Variational methods for targeted monitoring of atmospheric quality by specified cost criteria

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Abstract. The creation of problem-oriented monitoring strategies for the study of natural processes in the atmosphere-Earth system based on use of mathematical models in combination with observational data is discussed. Major objects of a modeling system are described. These are: a model of processes of transport and transformation of substances in the gas and aerosol state, data and models of observations. We develop a variational approach that provides formulation, construction, and implementation of solutions to direct and inverse problems. To formulate the variational principle, some target functionals are defined. They serve for forecasting, assimilating observational data, controlling atmospheric quality, etc. Data assimilation techniques play a significant role in successful management of environmental objectives. The result of the study is a version of the so-called “seamless” modeling technology in which five classes of the required functions are calculated. These are state functions, adjoint functions, uncertainty functions, and two functions of sensitivity with respect to variations of model parameters and monitoring data. We can solve inverse problems of strategic operational assessments of hazardous situations and identification of sources of intensive technogenic impacts to organize the targeted monitoring.

1. Introduction

This paper discusses the development of problem-oriented strategies for studying natural processes in the atmosphere-Earth system based on a combination of mathematical models for their description and observations of their real behavior. An important role in this is played by methods of assimilating information that are acceptable for work in the conditions of time and actual data shortages.

To date, various observational systems for terrestrial and aerospace sounding of the atmosphere have been created and are working in the world for monitoring natural processes of various scales, from local to global. In [1-3] there are reviews of the current state and prospects for the development of research on a wide range of issues related to the subject of the study. In particular, in [1] the fact is discussed that only about 20% from the majority of the satellite data are actually acquired in numerical models of weather forecasting. This is essentially a call for improvement and creation of new data assimilation methods, especially for high dimensionality of different-scale model state functions. In this situation, one can see a paradox: somewhere there is an excess of data, and somewhere they are
not enough. This means that, despite the relatively long history of development, the issues of creating effective methods for assimilating data and organizing operational strategies for targeted monitoring of various processes remain very relevant at the present time.

To solve environmental problems, we develop a variational approach that provides new opportunities in the formulation, construction, and implementation of solutions of direct and inverse problems [4,5]. With the help of data assimilation methods, it is possible to solve inverse problems, including strategic ones of operative assessment of the development of situations and identification of sources of intensive technogenic impacts.

2. Models of the processes

To specify the main issues of the developed methodology, we consider a system of equations of transport and transformation of substances in the gaseous and aerosol states, including the categories of moisture in the hydrological cycle of the atmosphere

$$L(X) = \frac{\partial \rho \phi}{\partial t} + \text{div} \rho \phi u - \text{div} \mu \rho \text{grad} \phi_i + \rho S_i(\phi) - (f_{\psi_i} + r_{\psi_i}) = 0, \quad i = 1, n. \quad (1)$$

Here $X = (\phi, Y, f, r)$ is the vector of functional arguments of the modeling system, $\phi(x, t) = (\phi, i = 1, n)$ are state vector-functions belonging to a real space $Q(D)$; $D_t = D \times [0, T]$ is the time interval; $x = (x, y, z)$ is the domain of space variable definition; $Y(x, t)$ is a vector of parameters including the velocity vector $u = (u, v, w)$, and $\mu = \{\mu_x, \mu_y, \mu_z\}$ is the tensor of the coefficients of turbulent exchange in coordinates $x, y, z$, respectively; $\rho$ is density, $f = \{f_i(x, t), i = 1, n\}$ are source functions; $r = \{r_i(x, t), i = 1, n\}$ are the functions which are subject to determination. They describe the uncertainties of the system (1) and are used in the assimilation of observations.

The initial and boundary conditions at the corresponding boundaries of the region $D_t$ are also considered as functional parameters of the system (1) in vector $Y$.

The operators $S_i$, representing the multiscale and multivariate processes of transformation of various substances and mechanisms participating in the modeling technology, are of fundamental significance in the system (1). They have the following structure:

$$S_i(\phi) = P_i(\phi) \phi_i - \Pi_i(\phi), \quad i = 1, n, \quad (2)$$

where $P_i(\phi)$ are the destruction operators and $\Pi_i(\phi)$ are the production operators in relation to the state function $\phi_i$. Note that all operators in (2) for the substances considered in (1) as gas and aerosol and for the moisture components have their internal structure. However, their main property

$$P_i(\phi) \geq 0, \quad \Pi_i(\phi) \geq 0 \quad \text{at} \quad \phi_i(x, t) \geq 0$$

provides the construction of stable monotonic numerical schemes of high order of accuracy within the framework of the variational principle in combination with the method of adjoint integrating factors.

Note that, according to the content, the system (1) is only a part of the general system of hydrothermodynamics and chemistry of the atmosphere [4].

3 Data and models of observations

Let the vector-function $\psi_m \in \{|\psi_m(D^m)| \subset D_t\}$ be the aggregate of the results of observations. Here the index $m$ marks the objects in the monitoring system, $D^m_t$ represents the area in which the results of observations in $D_t$ in different ranges of spectral sounding frequencies are identified. These are the contact (in situ) ground-based observations and measurements in the upper layers of the atmosphere.
Significant volumes of information are also provided by terrestrial and satellite remote sensing systems [1].

We determine the relationship between the monitoring data $\psi_m$ and the results of their calculation using the state functions $\varphi(x,t) \in Q(D_t)$ of the process model (1)-(2) with the help of the operator $H_m(\varphi)$ of the mathematical model of observations in the form

$$\psi_m = H_m(\varphi) + \eta_m, \quad (x,t) \in D_t^m \subset D_t. \quad (3)$$

The functions $\eta_m$ in (3) represent the estimation errors as a result of observations $\psi_m$ together with uncertainties in the mathematical representation of the operators of the model $H_m(\varphi)$. The observation operator in equation (3) defines the transformation

$$\{\psi_m(\varphi(x,t)) \Rightarrow Q(D_t)\} \Rightarrow \{\psi_m(\varphi(x,t)) \Rightarrow \Psi_m(D_t^m)\}.$$

The inverse transformation $\{\Psi_m(D_t^m) \Rightarrow Q(D_t)\}$ is realized by means of the operator $(\partial H_m(\varphi)/\partial \varphi)^*$, where the derivative is understood in the sense of Gateaux and the asterisk denotes the adjoint operator.

4 Functionals of forecasting goals

These functionals in a generalized form express the essence and aim of the case studies in the sense of environmental prediction and design. It is important to make a simulation system adaptable to specific customized problem statements and criteria. Based on these assumptions, we define the structure of the target functionals on the sets of state functions and model parameters in the form

$$F_k(\varphi) = \int_{D_t} F_k(\varphi) \chi_k(x,t) dDdt = (F_k, \chi_k)_{D_t}, \quad k = 1, K. \quad (4)$$

Here $F_k(\varphi, Y)$ are estimated functions limited and differentiable with respect to their functional arguments, and $\chi_k(x,t) \geq 0$ are non-negative weight functions different from zero at the points where the data and the corresponding measures of Radon or Dirac [6] satisfying the conditions of normalization $\int_{D_t} \chi_k(x,t) dDdt = 1$ are defined.

In variational principles, such measures allow uniform operation with both distributed and discrete objects in the regions $D_t$ and $D_t^m$. This is useful for assimilation of monitoring data from images of different types to point data, as well as for optimization and control problems with different settings.

4.1. Functional of data assimilation

In data assimilation technologies, the target functions for the functional (4) are defined as

$$F(\varphi) = (W_1, \eta) \Rightarrow \psi - H_m(\varphi), \quad \chi_k(x,t) \geq 0, \quad (x,t) \in D_t^m \subset D_t. \quad (5)$$

Here $W_1$ is the diagonal weight matrix of a block structure with non-negative elements, $\chi_k(x,t) \geq 0$ are non-negative weight functions different from zero at the points of the region $D_t^m$. They are zero in the rest of the region $D_t$. In this case, the functions of the form (4), (5) determine a measure of deviations between the results of the model calculations $\varphi$ and the monitoring data $\psi_m \in \Psi_m(D_t^m)$.

4.2. Functions for atmosphere quality management

For the organization of such functional, the conditions for the quality control of the atmosphere are determined. We will set them in the form of inequalities, expressing the conditions of environmental well-being in $D_t$:

$$U_i(\varphi, x, t) \leq C_i(x, t), \quad (x, t) \in D_t, \quad i = 1, n_U. \quad (6)$$
Here \( U_i \) are the operators of control functions; \( C_i \) are given functions that determine the maximum permissible levels of anthropogenic loads on the atmosphere of the region; \( n_r \) is the total number of restrictions. It is very problematic to work with such distributed constraints in high-dimensional problems. Therefore, we transform them to an equivalent integral form with functions of the type (4):
\[
\Phi_i(\varphi, U) = \int_{D_i} F_i(\varphi) \chi(x,t) dD dt = 0.
\]
(7)
Here \( F_i(\varphi) = |U_i - C_i| + (U_i - C_i) \geq 0 \), \( (x,t) \in D_i \), \( \chi_i \geq 0 \) are the given weight functions.

5. Formulation of the variational principle
We define an extended functional of the variational principle for working with objects (1) - (7) in the form
\[
\bar{\Phi}(Z) = \left( L(X), \varphi^* \right) + 0.5(W_r, r) + 0.5(W_f, r) + \sum_{k=1}^{K} \alpha_k \Phi_k(\varphi).
\]
(8)
Here \( Z(x,t) \) is the vector of functional arguments of the whole system which, in addition to the vector \( X \) from the system (1), includes components related to the results of observations and to the generalized functional of all the types (target, observations, control, etc.). In essence, equation (8) is a combination of process models (1), (2) and observational results (3) by means of the variational principle with the use of Lagrange multipliers. Let us denote the latter by \( \varphi^*(x,t) \in Q(D_t) \). They have the same structure as \( \varphi(x,t) \) in (1). In the technology of simulation they are solutions of adjoint problems. When uncertainties are included in the model (1), the variational principle is defined in the formulation with weak constraints. Its general structure and methods of implementation are presented in [4, 5]. Here, specifically, the first term in the right-hand side of (8) represents the integral identity functional for the process models (1). By analogy with [7], its structure is formulated in accordance with the definition of the equation of the energy balance of the system. The second and third terms are functionals for uncertainty estimates in the system (3)-(5) and in the system (1). The fourth term is a set of target functionals (6)-(7) with weight coefficients \( \alpha_i \geq 0 \).

The construction of numerical schemes for the approximation of objects in (1) - (7) included in the definition of the functional (8) is performed on the basis of splitting and decomposition methods. A finite element / volume technique is used in \( D_t \) in conjunction with a concept of adjoint integrating factors [8]. Numerical algorithms for solving the basic and adjoint problems, as well as the algorithms for finding the uncertainty functions and sensitivity functions of functionals and models to variations of model parameters and observational results, are obtained using the variations of an arbitrary order in the sense of Gateaux’s definition [9].

The uncertainty function \( r \) gives a quantification of the prediction error on the basis of the system of model - observation data (1)-(3). This means that we obtain, while making sequential data assimilation, a diagnostic assessment of the quality of the forecasting system and the degree of its predictability in relation to the data of monitoring of the studied processes with any set of used observations.

After calculating the functions \( \{ \varphi, \varphi^*, r \} \), the sensitivity functions (SF) of the target functionals of the system (1) - (8) to the variations of the model parameters \( Y \in R(D_f) \) (including initial data) and to the variations of the observation results \( \psi_m \in \Psi_m(D''_f) \) from (3) are calculated. The SFs are necessary for arranging the algorithms for solving inverse problems for identifying parameters \( Y \) using data (3) and for estimating the trends of the influence of uncertainties in observational data on forecast results. The number of such SFs is equal to the number of objects in the aggregate of functional components in the composition \( Y \in R(D_f) \) and in the set of measured data that are taken into account. We denote them
by \( S_\varphi \) and \( S_\psi \). If necessary, they also form the system sensitivity operators needed to solve the inverse problems.

As a result of the implementation of modeling technology based on the joint use of models and monitoring data \((1)-(3)\), we obtain a set of information spaces of the functions \( \{\varphi, \varphi^*, r, S_\varphi, S_\psi\} \). This is multivariate and multi-scale information about the evolution of the processes under study which can be further used for various purposes, for example, to analyze the degree of predictability of models \((1)\), to identify critical situations and centers of action in the system of objects under study, etc.

It should be noted that for quantitative assessment of the quality of forecasting systems and analysis of the sensitivity of the results to the initial state, some methods for calculating singular vectors of linearized operators of nonlinear dynamical systems are used (see, for example, \([10-11]\)).

The beginning of this line of research goes back to \([12]\). For modern models with high spatial-temporal resolution, this approach with the use of singular vectors turns out to be very expensive even for a relatively simple problem of studying the sensitivity of forecast errors to the initial conditions.

To study the dynamics and quality of the atmosphere, we develop methods for identifying the main factors and orthogonal decomposition of function spaces \( \{\varphi, \varphi^*, r, S_\varphi, S_\psi\} \). Since these spaces are generated by the models \((1)\) and related hydrodynamics models, we organize them as Krylov subspaces in the region \( D_r \). This is convenient for spectral decomposition with ordering of the basic subspaces by the eigenvalues of the corresponding matrices. For these purposes, methods of reduction of dimensions of multidimensional spaces with preservation of their informative value and methods of targeted monitoring \([13]\) are used for the organization of environmental strategies under conditions of natural and anthropogenic loads. In extreme conditions of man-made impacts for the detection of sources and risk assessments, methods of solving the corresponding inverse problems and continuation methods are used.

**Conclusions**

Thus, we have built the above-described version of the variational organization of the so-called "seamless" modeling technology. The presence of the desired function spaces \( \{\varphi, \varphi^*, r, S_\varphi, S_\psi\} \) in it simplifies the solution of the problem as a whole. Indeed, with their help and with the use of decomposition and splitting methods, we have built effective algorithms for solving various environmental problems, reducing high-dimensional systems to their analogues of low dimensionality \([13]\). The methods for solving these problems are correct and have a parallel organization of the calculations. In some cases, to combine models and observational data it is possible to construct sequential direct (without iterations) algorithms for variational data assimilation \([14]\), which are promising for solving problems of targeted monitoring by specified cost criteria.

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