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4D Technology of Variational Data Assimilation for Sea Dynamics Problems

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The technology aimed at high-performance computing is presented for modeling the sea dynamics problems based on 4D variational data assimilation technique developed at the Marchuk Institute of Numerical Mathematics, Russian Academy of Sciences (INM RAS). The technology is based on the multicomponent 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 with observation data and observation error covariances. Efficient algorithms for solving the variational data assimilation problems are presented based on modern iterative processes with a special choice of iterative parameters. The technology is illustrated for the Baltic Sea dynamics model with variational data assimilation to restore the initial states and the heat fluxes on the sea surface.

Keywords: sea dynamics modeling, variational data assimilation, observations, sea surface temperature.

Introduction

In recent years, there has been an increasing interest in research methods and numerical solution of inverse and data assimilation problems, which play a fundamental role in the theoretical understanding and mathematical modeling of processes and phenomena from various fields of knowledge. The data assimilation technique is widely used in geosciences to develop high-performance 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 assimilated into atmospheric and oceanic models in order to obtain the initial and/or boundary conditions (and other model parameters) for further modeling and forecasting [1, 7, 8, 12, 15, 16, 18, 22, 25].

A significant progress in solving data assimilation problems has been the use of variational methods and, in particular, optimal control methods. The development of this direction at the INM RAS was initiated by Academician Guriy I. Marchuk [18]. These approaches were the main content of research of G.I. Marchuk and his scientific school in various fields of mathematics and applications [1, 4, 5, 18, 25].

The variational data assimilation 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, which is very complicated from the computational point of view. The problem adjoint

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to the original nonlinear problem has a more complex form, and for solving the adjoint problem, it is required to store 4D arrays of the solutions of the direct problem in machine memory.

Ocean general circulation models are very complex systems, which are based on nonlinear differential equations describing the evolution of three-dimensional fields of currents, temperature and salinity, as well as pressure and density [9, 11, 13, 21], and require the development of efficient numerical methods for a long-time integration. This underlines the importance of high-performance computing for such problems. The ocean hydrodynamics INMOM model (INM ocean model) is described by primitive equations in the sigma-coordinate system, which is solved by finite-difference methods [11, 24, 27]. Its numerical implementation is based on the method of splitting according to physical processes and spatial coordinates [17, 27], 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 is based on the talk given at the Lomonosov Moscow State University Seminar "Supercomputer Modelling of the Earth System" (headed by V.A. Sadovnichy) and presents some approaches to solving the problems of variational data assimilation, developed at the INM RAS last year. 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 observation errors. On the basis of variational assimilation of observational data, algorithms are proposed for solving inverse problems of restoring initial conditions and heat fluxes on the sea surface. This is the novelty of this paper compared to the previous studies [3–6, 25]. The results of numerical experiments for the Baltic Sea area are discussed.

The article is organized as follows. Section 1 is devoted to the the mathematical model of sea dynamics using the splitting method. In Section 2 we give the statement of the variational data assimilation problem and formulate the algorithms for its solution. Section 3 contains the results of numerical experiments for the Baltic Sea water area. The main results are discussed in the Conclusions.

1. Mathematical Model of Sea Dynamics

We consider the system of equations of sea hydrothermodynamics in geographical coordinates under hydrostatics and Boussinesq approximations [2, 19], in the domain D of variables (x, y, z) for $t \in (0, \bar{t})$:

$$\begin{cases} \dfrac{d\vec{u}}{dt} + \begin{bmatrix} 0 & -f \\ f & 0 \end{bmatrix} \vec{u} - g\mathbf{grad}\zeta + A_u\vec{u} + (A_k)^2\vec{u} = \vec{F} - \dfrac{1}{\rho_0}\mathbf{grad}P_a - \\ \qquad -\dfrac{g}{\rho_0}\mathbf{grad}\displaystyle\int_0^z \rho_1(T,S)dz', \\ \dfrac{\partial\zeta}{\partial t} - m\dfrac{\partial}{\partial x}(\displaystyle\int_0^H \Theta(z)udz) - m\dfrac{\partial}{\partial y}(\displaystyle\int_0^H \Theta(z)\dfrac{n}{m}vdz) = f_3, \\ \dfrac{dT}{dt} + (\bar{U}, \mathbf{Grad})\,T + A_T T = f_T,\ \dfrac{dS}{dt} + (\bar{U}, \mathbf{Grad})S + A_S S = f_S, \end{cases} \tag{1}$$

where $\bar{U} = (u, v, w)$ is the velocity vector, ζ is the sea surface level function, T is the temperature, S is the salinity, $\vec{u}=(u, v)$, $\rho_1(T, S) = \rho_0\beta_T\left(T - T^{(0)}\right) + \rho_0\beta_S\left(S - S^{(0)}\right) + \gamma\rho_0\beta_{TS}(T, S)$ is the water density, P_a is the atmospheric pressure, $\vec{F} = (F_1, F_2)$ is the forcing, f_T, f_S are the functions of the 'internal' sources, $\rho_0 = const \approx 1$ is the mean density, $T^{(0)}$, $S^{(0)}$ 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, $\beta_T,\beta_S,\gamma,g=const, A_\varphi\varphi\equiv -\mathbf{Div}\,(\hat{a}_\varphi\mathbf{Grad}\varphi)$, $m=1/(r\cos y), n=1/r, r=R-z\approx R$, $\Theta(z)\equiv(R-z)/R\approx 1$, R is the Earth radius.

The operators $A_\varphi\varphi\equiv-\mathbf{Div}(\hat{a}_\varphi\mathbf{Grad}\varphi)$ involve $\hat{a}_\varphi=diag((a_\varphi)_{ii})$, 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 diffusion coefficients that are supposed to be positive bounded functions. The fourth order operator $(A_k)^2$, with A_k taken for $A_\varphi=A_k$, is defined by the matrix $\hat{k}=diag\{k_{ii}\}$ with nonnegative diagonal elements k_{ii} that are viscosity coefficients in respective directions. We consider $f=f(u)=l+mu\sin y\ \equiv l+f_1(u)$, where $l=l(y)$ is the Coriolis parameter $l=2\omega\sin y$, and ω is the Earth angular rotaton speed.

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. These functions are equal to 1 on the corresponding parts, otherwise they are equal to zero.

The unit outer normal vector to Γ is denoted by $\overrightarrow{N}\equiv(N_1,N_2,N_3)$, with $\overrightarrow{N}=(0,0,-1)$ on Γ_S and $\overrightarrow{N}=(N_1,N_2,0)$ on $\Gamma_w=\Gamma_{w,op}\bigcup\Gamma_{w,c}$, and $\vec{n}\equiv(N_1,N_2)\equiv(n_1,n_2)$ 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 $\bar{U}=(u,v,w)$ on the boundary Γ, the normal components are denoted by $U_n: U_n=\bar{U}\cdot\overrightarrow{N}=uN_1+vN_2+wN_3$. 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.

The hydrostatics approximation means that $\dfrac{\partial P}{\partial z}=g\rho$, where P is the pressure, $\rho=\rho_0+\rho_1$. This equation is used to find P after solving the system (1). Due to this relation, the pressure gradient in (1) is divided into three terms: the gradients of the atmospheric pressure, sea surface elevation, and water column pressure deviation.

We consider the equations (1) in $D\times(0,\bar{t})$ with the following boundary and initial conditions [2].

Boundary conditions on Γ_S:

$$\begin{cases}\left(\int\limits_0^H\Theta\vec{u}dz\right)\vec{n}=0\,\text{on}\,\partial\Omega,\\ U_n^{(-)}u-\nu\dfrac{\partial u}{\partial z}-k_{33}\dfrac{\partial}{\partial z}A_k u=\tau_x^{(a)}\Big/\rho_0,\ U_n^{(-)}v-\nu\dfrac{\partial v}{\partial z}-k_{33}\dfrac{\partial}{\partial z}A_k v=\tau_y^{(a)}\Big/\rho_0,\\ A_k u=0,\quad A_k v=0,\\ U_n^{(-)}T-\nu_T\dfrac{\partial T}{\partial z}+\gamma_T(T-T_a)=Q_T,\\ U_n^{(-)}S-\nu_S\dfrac{\partial S}{\partial z}+\gamma_S(S-S_a)=Q_S,\end{cases}\qquad(2)$$

where $\tau_x^{(a)}$, $\tau_y^{(a)}$ are the tangent wind stress components along the axes Ox and Oy, respectively, on the sea surface $z=0$, γ_T, γ_S are the coefficients of relaxation to the specified values of temperature T_a and salinity S_a, respectively, k_{33} is the vertical viscosity coefficient, ν is the turbulent exchange coefficient, and Q_T, Q_S are the surface heat and salinity fluxes, respectively.

We have also $U_n|_{z=0} = -w|_{z=0}$, where $w = w(u,v)$ is defined by the formula

$$w(x,y,z,t) = \frac{1}{r}\left(m\frac{\partial}{\partial x}\left(\int\limits_z^H rudz'\right) + m\frac{\partial}{\partial y}\left(\frac{n}{m}\int\limits_z^H rvdz'\right)\right),\ (x,y,t) \in \Omega \times (0,\bar{t}). \tag{3}$$

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

$$U_n = 0, \quad A_k\tilde{U} = 0, \quad \frac{\partial \tilde{U}}{\partial N_u}\cdot\tau_w + \left(\frac{\partial}{\partial N_u}A_k\tilde{U}\right)\cdot\tau_w = 0, \frac{\partial T}{\partial N_T} = 0, \frac{\partial S}{\partial N_S} = 0, \tag{4}$$

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

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

$$\begin{cases} U_n^{(-)}(\tilde{U}\cdot\vec{N}) + \dfrac{\partial\tilde{U}}{\partial N_u}\cdot\vec{N} = 0, \quad A_k\tilde{U} = 0 \\ U_n^{(-)}(\tilde{U}\cdot\tau_w) + \dfrac{\partial\tilde{U}}{\partial N_u}\cdot\tau_w + \left(\dfrac{\partial}{\partial N_u}A_k\tilde{U}\right)\cdot\tau_w = 0, \\ U_n^{(-)}T + \dfrac{\partial T}{\partial N_T} = Q_T,\, U_n^{(-)}S + \dfrac{\partial S}{\partial N_S} = Q_S, \end{cases} \tag{5}$$

where Q_T, Q_S are the heat and salinity fluxes, respectively.

Boundary conditions on Γ_H (on the bottom):

$$\begin{cases} w = um\dfrac{\partial H}{\partial x} + vn\dfrac{\partial H}{\partial y}, \quad A_k\tilde{U} = 0, \quad \dfrac{\partial T}{\partial N_T} = 0, \quad \dfrac{\partial S}{\partial N_S} = 0, \\ \dfrac{\partial\tilde{U}}{\partial N_u}\cdot\tau_x + \left(\dfrac{\partial}{\partial N_u}A_k\tilde{U}\right)\cdot\tau_x = \tau_x^{(b)}/\rho_0\,, \quad \dfrac{\partial\tilde{U}}{\partial N_u}\cdot\tau_y + \left(\dfrac{\partial}{\partial N_u}A_k\tilde{U}\right)\cdot\tau_y = \tau_y^{(b)}/\rho_0, \end{cases} \tag{6}$$

where τ_x, τ_y is the system of unit orthogonal vectors of the coordinate system corresponding to x and y directions; $\tau_x^{(b)}$, $\tau_y^{(b)}$ are the projections of the bottom friction vector on the axes Ox, Oy, respectively.

Initial conditions for u, v, T, S, ζ:

$$u = u^0, v = v^0, T = T^0, S = S^0, \zeta = \zeta^0, \text{ for } t = 0, \tag{7}$$

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 the system (1)–(7). If the functions u, v, ζ, T, S are found, then the function w is determined by formula (3).

The main features of the numerical model of sea dynamics INMOM are the simultaneous use of the splitting method [17, 27] and the σ-coordinate system [24, 27] for (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)–(7) before applying suitable splitting schemes and other numerical procedures [20].

In order to approximate the model (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)–(7) on (t_{j-1}, t_j), assuming that the vector of the approximate solution $\phi_k \equiv (u_k, v_k, \xi_k, T_k, S_k)$, $k = 1, 2, ..., j-1$ at the previous intervals, is already defined. To approximate the problem, we use one of the schemes of the total approximation method [17], which consists in the implementation of the following steps.

Step 1. Consider the problem

$$T_t + (\bar{U}, \mathbf{Grad})\, T - \mathbf{Div}\, (\hat{a}_T \cdot \mathbf{Grad}\, T) = f_T \;\text{ in }\; D \times (t_{j-1}, t_j) \tag{8}$$

under corresponding boundary and initial conditions.

Step 2. Solve the problem

$$S_t + (\bar{U}, \mathbf{Grad})S - \mathbf{Div}(\hat{a}_S \cdot \mathbf{Grad}\, S) = f_S \;\text{ in }\; D \times (t_{j-1}, t_j) \tag{9}$$

under appropriate boundary and initial conditions.

Step 3. The system

$$\begin{cases} \underline{u}_t^{(1)} + \begin{bmatrix} 0 & -l \\ l & 0 \end{bmatrix} \underline{u}^{(1)} - g\mathbf{grad}\zeta = \vec{F} - \dfrac{1}{\rho_0}\mathbf{grad}\left(P_a + g\int\limits_0^z \rho_1(\bar{T}, \bar{S})dz^{'} \right) \\ \qquad\qquad \text{in }\; D \times (t_{j-1}, t_j), \\ \zeta_t - \mathbf{div}\left(\int\limits_0^H \Theta \underline{u}^{(1)} dz \right) = f_3 \;\text{ in }\; \Omega \times (t_{j-1}, t_j), \\ \underline{u}^{(1)} = \underline{u}_{j-1},\; \zeta = \zeta_{j-1} \;\text{ for }\; t = t_{j-1},\; \underline{u}_j^{(1)} \equiv \underline{u}^{(1)}(t_j) \text{ in } D \end{cases} \tag{10}$$

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

$$\begin{cases} \underline{u}_t^{(2)} + \begin{bmatrix} 0 & -f_1(\bar{u}) \\ f_1(\bar{u}) & 0 \end{bmatrix} \underline{u}^{(2)} = 0 \;\text{ in }\; D \times (t_{j-1}, t_j), \\ \\ \underline{u}^{(2)} = \underline{u}_j^{(1)} \;\text{ for }\; t = t_{j-1},\; \underline{u}_j^{(2)} \equiv \underline{u}^{(2)}(t_j) \;\text{ in }\; D, \end{cases} \tag{11}$$

$$\begin{cases} \underline{u}_t^{(3)} + (\bar{U}, \mathbf{Grad})\underline{u}^{(3)} - \mathbf{Div}(\hat{a}_u \cdot \mathbf{Grad})\underline{u}^{(3)} + (A_k)^2 \underline{u}^{(3)} = 0 \;\text{ in }\; D \times (t_{j-1}, t_j)\,, \\ \\ \underline{u}^{(3)} = \underline{u}^{(2)} \;\text{ for }\; t = t_{j-1} \;\text{ in }\; D, \end{cases} \tag{12}$$

where $\underline{u}^{(3)} = (u^{(3)}, v^{(3)})$, $\bar{U}^{(3)} = (\underline{u}^{(3)}, w^{(3)}(u^{(3)}, v^{(3)}))$. After solving (12), the vector $\underline{u}^{(3)} \equiv \vec{u}_j \equiv (u_j, v_j)$ is taken as an approximation to the exact vector $\vec{u}$ 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 (3).

It is seen that step 3 consists of 3 substeps, and by the superscripts in parentheses we denote the value of the solution at the corresponding substeps. The underline stands for 2D vectors, and the overline stands for 3D vectors.

Steps 1 and 2 may be also subsplitted, each into several substeps, based on the method of splitting according to spatial coordinates [20, 27]. The differential operator of the three-dimensional transport-diffusion heat and salt problems (8) and (9) is represented as a sum of simpler non-negative operators, which allows to split the problems into a number of simpler ones and solve them in time using explicit or implicit schemes.

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 $\vec{u} = (u, v)$ and ζ. Therefore, the subproblems at these steps are independent of each other and may be solved in parallel. This is very important for high-performance computing.

2. Variational Data Assimilation Technology

Comprehensive monitoring of the main characteristics of natural environment and climate, which is important both for everyday life and for reducing the consequences of natural and man-made disasters, requires the 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 purpose 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 (deterministic or stochastic) involving cost functions associated with observations, and the minimization is considered on the trajectories (solutions) of the model under consideration [1, 4, 5, 15, 16, 18, 25].

We will demonstrate the data assimilation technology for the case when in problem (1)–(7) the initial state T^0 and the total heat flux function $Q = -\nu_T \dfrac{\partial T}{\partial z}$ on Γ_S are unknown and treated as additional "controls". The cost function is related to observations and has the form:

$$
\begin{gathered}
J(T^0, Q) = \frac{\alpha}{2} \int\limits_0^{\bar{t}} \int\limits_\Omega |Q - Q^{(0)}|^2 d\Omega dt + \frac{\beta}{2} \int\limits_D |T^0 - T^{(0)}|^2 dD + \frac{1}{2} \sum_{j=1}^{J} J_{0,j}, \\
J_{0,j} \equiv \int\limits_{t_{j-1}}^{t_j} \int\limits_\Omega (T|_{z=0} - T_{\text{obs}}) \mathcal{R}^{-1} (T|_{z=0} - T_{\text{obs}}) d\Omega dt,
\end{gathered}
\tag{13}
$$

where $Q^{(0)} = Q^{(0)}(x, y, t), T^{(0)} = T^{(0)}(x, y, z)$ are the given functions, T_{obs} is the function of observations on the sea surface Ω, $\mathcal{R}$ is the observation error covariance operator, and $\alpha, \beta = const > 0$ are the regularization parameters. The functions $Q^{(0)}, T^{(0)}$ are usually chosen as first approximations (so-called "background") for the unknown Q and T^0. The aim of variational data assimilation is, using $Q^{(0)}$ and $T^{(0)}$, to find better estimates for Q and T^0, 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)–(7) *and functions* T^0, Q, *such that functional* (13) *takes the minimum value*:

$$
J(T^0, Q) = \inf_{T^0, Q} J(T^0, Q).
$$

The gradient of the functional $J(T^0, Q)$ with respect to T^0, Q is defined by the adjoint state T^* as follows:

$$
\begin{aligned}
J'_Q &= \alpha \left(Q - Q^{(0)} \right) + T^* \ \text{ on } \ \Omega, \\
J'_{T^0} &= \beta \left(T^0 - T^{(0)} \right) + T^*|_{t=0} \ \text{ in } \ D.
\end{aligned}
\tag{14}
$$

The nesessary optimality condition $J'_Q = J'_{T^0} = 0$ 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)–(7), the adjoint problem, and the optimality conditions in the form:

$$
\begin{aligned}
\alpha \left(Q - Q^{(0)} \right) + T^* &= 0 \ \text{ on } \ \Omega, \\
\beta \left(T^0 - T^{(0)} \right) + T^*|_{t=0} &= 0 \ \text{ in } \ D.
\end{aligned}
\tag{15}
$$

Equations (14) are obtained by differentiating the cost function (13) with respect to T^0 and Q and using the classical representation of the result through the adjoint problem [18]. 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:

$$-{T^*}_t - \mathbf{Div}\,(\bar{U}T^*) - \mathbf{Div}\,(\hat{a}_T \cdot \mathbf{Grad}\, T^*) = 0 \text{ in } D \times (t_{j-1}, t_j)\,,$$

$$T^* = 0 \quad \text{for } t = t_j, \tag{16}$$

$$-\nu_T \frac{\partial T^*}{\partial z} = \mathcal{R}^{-1}(T|_{z=0} - T_{\text{obs}}) \quad \text{on } \Omega.$$

The adjoint problem (16) involves the observation data T_{obs} and the observation error covariance operator $\mathcal{R}$ 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 simultaneous determination of T^0, 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), and T^0_k is the approximation to T^0, then after solving the forward and adjoint problems with $Q \equiv Q_k, T^0 = T^0_k$, the next approximations Q_{k+1}, T^0_{k+1} are computed by:

$$Q_{k+1} = Q_k - \gamma_k(\alpha(Q_k - Q^{(0)}) + T^*) \text{ on } \Omega \times (t_{j-1}, t_j)\,, \tag{17}$$

$$T^0_{k+1} = T^0_k - \gamma_k(\beta(T^0_k - T^{(0)}) + T^*|_{t=0}) \text{ on } D \tag{18}$$

with the parameters γ_k chosen so that the iterative process (17)–(18) is convergent [3]. After computing Q_{k+1}, T^0_{k+1}, the solution of the direct and adjoint problems is repeated with the new approximations Q_{k+1}, T^0_{k+1}, and then Q_{k+2}, T^0_{k+2} are calculated, and so on. Iterations are repeated until a suitable convergence criterion is met.

The convergence properties of similar iterative algorithms were studied in previous works of the authors. For example, in the case $\beta = 0$, for γ_k one can take the parameters

$$\gamma_k = \frac{1}{2} \int_{t_{j-1}}^{t_j} \int_{\Omega} (T|_{z=0} - T_{\text{obs}}) \mathcal{R}^{-1} (T|_{z=0} - T_{\text{obs}}) d\Omega dt \Big/ \int_{t_{j-1}}^{t_j} \int_{\Omega} (T^*)^2|_{z=0} d\Omega dt$$

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. Each step of the assimilation procedure according to (17)–(18) requires solving the forward and adjoint problems. With the use of the σ-coordinate system, the model solution domain does not depend on time: its horisontal boundaries do not change, and the vertical coordinate changes from zero to unity. This allows using the uniform grid in the vertical direction, which is convenient for numerical implementation. The use of the method of splitting with respect to geometric coordinates makes it possible to numerically solve the subproblems independently of each other. These calculations can be done in parallel, which is important for high-performance computing.

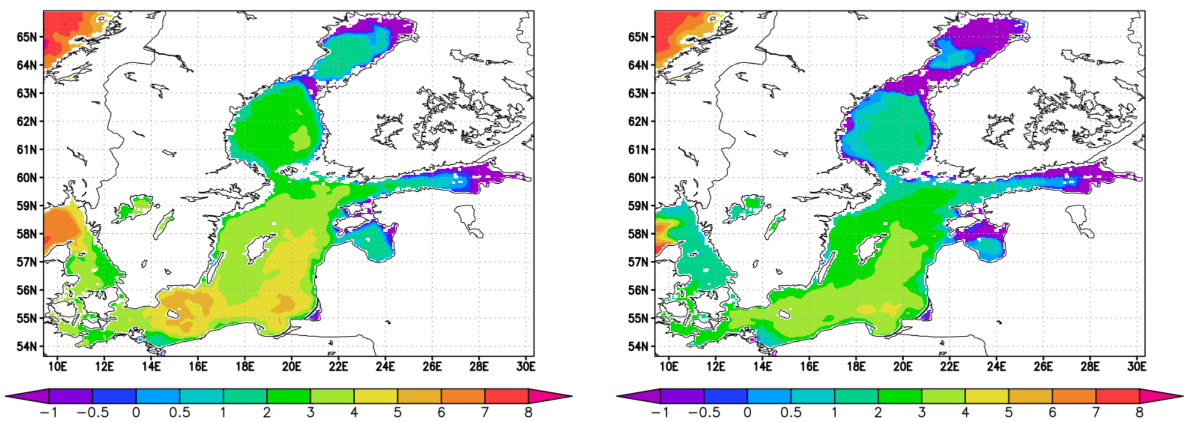
3. Numerical Experiments for the Baltic Sea Water Area

To carry out numerical experiments on the assimilation of satellite observation data on the sea surface temperature, the water area of the Baltic Sea was selected. In all experiments, the problem of recovering the initial and boundary conditions was considered in one iterative procedure of the form (17)–(18). The model of the dynamics of the Baltic Sea was chosen as the main model [26]. This model uses the method of splitting both in spatial variables and in physical processes, which greatly simplifies the application of the theory of adjoint equations for the formulation and solution of the data assimilation problems. It also allows the use of OpenMP technology for those processes that can be calculated independently of each other.

The second distinctive feature of the model considered is the use of the sigma-coordinate system. The approximation of the model on the "grid C" [26] was used. This model was supplemented by the variational data assimilation procedure described in the previous section. The model was started running with zero initial conditions and run with atmospheric forcing obtained from reanalysis, of about 20 years, and after that the result of calculation was taken as an initial condition for further running of the model. The assimilation procedure worked only during some time windows.

Meteorological characteristics were used to calculate the atmospheric impact in the INMOM model [10], including using the bulk formulas for calculating turbulent flows on the sea surface. The values of the mean climatic heat flow $Q^{(0)}$ calculated in this way were used in the data assimilation procedure as a background. To start the assimilation procedure, the function $T^{(0)}$ was taken as a model forecast for the previous time interval. For other functions in the boundary conditions their climatic values were taken.

The daily mean observations T_{obs} for the experiments were obtained from the Copernicus Marine Service (https://www.marine.copernicus.eu). Numerical calculations used the DMI Sea Surface Temperature reprocessed analysis aimed at providing daily gap-free maps of sea surface temperature, at 0.02° x 0.02° horizontal resolution, using satellite data from infra-red radiometers [14]. The data obtained were verified and interpolated on the computational grid of the numerical model [23]. Based on the observational data on the surface temperature, the covariance matrices of data errors $\mathcal{R}$ [6] were constructed, which are used to calculate the cost functional (13) and its gradient in the course of the numerical solution of the problem.



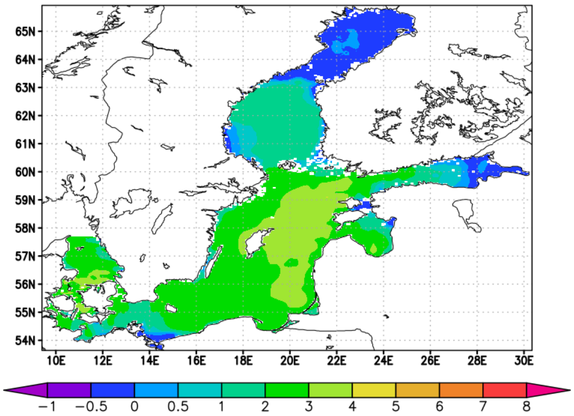
(a) Data for January 15, 2017 (b) Data for February 15, 2017

Figure 1. Daily mean SST observation data, °C

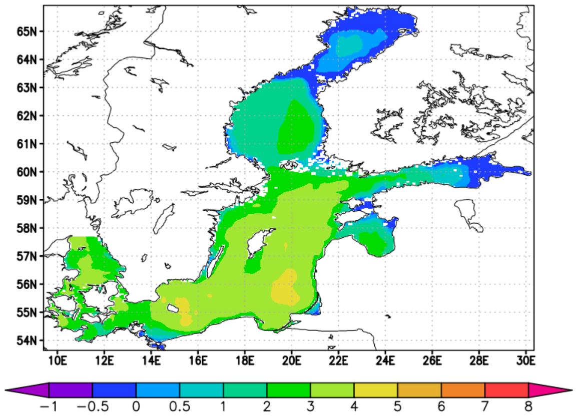
A number of calculations were made between January and March 2017. The grid step in the model was 3.5 km in space, with 27 vertical levels. The time step in the experiments was

5 minutes. In all experiments, the regularization parameters were chosen the same and equal to $\alpha = \beta = 10^{-5}$.

Let us consider some of the calculation results. Figure 1 shows the daily mean sea surface temperature (SST) fields for January 15 (Fig. 1a) and February 15 (Fig. 1b) obtained from Copernicus Marine Service and used as observational data in numerical experiments. In the model with the assimilation procedure, these data are used 2 times a day to adjust the initial and boundary conditions, i.e. the functions T^0 and Q.

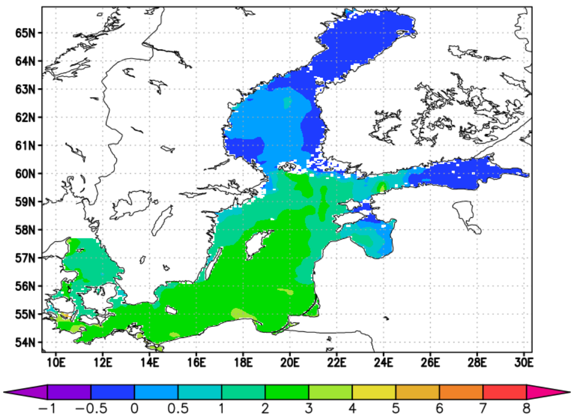


(a) Model calculation without assimilation

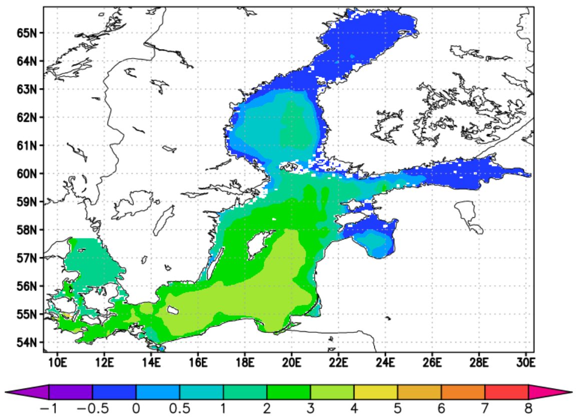


(b) Model calculation with data assimilation

Figure 2. Daily mean SST, January 15, 2017, °C



(a) Model calculation without assimilation



(b) Model calculation with data assimilation

Figure 3. Daily mean SST, February 15, 2017, °C

Figures 2 and 3 show the results of calculations using the model without variational data assimilation (Fig. 2a and 3a) and with temperature assimilation of sea surface data (Fig. 2b and 3b). It can be seen from the presented calculations that the use of the assimilation procedure makes it possible to correct the calculations of the model and bring them closer to the actually observed data. In wintertime, the sea ice block is used in the model [26], however, the assimilation does not use the points in the regions with ice, because we have no observation data at these points. Note that the model without assimilation in the southern part of the Baltic Sea and in the Gulf of Bothnia gives somewhat underestimated SST values, and the deviation from the observed values may reach 2.5°C. Application of the assimilation procedure allows bringing this deviation to 1–1.5°C. It is not possible to completely remove this deviation using only the daily averaged observational data, and it is necessary to use additional data sources for a more reliable correction of the model.

(a) Baroclinic kinetic energy (b) Barotropic kinetic energy

Figure 4. Difference in energies calculated without assimilation and using variational assimilation, cm^2/sec^2

Figure 4 shows the differences in the values of the baroclinic and barotropic kinetic energies of the system as a function of time, obtained from model calculations without using the data assimilation procedure and with using this procedure.

Numerical experiments show that the influence of assimilation on the value of the baroclinic and barotropic energies of the system is insignificant. According to the calculations, the difference in energies when calculated by the model without assimilation and using the assimilation procedure does not exceed 1%. So, the values of the baroclinic kinetic energy vary in the range from 4 cm^2/sec^2 to 28 cm^2/sec^2, while the difference in values at calculation according to the model with and without data assimilation lies in the range from –0.08 to 0.06 cm^2/sec^2 (see Fig. 4a). Similar results are obtained for barotropic kinetic energy. With values from 3 to 17 cm^2/sec^2, the difference in calculations with and without assimilation varies from –0.012 to 0.023 cm^2/sec^2 (see Fig. 4a).

From these and many other our numerical experiments it follows that when only the sea surface temperature is assimilated, the values of the velocities change faintly. Nevertheless, all hydrophysical fields obtained in the course of computations using the variational assimilation of observational data remain consistent and physical.

The iterative procedures used for the four-dimensional variational assimilation of the sea surface temperature in the Baltic Sea showed good convergence, and no more than 10 iterations were required to obtain the optimal heat flux Q and the initial state T^0. 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 has shown that the inclusion of the data assimilation procedure increases the calculation time by about 10%, which can be reduced by using parallelization. Due to the fact that some procedures of the numerical model use implicit schemes, it is quite difficult to build a full parallel model for the version used for experiments in this work. Nevertheless, where possible, the procedures were parallelized using the OpenMP methods. A series of calculations has been run to evaluate performance and acceleration when using the OpenMP technology. The Tab. 1 shows some test results calculated for 144 steps of the model.

Table 1. Test results

Number of threads	Computation time, s	Speed-up
1	178.37	1.00
2	118.93	1.49
4	77.31	2.31

When using the OpenMP methods, it was possible to speed up the model calculations by 2.3 times. The assimilation code has also been accelerated using the OpenMP technology. In the assimilation procedure, for all grid nodes in which there are observation data, the same operations are performed, therefore, such nodes were grouped into sets of 32, and the assimilation procedure was rewritten in such a way that each mathematical operation necessary for assimilation was performed in the most nested loop of 32 elements. On a 4-core Intel Core i7-3770K processor with 8 threads, the program code was accelerated by about 4 times due to parallel computations using the OpenMP technology.

Numerical experiments for the Baltic Sea dynamics model confirmed the feasibility of the presented computational technology and demonstrated that the assimilation can improve the predictive properties of the model.

Conclusions

The paper presents the results obtained by the INM RAS researchers on the 4D technology of variational data assimilation for sea dynamics problems, which is based on the development of efficient numerical algorithms for problems of variational assimilation of observation data for a model of marine hydrothermodynamics. Based on the variational assimilation of the observation data, we propose the algorithms for solving inverse problems to restore the heat fluxes on the sea surface and the initial states of the model under consideration. These 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 numerical experiments for the Baltic Sea dynamics model have shown the ability to apply 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. The reported technology belongs to a class of computational technologies that combine the flows of real data and hydrodynamic forecasts using mathematical models.

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