Inverse problems for the study of climatic and ecological processes under anthropogenic influences

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Abstract. This paper presents a description of algorithms for solving direct and inverse climatic and environmental problems based on a variational principle with weak constraints. The initial first-order system is supplemented by a system of equations in variations. It provides a calculation of all necessary components of the modeling system by combining the model and observation data and including first- and second-order functionals of sensitivity to variations in the model parameters, input data, and observation results.

1. Introduction: variety of inverse problems

To solve environmental problems, we are developing a variational approach that provides great opportunities in the formulation, construction, and implementation of solutions to direct and inverse problems [1-4].

Examples of direct problems are the well-known problems of forecasting the weather and quality of the atmosphere, the problem of climate research, etc. In mathematical sense, they are initial boundary value problems in which the result is obtained by successive propagation in time of the solution of the system of equations of the corresponding process models starting with initial data.

With this approach, it is believed that all necessary parameters of the models, including the initial data, as well as the sources of influences, are known in advance. However, with respect to the parameters and sources, it is not always obvious that they are set reliably. The fact is that usually the parameters are selected from a certain range of values, based on the previous knowledge and experience, which leaves an imprint on the quality of the solution. It is especially important to specify the initial data in cases when their impact on the result is significant, as, for example, in the weather and air quality forecasts.

Therefore, to improve the reliability of the result, researchers often refer to the methods of data assimilation, which are included in the modeling technology. In the history of weather forecasting for many years, several approaches to the methods of accounting for observational data have been developed. They are, for example, methods of subjective and objective analysis, nudging procedures, Kalman filtering methods, variational assimilation of data, etc. For contemporary reviews of works on this subject, see [5, 6] and the bibliography available there.

In fact, the construction of special procedures to obtain initial data for the state functions of the models are procedures for solving inverse problems. For example, we consider the process of data
assimilation as a sequential solution of interconnected inverse problems. Nowadays, the data assimilation methods make up the largest class of inverse problems used in climate and ecological studies. This is an illustrative example when inverse problems become an urgent need for successful solution of direct problems, justifying the expediency of their coordinated solution.

The methods of data assimilation do not exhaust the entire list of inverse problems used in such studies. Much attention has recently been given to the methods of identification of model parameters and, consequently, the parameters of the simulated processes. Identification of the sources of influence, reconstruction of the coefficients in the equations of models are among such problems. There are also performances of inverse problems which allow one to formulate the so-called continuation problems, which consist in the continuation of the solution from the inside of the region on its border and beyond.

In addition to these tasks, increased attention is paid to the problems of assessing the sensitivity of the models and simulated processes to changes in the parameters. For these purposes, a sensitivity theory is being developed, which makes it possible to indicate the range of changes in the results depending on the range of changes in the parameters. An essential point here is the adoption of the concept of model "flexibility", that is, the abandonment of the "rigid" formulation by including new sought-for functions, named uncertainty functions, in the process model and in the observation model. The benefit of introducing additional unknowns is also that they allow one to construct methods of real time data assimilation [2].

Among the methods gaining popularity in recent years, there are methods for exploring the sensitivity of the second order with special models in variations. Statements of problems of this type are discussed in [7, 8]. They present methods for estimating the sensitivity of the final state of the system (forecast) depending on perturbations in its initial state. For these purposes, methods of solving the spectral problem for the linearized operator in the first-order approximation are used. Accordingly, for approximation of the second order, the spectral methods are applied to matrices of the Hessian of the linearized operator in variations of the second order. In [9], using second-order methods, the sensitivity of the optimal solution and its functionals to errors in the observed data was studied. Despite the fact that methods of the second order are much more time-consuming than those of the first order, they serve to improve the accuracy of calculations. As shown in [8], they extend the predictability intervals in prognostic studies.

This paper presents a description of algorithms for solving direct and inverse climatic and environmental problems based on a variational principle with weak constraints developed at the Institute of Computational Mathematics and Mathematical Geophysics of the Siberian Branch of the Russian Academy of Sciences. The proposed approach provides the calculation of all necessary components of the modeling system by combining the model and observation data, including the study of the first- and second-order sensitivity of the functionals.

2. Key points
It is well-known that in problems of this class it is necessary to work in the conditions of uncertainty in the models of processes, in internal and external sources of influences, in estimates of the initial and current state of the environment, and in the results of observations. To combine all these objects in a mathematical modeling technology, we use the variational principles with weak constraints.

We define the main objects of the modeling technology in operator form [1, 2]:

\[ L(\psi, \mathbf{Y}, f, r) = \frac{\partial \psi}{\partial t} + G(\psi, \mathbf{Y}) - f - r = 0, \quad \varphi(\mathbf{x}, t) \in Q(D_{1}); \]  

\[ \varphi^{0} = \varphi^{0} + \xi, \quad t = 0; \]  

\[ \psi = H(\varphi) + \eta. \]  

\[ J(\varphi) = \int_{D_{1}} F(\varphi) \varphi(\mathbf{x}, t) dD dt. \]
Here \( L(\varphi, Y, f, r) \) is the model of processes, \( Q(D_r) \in \mathbb{R}(D_r) \) is the real space of the state functions \( \varphi(x, t) = \{ \varphi_i(x, t), i = 1, n \} \); \( G(\varphi, Y) \) is the nonlinear differential operator of the process model; \( f \) is the function of sources; \( Y \) is the vector of model parameters varying within acceptable values, \( \varphi_0 \) is the initial state, \( \varphi_0^0 \) is its a priori estimate; \( D_r = D \times [0, T] \), \( D \) is the area of change of the spatial coordinates \( x = (x, i = 1, 3) \), \( t \in [0, T] \) is the time interval; \( J(\varphi) \) is the target research (forecasting) functional; \( F(\varphi) \) is the estimated function; \( \chi(x, t) \) is a non-negative weight function defined in \( D_r \); \( \psi, H(\varphi) \) are the observed data and the observation model. The functions \( r, \xi, \eta \) in (1) - (4) describe the uncertainties and errors in the corresponding objects. The main components in the structure of the model (1) for the vector with components \( \varphi \) are represented by a system of equations describing the processes taking place in the region \( D_r \). The target functional \( J(\varphi) \) is responsible for the research objectives, for example, it can be the goals of weather forecasting taking into account the observational data, environmental safety assessments, etc.

We define the extended functional of the variational principle for combining all objects in equations (1) - (4) in the form

\[
\Phi(Z) = \left( L(X), \varphi_0 \right) + \alpha_0 J(\varphi) + 0.5 \left( \alpha_1 (M_1, \eta, \eta) + \alpha_2 (M_2, r, r) + \alpha_3 (M_3, \xi_1, \xi_2) \right).
\]

(5)

Here \( Z(x, t) \equiv (\varphi, \varphi', Y, f, r, \xi, \eta, \psi) \) is the vector of functional arguments of the entire system, which, in addition to the vector \( X \equiv (\varphi, Y, f, r) \) from the system (1), includes components related to the results of observations (3) and functionals of possible types, for example, target, observations, control, etc.; \( \varphi' (x, t) \in Q' (D_r) \), is the adjoint function representing the vectors of Lagrange multipliers, \( \alpha_i \) are real parameters, \( M_i, i = 1, 3 \) are the weight matrices in the definitions of functionals for estimating the uncertainty functions in equations (1) - (3). The first functional in the right-hand side of equation (5) is an integral identity of the energy type for the process models (1) - (2). Its structure is chosen so that when \( \varphi' = \varphi \) it determines the equation of energy balance of the system (1) - (2).

We construct numerical methods for the so-called “seamless” modeling technology for solving the problems (1) - (4) using the Gateaux definitions of variations of functionals and operators

\[
\delta^n \Phi(Z) = \left. \frac{d}{d \lambda^n} \{ \Phi(Z + \lambda \delta Z) \} \right|_{\lambda=0},
\]

(6)

where \( p \) is the order of variations and, based on them, the Taylor’s formulas

\[
\Phi(Z + \lambda \delta Z) = \Phi(Z) + \lambda \delta \Phi(Z) + \frac{\lambda^2}{2} \delta^2 \Phi(Z) + \cdots + \frac{\lambda^p}{p!} \delta^p \Phi(Z) + o(\lambda^p), \quad \lambda \to 0.
\]

(7)

To construct approximations of the numerical models, we use functional decomposition methods, operator splitting methods, finite element/volume methods, and adjoint integrating factor methods [1]-[4]. As a result, approximations are obtained that are generally agreed in the sense of the functional (5). The combination of applied splitting schemes allows us to efficiently use locally one-dimensional problems in the spatial coordinates and time.

Based on the first-order variations of the extended functional (5), we obtain systems of basic and adjoint equations for finding the functions \( \varphi, \varphi', r, \xi \) with assimilation of observational data and algorithms for calculating the set of spaces of sensitivity functions of the functionals to variations of the parameters and input data of the process models and to variations of the observation data. From the first three terms in (7), methods of sensitivity theory and methods of second-order forecasting are obtained, respectively.
2.1. Forward / inverse modeling algorithm

We write the forward/inverse modeling algorithm for a discrete analog of the process model operators [1-4], which is obtained from the stationary conditions of the functional (5) to the variations of the functions $\Phi, \Phi^*, r, \xi$ in accordance with the definition (6) for $p = 1$:

$$
\frac{\partial \Phi}{\partial t} + G^h(\Phi, Y) - f - r = 0, 
$$

$$
\Phi(x, 0) = \Phi_0(x) + \xi(x), \ x \in D, \ t = 0; 
$$

$$
- \frac{\partial \Phi^*}{\partial t} + A^\dagger(\Phi, Y)\Phi^* + d = 0, 
$$

$$
d = \frac{\partial}{\partial \Phi} \left( \alpha_0 J^h(\Phi) + 0.5\alpha_1 (M^h_{\alpha} \eta^h_{\alpha}) \right)^b = \alpha_0 \frac{\partial J^h(\Phi)}{\partial \Phi} + \left[ \frac{\partial H^h(\Phi)}{\partial \Phi} \right]^T \alpha_1 M^h_{\alpha} \eta^h_{\alpha}. 
$$

The superscript $h$ indicates discrete analogs of the corresponding objects. The system (8)-(15) is implemented sequentially in the time intervals $\left\{ [t_{j-1}, t_j], j = 1, J \right\} \in [0, T]$.

The system (8) - (15) allows us to find solutions to the direct and adjoint problems, $\Phi$ and $\Phi^*$, to calculate the uncertainty functions $r, \xi$. After the functions $\{\Phi, \Phi^*, r, \xi\}$ are calculated, they are used to obtain sensitivity functions of the target functionals of the system (1) - (4) to variations of the model parameters $Y \in R(D)$ and to variations of the observation results $\psi_m \in \Psi_m(D^m)$ from (3).

The sensitivity functions are derivatives of the target functionals (5) with respect to the variable parameters. These functions are necessary for organizing algorithms for solving inverse problems for identifying the parameters $Y$ using the data (3), for assessing trends in the influence of uncertainties in observational data on forecast results, etc.

2.2. Second order algorithms

To construct methods of forecasting and investigating the sensitivity of the second order, in the sense of the definition (6),(7), we use the idea of the method of neighboring extremals [10] and Newton's method for solving nonlinear problems [11]. For this purpose, the objects in the definitions of the second variation are calculated from the following system in perturbations (variations) in the vicinity of the trajectories of the solution of the system of equations (8)-(15):

$$
\frac{\partial \delta \Phi}{\partial t} + A(\Phi, Y)\delta \Phi - \delta f - \delta r = 0, 
$$

$$
\delta \Phi(x, 0) = \delta \Phi_0(x) + \delta \xi(x), \ x \in D, \ t = 0; 
$$

$$
- \frac{\partial \delta \Phi^*}{\partial t} + A^\dagger(\Phi, Y)\delta \Phi^* + \delta d = 0, 
$$

$$
\delta d = \left[ \alpha_0 \frac{\partial J^h(\Phi)}{\partial \Phi} + \left[ \frac{\partial H^h(\Phi)}{\partial \Phi} \right]^T \alpha_1 M^h_{\alpha} \eta^h_{\alpha} \right] \delta \Phi, 
$$

$$
\delta \Phi^*(x) \big|_{t, \tau} = 0; 
$$

$$
\delta r(x, t) = \alpha_2 M^h_{\alpha} \delta \Phi^*(x, t); 
$$
\[ \delta \xi(x) = \alpha^{-1} M^{-1} \delta \Phi (x, 0). \] (22)

In this system, \( \delta \Phi, \delta \Phi^*, \delta r, \delta \xi \) denote the variations of the corresponding objects. The system (16) - (22) has the structure and implementation schemes similar to those in (8) - (15).

Further, analyzing the solutions of the system for variations (16) - (22), we obtain an estimate of the solution of the original problem (1) - (4) with the second order of accuracy and estimates of other objects in the definition of variations (6) of the second order, for example, Hessian operators.

As a result of the implementation of our modeling technology (6) - (22) based on the joint use of models and monitoring data (1) - (5), we obtain a set of information spaces of functions \( \{ \Phi, \Phi^*, r, \xi, \delta \Phi, \delta \Phi^*, \delta r, \delta \xi \} \). Using these spaces, the set of functions of sensitivity of functionals and model operators in the system (1) - (5) to variations of its functional arguments and observation data \( \Psi \) taken into account in equation (3) is calculated. These calculations are performed according to the algorithm of formula (6). Denote them by \( \delta \Phi / \delta Y \) and \( \delta \Phi / \delta \Psi \).

Such multivariate and multi-scale information on the evolution of the studied processes is required for analyzing the predictability of models (1-4), identifying critical situations and centers of action in the system of studied objects, assessing the quality of models, assessing the influence of disturbances in various components of the modeling system, in the model parameters, in the results of observations, and in organizing targeted monitoring strategies, etc. For these purposes, we use the spectral decomposition methods of the above multidimensional spaces according to the characteristic scales of the processes. A detailed description of the implementation algorithms for such methods for the analysis of multidimensional spaces and some examples of their application to solving environmental forecasting and design tasks are given in [12].

Conclusions
Thus, this paper presented a general scheme for creating a modeling system for the study of climatic and environmental processes, environmental forecasting and design. The initial first-order system was supplemented by a system of equations in variations. The above technology is self-consistent in a variational sense and allows us to solve a wide range of direct and inverse problems.

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