Environmental forecasting on the base of online-integrated modeling technology

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Online-integrated modeling technology

- Models of hydrodynamics
- Models of atmospheric chemistry
- Data of observations / assimilation
- Technology of modeling
- New algorithms
- New mathematics/numerics

  (tera- (12), peta-(15), exa- (18)

Model of atmospheric dynamics

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u - fv + kw = -\frac{1}{\rho}\frac{\partial p}{\partial x} + F_u$$

$$\frac{\partial v}{\partial t} + \mathbf{v} \cdot \nabla v + fu = -\frac{1}{\rho}\frac{\partial p}{\partial y} + F_v$$

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla w - ku = -\frac{1}{\rho}\frac{\partial p}{\partial z} - g + F_w$$

$$\frac{\partial p}{\partial t} + \mathbf{v} \cdot \nabla p + \left(\frac{c_p}{c_v}\nabla \cdot \mathbf{v}\right)p = \left(\frac{c_p}{c_v} - 1\right)\rho c_p F_p + f_p$$

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T + \left(\frac{R_d}{c_v}(1+\alpha)\nabla \cdot \mathbf{v}\right)T = \frac{c_p}{c_v}F_T + f_T$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho\mathbf{v} = 0, \qquad \rho_a = p\left(R_d(1+\alpha)T\right)^{-1}$$

Transport and transformation of humidity

$$\frac{\partial q_v}{\partial t} + \mathbf{v} \cdot \nabla q_v = -\left(S_l + S_f\right) + F_{q_v}$$

$$\frac{\partial q_c}{\partial t} + \mathbf{v} \cdot \nabla q_c = S_c + F_{q_c}$$

$$\frac{\partial q_l}{\partial t} + \mathbf{v} \cdot \nabla q_l + \frac{1}{\rho}\frac{\partial}{\partial z}\rho q_l \left|v_{lT}\right| = S_l + F_{q_l}$$

$$\frac{\partial q_f}{\partial t} + \mathbf{v} \cdot \nabla q_f + \frac{1}{\rho}\frac{\partial}{\partial z}\rho q_f \left|v_{fT}\right| = S_f + F_{q_f}$$

Transport and transformation model
of gas pollutants and aerosols

$$\left(\mathrm{L}\boldsymbol{\varphi}\right)_{\mathrm{i}} \equiv \frac{\partial \boldsymbol{\pi} \boldsymbol{\varphi}_{\mathrm{i}}}{\partial \mathrm{t}} + \operatorname{div} \boldsymbol{\pi}(\boldsymbol{\varphi}_{\mathrm{i}} \mathbf{u} - \boldsymbol{\mu}_{\mathrm{i}} \operatorname{grad} \boldsymbol{\varphi}_{\mathrm{i}}) + \boldsymbol{\pi}((\mathrm{S}\boldsymbol{\varphi})_{\mathrm{i}} - \mathrm{f}_{\mathrm{i}}(\mathrm{x}, \mathrm{t}) - \mathrm{r}_{\mathrm{i}}) = 0,$$

Operators of transformation

$$\left\{\mathrm{S}_{\mathrm{g}}(\boldsymbol{\varphi}) = \mathrm{P}(\boldsymbol{\varphi}) - \boldsymbol{\Pi}(\boldsymbol{\varphi})\right\}_{\mathrm{i}} \equiv \sum_{\mathrm{q}=1}^{\mathrm{R}_{\mathrm{i}}} \left\{ \mathrm{k}(\mathrm{q}) \left(\mathrm{s}_{\mathrm{i}}(\mathrm{q}^{-}) - \mathrm{s}_{\mathrm{i}}(\mathrm{q}^{+}) \right) \prod_{\mathrm{j}=1}^{\mathrm{U}_{\mathrm{r}}} \boldsymbol{\varphi}_{\mathrm{j}}^{\mathrm{s}_{\mathrm{j}}(\mathrm{q}^{-})} \right\}$$

$$S_a\left(\varphi_i(\sigma)\right) = \frac{1}{2} \int_{\sigma_0}^{\sigma} \left[\sum_{k=1}^{M} \gamma_{ik} \varphi_k(\sigma_1) \left(\sum_{m=1}^{M} \alpha_{km} K(\sigma - \sigma_1, \sigma_1) \varphi_k(\sigma - \sigma_1) \right) \right] d\sigma_1$$

$$-\varphi_i(\sigma) \int_{\sigma_0}^{\sigma_M} K(\sigma, \sigma_1) \left(\sum_{k=1}^{M} \beta_{ik} \varphi_k(\sigma_1) \right) d\sigma_1 - \frac{\partial}{\partial \sigma} \left[e_i \varphi_i(\sigma) \right] + \frac{\partial^2}{\partial \sigma^2} \left[\nu_i \varphi_i(\sigma) \right]$$

$$-R_i \varphi_i(\sigma) + Q_i(\sigma), \quad i = \overline{1, M}$$

Goals

- Development of methodology for construction of integrated models of atmospheric dynamics and air quality in on(off)-line regimes with account of all accessible observational data
- Design of adequate/open modeling system

Variational principle as a tool for model integration

It presents the equations and relations describing the development of multi-component and multi-scale processes in a simple invariant form;

It holds the synthesis of continuum and discrete presentations of mathematical models and state functions;

Variational principle as a tool for model integration

It provides consistency for all technology stages of mathematical modeling;

- Euler, Lagrange, Jacobi, and Hamilton principles are interconnected among themselves: the stationary value of some definite integral (functional) is considered in each of them.

A CONCEPT
OF ENVIRONMENTAL MODELING

•variational principles

•combined use of models and observed data,
• forward and inverse modeling procedures,
• methodology for description of links between regional and global processes (including climatic changes) by means of orthogonal decomposition of functional spaces for analysis of data bases and phase spaces of dynamical systems

Theoretical background

•control theory,
•sensitivity theory,
•risk and vulnerability theory

Basic elements for concept implementation:

- models of processes
- data and models of measurements
- adjoint problems
- constraints on parameters and state functions
- functionals: objective, quality, control, restrictions etc.
- sensitivity relations for target functionals and constraints
- feedback equations for inverse problems

Statement of the problem

- **Mathematical model**

$$B\frac{\partial \vec{\varphi}}{\partial t} + G(\vec{\varphi}, \vec{Y}) - \vec{f} - \vec{r} = 0,$$

$$\vec{\varphi}^{\,0} = \vec{\varphi}_0^{\,0} + \vec{\xi}, \quad \vec{Y} = \vec{Y}_0 + \vec{\varsigma};$$

$\vec{\varphi} \in \Im(D_t)$ is the state function,

$\vec{Y} \in \Re(D_t)$ is the parameter vector.

G is the “space” operator of the model

- **A set of measured data** $\vec{\varphi}_m, \vec{\Psi}_m$ **on** D_t^m

$$\vec{\Psi}_m = [H(\vec{\varphi})]_m + \vec{\eta},$$

$[H(\vec{\varphi})]_m$ **is the model of observations.**

- $\vec{r}, \vec{\xi}, \vec{\varsigma}, \vec{\eta}$ **are the terms describing uncertainties and errors of the corresponding objects.**

Desired!

General form of functionals

$$\Phi_k(\vec{\varphi}) = \int_{D_t} F_k(\vec{\varphi})\chi_k(\vec{x},t)dDdt \equiv \left(F_k,\chi_k\right), \quad k = 1,\dots,K$$

F_k are the **Lipschitz's** functions of the given form, differentiable, bounded

$\chi_k dDdt$ are **Radon's or Dirac's** measures on D_t, $\chi_k \in \Im^*(D_t)$.

Quality functionals

$$\Phi_k(\vec{\varphi}) = \int_{D_t} (\Psi - H(\vec{\varphi}))_m^T M(\Psi - H(\vec{\varphi}))_m \chi_k(\vec{x},t)dDdt,$$

"Measurement" functionals

$$\Phi(\vec{\varphi}) = \sum_{k=1}^{K} \int_{D_t} \left[H(\vec{\varphi})\right]_{mk} \delta(\vec{x} - \vec{x}_{mk})dDdt, \quad \vec{x}_{mk} \in D_t^m$$

Restriction functionals

$\vec{\varphi}(\vec{x},t) \le N, \quad \vartheta_k(\vec{\varphi}(\vec{x},t) \le 0$ distributive constraints

$$\Phi_k(\vec{\varphi}) = \int_{D_t} (\vartheta_k(\vec{\varphi}) + |\vartheta_k(\vec{\varphi})|)\chi_k(\vec{x},t)dDdt$$

Differentiability in extended sense

Variational form of model's set: hydrodynamics+ chemistry+ hydrological cycle

$$I\left(\boldsymbol{\varphi},\mathbf{Y},\boldsymbol{\varphi}^*\right)\equiv\sum_{i=1}^{n}\left\{\left(\boldsymbol{\Lambda}\boldsymbol{\varphi},\boldsymbol{\varphi}^*\right)_i+\int_{D_t}\boldsymbol{\pi}((S\boldsymbol{\varphi})_i-f_i(x,t)-r_i)\boldsymbol{\varphi}^* dDdt\right\}+$$

$$\int_{D_t}\left\{\left(pp^*\operatorname{div}\mathbf{u}-p\operatorname{div}\mathbf{u}^*\right)+\left(\boldsymbol{\alpha}_p pp^*+\boldsymbol{\alpha}_T TT^*\right)\operatorname{div}\mathbf{u}\right\}dDdt+$$

$$\int_{D_t}\boldsymbol{\alpha}_{\rho}\left\{(\boldsymbol{\rho}-\boldsymbol{\rho}_a)^T W_a(\boldsymbol{\rho}-\boldsymbol{\rho}_a)\right\}dDdt+\int_{\boldsymbol{\Omega}_t}pu_n^* d\boldsymbol{\Omega}dt=0$$

Variational form of convection-diffusion operators

$$\left(\boldsymbol{\Lambda\varphi},\boldsymbol{\varphi}^*\right)_{\mathrm{i}} \equiv \left(\int_{\mathrm{D_t}} \left\{ \frac{1}{2} \left[\left(\boldsymbol{\varphi}^* \frac{\partial \boldsymbol{\pi\varphi}}{\partial \mathrm{t}} - \boldsymbol{\varphi} \frac{\partial \boldsymbol{\pi\varphi}^*}{\partial \mathrm{t}} \right) + \left(\boldsymbol{\varphi}^* \mathrm{div}\, \boldsymbol{\pi\varphi \mathrm{u}} - \boldsymbol{\varphi} \mathrm{div}\, \boldsymbol{\pi\varphi}^* \mathbf{u} \right) \right] \right.\right.$$

$$\left. + \boldsymbol{\pi\mu}_{\varphi}\, \mathrm{grad}\, \boldsymbol{\varphi}\ \mathrm{grad}\, \boldsymbol{\varphi}^* \right\} dDdt + \frac{1}{2}\int_D \boldsymbol{\varphi\varphi}^* \boldsymbol{\pi} dD \Big|_0^{\bar{t}} +$$

$$\left. \int_{\boldsymbol{\Omega}_t} \left[\left(\frac{1}{2} \boldsymbol{\varphi} u_n - \boldsymbol{\mu} \frac{\partial \boldsymbol{\varphi}}{\partial n} \right) + \boldsymbol{\alpha}_b \left(R_b \boldsymbol{\varphi} - q_b \right) \right] \boldsymbol{\varphi}^* \boldsymbol{\pi} d\boldsymbol{\Omega} dt \right)_i$$

$R_b\boldsymbol{\varphi} - q_b = 0$ boundary conditions on $\boldsymbol{\Omega}_t$

Augmented functional for construction of optimal algorithms and uncertainty assessment

$$\tilde{\Phi}^h(\vec{\varphi}) = \Phi_k^h(\vec{\varphi}) + 0.5\Big\{\alpha_1(\vec{\eta}^T M_1 \vec{\eta})_{D_t^m} + \alpha_2(\vec{r}^T M_2 \vec{r})_{D_t^h}$$

$$+\alpha_3(\vec{\xi}^T M_3 \vec{\xi})_{D^h} + \alpha_4(\vec{\zeta}^T M_4 \vec{\zeta})_{R^h(D_t^h)}\Big\}^h + \left[\mathbf{I}^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*)\right]_{D_t^h}$$

$M_i, (i = \overline{1,4})$ are the weight matrices,

$\alpha_i \geq 0, \ \sum_{i=1}^{4} \alpha_i = 1$ are the weight coefficients,

$\vec{\varphi}, \vec{\varphi}^*$ are the solutions of the direct and adjoint problems generated from

$$\mathbf{I}^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = 0$$

Additive aggregation of the functionals for decomposition

Variation of augmented cost functional. Consistency and optimization of algorithms

$$\delta\tilde{\Phi}_k^h(\vec{\varphi}) = \left(\frac{\delta\tilde{\Phi}_k^h(\vec{\varphi})}{\partial\vec{\varphi}^*}, \delta\vec{\varphi}^* \right) + \left(\frac{\delta\tilde{\Phi}_k^h(\vec{\varphi})}{\partial\vec{\varphi}}, \delta\vec{\varphi} \right) +$$

$$+ \left(\frac{\delta\tilde{\Phi}_k^h(\vec{\varphi})}{\partial r}, \delta r \right) + \left(\frac{\delta\tilde{\Phi}_k^h(\vec{\varphi})}{\partial \xi}, \delta \xi \right) + \left(\frac{\delta\tilde{\Phi}_k^h(\vec{\varphi})}{\partial Y}, \delta Y \right)$$

The universal algorithm
of forward & inverse modeling

$$\frac{\partial \tilde{\Phi}_k^h}{\partial \vec{\varphi}^*} \equiv B\Lambda_t \vec{\varphi} + G^h(\vec{\varphi}, \vec{Y}) - \vec{f} - \vec{r} = 0$$

$$\frac{\partial \tilde{\Phi}_k^h}{\partial \vec{\varphi}} \equiv (B\Lambda_t)^T \vec{\varphi}_k^* + A^T(\vec{\varphi}, \vec{Y})\vec{\varphi}_k^* + d_k = 0, \qquad \vec{\varphi}_k^*(\vec{x})\Big|_{t=\bar{t}} = 0$$

$$d_k = \frac{\partial}{\partial \vec{\varphi}}(\Phi_k^h(\vec{\varphi}) + 0.5\alpha_1(\vec{\eta}^T M_1 \vec{\eta})), \quad \vec{\varphi}^0 = \vec{\varphi}_a^0 + M_3^{-1}\vec{\varphi}_k^*(\vec{x},0), \quad t = 0$$

$$\vec{r}(\vec{x},t) = M_2^{-1}\varphi_k^*(\vec{x},t), \qquad \vec{Y} = \vec{Y}_a - M_4^{-1}\vec{\Gamma}_k$$

$$\vec{\Gamma}_k = \frac{\partial}{\partial \vec{Y}} I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}_k^*)$$

$$A(\vec{\varphi},\vec{Y})\delta\vec{\varphi} \equiv \frac{\partial}{\partial \alpha}\left[G^h(\vec{\varphi} + \alpha\,\delta\vec{\varphi}, \vec{Y})\right]_{\alpha=0}$$

$\Lambda_t \varphi$ is the approximation of time derivatives

Initial guess: $\vec{r}^{\,(0)} = 0$, $\vec{\varphi}^{0(0)} = \vec{\varphi}_a^0$, $\vec{Y}^{(0)} = \vec{Y}_a$

Algorithms of uncertainty calculation based on sensitivity analysis and data assimilation:

in model

$$\vec{r}(\vec{x},t) = M_2^{-1}\varphi_k^*(\vec{x},t),$$

in initial state

$$\vec{\xi} = M_3^{-1}\ \vec{\varphi}_k^*(\vec{x},0), \qquad t = 0$$

in model parameters and sources

$$\vec{\zeta} = M_4^{-1}\vec{\Gamma}_k = M_4^{-1}\frac{\partial}{\partial \vec{Y}} I^h(\vec{\varphi},\vec{Y},\vec{\varphi}_k^*)$$

$M_i, (i=\overline{2,4})$ are the weight matrices

Fundamental role of uncertainty functions

- integration of all technology components
- bringing control into the system
- regularization of inverse methods
- targeting of adaptive monitoring
- cost effective data assimilation

Some elements of optimal forecasting and design

The main sensitivity relations

$$\delta\Phi_k^h(\varphi) \equiv (\Gamma_k, \delta\,\mathrm{Y}) \equiv \frac{\partial}{\partial\alpha} I^h(\varphi, \mathrm{Y} + \alpha\ \ \delta\,\mathrm{Y},\ \varphi_k^*)\Big|_{\alpha=0}$$

Algorithm for calculation of sensitivity functions

$$\mathbf{\Gamma}_k = \frac{\partial}{\partial\delta\,\mathrm{Y}}\left(\frac{\partial}{\partial\alpha} I^h(\varphi, \mathrm{Y} + \alpha\ \ \delta\,\mathrm{Y}, \varphi_k^*)\Big|_{\alpha=0}\right)$$

The feed-back relations

$$\frac{dY_\alpha}{dt} = -\eta_\alpha \Gamma_{k\alpha}, \quad \alpha = \overline{1, N_\alpha}, \quad N_\alpha \le N$$

$\mathbf{\Gamma}_k = \{\Gamma_{ki}\}$ are the sensitivity functions

$\delta\,\mathbf{Y} = \{\delta Y_i\}$ are the parameter variations

$$k = \overline{1, K}, \ i = \overline{1, N}$$

ИВМиМГ

Realization
of main operator equations

Convection & diffusion

Idea and basic approximations

Differential operators of common type in the models

$$0=\int_{x_{i-1}}^{x_i}\left(L\varphi-f\right)\varphi^* dx=\int_{x_{i-1}}^{x_i} L^*\varphi^*\varphi dx+$$

$$\left(A\varphi,\varphi^*\right)\Big|_{x_{i-1}}^{x_i}-\int_{x_{i-1}}^{x_i} f(x)\varphi^*(x)dx=0$$

If $L^*\varphi^*=0,$ then

$$\left(A\varphi,\varphi^*\right)\Big|_{x_{i-1}}^{x_i}-\int_{x_{i-1}}^{x_i} f(x)\varphi^*(x)dx=0,\quad i=\overline{2,n_x}$$

$\varphi^{*(\alpha)}(x),\ x_{i-1}\le x\le x_i,\ \ \alpha=1,2$ integrating multipliers

Fundamental **analytical** solutions of local adjoint problems

$$\left\{\varphi_i^{*(1)}=1,\quad \varphi_{i+1}^{*(1)}=0\right\},\quad \left\{\varphi_i^{*(2)}=0,\quad \varphi_{i+1}^{*(2)}=1\right\},\ i=\overline{1,n_x-1}$$

Additive form of integral identity

$$I(\varphi,\varphi^{*}) = \int\limits_{D_t}\left(\frac{\partial\varphi}{\partial t} + \sum_{\alpha=1}^{r}\left(L_\alpha\varphi - f_\alpha\right)\right)\varphi^{*}dD\,dt = 0$$

Variational construction of additive schemes

$$I_t^h(\varphi,Y,\varphi^{*}) + \Phi_t^h(\varphi) =$$

$$\sum_{j=2}^{J}\int\limits_{D}\left\{\sum_{\alpha=1}^{r}\left\{\left[\Psi_\alpha^j - \varphi^{j-1} + \Delta\tau_\alpha^j\left(L_\alpha^j\Psi_\alpha^j - f_\alpha^j\right)\right]\Psi_\alpha^{*j} + \left[\Psi_\alpha^j - \left(\sigma_\alpha\varphi_\alpha^j - \left(1-\sigma_\alpha\right)\varphi^{j-1}\right)\right]\varphi_\alpha^{*j}\delta t_j\right\}\right.$$

$$\left. + \left(\varphi^j - \frac{1}{r}\sum_{\alpha=1}^{r}\varphi_\alpha^j\right)\varphi^{*j}\delta t_j\right\}dD + \sum_{j=2}^{J}\Phi^j(\varphi)$$

Decomposition of integral identity

$$I_{\alpha}^{j}(\varphi,\varphi^{*}) \equiv \int_{a}^{b}\left(\Psi + \Delta\tau^{j}\left(u\frac{\partial\Psi}{\partial x} - \frac{\partial}{\partial x}\mu\frac{\partial\Psi}{\partial x} + d\Psi \right) - W \right)\varphi^{*}dx = 0;$$

$$W = \varphi^{j-1} + \Delta\tau^{j} f^{j}$$

$$\Psi = \sigma\varphi^{j} + \left(1-\sigma\right)\varphi^{j-1},\ \ \Delta\tau^{j} = \sigma\Delta t_{j},\ \ \Delta t_{j} = t_{j} - t_{j-1},\ \ 0.5 \le \sigma \le 1$$

$$\varphi^{j} = \frac{1}{\sigma}\left(\Psi - \left(1-\sigma\right)\varphi^{j-1}\right)$$

Solutions of the local adjoint problems for convection-diffusion operators

$$L_i^* \omega_i^{(\alpha)}(x) = 0, \ \alpha = 1,2, \ x_i \le x \le x_{i+1}, \ \ i = \overline{1, n-1}.$$

$$\varphi_i^*(x) = \varphi_i^* \omega_i(x), \qquad \omega_i(x) = \begin{cases} \omega_{i-1}^{(1)}(x) & x_{i-1} \le x \le x_i \\ \omega_i^{(2)}(x) & x_i \le x \le x_{i+1} \end{cases}, \ \ i = \overline{1, n}$$

$$\omega_1(x) = \omega_1^{(2)}(x), \quad x_1 \le x \le x_2; \quad \omega_n(x) = \omega_{n-1}^{(1)}(x), \quad x_{n-1} \le x \le x_n$$

$$\omega_i^{(1)}(x) = A_i \left(e^{-\nu_1 x'} - e^{\nu_2(1-x') - \nu_1} \right) \qquad x' = (x_{i+1} - x)/\Delta x_i$$

$$\omega_i^{(2)}(x) = A_i \left(e^{\nu_2(1-x')} - e^{\nu_2 - \nu_1 x'} \right) \qquad A_i = \left(1/(1 - e^{(\nu_2 - \nu_1)}) \right)_i$$

$$\left\{ \nu_1 = \lambda_1 \Delta x, \ \nu_2 = \lambda_2 \Delta x, \ \lambda_1 \ge 0, \ \lambda_2 \le 0 \right\}_i$$

$$\left\{ \lambda^2 + \frac{u}{\mu}\lambda - \frac{1 + d\Delta\tau}{\mu\Delta\tau} = 0 \right\}_i^j$$

Three-point numerical scheme

$$-a_i\varphi_{i+1} + b_i\varphi_i - c_i\varphi_{i-1} = f_i$$

$$a_i \ge 0,\;\; c_i \ge 0,\;\; b_i = b_i^+ + b_i^-,\;\; b_i^+ \ge a_i,\;\; b_i^- \ge c_i,\;\; \text{при}\;\; \mu_i \ge 0$$

Properties of DA numerical schemes:

approximation, stability, monotonicity, transportivity, differentiability with respect to parameters and state functions , uniform schemes without flux-correction

$$CFL = \max_{\langle i\rangle}\left\{\frac{|u|\Delta\tau}{\Delta x} + \frac{2\mu\Delta\tau}{\Delta x^2} + d\Delta\tau\right\} < 1, \qquad \max\left\{\left(\nu_1 - \nu_2\right)_i, \left(|u|\Delta x/\mu\right)_i\right\} \le 10$$

Singular case $\mu = 0$

$$u\frac{\partial \varphi^j}{\partial x} + d\varphi^j = f$$

Numerical scheme

$$-u^{+}_{i-1/2}\exp(-\lambda^{(1)}_{i-1}\Delta x_{i-1})\varphi_{i-1} + \left(u^{+}_{i-1/2} + u^{-}_{i+1/2}\right)\varphi_i - u^{-}_{i+1/2}\exp(-\lambda^{(2)}_{i}\Delta x_i)\varphi_{i+1} =$$

$$\int_{x_{i-1}}^{x_i} f(x)\exp\left(-\lambda^{(1)}_{i-1}\left(x_i - x\right)\right)dx + \int_{x_i}^{x_{i+1}} f(x)\exp\left(-\lambda^{(2)}_{i}\left(x - x_i\right)\right)dx.$$

$$\Delta x_{i-1} = x_i - x_{i-1}; \qquad \Delta x_i = x_{i+1} - x_i;$$

$$\lambda^{(1)}_{i-1} = \left(d/u^{+}\right)_{i-1/2}; \quad \lambda^{(2)}_{i} = \left(d/u^{-}\right)_{i+1/2};$$

$$u^{+} = 0,5\left(|u| + u\right) > 0; \qquad u^{-} = 0,5\left(|u| - u\right) > 0.$$

Godunov's test problem
(С.К.Годунов Математический сборник, т. 47(89):3, 1959, с.271-306.)

$$\frac{\partial\varphi}{\partial t}+u\frac{\partial\varphi}{\partial x}=0,\quad \varphi\big|_{t=0}=\varphi^0(x),\quad u=const \qquad \text{(G1)}$$

Analytic solution

$$\varphi(x,t)=\left(\frac{x-ut}{\Delta x}-0,5\right)^2-0,25 \qquad \text{(G2)}$$

Difference-analytic scheme

$$\frac{3\varphi^{j} - 4\varphi^{j-1} + \varphi^{j-2}}{2\Delta t} + u\frac{\partial\varphi^{j}}{\partial x} = 0 \qquad \text{(G3)}$$

$$\frac{3\varphi^{j} - 4\varphi^{j-1} + \varphi^{j-2}}{2\Delta t} = -\frac{2u}{\Delta x}\left(\frac{x - ut^{j}}{\Delta x} - 0,5\right) = \left.\frac{\partial\varphi(x,t)}{\partial t}\right|_{t=t^{j}} \qquad \text{(G4)}$$

$$\frac{\partial\varphi}{\partial x} = \left.\frac{2}{\Delta x}\left(\frac{x - ut}{\Delta x} - 0,5\right)\right|_{t=t^{j}} \qquad \text{(G5)}$$

Chemical operators

Stiff differential systems

$$\dot{x}_1 + 1000x_1 = 0; \qquad x_1(0) = 1, \qquad x_1(t) > 0$$
$$\dot{x}_2 + x_2 = 0,999x_1; \qquad x_2(0) = 0,999, \qquad x_2(t) > 0$$

Analytical solution

$$x_1(t) = \exp(-1000t)$$

$$x_2(t) = -0,001\exp(-1000t) + \exp(-t)$$

Euler explicit scheme

$$x_1(t+\Delta t) = \left(1 - 1000\Delta t\right)x_1(t)$$
$$x_2(t+\Delta t) = \left(1 - \Delta t\right)x_2(t) + 0,999\Delta t x_1(t)$$

Euler implicit scheme

$$x_1(t+\Delta t) = x_1(t) / \left(1 + 1000\Delta t\right)$$
$$x_2(t+\Delta t) = \left(x_2(t) + 0,999\Delta t x_1(t)\right) / \left(1 + \Delta t\right)$$

Direct and adjoint operators for kinetics of chemical transformations

$$\left\{S_g(\vec{\boldsymbol{\varphi}}) = P(\vec{\boldsymbol{\varphi}})\boldsymbol{\varphi} - \boldsymbol{\Pi}(\vec{\boldsymbol{\varphi}})\right\}_i \equiv \sum_{q=1}^{R_i}\left\{k(q)\left(s_i(q^-) - s_i(q^+)\right)\prod_{j=1}^{U_r}\boldsymbol{\varphi}_j^{s_j(q^-)}\right\}$$

$$\left\{S_g^*(\vec{\boldsymbol{\varphi}}^*)\right\}_i \equiv \sum_{q=1}^{R_i}\left\{k(q)\frac{s_i(q^-)}{\boldsymbol{\varphi}_i}\prod_{j=1}^{U_q}\boldsymbol{\varphi}_j^{s_i(q^-)}\sum_{\boldsymbol{\alpha}=1}^{U_q}\left(s_{\boldsymbol{\alpha}}(q^-) - s_{\boldsymbol{\alpha}}(q^+)\right)\boldsymbol{\varphi}_{\boldsymbol{\alpha}}^*\right\}_i$$

Relations for reaction operators. Monotonicity and positivity properties

$$\int_{t_{j-1}}^{t_j} \left(\frac{\partial \varphi_\alpha}{\partial t} + \left(\mathrm{P}(\vec{\varphi}) \right)_\alpha \varphi_\alpha - \left(\Pi(\vec{\varphi}) \right)_\alpha - f_\alpha \right) \varphi_\alpha^{\ *} dt = 0$$

$$\vec{\varphi} = \{\varphi_\alpha\}, \ \ \alpha = \overline{1, n_\alpha}, \ \ \varphi_\alpha^*(t_j) = 1, \ \ j = \overline{2, J}, \ \ \vec{x} \in D_t^h$$

$$\varphi_\alpha \geq 0, \ \ \left(\mathrm{P}(\vec{\varphi}) \right)_\alpha \geq 0, \ \ \left(\Pi(\vec{\varphi}) \right)_\alpha \geq 0$$

Structure of aerosol operators

$$\frac{\partial \varphi_i(\sigma,t)}{\partial t} =$$

production

$$\frac{1}{2}\int_{\sigma_0}^{\sigma}\left[\sum_{k=1}^{M}\gamma_{ik}\varphi_k(\sigma_1)\left(\sum_{m=1}^{M}\alpha_{km}K(\sigma-\sigma_1,\sigma_1)\varphi_k(\sigma-\sigma_1)\right)\right]d\sigma_1$$

destruction

$$-\varphi_i(\sigma)\int_{\sigma_0}^{\sigma_M}K(\sigma,\sigma_1)\left(\sum_{k=1}^{M}\beta_{ik}\varphi_k(\sigma_1)\right)d\sigma_1 - R_i\varphi_i(\sigma)$$

condensation / evaporation

$$-\frac{\partial}{\partial\sigma}\left[e_i\varphi_i(\sigma)\right]+\frac{\partial^2}{\partial\sigma^2}\left[\nu_i\varphi_i(\sigma)\right]$$

diffusion

$$+Q_i(\sigma), \quad i=\overline{1,M}$$

sources / sinks

Variational principles for transformation models

$$\sum_{\alpha=1}^{n_\alpha}\left\{\int_{t_{j-1}}^{t_j}\left(\frac{\partial\varphi_\alpha}{\partial t}+\left(P(\vec{\varphi})\right)_\alpha-\left(\Pi(\vec{\varphi})\right)_\alpha-f_\alpha\right)\varphi_\alpha{}^{*}dt\right\}=0$$

$$\vec{\varphi}=\left\{\varphi_\alpha\right\},\ \ \alpha=\overline{1,n_\alpha},\ \ \ \varphi_\alpha^{*}(t_j)=1,\ \ j=\overline{2,J},\ \ \vec{x}\in D_t^h$$

$$\varphi_\alpha\geq 0,\ \ \left(P(\vec{\varphi})\right)_\alpha\geq 0,\ \ \left(\Pi(\vec{\varphi})\right)_\alpha\geq 0$$

Decomposition on reaction mechanisms

$$\int_{t_{j-1}}^{t_j}\left(\frac{\partial\varphi_\alpha}{\partial t}+\left(P(\vec{\varphi})\right)_\alpha-\left(\Pi(\vec{\varphi})\right)_\alpha-f_\alpha\right)\varphi_\alpha{}^{*}dt=0$$

$$\alpha=\overline{1,n_\alpha}$$

Variational principles for transformation models (2)

$$P_i(\boldsymbol{\varphi}) = \sum_{r=1}^{R_i}\left[k_i(r)s_i(r-)\prod_{\alpha=1}^{U_{ri}}\varphi_\alpha^{S_\alpha(r-)}\right], \qquad P_i(\boldsymbol{\varphi}) \equiv L_i(\boldsymbol{\varphi})\varphi_i$$

$$P_i(\boldsymbol{\varphi}) = \sum_{1}^{R_i}\left[k_i(r)s_i(r+)\prod_{\alpha=1}^{U_{ri}}\varphi_\alpha^{S_\alpha(r-)}\right].$$

$$F_i(\boldsymbol{\varphi}) = F_i(\boldsymbol{\varphi},\boldsymbol{\kappa},\mathbf{q}) = \Pi_i(\boldsymbol{\varphi}) + q_i$$

$$\boldsymbol{\kappa} = \left(k_1,\ldots,k_{n_\alpha}\right)^T$$

$$\mathbf{q} = \left(q_1,\ldots,q_{n_\alpha}\right)^T$$

Variational principles for transformation models (3)

$$\int_{t_j}^{t_{j+1}} \left(-\frac{\partial \psi_i^*}{\partial t} + L_i(\boldsymbol{\varphi})\psi_i^* \right) \varphi_i(t)\,dt - \int_{t_j}^{t_{j+1}} F_i(\boldsymbol{\varphi})\psi_i^*\,dt + \left(\varphi_i \psi_i^*\right)^{j+1} - \left(\varphi_i \psi_i^*\right)^{j} = 0$$

$$\psi_i^* \in Q^*(D_t)$$

Adjoint functions ψ_i^* are chosen as solutions of equations :

$$\frac{\partial \psi_i^*}{\partial t} - L_i(\boldsymbol{\varphi})\psi_i^* = 0, \quad t_j \le t \le t_{j+1}, \quad \psi_i^*\Big|_{t_{j+1}} = 1.$$

Variational principles for transformation models (4)

Using the idea of Euler integrating multipliers (factors), we get the system of integral equations

$$\varphi_i^{j+1} = \left(\varphi_i \psi_i^*\right)^j + \int_{t_j}^{t_{j+1}} F_i(\boldsymbol{\varphi}, t)\psi_i^*(t)dt$$

Finaly,

$$\varphi_i^{j+1} = \varphi_i^j e^{-b_i \Delta t_j} + \int_0^{\Delta t_j} F_i(\boldsymbol{\varphi}, \tau) e^{-b_i(\Delta t_j - \tau)} d\boldsymbol{\tau}$$

$$b_i = L_i^j(\boldsymbol{\varphi}^j)$$

Methane transformation in the atmosphere

$$CH_4 \xrightarrow{OH} CH_3 \xrightarrow{O_2} CH_3O_2 \xrightarrow{NO} CH_{3}0 \xrightarrow{O_2} H_2CO \xrightarrow{OH,h\nu} HCO \xrightarrow{O_2} CO \xrightarrow{OH} CO_2$$

$$CH_3O_2 \xrightarrow{HO_2} CH_3OOH$$

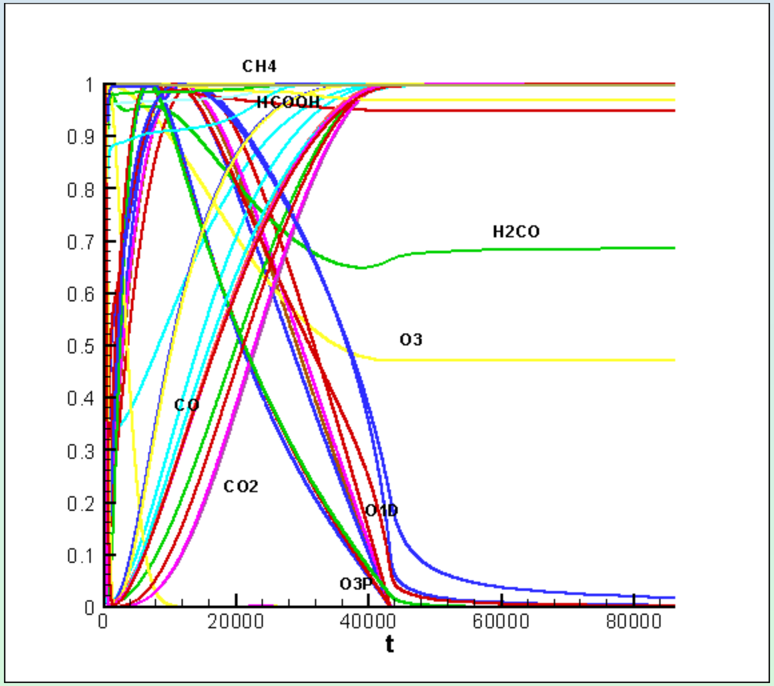
$$CH_3O_2 \xrightarrow{NO_2} CH_3O_2NO_2$$

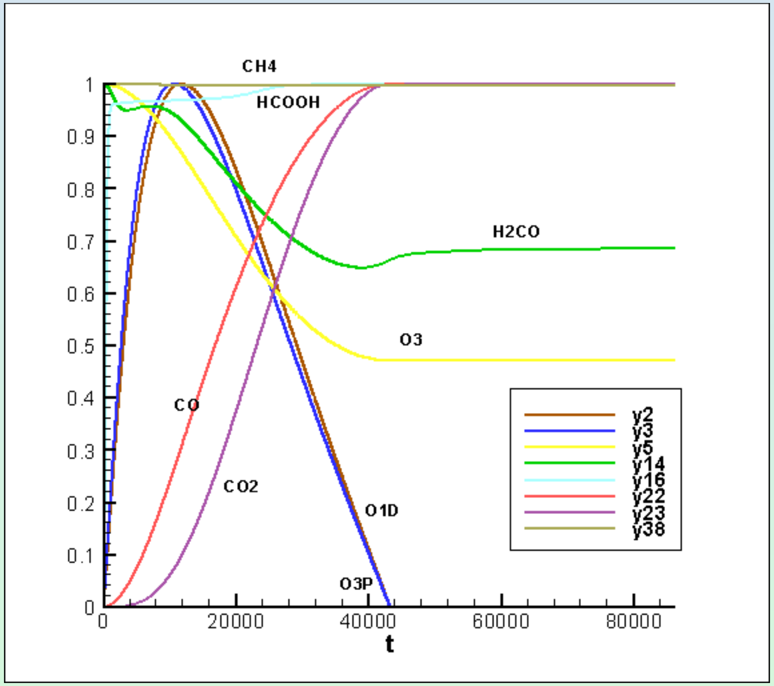
$$CH_{3}0 \xrightarrow{NO_2} CH_3ONO_2$$

$$CH_{3}0 \xrightarrow{HO_2,CH_2O} CH_3OH$$

$$H_2CO \xrightarrow{HO_2} HOCH_2O_2 \xrightarrow{NO} HOCH_2O \xrightarrow{O_2} HCOOH$$

Daily behavior of transformation products in methane-nitrogen-sulfur cycle





54 substances and 170 equations

Sensitivity relations for the problems of atmospheric chemistry

$$\delta\Phi\left(\boldsymbol{\varphi}\right)=\sum_{j=0}^{J}\left\{\sum_{i=1}^{n}\left\{\sum_{\gamma=1}^{\gamma_k}\left[\left(\frac{\partial F_i^j\left(\boldsymbol{\eta}_\gamma^j,\boldsymbol{\kappa}^j,q^j\right)}{\partial\mathbf{k}^j},\delta\mathbf{k}^j\right)+\delta q_i^j\right]f_{\gamma i}^{*j}+\right.\right.$$

$$\left.\left.\left(\frac{\partial L_i^j\left(\boldsymbol{\eta}_\gamma^j,\boldsymbol{\kappa}^j\right)}{\partial\mathbf{k}^j},\delta\mathbf{k}^j\right)b_i^{*j}\right\}\Delta t_j\right\}-\sum_{i=1}^{n}\left(\delta\varphi_{ai}^0\varphi_i^{*0}\right)$$

Stability and convergence of DA schemes

Let us consider an example:

$$\varphi_t - \Delta\varphi = 0, \quad \varphi\big|_{t=0} = \varphi^0, \ \varphi(\mathbf{x},t) \in D_t \quad (1)$$

$$\varphi_t - \Delta^h\varphi = 0, \quad \varphi\big|_{t=0} = \varphi^0, \ \varphi^h(\mathbf{x},t) \in D_t^h \quad (2)$$

For one-step schemes

$$\varphi^j = S(\Delta t\, \Delta^h)^j \varphi^0; \qquad j = 1,2,...., \quad (3)$$

$S(\ \ )$ Transition operator (TO), its spectral form

$S(\Delta t\lambda)$ corresponds to TO of the model problem

$$\psi_t + \lambda\psi = 0, \quad \psi\big|_{t=0} = \psi^0, \ \lambda \in £ \quad (4)$$

L-stability

<u>Definition</u>. The method is called L-stable,

if $\quad |S(z)| \le 1, \ \ for \ \ all \ z = \lambda \Delta t \in £ \ \ c \ \ \boldsymbol{Re}(z) \ge 0 \ \ u \ \ S(\infty) = 0$

Typical cases:

1. Implicit scheme $\quad S(z) = (1+z)^{-1} \Rightarrow S(\infty) = 0$

2. Explicit scheme $\quad S(z) = (1-z) \Rightarrow S(\infty) = -\infty$

3. Weighted scheme

$$S(z) = (1-\alpha_1 z)(1+(1-\alpha_1)z)^{-1}, \ \ 0 \le \alpha_1 \le 1 \Rightarrow S(\infty) = -\frac{\alpha_1}{(1-\alpha_1)}$$

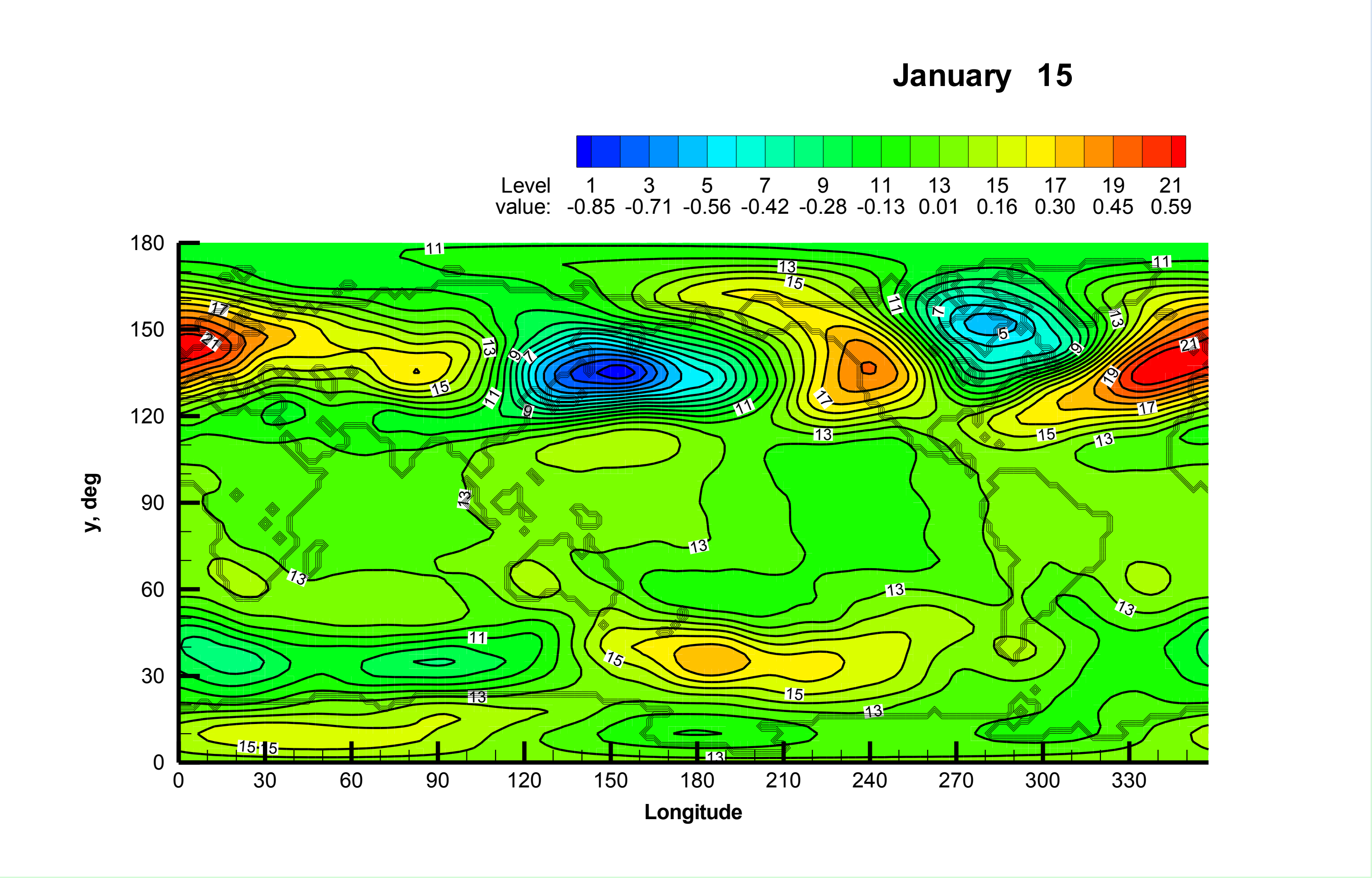
4. Implicit two-step Euler scheme

$$\left(3\psi^{j} - 4\psi^{j-1} + \psi^{j-2}\right) + 2\Delta t\, \lambda \psi^{j} = 0 \Rightarrow S(\infty) = 0$$

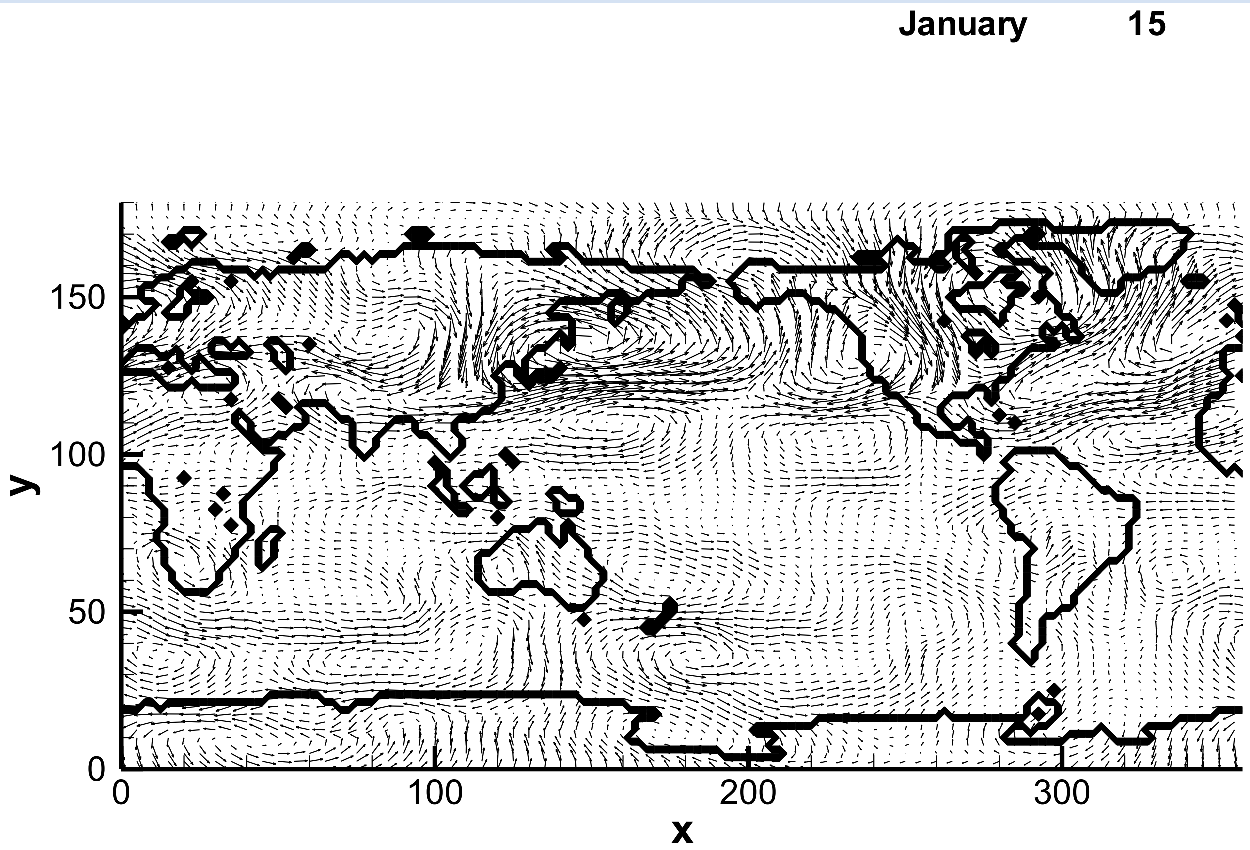
$$\psi^{j} = \left(\xi\right)^{j}; \ \ \xi_{1,2} = \left(2 \pm \sqrt{1+2z}\right)^{-1}; \ \ \left|\xi_{1,2}\right| < 1$$

Scenario forecasts of climate-caused risks by inverse methods

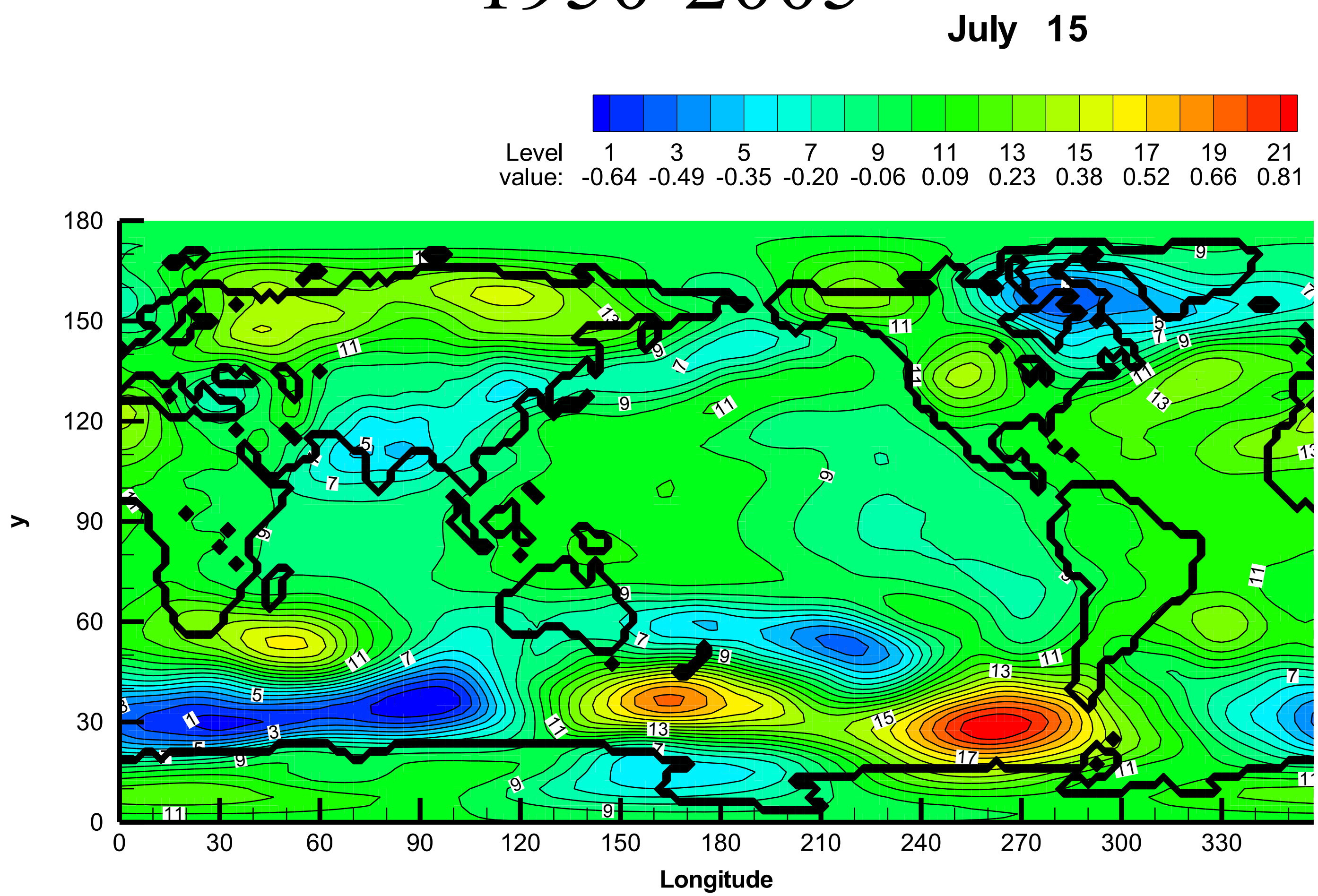
Winter pattern of the global 500-hPa geopotential height (the 1st main factor) 1950-2005



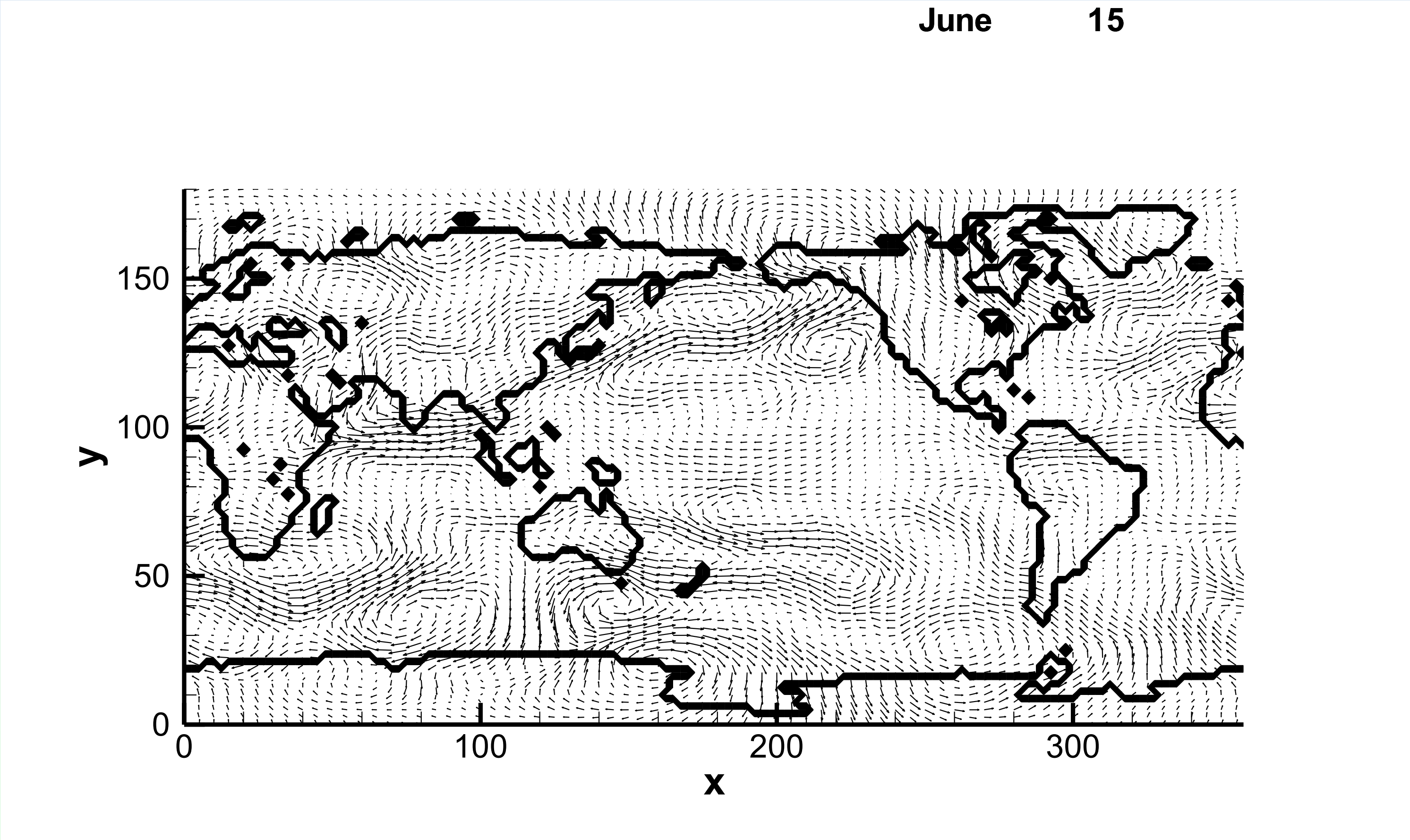
Winter pattern of global circulation (the 1st main factor) 1950-2005

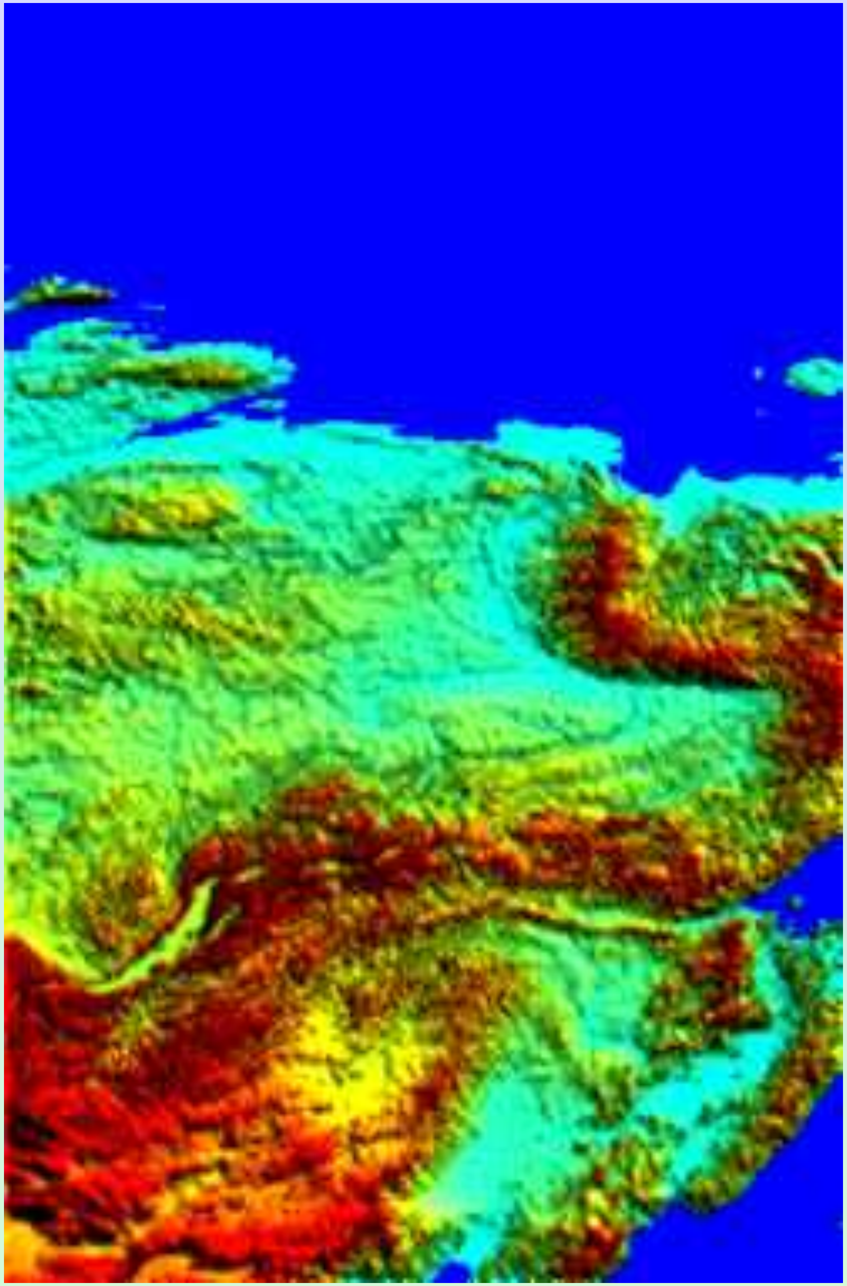


Summer pattern of the global 500-hPa geopotential height (the 1st main factor) 1950-2005



Summer pattern of global circulation (the 1st main factor) 1950-2005

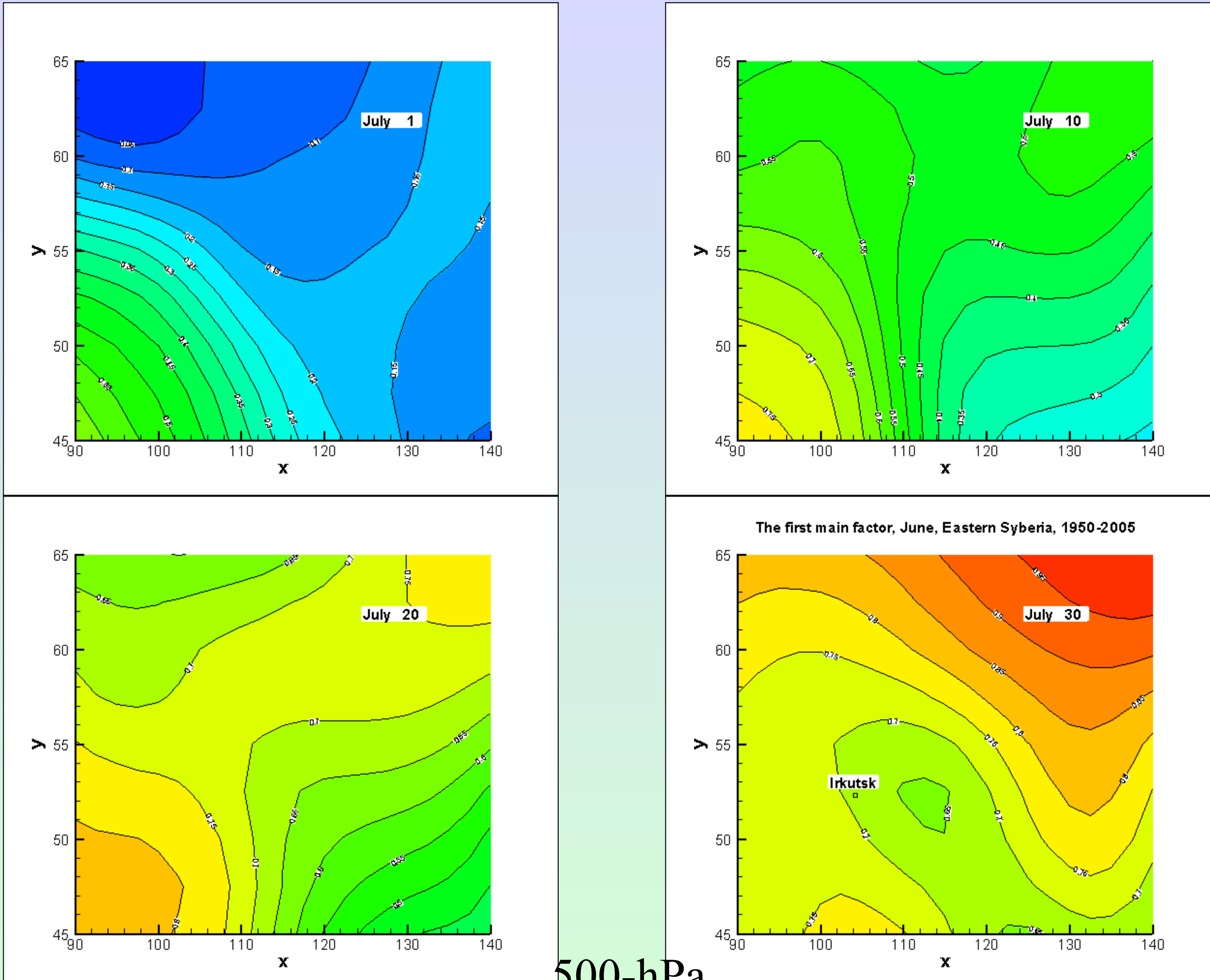




East Siberia Region

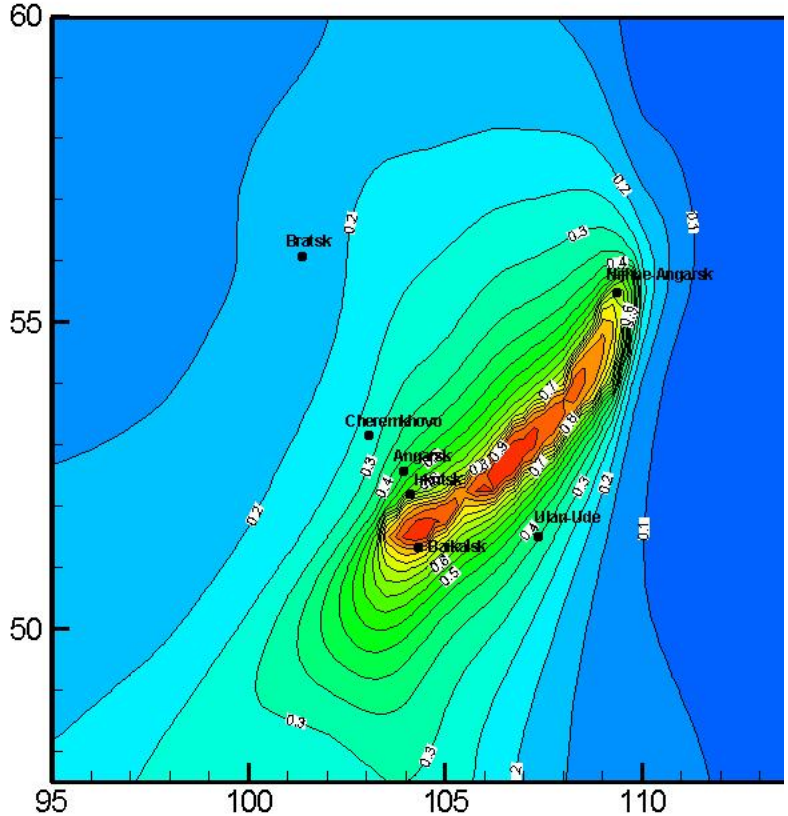
90-140 E, 45-65 N

June 1950-2005

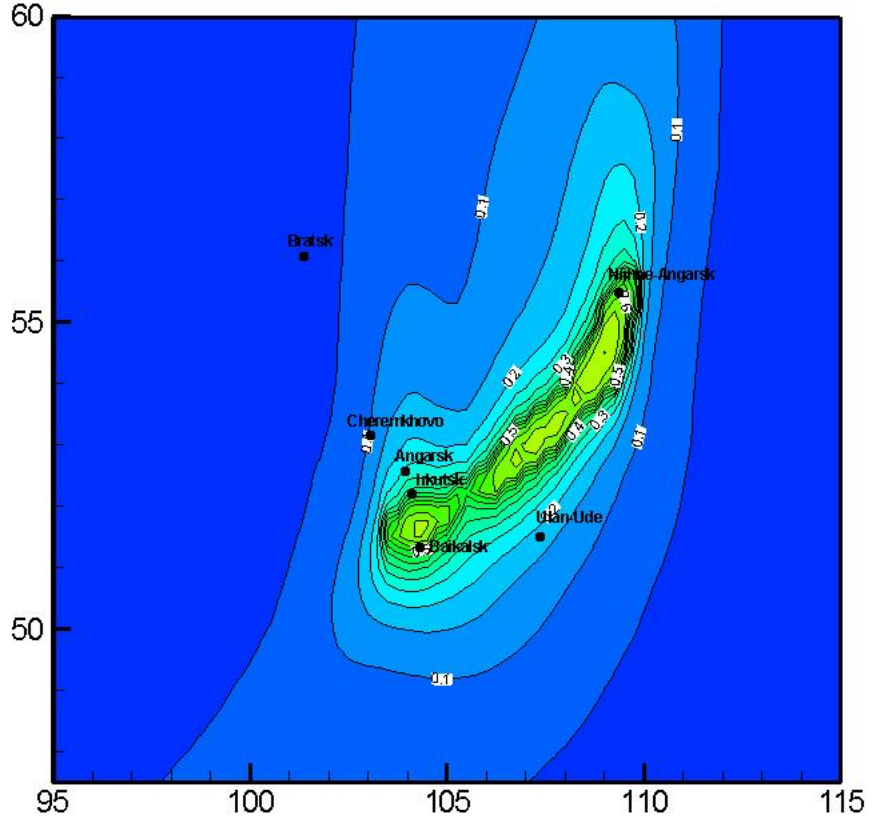

July 1
July 10
July 20
The first main factor, June, Eastern Syberia, 1950-2005
July 30
Irkutsk
y
x
65
60
55
50
45
90
100
110
120
130
140

500-hPa

Monthly risk functions for Lake Baikal



July



December

Optimal forecasting and design

Optimality is meant in the sense that estimations of the goal functionals do not depend on the variations :

- of the sought functions in the phase spaces of the dynamics of the physical system under study
- of the solutions of corresponding adjoint problems that generated by variational principles
- of the uncertainty functions of different kinds which explicitly included into the extended functionals

Advantage of the approach

- Consistency of all technology elements
- Optimality of numerical schemes based on discrete-analytical approximations(without flux-correction procedures)
- Cost-effectiveness of computational technology

Conclusion

Variational principle

is the universal tool for construction of numerical models, algorithms, and

integrated modeling technology

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Thank you for your time!