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Variational assimilation with covariance matrices of observation data errors for the model of the Baltic Sea dynamics

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Abstract: The mathematical model of the Baltic Sea dynamics developed at the Institute of Numerical Mathematics of RAS is considered. The problem of variational assimilation of average daily data for the sea surface temperature (SST) is formulated and studied with the use of covariance matrices of observation data errors. Based on variational assimilation of satellite observation data, we propose an algorithm for solving the inverse problem of the heat flux reconstruction on the sea surface. The results of numerical experiments on reconstruction of the heat flux function are presented for the problem of variational assimilation of observation SST data.

Keywords: Variational assimilation, covariance matrices, numerical algorithm, determination of heat fluxes, sea surface temperature.

MSC 2010: 49K20, 65K10

Reliable monitoring and forecasting of oceanic and marine circulation require the establishment of a data assimilation system, and one of its main components should be a physically complete and verified model that can be used to calculate circulation in various water areas. At the present stage of research it is necessary to combine real observation data and computational experiments with mathematical models, improve the accuracy of modelling and forecasting of physical processes in the natural environment.

The most universal and perspective technology of solution to problems of monitoring and analysis of the natural environment state is the four-dimensional variational data assimilation [1, 7–9]. One of approaches to construction of the efficient assimilation algorithms is the study of covariance matrices of observation errors and their inclusion into the initial cost functional [13]. In this paper we formulate the inverse problem of sea surface temperature data assimilation using the covariance matrices of observation errors for the Baltic Sea dynamics model. It is worth noting that observations of sea surface temperature from satellites allow us to monitor various values on the sea surface in real time. Note that in formulation of variational assimilation problems for the data mentioned above we introduce only those additional unknowns ('controls') which can be uniquely determined by means of observable functions, but not an arbitrary set of additional unknowns.

The basis of the sea circulation model used in this paper is formed by the hydrothermodynamic numerical model of the Baltic Sea developed at the INM RAS [18, 19] with the use of the splitting method [11, 12, 17] and supplied with the block of variational data assimilation for the sea surface temperature [3, 4] taking into account the covariance matrices of observation errors. We propose an algorithm for numerical solution of the formulated variational data problem and present the results of numerical experiments for the considered model of the Baltic Sea dynamics.

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1 Equations of the model

Let us consider the problem of sea hydrothermodynamics in the form [5, 10]:

$$
\begin{gathered}
T_t + (\bar{U}, \mathrm{Grad})T - \mathrm{Div}(\hat{a}_T \cdot \mathrm{Grad}\ T) = f_T \quad \text{in} \ D \times (0, \bar{t}) \\
T = T_0 \quad \text{for } t = 0 \ \text{ in } \ D \\
-\nu_T \frac{\partial T}{\partial z} = Q \quad \text{on} \ \Gamma_S \times (0, \bar{t}), \qquad \frac{\partial T}{\partial N_T} = 0 \ \text{ on } \ \Gamma_{w,c} \times (0, \bar{t}) \\
\bar{U}_n^{(-)}\, T + \frac{\partial T}{\partial N_T} = \bar{U}_n^{(-)}\, d_T + Q_T \quad \text{on} \ \Gamma_{w,op} \times (0, \bar{t}) \\
\frac{\partial T}{\partial N_T} = 0 \quad \text{on} \ \Gamma_H \times (0, \bar{t})
\end{gathered} \tag{1.1}
$$

where $T = T(x, y, z, t)$ is the unknown temperature function, $t \in (0, \bar{t})$, $(x, y, z) \in D = \Omega \times (0, H)$, $\Omega \subset R^2$, $H = H(x, y)$ is the bottom relief function, $Q = Q(x, y, t)$ is the total heat influx, $\bar{U} = (u, v, w)$, $\hat{a}_T = \mathrm{diag}((a_T)_{ii})$, $(a_T)_{11} = (a_T)_{22} = \mu_T$, $(a_T)_{33} = \nu_T$, $f_T = f_T(x, y, z, t)$ are the given functions. The boundary $\Gamma \equiv \partial D$ of the domain is represented as a union of four nonintersecting parts Γ_S, $\Gamma_{w,\mathrm{op}}$, $\Gamma_{w,c}$, Γ_H, where $\Gamma_S = \Omega$ is the unperturbed sea surface, $\Gamma_{w,\mathrm{op}}$ is the liquid (open) part of the vertical boundary, $\Gamma_{w,c}$ is the solid part of the vertical lateral boundary, Γ_H is the sea bottom. For other notations and detailed formulation of the problem see [2, 3, 18].

Problem (1.1) can be written in the form of the following operator equation in $(W_2^1(D))^*$:

$$
\begin{gathered}
T_t + LT = F + BQ \quad \text{for a.e. } \ t \in (0, \bar{t}) \\
T = T_0 \quad \text{for } \ t = 0
\end{gathered} \tag{1.2}
$$

where the equality is understood in the weak sense, i.e.,

$$
(T_t, \widehat{T}) + (LT, \widehat{T}) = F(\widehat{T}) + (BQ, \widehat{T}) \quad \forall \widehat{T} \in W_2^1(D) \tag{1.3}
$$

and L, F, and B are defined by the following relations:

$$
(LT, \widehat{T}) \equiv \int_D (-T\mathrm{Div}(\bar{U}\widehat{T}))\mathrm{d}D + \int_{\Gamma_{w,\mathrm{op}}} \bar{U}_n^{(+)}\, T\widehat{T}\mathrm{d}\Gamma + \int_D \hat{a}_T \,\mathrm{Grad}(T) \cdot \mathrm{Grad}(\widehat{T})\mathrm{d}D
$$

$$
F(\widehat{T}) = \int_{\Gamma_{w,\mathrm{op}}} (Q_T + \bar{U}_n^{(-)}\, d_T)\widehat{T}\mathrm{d}T + \int_D f_T \widehat{T}\mathrm{d}D
$$

$$
(T_t, \widehat{T}) = \int_D T_t \widehat{T}\mathrm{d}D, \qquad (BQ, \widehat{T}) = \int_\Omega Q\widehat{T}|_{z=0}\mathrm{d}\Omega
$$

and the functions $\hat{a}_T$, Q_T, f_T, and Q are such that equality (1.3) makes sense.

It was shown in [3] that the operator L can be represented as the sum of nonnegative operators L_1 and L_2:

$$
L = L_1 + L_2
$$

where $L_1 = L - L_2$,

$$
(L_2 T, \widehat{T}) \equiv \int_D \left(-T\frac{1}{2}\Big(w_1 \frac{\partial T}{\partial z} + \frac{1}{r^2}\, \frac{\partial (r^2 w_1 T)}{\partial z}\Big) + \nu_T \frac{\partial T}{\partial z}\frac{\partial \widehat{T}}{\partial z} \right) \mathrm{d}D + \int_\Omega (\bar{U}_n^{(+)} + \gamma_T) T\widehat{T}\Big|_{z=0} \mathrm{d}\Omega.
$$

The operators L_1 and L_2 are nonnegative, which allows us to apply for equation (1.2) one of the splitting methods of *total approximation* (see [11]):

$$
\begin{gathered}
(T_1)_t + L_1 T_1 = F_1, \quad t \in (t_{j-1}, t_j) \\
T_1 = T_{j-1} \quad \text{for } \ t = t_{j-1}
\end{gathered} \tag{1.4}
$$

$$
\begin{aligned}
(T_2)_t + L_2 T_2 &= F_2 + BQ, \quad t \in (t_{j-1}, t_j) \\
T_2(t_{j-1}) &= T_1(t_j), \quad j = 1, 2, \dots, J
\end{aligned}
\tag{1.5}
$$

where

$$F_1 = F - F_2, \qquad F_2(\widehat{T}) = \int_D f_T \widehat{T} \mathrm{d}D, \quad t_0 = 0, \quad t_J = \bar{t}.$$

After solving subproblem (1.5), the function $T_2(t_j)$ is taken as an approximate solution to problem (1.2) for $t = t_j$:

$$T_2(t_j) \equiv T_j \cong T.$$

System of equations (1.4)–(1.5) considered on $\{(t_{j-1}, t_j)\}$ specifies the approximation of original problem (1.2) constructed by the splitting method. The equations for velocities, salinity, and sea level are approximated similarly [3].

2 Variational data assimilation problem for the sea surface temperature

We consider the sea surface temperature assimilation problem (see [3]). Suppose the function $Q \in L_2(\Omega \times (0, \bar{t}))$ is unknown in problem (1.1). Let the observation data function $T_{\mathrm{obs}}(x, y, t)$ be given on $\bar{\Omega} \equiv \Omega \cup \partial\Omega$ for $t \in (0, \bar{t})$, and in its physical sense this function is an approximation to the surface temperature function on Ω, i.e., to $T|_{z=0}$. Suppose $T_{\mathrm{obs}} \in L_2(\Omega \times (0, \bar{t}))$, however, the function T_{obs} may not possess a greater smoothness and hence it cannot be used as a boundary condition on Γ_S. We admit the case when T_{obs} is available only on a certain subset from $\Omega \times (0, \bar{t})$ whose characteristic function is denoted here by m_0. For definiteness sake, assume that T_{obs} is trivial outside this subset.

It should be noted that in this paper for T_{obs} we take the function of *mean daily observations* of the sea surface temperature on account of just this parameter is often available for assimilation. Note also that in problem (1.1) with the unknowns T and Q the closure equation has the form

$$T = T_{\mathrm{obs}} \quad \text{on } \Gamma_S \quad \text{for } t \in (0, \bar{t}). \tag{2.1}$$

If T_{obs} is taken as mean daily observations (i.e., the function T_{obs} is piecewise-constant on $(0, \bar{t})$), then we easily see that *such problem for determination of T and Q is ill posed* because the closure equation taken in this way, generally speaking, does not hold on $(0, \bar{t})$. However, we can present arguments allowing us to use it in variational assimilation problems. Thus, according to some sources (see, e.g., [14]), the surface temperature varies insignificantly within a day (often, this is several tenth of a degree). If we take into account that the calculation of sea temperature variations reach several degrees even with the use of modern models (without observation data assimilation), then the choice of the closure equation in form (2.1) looks quite reasonable, one should only write it in the 'least squares' sense (which, as a rule, is done in the theory of ill posed problems) with possible introduction of 'regularization'. Just this approach is applied in the present paper.

Below we assume that the observation data T_{obs} are given with errors, namely,

$$T_{\mathrm{obs}} = m_0 T^t|_{z=0} + \xi_{\mathrm{obs}}$$

where T^t is the exact solution to problem (1.1) for some $Q = Q^t$, and $\xi_{\mathrm{obs}} \in Y_{\mathrm{obs}} = L_2(\Omega \times (0, \bar{t}))$ can be considered as observation error. We assume that the errors ξ_{obs} are random and distributed according to the normal (Gaussian) law with zero mathematical expectation and the covariation operator $R\cdot = E[(\cdot, \xi_{\mathrm{obs}})\xi_{\mathrm{obs}}]$, $R : Y_{\mathrm{obs}} \to Y_{\mathrm{obs}}$, where E is the mathematical expectation. Covariance matrices of observation errors play an important role in variational data assimilation, their inverse matrices are included as weigh operators into the original cost functional. Below we assume that R is positive definite and hence invertible.

Thus, instead of the problem on determination of T and Q given by relations (1.1), (2.1), we consider the following problem of variational assimilation (see [3]): determine T and Q so that

$$\begin{cases} T_t + LT = F + BQ & \text{for a.e. } t \in (0, \bar{t}) \\ T = T_0 & \text{for } t = 0 \\ J_\alpha(Q) = \inf_Q J_\alpha(Q) \end{cases} \tag{2.2}$$

where

$$J_\alpha(Q) = \frac{\alpha}{2} \int_0^{\bar{t}} \int_\Omega |Q - Q^{(0)}|^2 \mathrm{d}\Omega \mathrm{d}t + \frac{1}{2} \sum_{j=1}^{J} J_{0,j}$$

$$J_{0,j} \equiv \int_{t_{j-1}}^{t_j} \int_\Omega (m_0 T|_{z=0} - T_{\text{obs}}) R^{-1} (m_0 T|_{z=0} - T_{\text{obs}}) \mathrm{d}\Omega \mathrm{d}t$$

and $Q^{(0)} = Q^{(0)}(x, y, t)$ is a given function, $\alpha = \text{const} > 0$.

For $\alpha > 0$ this problem of variational data assimilation has a unique solution. The existence of the optimal solution follows from classic results of the theory of extremal problems because it is not difficult to prove that the solution to problem (1.2) continuously depends on the flux Q (there are a priori estimates in the corresponding functional spaces).

For $\alpha = 0$ the problem does not always have a solution. However, as was shown in [3], for $R = I$ we have the unique and dense solvability, which allows us to construct a sequence of regularizing solutions minimizing the functional.

Instead of (1.2), we consider its approximation (1.4)–(1.5) by the splitting method. It was shown in [3] that the optimality system determining the solution to the formulated problem of variational data assimilation is reduced according to the necessary condition grad $J_\alpha = 0$ to sequential solution of some subproblems on (t_{j-1}, t_j), $j = 1, 2, \dots, J$. We present these subproblems on the interval (t_0, t_1) only.

On the interval (t_0, t_1) we have to solve the system of variational equations appearing in the minimization of the functional J_α on solutions of equations of the splitting method and consisting of (1.4)–(1.5), the system of adjoint equations

$$\begin{gathered} (T_2^*)_t + L_2^* T_2^* = BR^{-1}(m_0 T|_{z=0} - T_{\text{obs}}) \quad \text{for a.e. } t \in (t_0, t_1) \\ T_2^* = 0 \quad \text{for } t = t_1 \end{gathered} \tag{2.3}$$

$$\begin{gathered} (T_1^*)_t + L_1^* T_1^* = 0 \quad \text{for a.e. } t \in (t_0, t_1) \\ T_1^* = T_2^*(t_0) \quad \text{for } t = t_1 \end{gathered} \tag{2.4}$$

and the following optimality condition:

$$\alpha(Q - Q^{(0)}) + B^* T_2^* = 0 \quad \text{a.e. on } \Omega \times (t_0, t_1) \tag{2.5}$$

where L_1^*, L_2^*, and B^* are the operators adjoint to L_1, L_2, and B, respectively.

After that, the functions T_2, $Q(t_1)$ are taken as approximations to the components T, Q of the total solution to the problem for $t > t_1$, and $T_2(t_1) \cong T(t_1)$ is taken as the initial condition for T in the solution of problems on (t_1, t_2).

Let us consider the case $\alpha = 0$ separately. Let $t \in (t_0, t_1)$. In order to establish the unique solvability of the problem for $\alpha = 0$, we consider the homogeneous system

$$\begin{gathered} (T_1)_t + L_1 T_1 = 0, \quad t \in (t_0, t_1) \\ T_1 = 0 \quad \text{for } t = t_0 \end{gathered}$$

$$\begin{gathered} (T_2)_t + L_2 T_2 = BQ, \quad t \in (t_0, t_1) \\ T_2(t_0) = T_1(t_1) \end{gathered}$$

$$m_0 T_2 = 0 \quad \text{on} \quad \Omega \quad \text{for} \quad t \in (t_0, t_1)$$

assuming $\operatorname{supp}(m_0) = \bar{\Omega} \times [t_0, t_1]$. In this case it is easy to see that $T_1 \equiv 0$ in $D \times (t_0, t_1)$. After that, replacing the Neumann condition by the homogeneous Dirichlet condition on Ω (due to the last relation), we conclude that $T_2 \equiv 0$ in $D \times (t_0, t_1)$ and hence $Q = 0$ on $\Omega \times (t_0, t_1)$. Thus, the considered assimilation problem is uniquely solvable for any $\alpha \geqslant 0$.

Note that if $\operatorname{mes}(\Omega \times (t_0, t_1) \setminus \operatorname{supp}(m_0)) > 0$, then in the general case there is no uniqueness of the solution to the considered problem for $\alpha = 0$. However, this property will be valid again if Q is sought not on $\Omega \times (t_0, t_1)$, but on the same set where the observation data T_{obs} are presented.

In order to answer the question on the dense solvability of the problem for $\operatorname{supp}(m_0) = \bar{\Omega} \times [t_0, t_1]$, consider (2.3) for $w \equiv R^{-1} m_0 (T - T_{\text{obs}})$ with unknown w and condition (2.5) for $\alpha \equiv 0$. Note that (2.5) is the boundary condition in problem (2.3) for $z = 0$. In this case we conclude that $T_2^* \equiv 0$ in $D \times (t_0, t_1)$ and $w = 0$. Therefore, according to the theory of solvability of operator equations and problems of variational data assimilation (see [1]), the assimilation problem considered here (for $\alpha = 0$) is densely solvable and for the sequence of regularized solutions minimizing the functional J_0 we can take the sequence of solutions of variational data assimilation for $\alpha \to +0$, in this case we have $\inf J_{0,1} = 0$.

The assertion on the dense solvability of the problem on $D \times (t_0, t_1)$ remains valid in the case when Q is sought on the same set where T_{obs} is given. However, one can easily see that if for the unknown function Q we have $\operatorname{mes}(\operatorname{supp}(T_{\text{obs}}) \setminus \operatorname{supp}(Q)) > 0$, then the property of dense solvability of the assimilation problem (for $\alpha = 0$) is absent. In this case, generally speaking, we have $J_{0,1} > 0$ on the sequence of solution to the system of variational equations for $\alpha \to +0$.

The proof of the assertions formulated here on other intervals (t_{j-1}, t_j) is performed similarly and thus we prove the assertion on the whole interval $(0, \bar{t})$.

The assertion proved above allows us to formulate the corollary being principal for formulation and implementation of the numerical solution algorithm, i.e., *under the conditions of unique and dense solvability of the variational assimilation problem on* $\{(t_{j-1}, t_j)\}$, *the solution to the original assimilation problem on* $(0, \bar{t})$ *is reduced to sequential solution of the corresponding problems on the intervals* (t_{j-1}, t_j).

Consider one of solution algorithms for the problem studied here. We can approximately solve the complete numerical model on determination of the flux Q using the procedure of variational assimilation of the sea surface temperature in the following way: Let $Q^{(k)}$ be the approximation already constructed for Q, then, solving the direct problem for $Q \equiv Q^{(k)}$, we solve the corresponding adjoint problem and after that calculate the next approximation $Q^{(k+1)}$, i.e.,

$$Q^{(k+1)} = Q^{(k)} - \gamma_k (\alpha (Q^{(k)} - Q^{(0)}) + B^* T^*) \quad \text{a.e. on} \quad \Omega \times (t_0, t_1) \tag{2.6}$$

with the parameter γ_k providing the convergence of this iterative process [1]. After calculation of $Q^{(k+1)}$ we repeat the solution of the direct and adjoint problems with the new approximation $Q^{(k+1)}$, and after that calculate $Q^{(k+2)}$, etc. The iterations repeat until fulfillment of an appropriate convergence criterion.

Due to the property of dense solvability, for $\{\gamma_k\}$ we can take the parameters calculated by the following formula for $\alpha \approx +0$ (see [1]):

$$\gamma_k = \frac{1}{2} \int_{t_0}^{t_1} \int_{\Omega} (m_0 T|_{z=0} - T_{\text{obs}}) R^{-1} (m_0 T|_{z=0} - T_{\text{obs}}) \, \mathrm{d}\Omega \mathrm{d}t \Big/ \int_{t_0}^{t_1} \int_{\Omega} (T_2^*)^2 \Big|_{z=0} \mathrm{d}\Omega \mathrm{d}t$$

which may essentially accelerate the convergence of the iterative process.

Remark 2.1. Since we used mean daily data for T_{obs} in numerical experiments, then by the mean value theorem there exists at least one point t_{j_k} such that the value T_{obs} at that point is close to the mean daily value for the kth day. Given the points $\{t_{j_k}\}$, $k = 1, \dots, K$, we may use the following characteristic function m_0 for the assimilation procedure:

$$m_0 = \begin{cases} 1, & \text{for} \quad t \in \bigcup_{k=1}^{K} (t_{j_k - 1}, t_{j_k}) \\ 0, & \text{otherwise.} \end{cases}$$

Following [3], one can easily see that the properties of unique and dense solvability of the assimilation problem remain valid for this case as well if we seek for Q on the same set where T_{obs} is given.

3 Results of numerical experiments

In this section we present the results of numerical experiments for solution of the inverse problem on reconstruction of the heat flux function Q in the water area of the Baltic Sea by variational assimilation of the sea surface temperature data with the use of the covariance matrix of observation errors.

In these numerical experiments we used the modifications of boundary conditions and their coefficients in accordance to [17, 19].

The model domain of the Baltic Sea is positioned from 9.375 E to 30.375 E and from 53.625 N to 65.9375 N. The spatial distribution of the model is 1/16°×1/32°×25 in the longitude, latitude, and vertical direction, respectively. The grid domain contains 336×394 nodes in the horizontal plane and σ-levels are nonuniformly distributed over depth. The step in time is 5 min. The domain with topography of the Baltic Sea is presented in Fig. 1.

The values of T_{obs} corresponded to mean daily values of the Baltic Sea surface temperature according to the data of the Danish Meteorological Institute measured by radiometers (AVHRR, AATSR, AMSRE) and spectral radiometers (SEVIRI and MODIS) [6]. The observation data were recalculated on the calculation grid of the numerical model of the Baltic Sea thermodynamics using data interpolation algorithms [15, 16].

In our experiments for weight coefficients in the cost functional in solution of the data assimilation problem we took the diagonal elements of the covariance matrix R calculated based on the statistical properties of observation data.

In the finite-dimensional case the covariation operator R is a covariance matrix and is determined by the formula

$$R = E[\xi_{\text{obs}}\xi_{\text{obs}}^T] = E[(T_{\text{obs}} - \bar{T}_{\text{obs}})(T_{\text{obs}} - \bar{T}_{\text{obs}})^T]$$

where $\bar{T}_{\text{obs}}$ is the mathematical expectation of the observation data function.

If $\xi_{\text{obs}} = (\xi_1, \dots, \xi_N)^T$, then the elements of the matrix R can be written in the form

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

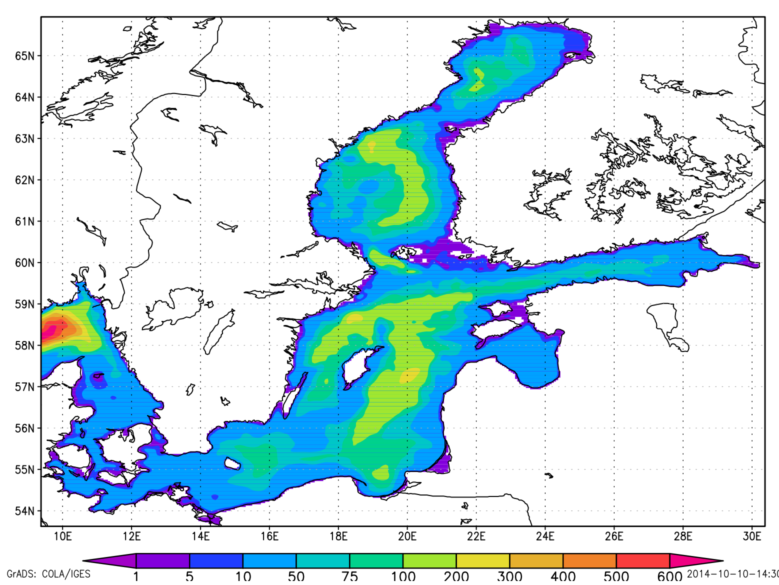


Fig. 1: Computational domain of the Baltic Sea with depths, m.

The values r_{jk} are the covariation coefficients between the jth and kth coordinates of the random vector ξ_{obs}. For $j = k$ we get

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

where $D\xi_j$ is the variance of the random variable ξ_j (the second central moment of the distribution), i.e.,

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

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

Therefore, the diagonal elements of the matrix R are the variances $D\xi_j$, and they play an important role in the weight adjustment of the cost functional in the variational data assimilation. In practice, in variational assimilation one often assumes [13] that the matrix R is diagonal with the elements $D\xi_j$ calculated based on the statistical properties of observation data. Thus, if $\xi^{(1)}, \dots, \xi^{(n)}$ is the sequence of implementations 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 (sample mean)

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

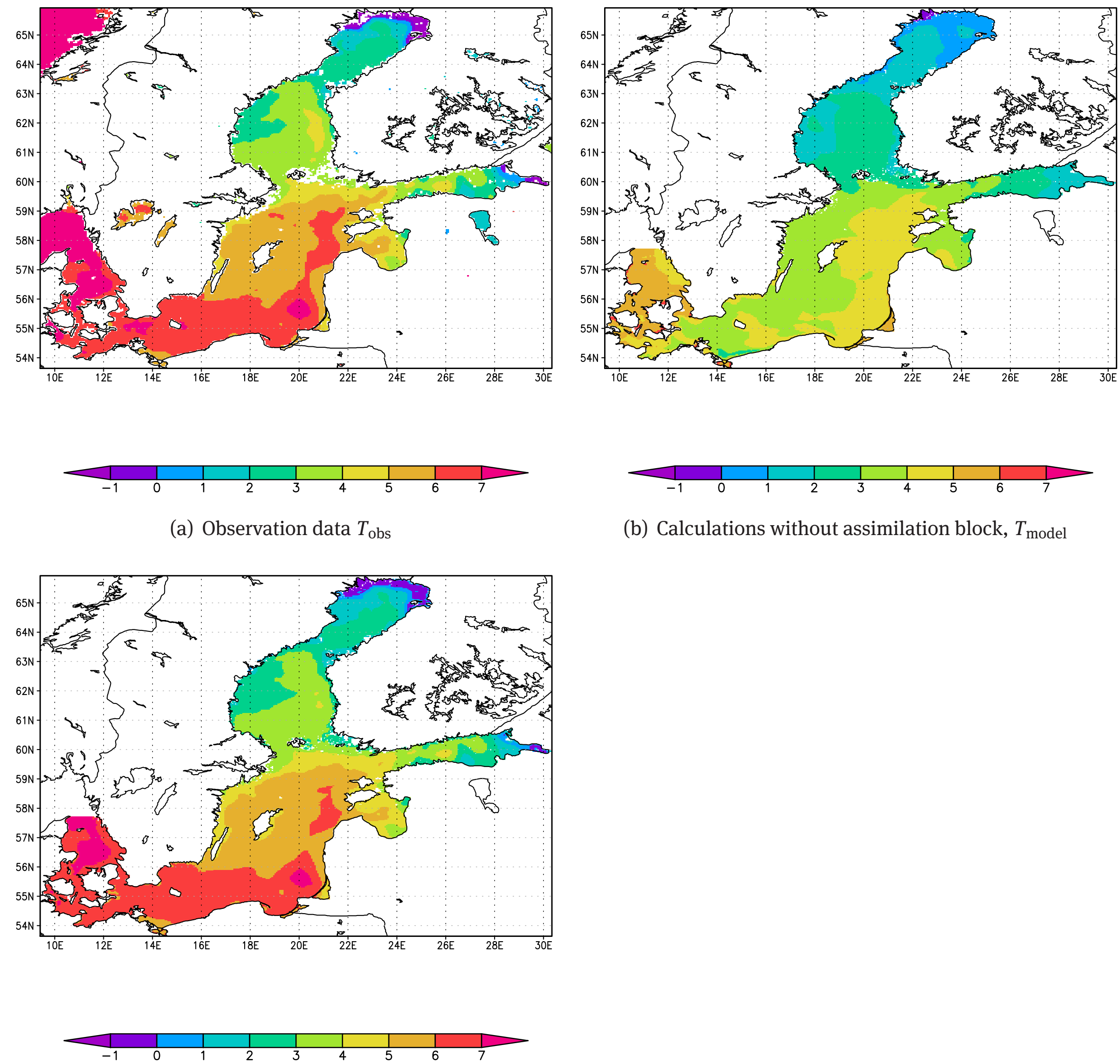
Due to the assumption $E\xi_{\text{obs}} = 0$, is it easy to see that $DT_{\text{obs}} = D\xi_{\text{obs}}$, i.e., the variance of the observation data errors equals the variance of observation data and hence in our case it can be calculated based on the SST data for a long period of time. In this work we calculated statistical averaging $\bar{T}_{\text{obs}}$ and mean square deviations σ of SST in the Baltic Sea water area. The statistical characteristics were calculated based on the observation data for 27 years beginning from 1982 to 2009 (Copernicus Marine environment monitoring service, Product ID SST_Bal_SST_L4_rep_observation_010_016) separately for each day of the year.

Let us present the results of numerical calculations (on the example of the Baltic Sea water area) for the inverse problem on reconstruction of the heat flux function Q by variational assimilation of sea surface temperature data using covariance matrices of observation data errors.

Using the model of sea hydrothermodynamics presented above and supplied with the 'assimilation procedure' for the sea surface temperature T_{obs}, we carried out calculations using the assimilation algorithm. The calculations included assimilation of T_{obs} for the period of 5 days (January 2007).

Figure 2 presents the results of this experiment. Figure 2a shows the mean value of the temperature field on January 5 according to the satellite data. The mean value of the sea surface temperature (SST) on the fifth calculation day (daily mean) obtained by the model without assimilation block is shown in Figure 2b, and Figure 2c shows the mean SST field for the same day calculated with the use of the assimilation procedure and with the use of the covariance matrix of observation errors. Figure 3 presents differences of mean daily values of SST on the last calculation day (January 5). Thus, Figure 3a shows the deviation of the mean daily SST field calculated by the model without the assimilation block (T_{model}) from the observation data T_{obs}. Figure 3b presents the deviation of the observation data for the SST field calculated with the assimilation block and using the covariance matrix of observation errors (T_{cov}). The difference between the calculations by the models without assimilation and with assimilation block using elements of the covariance matrix of observation errors is presented in Figure 3c. We also carried out calculations with assimilation block, but without covariance matrix of observation errors (i.e., when $R = E$), the obtained SST field is denoted in Fig. 3d by T_{assim}.

As can be seen in Fig. 3, the use of the observation data assimilation block in the model essentially improves predictive properties of the model. One can also see that the calculation with the assimilation block and without the covariance matrix differs insignificantly from the calculation with the use of elements of the covariance matrix, although certain corrections to the solution appear in some parts of the water area.



(a) Observation data T_{obs}

(b) Calculations without assimilation block, T_{model}

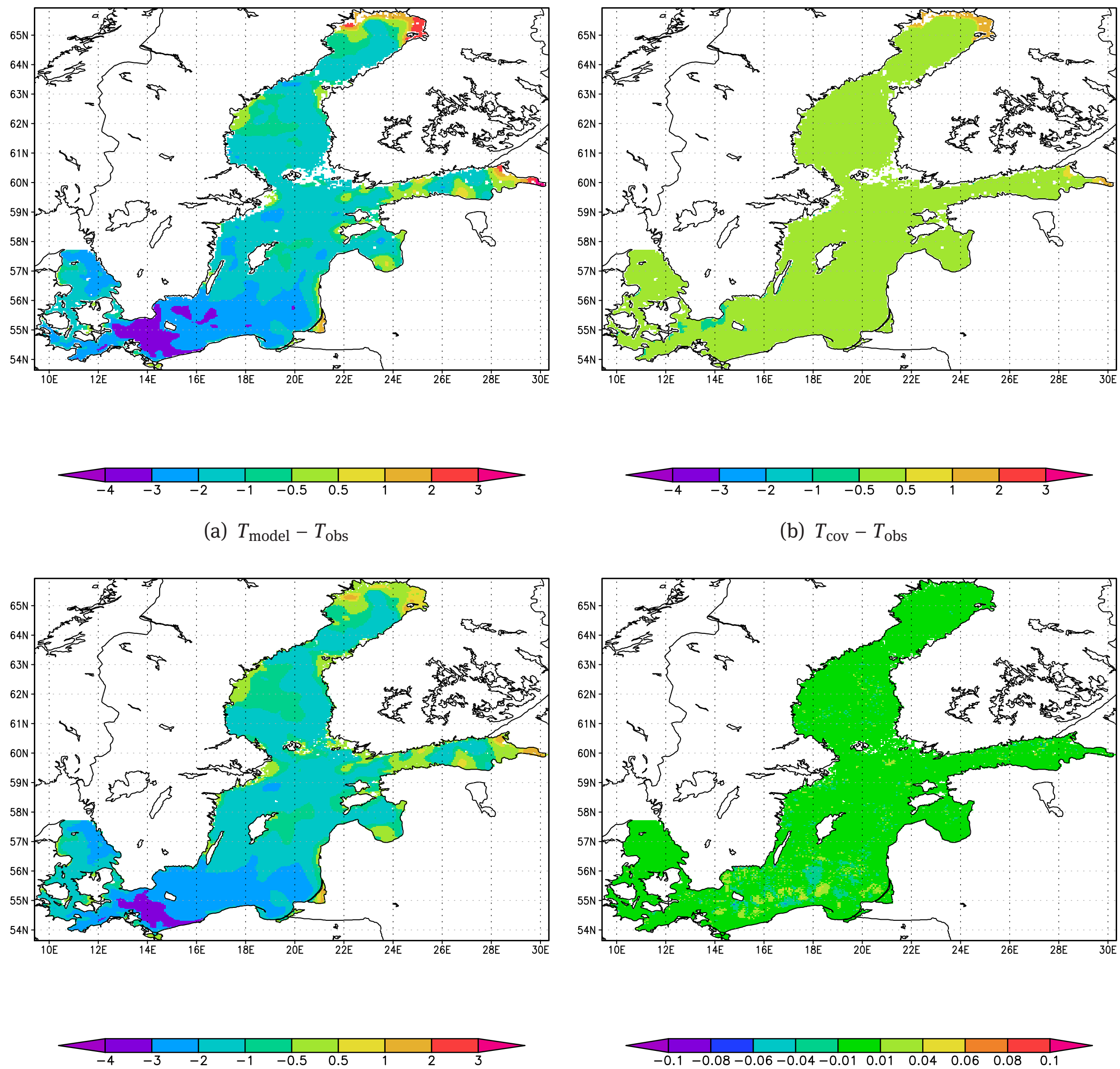
(c) Calculations with assimilation block, T_{cov}

Fig. 2: Numerical calculations for 5 days. Mean value of T on the 5th day, °C.

Figure 4 presents the values of the mean daily temperature on the fifth day in the section of the Baltic Sea water area along 20°N. The section of the temperature field along 56°N for the same period of time is presented in Fig. 5.

Figures 4c and 5c show the differences between the calculations by the model without assimilation and with assimilation using the covariation matrix. One can see that with the SST assimilation procedure the changes in temperature can be found on the surface layer while the temperature values in other layers remain practically unchanged. Thus, we may conclude that the depth temperature values calculated by the model can be 'corrected' only in the presence of observation data in depth.

The use of the diagonal elements of the observation data covariance matrix weakly affect the data assimilation procedure, as shown in Fig. 6. The mean daily value of SST on the 5th day of calculation in the section along 55°N calculated with the use of the observation data covariance matrix are presented in Fig. 6a, the calculations without the covariance matrix are shown in Fig. 6b, their difference is shown in Fig. 6c.



(a) $T_{\text{model}} - T_{\text{obs}}$

(b) $T_{\text{cov}} - T_{\text{obs}}$

(c) $T_{\text{model}} - T_{\text{cov}}$

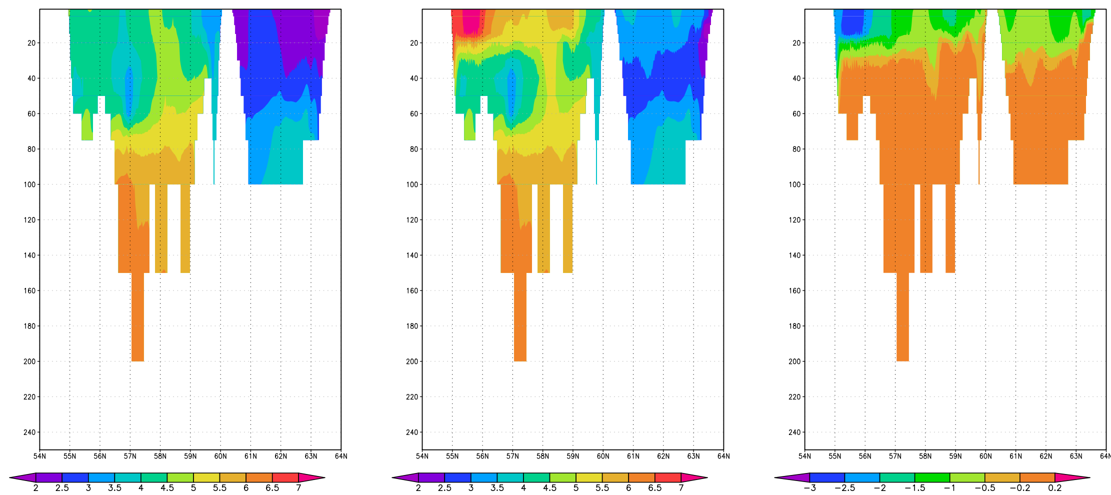
(d) $T_{\text{assim}} - T_{\text{cov}}$

Fig. 3: Numerical calculations for 5 days. Difference of mean values of T on the 5th day, $^\circ$C.

The results of numerical experiments also showed that the SST assimilation procedure weakly affects other components of the full solution to the problem such as salinity, flow velocities, and level surface. Thus, Figure 7 presents mean daily values of the salinity in the Baltic Sea water area on the 5th calculation day. Figures 7a and 7b correspond to the section along 20°E and Figures 7c and 7d correspond to the section along 56°N. Here S_{model} is the salinity calculated without the SST assimilation block and $S_{T_{cov}}$ are the obtained values of the salinity with the SST assimilation block and the use of observation error covariance matrix.

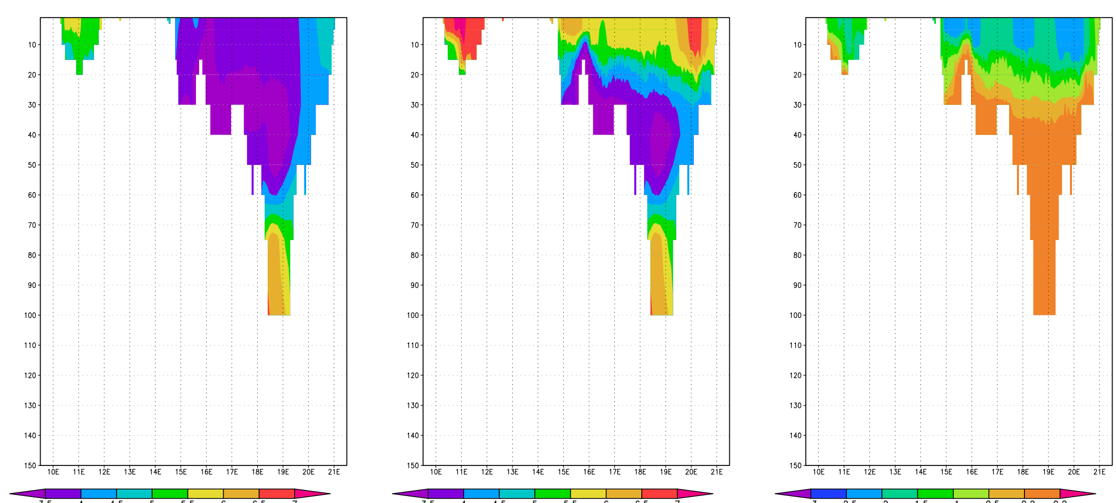
4 Conclusion

The numerical algorithm for solving the problem of variational assimilation of the sea surface temperature data for reconstruction of heat fluxes on the surface using the three-dimensional model of the Baltic Sea hydrothermodynamics developed at the INM RAN (V. B. Zalesny, N. A. Dianskii, A. V. Gusev) is formulated and studied in the paper. The diagonal elements of the observation errors covariance matrix calculated based on



(a) Calculations without assimilation (b) Calculations with assimilation block (c) Difference $T_{\text{model}} - T_{\text{cov}}$

Fig. 4: Numerical calculations for 5 days. The section along 20° E. Temperature, °C.

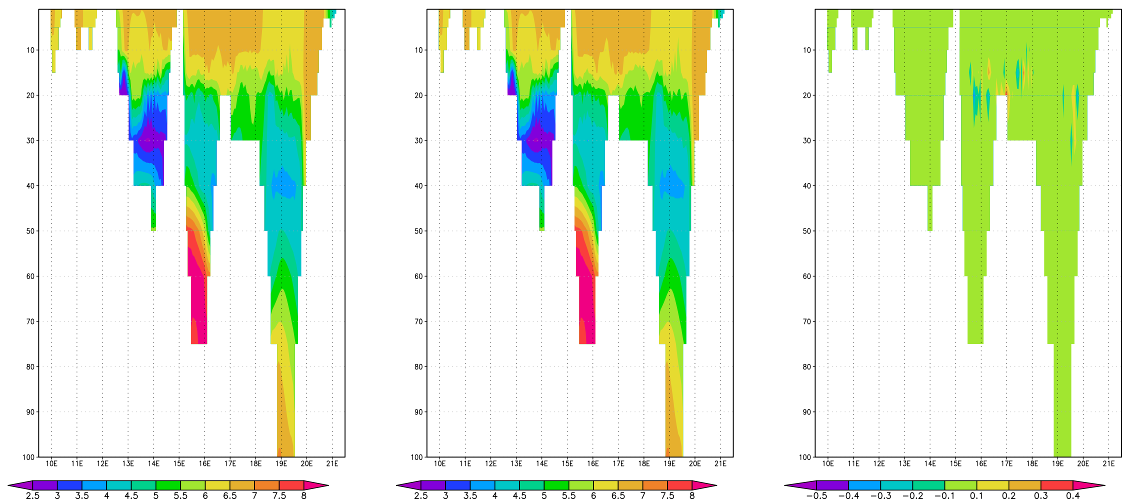


(a) Calculations without assimilation (b) Calculations with assimilation block (c) Difference $T_{\text{model}} - T_{\text{cov}}$

Fig. 5: Numerical calculations for 5 days. The section along 56°N. Temperature, °C.

statistical properties of observation data are used as weight functions of the cost functional in the assimilation problem.

The results of numerical calculations allow us to conclude about the efficiency of the model using variational assimilation procedures with inclusion of the observation error covariance matrix. We adjust the work of the model and obtain results close to observed data by using the assimilation procedure. However, it is worth noting that the SST assimilation procedure has a weak influence on other components of the full solution to the problem. Therefore, for more accurate calculation of thermodynamic parameters it is necessary to have a more complete set of observation data not only for the temperature on the surface but in depth and also for the salinity, flow velocities, and sea level. In this case, the predictive properties of the model can be significantly improved.

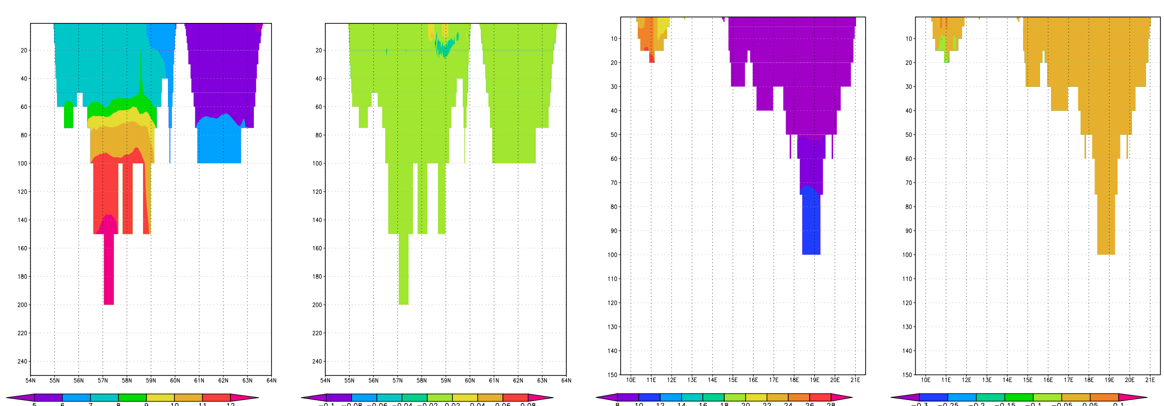


(a) Calculations with covariance matrix

(b) Calculations without covariance matrix

(c) Difference $T_{\text{cov}} - T_{\text{assim}}$

Fig. 6: Numerical calculations for 5 days. The section along 55°N. Assimilation of temperature, °C.



(a) Section along 20°E. Calculations with assimilation block

(b) Section along 20°E. Difference $S_{\text{model}} - S_{T_{\text{cov}}}$

(c) Section along 56°N. Calculations with assimilation block

(d) Section along 56°N. Difference $S_{\text{model}} - S_{T_{\text{cov}}}$

Fig. 7: Numerical calculations for 5 days. The sections in the Baltic Sea water area. Salinity, ‰.

The iterative procedures used in the data assimilation block demonstrated rather good convergence. We applied 3–5 iterations to achieve the required accuracy for the flux with the use of an especially calculated optimal iteration parameter. However, due to a large number of spatial steps of the grid, the complete calculation in the whole water area of the Baltic Sea required considerable time. This problem may be solved by applying parallel computation algorithms because the implementation peculiarities of the assimilation procedure allow us to use independent parallel calculations of assimilation parameters for all grid points simultaneously.

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References

[1] V. I. Agoshkov, *Methods of Optimal Control and Adjoint Equations in Problems of Mathematical Physics*. INM RAS, Moscow, 2003 (in Russian).

[2] V. I. Agoshkov, A. V. Gusev, N. A. Dianskii, and R. V. Oleinikov, An algorithm for the solution of the ocean hydrothermodynamics problem with variational assimilation of the sea level function data. *Russ. J. Numer. Anal. Math. Modelling* **22** (2007), No. 2, 1–10.

[3] V. I. Agoshkov, E. I. Parmuzin, and V. P. Shutyaev, Numerical algorithm for variational assimilation of sea surface temperature data. *Comp. Math. Math. Phys.* **48** (2008), No. 8, 1293–1312.

[4] V. I. Agoshkov, E. I. Parmuzin, V. B. Zalesny, V. P. Shutyaev, N. B. Zakharova, and A. V. Gusev, Variational assimilation of observation data in the mathematical model of the Baltic Sea dynamics. *Russ. J. Numer. Anal. Math. Modelling* **30** (2015), No. 4, 203–212.

[5] V. V. Alekseev and V. B. Zalesny, Numerical model of large-scale ocean dynamics. In: *Vychislitelnye processy i sistemy* (Computational processes and systems), Nauka, Moscow, 1993, pp. 232–253 (in Russian).

[6] I. Karagali, J. Hoyer, and C. B. Hasager, SST diurnal variability in the North Sea and the Baltic Sea. *Remote Sensing of Environment* **121** (2012), 159–170. doi: 10.1016/j.rse.2012.01.016.

[7] F. X. Le Dimet and O. Talagrand, Variational algorithms for analysis and assimilation of meteorological observations: theoretical aspects. *Tellus* **38A** (1986), 97–110.

[8] J. L. Lions, *Contrôle Optimal des Systèmes Gouvernés par des Équations aux Dérivées Partielles*. Dunod, Paris, 1968.

[9] G. I. Marchuk, *Adjoint Equations and Analysis of Complex Systems*. Kluwer, Dordrecht, 1995.

[10] G. I. Marchuk, V. P. Dymnikov, and V. B. Zalesny, *Mathematical Models in Geophysical Fluid Dynamics and Numerical Methods for Their Implementation*. Gidrometeoizdat, Leningrad, 1987 (in Russian).

[11] G. I. Marchuk, Splitting and alternative direction methods. In: *Handbook of Numerical Analysis* (Eds. P. G. Ciarlet and J. L. Lions). North-Holland, Amsterdam, 1990, Vol. 1, pp. 197–462.

[12] G. I. Marchuk, A. S. Rusakov, V. B. Zalesny, and N. A. Dianskii, Splitting numerical technique with application to the high resolution simulation of the Indian ocean circulation. *Pure and Applied Geophysics* **162** (2005), 1407–1429.

[13] K. Mogensen, M. A. Balmaseda, A. T. Weaver, M. Martin, and A. Vidard, *NEMOVAR: A Variational Data Assimilation System for the NEMO Ocean Model*. ECMWF Technical Memorandum No. 120, 2009.

[14] H. U. Roll, *Physics of the Marine Atmosphere*. Academic Press, New York, 1965.

[15] N. B. Zakharova, Verification of the sea surface temperature observation data. *Current Problems of Remote Sensing of the Earth from Space* **13** (2016), No. 3. 106–113.

[16] N. B. Zakharova, V. I. Agoshkov, and E. I. Parmuzin, The new method of ARGO buoys system observation data interpolation. *Russ. J. Numer. Anal. Math. Modelling* **28** (2013), No. 1, 67–84.

[17] V. B. Zalesny, G. I. Marchuk, V. I. Agoshkov, A. V. Bagno, A. V. Gusev, N. A. Dianskii, S. N. Moshonkin, R. Tamsalu, and E. M. Volodin, Numerical simulation of large-scale ocean circulation based on multicomponent splitting method. *Russ. J. Numer. Anal. Math. Modelling* **25** (2010), No. 6, 581–609.

[18] V. B. Zalesny, A. V. Gusev, V. O. Ivchenko, R. Tamsalu, and R. Aps, Numerical model of the Baltic Sea circulation. *Russ. J. Numer. Anal. Math. Modelling* **28** (2013), No. 1, 85–100.

[19] V. B. Zalesny, A. V. Gusev, S. Yu. Chernobai, R. Aps, R. Tamsalu, P. Kujala, and J. Rytkönen, The Baltic Sea circulation modelling and assessment of marine pollution. *Russ. J. Numer. Anal. Math. Modelling* **29** (2014), No. 2, 129–138.