Variational organization of a modeling technology for environmental problems

Vladimir V. Penenko, Elena A. Tsvetova, Alexey V. Penenko
Institute of Computational Mathematics and Mathematical Geophysics SB RAS, Novosibirsk, Russia
penenko@sscc.ru, e.tsvetova@ommgp.sscc.ru, a.penenko@gmail.com

Abstract

Methods for the combined use of mathematical models and observational data for studying and forecasting the evolution of natural processes in the atmosphere and environment are presented. Theoretical background for the methods are variational principles for estimation of functional defined on a set of state functions, parameters and sources of processes models. In the approach mathematical models with allowance for different kinds of uncertainty are considered as constraints to the class of state functions.

Modeling technology outline [1]

- Form an informative base of orthogonal base vectors (OBV) from historical meteorology data.
- Build typical scenarios taking into account component variability.
- Asses risks for the typical scenarios.
- Assimilate incoming data.

Pollution risk assessment case study

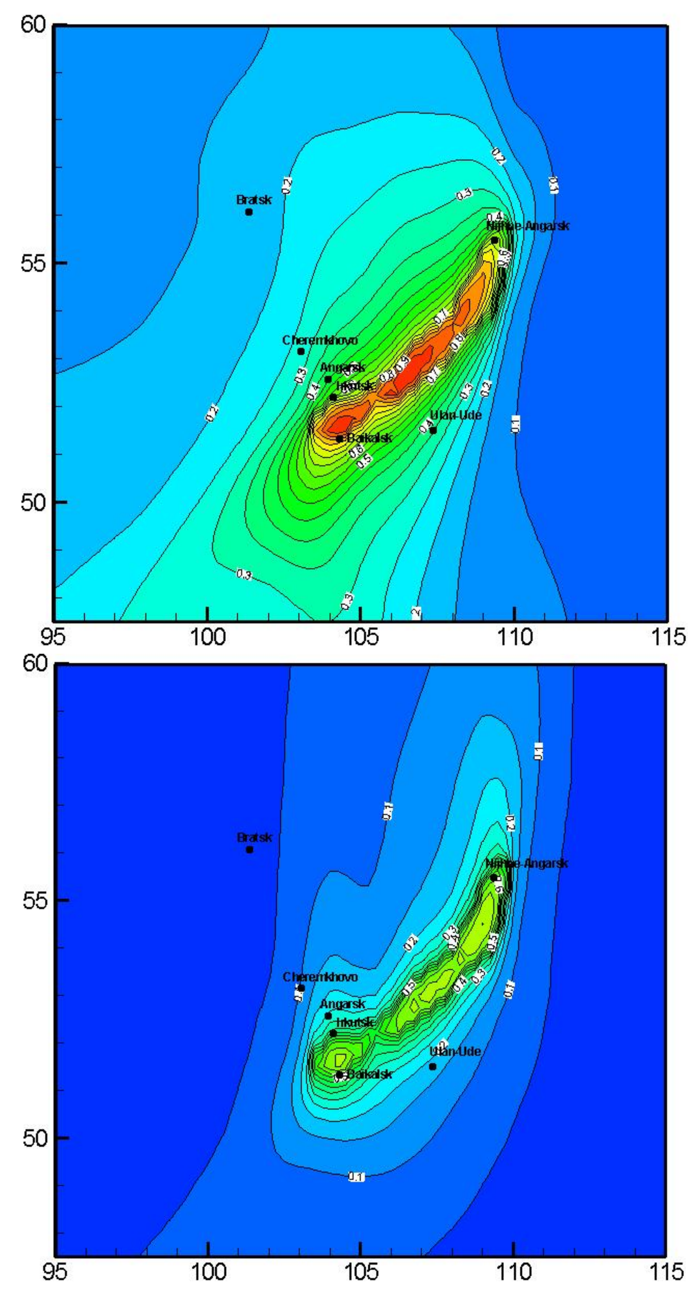

Fig. 2: Lake Baikal sensitivity function [1] to cumulative emissions of climatic (for 56 years) July (upper) and December (lower).

The sensitivity function has a 4D space-time structure. Its values show which part of the total emission from the sources may enter into the receptor zone. The greater the value of sensitivity function in a grid point, the more the risk to get the input into the quality functional from the source situated in this point.

Real-time data assimilation case study

Considered in [4] real-time data assimilation algorithm is a special case of general data assimilation scheme with splitting method applied and

$$\vec{\phi} = \phi^{j+1}, \quad \Lambda_t = Id/\tau, \quad f_a = \bar{f}_a + \phi^j/\tau.$$

where ϕ^j is the state function on j-th timestep, $\bar{f}_a$ are *a priori* sources and τ is the timestep.

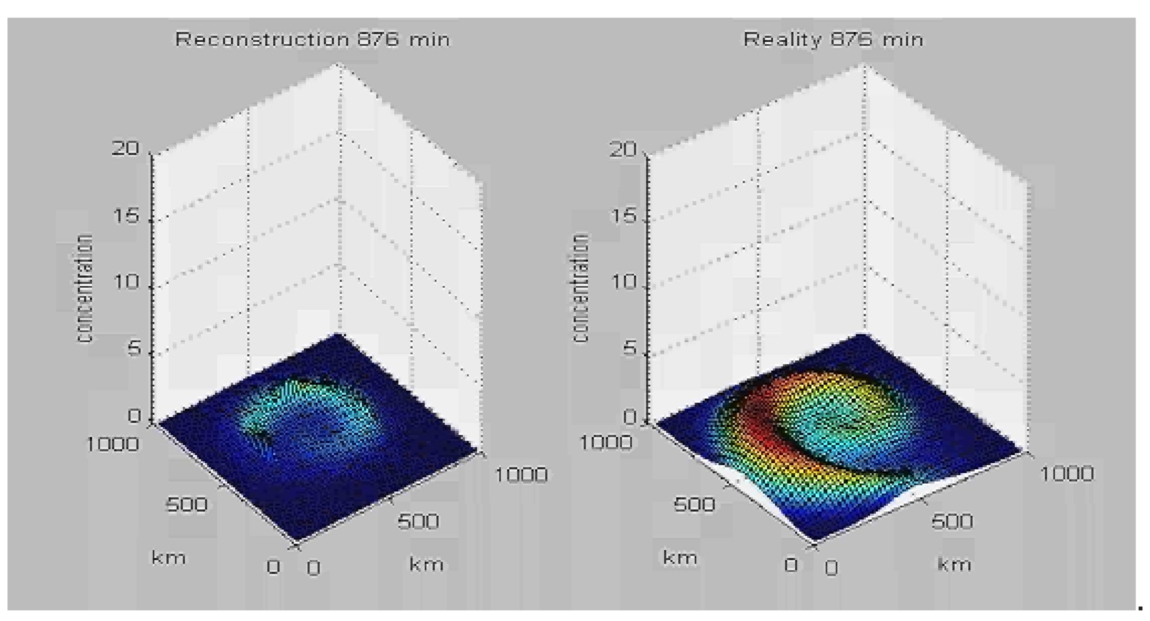

Fig. 3: Data assimilation result (left) for artificial data (right). Four fixed observers, circular wind field and zero value *a priori* data on sources.

References

[1] V. Penenko, A. Baklanov, E. Tsvetova, A. Mahura *Direct and Inverse Problems in a Variational Concept of Environmental Modeling*, Pure Appl. Geophys. (2012) 169:447-465

[2] V. V. Penenko *Variational methods of data assimilation and inverse problems for studying the atmosphere, ocean, and environment* Num. Anal. and Appl., 2009 V 2 No 4, 341-351.

[3] V. Penenko, E. Tsvetova, *Orthogonal decomposition methods for inclusion of climatic data into environmental studies*, Ecol.modelling v.217, (2008) 279-291.

[4] A. Penenko *Some theoretical and applied aspects of sequential variational data assimilation (In Russian)*, Comp. tech. v.11, Part 2, (2006) 35-40.

Acknowledgements

This study is supported by Presidium of RAS (Program N 4), the Department of Mathematical Sciences of RAS (Program N 3), and the Russian Foundation for Basic Research (grant 11-01-00187).

Orthogonal vector spaces for long-term environmental studies [3]

We suggest a methodology for a quantitative description of the behavior of a dynamic system for a long time interval in a generalized form. Following it, the necessary information, intended to be used for the construction of scenarios, is extracted from a database containing measured and/or calculated data on hydrodynamic state functions. Calculations are made with the help of a method of orthogonal decomposition of functional spaces formed by multivariate, multidimensional state functions from a database. A two-level data structuring with allowance for given goal criteria is firstly produced. This provides an efficient realization of the methodology practically without restrictions upon the amount of data and component content of the database. The targeted structuring is just the element which differs the methodology proposed from the traditional approaches to data decomposition.
The NCEP/NCAR reanalysis database for 56 years (1950-2005) is used to demonstrate the possibilities of the methodology. The method of orthogonal decomposition results in the subspaces which correspond to the processes on different scales: from global climatic processes to weather noises. These subspaces serve as informative bases for analysis of the climatic system behavior. Moreover, the subspaces are key elements for the construction of deterministic-stochastic scenarios to obtain an atmospheric background for problems of environment protection and design, ecological risk/vulnerability assessment and control, etc.

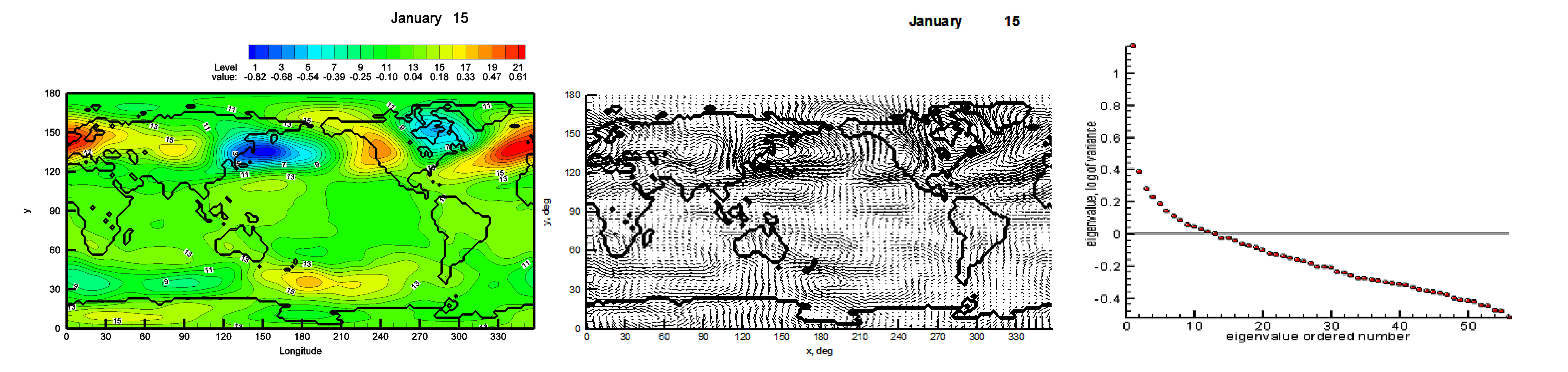

Fig. 1.a: One of 62 fragments corresponding to the 15th day of the first OBV for 500-hPa geopotential hight (left) and wind velocities (center), eigenvalues of Gram matrix for 500-hPa geopotential height(right) for monthly vectorized data corresponding to January for 1950-2005 years.

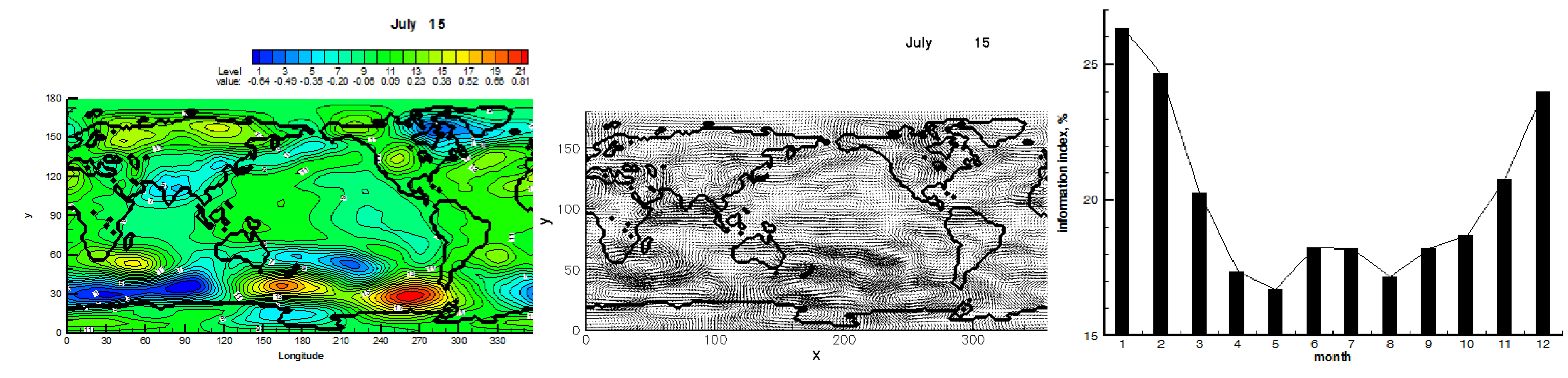

Fig. 1.b: One of 62 fragments corresponding to the 15th day of the first OBV for 500-hPa geopotential hight(left) and wind velocities (right) monthly vectorized data corresponding to June for 1950-2005 years. Seasonal variability of the information index of the OBV-1.

Model

4D models describing the processes of heat, moisture, radiation, and pollutants transport and transformation in the atmosphere have the generic structure:

$$L(\phi, \mathbf{Y}) \equiv \frac{\partial \rho\phi}{\partial t} + \operatorname{div}\rho(\phi\mathbf{u} - \mu \operatorname{grad}\phi) + \rho((\mathbf{H}\phi) - \mathbf{f_a} - \mathbf{r}) = \mathbf{0},$$

$$\phi^0 = \phi^0_a + \xi, \quad R_{bound}(\phi) = g_a + \varepsilon, \quad Y = Y_a + \zeta.$$

Incoming measurement data is connected with the state function with measurement operator $\mathbf{W}$

$$\Psi_m = [\mathbf{W}(\phi)]_m + \eta,$$

Here ϕ is model state function, $\{\rho, u, \mu\} = Y$ are model parameters that can be composed of extracted OVB, H is transformation operator, f_a, g_a, ϕ^0_a are *a priori* values of sources and initial data, r, ξ, ε, ζ, η are flexibility (uncertainty) functions introduced in the rigid model structure.

Variational framework

The Model is represented in the weak form with introduction of the adjoint function

$$I(\phi, Y, \phi^*) \equiv (L(\phi, Y), \phi^*).$$

With the functional to be estimated

$$\Phi_k(\phi) = \int_{D_t} F_k(\phi)\chi_k(\mathbf{x}, t)dDdt = (F_k, \chi_k),$$

all structures are aggregated to an augmented functional and then the latter is discretized with the use of splitting and decomposition techniques

$$\tilde{\Phi}^h_k(\phi, \phi^*, \mathbf{Y}, \eta, \mathbf{r}, \xi, \zeta) = \alpha_0\Phi^h_k(\phi) + \frac{1}{2}\left\{\alpha_1(\eta^T M_1\eta)_{D^m_t} + \alpha_2(\mathbf{r}^T M_2\mathbf{r})_{D^h_t} + \alpha_3(\xi^T M_3\xi)_{D^h} + \alpha_4(\varepsilon^T M_4\varepsilon)_{D^h_t} + \alpha_5(\zeta^T M_5\zeta)_Y\right\}^h + \left[I^h(\phi, Y, \phi^*)\right]_{D^h_t},$$

$$\delta\tilde{\Phi}^h_k = \left(\frac{\delta\tilde{\Phi}^h_k}{\partial\vec{\phi}^*}, \delta\vec{\phi}^*\right) + \left(\frac{\delta\tilde{\Phi}^h_k}{\partial\vec{\phi}}, \delta\vec{\phi}\right) + \left(\frac{\delta\tilde{\Phi}^h_k}{\partial r}, \delta r\right) + \left(\frac{\delta\tilde{\Phi}^h_k}{\partial\xi}, \delta\xi\right) + \left(\frac{\delta\tilde{\Phi}^h_k}{\partial Y}, \delta Y\right).$$

Within the framework, different tasks can be accomplished.

Data assimilation $(\alpha_0 = 0, \alpha_4 = 0, \varepsilon \equiv 0, \alpha_5 = 0, \zeta \equiv 0)$

Data assimilation is the process that improves forecast with the use of incoming measurement data. The general algorithm for data assimilation [2] has the form

$$\frac{\partial\tilde{\Phi}^h_k}{\partial\vec{\phi}^*} \equiv \Lambda_t\vec{\phi} + G^h(\vec{\phi}, \vec{Y}) - \vec{f} - \vec{r} = 0, \quad \phi^0 = \phi^0_a + \xi. \quad (Direct/Forward\ problem)$$

$$\frac{\partial\tilde{\Phi}^h_k}{\partial\vec{\phi}} \equiv (\Lambda_t)^T\vec{\phi}^*_k + A^T(\vec{\phi}, \vec{Y})\vec{\phi}^*_k + \frac{\partial}{\partial\vec{\phi}}\left(\frac{1}{2}\alpha_1(\vec{\eta}^T M_1\vec{\eta})\right) = 0, \quad A(\vec{\phi}, \vec{Y})\delta\vec{\phi} \equiv \frac{\partial}{\partial\alpha}\left[G^h(\vec{\phi} + \alpha\,\delta\vec{\phi}, \vec{Y})\right]_{\alpha=0}, \quad \vec{\phi}^*_k|_{t=\bar{t}} = 0. \quad (Adjoint\ problem)$$

$$\frac{\partial\tilde{\Phi}^h_k}{\partial\xi} \equiv \alpha_3 M_3\xi - \rho\vec{\phi}^*_k|_{t=0} = 0 \rightarrow \xi = \frac{1}{\alpha_3}{M_3}^{-1}\rho\vec{\phi}^*_k|_{t=0}, \quad \frac{\partial\tilde{\Phi}^h_k}{\partial r} \equiv \alpha_2 M_2 r - \vec{\phi}^*_k = 0 \rightarrow \quad r = \frac{1}{\alpha_2}{M_2}^{-1}\vec{\phi}^*_k. \quad (Flexibility/uncertainy\ estimation)$$

Here Λ_t is a time derivative discretization and G^h is the discretization of transport-diffusion-reaction operator. Assimilation window is a parameter of the data-assimilation procedure. Real-time data assimilation can be carried out when assimilation window is equal to one time step for model of processes.

Receptor territory pollution risk assessment $(\alpha_1 = 0, \alpha_2 = 0, \alpha_3 = 0, \xi \equiv 0, \alpha_4 = 0, \varepsilon \equiv 0, \alpha_5 = 0, \zeta \equiv 0)$

To assess the risk we need the quantity values of the sensitivity functions of the goal functional describing an accumulated pollution of the receptor territory WRT the variations r of the sources f_a which are explicitly included in the model description. The algorithm for calculation of the sensitivity function is

$$\frac{\delta\tilde{\Phi}^h_k}{\partial\vec{\phi}^*} = 0, \quad \frac{\partial\tilde{\Phi}^h_k}{\partial\vec{\phi}} \equiv (\Lambda_t)^T\vec{\phi}^*_k + A^T(\vec{\phi}, \vec{Y})\vec{\phi}^*_k + \frac{\partial}{\partial\vec{\phi}}(\alpha_0\Phi^h_k(\phi)) = 0, \quad \delta\tilde{\Phi}^h_k = \left(\frac{\delta\tilde{\Phi}^h_k}{\partial r}, \delta r\right).$$