Parallel implementation of substance transport problems for restoration the salinity field based on schemes of high order of accuracy

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Abstract

Paper covers the research of discrete analogs of convective and diffusion transfer operators of the fourth order of accuracy in the case of partial cell occupancy. According to the comparison of calculation results of substance transport problem based on schemes of the second and fourth orders of accuracy, the accuracy was increased in 66.7 times for diffusion problem, and in 48.7 times for diffusion-convection problem. A library of two-layer iterative methods was designed for solving two-dimensional diffusion-convection problem based on schemes of high order of accuracy. It has intended to solve the nine-diagonal grid equations on a multiprocessor computer system. A mathematical algorithm was designed and numerically implemented for restoration the water salinity field based on hydrographic information (water salinity at separate points or level isolines). The map of salinity of the Azov Sea was obtained using the proposed solution method.

1 Introduction

One of the main problems of computational mathematics is the problem of solving systems of linear algebraic equations. Direct and iterative methods are used to obtain an approximate solution of systems of equations. One of the most successful method among the two-layer iterative methods is the alternately triangular method (ATM) proposed by A.A. Samarsky [Sam89]. Later, the academician A.N. Konovalov developed an adaptive version of ATM [Kon02]. The technique for increasing the convergence rate of ATM with a priori information by refining the spectral estimates of the preconditioned operator are presented in [Suk84].

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Often in applied problems, for example, in mathematical modeling of hydrodynamics [Suk11, Ka17, Rue05], heat and mass transfer [Suk18, Suk18'], geofiltration, population dynamics [Suk05], seismic exploration [Mur13] and other processes, it is necessary to solve the equations of convection-diffusion type. In the case of implicit schemes and schemes with weights, such problems lead to linear algebraic equations with a non-self-adjoint operator. One of approaches to solving such problems is the Gaussian symmetry method. The disadvantage of this method is the squared increase of the condition number of operator, which leads to a decrease the convergence rate of iterative methods for solving grid equations. This fact contributed to the creation by the author's team the version of the modified iterative alternating triangular method of minimum corrections for solving grid equations with non-self-adjoint operator [Suk12'].

The use of rapidly converging iterative method as well as the use of parallal computations [Che06, Iak05] and the choice of difference schemes are effective ways to reduce the running time of the algorithm.

To increase the time step, we can use schemes with the optimal value of weight parameter [Suk14]. In addition, we can use the splitting computational grids, but it leads to increasing the calculation time. To increase the accuracy of calculations, it is possible to use schemes of higher order of accuracy [Pet13, Lad09] and schemes that take into account the filling of cells [Suk15]. In the second case, the accuracy is increased due to a better approximation of the boundary of computational domain.

Within the framework of this research, a library of iterative methods was designed to solve grid equations with self-adjoint and non-self-adjoint operators, arising in the solution of applied problems, schemes of high order of accuracy, taking into account the fullness of cells on a multiprocessor computing system.

2 Problem Statement

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

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

with boundary conditions:

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

where u,v are components of the velocity vector; μ is the turbulent exchange coefficient; f is a function, describing the intensity and distribution of sources.

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

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

where τ is a time step; h_x, $h_y$are spatial steps; N_t is an upper boundary on time; N_x, N_y are space boundaries.

Discrete analogues of convective uc'_x and diffusive $\left(\mu c'_x\right)'_x$transfer operators of the second order of approximation error in the case of partially filled cells can be written as:

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

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

$$- \left|\left(q_1\right)_{i,\,j} - \left(q_2\right)_{i,\,j}\right| \mu_{i,\,j} \frac{\alpha_x c_{i,\,j} + \beta_x}{h_x},$$

where q_i are coefficients, describing the fullness of control domain [Suk15].

3 Schemes of High Order of Accuracy for Convective and Diffusive Transfer Operators

Expressions (1)-(2) can be considered in the case if $\left(q_1\right)_{i,\,j} = \left(q_2\right)_{i,\,j} = 1$. To increase the approximation order of equations (1)-(2), it's necessary to research the following difference schemes:

- the discrete analogue of the convective transport operator in absence of influence of domain boundary:

$$uc'_x \simeq u_{i+1/2,\,j} \frac{c_{i+1,\,j} - c_{i,\,j}}{2h_x} + u_{i-1/2,\,j} \frac{c_{i,\,j} - c_{i-1,\,j}}{2h_x}, \tag{3}$$

- the discrete analogue of the diffusive transport operator in absence of influence of domain boundary:

$$\left(\mu c'_x\right)'_x \simeq \mu_{i+1/2,\,j}\frac{c_{i+1,\,j}-c_{i,\,j}}{h_x^2}-\mu_{i-1/2,j}\frac{c_{i,\,j}-c_{i-1,\,j}}{h_x^2}, \tag{4}$$

The approximation error of expression (3) will take the following form:

$$u_{i+1/2,\,j}\frac{c_{i+1,\,j}-c_{i,\,j}}{2h_x}+u_{i-1/2,\,j}\frac{c_{i,\,j}-c_{i-1,\,j}}{2h_x}=$$

$$=u_{i,\,j}\left(c_{i,\,j}\right)'+\frac{\left(c_{i,\,j}\right)'\left(u_{i,\,j}\right)''}{4}h_x^2+\frac{u_{i,\,j}\left(c_{i,\,j}\right)'''}{6}h_x^2+\frac{\left(u_{i,\,j}\right)'\left(c_{i,\,j}\right)''}{4}h_x^2+O\left(h_x^4\right).$$

Therefore, for approximation the convective transport operator uc' by difference scheme of the fourth order of accuracy we have to approximate the operator $uc'-c'u''h^2/4-uc'''h^2/6-u'c''h^2/4$ by the scheme of the second order of accuracy.

The approximation of the convective transport operator uc' by difference scheme of the fourth order of accuracy has the form:

$$\begin{aligned}\left(q_0\right)_i L\left(c\right) = &-\left(q_1\right)_i\frac{u_{i+1/2}}{12h}\frac{\left(q_1\right)_{i+1}}{\left(q_0\right)_{i+1}}c_{i+2}-\left(-\left(q_1\right)_i\frac{u_{i+1/2}}{12h}\left(2+\frac{\left(q_1\right)_i}{\left(q_0\right)_i}\right)+\right.\\
&\left.+\left(q_2\right)_i\frac{u_{i-1/2}}{12h}\frac{\left(q_1\right)_i}{\left(q_0\right)_i}+\left(q_1\right)_i\left(-\frac{u_{i+1/2}}{2h}+k_i^{(1)}+k_i^{(2)}\right)\right)c_{i+1}+\left(-\left(q_1\right)_i\frac{u_{i+1/2}}{12h}\left(2+\frac{\left(q_2\right)_{i+1}}{\left(q_0\right)_{i+1}}\right)+\right.\\
&\left.+\left(q_2\right)_i\frac{u_{i-1/2}}{12h}\left(2+\frac{\left(q_1\right)_{i-1}}{\left(q_0\right)_{i-1}}\right)+\left(q_2\right)_i\frac{u_{i-1/2}}{2h}-\left(q_1\right)_i\frac{u_{i+1/2}}{2h}-\left(\left(q_2\right)_i-\left(q_1\right)_i\right)k_i^{(1)}+\left(\left(q_2\right)_i+\left(q_1\right)_i\right)k_i^{(2)}\right)c_i+\\
&-\left(-\left(q_1\right)_i\frac{u_{i+1/2}}{12h}\frac{\left(q_2\right)_i}{\left(q_0\right)_i}+\left(q_2\right)_i\frac{u_{i-1/2}}{12h}\left(2+\frac{\left(q_2\right)_i}{\left(q_0\right)_i}\right)+\left(q_2\right)_i\left(\frac{u_{i-1/2}}{2h}+k_i^{(2)}-k_i^{(1)}\right)\right)c_{i-1}-\\
&-\left(-\left(q_2\right)_i\frac{u_{i-1/2}}{12h}\frac{\left(q_2\right)_{i-1}}{\left(q_0\right)_{i-1}}\right)c_{i-2},\end{aligned} \tag{5}$$

where $k_i^{(1)}=\left(\frac{\left(q_1\right)_i}{\left(q_0\right)_i}\left(u_{i+1}-u_{i,}\right)-\frac{\left(q_2\right)_i}{\left(q_0\right)_i}\left(u_i-u_{i-1}\right)\right)/\left(8h\right)$, $k_i^{(2)}=\frac{\left(q_1\right)_i}{\left(q_0\right)_i}\frac{u_{i+1}-u_i}{8h}+\frac{\left(q_2\right)_i}{\left(q_0\right)_i}\frac{u_i-u_{i-1}}{8h}$.

The approximation error of expression (4) will take the following form:

$$\mu_{i+1/2,\,j}\frac{c_{i+1,\,j}-c_{i,\,j}}{h_x^2}-\mu_{i-1/2,j}\frac{c_{i,\,j}-c_{i-1,\,j}}{h_x^2}=\left(\mu_{i,\,j}\left(c_{i,\,j}\right)'\right)'+\mu_{i,\,j}\left(c_{i,\,j}\right)^{(IV)}\frac{h_x^2}{12}+$$

$$+\left(\mu_{i,\,j}\right)''\left(c_{i,\,j}\right)''\frac{h_x^2}{4}+\left(\mu_{i,\,j}\right)'\left(c_{i,\,j}\right)'''\frac{h_x^2}{6}+\left(\mu_{i,\,j}\right)'''\left(c_{i,\,j}\right)'\frac{h_x^2}{6}+O\left(h_x^4\right).$$

Therefore, for approximation the diffusive transport operator $\left(\mu c'\right)'$ by difference scheme of the fourth order of accuracy we have to approximate the operator $\left(\mu c'\right)'-\mu c^{(IV)}h^2/12-\mu''c''h^2/4-\mu'c'''h^2/6-\mu'''c'h^2/6$ by the scheme of the second order of accuracy.

The diffusive transport operator $\left(\mu c'\right)'$ by difference scheme of the fourth order of accuracy can be written as:

$$\left(q_0\right)_i L\left(c\right)=-A_ic_i+B_{1,i}c_{i+1}+B_{2,i}c_{i-1}+B_{3,i}c_{i+2}+B_{4,i}c_{i-2}. \tag{6}$$

$$B_{1,i}=\left(q_1\right)_i\frac{\mu_{i+1/2}}{h^2}+\left(q_1\right)_i\frac{\mu_{i+1}}{12h^2}\left(\frac{\left(q_1\right)_i}{\left(q_0\right)_i}+2\right)+\left(q_2\right)_i\frac{\mu_{i-1}}{12h^2}\frac{\left(q_1\right)_i}{\left(q_0\right)_i}-\left(q_1\right)_ik_i^{(3)}-\left(q_1\right)_i\frac{\mu''_{i+1}-\mu''_i}{12},$$

$$B_{2,i}=\left(q_2\right)_i\frac{\mu_{i-1/2}}{h^2}+\left(q_1\right)_i\frac{\mu_{i+1}}{12h^2}\frac{\left(q_2\right)_i}{\left(q_0\right)_i}+\left(q_2\right)_i\frac{\mu_{i-1}}{12h^2}\left(\frac{\left(q_2\right)_i}{\left(q_0\right)_i}+2\right)-\left(q_2\right)_ik_i^{(3)}-\left(q_2\right)_i\frac{\mu''_i-\mu''_{i-1}}{12},$$

$$B_{3,i}=-\left(q_1\right)_i\frac{\mu_{i+1}}{12h^2}\frac{\left(q_1\right)_{i+1}}{\left(q_0\right)_{i+1}},B_{4,i}=-\left(q_2\right)_i\frac{\mu_{i-1}}{12h^2}\frac{\left(q_2\right)_{i-1}}{\left(q_0\right)_{i-1}},$$

$$A_i=\left(q_1\right)_i\frac{\mu_{i+1/2}}{h^2}+\left(q_2\right)_i\frac{\mu_{i-1/2}}{h^2}-\left(\left(q_1\right)_i+\left(q_2\right)_i\right)k_i^{(3)}+\left(q_1\right)_i\frac{\mu_{i+1}}{12h^2}\left(\frac{\left(q_2\right)_{i+1}}{\left(q_0\right)_{i+1}}+2\right)+$$

$$+\left(q_2\right)_i \frac{\mu_{i-1}}{12h^2}\left(\frac{\left(q_1\right)_{i-1}}{\left(q_0\right)_{i-1}}+2\right)-\left(q_2\right)_i \frac{\mu_i''-\mu_{i-1}''}{12}-\left(q_1\right)_i \frac{\mu_{i+1}''-\mu_i''}{12}+\left(q_2\right)_i \frac{\mu_{i-1}}{12h^2}\frac{\left(q_1\right)_i}{\left(q_0\right)_i}+$$

$$+\left(q_1\right)_i \frac{\mu_{i+1}}{12h^2}\frac{\left(q_2\right)_i}{\left(q_0\right)_i}-\left(q_1\right)_i \frac{\mu_{i+1}}{12h^2}\frac{\left(q_1\right)_{i+1}}{\left(q_0\right)_{i+1}}-\left(q_2\right)_i \frac{\mu_{i-1}}{12h^2}\frac{\left(q_2\right)_{i-1}}{\left(q_0\right)_{i-1}},$$

where $k_i^{(3)}=\frac{(q_1)_i}{(q_0)_i}\frac{\mu_{i+1}-\mu_i}{4h^2}-\frac{(q_2)_i}{(q_0)_i}\frac{\mu_i-\mu_{i-1}}{4h^2}$, $\mu_i''=\left(\frac{(q_1)_i}{(q_0)_i}c_{i+1}-2c_i+\frac{(q_2)_i}{(q_0)_i}c_{i-1}\right)/h^2$.

4 Comparison of Calculation Results of Substance Transport Problem Based on Schemes of the Second and Fourth Orders of Accuracy

The field, describing the error of calculations obtained as the difference between the analytical and numerical solution of substance transport problem, is given in Fig. 1. The initial distribution was determined by the function:

$$C\left(x,y\right)=\begin{cases}\sin\left(\pi\left(x-10\right)\right)\cos\left(\pi\left(y-10\right)\right), & \{x,y\}\in D, \quad D:\{x\in[10,20], y\in[10,20]\}.\\ 0, \ \{x,y\}\notin D, & \end{cases}$$

Simulation was performed on the grid by dimension of 100x100 computational nodes. Simulation parameters: the dimensions of the computational domain *lx=100 m, ly=100 m,* and the time step is *ht=0.001 s;* the time period is 100 *s*; the horizontal component is 4 m/s, vertical – 3 m/s; the coefficient of turbulent exchange is 2 m^2/s.

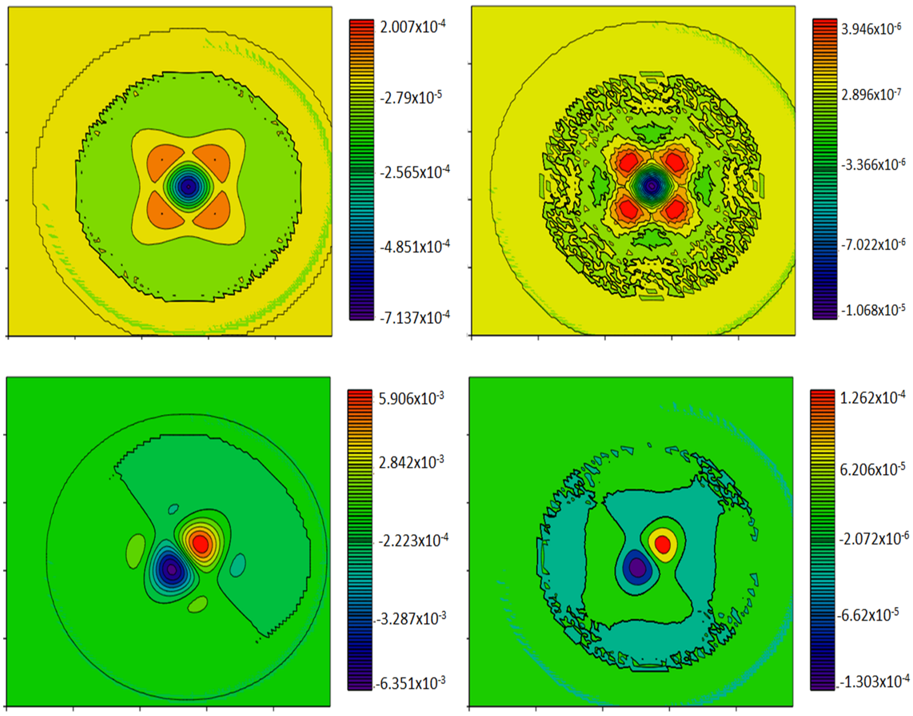

Figure 1: Computational accuracy of substances: overhand – for diffusion problem; below – for diffusion-convection problem (schemes of the second order of accuracy on the left, the fourth – on the right

According to the comparison of results of numerical experiments based on schemes of the second and fourth orders of accuracy (see Fig. 1), the accuracy was increased in 66.7 times for solution the diffusion problem, and in 48.7 times – for solution the diffusion problem-convection.

5 Parallel Implementation of Diffusion-Donvection Problem Solution

A library of two-layer iterative methods for solution the nine-diagonal grid equations was designed for solution the two-dimensional diffusion-convection problem based on the schemes of high order of accuracy. This library

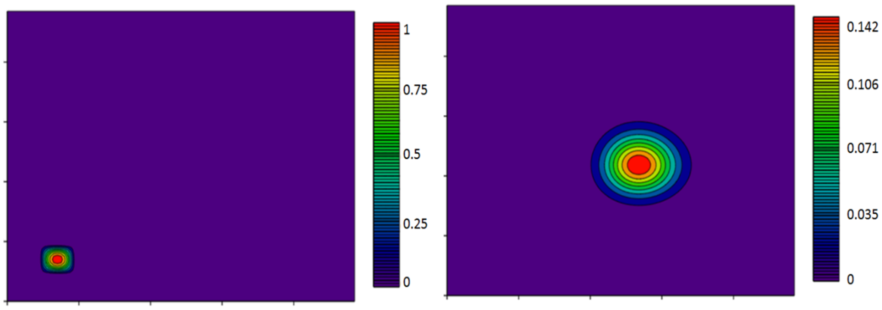

Figure 2: Values of substance concentration at initial and final time moments

for solution the systems of linear algebraic equations (SLAE) include the following methods: the Jacobi method; the method of minimal corrections; the method of steepest descent; the Seidel method; the method of upper relaxation; the adaptive MATM of variation type.

Dependences of the number of iterations, required to solve the model problem on the time variable step, are given in the Table 1.

Table 1: Dependences of amount iteration for SLAE solution by iteration methods from the time step

Time step	Number of iterations					
	Jacobi method	Minimal correction method	Method of steepest descent	Zeidel method	Upper relaxation method	MATM
0.001	6	6	6	5	43	5
0.005	8	8	8	8	43	6
0.01	10	10	10	8	45	6
0.05	23	23	23	15	56	10
0.1	37	36	37	22	61	12
0.5	138	134	138	70	60	27
1	256	247	256	126	60	28
5	1138	1077	1138	558	131	50
10	2233	2110	2233	1073	246	72
50	10160	9523	10160	4774	1074	158
100	19966	18625	19966	9320	2096	218
500	99651	92789	99651	46383	10399	1281
1000	199295	185529	199295	92739	20781	4382

The idea of parallel algorithm of iterative methods with preconditioners of triangular type [Suk12'] (Zeidel method, upper relaxation method, alternative triangular method) on a system with distributed memory is as follows: at the first step, each processor receives a subdomain, obtained by partition of the source domain into parts in one or more coordinate directions with an intersection of two nodes in each direction. Then, the SLAE solution with the upper-triangular operator is carried out, as a result of which the vector of solutions is calculated at the next iteration. The order of traversal of grid nodes in calculations and data exchanges in the case of decomposition in one spatial direction are shown in Fig. 3 and denoted by arrows. On the next step the residual vector and its uniform norm (the maximum modulo element) is calculated. In this case, each processor determines the maximum modulo element of the residual vector and transfers its value to all other processors. After data exchanges, processors calculate the maximum element in which the norm of the residual vector will be stored. If the norm of the residual vector is greater than the specified error, then the return to the calculation of the residual is performed.

At calculation the value of the solution vector, only the first processor does not require additional information and can process its part of the region independently of other calculators; other processors are waiting for data transfer from the previous one.

Data transfer for one element is not optimal, because there're time costs associated with the organization of transfers. It can be minimized by increasing the size of data package; but it increases the delay time of the start

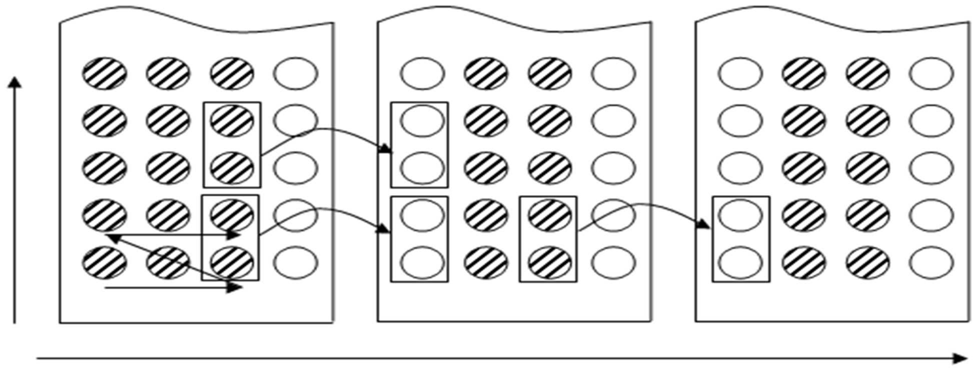

Figure 3: Scheme for calculation the values of solution vector on the next time layer

of processors. Thus, the problem of calculation (selection) the optimal amount of transferred data package occur.

Values of acceleration and efficiency of parallel implementation of the software, designed to solve the two-dimensional diffusion-convection problem on the basis of high order accuracy schemes, are given in the Table 2. The grid equations were solved by the modified alternating-triangular method. The computational grid consist of 2000x2000 nodes. Parallel implementation of the developed algorithms was based on Message Passing Interface (MPI) technologies. The peak performance of the multiprocessor computer system (MCS) is 18.8 TFlops. As computing nodes 128 one-type16-core HP ProLiant BL685c Blade-servers were used, each of which is equipped with four 4-core processors AMD Opteron 8356 2.3 GHz and 32GB RAM.

Table 2:

Number of processors	Time, s.	Acceleration	Efficiency
1	1447.415	1	1
2	734.728	1.97	0.985
4	387.009	3.74	0.935
8	199.643	7.25	0.906
16	109.653	13.2	0.825
32	62.659	23.1	0.722
64	36.643	39.5	0.617

According to the table 2, the parallel algorithm of the modified alternating-triangular method can be applied to solve real problems, and the use of parallel technologies makes a significant contribution to reduce the calculation time.

6 Use the High Order Accuracy Schemes for Reconstruction the Salinity Field and Comparison of Interpolation Results With Other Algorithms

One of the urgent problems that arise at mathematical modeling of hydrodynamics of shallow waters [Suk18'] is the problem of hydrographic information processing. Typically, the salinity is specified at separate points or level isolines (see Fig. 4).

Using these maps for construction the computational grids is undesirable because of the error of calculations related to the "coarse" setting geometry of computational domain. Thus, for increasing the accuracy of calculations of hydrodynamic processes, it is necessary to approximate the function of two variables describing the salinity field by more stable functions.

Formulation the problem of calculation the salinity field. To determine the salinity function, we use the diffusion equation solution to which the Saint-Venant equation describing the transport of bottom materials is reduced [Sid17]. The solution of the diffusion problem for a long time intervals is reduced to the solution of the Laplace equation:

$$\Delta H = 0, \tag{7}$$

where H is a water salinity.

Figure 4: The original image of salinity isolines' level in the Azov Sea

This approach has a significant disadvantage due to the lack of smoothness at points where the salinity field values are specified. To resolve this problem, we can use the following equation:

$$\Delta^2 H = 0. \tag{8}$$

The disadvantages of this approach include large outliers (deviation from the linear function). With the first two approaches, we can get functions that do not have a direction, but each approach has disadvantages.

To determine a smooth salinity function, we can also apply the equation solution used to obtain schemes of the high order of accuracy for the Laplace equation:

$$\Delta H - \frac{h^2}{12}\Delta^2 H = 0. \tag{9}$$

Note that, the operator for the third problem can be written as a linear combination of operators for the first and second problems.

The fundamental system of solutions for equation (7) is the following function:

$$H_1(x) = 1,\ H_2(x) = x, \tag{10}$$

for equation (8):

$$H_1(x) = 1,\ H_2(x) = x, H_3(x) = x^2, H_4(x) = x^3, \tag{11}$$

for equation (9):

$$H_1(x) = 1,\ H_2(x) = x, H_3(x) = ch\,(kx)\,, H_4(x) = sh\,(kx)\,,\ k = \sqrt{12}/h. \tag{12}$$

In the first case, the interpolation is performed by segments of lines passing through neighboring points; in the second case, the interpolation is based on cubic splines; in the third case – on function splines (12). The algorithm for one-dimensional interpolation based on the function (12) is described below, and the proposed approaches are compared.

Results of salinity field restoration. The proposed mathematical algorithm for determine the water salinity field was numerically implemented. The salinity isolines were obtained using the recognition algorithm (Fig. 5a) The salinity field was obtained using the describing above interpolation algorithm in a rectangle (Fig. 5b). The map of salinity of the Azov Sea was obtained by applying the boundaries of the region (Fig. 6).

Note that the proposed algorithm has a sufficient degree of smoothness at points of gluing functions and lower emissions compared to the cubic function used in the calculations.

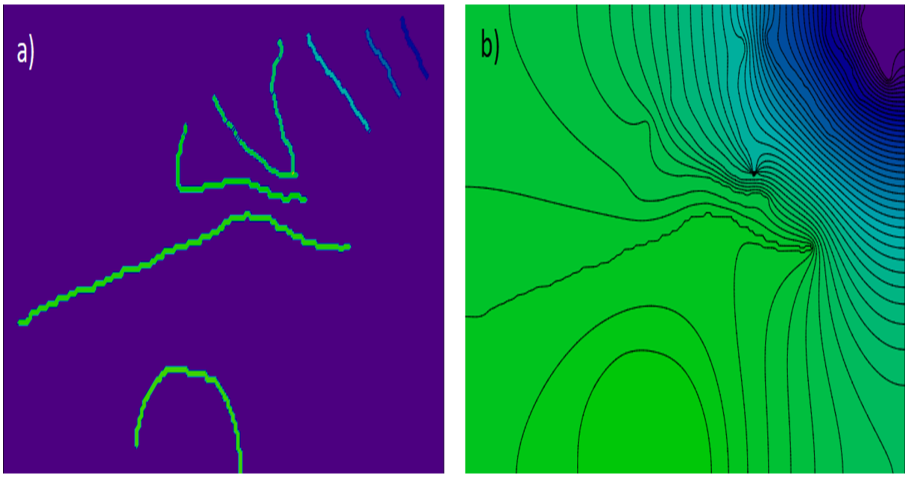

Figure 5: a) Isolines of salinity of the Azov Sea; b) the result of interpolation by the proposed method

Figure 6: Restored salinity field of the Azov Sea

7 Conclusion

Schemes of high (fourth) order of accuracy for the convective and diffusive transfer operators, taking into account the filling of the cells, were constructed. A library of two-layer iterative methods was designed and implemented on MCS for solution the two-dimensional diffusion-convection problem based on the schemes of high order of accuracy.

The comparison of calculation results of substance transport problem on the basis of schemes of the second and fourth orders of accuracy was performed. According to the comparison of results of numerical experiments, the accuracy was increased in 66.7 times for solution the diffusion problem, and in 48.7 times – for solution the diffusion problem-convection. The algorithms description of parallel implementation of iterative methods with preconditioners of triangular type and value of acceleration and efficiency of parallel variant of algorithm of the modified alternative triangular method is given. A mathematical algorithm was proposed to restore the water salinity field on the basis of hydrographic information (water salinity at separate points or level isolines), and its numerical implementation was performed. The map of the salinity of the Azov Sea was obtained and based on the proposed method for solving the problem. The developed algorithm has a sufficient degree of smoothness at points of gluing functions and lower emissions in the one-dimensional case compared to the cubic function used in calculations. Note that the proposed schemes were also used for development a software package designed to calculate the three-dimensional velocity flow fields in shallow waters [Suk11]. In the future, the developed schemes will be software implemented for calculation the biological kinetic problems [Gus18] and transport of bottom materials [Sid17].

7.0.1 Acknowledgements

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