Global and regional principal components of the climatic system and their application to environmental studies

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Separation of principal components characterized by a long-term climate dynamics and their application to diagnostics and prognosis is considered. Principal factors are multicomponent 4D (space and time) constructions. They are calculated based on many-year data on the climatic system behavior and sensitivity characteristics using factor analysis algorithms. Reanalysis NCEP/NCAR 40-year database is invoked into calculations. Two types of principal components of global and regional scale are constructed. The results of comparative analysis of their information quality are given. The principles of construction of climatic and ecological scenarios with the use of databases, factor solutions, and numerical models of the processes under study are formulated.

Introduction

The use of mathematical simulation to study natural processes evolving under a joint effect of natural and anthropogenic factors opens a possibility to solve the problems of climatic and ecological variations of environmental conditions. Mathematical models needed for such investigations are the complex developed structures describing various mechanisms of phenomena under study.

This paper considers some aspects of mathematical simulation in diagnostics of priority factors in climate dynamics as applied to the study of ecological responses to anthropogenic impacts.

To study the scales of interactions between various processes in a climatic-ecological system, diagnostics and prediction of their development, a set of generalized characteristics is introduced. As these characteristics, it is convenient to use basic elements of factor analysis and functionals determined in a space of state functions of the system under study. The functions of the functionals' sensitivity to variations of the internal and external parameters bear the information on the tendencies of changes in the system under the effect of variation of each individual parameter. In contrast to them, the principal factors reflect general regularities in formation of the processes under study and give their decomposition by scales.

Thus, on the one hand, ranking of model parameters and zoning of territories by the intensity of the sensitivity functions is performed and, on the other hand, decomposing the spaces of the state functions by scales in terms of integral representations of factor analysis. This allows one to join the concept of identification of the centers of influence in the global climatic system with the problem of revealing the areas of risk/vulnerability for individual regions.

Up-to-date databases on the state of the climatic system and methods of joint use of models and actual information open a possibility of developing the proposed technique and algorithms for its practical implementation.

To get the quantitative and qualitative impression on relations between global and regional processes, we have performed multidimensional multicomponent factor analysis of the state functions of the global climatic system and its regional part corresponding to the southern part of Eastern Siberia. The region was chosen due to its ecologically important and climate-forming natural object – Lake Baikal.

In the analysis, we used a complex of mathematical models and simulation technology developed at the Institute of Computational Mathematics and Mathematical Geophysics for solution of ecological problems in modifications oriented at diagnostics and prediction of possible climatic and ecological changes.

1. Problem formulation

Basic and applied aspects of factor analysis and principal component analysis are of interest for researchers in various fields and they are discussed in a large number of papers. Systematic consideration of the fundamentals of these methods and some of their applications can be found, for example, in Refs. 1–3. These works include, in particular, an extensive bibliography and the review of the method's evolution starting from 1873. Different methods of principal factor analysis are actively used in recent years in meteorology and oceanology for studying the structure and variability of the processes with the wide spectrum of spatial and temporal scales.[2–7]

We develop algorithms of multidimensional multicomponent factor analysis in climatic and ecological investigations and formation of scenarios

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for ecological prediction and design. The peculiarity of problems of this class is that the organization of scenarios requires functional spaces with a detailed structure of representation of their elements in 3D space and time. The results presented below continue the investigations described in Refs. 4 and 5, therefore we present here only key elements of the algorithms, which demonstrate mutual dependences between the studied fields of functions and orthogonal factor bases for their representation with the preset degree of informativeness.

Let

$$\Phi = \left\{\varphi_\beta \equiv \varphi_\beta(\mathbf{x},t,q),\ \beta = \overline{1,n},\ n \geq 1,\ q = \overline{1,Q},\ Q \geq 1\right\}, \quad (1)$$

be the initial set of vectors of the dimension N, centered about their component-wise mean values, and normalized to unity. Here $(\mathbf{x}, t) \in D_t^h$, D_t^h is the domain of variability of spatial coordinates and the time in the discrete representation. The integer-valued parameter $q \geq 1$ marks the components of the state functions with different physical content. This set can be considered as $N \times n$ matrix with $n \leq N$. The internal block structure of the vectors φ_β can be arbitrary in the physical meaning, information content, and the number of components. It is formed depending on the objectives of investigation. Its specificity is taken into account in the definition of the scalar product for calculation of the Gram matrix elements

$$H = \left\{H_{\alpha\beta} \equiv (\varphi_\alpha, \varphi_\beta),\ \ \alpha,\beta = \overline{1,n}\right\} \quad (2)$$

and the generated by it metric for normalization of vectors from the initial set in the discrete representation. For the problems of the considered class, it is convenient to use the energy scalar product introduced for constructing variational formulations of models and the sensitivity theory relations for functionals.[4] In this case, the domain D_t^h is so chosen that it coincides with the grid area for discrete analogs of models of the studied processes.

The main idea of factor analysis consists in the optimal choice of the representation

$$\varphi_\beta \approx \sum_{p=1}^{m} a_{\beta p}\mathbf{F}_p,\ \ m \leq\ n,\ \ \beta = \overline{1,n}, \quad (3)$$

where $\mathbf{F}_p$ are sought orthonormal basis functions (factors, UOF) with the internal structure identical to the structure of the vectors φ_β; $a_{\beta p}$ are the decomposition coefficients or so-called factor loads reflecting a contribution of corresponding factors to φ_β; m is the number of factors participating in the decomposition in accordance with the preset level of informativeness (3) in comparison with the initial set of vectors.

The basis functions are calculated from the initial set by the algorithm

$$\mathbf{F}_p = \sum_{\beta=1}^{n} \frac{a_{\beta p}}{\lambda_p}\varphi_\beta,\ \ p = \overline{1,m}. \quad (4)$$

$\mathbf{a}_p \equiv \{a_{\beta p},\ \beta = \overline{1,n}\}$, $p = \overline{1,n}$ are $n \times n$ eigenvectors of the Gram matrix (2), and λ_p are the corresponding eigenvalues in the decreasing order $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

The full spectral problem for the Gram matrix is solved under conditions of consecutive maximization of the values

$$\lambda_p = \sum_{\beta=1}^{n} a_{\beta p}^2,\ \ p = \overline{1,n}. \quad (5)$$

These conditions are also used for normalization of eigenvectors, whose elements take part in Eqs. (3) and (4). Calculations by Eq. (4) involve all the initial φ_β, $\beta = \overline{1,n}$. The function $f_i(\lambda) = \sum_{k=1}^{i}\lambda_k,\ i \leq n,$ can be considered as a measure of informativeness for a set of the first i basis functions relative to the initial set (1); $f_n(\lambda) = n$. Note that the spur of the Gram matrix (2) is also equal to n. The number of basis functions m for Eq. (4) is chosen based on the rate of decrease of the eigenvalues and the behavior of $f_i(\lambda)$. The fulfillment of the orthonormality conditions for the basis $\{\mathbf{F}_p\}$ is checked directly.

The parameter $b_p = \lambda_p/n$ characterizes the informativeness of the pth factor, i.e., a summary measure of relative contribution of the factor with the number p to representation of the whole set by Eq. (3). Descending ordering of the eigenvalues gives the representation (3) under the conditions (5) with consecutive exhaustion of the initial set with maximization of the factors' contribution (4) at every step. In this case, the process of calculation of the factors (4) in accordance with the levels of informativeness (5) gives a decomposition of the initial space (1) by the scales of the processes. The first m factors in Eq. (3) corresponding to large eigenvalues and, consequently, having a higher measure of informativeness are usually called the principal factors. Vectors with $\lambda_p > 1$ also fall in this category. This means that the informativeness of the selected principal factors should not be less than the informativeness of each initial vector.

At a large length of the sample (1), realization of the algorithms of the component separation and factor analysis is a complicated and time-consuming computational problem. In practice, these algorithms are very sensitive to the problem's dimension increase. These aspects are considered in detail in Ref. 3. In particular, it is proposed to use the procedures with decomposition of vectors of the initial set by subzones, as well as some other tricks aimed at the dimension decrease. Thus, to study interannual climatic variations, the monthly, seasonally, and annually means of the state function fields are used.[3,6,7]

To overcome the difficulties arising from high dimensions of the analyzed spaces, we modify the algorithms so that, when solving spectral problems, all the internal degrees of freedom in vectors (1) close on themselves in the elements of the Gram matrix (2). And only at tabulation of the basis functions (4) the vectors (1) take part in the full form. The parallel structure algorithms turn out to be extremely efficient in these calculations. They provide for a high efficiency of the computational algorithm as a whole at any size of the vectors. Note that from the viewpoint of the numerical simulation of natural processes, the algorithms with the Gram matrices with the specialized structure of scalar products are more efficient in operating with multidimensional multicomponent spaces of functions than the algorithms with covariance matrices, which are traditionally used in the methods of factor analysis.

2. Global-scale principal factors

Of particular interest is a study of interannual variability of the seasonal and annual spatiotemporal behavior of the climatic system. For such investigations, the initial set (1) is organized in the corresponding way, that is, the internal structure of vectors in Eq. (1) and in factor aggregates (4) is specified and the scalar product is introduced.

For development of the algorithms and solution of specific problems, we use the Reanalysis database for 40 years[8] and the system of the information preparation for numerical models.[9] In accordance with our purposes of climatic-ecological investigations, we select a set of the type (1) with the number of initial vectors equal to the number of years in the used Reanalysis database. In our case we take $n = 40$. The parameter n is a key parameter for development of the algorithms, since the efficiency of their realization and the character of interpretation of results depend on its value. As to setting the internal structure of the vectors, a lot of different versions are possible. In the general case, they are block vectors. The physical meaning and information content impose no restrictions on the number of blocks and the common dimension N. The magnitude of N is specified based on either the number of data available for analysis or the capability of the computers used. In tabulation of the Gram matrix (2) elements, it is important that the informativeness of the scalar products keeps constant for all their vector components taken into account.

In our particular case, when forming the structure of the set (1) and factor aggregates (4), the one-month interval with a 12-hour discretization step is taken as a reference time interval. The spatial structure of these vectors is determined in accordance with the structure of grids in the computer model consistent with the structure of the spatially distributed information in the database. The component composition of the vectors is specified depending on the investigation objectives in accordance with a set of the components of the state functions of the mathematical model and the sensitivity functions used to study the set of functionals.

Separation of monthly intervals is convenient for studying the interannual variability and for interpreting the results of analysis. To analyze the specificity of changes in the seasonal and annual behavior, it is sufficient to consider 12 monthly intervals. Thus, the whole many-year database can be represented as 12 similar arrays (by the number of months in a year). By the way, it should be noted that in this case the algorithms also have a large-block parallel structure, in which the number of parallel branches is equal to the number of the analyzed months. As a result, we obtain 12 sets of UOF's and the corresponding sets of factor load vectors $\mathbf{a}_p$, ($p = \overline{1,n}$) allowing us to study the behavior of the global climatic system in dynamics.

By the idea itself and the structure, the factor analysis algorithms realize the decomposition of the initial space of functions by the informativeness scales of each basis vector contribution. The components of $\mathbf{a}_p$ at the chosen representation of the inner structure of φ_β give quantitative estimates of the variability of the studied processes with respect to the constructed bases. From the viewpoint of numerical simulation, such generalized description of the climatic system dynamics form a constructive basis for development of new algorithms needed for solving practical problems.

The use of multidimensional multicomponent factors with the spatiotemporal structure consistent with the database structure and the state functions of the models significantly simplifies the analysis of the common tendencies in the behavior of the global climatic system and its regional parts. The construction of factor aggregates chosen by us gives a simple method for orientation in multidimensional spaces. In essence, the multidimensional character is hidden in the bases, while the interannual variability is analyzed in the formally one-dimensional space, where the current number of a year serves an independent variable and the analyzed characteristics are the components of the factor load vectors in the decomposition (3). In its turn, each of the basis factors (4) is valuable in itself as well, since it is a spatially global construction with the monthly dynamics in time in order of decreasing informativeness in terms of Eq. (5).

In particular, the use of principal factors allows an efficient solution of the following problems:

– few-component representation of the initial set of vectors with the preset degree of informativeness;

– separation of the centers of influence in the climatic system, identification of their spatial arrangement, and study of variability;

– typification of the many-year dynamics of the studied system in accordance with the intensity of factor loads with respect to the subset of UOF's having an increased informativeness;

– formation of informative phase subspaces for organization of determinately stochastic scenarios based on fluid dynamics and pollutant transport models.

Let us present an example of the analysis of the climatic system behavior for 40 years from 1960 to 1999 based on the Reanalysis data.[8] The calculations involved the geopotential and temperature fields. Here we demonstrate some calculation fragments for global geopotential fields in the isobaric coordinates on the spherical Earth on the surface corresponding to a pressure of 500 mbar. In this case, the total number of vectors is $n = 40$, and the internal dimension of the initial and basis vectors is $N = 144 \cdot 74 \cdot 60$. In accordance with the scheme described above, we have calculated 12 sets of UOF's. They have the spatiotemporal structure with a resolution of 2.5×2.5 on the sphere surface and the duration of one month with a discreteness of 12 h. Each set consists of 40 UOF's. Such representation is a compromise from the viewpoint of computational expenses and informativeness for analysis of the annual and seasonal behavior in the mode of interannual variability of the global behavior of the climatic system and its parts.

Table presents the characteristics of informativeness (%) of the first basis vectors for each of 12 sets. It is seen that the informativeness has the seasonal behavior with maximum in January and minimum in May. For the 40-year period, the first factors prevail in all months. This means that they can be used for separation of the climatic component in the studied fields. Relative contributions of other individual basis vectors are much smaller.

Figure 1 depicts two fragments of the first global-scale principal factors for June and January. Further, Fig. 2*a* shows the behavior of factor loads for the first June basis vector for the 40-year period. It demonstrates the character of the interannual variability of the global atmospheric circulation with respect to this factor.

Comparative analysis of the generalized characteristics of the many-year atmospheric dynamics represented by the principal factors shows well-known differences in circulation mechanisms for the summer and winter seasons.

3. Regional-scale principal factors

Unlike the global-scale principal factors, regional factors show a higher informativeness in interannual variations. This is caused by the fact that in relatively small regions the geophysical conditions are more homogeneous and the quasiperiodic component in the many-year behavior shows itself more clearly. Thus, for example, for the southern part of Eastern Siberia (95–115°E, 47.5–60°N) the first basis vector corresponding to the maximum eigenvalue provides for 97% significance for June and 93% for November. For the global-scale factors, these values are, respectively, 17.5 and 20.3%. Reference 5 presents UOF's of the geopotential field in the Northern Hemisphere in the mode of interdiurnal variations for December 1998. The informativeness of the first factor is 42%. Comparing these data, we can conclude that regional climates can be described using the spatiotemporal UOF aggregates with rather high degree of informativeness.

Figure 2*b* depicts the factor loads for the first June UOF in different years. Having specified some significance interval for typification, we can distinguish the abnormal years with respect to the principal factors. In our case, they are Junes of 1969 and 1990. In other years the June values fall in the range of typical values with respect to the principal factor.

Figure 3 depicts four fragments of the first principal factor of the geopotential field on the 500 mbar surface corresponding to 00 GMT for June 1, 10, 20, and 30. It is seen that the principal factors vary widely during the month. The joint analysis of the regional and global factors in dynamics suggests that the regional factors agree in the structure with the global ones, but reflect the seasonal variability with a higher degree of informativeness. This is important for analysis of regional processes in the many-year dynamics and for development of numerical models for diagnostics and prediction.

As to the Lake Baikal region (the lake center lies roughly at 107.5°E, 52.5°N), the main conclusion is that in the structure of global and regional principal factors, it is in an unstable transient zone between the large-scale thermobaric formations of the quasi-stationary character: by the latitude in summer and by the longitude in winter. As a consequence, the climatic-ecological processes in the region have a high spatiotemporal variability as can be seen from Fig. 3.

4. Principles of scenario formation

The factor analysis methods extend the capabilities of mathematical models for investigation of natural processes. The use of the information about principal factors in ecological investigations allows an efficient solution of the problems concerning the proper choice of the methods for description of meteorological situations serving as a background for formation of the long-period processes of humidity and pollutant transport and transformation.

Analysis of the global- and regional-scale principal factors along with analysis of the sensitivity functions and domains of influence for models and functionals shows that it is impossible to reconstruct adequately the dynamics of regional processes without taking into account their relations with global processes. This is clearly seen, for example, when estimating the areas of ecological risks and vulnerability in the region under study with respect to the anthropogenic impact.[10–12]

Month	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
b_1, %	30.4	27.5	22.5	16.8	16.5	17.5	20.0	18.1	18.0	17.6	20.3	26.4

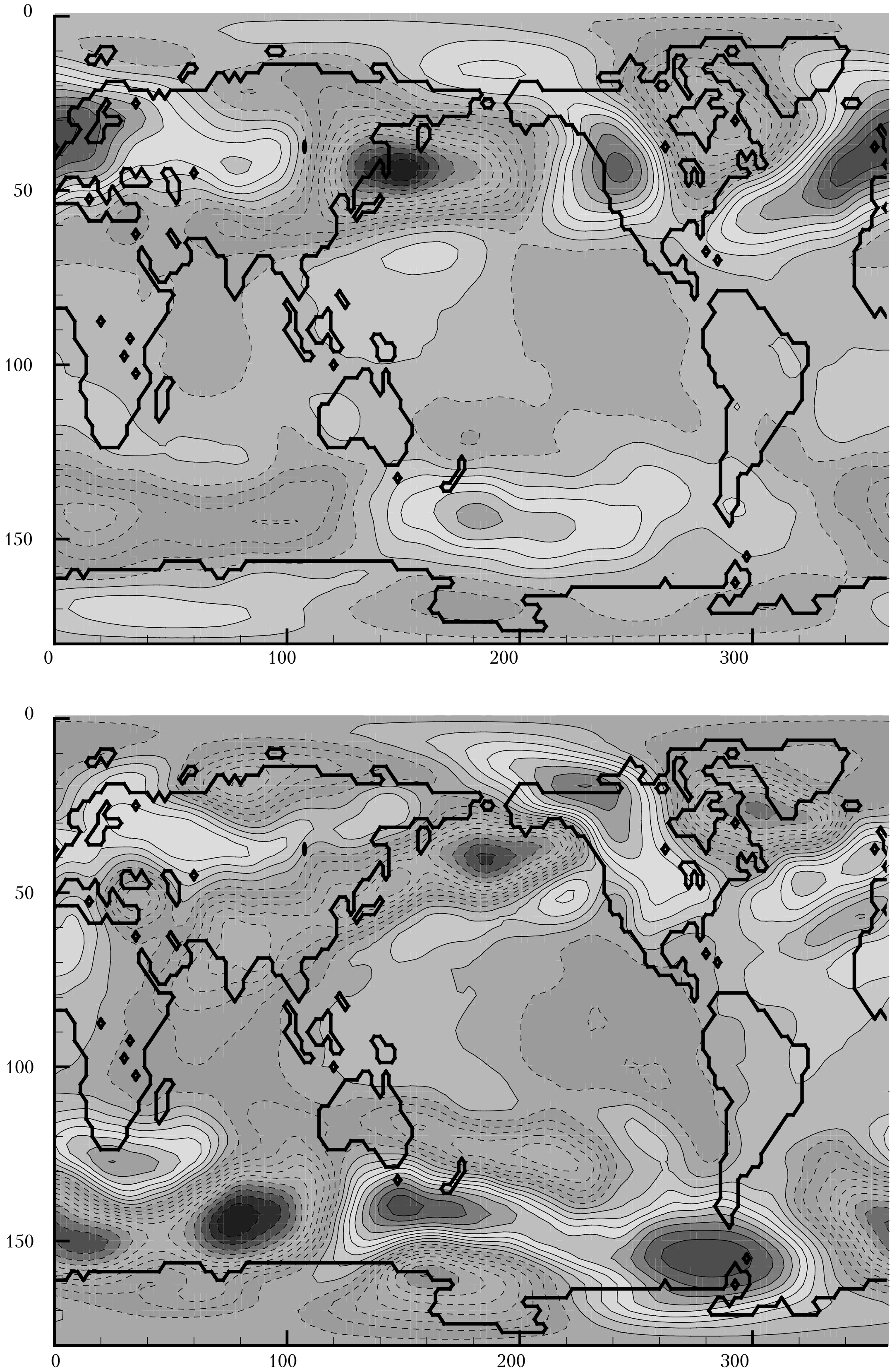

Fig. 1. Global-scale principal factors for the geopotential field at the 500 mbar surface at 00:00 GMT on January 15 (top) and June 15 (bottom); zones of positive values are shown by solid curves and those of negative values are shown by dashed curves.

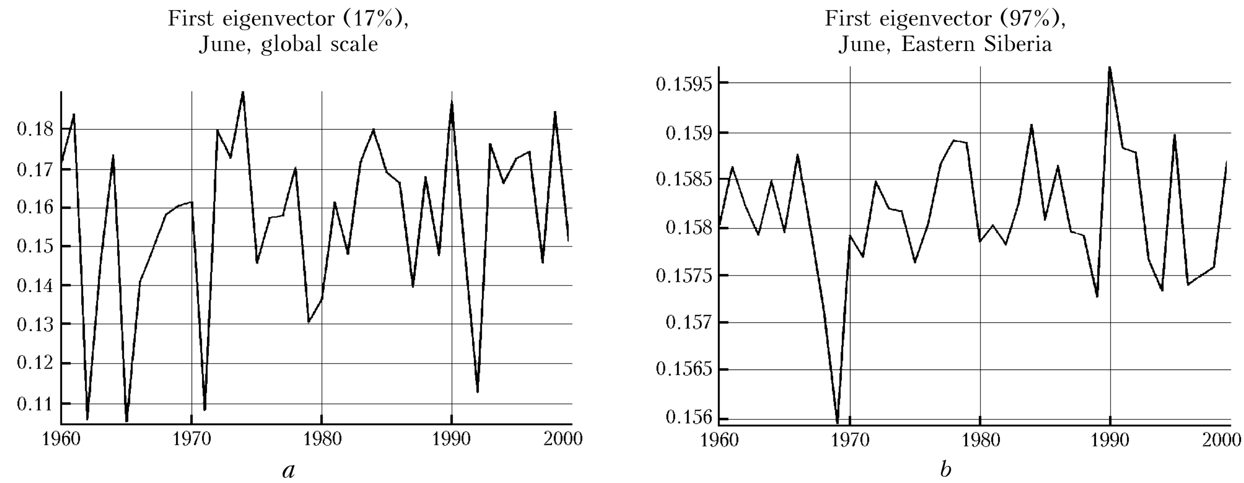

Fig. 2. Annual behavior of factor loads for the first June basis vector for the 40-year period (1960–1999): global factor (*a*) and regional factor (*b*).

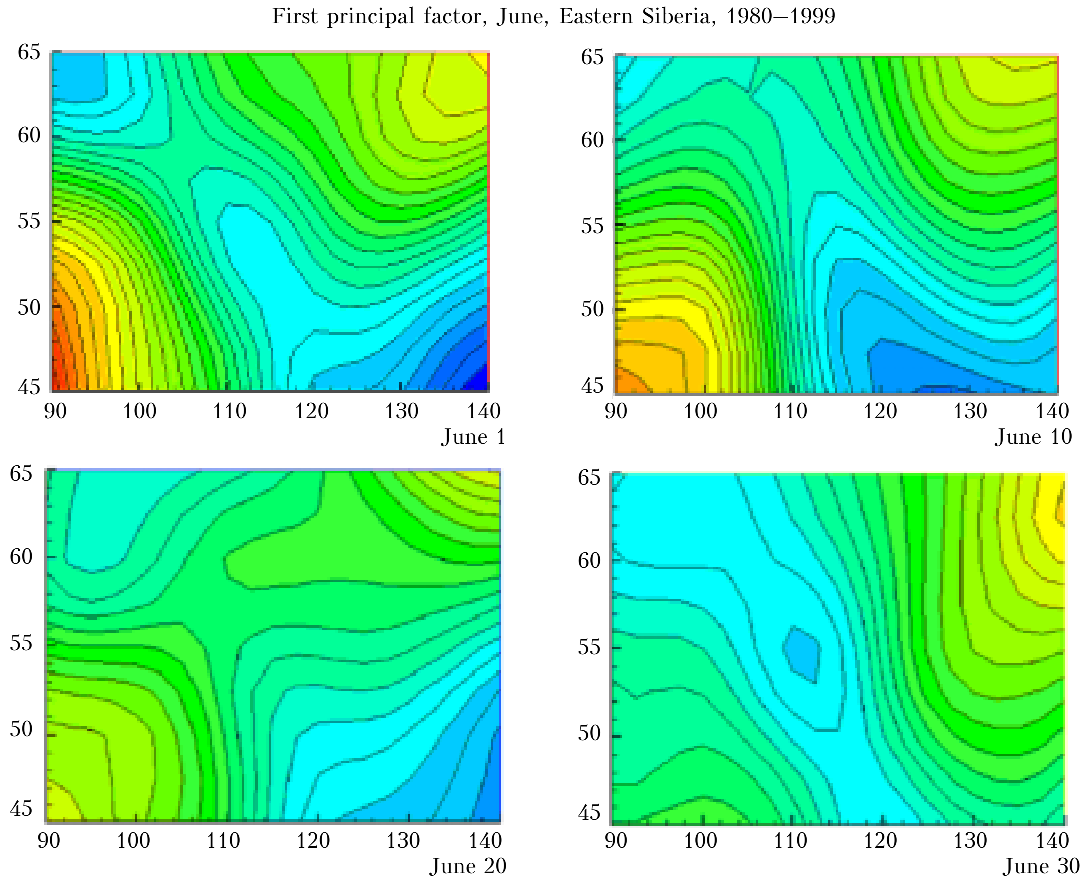

Fig. 3. Principal factor of the geopotential field (500 mbar surface) of regional scale for the southern part of East Siberia.

Based on the above prerequisites, the simulation technology is organized on the principles of integration of different-scale models and decomposition of the state functions into background and perturbation components in accordance with the process scales. The essence of this technology is in the following. New elements, namely, the guiding phase spaces are introduced in the model. They are multicomponent fields of the spatiotemporal structure providing for description of background processes with the preset degree of informativeness with respect to the observed states of the global climatic system. The component composition is determined by the form and content of the model state functions.

To form the guiding spaces, we develop two approaches within the hypothesis of the relative stability of climate. The first approach has a simple scheme and consists in generation of background fields by the technology described in Ref. 9, using directly the Reanalysis database[8] of many-year behavior of the climatic system. In this case, particular situations for organization of scenarios are selected taking into account the typification with respect to the principal factors. Another approach is based on the factor analysis methods described above. They are used to construct informative bases and to separate principal factors, as well as to form phase subspaces by the preset criterion of informativeness. Just these constructions provide for description of the background climatic processes. The detailed structure of the fields is calculated with a set of mathematical models. Regional investigations assume a synchronous use of the global and regional models.[10–11] Different-scale models are integrated and the guiding phase spaces in them are taken into account in the simulation rate at every time step with the fast data-assimilation procedures developed by us.[13] It is important for all information arrays to be presented on the structure-consistent grid areas. This facilitates the embedding procedure without loss in informativeness and accuracy of the fields' representation.

The simulation scenarios are organized using the set of models described in Ref. 10 and supplemented with the factor analysis algorithms, fast data-assimilation procedures, and methods of the model sensitivity theory. The scenarios are realized in the modes of direct and inverse simulation.[11,12] In particular, when the processes of pollutant spread in the atmosphere from regional sources are studied, the methods of direct simulation are used. The regional models in them fully describe the process until the distortions generated by the sources reach the region boundaries. To follow the behavior of these distortions beyond the region, if necessary, the global models are invoked. If the ecological situation in the region is estimated in the mode of inverse simulation, then the composition of the set of models is organized depending on the behavior of functions of sensitivity of the environment quality functionals. That is, if the sensitivity regions reach the boundary, this is a signal of the need to invoke the global-scale model for estimation of the domain of influence and transborder sources.

Due to the use of guiding spaces, such organization of simulation allows us to calculate the long-term scenarios of the regional atmospheric circulation and pollutant transport with retention of predictability and informativeness. This is achieved through assimilation of the background space elements accounting for the dynamics of global processes in the models. Besides, this approach provides for correct solution of the problems connected with an uncertainty in setting the boundary conditions for regions on a bounded territory. In this context, the models give, in essence, a detailed description of the processes inside some region with allowance for background global processes.

Conclusion

The factor analysis methods and algorithms for separation of the principal components are an efficient tool for studying the variability of natural processes and, especially, the variability of many-year dynamics of the climatic system. Special organization of information arrays and calculations allows us to obtain a contracted representation in terms of decomposition of the dimension of multidimensional and multicomponent fields, leaving for analysis most significant direction of changes from the investigator's point of view. For example, in the climatic dynamics we have chosen as the variable the time with the discreteness of one year. Its parametric representation is the number of a year in the relative scale of readings. The month's number in a year is specified as a parameter of seasonal behavior, while other variables, including the time during a month, pass into the internal structure of characteristics of the studied fields.

Numerical experiments on selection of the internal structure of vectors have shown that taking into account both spatial and temporal behaviors increases the field analysis informativeness in general and makes its results more convenient for interpretation and use in formation of scenarios.

The results of analysis of the global and regional processes show that the first principal factors with relatively high degree of informativeness are distinguished in factor solutions. This is especially pronounced in regional scenario estimates. Thus, for the Baikal region, in the global circulation structure, in particular, in the geopotential fields on the 500 mbar isobaric surface, we can separate the principal factors with the measure of informativeness higher than 90%, which can be interpreted as regional manifestations of the global climatic background.

Analysis of the climatic system's centers of influence by the results of factor analysis of the monthly structures of many-year data on the global-scale atmospheric circulation shows that the Baikal region is between the large-scale thermobaric formations. This leads to formation of locally unstable circulations in the region, which is indicated, in particular, by the presence of the Sayano-Altai energoactive zone characterized by a high intensity of summer cyclogenesis.

Thus, the integrated use of the qualitative and quantitative information about the structure of the principal factors in the dynamics of the climatic system and about the sensitivity functions of this system to perturbations of its governing parameters gives new possibilities for constructing the models and scenarios for climatic-ecological investigations adequately reflecting both general and specific features of the studied phenomena.

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