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# Application of high-performance computing for modeling the hydrobiological processes in shallow water*

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# Relevance

- The development of two mathematical modeling directions of biological kinetics processes taking into account the compensation of a priori uncertainty arising from the non-stationary and stochastic nature of environmental systems: methods for solving the problems of identification and verification as a sequential process of determining and refining the numerical values of the coefficients of hydrobiological models; search for hidden patterns of the simulated system of interaction of different types of phytoplankton and their integration into the model.
- Primary production in waters is synthesized by phytoplankton, macrophytes and phytobenthos. Destruction is a set of stages of the production process, representing the stages of destruction and mineralization of organic substances, accompanied by oxygen consumption and energy dissipation. Distributions of real observed random variables (in particular, biological data) in the vast majority of cases are different from normal (Gaussian).
- The results of statistical analysis of natural hydrological and hydrochemical information obtained in the course of long-term expeditionary studies of the coastal system on the example of the Azov sea, is the finding of analytical curves of security for mathematical modeling of production and destruction processes of phytoplankton. These processes can be considered as an indicator of the development of natural and anthropogenic eutrophication of the reservoir, they also become an indicator of pollution of the reservoir, when the total content of nitrogen and phosphorus exceeds the concentration of carbon in the water.
- Creation of a model of formation of production-destructive relations in aquatic ecosystem involves taking into account the influence of physical, chemical and biological factors on the formation of primary products and destruction, with its help an integrated approach to solving the problem.
- Water pollution by biogenic elements coming from river flows, as well as from the widespread abrasion of the shores, construction, expansion and technical re-equipment of sea ports, dredging, increasing intensity of navigation, deep-water releases of treated wastewater, storm drains, interaction and deposition of pollutants on the water surface from the air, is considered as a probabilistic process. Stochasticity is caused by many factors-anthropogenic, climatic, biological, morphological, determining the concentration of pollutants and phytoplankton in the control range.

# Relevance

- Petroleum products are among the priority pollutants and included in the list of mandatory indicators, which are controlled at water pollution monitoring in accordance with Russian and international regulations. The danger of water oil pollution is associated with the presence of compounds, dangerous both to the life of aquatic organisms and to their functional situation. Oil spills lead to the toxic conversion and death of plankton organisms since the oxygen supply stops, fish and fry destruction of rivers, streams, lakes and seas. The oil has a toxic effect on phytoplankton at concentrations of $10^{-8} – 10^{-3}$ mg/l (cell division slows down or stops, the main production decreases). Primary production of marine phytoplankton with the oil concentration of 0.05 – 0.5 mg/l is reduced on 50%. Many hydrobionts are characterized by the cumulative effect, the accumulation in a toxicant, and as a result they become toxic dangerous.
- Processing the most contaminated coastal zones, water vegetation may be performed by the oxidizing biologic product of the ``Oleovarin'' family and mineral fertilizers, installation of biofilter cascade with immobilized cells biopreparation and fertilizers, and the lemna and chlorella algae introduction for water phytoremediation on the limited areas, enabling to intensify the oxidation of diesel fuel in the surface water layer. Such technologies result for destruction of hydrocarbons in water at high concentrations, regardless of partial water eutrophy and are relatively cheap at the same time. Biosorbent include the hydrophobic oil sorbent as a carrier based on peat, and the oil-oxidizing microorganisms immobilized on the carrier in an effective amount.
- The microorganism immobilization is carried out by the adsorption method with obtaining individual sorbents: the bacterial sorbent with the *Rhodococcus eqvi* P-72-00 culture; the yeast sorbent with the *Rhodotorula glutinis* 2-4M culture; the mushroom sorbent with the *Trichoderma lignorum* F-98 mycelial fungi. The biosorbent is used in conjunction with the concentrated culture of *Chlorella vulgaris Beijer* microalgae with the ratio of components on the dry matter, wt.: the biosorbent of 90 – 97%; the biomass of *Chlorella vulgaris Beijer* microalgae of 3 – 10%.

# Relevance

- Shallow waters are suffered the great anthropogenic influence. But most of them is the unique 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 of suffocation.
- The most important technogenic factors that have a significant impact on the ecosystem of the reservoir are: metallurgical and chemical waste of industrial activity, as well as municipal contaminated waste water; oil and oil products; bottom trawling, destroying bottom biocenoses; difficult to control fishing by poachers; construction of reservoirs; saturated chemization, soil and water pollution, salinization of the reservoir; increase of uncontrolled discharge of pesticides into the reservoir, which entails «water blooming»; enhanced construction of facilities along the coast, not in accordance with environmental standards; dumping, etc.
- The research topic develops the important subject area – mathematical modeling of complex system. The development of multi-species models of hydrobiological processes will make it possible to build a model of a complete shallow-water reservoir ecosystem in the future.
- According to the Federal Law from 10.01.2002, No.7-FL (amended from July 3, 2016) «About the Environmental Protection»; The Water Code of the Russian Federation; Order of the Government of the Russian Federation of December 4, 2014 No.2462-r; Decree of the Government of the Russian Federation No.794 of December 30, 2003 (amended from October 19, 2016) «On a unified state system for the prevention of emergencies», the time for making decisions and eliminating contingencies of technogenic or natural characters should be from several hours to two to three days . Therefore, the time allotted to the construction of forecasts of the ecological state of coastal systems in the event of emergencies is limited.
- Several researches in mathematical modeling of processes of hydrophysics and biological kinetics are devoted to the parallel implementation of problems of this class. Although the conditions for the development of catastrophic and unfavorable phenomena in shallow waters, it is necessary to forecast the development of such phenomena and make decisions within tens of minutes - units of hours. It, in turn, requires the modeling of hydrobiological processes on multiprocessor computer systems on the accelerated time mode.

# Research goal and tasks

**Purpose of research:** development and numerical implementation on supercomputer the models of hydrobiological process in coastal system. For numerical solution it's necessary to develop conservative difference schemes of high order of accuracy taking into account the degree of cell occupancy for obtaining a detailed description of researching values of contaminant concentrations, petroleum hydrocarbons' pollution, phytoplankton for a given number of nodes of the used computational grid.

⇩

**Research problems:** development of stochastic mass transfer velocities models are included the designing of production velocity model of organic matter (OM) in water, and OM destruction models by the bacteria and phytoplankton. The relative velocity of mass transfer were considered as dependent from climate factors, as well as components of chemical-biological model. The Mitscherlich hypothesis about simultaneous influence of factors (water temperature, illumination and content of biogenic elements in the water, etc.) on the mass transfer velocity was used. Each factor decrease and increase the maximum specific growth rate due to the its lack or excess in the system. So, the generalized response function is used in this research. The main method for constructing the model is the selection of algorithms for calculation particular response functions (dependence functions of the concrete indicator values on one ecological factor). The generalized response function is the dependence functions of the k-th value or process from all considered environmental factors (combination of specific response functions). The total biomass for each individual phytoplankton species is used as a generalized response function.

# Analysis of existing complexes and models of hydrobiological processes

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, 2001г.); PISCATOR (2002г.); 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 and forecasting systems

- Universal modeling packages of hydrodynamical processes (FlowVision, FLUENT, GAS DYNAMICS TOOL, PHOENICS, Star-CD, etc.) are focused on multiprocessor systems, but the versatility of these packages is to use the limited number of models, algorithms and methods to variety of different cases. Programs, aimed for solving the particular problems, have the potential to address these challenges more effectively.
- Most of the known specialized software (ADAM, CAL3QHC, Chensi, TASCflow, ISC-3, PANACHE, REMSAD, UAM-IV, ЭКОЛОГ, ПРИЗМА, VITECON), designed for calculation the pollution spread, is focused on single-processor systems. Only separate modules of specialized software systems (for example, ECOSIM и MAQSIP), adapted to perform on multiprocessor systems, are parallelized. This fact does not allow to achieve high efficiency computing in some cases.

These methods:

- use simplified models of hydro-biological processes for water objects with the slightly varying salinity, and, in most cases, with the varying depth.
- do not provide the operational forecasts of the environmental situation of shallow waters after the disaster.
- can not be replicated to other aquatic ecosystems, as focused on the description of the biogeochemical cycles and species composition of biological plankton populations and their interactions in single water objects.

# Hydrodynamic mathematical model of shallow waters

**Motion equation (the Navier – Stokes equation)**

$$u'_t + uu'_x + vu'_y + wu'_z = -p'_x / \rho + \left(\mu u'_x\right)'_x + \left(\mu u'_y\right)'_y + \left(\nu u'_z\right)'_z + 2\Omega(v\sin\theta - w\cos\theta)$$

$$v'_t + uv'_x + vv'_y + wv'_z = -p'_y / \rho + \left(\mu v'_x\right)'_x + \left(\mu v'_y\right)'_y + \left(\nu v'_z\right)'_z - 2\Omega u\sin\theta$$

$$w'_t + uw'_x + vw'_y + ww'_z = -p'_z / \rho + \left(\mu w'_x\right)'_x + \left(\mu w'_y\right)'_y + \left(\nu w'_z\right)'_z + 2\Omega u\cos\theta + g\left(\rho_0 / \rho - 1\right)$$

**Continuity equation in the case of variable density**

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

where $\mathbf{u} = \{u, v, w\}$ 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.

**Boundary conditions**

- at the entrance (the mouth of the Don and Kuban rivers):

$\mathbf{u} = \mathbf{u}_0$, $p'_{\mathbf{n}} = 0$,

- the lateral boundary (the bank and the bottom):

$\rho_v \mu(\mathbf{u})'_{\mathbf{n}} = -\boldsymbol{\tau}$, $\mathbf{u}_{\mathbf{n}} = 0$, $p'_{\mathbf{n}} = 0$,

- the upper boundary:

$\rho\mu(\mathbf{u}_{\boldsymbol{\tau}})'_{\mathbf{n}} = -\boldsymbol{\tau}$, $w = -\omega - p'_t / \rho g$, $p'_{\mathbf{n}} = 0$,

- output (Kerch Strait):

$p'_{\mathbf{n}} = 0$, $\mathbf{u}'_{\mathbf{n}} = 0$,

where $\omega$ is the rate of evaporation of the liquid; $\boldsymbol{\tau} = \{\tau_x, \tau_y\}$ is the tangential stress vector, $\mathbf{u}_{\mathbf{n}}$, $\mathbf{u}_{\boldsymbol{\tau}}$ are normal and tangential components of the water flow velocity vector; $\rho_v$ is the density suspension.

# Hydrodynamic mathematical model of shallow waters

Components of the tangential stress may

- for the free surface

$\boldsymbol{\tau} = \rho_a Cd_s |\mathbf{w}|\mathbf{w}$, $Cd_s = 0.0026$, $\mathbf{w}$ is the vector of the wind speed relative to the water, $\rho_a$ is the density of the atmosphere, $Cd_s$ is dimensionless surface drag coefficient, which depends on the wind speed, was considered in the range 0.0016 – 0.0032.

- for the bottom

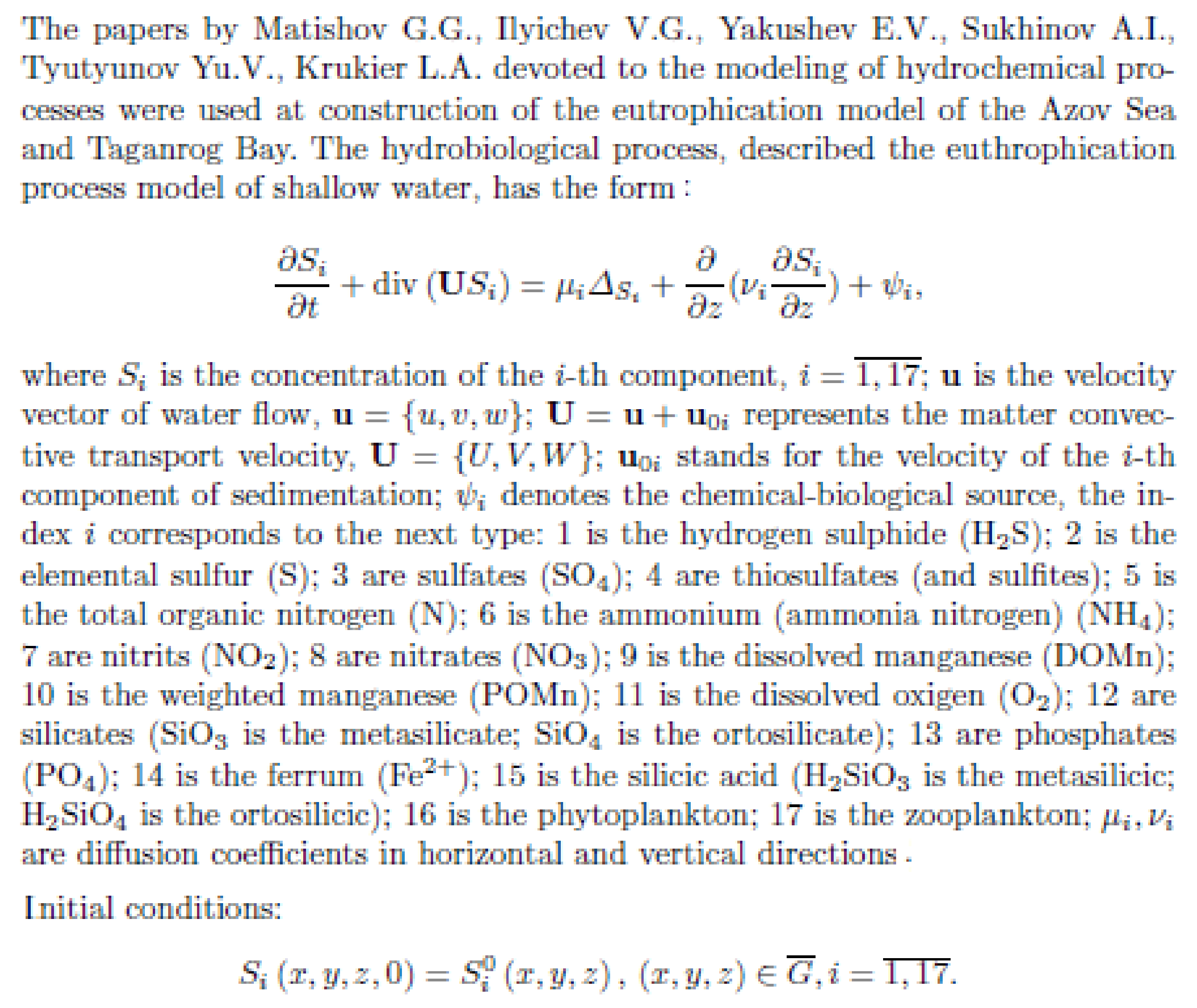
$\boldsymbol{\tau} = \rho Cd_b |\mathbf{u}|\mathbf{u}$, $Cd_b = gk^2 / h^{1/3}$, where $k = 0.04$, $k$ is the group coefficient of roughness in Manning's formula, $k \in [0.025, 0.2]$; $h=H+\eta$, h is the total depth of the water area, [m]; H is the depth to undisturbed surface, [m]; $\eta$ is the height of the free surface relative to the geoid (Sea level), [m].

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

$$\nu = C_s^2 \Delta^2 \frac{1}{2} \sqrt{\left(\frac{\partial \overline{U}}{\partial z}\right)^2 + \left(\frac{\partial \overline{V}}{\partial z}\right)^2}$$

where $\overline{U}, \overline{V}$ are the time-averaged pulsations of the horizontal velocity components, $\Delta$ is the characteristic scale of the grid, $C_s$ is Smagorinsky dimensionless empirical constant whose value is usually determined on the basis of calculating the decay process of homogeneous isotropic turbulence.

# Modeling of hydrobiological processes in shallow system



The papers by Matishov G.G., Ilyichev V.G., Yakushev E.V., Sukhinov A.I., Tyutyunov Yu.V., Krukier L.A. devoted to the modeling of hydrochemical processes were used at construction of the eutrophication model of the Azov Sea and Taganrog Bay. The hydrobiological process, described the euthrophication process model of shallow water, has the form :

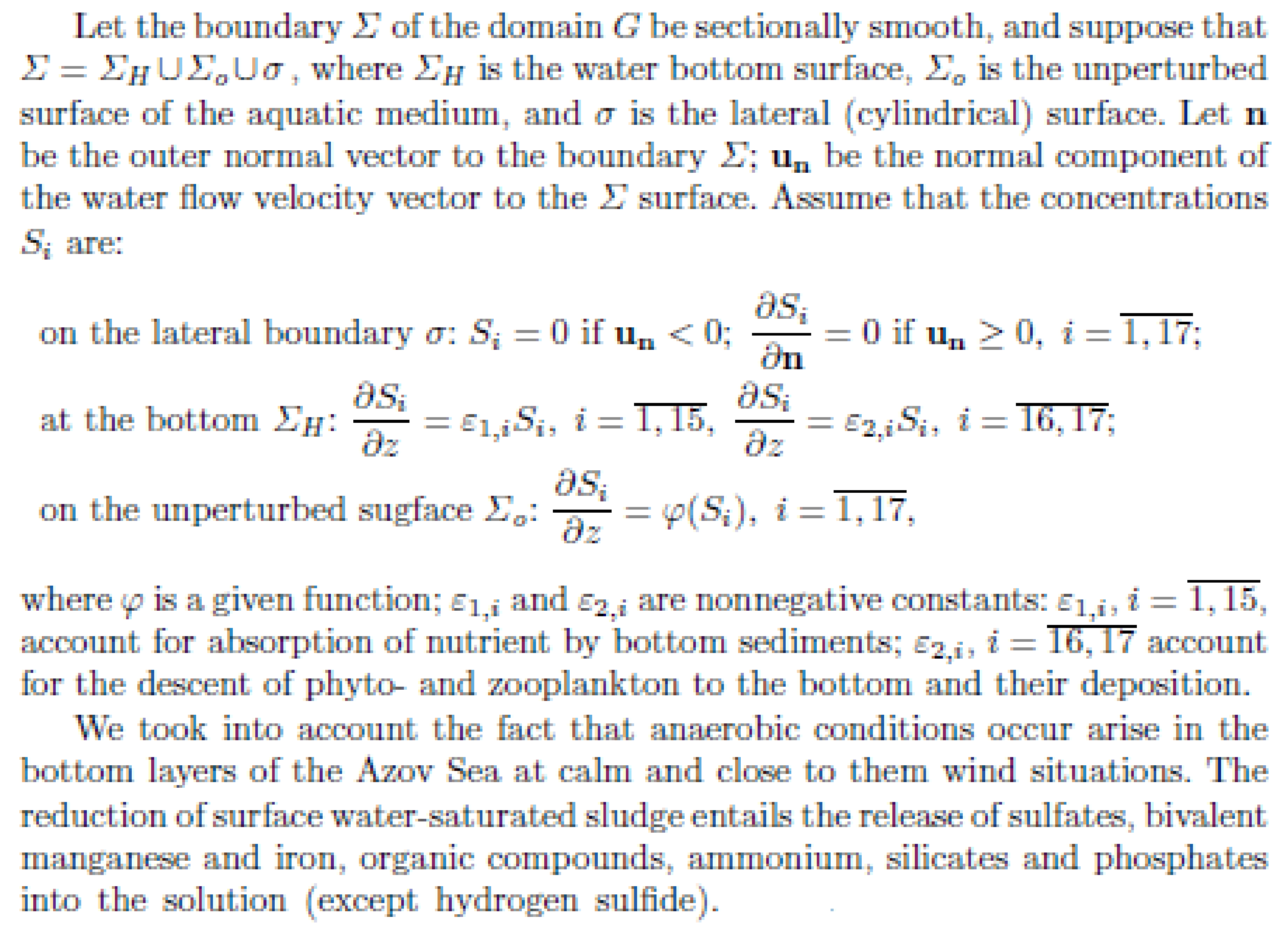
$$\frac{\partial S_i}{\partial t} + \operatorname{div}(\mathbf{U}S_i) = \mu_i \Delta_{S_i} + \frac{\partial}{\partial z}\left(\nu_i \frac{\partial S_i}{\partial z}\right) + \psi_i,$$

where $S_i$ is the concentration of the $i$-th component, $i = \overline{1,17}$; $\mathbf{u}$ is the velocity vector of water flow, $\mathbf{u} = \{u, v, w\}$; $\mathbf{U} = \mathbf{u} + \mathbf{u}_{0i}$ represents the matter convective transport velocity, $\mathbf{U} = \{U, V, W\}$; $\mathbf{u}_{0i}$ stands for the velocity of the $i$-th component of sedimentation; $\psi_i$ denotes the chemical-biological source, the index $i$ corresponds to the next type: 1 is the hydrogen sulphide ($H_2S$); 2 is the elemental sulfur (S); 3 are sulfates ($SO_4$); 4 are thiosulfates (and sulfites); 5 is the total organic nitrogen (N); 6 is the ammonium (ammonia nitrogen) ($NH_4$); 7 are nitrits ($NO_2$); 8 are nitrates ($NO_3$); 9 is the dissolved manganese (DOMn); 10 is the weighted manganese (POMn); 11 is the dissolved oxigen ($O_2$); 12 are silicates ($SiO_3$ is the metasilicate; $SiO_4$ is the ortosilicate); 13 are phosphates ($PO_4$); 14 is the ferrum ($Fe^{2+}$); 15 is the silicic acid ($H_2SiO_3$ is the metasilicic; $H_2SiO_4$ is the ortosilicic); 16 is the phytoplankton; 17 is the zooplankton; $\mu_i, \nu_i$ are diffusion coefficients in horizontal and vertical directions .

Initial conditions:

$$S_i\left(x,y,z,0\right) = S_i^0\left(x,y,z\right),\ (x,y,z) \in \overline{G}, i = \overline{1,17}.$$

# Modeling of hydrobiological processes in shallow system



Let the boundary $\Sigma$ of the domain $G$ be sectionally smooth, and suppose that $\Sigma = \Sigma_H \cup \Sigma_o \cup \sigma$, where $\Sigma_H$ is the water bottom surface, $\Sigma_o$ is the unperturbed surface of the aquatic medium, and $\sigma$ is the lateral (cylindrical) surface. Let $\mathbf{n}$ be the outer normal vector to the boundary $\Sigma$; $\mathbf{u_n}$ be the normal component of the water flow velocity vector to the $\Sigma$ surface. Assume that the concentrations $S_i$ are:

on the lateral boundary $\sigma$: $S_i = 0$ if $\mathbf{u_n} < 0$; $\dfrac{\partial S_i}{\partial \mathbf{n}} = 0$ if $\mathbf{u_n} \geq 0$, $i = \overline{1,17}$;

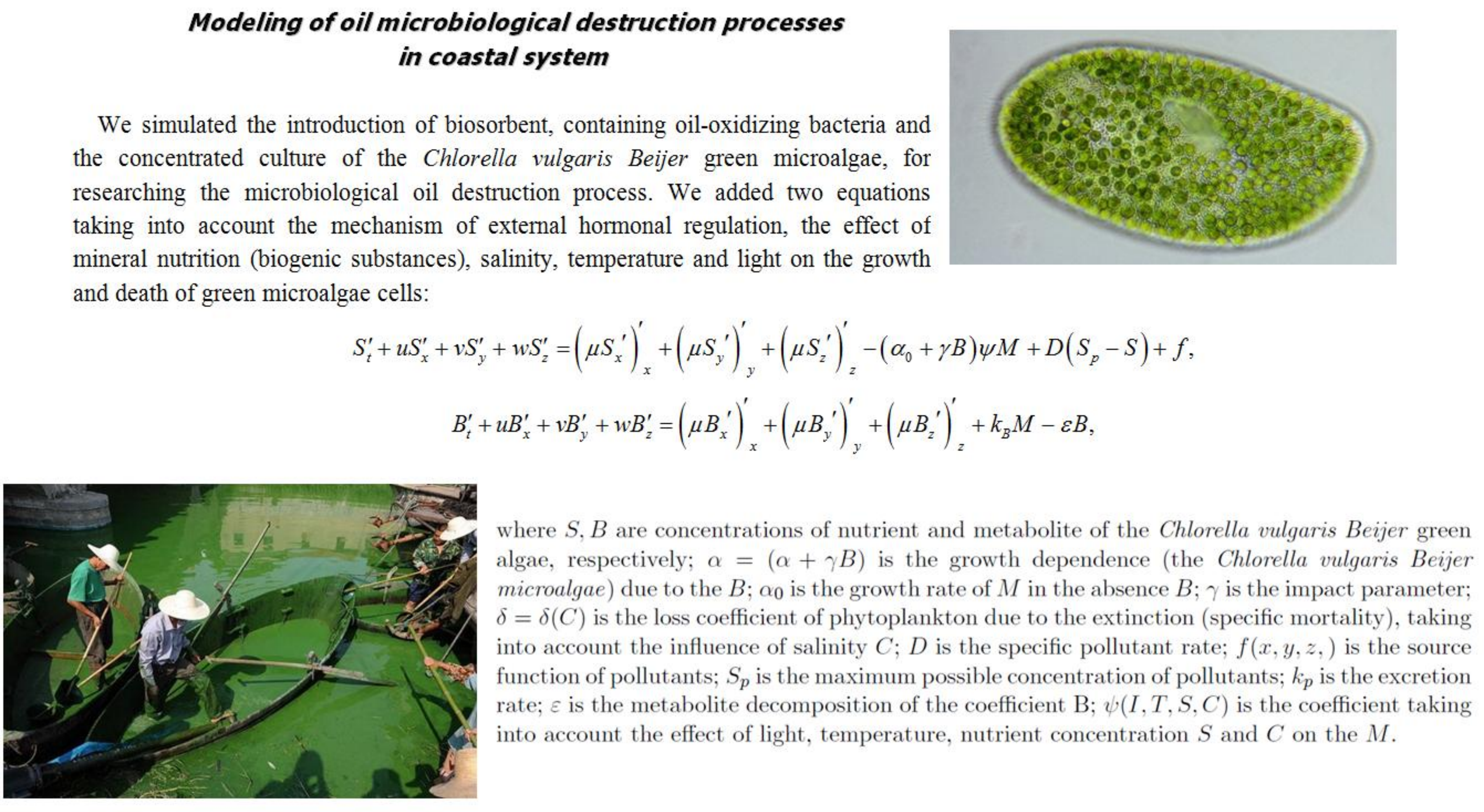
at the bottom $\Sigma_H$: $\dfrac{\partial S_i}{\partial z} = \varepsilon_{1,i} S_i$, $i = \overline{1,15}$, $\dfrac{\partial S_i}{\partial z} = \varepsilon_{2,i} S_i$, $i = \overline{16,17}$;

on the unperturbed sugface $\Sigma_o$: $\dfrac{\partial S_i}{\partial z} = \varphi(S_i)$, $i = \overline{1,17}$,

where $\varphi$ is a given function; $\varepsilon_{1,i}$ and $\varepsilon_{2,i}$ are nonnegative constants: $\varepsilon_{1,i}$, $i = \overline{1,15}$, account for absorption of nutrient by bottom sediments; $\varepsilon_{2,i}$, $i = \overline{16,17}$ account for the descent of phyto- and zooplankton to the bottom and their deposition.

We took into account the fact that anaerobic conditions occur arise in the bottom layers of the Azov Sea at calm and close to them wind situations. The reduction of surface water-saturated sludge entails the release of sulfates, bivalent manganese and iron, organic compounds, ammonium, silicates and phosphates into the solution (except hydrogen sulfide).

# Modeling of oil microbiological destruction processes in coastal system



**Modeling of oil microbiological destruction processes in coastal system**

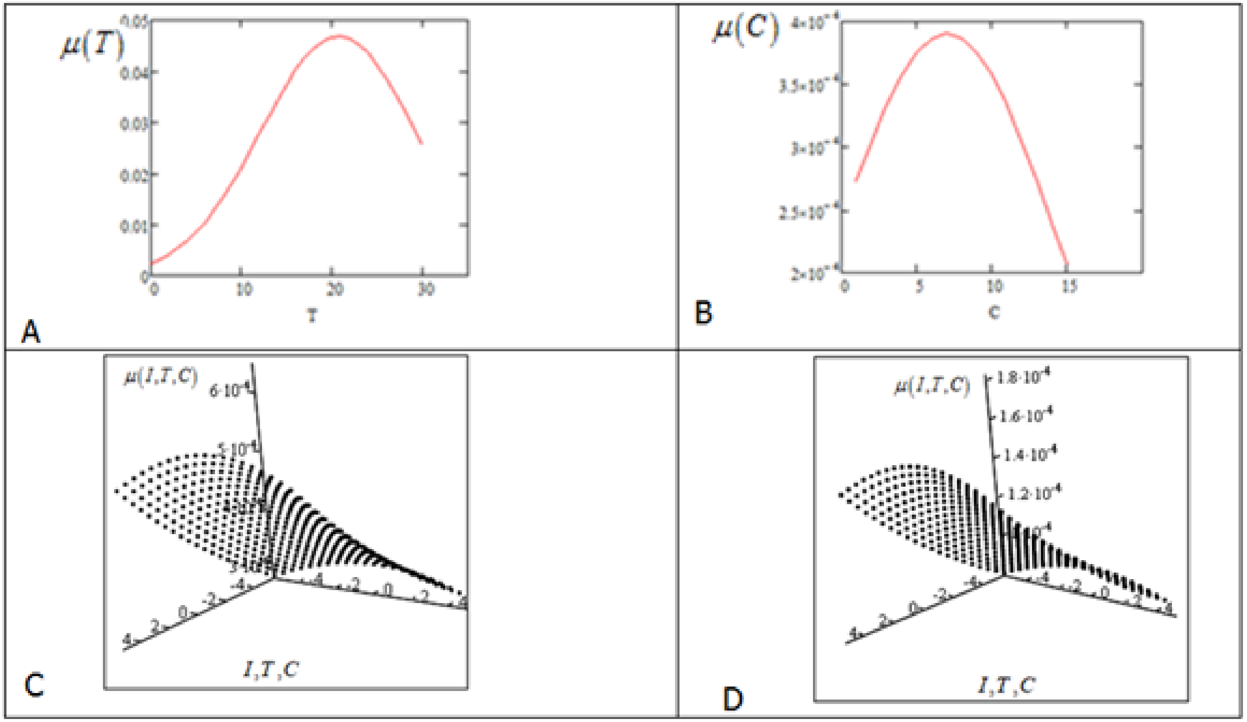
We simulated the introduction of biosorbent, containing oil-oxidizing bacteria and the concentrated culture of the *Chlorella vulgaris Beijer* green microalgae, for researching the microbiological oil destruction process. We added two equations taking into account the mechanism of external hormonal regulation,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

$$S'_t + uS'_x + vS'_y + wS'_z = \left(\mu S_x{}'\right)'_x + \left(\mu S_y{}'\right)'_y + \left(\mu S_z{}'\right)'_z - (\alpha_0 + \gamma B)\psi M + D\left(S_p - S\right) + f,$$

$$B'_t + uB'_x + vB'_y + wB'_z = \left(\mu B_x{}'\right)'_x + \left(\mu B_y{}'\right)'_y + \left(\mu B_z{}'\right)'_z + k_B M - \varepsilon B,$$

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 $B$; $\alpha_0$ is the growth rate of $M$ in the absence $B$; $\gamma$ 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; $\varepsilon$ 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 $M$.

# Functional dependency models observations



A) $\mu(T)=\mu_0\exp\left[-\{(T-T_{opt})/\sigma_T\}^2-\mu_1T+\mu_2\right]$, $T_{opt}=25$, $\sigma_T=12$, $\mu_0=0.12$, $\mu_1=0.06$, $\mu_2=0.43$;

B) $\mu(C)=\mu_0\exp\left[-\{(C-C_{opt})/\sigma_c\}^2-\mu_1C+\mu_2\right]$, $C_{opt}=12$, $\sigma_C=10$, $\mu_0=0.001$, $\mu_1=0.1$, $\mu_2=0.01$;

C) $\mu(I,T,C)=\alpha_0\exp(aT)(I/I_{opt})\exp(1-I/I_{opt})\eta_0\exp\left[-\{(C-C_{opt})/\sigma_c\}^2-\eta_1C+\eta_2\right]$, $\alpha_0=0.8$, $a=0.063$, $I=I_{opt}=86$, $C_{opt}=12$, $\sigma_C=15$, $\eta_0=0.001$, $\eta_1=0.1$, $\eta_2=0.1$; D) $I=10$, $I_{opt}=86$.

# Discretization of models of hydrobiological processes

Sediment transport problem can be represented by the convection-diffusion-reaction equation:

$$c'_t + uc'_x + vc'_y = \left(\mu c'_x\right)'_x + \left(\mu c'_y\right)'_y + f$$

with the boundary conditions: $c'_n\left(x,y,t\right) = \alpha_n c + \beta_n$,
where *u*,*v* are components of the velocity vector; f is the function of intensity and distribution of sources; μ is the coefficient of diffusion (turbulent) exchange.

We have introduced a uniform grid for the numerical implementation of the discrete mathematical model:

$$w_h = \left\{t^n = n\tau, x_i = ih_x, y_j = jh_y;\ n = \overline{0,N_t}, i = \overline{0,N_x}, j = \overline{0,N_y};\ N_t\tau = T, N_x h_x = l_x, N_y h_y = l_y\right\},$$

где $\tau$ is the time step; $h_x, h_y$ are space steps; $N_t$ is an upper time boundary; $N_x, N_y$ are space bounds.

**Approximation of operators the diffusion and convection transports:**

$$\left(q_0\right)_{i,j} uc'_x \ ;\ \left(q_1\right)_{i,j} u_{i+1/2,j} \frac{c_{i+1,j} - c_{i,j}}{2h_x} + \left(q_2\right)_{i,j} u_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{2h_x},$$

$$\left(q_0\right)_{i,j} \left(\mu c'_x\right)'_x \ ;\ \left(q_1\right)_{i,j} \mu_{i+1/2,j} \frac{c_{i+1,j} - c_{i,j}}{h_x^2} - \left(q_2\right)_{i,j} \mu_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{h_x^2} - \left|\left(q_1\right)_{i,j} - \left(q_2\right)_{i,j}\right| \mu_{i,j} \frac{\alpha_x c_{i,j} + \beta_x}{h_x},$$

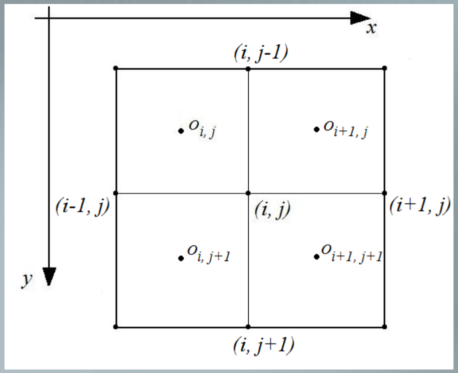
in the case of boundary conditions of the first kind: $u'_n(x,y,t) = \alpha u + \beta$
Filling coefficients of control domains $q_m$, $m = \overline{0,4}$

$$\left(q_m\right)_{i,j} = \frac{S_{\Omega_m}}{S_{D_m}}, \left(q_0\right)_{i,j} = \frac{o_{i,j} + o_{i+1,j} + o_{i+1,j+1} + o_{i,j+1}}{4},$$

$$\left(q_1\right)_{i,j} = \frac{o_{i+1,j} + o_{i+1,j+1}}{2}, \left(q_2\right)_{i,j} = \frac{o_{i,j} + o_{i,j+1}}{2},$$

$$\left(q_3\right)_{i,j} = \frac{o_{i+1,j+1} + o_{i,j+1}}{2}, \left(q_4\right)_{i,j} = \frac{o_{i,j} + o_{i+1,j}}{2}.$$

$o_{i,j}$ is the filling of $(i,j)$ cell.



**Location units relative to cells**

# Discretization of model

Each equation of the system can be represented by the diffusion-convection equation in the two-dimensional case:

$$c'_t+uc'_x+vc'_y=\left(\mu c'_x\right)'_x+\left(\mu c'_y\right)'_y+f$$

with boundary conditions:

$$c'_n\left(x,y,t\right)=\alpha_n c+\beta_n .$$

The uniform grid was defined for numerical implementation of the discrete mathematical model:

$w_h=\left\{t^n=n\tau, x_i=ih_x, y_j=jh_y;\ n=\overline{0,N_t}, i=\overline{0,N_x}, j=\overline{0,N_y};\ N_t\tau=T, N_xh_x=l_x, N_yh_y=l_y\right\}$, where $\tau$ is the time step; $h_x$, $h_y$ are spatial steps; $N_t$ is the upper time boundary; $N_x$, $N_y$ are spatial boundaries; $l_x$, $l_y$ are characteristic dimensions of the computational domain.

**Discrete analog of the diffusion-convection equation (splitting scheme for the space) taking into account the partial filling of computational nodes:**

$$\frac{q^{n+1/2}_{i,j}-q^{n}_{i,j}}{\tau}+\psi_{xL}\frac{q^{n-1/2}_{i-1,j}-q^{n-1}_{i-1,j}}{2\tau}+\psi_{xR}\frac{q^{n-1/2}_{i+1,j}-q^{n-1}_{i+1,j}}{2\tau}+u\frac{q^{n}_{i+1,j}-q^{n}_{i-1,j}}{4h_x}+$$

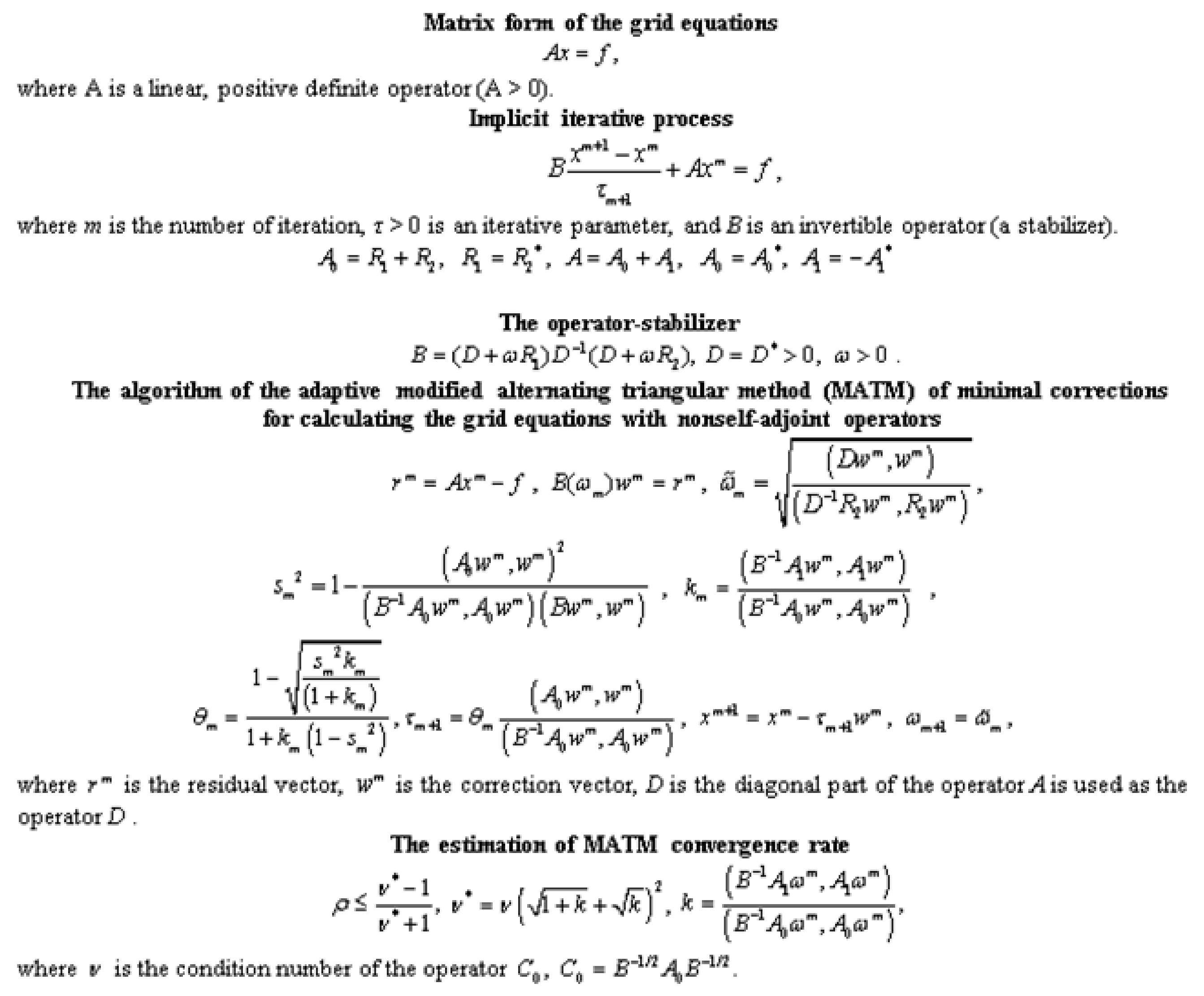
$$+\psi_{xL}u\frac{q^{n}_{i,j}-q^{n}_{i-1,j}}{h_x}+\psi_{xR}u\frac{q^{n}_{i+1,j}-q^{n}_{i,j}}{h_x}=\frac{3}{2}\mu\frac{q^{n}_{i+1,j}-2q^{n}_{i,j}+q^{n}_{i-1,j}}{h_x^2}+\frac{1}{2}\left(g\left(q^{n}_{i,j}\right)+\eta^{n}_{i,j}\right);$$

$$\frac{q^{n+1}_{i,j}-q^{n+1/2}_{i,j}}{\tau}+\psi_{yL}\frac{q^{n}_{i,j-1}-q^{n-1/2}_{i,j-1}}{2\tau}+\psi_{yR}\frac{q^{n}_{i,j+1}-q^{n-1/2}_{i,j+1}}{2\tau}+v\frac{q^{n+1/2}_{i,j+1}-q^{n+1/2}_{i,j-1}}{4h_y}+$$

$$+\psi_{yL}v\frac{q^{n+1/2}_{i,j}-q^{n+1/2}_{i,j-1}}{h_y}+\psi_{yR}v\frac{q^{n+1/2}_{i,j+1}-q^{n+1/2}_{i,j}}{h_y}=\frac{3}{2}\mu\frac{q^{n+1/2}_{i,j+1}-2q^{n+1/2}_{i,j}+q^{n+1/2}_{i,j-1}}{h_y^2}+\frac{1}{2}\left(g\left(q^{n}_{i,j}\right)+\eta^{n}_{i,j}\right),$$

$=0$ 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 $v<0$.

# Modified alternating triangular method



### Matrix form of the grid equations

$$Ax = f,$$

where A is a linear, positive definite operator (A > 0).

### Implicit iterative process

$$B\frac{x^{m+1}-x^m}{\tau_{m+1}} + Ax^m = f,$$

where $m$ is the number of iteration, $\tau > 0$ is an iterative parameter, and $B$ is an invertible operator (a stabilizer).

$$A_0 = R_1 + R_2,\ \ R_1 = R_2^*,\ \ A = A_0 + A_1,\ \ A_0 = A_0^*,\ \ A_1 = -A_1^*$$

### The operator-stabilizer

$$B = (D + \omega R_1)D^{-1}(D + \omega R_2),\ D = D^* > 0,\ \ \omega > 0\ .$$

### The algorithm of the adaptive modified alternating triangular method (MATM) of minimal corrections for calculating the grid equations with nonself-adjoint operators

$$r^m = Ax^m - f\ ,\ \ B(\omega_m)w^m = r^m,\ \ \tilde{\omega}_m = \sqrt{\frac{\left(Dw^m, w^m\right)}{\left(D^{-1}R_2w^m, R_2w^m\right)}},$$

$$s_m^{\ 2} = 1 - \frac{\left(A_0w^m, w^m\right)^2}{\left(B^{-1}A_0w^m, A_0w^m\right)\left(Bw^m, w^m\right)}\ ,\ \ k_m = \frac{\left(B^{-1}A_1w^m, A_1w^m\right)}{\left(B^{-1}A_0w^m, A_0w^m\right)}\ ,$$

$$\theta_m = \frac{1 - \sqrt{\dfrac{s_m^{\ 2}k_m}{\left(1 + k_m\right)}}}{1 + k_m\left(1 - s_m^{\ 2}\right)},\ \tau_{m+1} = \theta_m\frac{\left(A_0w^m, w^m\right)}{\left(B^{-1}A_0w^m, A_0w^m\right)},\ \ x^{m+1} = x^m - \tau_{m+1}w^m,\ \ \omega_{m+1} = \tilde{\omega}_m,$$

where $r^m$ is the residual vector, $w^m$ is the correction vector, $D$ is the diagonal part of the operator $A$ is used as the operator $D$.

### The estimation of MATM convergence rate

$$\rho \le \frac{\nu^* - 1}{\nu^* + 1},\ \nu^* = \nu\left(\sqrt{1 + k} + \sqrt{k}\right)^2,\ k = \frac{\left(B^{-1}A_1\omega^m, A_1\omega^m\right)}{\left(B^{-1}A_0\omega^m, A_0\omega^m\right)},$$

where $\nu$ is the condition number of the operator $C_0$, $C_0 = B^{-1/2}A_0B^{-1/2}$.

# Multiprocessor computer system

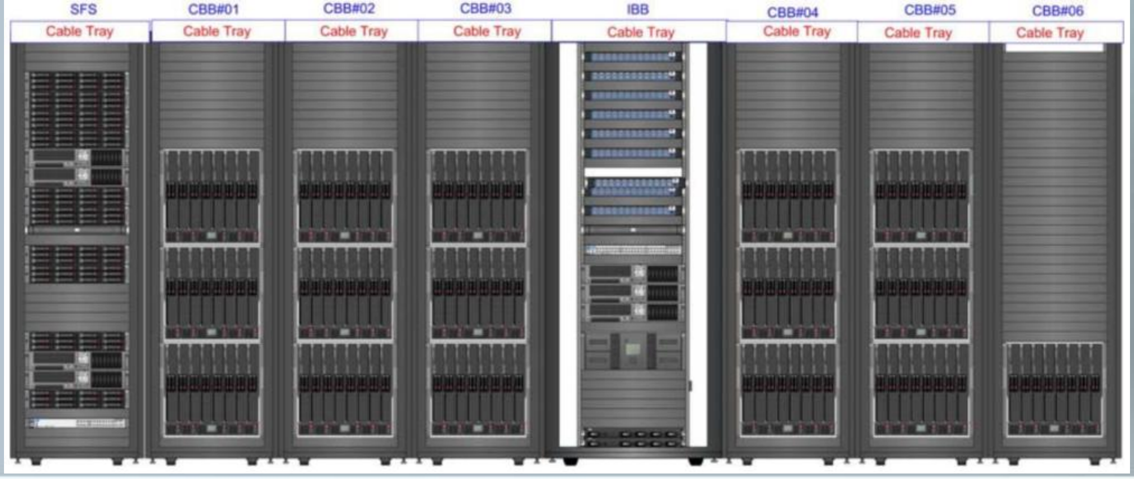
**Technical specifications**

- 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

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 rectangular grids by dimensions:

$$251\times351\times15,\ \ 502\times702\times30,\ \ 1004\times1404\times60.$$

Physical dimensions of the computational domain: the surface area - 37605 km²,
the length - 343 km,
the width - 231 km.



# Parallel implementation on graphic accelerator

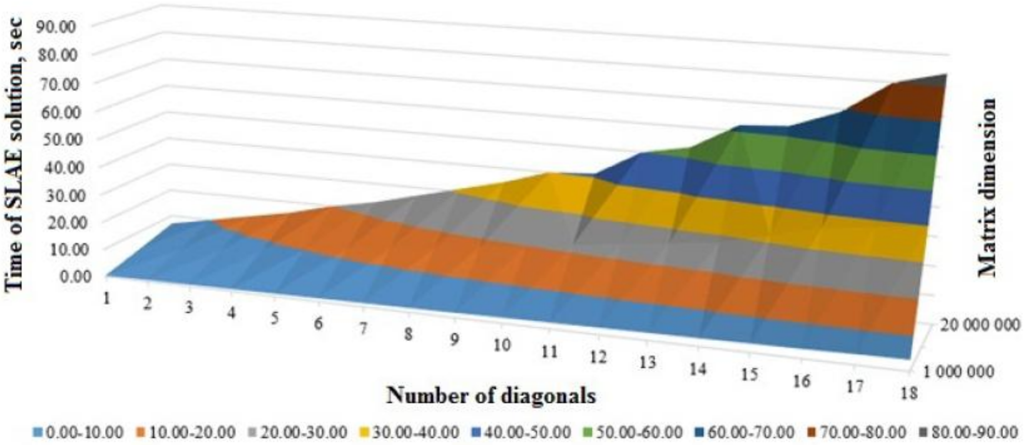
For numerical implementation of proposed interrelated mathematical models of biological kinetics, we developed parallel algorithms which will be adapted for hybrid computer systems using the NVIDIA CUDA architecture.

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 of RAM 32 GB, the NVIDIA GeForce GTX 750 Ti video card of 2GB, 640 CUDA cores.

# Parallel implementation on graphic accelerator

The dependence of the SLAE solution time on the matrix dimension and the number of nonzero diagonals was obtained for implementation the corresponding algorithm.

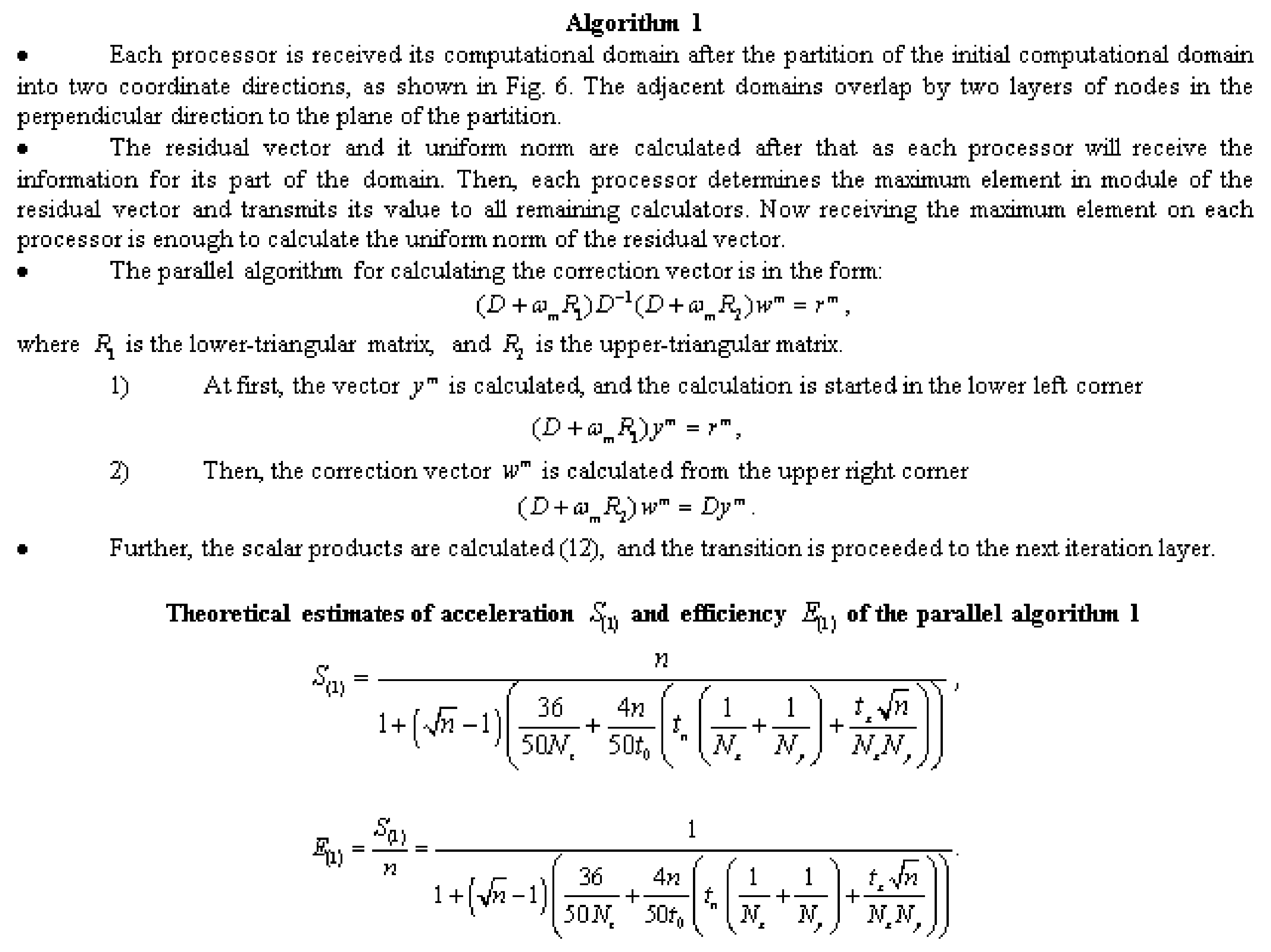


The dependence of SLAE solution time on matrix dimension and the number of nonzero diagonals

Due to it, in particular, we can choose the grid size and to determine the time for solving the SLAE based on the amount of nonzero matrix diagonals.

Analysis of the CUDA architecture characteristics showed the algorithms for numerical implementation of the developed mathematical model of hydrobiological processes can be applied for designing high-performance information systems on a personal computer.

# Parallel implementation of the modified alternating triangular method



**Algorithm 1**

- Each processor is received its computational domain after the partition of the initial computational domain into two coordinate directions, as shown in Fig. 6. The adjacent domains overlap by two layers of nodes in the perpendicular direction to the plane of the partition.
- The residual vector and it uniform norm are calculated after that as each processor will receive the information for its part of the domain. Then, each processor determines the maximum element in module of the residual vector and transmits its value to all remaining calculators. Now receiving the maximum element on each processor is enough to calculate the uniform norm of the residual vector.
- The parallel algorithm for calculating the correction vector is in the form:

$$(D+\omega_m R_1)D^{-1}(D+\omega_m R_2)w^m = r^m,$$

where $R_1$ is the lower-triangular matrix, and $R_2$ is the upper-triangular matrix.

1) At first, the vector $y^m$ is calculated, and the calculation is started in the lower left corner

$$(D+\omega_m R_1)y^m = r^m,$$

2) Then, the correction vector $w^m$ is calculated from the upper right corner

$$(D+\omega_m R_2)w^m = Dy^m.$$

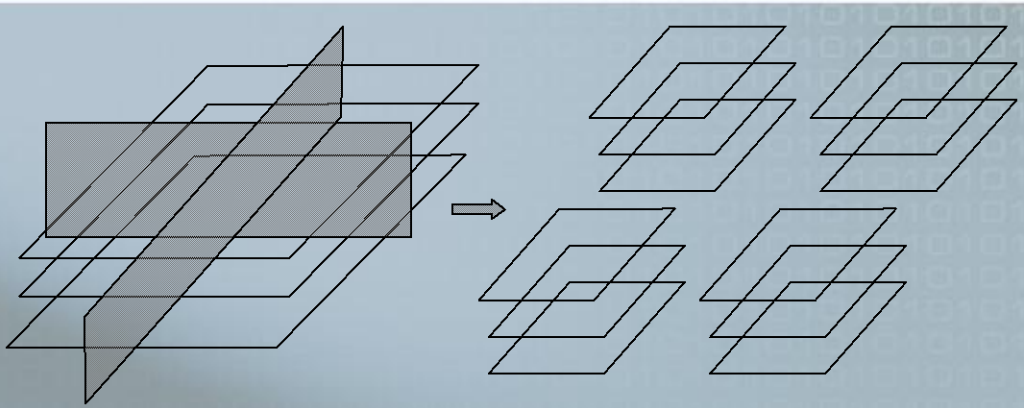
- Further, the scalar products are calculated (12), and the transition is proceeded to the next iteration layer.

**Theoretical estimates of acceleration $S_{(1)}$ and efficiency $E_{(1)}$ of the parallel algorithm 1**

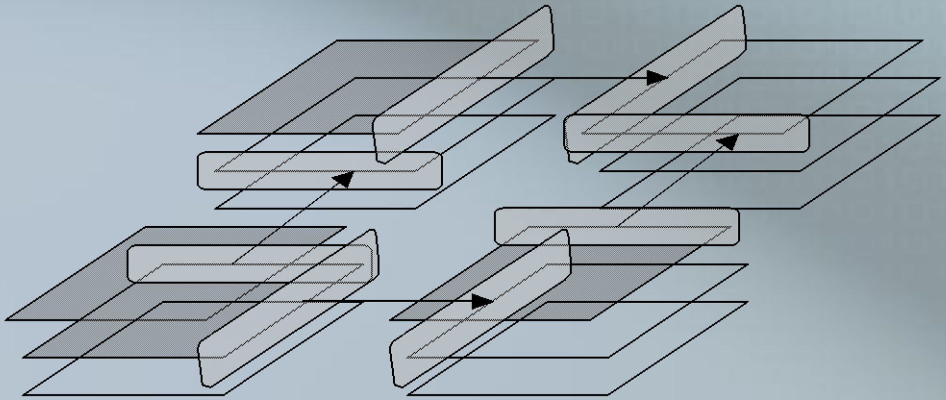
$$S_{(1)} = \frac{n}{1+\left(\sqrt{n}-1\right)\left(\frac{36}{50N_c}+\frac{4n}{50t_0}\left(t_n\left(\frac{1}{N_x}+\frac{1}{N_y}\right)+\frac{t_x\sqrt{n}}{N_xN_y}\right)\right)},$$

$$E_{(1)} = \frac{S_{(1)}}{n} = \frac{1}{1+\left(\sqrt{n}-1\right)\left(\frac{36}{50N_c}+\frac{4n}{50t_0}\left(t_n\left(\frac{1}{N_x}+\frac{1}{N_y}\right)+\frac{t_x\sqrt{n}}{N_xN_y}\right)\right)}.$$

# Parallel implementation of the modified alternating triangular method

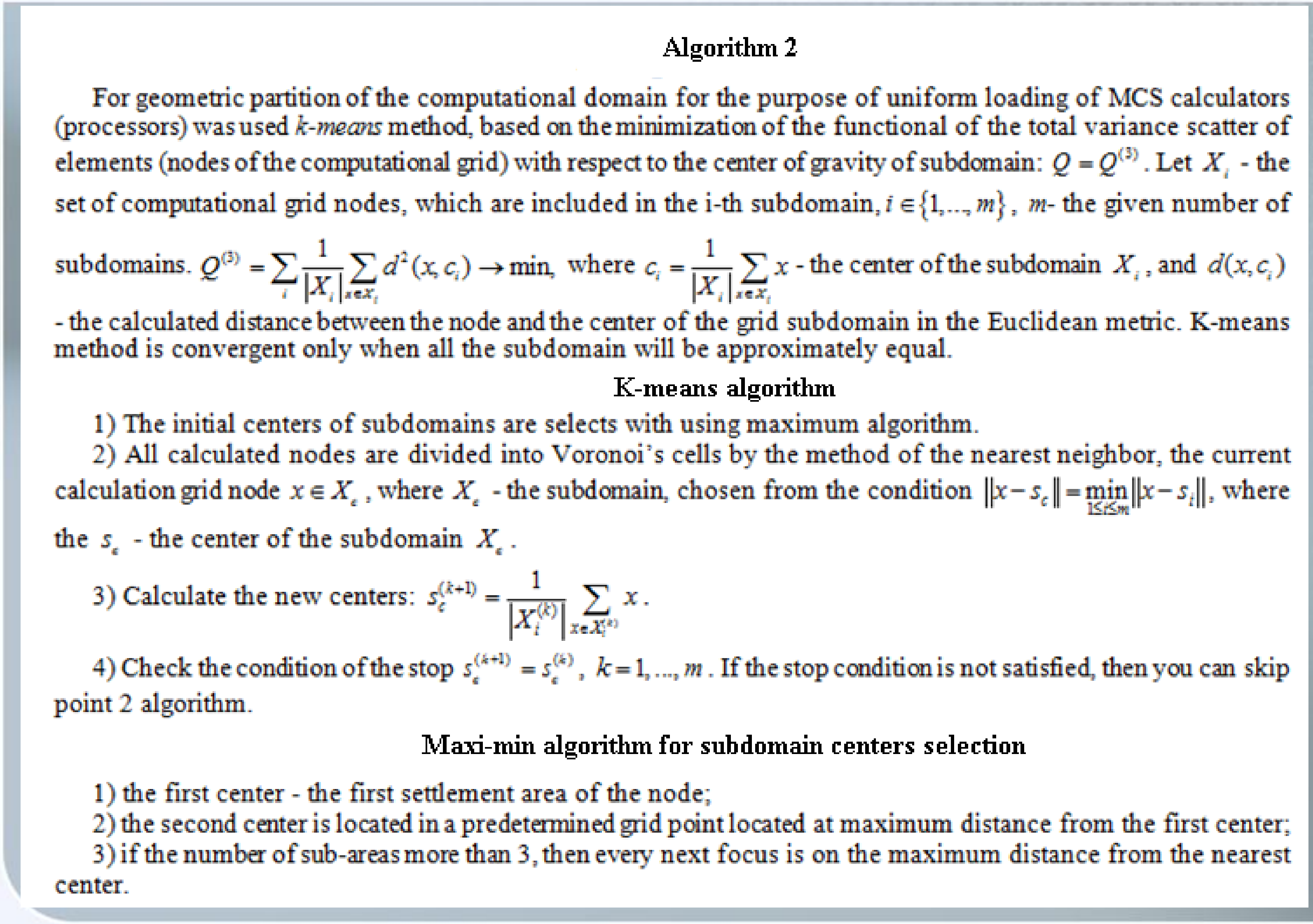


**Domain decomposition**



**Scheme for calculation the vector $y^m$ (the transfer of components after calculation of the two layers by the first processor)**

# Parallel implementation of grid equations using k-means method



## Algorithm 2

For geometric partition of the computational domain for the purpose of uniform loading of MCS calculators (processors) was used *k-means* method, based on the minimization of the functional of the total variance scatter of elements (nodes of the computational grid) with respect to the center of gravity of subdomain: $Q = Q^{(3)}$. Let $X_i$ - the set of computational grid nodes, which are included in the i-th subdomain, $i \in \{1,..., m\}$, $m$- the given number of subdomains. $Q^{(3)} = \sum_i \frac{1}{|X_i|} \sum_{x \in X_i} d^2(x, c_i) \to \min$, where $c_i = \frac{1}{|X_i|} \sum_{x \in X_i} x$ - the center of the subdomain $X_i$, and $d(x, c_i)$ - the calculated distance between the node and the center of the grid subdomain in the Euclidean metric. K-means method is convergent only when all the subdomain will be approximately equal.

### K-means algorithm

1) The initial centers of subdomains are selects with using maximum algorithm.

2) All calculated nodes are divided into Voronoi's cells by the method of the nearest neighbor, the current calculation grid node $x \in X_c$, where $X_c$ - the subdomain, chosen from the condition $\|x - s_c\| = \min_{1 \le i \le m} \|x - s_i\|$, where the $s_c$ - the center of the subdomain $X_c$.

3) Calculate the new centers: $s_c^{(k+1)} = \frac{1}{|X_i^{(k)}|} \sum_{x \in X_i^{(k)}} x$.

4) Check the condition of the stop $s_c^{(k+1)} = s_c^{(k)}$, $k = 1, ..., m$. If the stop condition is not satisfied, then you can skip point 2 algorithm.

### Maxi-min algorithm for subdomain centers selection

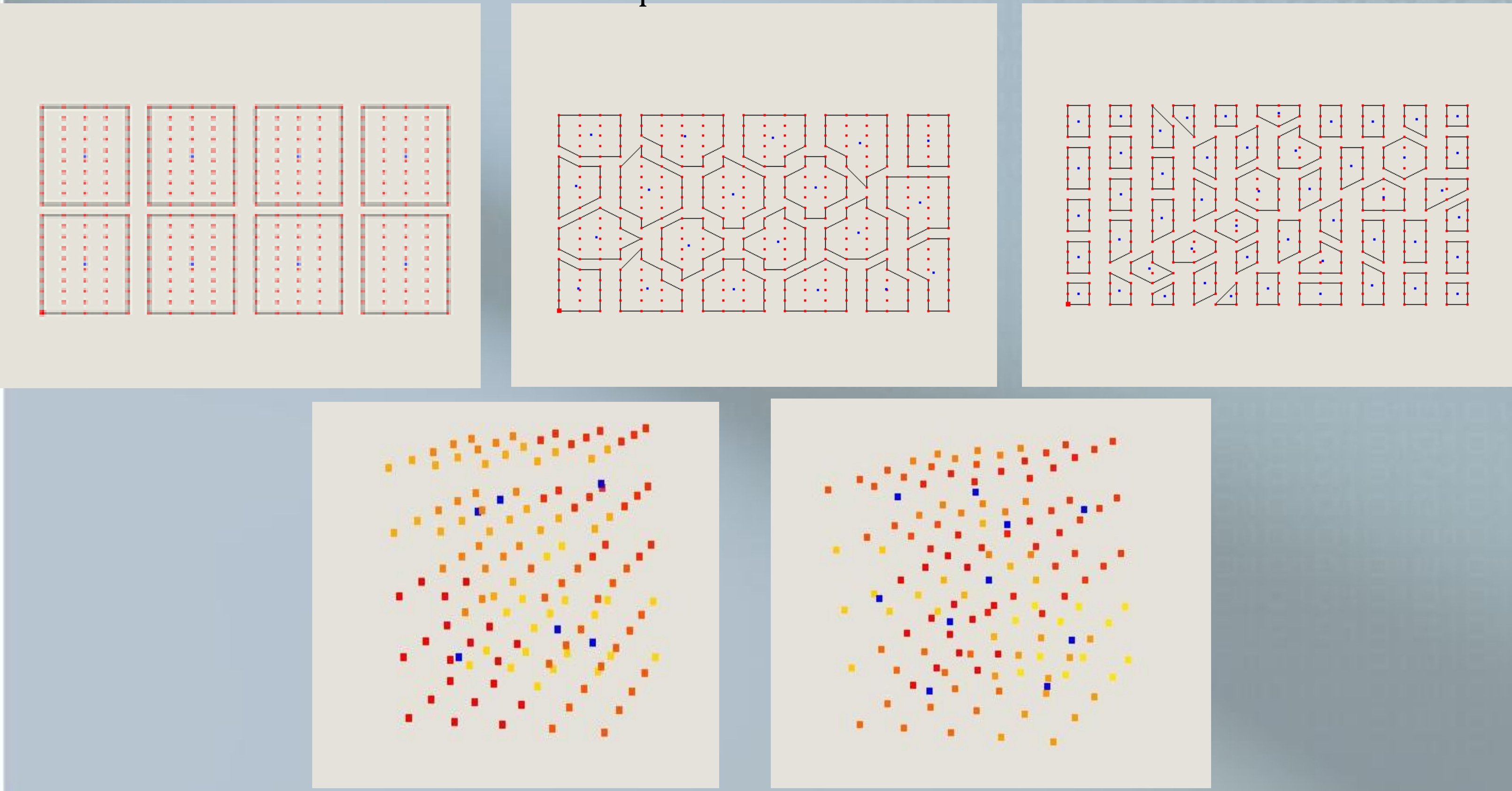
1) the first center - the first settlement area of the node;

2) the second center is located in a predetermined grid point located at maximum distance from the first center;

3) if the number of sub-areas more than 3, then every next focus is on the maximum distance from the nearest center.

# Results of k-means algorithm

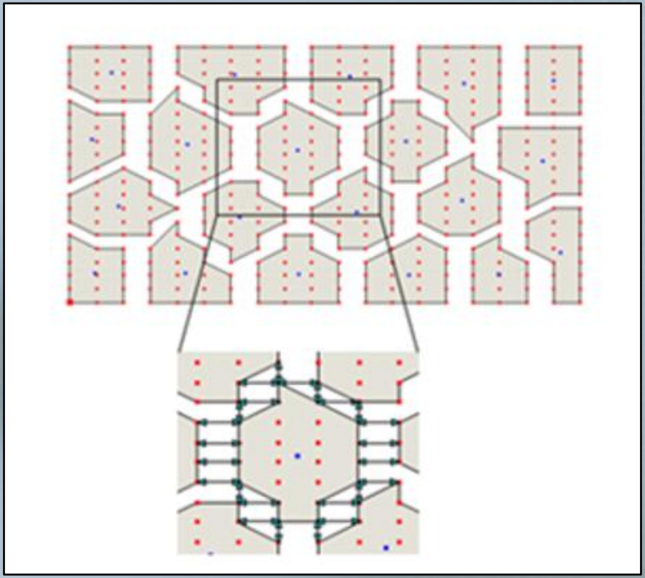
It’s necessary to define all points on the boundary of each subdomain for data exchange in computational process. For this, the Jarvis algorithm (the construction of a convex hull) was used. A list of neighboring subdomains for each subdomain was formed, and an algorithm for data transfer between subdomains 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 of the algorithm 2**

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

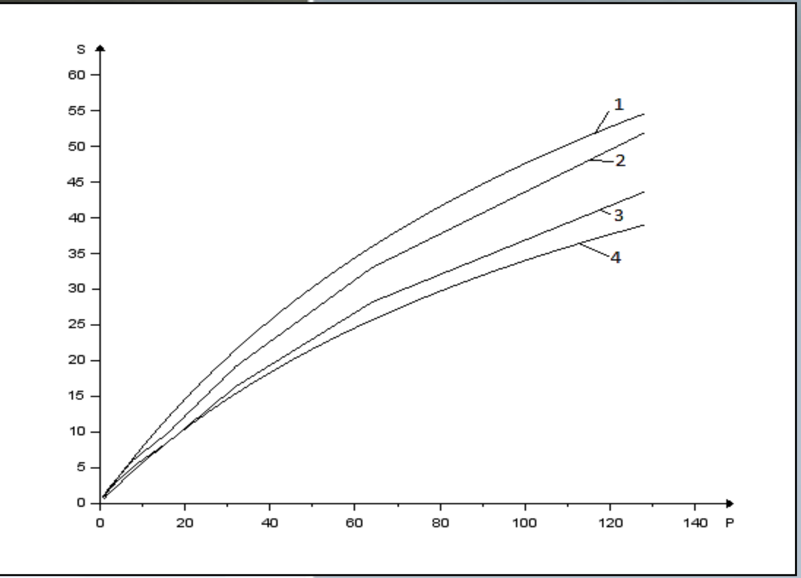
$$E_{(2)} = \frac{S_{(2)}}{n} = \frac{\chi}{1 + \left(\sqrt{n} - 1\right)\left(\dfrac{36}{50N_z} + \dfrac{4n}{50t_0}\left(t_n\left(\dfrac{1}{N_x} + \dfrac{1}{N_y}\right) + \dfrac{t_x\sqrt{n}}{N_x N_y}\right)\right)},$$

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

# Results of experimental researches

**The estimation is used for comparison the performance values of the algorithm 1 and algorithm 2, obtained practically:**

$$\delta = \sqrt{\sum_{k=1}^{n}\left(E_{(2)k} - E_{(1)k}\right)^2} \bigg/ \sqrt{\sum_{k=1}^{n} E_{(2)k}^2} = 0.154$$



**Graphs of accelerations for the developed parallel algorithms:**
**1 – the theoretical estimation of the acceleration of the algorithm 1;**
**2 – the acceleration of the algorithm 2;**
**3 – the acceleration of the algorithm 1;**
**4 – theoretical estimations of the acceleration of the algorithm 2**

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

| $n$ | $t_{(1)}, c$ | $S^t_{(1)}$ | $S_{(1)}$ | $t_{(2)}, c$ | $E^t_{(2)}$ | $E_{(2)}$ |
|---|---|---|---|---|---|---|
| **1** | 7.490639 | 1.0 | 1.0 | 6.072899 | 1.0 | 1.0 |
| **2** | 4.151767 | 1.653577 | 1.804205 | 3.121229 | 1.181126 | 1.945675 |
| **4** | 2.549591 | 3.256077 | 2.937976 | 1.810628 | 2.325769 | 3.354028 |
| **8** | 1.450203 | 6.317738 | 5.165234 | 0.996729 | 4.512670 | 6.092825 |
| **16** | 0.88242 | 11.928279 | 8.488745 | 0.619345 | 8.520199 | 9.805356 |
| **32** | 0.458085 | 21.482173 | 16.352072 | 0.317173 | 15.344409 | 19.146924 |
| **64** | 0.265781 | 35.954877 | 28.18350 | 0.183929 | 25.682055 | 33.017611 |
| **128** | 0.171535 | 54.617841 | 43.668283 | 0.116936 | 39.012744 | 51.933099 |

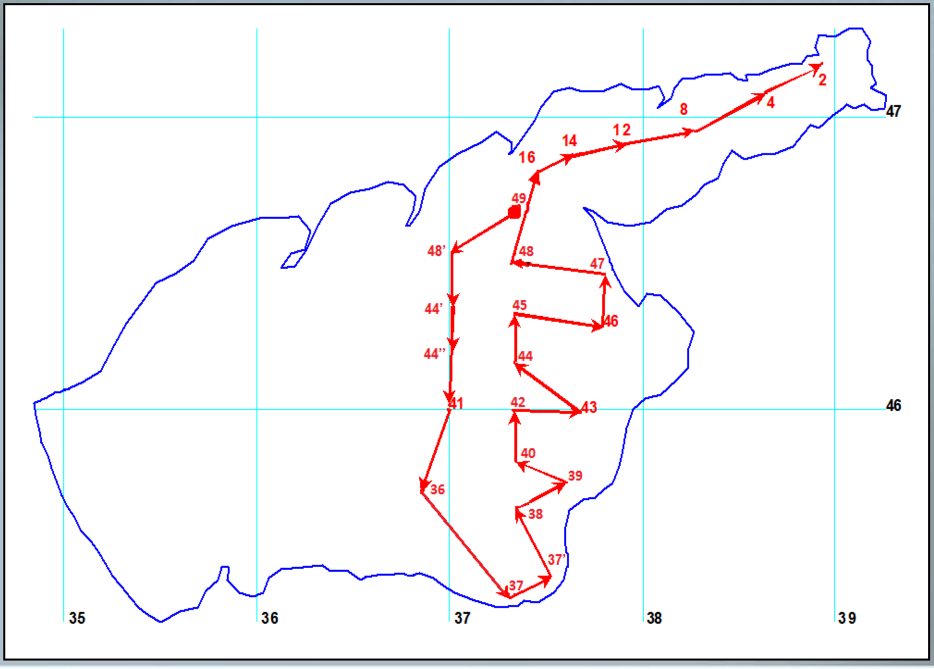
where $n$ is the number of processor; $t_{(k)}, S_{(k)}, E_{(k)}$ are the calculation time, acceleration and efficiency values of *k*-th algorithm, *k=1,2*;
$S^t_{(k)}, E^t_{(k)}$ are the theoretical comparison of acceleration and efficiency values of *k*-th algorithm.

# *Expedition researches, SRV «Deneb», 2017*

**In July 2017, employees of the Don State Technical University, the Southern Federal University, the southern Scientific Center of the Russian Academy of Sciences were carried out a voyage on the research vessel «Deneb» in the Azov sea.**

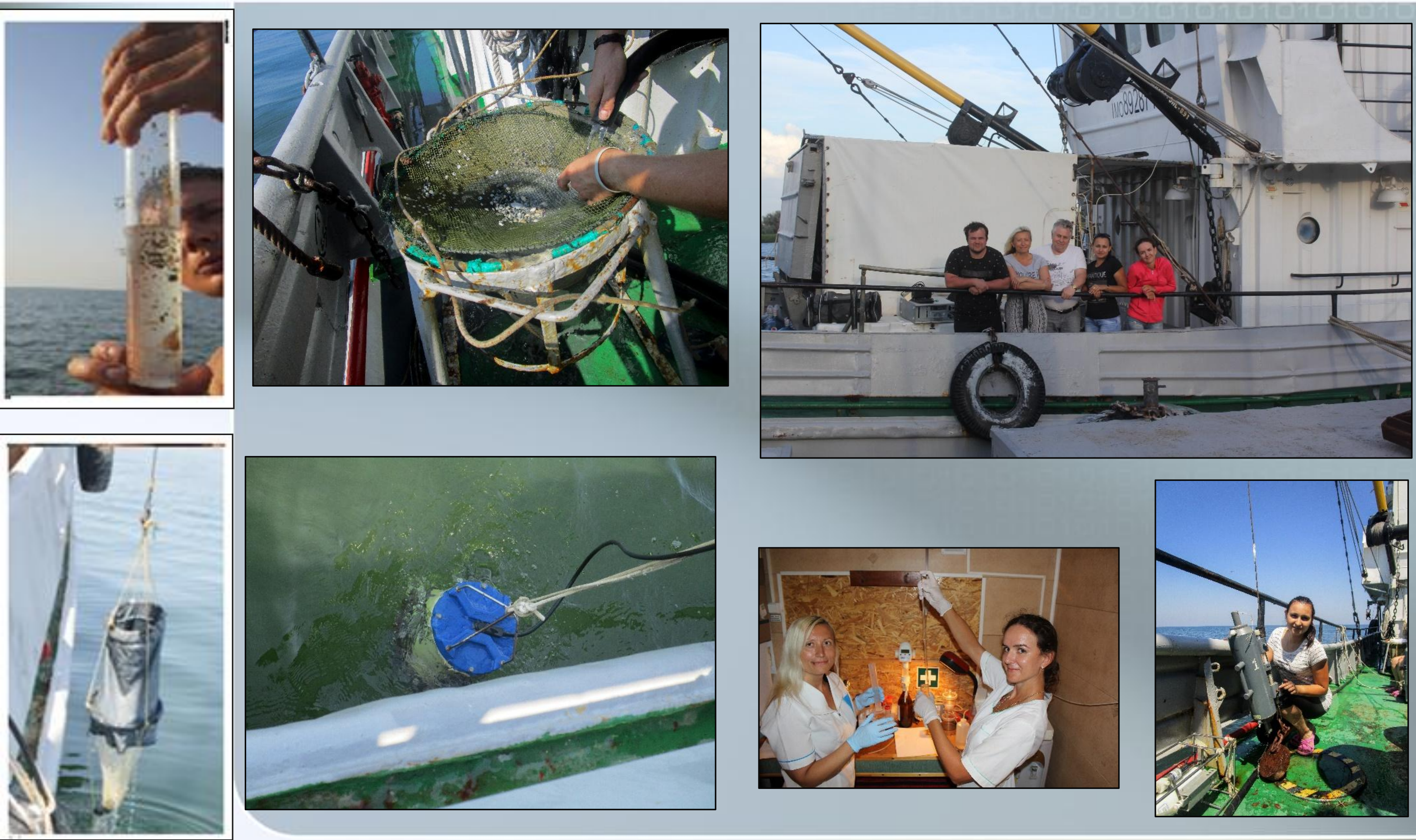
**The main problem of expedition research** is the complex researching the current situation and dimension-time changes of hydrobiological, hydrological and hydrochemical regimes of the Azov Sea and the Taganrog Bay. During the expedition, more than 20 integrated oceanographic stations were investigated, water probe, plankton and benthic samples probe were taken, ship observations of birds and marine mammals were carried out.

**Scientific-research vessel «Deneb»**



**Expedition route**

# Expedition researches, SRV «Deneb», 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).
- San++ automatic flow analyzer with the SA1100 sampler, that holds 2 x 50 positions for samples.
- 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 trol - 28 m in horizontal, 8 m in vertical).
- SBE19 plus hydro-probe.
- SBE43 dissolved oxygen sensor.
- PC (personal computer) with software for connecting the hydro-probes.
- 3 l and 5 l bathometers and equipment for measuring the oxygen concentration by Winkler method.
- WHS 600 (ADCP) profilograph.

# Scientific-research equipment for model verification

**Sea Bird Electronics 19 Plus V2**

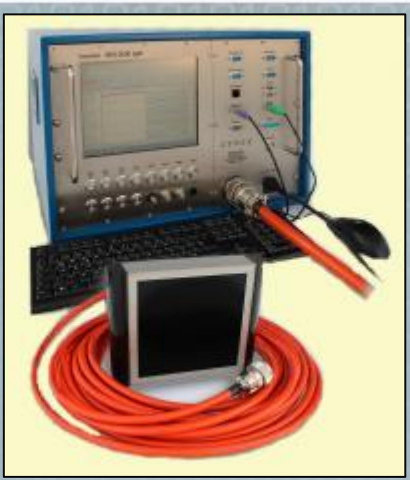
SBE 43 dissolved oxygen sensor

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**

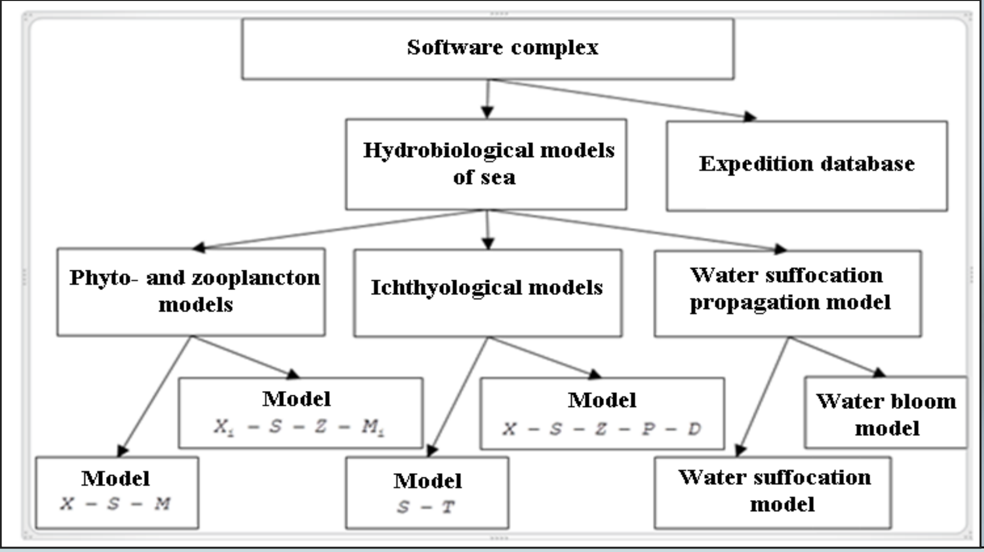
Immersion depth up to 70 m

Frequency 600 kHz

Accuracy of measurements 0.25%

# Software complex

**Software complex, oriented on the MCS, for calculation the fields of water flow velocities, nutrient concentrations, oil pollution, bacteria and phytoplankton in the areas of complex shapes**



Software complex

Hydrobiological models of sea

Expedition database

Phyto- and zooplancton models

Ichthyological models

Water suffocation propagation model

Model $X_1 - S - Z - M_1$

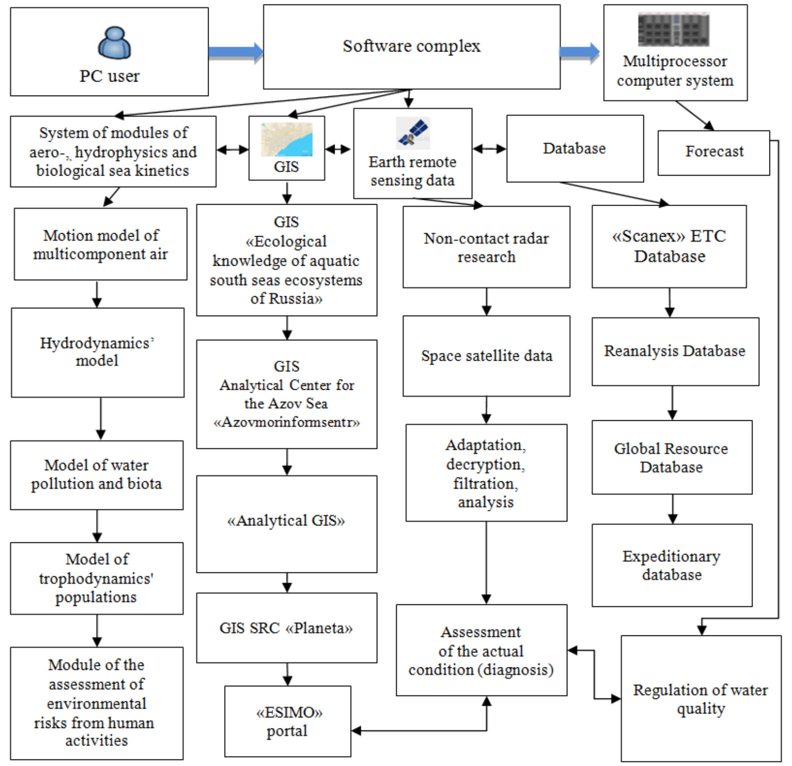
Model $X - S - Z - P - D$

Water bloom model

Model $X - S - M$

Model $S - T$

Water suffocation model



PC user

Software complex

Multiprocessor computer system

System of modules of aero-, hydrophysics and biological sea kinetics

GIS

Earth remote sensing data

Database

Forecast

Motion model of multicomponent air

Hydrodynamics' model

Model of water pollution and biota

Model of trophodynamics' populations

Module of the assessment of environmental risks from human activities

GIS «Ecological knowledge of aquatic south seas ecosystems of Russia»

GIS Analytical Center for the Azov Sea «Azovmorinformsentr»

«Analytical GIS»

GIS SRC «Planeta»

«ESIMO» portal

Non-contact radar research

Space satellite data

Adaptation, decryption, filtration, analysis

Assessment of the actual condition (diagnosis)

«Scanex» ETC Database

Reanalysis Database

Global Resource Database

Expeditionary database

Regulation of water quality

**Advantages of developed complex of programs :**

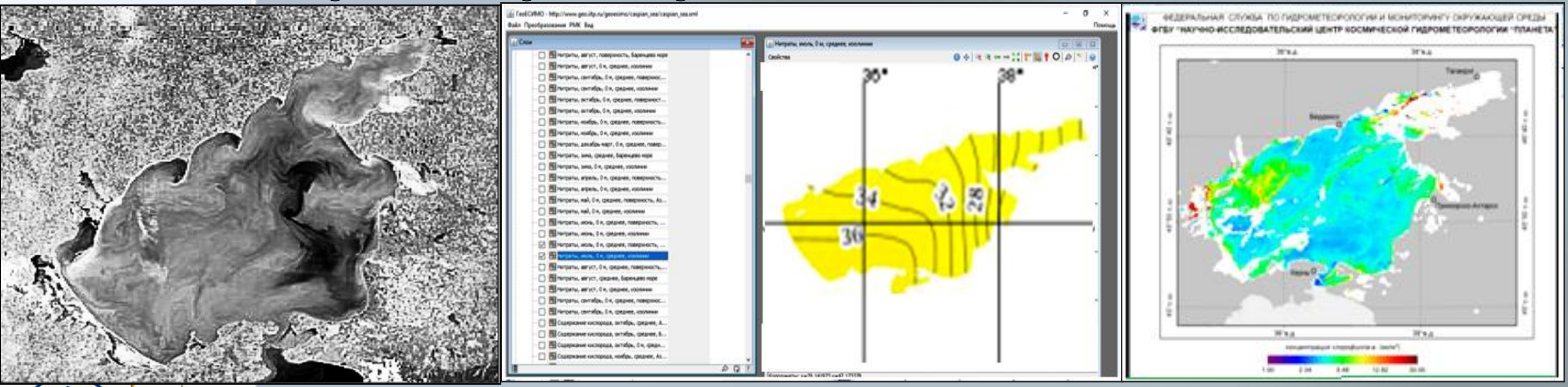
- improvement and implementation the integrated fisheries monitoring system in the water (monitoring, evaluation and prediction of the mode of ecosystems, fodder stocks and fishing sites); development, negotiation of proposals and measures for ensuring an optimal regime, biodiversity, fisheries resources, ecosystems of shallow ponds;
- improvement of environmental research methodology, development of new, testing and implementation of promising methods for studying the state of aquatic ecosystems and individual components;
- development and improvement of methods of diagnostics of toxic effects of nutrients on hydrobionts, including early and differential diagnosis of toxicosis, as well as the search for antidote protection of aquatic ecosystems;
- organization and carrying out research to identify trends and patterns of changes in the state of aquatic ecosystems under the influence of anthropogenic factors, development of proposals and measures to reduce and prevent such impacts;
- assessment of damage to fisheries caused by different types of economic activities, development of proposals for the prevention, reduction and adequate compensation of damage.

# Earth distance scan data

**To control the quality of modeling of hydrodynamics and biological kinetics processes, we used the following:**

- results of expeditionary research;
- NOAA database (National Oceanic and Atmospheric Administration);
- Earth satellite monitoring data, obtained by the SRC «Planeta»;
- «Analytical GIS» portal systems, developed by the Institute for Information Transmission Problems of the Russian Academy of Sciences (IITP RAS, Moscow) for complex geoinformational analysis of space-time processes and phenomena;
- data of the Unified state system of information on the situation in the world ocean «ESIMO» portal;
- data of the Azov scientific-research institute of fishers («AzNIIRKH»).

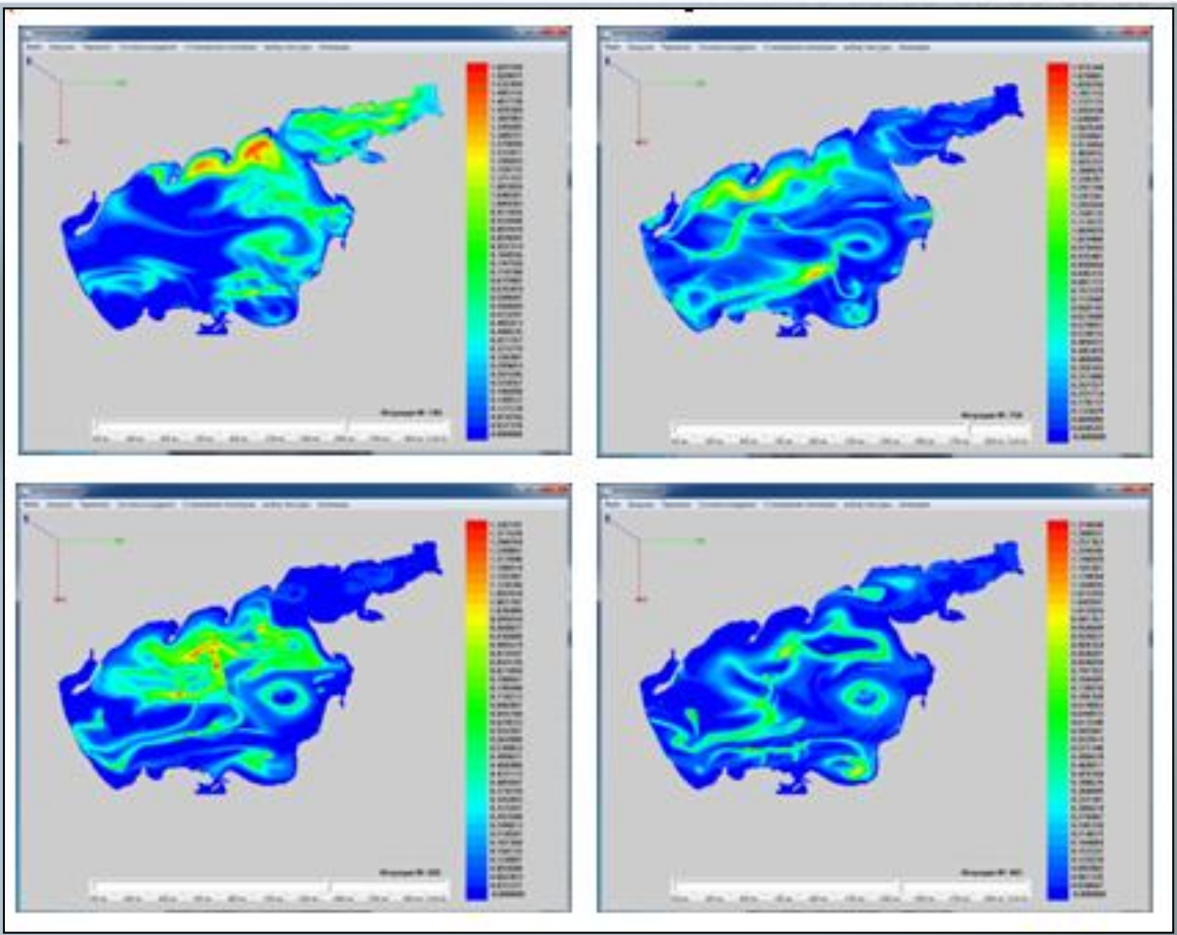
Due to the analysis of satellite data, we can identify water areas, which are the most vulnerable to biological and technogenic challenges.



**A** **B** **C**

**A: satellite image of the Azov Sea in the ultraviolet spectrum, which is taken from the NASA site (http://veimages.gsfc.nasa.gov/1326/S1998282101838.jpg);**
**B: «ESIMO» portal data; C: satellite image of the Azov Sea by the SRC «Planeta»**

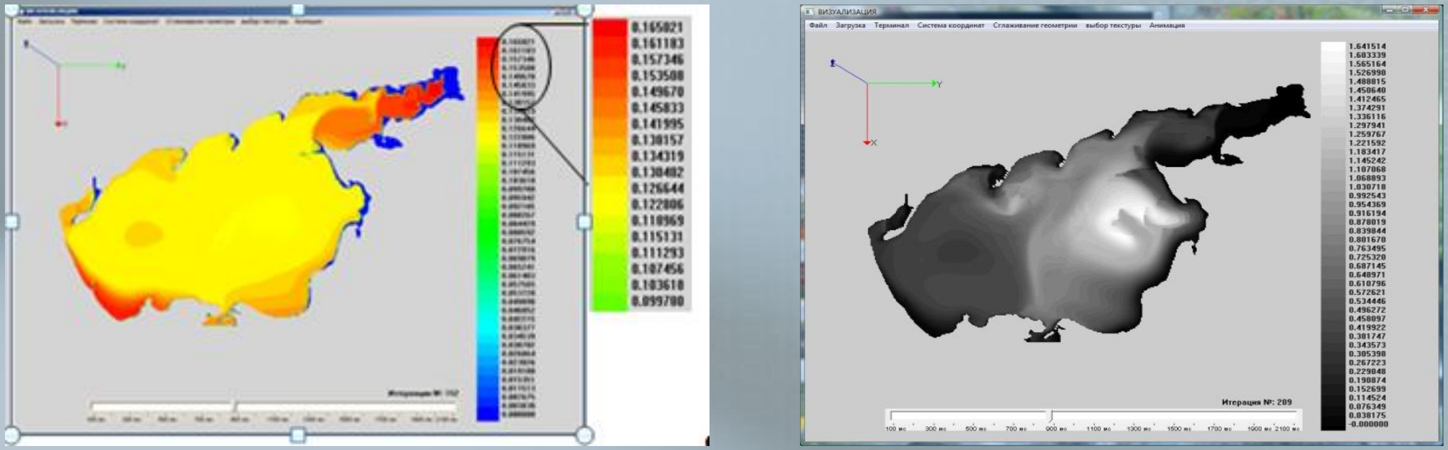
# Results of numerical experiments



Dynamics in phytoplankton concentration in the Azov Sea,

$$\mu_2 = 5 \times 10^{-11},\ \nu_2 = 10^{-11}$$

# Results of numerical experiments



a) b)

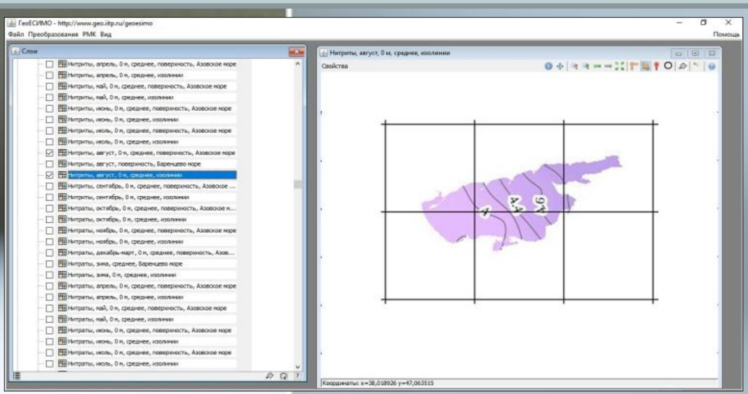
a) the change in the concentration of polluting nutrients;
(b) changes in the concentration of green microalgae *Chlorella vulgaris Beijer*

The time period is 28 days from the date of introduction of algae into the pond. Value of coefficient:

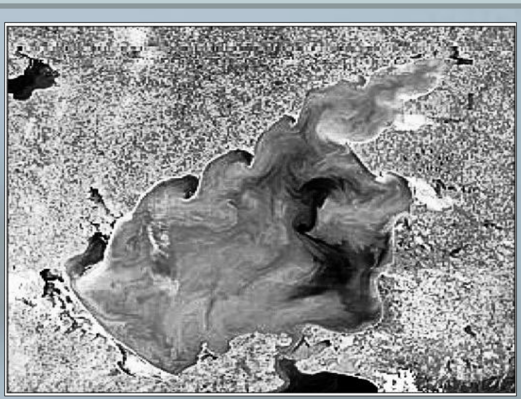
$$\mu = 5\cdot 10^{-10};\ D = 0,001;\ S_p = 1;\ \ f = 3;\ \ \tau_\varphi = 0,1;\ \ \varphi \in \{S, B\};\ \ \kappa = 0,3;\ \ \varepsilon = 0,8;\ \alpha_0 = 0,1;\ \gamma = 0,0416.$$

# The Earth remote sensing data

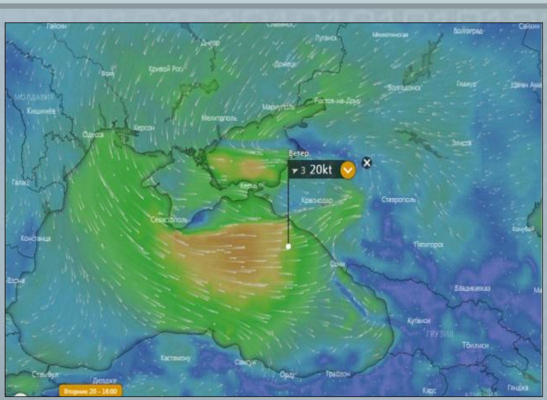
For calibration and verification of the developed hydrophysical models, included in the SC, we used the data of the Unified state system of information on the situation in the World ocean («ESIMO»), the «Analytical GIS» portal. Data of the Scientific Research Center of space hydrometeorology «Planeta», the Azov Fisheries Research Institute («AzNIIRH»), the FSI «Azovmorinformtsentr» were used as input data for modeling the hydrophysical processes in addition to the expedition data, literature sources.



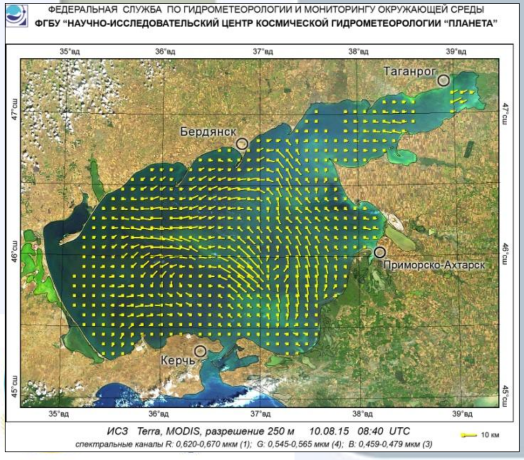
**Navigation panel of the «ESIMO» portal, data on polluting nutrients (nitrites) in the Azov Sea**



**The Earth remote sensing data: satellite image of the Azov Sea in the ultraviolet spectrum**



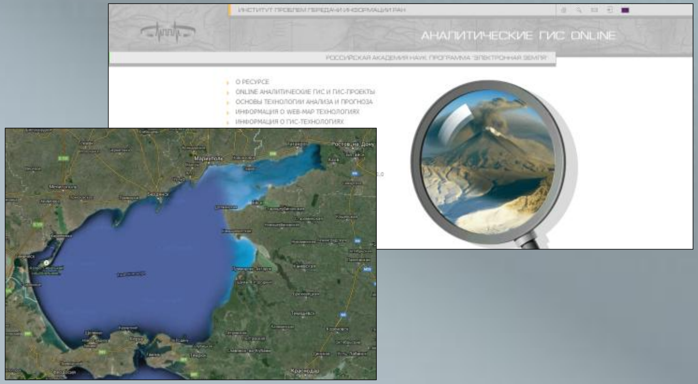
**The Earth remote sensing data: wind speed and direction in the Azov-Black sea basin (взято http://hobitus.com/noaa)**



**(A)**

**(B)**

**Maps of large-scale movement of water masses in the Azov ыea, combined with color-synthesized image (a) (SRC «Planeta») , and distribution diagrams of velocities and directions transfer (b) (SRC «Planeta»)**



**The map of the Azov Sea («Analytical GIS»)**

# Adequacy of the developed probabilistic models

**The algorithm for verification the developed probabilistic observation models**

1. Calculation the organic matter $P$ growth rate.

2. Checking the convergence of natural (measured) and calculated (simulated) values according to the following criteria:

2.1 – The criterion of randomness

$$\delta = D_\Delta / D,$$

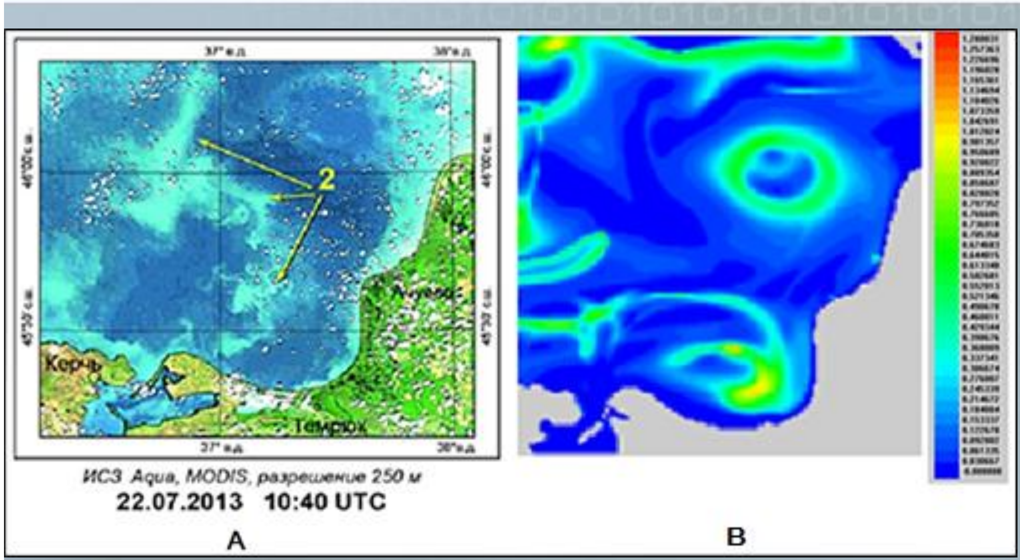
where $D, D_\Delta$ are dispersions of a number of actual values of the parameter and its random component caused by the influence of random elements.

If $\delta < 0.7$, the value is taken to be satisfactory.

2.2 – The coincidence of the calculated value with the actual value is considered satisfactory, if the difference does not exceed the absolute value $0.7\sigma$, where $\sigma$ is a standard deviation of the original actual series.

3. Checking the sensitivity of the model parameters.

4. The input data correction, if this is necessary. If the production rate $P$ was calculated with sufficient accuracy, so the calculation the total destruction velocity by the plankton are necessary for improvements.



**Comparison of the software complex results with the satellite data**

A: satellite image of the Azov Sea by the SRC «Planeta»;
B: results of the software complex
(the dynamics of phytoplankton concentration
in the Azov Sea)

# Conclusion

- The stochastic model of seasonal changes in biomass for each main type of phytoplankton (*Chlorella vulgaris, Aphanizomenon flos-aquae и Sceletonema costatum*) was developed with taking into account the changes in the rate of production and destruction of organic matter, taking into account the change in the concentration of plant pigment (chlorophyll) from water temperature, salinity, dissolved oxygen and carbon dioxide, nitrites, nitrates, phosphates, silica, iron, and labile dissolved organic matter, active reaction of environment, which allowed to investigate the influence of various factors on the growth rate of phytoplankton. The combination of principles of the combined action of the Mitcherlich factors and the Libich limiting factor law were used. The dependences of Benndorf, Mono-Goldoni, Romanovsky Yu. M., Berger, Country, Tutunova Yu. were researched. The stochastic model of the organic matter destruction process taking into account costs of exchange of phyto -, zooplankton and bacteria, associated with detritus. According to the production-destructive P/D ratio, we can the ability of the water ecosystem to self-purification: if the ratio is close to 1, the system produces more organic matter than it can decompose.
- The developed empirical-statistical models of biological kinetics for phytoplankton combine almost all biometric methods of primary processing of experimental information and can be used to develop schemes for sustainable development of the coastal system.
- Numerical implementation of the developed model was performed on the multiprocessor computer system (MCS) with distributed memory. Theoretical calculations of acceleration and efficiency of parallel algorithms were performed. The experimental software is designed for mathematical modeling of possible scenarios for the development of ecosystems of shallow water bodies on the example of the Azov-black Sea basin. In parallel implementation, the decomposition methods of grid domains were used for computationally time-consuming diffusion-convection problems, taking into account the architecture and parameters of MCS. An algorithm based on the k-means method was developed for optimal data distribution between processors, due to which the efficiency was increased for solution the problem on 10-20%, compared to the algorithm with the standard domain partition.
- The literature and expedition data, as well as data of remote sensing of the Earth were used for calibration and verification of the developed mathematical models of water ecology.
- The developed software complex on the MVS is intended for solving numerically model problems of water ecology, as well as for conducting numerical experiments in various hydrometeorological situations. Due to the application on the MCS, the calculation time was decreased and the accuracy was preserved that required for modeling of hydrobiological processes occurring in the shallow waters. It is important in aquatic ecology problems.

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# Certificates of program registration

РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

№ 2012614677

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

о государственной регистрации программы для ЭВМ

№ 2016661550

**Программа для решении сеточных уравнений многосеточным методом**

Правообладатель: *федеральное государственное автономное образовательное учреждение высшего образования «Южный федеральный университет» (Южный федеральный университет) (RU)*

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Заявка № 2016618901

Дата поступления 17 августа 2016 г.

Дата государственной регистрации

в Реестре программ для ЭВМ *13 октября 2016 г.*

*Руководитель Федеральной службы по интеллектуальной собственности*

*Г.П. Ивлиев*

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

о государственной регистрации программы для ЭВМ

№ 2015616787

**Программа для решения сеточных уравнений итерационными методами на многопроцессорной вычислительной системе**

Правообладатель: *федеральное государственное автономное образовательное учреждение высшего образования «Южный федеральный университет» (Южный федеральный университет) (RU)*

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Заявка № 2015613749

Дата поступления 05 мая 2015 г.

Дата государственной регистрации

в Реестре программ для ЭВМ *23 июня 2015 г.*

*Врио руководителя Федеральной службы по интеллектуальной собственности*

*Л.Л. Кирий*

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

о государственной регистрации программы для ЭВМ

№ 2015617008

**Программа решения задачи диффузии-конвекции-реакции на основе схем повышенного порядка точности**

Правообладатель: *федеральное государственное автономное образовательное учреждение высшего образования «Южный федеральный университет» (Южный федеральный университет) (RU)*

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Заявка № 2015613797

Дата поступления 05 мая 2015 г.

Дата государственной регистрации

в Реестре программ для ЭВМ *26 июня 2015 г.*

*Врио руководителя Федеральной службы по интеллектуальной собственности*

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

о государственной регистрации программы для ЭВМ

№ 2016661533

**Программа для моделирования процессов биологической реабилитации мелководного водоема**

Правообладатель: *федеральное государственное автономное образовательное учреждение высшего образования «Южный федеральный университет» (Южный федеральный университет) (RU)*

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Заявка № 2016618881

Дата поступления 17 августа 2016 г.

Дата государственной регистрации

в Реестре программ для ЭВМ *12 октября 2016 г.*

*Руководитель Федеральной службы по интеллектуальной собственности*

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

№ 2012614681

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

№ 2012614678

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

**СВИДЕТЕЛЬСТВО**

о государственной регистрации программы для ЭВМ

№ 2018613121

**Решение задачи переноса веществ при больших числах Пекле**

Правообладатель: *федеральное государственное бюджетное образовательное учреждение высшего образования «Донской государственный технический университет» (ДГТУ) (RU)*

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Заявка № 2018610088

Дата поступления 09 января 2018 г.

Дата государственной регистрации

в Реестре программ для ЭВМ *02 марта 2018 г.*

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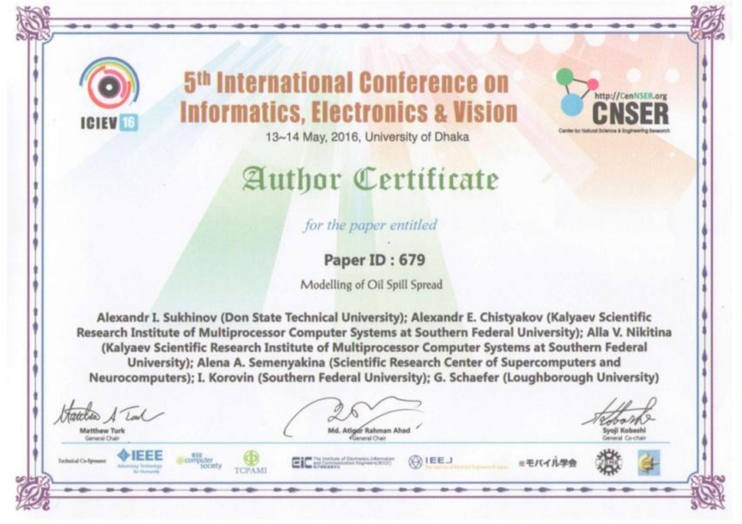

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Modelling of Oil Spill Spread

**Alexandr I. Sukhinov (Don State Technical University); Alexandr E. Chistyakov (Kalyaev Scientific Research Institute of Multiprocessor Computer Systems at Southern Federal University); Alla V. Nikitina (Kalyaev Scientific Research Institute of Multiprocessor Computer Systems at Southern Federal University); Alena A. Semenyakina (Scientific Research Center of Supercomputers and Neurocomputers); I. Korovin (Southern Federal University); G. Schaefer (Loughborough University)**

Matthew Turk
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№ 2012614680

*Thank you for attention!*