# Advanced variational modeling technologies for environmental studies

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# Objectives

1. Variational technology for integrated systems (direct and feedback relations)
2. New algorithms of realization: hybrid discrete-analytical numerical schemes

   ( the idea of Euler's integrating factors) for

   - convection-diffusion operators
   - chemical transformation operators

# MODELS

# Model of atmospheric dynamics

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

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

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

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

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

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

# Transport and transformation of humidity

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

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

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

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

$q_v$ -vapor   $q_c$ -cloud water   $q_r$ -rain   $q_f$ - ice crystals & snow

$S_l, S_f, S_c$ - phase transitions   $F_{q_v}, F_{q_l}, F_{q_f}$- sources

# Chemistry transport and transformation model

$$\frac{\partial \boldsymbol{\varphi}_i}{\partial t} + \mathrm{div}(\boldsymbol{\varphi}_i \mathbf{u} - \boldsymbol{\mu}_i \mathrm{grad}\, \boldsymbol{\varphi}_i) + (S\boldsymbol{\varphi})_i - f_i(x,t) - r_i = 0,$$

$$i = \overline{1, n_g};$$

Operators of transformation

destruction

$$S_i(\boldsymbol{\varphi}) = P_i(\boldsymbol{\varphi})\varphi_i - \boldsymbol{\Pi}_i(\boldsymbol{\varphi}) \equiv \sum_{q=1}^{R_i} \left\{ k(q)\Big(s_i(q^-) - s_i(q^+)\Big) \prod_{j=1}^{U_q} \varphi_j^{s_j(q^-)} \right\}$$

production

$$i = \overline{1, n_g}$$

! Important properties

$$\boldsymbol{\varphi} \geq 0; \qquad P_i(\boldsymbol{\varphi}) \geq 0; \qquad \boldsymbol{\Pi}_i(\boldsymbol{\varphi}) \geq 0$$

# MODEL AGGREGATION VIA VARIATIONAL APPROACH

# Integral identity is a variational form of integrated system: hydrodynamics+ chemistry+ hydrology

Integral identity

Convection-diffusion

transformation

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

$$\int_{D_t} \left\{ \left( p^* \operatorname{div} \mathbf{u} - p \operatorname{div} \mathbf{u}^* \right) + \left( \alpha_p p p^* + \alpha_T T T^* \right) \operatorname{div} \mathbf{u} \right\} dDdt +$$

$$\int_{D_t} \alpha_{\boldsymbol{\rho}} \left\{ \left(\rho - \rho_a\right)^T W_a \left(\rho - \rho_a\right) \right\} dDdt + \int_{\boldsymbol{\Omega}_t} p \mathbf{u}_n^* d\boldsymbol{\Omega} dt = 0$$

$\boldsymbol{\varphi} \in Q(D_t)$ state vector-functions

$\boldsymbol{\varphi}^* \in Q^*(D_t)$ adjoint vector-functions

$I\left(\boldsymbol{\varphi}, \mathbf{Y}, \boldsymbol{\varphi}\right) = 0$ equation of the energy balance for the system

# Variational forms corresponding to convection-diffusion operators

There are 12$_{(\text{ dynamics+hydrology})}$+n$_{(\text{gas})}$+m$_{(\text{aerosol})}$ types for different state functions $\varphi_i$

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

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

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

$R_b\boldsymbol{\varphi}-\mathbf{q}_b=0$ boundary conditions on $\boldsymbol{\Omega}_t$

# Convection-diffusion-reaction model

$G(\boldsymbol{\varphi}, \mathbf{Y})$

$$\frac{\partial \boldsymbol{\varphi}}{\partial t} + \sum_{\alpha=1}^{4} L_\alpha \boldsymbol{\varphi} = \mathbf{f}(\mathbf{x}, t) \quad (\mathbf{x}, t) \in D_t,$$

$$L_\alpha \boldsymbol{\varphi} \equiv -\frac{\partial}{\partial x_\alpha} \mu_\alpha(\mathbf{x}, t) \frac{\partial \boldsymbol{\varphi}}{\partial x_\alpha} + u_\alpha(\mathbf{x}, t) \frac{\partial \boldsymbol{\varphi}}{\partial x_\alpha} + d_\alpha(\mathbf{x}, t) \boldsymbol{\varphi},$$

$$\mu_\alpha \geq 0, d_\alpha \geq 0, \quad \alpha = \overline{1,3}$$

decomposition on reaction mechanisms

destruction

production

$$\mathrm{L}_4 \boldsymbol{\varphi} \equiv \left\{ \mathrm{S}_\mathrm{g}(\boldsymbol{\varphi}) \right\}_\mathrm{i} = \mathrm{P}_\mathrm{i}(\boldsymbol{\varphi}) \varphi_\mathrm{i} - \boldsymbol{\Pi}_\mathrm{i}(\boldsymbol{\varphi}) \equiv \sum_{\mathrm{q}=1}^{\mathrm{R}_\mathrm{i}} \left\{ \mathrm{k}(\mathrm{q}) \left( \mathrm{s}_\mathrm{i}(\mathrm{q}^-) - \mathrm{s}_\mathrm{i}(\mathrm{q}^+) \right) \prod_{\mathrm{j}=1}^{\mathrm{U}_\mathrm{r}} \varphi_\mathrm{j}^{\mathrm{s}_\mathrm{j}(\mathrm{q}^-)} \right\}$$

$\mathbf{x} \in D_t^h$

reaction rates

stoichiometric coefficients

# DISCRETE ANALYTICAL SCHEME FOR CONVECTION DIFFUSION MODELS

# Process-level splitting

$$I(\varphi,\varphi^{*}) \equiv$$

$$\equiv \int_0^T \left\{ \int_D \sum_{\alpha=1}^{3} \left( \left( \gamma_\alpha \frac{\partial \varphi}{\partial t} + L_\alpha \varphi - f_\alpha \right) \varphi^{*} \right) dD \right\} dt = 0$$

$\Longrightarrow$

$$I(\varphi,\varphi^{*}) \equiv$$

$$\equiv \int_0^T \left\{ \int_D \sum_{\alpha=1}^{3} \left( \left( \gamma_\alpha \frac{\partial \varphi}{\partial t} + L_\alpha \varphi - f_\alpha \right) \varphi_\alpha^{*} \right) dD \right\} dt = 0$$

# Domain decomposition

$$\bar{D}_t^h = \omega_t^h \times \omega_{x_1}^h \times \ldots \times \omega_{x_p}^h$$

$$\omega_t^h = \left\{ \bigcup_{j=1}^{J} \left[ t_{j-1}, t_j \right];\ t_j = t_{j-1} + \Delta t_j,\ j = \overline{0, J}, t_0 = 0, t_J = \bar{t} \right\}$$

$$\omega_x^h = \left\{ \begin{array}{l} \bigcup_{i=1}^{N_x} \left[ x_{i-1}, x_i \right];\ x_i = x_{i-1} + \Delta x_i, i = \overline{0, N_x}, \\ x_0 = 0, x_{N_x} = X_x \end{array} \right\}$$

# Temporal and spatial approximation

$$I(\varphi,\varphi^*) \equiv$$

$$\equiv \sum_{j=1}^{J} \int_{t_{j-1}}^{t_j} \left\{ \int_D \sum_{\alpha=1}^{3} \left( \left( \gamma_\alpha \frac{\partial \varphi}{\partial t} + L_\alpha \varphi - f_\alpha \right) \varphi_\alpha^* \right) dD \right\} dt = 0$$

$$\longrightarrow \sum_{j=1}^{J} \int_{t_{j-1}}^{t_j} \left\{ \sum_{\alpha=1}^{3} \int_{S_\alpha} \left\{ \sum_{\omega_\alpha^h} \int_{x_{\alpha_{i-1}}}^{x_{\alpha_i}} \left( \gamma_\alpha \frac{\left(\varphi_\alpha^j - \varphi_\alpha^{j-1}\right)}{\Delta t_\alpha} + \right. \right. \right.$$

$$\left. \left. \left. + L_\alpha \varphi_\alpha^j - f_\alpha^j \right) \varphi_\alpha^{*j} \right) dx_\alpha \right\} dS_\alpha \right\} dt = 0$$

$$D^h = \omega_\alpha^h \times S_\alpha^h,\ dD = dx_\alpha dS_\alpha,\ \alpha = \overline{1,3}, i = \overline{1,n_\alpha}, j = \overline{1,J}$$

# Idea: Euler's integrating factors in frames of variational principle

$$\Lambda\varphi = f, \quad x_{i-1} \le x \le x_i, \tag{1}$$

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

If $\varphi^*$ is a solution of $\Lambda^*\varphi^* = 0$, (3)

then the solution of (1) is obtained from

$$\left(A\varphi, \varphi^*\right)\Big|_{x_{i-1}}^{x_i} - \int_{x_{i-1}}^{x_i} f(x)\varphi^*(x)dx = 0, \tag{4}$$

$\varphi^*(x)$ is the integrating factor for (1)

Penenko V., Tsvetova E. Discrete-analytical methods for the implementation of variational principles in environmental applications// Journal of computational and applied mathematics, 2009, v. 226, 319-330.

# Discrete-analytical (DiAn) schemes for convection-diffusion problems

Local adjoint problems ( with piece-wise coefficients)

$$L^{*}\varphi^{*(\alpha)} = 0,\ \ \alpha = 1,2,\ \ x_{i-1} \le x \le x_i, i = \overline{2, n_x}$$

$\varphi^{*(\alpha)}(x)$ integrating factors

Fundamental **analytical** solutions of local adjoint problems

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

**Properties of DiAn numerical schemes for convection-diffusion:**

Three-point schemes in each direction, exact in space, stable, monotonic, transportive, differentiable with respect to parameters and state functions, uniform construction for each grid element, without flux correctors!

# Basic integral identity in convection-diffusion case

$$\left( L\varphi - f, \varphi^{*} \right) = 0$$

$$\int_a^b \left( -\frac{\partial}{\partial x}\mu(x)\frac{\partial \varphi}{\partial x} + u(x)\frac{\partial \varphi}{\partial x} + d(x)\varphi - f(x) \right)\varphi^{*} dx = 0$$

$$\int_a^b \left( \mu(x)\frac{\partial \varphi}{\partial x}\frac{\partial \varphi^{*}}{\partial x} + u(x)\varphi^{*}\frac{\partial \varphi}{\partial x} + d(x)\varphi\varphi^{*} - f(x)\varphi^{*} \right) dx$$

$$- \mu\varphi^{*}\frac{\partial \varphi}{\partial x}\Big|_a^b = 0,$$

# Locally adjoint problems

$$L^{*}\varphi^{*} \equiv \mu_{i-1/2}\left(-\frac{\partial^{2}\varphi^{*}}{\partial x^{2}}-\left(\frac{u}{\mu}\right)_{i-1/2}\frac{\partial\varphi^{*}}{\partial x}+\frac{d}{\mu}\varphi^{*}\right)=0,$$

$$x_{i-1} \le x \le x_{i},\ i=\overline{2,n}$$

On the left subinterval

$$\varphi^{*(1)}(x_{i-1})=0,$$

$$\varphi^{*(1)}(x_{i})=1;$$

On the right subinterval

$$\varphi^{*(2)}(x_{i-1})=1,$$

$$\varphi^{*(2)}(x_{i})=0$$

$$\varphi^{*}(x)=e^{\lambda x}$$

# Characteristic equation

$$\lambda^2 + \frac{u}{\mu}\lambda - \frac{d}{\mu} = 0$$

$$\lambda^{(1)} = -\frac{u}{2\mu} + \sqrt{\left(\frac{u}{2\mu}\right)^2 + \frac{d}{\mu}} \geq 0,$$

$$\lambda^{(2)} = -\frac{u}{2\mu} - \sqrt{\left(\frac{u}{2\mu}\right)^2 + \frac{d}{\mu}} \leq 0$$

# Fundamental solutions

$$\varphi^{*(1)}(x) = A\left(e^{-\lambda^{(1)}(x_i - x)} - e^{\lambda^{(2)}(x - x_{i-1})}e^{-\nu^{(1)}}\right)$$

$$\varphi^{*(2)}(x) = A\left(e^{\lambda^{(2)}(x - x_{i-1})} - e^{-\lambda^{(1)}(x_i - x)}e^{\nu^{(2)}}\right)$$

$$A = 1/\left(1 - e^{\nu^{(2)} - \nu^{(1)}}\right);$$

$$\nu^{(k)} = \lambda^{(k)}\Delta x_{i-1},\ k = 1,2$$

# Resulting tridiagonal system

$$c_i^{(2)}\varphi_i - r_i\varphi_{i+1} = f_i^{(2)}$$

$$-l_i\varphi_{i-1} + \left(c_i^{(1)} + c_i^{(2)}\right)\varphi_i - r_i\varphi_{i+1} = f_i^{(1)} + f_i^{(2)}$$

$$-l_i\varphi_{i-1} + c_i^{(1)}\varphi_i = f_i^{(1)}$$

$$c_i^{(1)} = \mu_{i-1/2}\left(\frac{\partial\varphi^{*(1)}}{\partial x} + \left(\frac{u}{\mu}\right)_{i-1/2}\varphi^{*(1)}\right)_{i-0} \qquad c_i^{(2)} = -\mu_{i+1/2}\left(\frac{\partial\varphi^{*(2)}}{\partial x} + \left(\frac{u}{\mu}\right)_{i+1/2}\varphi^{*(2)}\right)_{i+0}$$

$$l_i = \left(\mu_{i-1/2}\frac{\partial\varphi^{*(1)}}{\partial x}\right)_{i-1} \qquad r_i = \left(\mu_{i+1/2}\frac{\partial\varphi^{*(2)}}{\partial x}\right)_{i+1}$$

$$f_i^{(\alpha)} = \int_{x_{i-1}}^{x_i} f(x)\varphi^{*(\alpha)}(x)dx$$

# Properties of the scheme

***The numerical scheme has the following properties:***

- ***The coefficients are nonnegative;***
- ***Coefficient matrix is diagonally dominant:***
- ***The scheme is transportive in the direction of convective transport;***
- ***Coefficient matrix is monotone, it is nodegenerate and is an M-matrix***
- ***Elements of the inverse matrix are positive;***
- ***Numerical scheme is precise with piecewise-constant coefficients and exact calculation of integrals in the right hand side;***
- ***Boundary conditions of all the three types are satisfied exactly.***

# Parallel organization of algorithms for DiAn-schemes

$$\int_{x_{\alpha_{i-1}}}^{x_{\alpha_i}} \left( \gamma_\alpha \frac{\left(\varphi_\alpha^j - \varphi_\alpha^{j-1}\right)}{\Delta t_\alpha} + L_\alpha \varphi_\alpha^j - f_\alpha^j \right) \varphi_\alpha^{*j} dx_\alpha$$

bilinear form

$$= \int_{x_{\alpha_{i-1}}}^{x_{\alpha_i}} L_\alpha^* \varphi_\alpha^{*j} \varphi_\alpha^j dx_\alpha + \left[ A_\alpha \varphi_\alpha^j \varphi_\alpha^{*j} \right]_{x_{\alpha_{i-1}}}^{x_{\alpha_i}} - \int_{x_{\alpha_{i-1}}}^{x_{\alpha_i}} f_\alpha^j \varphi_\alpha^{*j} dx_\alpha$$

$$L_\alpha^* \varphi_\alpha^{*j} = 0; \quad \left[ A_\alpha \varphi_\alpha^j \varphi_\alpha^{*j} \right]_{x_{\alpha_{i-1}}}^{x_{\alpha_i}} - \int_{x_{\alpha_{i-1}}}^{x_{\alpha_i}} f_\alpha \varphi_\alpha^{*j} dx_\alpha = 0$$

$$\varphi_\alpha^{j-1} = \varphi^{j-1}, \ \varphi^j = \sum_{\alpha=1}^{3} \gamma_\alpha \varphi_\alpha^j, \ \alpha = \overline{1,3}, \ i = \overline{1, n_\alpha}, \ j = \overline{1, J}$$

# Hopf equation test

•Consider nonstationary Hopf equation with Dirichlet boundary conditions

$$\frac{\partial \varphi}{\partial t} + \varphi \frac{\partial \varphi}{\partial x} - \mu \frac{\partial^2 \varphi}{\partial x^2} = 0,$$

•Parameter μ=1

•Domain

$$D_t = \{0 \le x \le 1, 0 \le t \le 2\},$$

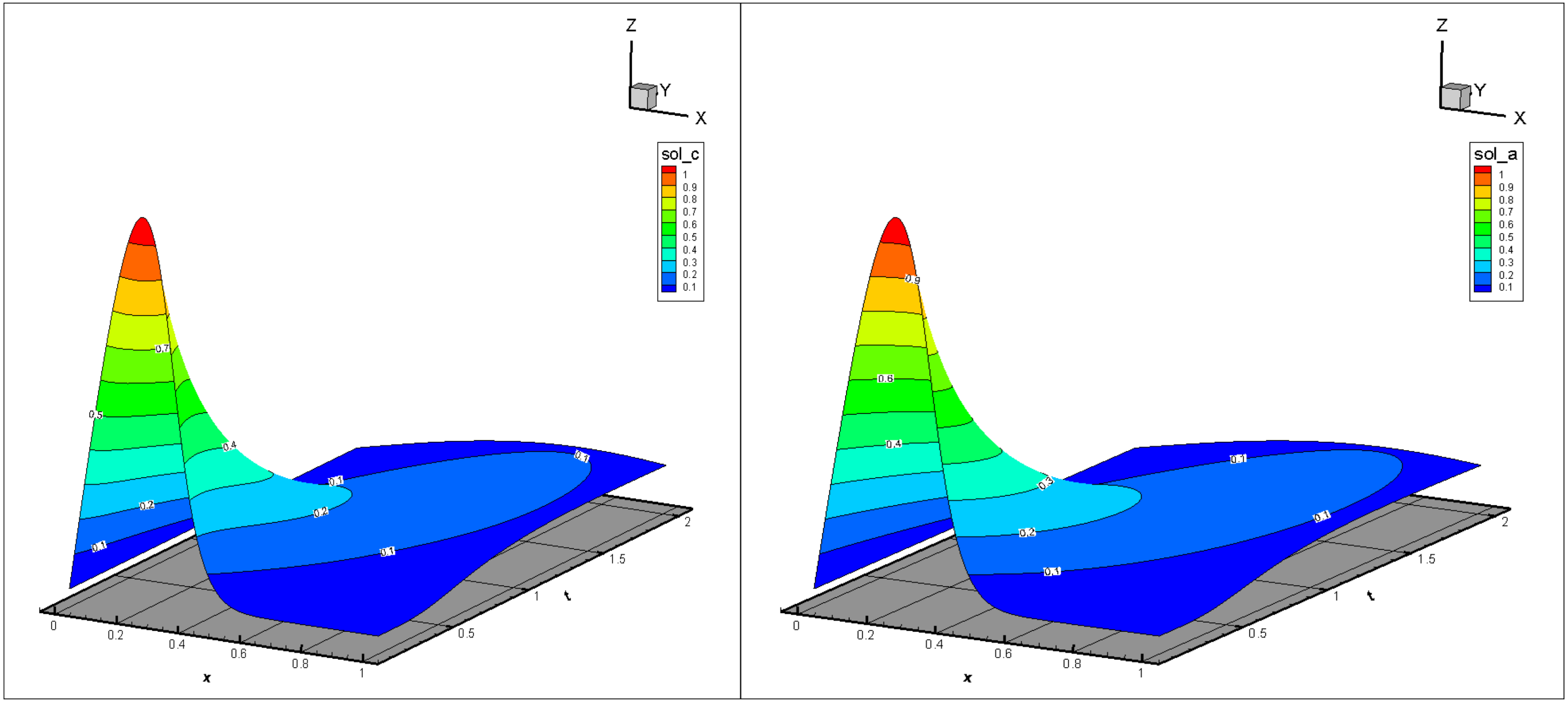
•Exact solution

$$\varphi(x,t) = \frac{x}{t(1 + \sqrt{t}\exp(x^2/(4\mu t)))},$$

•Grid domain: 101x201 points in space in time

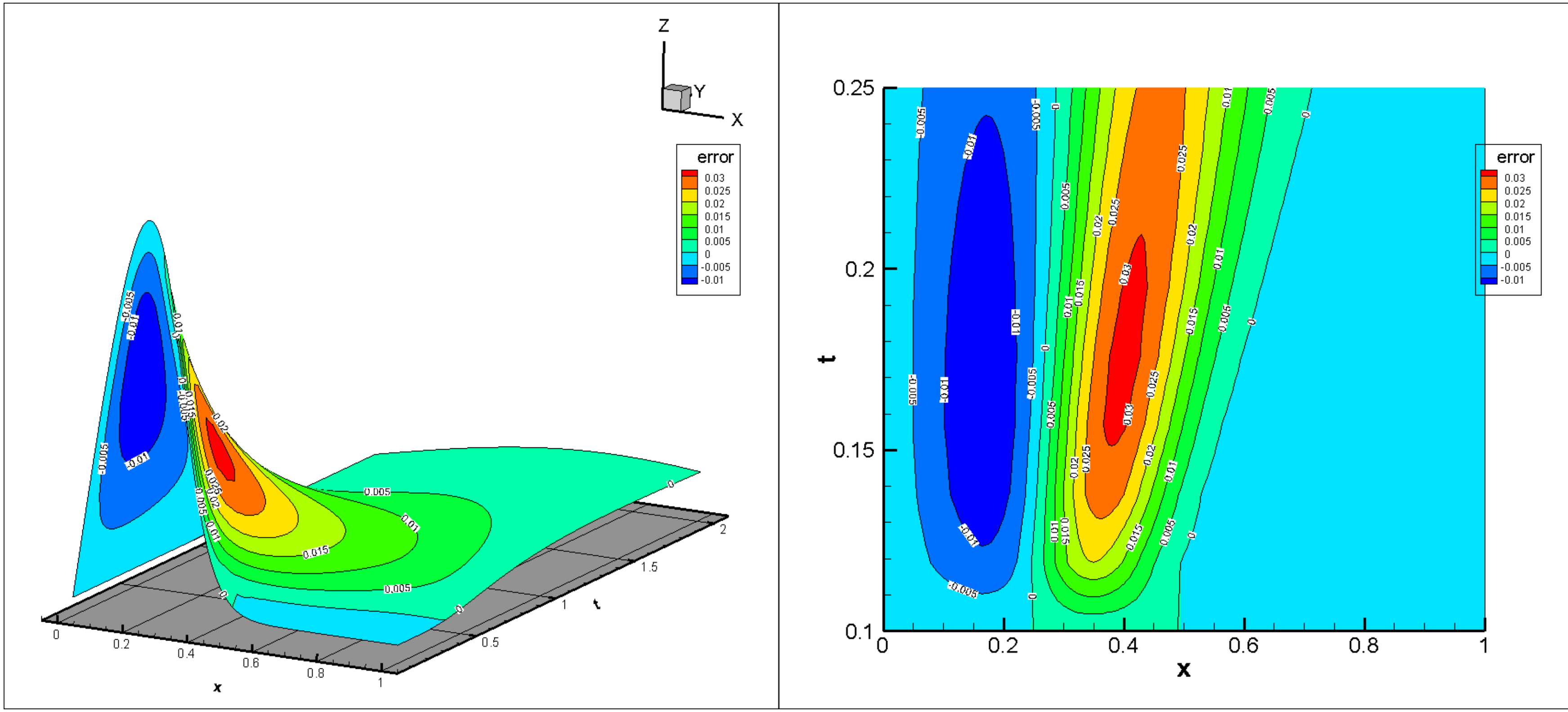
•Nonlinear term is approximated from the previous time step

# Hopf equation test




Exact solution on left and DiAn scheme on the right

# Hopf equation test




Absolute error

# DISCRETE ANALYTICAL SCHEME FOR CHEMICAL KINETICS MODELS

# Direct and adjoint operators for kinetics of chemical transformations

quasi-linear presentation

decomposition on reaction mechanisms

$$S_i(\boldsymbol{\varphi}) = P_i(\boldsymbol{\varphi})\varphi_i - \boldsymbol{\Pi}_i(\boldsymbol{\varphi}) \equiv \sum_{q=1}^{R_i} \left\{ k(q)\left(s_i(q^-) - s_i(q^+)\right) \prod_{j=1}^{U_q} \varphi_j^{s_j(q^-)} \right\}$$

reaction rates

stoichiometric coefficients

http://link.springer.com/article/10.1134%2FS199542391303004X

$$P_i(\boldsymbol{\varphi}), \Pi_i(\boldsymbol{\varphi}) \geq 0; \;\; i = \overline{1, n_g}, \;\; n_g \geq 1, \;\; \forall \mathbf{x} \in D_t^h$$

Adjoint operator

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

**Penenko V. V., Tsvetova E. Variational methods for constructing the monotone approximations for atmospheric chemistry models // Numerical Analysis and Applications, 2013, No 3 , pp 210-220.**

# Discrete-analytical schemes for atmospheric chemistry

Local adjoint problems in time
( quasi-linear destructive operator, decomposition on reaction mechanisms )

(1) $$\frac{\partial \varphi_i^*}{\partial t} - P_i(\boldsymbol{\varphi})\varphi_i^* = 0,\ i = \overline{1, n_g},\ t_j \le t \le t_{j+1},\ j = \overline{1, J-1},\ \varphi_i^*\Big|_{t_{j+1}} = 1.$$

(2) $\varphi_i^*(t)$ integrating factor of (1) within $\left[\, t_j, t_{j+1} \right]$

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

Finally, the system of integral equations is obtained

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

$$b_i = P_i^j(\boldsymbol{\varphi}^j),\quad \mathrm{F_i}(\boldsymbol{\varphi}, \mathrm{t}) = \boldsymbol{\Pi}_\mathrm{i}(\boldsymbol{\varphi}) + \mathrm{f_i}$$

# Discrete-analytical schemes for atmospheric chemistry

Integral equation

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

$$b_i = P_i^j(\boldsymbol{\varphi}^j), \quad \mathrm{F_i}(\boldsymbol{\varphi}, \mathrm{t}) = \boldsymbol{\Pi}_\mathrm{i}(\boldsymbol{\varphi}) + \mathrm{f_i}$$

First order approximation

$$\varphi_{1i}^{j+1} = \varphi^j \mathrm{e}^{-a_i^j \Delta t_j} + \frac{1 - \mathrm{e}^{-a_i^j \Delta t_j}}{a_i^j \Delta t_j} \mathrm{F_i}(\boldsymbol{\varphi}^j) \Delta t_j,$$

Second order approximation

$$\varphi_{2i}^{j+1} = \varphi_i^j \mathrm{e}^{-a_i^j \Delta t_j} + \frac{1 - \mathrm{e}^{-a_i^j \Delta t_j / 2}}{a_i^j \Delta t_j / 2} \left( \mathrm{F_i}(\boldsymbol{\varphi}^j) \mathrm{e}^{-a_i^j \Delta t_j / 2} + \mathrm{F_i}(\boldsymbol{\varphi}_1^{j+1}) \right)$$

# Chemical kinetics equations test

$\mathrm{C10H15Oo}'(t) = \mathrm{C5H7Oo}(t)\,\mathrm{C5H8}(t)\,k\llbracket 9\rrbracket - \mathrm{C10H15Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 10\rrbracket$

$\mathrm{C10H15Oo3}'(t) = \mathrm{C10H15Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 10\rrbracket - \mathrm{C10H15Oo3}(t)\,\mathrm{C10H17Oo3}(t)\,k\llbracket 13\rrbracket$

$\mathrm{C10H17Oo}'(t) = \mathrm{C5H8}(t)\,\mathrm{C5H9Oo}(t)\,k\llbracket 11\rrbracket - \mathrm{C10H17Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 12\rrbracket$

$\mathrm{C10H17Oo3}'(t) = \mathrm{C10H17Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 12\rrbracket - \mathrm{C10H15Oo3}(t)\,\mathrm{C10H17Oo3}(t)\,k\llbracket 13\rrbracket$

$\mathrm{C20H32Oo6}'(t) = \mathrm{C10H15Oo3}(t)\,\mathrm{C10H17Oo3}(t)\,k\llbracket 13\rrbracket$

$\mathrm{C4H5Oo2}'(t) = \mathrm{C5H7Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 15\rrbracket$

$\mathrm{C4H6Oo2}'(t) = \mathrm{C5H8}(t)\,\mathrm{Oo3}(t)\,k\llbracket 14\rrbracket$

$\mathrm{C5H7}'(t) = \mathrm{C5H8}(t)\,\mathrm{OoH}(t)\,k\llbracket 6\rrbracket - \mathrm{C5H7}(t)\,\mathrm{Oo2}(t)\,k\llbracket 7\rrbracket$

$\mathrm{C5H7Oo}'(t) = \mathrm{C5H7Oo2}(t)\,\mathrm{NOo}(t)\,k\llbracket 8\rrbracket - \mathrm{C5H7Oo}(t)\,\mathrm{C5H8}(t)\,k\llbracket 9\rrbracket - \mathrm{C5H7Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 15\rrbracket$

$\mathrm{C5H7Oo2}'(t) = \mathrm{C5H7}(t)\,\mathrm{Oo2}(t)\,k\llbracket 7\rrbracket - \mathrm{C5H7Oo2}(t)\,\mathrm{NOo}(t)\,k\llbracket 8\rrbracket$

$\mathrm{C5H8}'(t) = -\mathrm{C5H8}(t)\,\mathrm{OoH}(t)\,k\llbracket 5\rrbracket - \mathrm{C5H8}(t)\,\mathrm{OoH}(t)\,k\llbracket 6\rrbracket - \mathrm{C5H7Oo}(t)\,\mathrm{C5H8}(t)\,k\llbracket 9\rrbracket - \mathrm{C5H8}(t)\,\mathrm{C5H9Oo}(t)\,k\llbracket 11\rrbracket - \mathrm{C5H8}(t)\,\mathrm{Oo3}(t)\,k\llbracket 14\rrbracket$

$\mathrm{C5H9Oo}'(t) = \mathrm{C5H8}(t)\,\mathrm{OoH}(t)\,k\llbracket 5\rrbracket - \mathrm{C5H8}(t)\,\mathrm{C5H9Oo}(t)\,k\llbracket 11\rrbracket$

$\mathrm{COo}'(t) = \mathrm{HCOo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 18\rrbracket$

$\mathrm{H2COo}'(t) = \mathrm{C5H8}(t)\,\mathrm{Oo3}(t)\,k\llbracket 14\rrbracket + \mathrm{C5H7Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 15\rrbracket - \mathrm{H2COo}(t)\,\mathrm{OoH}(t)\,k\llbracket 16\rrbracket - \mathrm{H2COo}(t)\,\mathrm{HOo2}(t)\,k\llbracket 20\rrbracket$

$\mathrm{H2Oo}'(t) = -\mathrm{H2Oo}(t)\,\mathrm{Oo}(t)\,k\llbracket 4\rrbracket + \mathrm{C5H8}(t)\,\mathrm{OoH}(t)\,k\llbracket 6\rrbracket + \mathrm{H2COo}(t)\,\mathrm{OoH}(t)\,k\llbracket 16\rrbracket$

$\mathrm{HCOo}'(t) = \mathrm{H2COo}(t)\,\mathrm{OoH}(t)\,k\llbracket 16\rrbracket - \mathrm{HCOo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 17\rrbracket - \mathrm{HCOo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 18\rrbracket - \mathrm{HCOo}(t)\,\mathrm{HOo2}(t)\,k\llbracket 19\rrbracket$

$\mathrm{HCOoOo2}'(t) = \mathrm{HCOo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 17\rrbracket$

$\mathrm{HCOoOoH}'(t) = \mathrm{HOoCH2Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 22\rrbracket$

$\mathrm{HCOoOoOoH}'(t) = \mathrm{HCOo}(t)\,\mathrm{HOo2}(t)\,k\llbracket 19\rrbracket$

$\mathrm{HOo2}'(t) = \mathrm{HCOo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 18\rrbracket - \mathrm{HCOo}(t)\,\mathrm{HOo2}(t)\,k\llbracket 19\rrbracket - \mathrm{H2COo}(t)\,\mathrm{HOo2}(t)\,k\llbracket 20\rrbracket + \mathrm{HOoCH2Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 22\rrbracket$

$\mathrm{HOoCH2Oo}'(t) = \mathrm{HOoCH2OoOo}(t)\,\mathrm{NOo}(t)\,k\llbracket 21\rrbracket - \mathrm{HOoCH2Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 22\rrbracket$

$\mathrm{HOoCH2OoOo}'(t) = \mathrm{H2COo}(t)\,\mathrm{HOo2}(t)\,k\llbracket 20\rrbracket - \mathrm{HOoCH2OoOo}(t)\,\mathrm{NOo}(t)\,k\llbracket 21\rrbracket$

$\mathrm{NOo}'(t) = \mathrm{NOo2}(t)\,k\llbracket 1\rrbracket - \mathrm{C5H7Oo2}(t)\,\mathrm{NOo}(t)\,k\llbracket 8\rrbracket - \mathrm{HOoCH2OoOo}(t)\,\mathrm{NOo}(t)\,k\llbracket 21\rrbracket$

$\mathrm{NOo2}'(t) = -\mathrm{NOo2}(t)\,k\llbracket 1\rrbracket + \mathrm{C5H7Oo2}(t)\,\mathrm{NOo}(t)\,k\llbracket 8\rrbracket + \mathrm{HOoCH2OoOo}(t)\,\mathrm{NOo}(t)\,k\llbracket 21\rrbracket$

$\mathrm{Oo}'(t) = \mathrm{NOo2}(t)\,k\llbracket 1\rrbracket - \mathrm{Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 2\rrbracket + \mathrm{Oo3}(t)\,k\llbracket 3\rrbracket - \mathrm{H2Oo}(t)\,\mathrm{Oo}(t)\,k\llbracket 4\rrbracket$

$\mathrm{Oo2}'(t) = -\mathrm{Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 2\rrbracket + \mathrm{Oo3}(t)\,k\llbracket 3\rrbracket - \mathrm{C5H7}(t)\,\mathrm{Oo2}(t)\,k\llbracket 7\rrbracket - \mathrm{C10H15Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 10\rrbracket - \mathrm{C10H17Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 12\rrbracket - \mathrm{C5H7Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 15\rrbracket - \mathrm{HCOo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 17\rrbracket - \mathrm{HCOo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 18\rrbracket - \mathrm{HOoCH2Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 22\rrbracket$

$\mathrm{Oo3}'(t) = \mathrm{Oo}(t)\,\mathrm{Oo2}(t)\,k\llbracket 2\rrbracket - \mathrm{Oo3}(t)\,k\llbracket 3\rrbracket - \mathrm{C5H8}(t)\,\mathrm{Oo3}(t)\,k\llbracket 14\rrbracket$

$\mathrm{OoH}'(t) = 2.\,\mathrm{H2Oo}(t)\,\mathrm{Oo}(t)\,k\llbracket 4\rrbracket - \mathrm{C5H8}(t)\,\mathrm{OoH}(t)\,k\llbracket 5\rrbracket - \mathrm{C5H8}(t)\,\mathrm{OoH}(t)\,k\llbracket 6\rrbracket - \mathrm{H2COo}(t)\,\mathrm{OoH}(t)\,k\llbracket 16\rrbracket$

$\mathrm{H2Oo}(0) = 2.\times 10^{19}$

$\mathrm{NOo2}(0) = 8.\times 10^{10}$

$\mathrm{NOo}(0) = 7.\times 10^{9}$

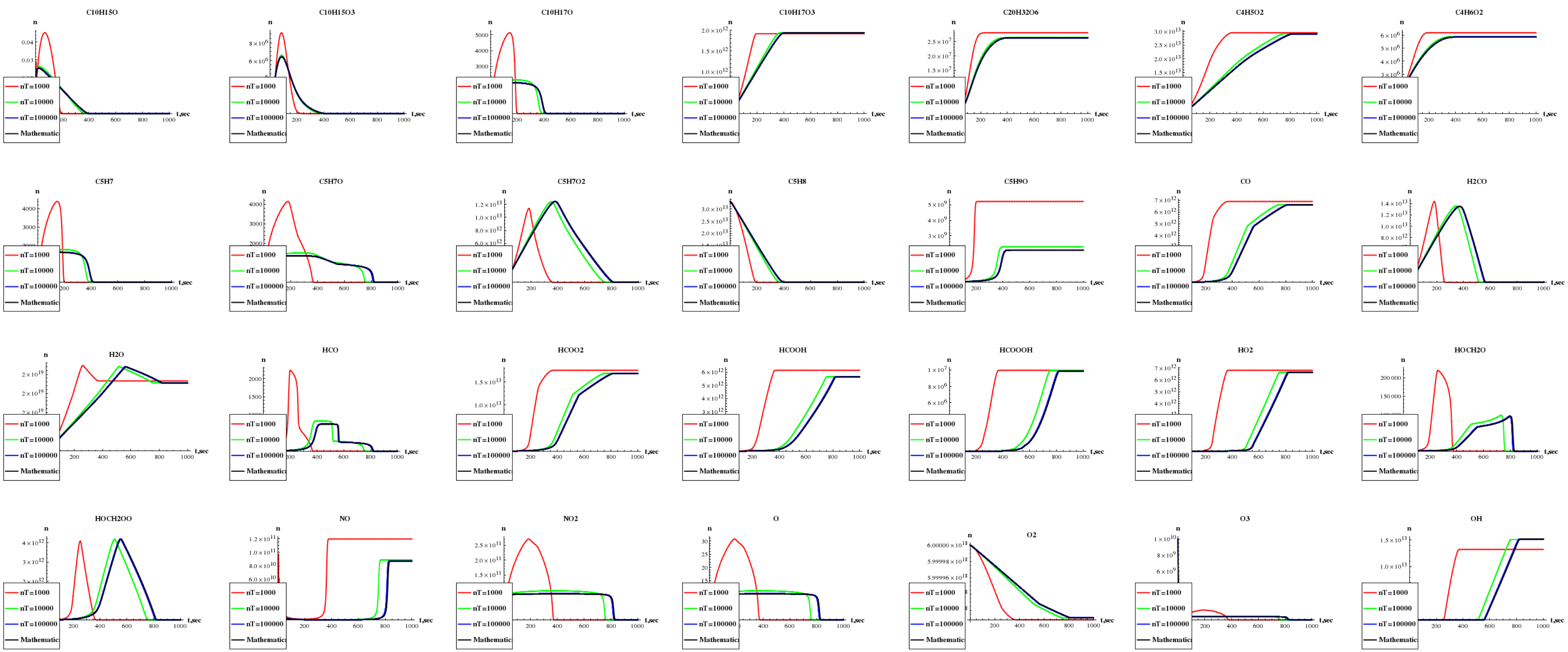
$\mathrm{C5H8}(0) = 3.3\times 10^{13}$

$\mathrm{Oo2}(0) = 6.\times 10^{18}$

$\mathrm{Oo3}(0) = 1.\times 10^{10}$

Prepared by Dultseva G.G. ICK&C SB RAS  Project 35 SB RAS

# Chemical kinetics equations test




Numerical convergence study of the first-order scheme. T = 1000 sec. Nt=1e+3 (Red), 1e+4 (Green), 1e+5 (Blue), Wolfram Research Mathematica 9 ODE Solver (Black).

# VARIATIONAL DATA ASSIMILATION AND MODEL TUNNING (INVERSE MODELING) ALGORITHMS

# Two main components: model and data

- **Mathematical model(s) of processes**

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

$$\boldsymbol{\varphi}^0 = \boldsymbol{\varphi}_0^0 + \boldsymbol{\xi}, \quad Y = Y_0 + \boldsymbol{\varsigma},$$

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

$D_t = D \times [0, t] \in R_4,$

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

G is the “space-time” operator of the model

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

$$\boldsymbol{\Psi}_m = H(\boldsymbol{\varphi}) + \boldsymbol{\eta},$$

$H(\boldsymbol{\varphi})$ **is the model of observations**.

- $r, \boldsymbol{\xi}, \boldsymbol{\varsigma}, \boldsymbol{\eta}$ **uncertainties.**

# Functionals for inverse problems (data assimilation, environmental control, etc.)

## General form

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

$F_k$ are evaluated 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 functional for data assimilation

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

# Augmented functional for construction of optimal algorithms and uncertainty assessment

cost functional

misfit in observations

model's uncertainty

$$\tilde{\Phi}_k^h(\boldsymbol{\varphi}, \boldsymbol{\varphi}^*, \mathbf{Y}, \mathbf{r}, \boldsymbol{\xi}) = \Phi_k^h(\boldsymbol{\varphi}) + 0.5\Big\{\alpha_1(\boldsymbol{\eta}^T \mathbf{M}_1 \boldsymbol{\eta})_{D_t^m} + \alpha_2(\mathbf{r}^T \mathbf{M}_2 \mathbf{r})_{D_t^h}$$

$$+\alpha_3(\boldsymbol{\xi}^T \mathbf{M}_3 \boldsymbol{\xi})_{D^h} + \alpha_4(\boldsymbol{\zeta}^T \mathbf{M}_4 \boldsymbol{\zeta})_{R^h(D_t^h)}\Big\}^h + \Big[\mathbf{I}^h(\boldsymbol{\varphi}, \mathbf{Y}, \boldsymbol{\varphi}_k^*)\Big]_{D_t^h}$$

initial data unc.

parameters unc.

integral identity

$\mathbf{M}_i, (i = 1, 4)$, $\boldsymbol{\alpha}_i \geq 0$ are weight matrices and coefficients for scaling,

$\boldsymbol{\varphi}, \boldsymbol{\varphi}_k^*$ are the solutions of the direct and adjoint problems generated by variational principle.

Symbol $()^h$ denotes discrete analogs. For approximation, finite volumes, decomposition and splitting methods are used.

$D_t^h \in D_t$ is the grid domain

**Penenko V. V. Variational methods of data assimilation and inverse problems for studying the atmosphere, ocean, and environment // Numerical Analysis and Applications, 2009 V 2 No 4, 341-351.**

# Variations of the augmented cost functional

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

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

**Stationary conditions**

$$\frac{\partial\tilde{\Phi}_k^h}{\partial\boldsymbol{\varphi}^*} = 0,\ \frac{\partial\tilde{\Phi}_k^h}{\partial\boldsymbol{\varphi}} = 0,\ \frac{\partial\tilde{\Phi}_k^h}{\partial\mathbf{r}} = 0,\ \frac{\partial\tilde{\Phi}_k^h}{\partial\boldsymbol{\xi}} = 0 \quad\Rightarrow$$

**Sensitivity relations**

$$\delta\tilde{\Phi}_k^h = \left(\frac{\partial\tilde{\Phi}_k^h}{\partial\mathbf{Y}}, \delta\mathbf{Y}\right)$$

# The generic algorithm of forward & inverse modeling

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

$$\frac{\partial \tilde{\Phi}_k^h}{\partial \boldsymbol{\varphi}} \equiv (\Lambda_t)^T \boldsymbol{\varphi}_k^* + A^T(\boldsymbol{\varphi}, \mathbf{Y})\boldsymbol{\varphi}_k^* + \mathbf{d}_k = 0,$$

$$\mathbf{d}_\mathrm{k} = \frac{\partial}{\partial \boldsymbol{\varphi}}(\boldsymbol{\Phi}_\mathrm{k}^\mathrm{h}(\boldsymbol{\varphi}) + 0.5\alpha_1(\boldsymbol{\eta}^\mathrm{T} \mathrm{M}_1 \boldsymbol{\eta})), \qquad \varphi_k^*(\vec{x})\Big|_{t=\bar{t}} = 0$$

$$\boldsymbol{\varphi}^0 = \boldsymbol{\varphi}_\mathrm{a}^0 + \mathrm{M}_3^{-1} \boldsymbol{\varphi}_\mathrm{k}^*(\mathbf{x}, 0), \ \ \mathrm{t} = 0,$$

$$\mathbf{r}(\mathbf{x}, \mathrm{t}) = \mathrm{M}_2^{-1} \boldsymbol{\varphi}_\mathrm{k}^*(\mathbf{x}, \mathrm{t}),$$

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

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

Initial guess: $\mathbf{r}^{(0)} = 0, \ \boldsymbol{\varphi}^{0(0)} = \boldsymbol{\varphi}_\mathrm{a}^0, \ \ \mathbf{Y}^{(0)} = \mathbf{Y}_\mathrm{a}$

# Some elements
# of optimal forecasting and design

## The main sensitivity relations

Sensitivity functions

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

## Feed-back relations

$$\mathbf{Y} = \mathbf{Y}_{\mathrm{a}} - \mathrm{M}_4^{-1}\boldsymbol{\Gamma}_{\mathrm{k}},$$

$$\frac{\partial Y_\alpha}{\partial \mathrm{t}} = -\eta_\alpha \mathrm{grad}_{Y_\alpha} \boldsymbol{\Phi}_{\mathrm{k}}^{\mathrm{h}}(\varphi), \quad \alpha = \overline{1, \mathrm{N}_\alpha}, \quad \mathrm{N}_\alpha \le \mathrm{N}$$

$\boldsymbol{\Gamma}_{\mathrm{k}} = \{\Gamma_{\mathrm{ki}}, \ \mathrm{i} = \overline{1, \mathrm{N}}\}$ are the sensitivity functions

$\boldsymbol{\delta}\mathrm{Y} = \{\boldsymbol{\delta}\mathrm{Y}_{\mathrm{i}}, \mathrm{i} = \overline{1, \mathrm{N}}\}$ are the parameter variations

# Conclusion

Variational principle is the universal tool for construction of numerical models, algorithms, and integrated modeling technology

## 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

# References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# Thank you!