp\left(-\beta \left(\frac{S - S_{opt}}{S_{opt}}\right)^2\right)$$

Results of numerical simulation for the eutrophication problem of shallow water system (the Azov sea)



Distribution of nitrate concentrations (initial distribution of flow fields at the north wind)

$$\mu_7 = 5 \times 10^{-10}, v_7 = 10^{-10}$$

Results of numerical simulation for the eutrophication problem of shallow water system (the Azov sea)



Dynamics of phytoplankton concentration in the Azov Sea,

$$\mu_2 = 5 \times 10^{-11}, v_2 = 10^{-11}$$

Results of numerical experiments



Distribution of pollution and plankton concentrations:

a) the nitrite; b) the phosphates; c) the phytoplankton

Results of numerical experiments



d) e) f) Distribution of phytoplankton and forms of phosphorus taking into account the influence of salinity and temperature:

a) green algae; b) bluegreen algae; c) diatom algae;

d) suspended organic phosphorus; e) dissolved organic phosphorus; f) phosphates

Results of numerical experiments



influence of salinity and temperature:

a) green algae; b) bluegreen algae; c) diatom algae; d) ammonium: c) pitritos: f) pitratos

d) ammonium; e) nitrites; f) nitrates

Additional part of report. Mathematical model of oil pollution dynamics in coastal system and bioremediation

Mathematical model of oil products transport taking into account the evaporation of light, neutral and no-evaporating pseudofractions of oil spot, dissolution of oil slick and biodegradation



$$(c_{i})'_{t} + u(c_{i})'_{x} + v(c_{i})'_{y} = \left(\mu^{*}(c_{i})'_{x}\right)'_{x} + \left(\mu^{*}(c_{i})'_{y}\right)'_{y} - \alpha_{i}(T) - \beta_{i}(c_{i})M, \quad (c_{i})'_{n}\Big|_{(x,y)\in\gamma} = 0$$

$$M'_{t} + (u + u_{M})M'_{x} + (v + v_{M})M'_{y} = (\mu M'_{x})'_{x} + (\mu M'_{y})'_{y} + \gamma_{M}(c_{i})M - \lambda M, \quad M'_{n}\Big|_{(x,y)\in\gamma} = 0,$$

$$(\varphi_{i})'_{t} + u(\varphi_{i})'_{x} + v(\varphi_{i})'_{y} + w(\varphi_{i})'_{z} = \left(\mu(\varphi_{i})'_{x}\right)'_{x} + \left(\mu(\varphi_{i})'_{y}\right)'_{y} + \left(\mu(\varphi_{i})'_{z}\right)'_{z},$$

$$(\varphi_{i})'_{n}\Big|_{(x,y,z)\in\Gamma\setminus(z=0)} = 0, \quad (\varphi_{i})'_{z}\Big|_{z=0} = \varphi_{i0},$$

Mathematical model of oil products transport in coastal systems



Changes of the oil initial solubility are described by the equation:

$$S_i = S_{i0}e^{-0.1t},$$

where S_{i0} is an initial oil solubility; t is the time, [day]. The coefficient of horizontal turbulent diffusion depends on the hydrodynamic and climatic conditions in which the process takes place. The coefficient of horizontal turbulent diffusion will be subject to the law of the "four thirds" by Richardson for difficult hydrodynamic and climatic conditions of the Azov-Black Sea area

$$\mu \approx \varepsilon^{1/3} L^{4/3},$$

where L is the characteristic size of diffusing spots; ε is the rate of turbulent energy dissipation. It is equalled to the order of $10^{-1} - 1 \ cm^2/s^3$ at the surface and decreased at the average with depth to values of the order of $10^{-4} - 10^{-3} \ cm^2/s^3$. Boundary and initial conditions for the one-shot volley oil spill were determined for solving the above systems of equations:

$$c_i|_{t=0,(x,y)\in S_0} = c_{i0}, \ c_i|_{t=0,(x,y)\notin S_0} = 0,$$

where S_0 is an area, covered by the spot; c_{i0} is the oil concentration in the considered area.

Modeling of oil microbiological destruction processes in coastal systems

The bioremediation process of oil slick, including the evaporation, dissolution, biological oxidation by microorganisms

Functional dependencies (observation models) were introduced to the system for researching the bioremediation processes of oil slick, including the evaporation, dissolution, biological oxidation by microorganisms: $\gamma(c_i) = \mu_m c_i / (c_i + K_S)$, where $\mu_m(T, C, I)$ is the maximum velocity of microorganism growth; T is an ambient temperature over the spill surface; C is the water salinity; water illumination; K_S is $_{\mathrm{the}}$ saturation coefficient: \mathbf{the} \mathbf{is} $\alpha_i(T) = (K_E P_i/(RT) + K_D S_i) A X_i M_i^m, K_E = 2.5 \cdot 10^{-3} U^{0.78}$ is the mass transport coefficient for hydrocarbon, [m/s]; U is the wind velocity, relatively to the water, [m/s]; X_i is the mole fraction of i-th component, equaled to $v_i / \sum v_i$; v_i is an amount of i-th component substance, [mol]; P_i is the vapor pressure of i-th component, [Pa]; R is the universal gas constant, R = 8.314 J/mol; A is an area of oil spill, $[m^2]$; M_i^m is the molar mass of i-th component, [kg/mol]; $K_D = kK_{D0}$ is the coefficient of mass transport of dissolution; K_{D0} is the initial value of the mass transport coefficient of dissolution; k is the coefficient, depending on the water situation; S_i is the dissolubility of i-th component in water, $[kg/m^3]$; $\varphi_{i0} = K_D S_i X_i M_i^m$; $\beta_i(c_i) = \gamma(c_i)/q$, q is the proportion coefficient between the amount of microorganisms and the absorbed substrate.



Accounting the food taxis (movement of microorganisms in direction of increasing the food concentration – oil fractions)



The number of microorganisms increases as much as possible at movement along the gradient c_i

$$(\mathbf{u}_{M})_{t}' + (u+u_{M})(\mathbf{u}_{M})_{x}' + (v+v_{M})(\mathbf{u}_{M})_{y}' = \left(\mu(\mathbf{u}_{M})_{x}'\right)_{x}' + \left(\mu(\mathbf{u}_{M})_{y}'\right)_{y}' - \alpha_{u}\mathbf{u}_{M} + k_{i}gradc_{i},$$

 α_u is the coefficient of inertial motion of microorganisms (M – bacteria); k_i is the ratio of taxis.

Modeling of oil microbiological destruction processes in coastal system

Modeling of oil microbiological destruction processes in coastal system

We simulated the introduction of biosorbent, containing oil-oxidizing bacteria and the concentrated culture of the *Chlorella vulgaris Beijer* green microalgae, for researching the microbiological oil destruction process. We added two equations taking into account the mechanism of external hormonal regulation, the effect of mineral nutrition (biogenic substances), salinity, temperature and light on the growth and death of green microalgae cells:



$$S'_{t} + uS'_{x} + vS'_{y} + wS'_{z} = \left(\mu S'_{x}\right)'_{x} + \left(\mu S'_{y}\right)'_{y} + \left(\mu S'_{z}\right)'_{z} - (\alpha_{0} + \gamma B)\psi M + D(S_{p} - S) + f,$$

$$B'_{t} + uB'_{x} + vB'_{y} + wB'_{z} = \left(\mu B'_{x}\right)'_{x} + \left(\mu B'_{y}\right)'_{y} + \left(\mu B'_{z}\right)'_{z} + k_{B}M - \varepsilon B,$$



where S, B are concentrations of nutrient and metabolite of the *Chlorella vulgaris Beijer* green algae, respectively; $\alpha = (\alpha + \gamma B)$ is the growth dependence (the *Chlorella vulgaris Beijer microalgae*) due to the B; α_0 is the growth rate of M in the absence B; γ is the impact parameter; $\delta = \delta(C)$ is the loss coefficient of phytoplankton due to the extinction (specific mortality), taking into account the influence of salinity C; D is the specific pollutant rate; f(x, y, z,) is the source function of pollutants; S_p is the maximum possible concentration of pollutants; k_p is the excretion rate; ε is the metabolite decomposition of the coefficient B; $\psi(I, T, S, C)$ is the coefficient taking into account the effect of light, temperature, nutrient concentration S and C on the M. 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 result of SC "Azov3d" (changing of petroleum hydrocarbons concentration): a) initial distribution of light oil fraction ; b) distribution of light oil fraction, N=121; C) initial distribution of heavy oil fraction;
d) distribution of heavy oil fraction, N=148. The time period is 30 days. With the initial oil pollution (two oil slicks), a decrease in the content of sorbed oil by 40% was obtained, which corresponds to the process of oil distribution in the water at the qualitative and quantitative levels.

The comparison of numerical results of the concentration of light oil in the coastal system using SC "Azov3d" with the results of satellite image locations a catastrophic oil spill. The forecast time is 4 days after the spill.



Dynamics of crude oil degradation



RS3 Radarsat-1, November 15, 2007

Wind speed by the data of Kerch weather station was equaled to 2 m/sec

RS3 Radarsat-1, November 16, 2007

Wind speed by the data of Kerch weather station was equaled to 3 m/sec. The total area of the films of oil pollution 117,6 km²

Radar oil spill during the catastrophic oil spill



Wind velocity in the Kerch Strait



Modeling of an emergency oil spill using Azov3d SC

Calibration and verification of results



Decoding of oil sliks on the radar image of IS3 Envisat

SRC «Planeta» data, decoding of oil pollution in the Azov-Black Sea basin

Parallel implementation in hydrobiological modeling of the adaptive modified alternating triangular method for grid equations



Scheme for calculation the correction vector (the transfer of elements after calculation of two layers by the first processor)

Results of k-means algorithm

It's necessary to define all points on the boundary of each subdomain for data exchange in computational process. For this, the Jarvis algorithm (the construction of a convex hull) was used. A list of neighboring subdomains for each subdomain was formed, and an algorithm for data transfer between subdomains was developed.



Results of k-means algorithm for partition of the 2D computational domain into 9, 38, 150 subdomains; 3D computational domain into 6 and 10 subdomains

Parallel implementation of grid equations using k-means method

Domain decomposition



Theoretical estimates of the acceleration and efficiency

$$\begin{split} S_{(2)} &= \frac{n \cdot \chi}{1 + \left(\sqrt{n} - 1\right) \left(\frac{36}{50N_z} + \frac{4n}{50t_0} \left(t_n \left(\frac{1}{N_x} + \frac{1}{N_y}\right) + \frac{t_x \sqrt{n}}{N_x N_y}\right)\right)}{E_{(2)}} \\ E_{(2)} &= \frac{S_{(2)}}{n} = \frac{\chi}{1 + \left(\sqrt{n} - 1\right) \left(\frac{36}{50N_z} + \frac{4n}{50t_0} \left(t_n \left(\frac{1}{N_x} + \frac{1}{N_y}\right) + \frac{t_x \sqrt{n}}{N_x N_y}\right)\right)} \end{split}$$

 $\mathcal X$ is the ratio of the number of computational nodes to the total number of nodes (computational and fictitious).

Hardware resource

For mathematical modeling of hydrodynamic and chemical-biological processes in the three-dimensional domain of complex shape the Azov Sea and the Taganrog Bay – we used sequentially condensed prismatic boundary adaptive grids by dimensions:

 $251 \times 351 \times 15$, $502 \times 702 \times 30$, $1004 \times 1404 \times 60$.

the surface area - 37605 km^2 .

the length - 343 km,

the width - 231 km.

Multiprocessor computer system

Technical specifications

- HP BladeSystem c-class with integrated communication modules, power supply and cooling systems
- HP StorageWorks SFS data storage system, 12 TB
- 8 computer racks
- MSL4048 tape library for data backup, 50 TB
- XC System Software
- Peak performance is 18.8 TFlops
- As computing nodes 512 single-type 16-core Blade servers HP ProLiant BL685c were used, each of which is equipped with four 4-core AMD Opteron 8356 processors 2.3 GHz and 32 GB RAM
- 3 HP ProLiant DL385G5 control servers
- 2048 computing cores, 4 TB total amount of RAM
- 4 4-core processors Intel Core i7-3770K 3.5 GHz



Results of experimental researches

The estimation is used for comparison the performance values of the algorithm 1 (standard)

and algorithm 2 (based on *k-means*), obtained practically s 60 -55 50 Graphs of accelerations for the developed 45 parallel algorithms: 40 1 - the theoretical estimation of the 35 acceleration of the algorithm 1; 2 - the acceleration of the algorithm 2; 30 3 - the acceleration of the algorithm 1; 25 4 - theoretical estimations of the 20 acceleration of the algorithm 2 S(2) 15 10 5 0 10 20 130

The use of the algorithm 2 based on k-means method are increased the efficiency of problem solution on 15% at comparison with the algorithm 2.

Results of experimental researches

Comparison of acceleration and efficiency values of parallel algorithm

p	t ₍₁₎ , s	S'(1)	<i>S</i> ₍₁₎	$E'_{(1)}$	E ₍₁₎	t ₍₂₎ , s	$S_{(2)}^t$	<i>S</i> ₍₂₎	$E_{(2)}^{t}$	E ₍₂₎
1	7,491	1,0	1,0	1,0	1,0	6,073	1,0	1,0	1,0	1,0
2	4,152	1,654	1,804	0,827	0,902	3,121	1,181	1,946	0,59	0,973
4	2,550	3,256	2,938	0,814	0,7345	1,811	2,326	3,354	0,582	0,839
8	1,450	6,318	5,165	0,7897	0,6456	0,997	4,513	6,093	0,654	0,762
16	0,882	11,928	8,489	0,7455	0,5306	0,620	8,520	9,805	0,533	0,613
32	0,458	21,482	16,352	0,6713	0,511	0,317	15,344	19,147	0,48	0,598
64	0,266	35,955	28,184	0,5618	0,4404	0,184	25,682	33,018	0,401	0,516
128	0,172	54,618	43,668	0,4267	0,3411	0,117	39,013	51,933	0,305	0,406

where *p* is the number of processor; $t_{(k)}, S_{(k)}, E_{(k)}$ are the calculation time, acceleration and efficiency values of *k*-th algorithm, *k*=1,2;

 $S_{(k)}^{t}, E_{(k)}^{t}$ are the theoretical comparison of acceleration and efficiency values of *k*-th algorithm.

Information about recent expedition researches (2017)

Scientific expeditions were performed by the employees of the Don State Technical University, the Southern Federal University, the Southern Scientific Center of the Russian Academy of Science in waters of the Azov Sea on the research vessel «Deneb» in July 2017.

The main objective of the expedition research is a comprehensive research of the current situation and spatial-temporal changes in the hydrobiological, hydrological and hydrochemical regimes of the Azov Sea and the Taganrog Bay. During the expedition, more than 20 integrated oceanographic stations were investigated; water, plankton and benthic samples were taken, and ship observations of birds and marine mammals were carried out.



Scientific-research vessel «Deneb»

Expedition researches, 2017



Expedition equipment

- SEACAT SBE19 Hydrological CDT-probe.
- RCM 9LW current recorder.
- SES-2000 light escaladieu parametric profilograph (Innomar Technologie GmbH).
- 13.540 B gravity ground tube with the possibility
- of establishing a piston system (Piston/Gravity corer Model 13.540B).
- $\circ~$ San++ automatic flow analyzer with the SA1100 sampler, that holds 2x50 positions for samples.
- o Deep-water sampling complex of carousel type.
- Equipment for hydrological and lithological researches:
 - the Molchanov sampler for water sampling;
 - the Niskin sampler 5.0 л for water sampling;
 - the Petersen grab for sampling of bottom sediments;
 - the Van-Viin grab for sampling of bottom sediments;
 - benthic drag;
 - the Apstein plankton net for plankton sampling;
 - the Jedi plankton net for plankton sampling;
 - caviar net for ichthyoplankton sampling;
 - the net and drag to conduct ichthyological research;
 - ground straight-flow tube with the possibility of taking the precipitation column 2-2.5 m.
- Equipment for hydrochemical researches, laboratory for performing the full range of field analyses (oxygen, biogenic elements, pH, hydrogen sulfide, plant pigments, products-destruction).
- Equipment for fisheries research (demersal trawl; pelagic spacer trawl 28 m in horizontal, 8 m in vertical).
- SBE19 plus hydro-probe.
- $\circ~$ SBE43 dissolved oxygen sensor.
- $\circ~$ PC (personal computer) with software for connecting the hydro-probes.
- $\circ~$ 3 l and 5 l bathometers and equipment for measuring the oxygen concentration by the Winkler method.
- WHS 600 (ADCP) profilograph.



Scientific-research equipment for model verification



Sea Bird Electronics 19 Plus V2

SBE 43 dissolved oxygen sensor

Turbidity sensor

Pressure sensor

Temperature sensor

Salinity sensor



SES-2000 light

Depth range 1 m...400 m

Multiple object resolution: > 5 cm (depending on the frequency and recording range)

Accuracy:

100 kHz: 0,02 m + 0,02% from water depth

10 kHz: 0,04 m + 0,02% from water depth



ADCP Workhorse 600 Sentinel

Immersion depth up to 70 m

Frequency 600 kHz

Accuracy of measurements 0.25%

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Thank you for attention!