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Variational data assimilation for a sea dynamics model

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Abstract — The 4D variational data assimilation technique is presented for modelling the sea dynamics problems, developed at the Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences (INM RAS). The approach is based on the splitting method for the mathematical model of sea dynamics and the minimization of cost functionals related to the observation data by solving an optimality system that involves the adjoint equations and observation and background error covariances. Efficient algorithms for solving the variational data assimilation problems are presented based on iterative processes with a special choice of iterative parameters. The technique is illustrated for the Black Sea dynamics model with variational data assimilation to restore the sea surface heat fluxes.

Keywords: Sea dynamics modelling, variational data assimilation, observations, sea surface temperature

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Comprehensive monitoring of the main features of natural environment and climate, which is important both for everyday life and for reducing the consequences of natural and man-made disasters, requires a new effective methods and algorithms for the variational assimilation of remote sensing data in atmospheric, ocean and climate models to be developed for high-performance computing.

The data assimilation methods are widely used in geosciences to develop computational technologies that combine the flows of real data and hydrodynamic forecasts using mathematical models. It received the greatest applications in meteorology and oceanography, where observations of the atmosphere and ocean are assim-

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ilated into atmospheric and oceanic models in order to obtain the initial or boundary conditions and other model parameters for further modelling and forecasting [6, 7, 11, 15, 16, 19, 22, 24].

The development of numerical algorithms for solving variational data assimilation problems by optimal control methods using adjoint equations at the INM RAS was initiated by Academician Guriy I. Marchuk [19]. This approach was the main content of research of G. I. Marchuk and his scientific school at the INM RAS in various fields of mathematics and applications [1, 4, 5, 19, 28]. This approach allows, on a unified methodological basis, to solve the problems of initializing hydrophysical fields, assessing the sensitivity of a model solution, identifying model parameters, etc. The main idea of the method is to minimize some functional that describes the deviation of the model solution from the observational data, and the minimum of this functional is sought on the model trajectories, in other words, in the subspace of model solutions. The problem is formulated in a four-dimensional space–time domain and requires the solution of a coupled system of direct and adjoint equations in forward and backward time, respectively.

Ocean general circulation models are based on nonlinear differential equations describing the evolution of three-dimensional fields of currents, temperature and salinity, as well as pressure and density [8, 10, 12, 23], and require the development of efficient numerical methods for a long-time integration. The ocean hydrodynamics INMOM model developed at INM RAS is described by primitive equations in the sigma-coordinate system, which is solved by finite-difference methods [10, 27, 30]. Its numerical implementation is based on the method of splitting according to physical processes and spatial coordinates [18, 30], which allows us to split the complex problem into a number of simpler ones and solve it in time using explicit or implicit schemes.

This paper presents some results for solving the problems of variational data assimilation, developed at the INM RAS last years. As an application, a mathematical model of sea dynamics is considered with a block of variational assimilation of data on sea surface temperature taking into account the covariance matrices of background and observation errors. On the basis of variational assimilation of observational data, algorithms are proposed for solving inverse problems to restore heat fluxes on the sea surface. The results of numerical experiments for the Black Sea dynamics model are discussed.

1. Mathematical model of sea dynamics

We consider the system of equations of sea hydrothermodynamics in geographical coordinates under hydrostatics and Boussinesq approximations [20], with the Lame coefficients for a spherical coordinate system [2], in the domain D of variables (x,y,z) for $t \in (0,\bar{t})$:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} + \begin{bmatrix} 0 & -f \\ f & 0 \end{bmatrix} \mathbf{u} - g\,\mathbf{grad}\zeta + A_u\mathbf{u} + (A_k)^2\mathbf{u} = \mathbf{f} - \dfrac{1}{\rho_0}\mathbf{grad}P_a \\ \qquad - \dfrac{g}{\rho_0}\mathbf{grad}\displaystyle\int_0^z \rho_1(T,S)\,\mathrm{d}z' \\ \dfrac{\partial\zeta}{\partial t} - m\dfrac{\partial}{\partial x}\left(\displaystyle\int_0^H \Theta(z)u\,\mathrm{d}z\right) - m\dfrac{\partial}{\partial y}\left(\displaystyle\int_0^H \Theta(z)\dfrac{n}{m}v\,\mathrm{d}z\right) = f_3 \\ \dfrac{\mathrm{d}T}{\mathrm{d}t} + (\mathbf{U},\mathbf{Grad})T + A_T T = f_T, \quad \dfrac{\mathrm{d}S}{\mathrm{d}t} + (\mathbf{U},\mathbf{Grad})S + A_S S = f_S \end{cases} \tag{1.1}$$

where $\mathbf{U} = (u,v,w)$ is the velocity vector, ζ is the sea surface level function, T is the temperature, S is the salinity, $\mathbf{u} = (u,v)$, $\rho_1(T,S) = \rho_0\beta_T\left(T - T^{(0)}\right) + \rho_0\beta_S\left(S - S^{(0)}\right) + \gamma\rho_0\beta_{TS}(T,S) + f_P$ is the water density, P_a is the atmospheric pressure, $\mathbf{f} = (f_1, f_2)$ is the forcing, f_T, f_S, f_P are the functions of the 'internal' sources, $\rho_0 = \text{const} \approx 1$ is the mean density, $T^{(0)}$ and $S^{(0)}$ are the reference values of temperature and salinity, $\beta_{TS}(T,S)$ is the sum of all other terms of the expansion of the function of state $\rho = \rho(T,S)$, $f_3 \equiv f_3(x,y,t)$ is the function related to the tide-generating forces, $\beta_T, \beta_S, \gamma, g = \text{const}, A_\varphi\varphi \equiv -\mathbf{Div}\left(\widehat{a}_\varphi\mathbf{Grad}\varphi\right)$, $m = 1/(r\cos y), n = 1/r, r = R - z \approx R$, $\Theta(z) \equiv (R-z)/R \approx 1$, R is the Earth radius.

The operators $A_\varphi\varphi \equiv -\mathbf{Div}(\widehat{a}_\varphi\mathbf{Grad}\varphi)$ involve $\widehat{a}_\varphi = \mathrm{diag}((a_\varphi)_{ii})$, where $(a_\varphi)_{11} = (a_\varphi)_{22} \equiv \mu_\varphi, (a_\varphi)_{33} \equiv \nu_\varphi$, and φ may take the values u,v,T,S. We assume that $\mu_u = \mu_v \equiv \mu$, $\nu_u = \nu_v \equiv \nu$, and μ, ν, μ_T, μ_S, ν_T, ν_S are given positive bounded functions. The fourth order operator $(A_k)^2$, with A_k taken for $A_\varphi = A_k$, is defined by the matrix $\widehat{k} = \mathrm{diag}\{k_{ii}\}$ with nonnegative diagonal elements k_{ii}. By $l = l(y)$ we denote the Coriolis parameter $l = 2\omega\sin y$, where ω is the Earth angular rotation speed, and $f(u) = l + mu\sin y \equiv l + f_1(u)$.

The boundary $\Gamma \equiv \partial D$ of the domain D is represented as a union of four disjoint parts Γ_S, $\Gamma_{w,op}$, $\Gamma_{w,c}$, and Γ_H, where $\Gamma_S \equiv \Omega$ is the 'unperturbed' sea surface, $\Gamma_{w,op}$ is the liquid (open) part of the vertical lateral boundary, $\Gamma_{w,c}$ is the solid part of the vertical lateral boundary, and Γ_H is the sea bottom. The characteristic functions (indicator functions) of the parts Γ_S, $\Gamma_{w,op}$, $\Gamma_{w,c}$, and Γ_H of the boundary Γ are denoted by m_S, $m_{w,op}$, $m_{w,c}$, and m_H, respectively.

The unit outer normal vector to Γ is denoted by $\mathbf{N} \equiv (N_1,N_2,N_3)$, with $\mathbf{N} = (0,0,-1)$ on Γ_S and $\mathbf{N} = (N_1,N_2,0)$ on $\Gamma_w = \Gamma_{w,op} \cup \Gamma_{w,c}$, and $\mathbf{n} \equiv (N_1,N_2) \equiv (n_1,n_2)$ is the unit outer normal vector to $\partial\Omega$. We assume also that $|N_3| > 0$ on Γ_H. The components N_1,N_2,N_3 are defined by the chosen parametric representation of the corresponding part of the boundary. For the velocity vector $\mathbf{U} = (u,v,w)$ on the boundary Γ, the normal components are denoted by $U_n : U_n = \mathbf{U}\cdot\mathbf{N} = uN_1 + vN_2 + wN_3$. Below we put $U_n^{(+)} \equiv (|U_n| + U_n)/2$, $U_n^{(-)} \equiv (|U_n| - U_n)/2$, with $U_n = U_n^{(+)} - U_n^{(-)}$ on Γ.

We consider the equations (1.1) in $D\times(0,\bar{t})$ with the following boundary and initial conditions [2].

Boundary conditions on Γ_S:

$$\begin{cases} \left(\int\limits_0^H \Theta\mathbf{u}\,\mathrm{d}z\right)\mathbf{n}+\beta_0 m_{op}\sqrt{gH}\,\zeta = m_{op}\sqrt{gH}\,d_s \quad \text{on } \partial\Omega \\ U_n^{(-)}u-\nu\dfrac{\partial u}{\partial z}-k_{33}\dfrac{\partial}{\partial z}A_k u = \tau_x^{(a)}\Big/\rho_0, \quad U_n^{(-)}v-\nu\dfrac{\partial v}{\partial z}-k_{33}\dfrac{\partial}{\partial z}A_k v = \tau_y^{(a)}\Big/\rho_0 \\ A_k u = 0, \quad A_k v = 0 \\ U_n^{(-)}T-\nu_T\dfrac{\partial T}{\partial z}+\gamma_T(T-T_a) = Q_T+U_n^{(-)}d_T \\ U_n^{(-)}S-\nu_S\dfrac{\partial S}{\partial z}+\gamma_S(S-S_a) = Q_S+U_n^{(-)}d_S \end{cases} \tag{1.2}$$

where $\tau_x^{(a)}$ and $\tau_y^{(a)}$ are the tangent wind stress components along the axes Ox and Oy, respectively, on the sea surface $z=0$, and γ_T, γ_S, T_a, S_a, Q_T, Q_S, d_T, d_S are the given functions. We have also $U_n|_{z=0}=-w|_{z=0}$, where $w = w(u,v)$ is defined by the formula

$$w(x,y,z,t) = \frac{1}{r}\left(m\frac{\partial}{\partial x}\left(\int\limits_z^H ru\,\mathrm{d}z'\right)+m\frac{\partial}{\partial y}\left(\frac{n}{m}\int\limits_z^H rv\,\mathrm{d}z'\right)\right), \quad (x,y,t)\in\Omega\times(0,\bar{t}). \tag{1.3}$$

Boundary conditions on $\Gamma_{w,c}$ (*on the 'solid' part lateral wall*):

$$U_n = 0, \quad A_k\widetilde{U} = 0, \quad \frac{\partial\widetilde{U}}{\partial N_u}\cdot\tau_w+\left(\frac{\partial}{\partial N_u}A_k\widetilde{U}\right)\cdot\tau_w = 0, \quad \frac{\partial T}{\partial N_T} = 0, \quad \frac{\partial S}{\partial N_S} = 0 \tag{1.4}$$

where $\tau_w = (-N_2,\ N_1,\ 0)$, $\widetilde{U}\equiv(u,v,0)\equiv(\mathbf{u},0), \partial\varphi/\partial N_\varphi \equiv \mathbf{N}\cdot\widehat{a}_\varphi\cdot\mathbf{Grad}\varphi,\ \varphi = u,T,S$.

Boundary conditions on $\Gamma_{w,op}$ (*on the 'liquid' part lateral wall*):

$$\begin{cases} U_n^{(-)}(\widetilde{U}\cdot\mathbf{N})+\dfrac{\partial\widetilde{U}}{\partial N_u}\cdot\mathbf{N} = U_n^{(-)}d, \quad A_k\widetilde{U} = 0 \\ U_n^{(-)}(\widetilde{U}\cdot\tau_w)+\dfrac{\partial\widetilde{U}}{\partial N_u}\cdot\tau_w+\left(\dfrac{\partial}{\partial N_u}A_k\widetilde{U}\right)\cdot\tau_w = 0 \\ U_n^{(-)}T+\dfrac{\partial T}{\partial N_T} = U_n^{(-)}d_T+Q_T,\ U_n^{(-)}S+\dfrac{\partial S}{\partial N_S} = U_n^{(-)}d_S+Q_S \end{cases} \tag{1.5}$$

where d, d_T, d_S, Q_T, Q_S are the given functions.

Boundary conditions on the bottom Γ_H:

$$\begin{cases} w = um\dfrac{\partial H}{\partial x} + vn\dfrac{\partial H}{\partial y}, \quad A_k\widetilde{U} = 0, \quad \dfrac{\partial T}{\partial N_T} = 0, \quad \dfrac{\partial S}{\partial N_S} = 0 \\ \dfrac{\partial \widetilde{U}}{\partial N_u}\cdot\tau_x + \left(\dfrac{\partial}{\partial N_k}A_k\widetilde{U}\right)\cdot\tau_x = \dfrac{\tau_x^{(b)}}{\rho_0}, \quad \dfrac{\partial \widetilde{U}}{\partial N_u}\cdot\tau_y + \left(\dfrac{\partial}{\partial N_u}A_k\widetilde{U}\right)\cdot\tau_y = \dfrac{\tau_y^{(b)}}{\rho_0} \end{cases} \tag{1.6}$$

where τ_x and τ_y is the system of unit orthogonal vectors on the sea surface $z = 0$; $\tau_x^{(b)}$ and $\tau_y^{(b)}$ are the projections of the bottom friction vector on the axes Ox and Oy, respectively.

Initial conditions for u, v, T, S, ζ:

$$u = u^0, \quad v = v^0, \quad T = T^0, \quad S = S^0, \quad \zeta = \zeta^0 \quad \text{for } t = 0 \tag{1.7}$$

where u^0, v^0, T^0, S^0, ζ^0 are the given functions.

The problem of large-scale sea dynamics in terms of the functions u, v, w, ζ, T, S consists in solving problem (1.1)–(1.7). If the functions u, v, ζ, T, S are found, then the function w is determined by formula (1.3).

The main features of the numerical model of sea dynamics developed at the Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences are the simultaneous use of the splitting method [30, 18] and the transition to the σ-coordinate system [27, 30] for (1.1)–(1.7). These two components are used in tandem to build efficient computer technology for 4DVAR ocean data assimilation.

The transition to the σ-system can be carried out at the stage of considering the original problem (1.1)–(1.7) before applying suitable splitting schemes and other numerical procedures [21].

In order to approximate the model (1.1)–(1.7) in time, we use the splitting method that allows us to represent the solution of the original nonlinear system by subsequent solutions of simpler problems (steps of the splitting method). Let us introduce the grid on $[0;\bar{t}]$: $0 = t_0 < t_1 < ... < t_{J-1} < t_J = \bar{t}$, $\Delta t_j = t_j - t_{j-1}$ and consider problem (1.1)–(1.7) on (t_{j-1}, t_j), assuming that the vector of the approximate solution $\varphi_k \equiv (u_k, v_k, \xi_k, T_k, S_k)$, $k = 1, 2, ..., j-1$ at the previous intervals, is already defined. To approximate the problem, we use one of the schemes of the total approximation method [18], which consists in the implementation of the following steps.

Step 1. Consider the problem

$$T_t + (\mathbf{U}, \mathbf{Grad})\,T - \mathbf{Div}\,(\widehat{a}_T \cdot \mathbf{Grad}\;T) = f_T \quad \text{in } D \times (t_{j-1}, t_j) \tag{1.8}$$

under corresponding boundary and initial conditions.

Step 2. Solve the problem

$$S_t + (\mathbf{U}, \mathbf{Grad})S - \mathbf{Div}(\widehat{a}_S \cdot \mathbf{Grad}\;S) = f_S \quad \text{in } D \times (t_{j-1}, t_j) \tag{1.9}$$

under appropriate boundary and initial conditions.

Step 3. The system

$$\begin{cases} \underline{u}_t^{(1)} + \begin{bmatrix} 0 & -l \\ l & 0 \end{bmatrix} \underline{u}^{(1)} - g\,\mathbf{grad}\xi = \mathbf{f} - \dfrac{1}{\rho_0}\mathbf{grad}\left(P_a + g\int\limits_0^z \rho_1(\bar{T},\bar{S})\,\mathrm{d}z'\right) \\ \qquad\qquad\text{in } D\times(t_{j-1},t_j) \\ \xi_t - \mathbf{div}\left(\int\limits_0^H \Theta\underline{u}^{(1)}\,\mathrm{d}z\right) = f_3 \quad \text{in } \Omega\times(t_{j-1},t_j) \\ \underline{u}^{(1)} = \underline{u}_{j-1},\ \xi = \xi_{j-1} \text{ for } t = t_{j-1},\ \underline{u}_j^{(1)} \equiv \underline{u}^{(1)}(t_j) \quad \text{in } D \end{cases} \tag{1.10}$$

is solved under corresponding boundary conditions, and the function $\xi_j \equiv \xi^{(1)}$ is taken as an approximation to ξ on (t_{j-1},t_j). Then the following problems are solved:

$$\begin{cases} \underline{u}_t^{(2)} + \begin{bmatrix} 0 & -f_1(\bar{u}) \\ f_1(\bar{u}) & 0 \end{bmatrix} \underline{u}^{(2)} = 0 \quad \text{in } D\times(t_{j-1},t_j) \\ \underline{u}^{(2)} = \underline{u}_j^{(1.1)} \quad \text{for } t = t_{j-1}, \quad \underline{u}_j^{(2)} \equiv \underline{u}^{(2)}(t_j) \quad \text{in } D \end{cases} \tag{1.11}$$

$$\begin{cases} \underline{u}_t^{(3)} + (\mathbf{U},\mathbf{Grad})\underline{u}^{(3)} - \mathbf{Div}(\widehat{a}_u\cdot\mathbf{Grad})\underline{u}^{(3)} + (A_k)^2\underline{u}^{(3)} = 0 \quad \text{in } D\times(t_{j-1},t_j) \\ \underline{u}^{(3)} = \underline{u}^{(2)} \quad \text{for } t = t_{j-1} \quad \text{in } D \end{cases} \tag{1.12}$$

where $\underline{u}^{(3)} = (u^{(3)},v^{(3)})$ and $\mathbf{U}^{(3)} = (\underline{u}^{(3)}, w^{(3)}(u^{(3)},v^{(3)}))$. After solving (1.12), the vector $\underline{u}^{(3)} \equiv \mathbf{u}_j \equiv (u_j,v_j)$ is taken as an approximation to the exact vector $\mathbf{u}$ on $D\times(t_{j-1},t_j)$, and the approximation $w_j \equiv w(u_j,v_j)$ to the vertical component of the velocity vector is calculated by (1.3) .

When Steps 1–3 are implemented, after the first step we get an approximation to T, after the second an approximation to S, and after the third step we get an approximation to $\mathbf{u} = (u,v)$ and ξ. Therefore, the subproblems at these steps are independent of each other and may be solved in parallel.

2. Variational data assimilation

The purpose of data assimilation is to estimate the unknown model inputs: the initial state of the system, the boundary conditions, the source terms, distributed coefficients, etc. The problems are formulated as optimal control problems involving cost functions associated with observations, and the minimization is considered on the trajectories (solutions) of the model under consideration [6, 7, 11, 15, 16, 19, 22, 24].

We will demonstrate the data assimilation technique for the case when in problem (1.1)–(1.7) the total heat flux function $Q = -\nu_T\,\partial T/\partial z$ on Γ_S is unknown and treated as an additional 'control'. The cost function is related to observations and has the form:

$$
\begin{aligned}
J(Q) &= \frac{1}{2}\int_0^{\bar{t}}\int_\Omega (Q-Q^{(0)})\mathscr{B}^{-1}(Q-Q^{(0)})\,\mathrm{d}\Omega\,\mathrm{d}t + \frac{1}{2}\sum_{j=1}^{J} J_{0,j} \\
J_{0,j} &\equiv \int_{t_{j-1}}^{t_j}\int_\Omega (T|_{z=0}-T_{\mathrm{obs}})\mathscr{R}^{-1}(T|_{z=0}-T_{\mathrm{obs}})\,\mathrm{d}\Omega\,\mathrm{d}t
\end{aligned}
\tag{2.1}
$$

where $Q^{(0)} = Q^{(0)}(x,y,t)$ is a given functions, T_{obs} is the function of observations on the sea surface Ω, $\mathscr{R}$ is the observation error covariance operator, $\mathscr{B}$ is the background error covariance operator. The function $Q^{(0)}$ is usually chosen as the first approximation (so-called ‘background’) for the unknown heat flux Q. The aim of variational data assimilation is, using $Q^{(0)}$, to find better estimate for Q, consistent with the model solution and observations, for further modelling and forecast.

We consider the following variational data assimilation problem: *Find a solution to* (1.1)–(1.7) *and the function Q, such that functional* (2.1) *takes the minimum value*:

$$
J(Q) = \inf_Q J(Q).
$$

The gradient of the functional $J(Q)$ with respect to Q is defined by the adjoint state T^* as follows:

$$
J'_Q = \mathscr{B}^{-1}\left(Q-Q^{(0)}\right) + T^* \quad \text{on } \Omega. \tag{2.2}
$$

The necessary optimality condition $J'_Q = 0$ leads to the optimality system, which determines the solution of the formulated problem of variational data assimilation. The optimality system includes the direct problem (1.1)–(1.7), the adjoint problem, and the optimality conditions in the form:

$$
\mathscr{B}^{-1}\left(Q-Q^{(0)}\right) + T^* = 0 \quad \text{on } \Omega. \tag{2.3}
$$

The adjoint state T^* is the solution of the adjoint problem, which in the case of applying the splitting method is determined at Step 1 in the form:

$$
\begin{aligned}
-T^*{}_t - \mathbf{Div}\,(\mathbf{U}T^*) - \mathbf{Div}\,(\widehat{a}_T \cdot \mathbf{Grad}\,T^*) &= 0 \quad \text{in } D\times(t_{j-1},t_j) \\
T^* &= 0 \quad \text{for } t = t_j \\
-\nu_T \frac{\partial T^*}{\partial z} &= \mathscr{R}^{-1}(T|_{z=0}-T_{\mathrm{obs}}) \quad \text{on } \Omega.
\end{aligned}
\tag{2.4}
$$

The adjoint problem (2.4) involves the observation data T_{obs} and the observation error covariance operator $\mathscr{R}$ in the boundary condition on the sea surface.

The optimality system that determines the solution of the formulated problem of variational data assimilation reduces to the sequential solution of the subproblems on $t \in (t_{j-1},t_j)$, $j = 1,2,\ldots,J$.

To find an approximate solution of the optimality system, with the determination of Q by variational assimilation of T_{obs} we can use the following iterative algorithm. If $Q^{(k)}$ is the already constructed approximation to Q on (t_{j-1}, t_j), then after solving the forward and adjoint problems with $Q \equiv Q^{(k)}$, the next approximation $Q^{(k+1)}$ is computed by:

$$Q^{(k+1)} = Q^{(k)} - \gamma_k(\mathscr{B}^{-1}(Q^{(k)} - Q^{(0)}) + T^*) \;\text{ on }\; \Omega \times (t_{j-1}, t_j) \tag{2.5}$$

with the parameters γ_k chosen so that the iterative process (2.5) is convergent [3]. After computing $Q^{(k+1)}$, the solution of the direct and adjoint problems is repeated with the new approximation $Q^{(k+1)}$, and then $Q^{(k+2)}$ is calculated, and so on. Iterations are repeated until a suitable convergence criterion is met.

For example, in some cases one can take the parameters

$$\gamma_k = \frac{1}{2}\int_{t_{j-1}}^{t_j}\int_{\Omega}(T|_{z=0} - T_{\mathrm{obs}})\mathscr{R}^{-1}(T|_{z=0} - T_{\mathrm{obs}})\,\mathrm{d}\Omega\,\mathrm{d}t \Big/ \int_{t_{j-1}}^{t_j}\int_{\Omega}(T_2^*)^2|_{z=0}\,\mathrm{d}\Omega\,\mathrm{d}t$$

which may significantly accelerate the convergence of the iterative process [3].

The formulated algorithm allows us to solve the considered four-dimensional variational data assimilation problem.

In what follows, we will assume that the first approximation (background) function $Q^{(0)}$ is specified with some error, namely,

$$Q^{(0)} = \bar{Q}^{(0)} + \xi_Q$$

where $\bar{Q}^{(0)}$ is some average (exact) value of the surface flux $Q^{(0)}$, and ξ_Q can be seen as a background error. We will assume that the errors ξ_Q are random and they are distributed according to the normal law (Gaussian) with zero mathematical expectation and the covariance operator $\mathscr{B}\cdot = E[(\cdot, \xi_Q)\xi_Q]$, where E is the expectation. Covariance matrices of background and observation errors play an important role in variational data assimilation: their inverse matrices are included as weight operators in the original cost functional [11].

Due to the fact that

$$E[Q^{(0)}] = E[\bar{Q}^{(0)}] + E[\xi_Q] = \bar{Q}^{(0)}$$

we can assume that $\bar{Q}^{(0)}$ is the expectation of the first approximation (background) function, which can be calculated using the standard formula for mean values.

In the finite-dimensional case, the covariance operator $\mathscr{B}$ is a covariance matrix and is defined by the formula

$$\mathscr{B} = E[\xi_Q \xi_Q^T] = E[(Q^{(0)} - \bar{Q}^{(0)})(Q^{(0)} - \bar{Q}^{(0)})^T].$$

If $\xi_Q = (\xi_1, \ldots, \xi_N)^T$, then the elements of the matrix $\mathscr{B}$ can be written in the form

$$b_{jk} = E[(\xi_j - E\xi_j)(\xi_k - E\xi_k)] = E[\xi_j \xi_k] - E[\xi_j]E[\xi_k] = E[\xi_j \xi_k].$$

The quantities b_{jk} are called the coefficients of covariance between the jth and kth coordinates of the random vector ξ_Q and are denoted by $\mathrm{cov}(\xi_j, \xi_k)$.

For $j = k$ we get

$$b_{jj} = D\xi_j = \sigma_j^2$$

where $D\xi_j$ is the variance of the random variable ξ_j (the second central moment of the distribution):

$$D\xi_j = E[(\xi_j - E\xi_j)^2] = E[\xi_j^2] - (E[\xi_j])^2$$

and σ_j is the mean square deviation, or standard deviation, with $\sigma_j = \sqrt{D\xi_j}$.

Thus, the diagonal elements of the matrix $\mathscr{B}$ are the variances $D\xi_j$, and they play an important role in weighting the cost functional under variational data assimilation. In practice, variational assimilation often assumes that the matrix $\mathscr{B}$ is diagonal with elements $D\xi_j$, which are calculated based on the statistical properties of background data. Thus, if $\xi^{(1)}, \ldots, \xi^{(n)}$ is a sequence of realizations of the random variable ξ_j, then $D\xi_j$ is calculated by the formula:

$$D\xi_j = \frac{1}{n} \sum_{i=1}^{n} (\xi^{(i)} - E[\xi_j])^2$$

where $E[\xi_j]$ is the mathematical expectation (mean of the sample):

$$E[\xi_j] = \frac{1}{n} \sum_{i=1}^{n} \xi^{(i)}.$$

By virtue of the assumption $E\xi_Q = 0$, it is easy to see that $DQ^{(0)} = D\xi_Q$, therefore, to calculate the dispersion, one can take the values of the surface flux over a long observation period as realizations of a random variable. The resulting variances are the diagonal elements of the covariance matrix $\mathscr{B}$ of the first approximation (background) errors.

3. Numerical experiments for the Black Sea water area

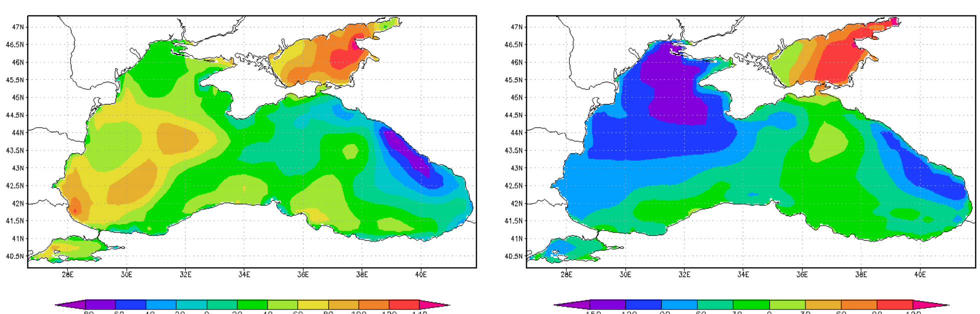
The numerical experiments were performed using the three-dimensional numerical model of the Black and Azov seas hydrothermodynamics developed at the INM RAS on the base of the splitting method [29] and supplied with the assimilation procedure for the sea surface temperature (SST) in order to reconstruct the heat fluxes Q.

The object of simulation is the water area of the Black and Azov seas. The parameters of the considered domain and its geographic coordinates can be described in the following way: σ-grid is $306 \times 200 \times 27$ (the latitude, longitude, and depth, respectively). The first point of the 'grid C' [9] has the coordinates 26.65°E and 40.15°N. The mesh sizes in x and y are constant and equal to 0.05 and 0.036 degrees, respectively. The time step is $\Delta t = 2.5$ minutes.

The SST observation data were provided by the 'See the Sea' satellite service being a part of the CKP 'IKI Monitoring', which collects and processes various data on the state of the Earth surface and focuses on working with satellite observations [17]. The SST data from the VIIRS spectrometer on the SNPP satellite and MODIS spectrometer on the Aqua and Terra satellites were selected (several measurements per day at certain points in time) as T_{obs} in this experiment. The SST data for the dates from January 1 to June 30, 2019 were recalculated on the numerical model grid [26]. Meteorological characteristics were used to calculate the atmospheric impact in the model, including the bulk formulas for calculating turbulent flows on the sea surface. The values of the mean climatic heat flow $Q^{(0)}$ calculated in the same way were used in the data assimilation procedure as a background.

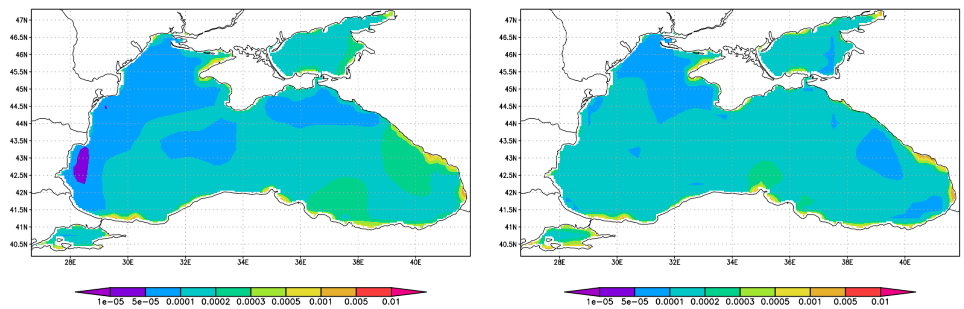
When solving problems of variational assimilation of satellite observation data, the question arises of setting the regularization parameter. One solution to this issue is to introduce into consideration the background error covariance matrix $\mathscr{B}^{-1}$ that occurs in the first term of the cost functional (2.1).

To calculate the diagonal elements of the covariance matrix $\mathscr{B}$, we obtained data on the heat flux on the sea surface. The heat flux on the sea surface was calculated using Era 5 reanalysis data (www.ecmwf.int/en/forecasts/datasets/reanalysis-datasets/era5) [13] for the period from 1979 to 2020. The following characteristics on the sea surface were used for the calculation: latent heat flux; sensible heat flux; the total flux of shortwave radiation; the total flux of long-wave radiation. For the problem of calculating the heat flux on the sea surface, the penetrating role of shortwave radiation was taken into account [14]. The Era 5 data were uploaded with a temporal resolution of 12 hours, which makes it possible to consider the daily course of changes, to separate day and night heat fluxes. In Fig. 1, to illustrate the



(a) 12:00 01.01.1979 (day) (b) 00:00 02.01.1979 (night)

Figure 1. Heat flux on the surface of the Black and Azov Seas at 12:00 01.01.1979 (a) and 00:00 02.01.1979 (b), $\mathrm{W/m^2}$.



(a) Regularization parameters for February 28, 2019

(b) Regularization parameters for June 28, 2019

Figure 2. Region of the Black Sea area.

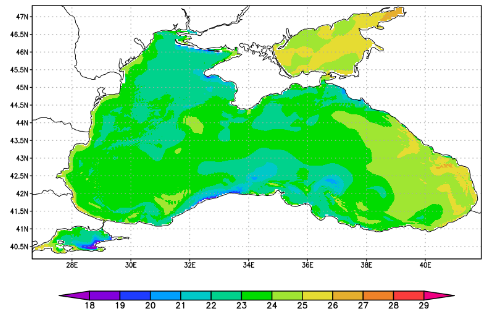
daily course of the heat flux, the data fields of the heat flux on the surface of the Black and Azov Seas on January 1 (daily) and 2 (night), 1979 are presented.

The axis is directed so that positive values mean that the sea receives heat, negative values mean that the sea gives off heat (mainly at night). Based on data for 1979–2020 the mean values and variances of the heat flux are calculated from daytime and nighttime data for each day of the year. The resulting variances are the diagonal elements b_{jj} of the covariance matrix of first approximation (background) errors.

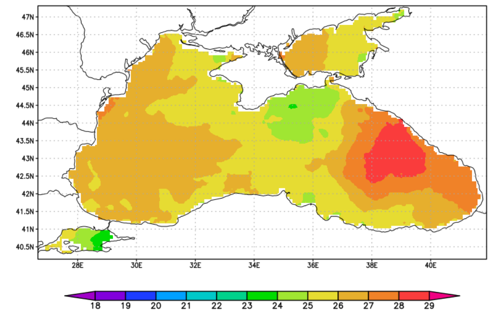
In the numerical experiments the value of the regularization parameter calculated on the basis of the diagonal elements of this covariance matrix sometimes differs by several orders of magnitude from the previously used constant parameter $\mathscr{B}^{-1} = 5 \cdot 10^{-5} \times I$, where I is the identity matrix. Note that the regularization parameter depends now on coordinates and time. Thus, Figure 2 shows the values of the parameter calculated on the basis of the matrix $\mathscr{B}^{-1}$ on February 28 and on June 28, 2019.

To confirm the possibility of using $\mathscr{B}^{-1}$ as a regularization parameter, numerical experiments were carried out to solve the problem of variational assimilation of satellite observation data. The duration of the calculation was six months. The results of numerical calculations were then compared with observation data obtained from the Copernicus service (product ID sst_eur_sst_l3s_nrt_observations_010_009_a) for the same period of time. Note that the data used in the assimilation procedure are quasi-operational, that is, assimilated at certain points in time, and the Copernicus data are average daily data. Therefore, for a correct comparison, the calculation data were averaged over a day.

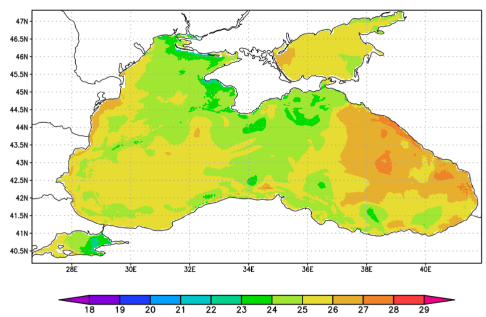
Figure 3 shows the calculation results on June 28, 2019. Thus, Figure 3a shows the average value of the sea surface temperature when calculated by the model without the assimilation block, Figure 3b shows the data obtained from the Copernicus service, Figure 3c presents the calculated SST based on assimilation with a constant regularization parameter, and Figure 3d presents the calculated SST based on assimilation using the background error covariance matrix.



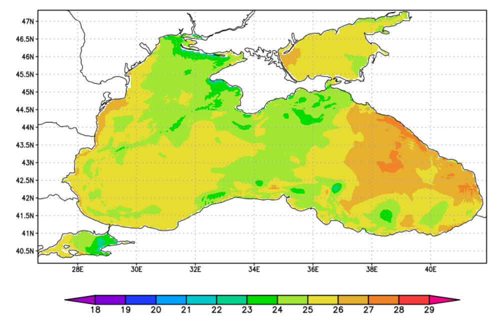
(a) Model calculation without assimilation procedure



(b) Average daily observational data of the Copernicus service



(c) Calculation with assimilation for $\mathscr{B}^{-1} = 5 \cdot 10^{-5} \times I$

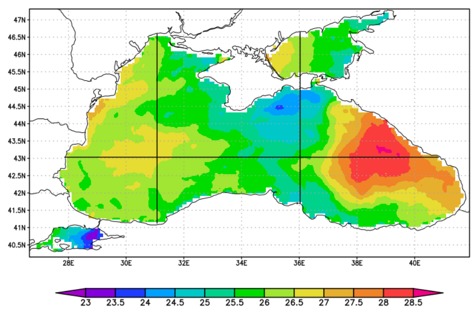


(d) Calculation with assimilation involving $\mathscr{B}^{-1}$

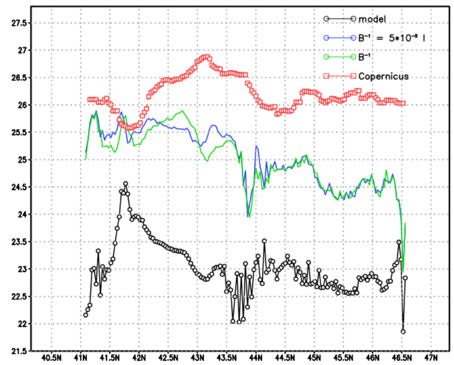
Figure 3. Average SST, June 28, 2019, $^{\mathrm{o}}$C.

Comparing the results of calculations, it can be seen that the model without the assimilation procedure somewhat underestimates the sea surface temperature in the considered period of time, and the discrepancy with the observational data can reach up to 3$^{\mathrm{o}}$C. The use of the data assimilation procedure makes it possible to reduce this difference to 1–2$^{\mathrm{o}}$C practically throughout the Black and Azov Seas. Note that the calculations with a constant regularization parameter and those calculated on the basis of the matrix $\mathscr{B}^{-1}$ showed very close results.

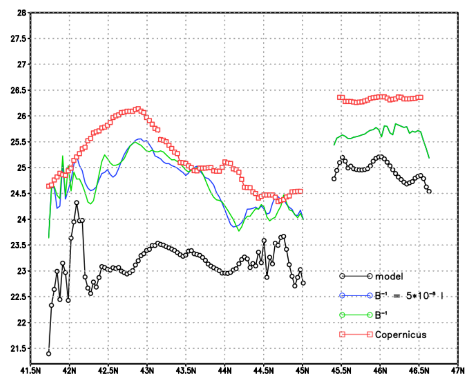
Figure 4 shows sections along 31$^{\mathrm{o}}$E (Fig. 4b), 36$^{\mathrm{o}}$E (Fig. 4c), and 43$^{\mathrm{o}}$N (Fig. 4d) for sea surface temperature. In all plots, the line with black circles is the calculation according to the model without the data assimilation block, the blue line is the calculation according to the model with data assimilation and constant regularization parameter, the green line is the calculation according to the model with assimilation and regularization parameters built on the basis of the matrix $\mathscr{B}^{-1}$, line with red squares – average daily data from the Copernicus service. Based on the results presented in Fig. 4, we note that the inclusion of the data assimilation procedure allows improving the behavior of the model and, after calculation, the SST values become closer to the observed ones. Note that in the Sea of Azov (see Fig. 4c)



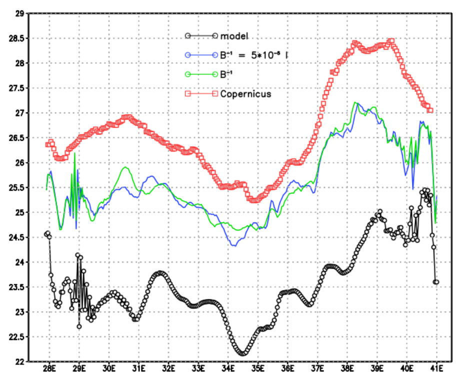
(a) Cross-sections for SST



(b) SST along 31°E



(c) SST along 36°E



(d) SST along 43°N

Figure 4. Cross-sections of SST: red square is Copernicus data, black circle – model without assimilation, green line – regularization with $\mathscr{B}^{-1}$, blue line – constant regularization, June 28, 2019, °C.

the calculation results with a constant value of the regularization parameter and the parameter calculated on the basis of the matrix $\mathscr{B}^{-1}$ turned out to be identical. In the rest of the study region, they differ by a small amount.

The iterative procedures used for the four-dimensional variational assimilation of the sea surface temperature in the Black Sea showed good convergence, and no more than 10 iterations were required to obtain the optimal heat flux Q. In some experiments, the parameters of the iterative process can be calculated based on the features of the system itself, and in this case it is possible to achieve convergence of the process in 3–5 iterations.

Numerical experiments for the Black Sea dynamics model confirmed the efficiency of the presented computational technique and demonstrated that the assimilation improves the predictive properties of the model.

4. Conclusions

The results on the development of efficient numerical algorithms for problems of variational assimilation of observation data for a model of sea dynamics are presented. The algorithms for solving inverse problems to restore the heat fluxes on the sea surface for the model under consideration are proposed. The algorithms have shown their efficiency for the models based on the use of the method of splitting with respect to physical processes and geometric coordinates, which made considered problems easier at each implementation step.

The research shows the possibility of choosing a regularization parameter based on the background error covariance matrix. The numerical experiments for the Black Sea dynamics model have confirmed the efficiency of this approach in the proposed variational assimilation algorithms to modelling hydrothermodynamics problems of marine areas and demonstrated a good proximity of the obtained solutions to real observation data.

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