Вариационные методы построения дискретно-аналитических схем с использованием техники интегрирующих множителей

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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, $F_{q_v}, F_{q_c}, F_{q_l}, F_{q_f}$ - turbulent operators

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

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

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

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

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

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

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

Variational forms corresponding to convection-diffusion operators

There are 12(dynamics+hydrology)+n(gas)+m(aerosol) types for different state functions φ_i

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

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

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

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

Convection-diffusion-reaction operators

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

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

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

destruction

production

decomposition on reaction mechanisms

$$\mathrm{L}_4 \boldsymbol{\varphi} \equiv \left\{ \mathrm{S_g}(\boldsymbol{\varphi}) \right\}_{\mathrm{i}} = \mathrm{P_i}(\boldsymbol{\varphi})\varphi_{\mathrm{i}} - \boldsymbol{\Pi}_{\mathrm{i}}(\boldsymbol{\varphi}) \equiv \sum_{\mathrm{q}=1}^{\mathrm{R_i}} \left\{ \mathrm{k(q)} \left(\mathrm{s_i(q^-)} - \mathrm{s_i(q^+)} \right) \prod_{\mathrm{j}=1}^{\mathrm{U_r}} \varphi_{\mathrm{j}}^{\mathrm{s_j(q^-)}} \right\}$$

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

reaction rates

stoichiometric coefficients

VARIATIONAL FORMS FOR CONVECTION- DIFFUSION – REACTION MODELS

Process-level decomposition/splitting

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

$$\equiv\int_0^{\bar{t}}\left\{\int_D\sum_{\alpha=1}^{4}\left(\left(\gamma_\alpha\frac{\partial\varphi}{\partial t}+L_\alpha\varphi-f_\alpha\right)\varphi^*\right)dD\right\}dt=0$$

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

$$\equiv\int_0^{\bar{t}}\left\{\int_D\sum_{\alpha=1}^{4}\left(\left(\gamma_\alpha\frac{\partial\varphi}{\partial t}+L_\alpha\varphi-f_\alpha\right)\varphi_\alpha^*\right)dD\right\}dt=0$$

Domain decomposition

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

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

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

Decomposition+ splitting for temporal and spatial approximations

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

$$\equiv \sum_{j=1}^{J} \int_{t_{j-1}}^{t_j} \left\{ \int_D \sum_{\alpha=1}^{4} \left(\left(\gamma_\alpha \frac{\partial \varphi}{\partial t} + L_\alpha \varphi - f_\alpha \right) \varphi_\alpha^{*} \right) dD \right\} dt = 0$$

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

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

$$\sum_{\langle D^h \rangle} \left\{ \int_{\Delta D^h} \left\{ \int_{t_{j-1}}^{t_j} \left(\gamma_4 \frac{\partial \varphi}{\partial t} + L_4 \varphi - f_4 \right) \varphi_4^{*} dt \right\} dD \right\} \right\} = 0$$

Decomposition+ splitting for temporal and spatial approximations (2)

$$\varphi_{\alpha}^{j-1} = \varphi^{j-1},$$

$$\varphi^{j} = \sum_{\alpha=1}^{s} \gamma_{\alpha} \varphi_{\alpha}^{j}$$

$$D^{h} = \omega_{\alpha}^{h} \times S_{\alpha}^{h} = \bigcup \Delta D^{h}, \; dD = dx_{\alpha} dS_{\alpha},$$

$$\alpha = \overline{1,3}, i = \overline{1, n_{\alpha}}, \; j = \overline{1, J}$$

Basic integral identity in convection-diffusion case

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

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

$$\int_a^b \left(\mu\frac{\partial \varphi}{\partial x}\frac{\partial \varphi^*}{\partial x} + u\varphi^*\frac{\partial \varphi}{\partial x} + d\varphi\varphi^* - f\varphi^* \right)dx - \mu\varphi^*\frac{\partial \varphi}{\partial x}\Big|_a^b = 0, \quad \text{(B)}$$

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

$$+\left[\mu\varphi^*\frac{\partial \varphi}{\partial x} - \mu\varphi\frac{\partial \varphi^*}{\partial x} + u\varphi\varphi^* \right]\Big|_a^b + \int_a^b f\varphi^* dx \quad \text{(C)}$$

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

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

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

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

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

then the solution of (1) is obtained from

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

$\varphi^*(x)$ 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!

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

$$\varphi^{*(2)}(x_i) = 1,$$

$$\varphi^{*(2)}(x_{i+1}) = 0$$

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

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

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

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

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

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

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

$$f_i^{(\alpha)} = \int_{x_{i-1}}^{x_i} f(x)\varphi^{*(\alpha)}(x)\,dx,\ \alpha = 1,2$$

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.

DISCRETE ANALYTICAL SCHEME FOR CHEMICAL KINETICS MODELS

Direct and adjoint operators
for kinetics of chemical transformations

quasi-linear presentation

decomposition on reaction mechanisms

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

reaction rates

stoichiometric coefficients

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

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.

Variational principles for transformation models

Monotonicity and positivity properties

$$\sum_{i=1}^{n_i}\left\{\int_{t_{j-1}}^{t_j}\left(\frac{\partial \varphi_i}{\partial t}+\left(P(\boldsymbol{\varphi})\right)_i\varphi_i-\left(\Pi(\boldsymbol{\varphi})\right)_i-\tilde{f}_i\right)\varphi_i^{*}dt\right\}=0$$

$$\boldsymbol{\varphi}=\{\varphi_i\},\ \ i=\overline{1,n_i},\ \ \varphi_i^{*}(t_j)=1,\ \ j=\overline{2,J},\ \ \vec{x}\in D_t^h$$

Decomposition on reaction mechanisms

$$\int_{t_{j-1}}^{t_j}\left(\frac{\partial \varphi_i}{\partial t}+\left(P(\boldsymbol{\varphi})\right)_i\varphi_i-\left(\Pi(\boldsymbol{\varphi})\right)_i-\tilde{f}_i\right)\varphi_i^{*}dt=$$

$$\int_{t_{j-1}}^{t_j}\left(\left(-\frac{\partial \varphi_i^{*}}{\partial t}+P_i(\boldsymbol{\varphi})\varphi_i^{*}\right)\varphi_i-\left(\varphi_i^{*}\left(\Pi(\boldsymbol{\varphi})+\tilde{f}\right)_i\right)\right)dt+\varphi_i\varphi_i^{*}\Big|_{t_{j-1}}^{t_j}=0$$

$i=\overline{1,n_i}$ n_i is the number of gaseous pollutants

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

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

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

Discrete-analytical schemes for atmospheric chemistry

Integral equation

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

$$b_i = P_i^j(\varphi^j), \quad F_i(\varphi, t) = \Pi_i(\varphi) + f_i$$

First order approximation

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

Second order approximation

$$\varphi_{2i}^{j+1} = \varphi_i^j e^{-a_i^j \Delta t_j} + \frac{1 - e^{-a_i^j \Delta t_j / 2}}{a_i^j \Delta t_j / 2} \left(F_i(\varphi^j) e^{-a_i^j \Delta t_j / 2} + F_i(\varphi_1^{j+1}) \right)$$

Variations of the augmented cost functional

$$\tilde{\Phi}_k^h(,\ldots,) = \Phi_k^h(\boldsymbol{\varphi}) + I^h(\boldsymbol{\varphi}, \mathbf{Y}, \boldsymbol{\varphi}^*)$$

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

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

Stationary conditions

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

⇒

Sensitivity relations

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

Параллельная организация алгоритмов

Многовариантность :

- по процессам (перенос+диффузия, трансформация);
- по координатным направлениям;
- по механизмам реакций в химии и гидрологическом цикле;

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

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Thank you!

Вырожденный случай $\mu = 0$

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

Численная схема

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

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

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

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

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

Тест для анализа дискретно-аналитических схем: пример С.К.Годунова

(Математический сборник, т. 47(89):3, 1959, с.271-306.)

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

Точное решение

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

Рассмотрим схему дискретную по времени и аналитическую по пространству вида:

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

$$u\frac{\partial \varphi^{j}}{\partial x} + \frac{3}{2\Delta t}\varphi^{j} = \frac{4\varphi^{j-1} - \varphi^{j-2}}{2\Delta t}$$

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

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

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

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

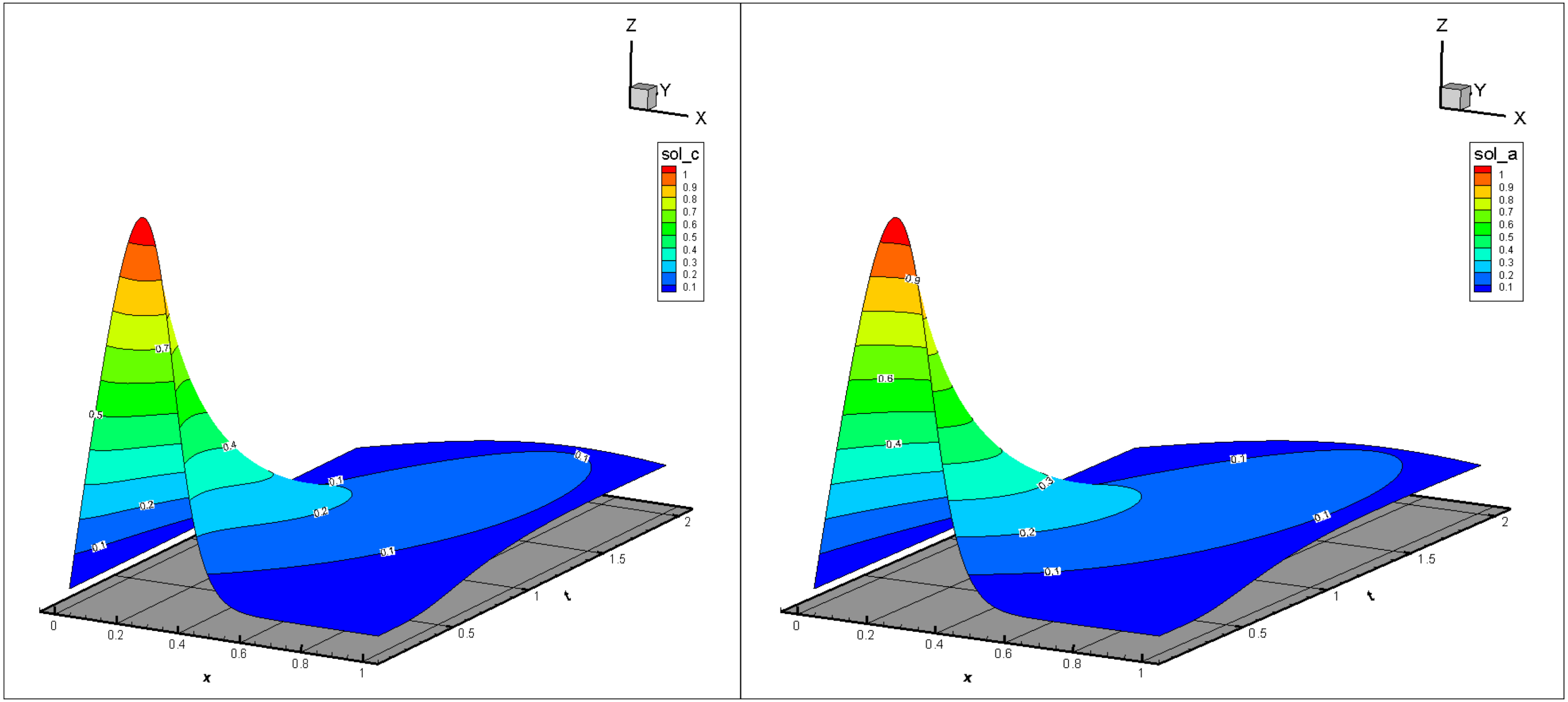
•Exact solution

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

•Grid domain: 101x201 points in space in time

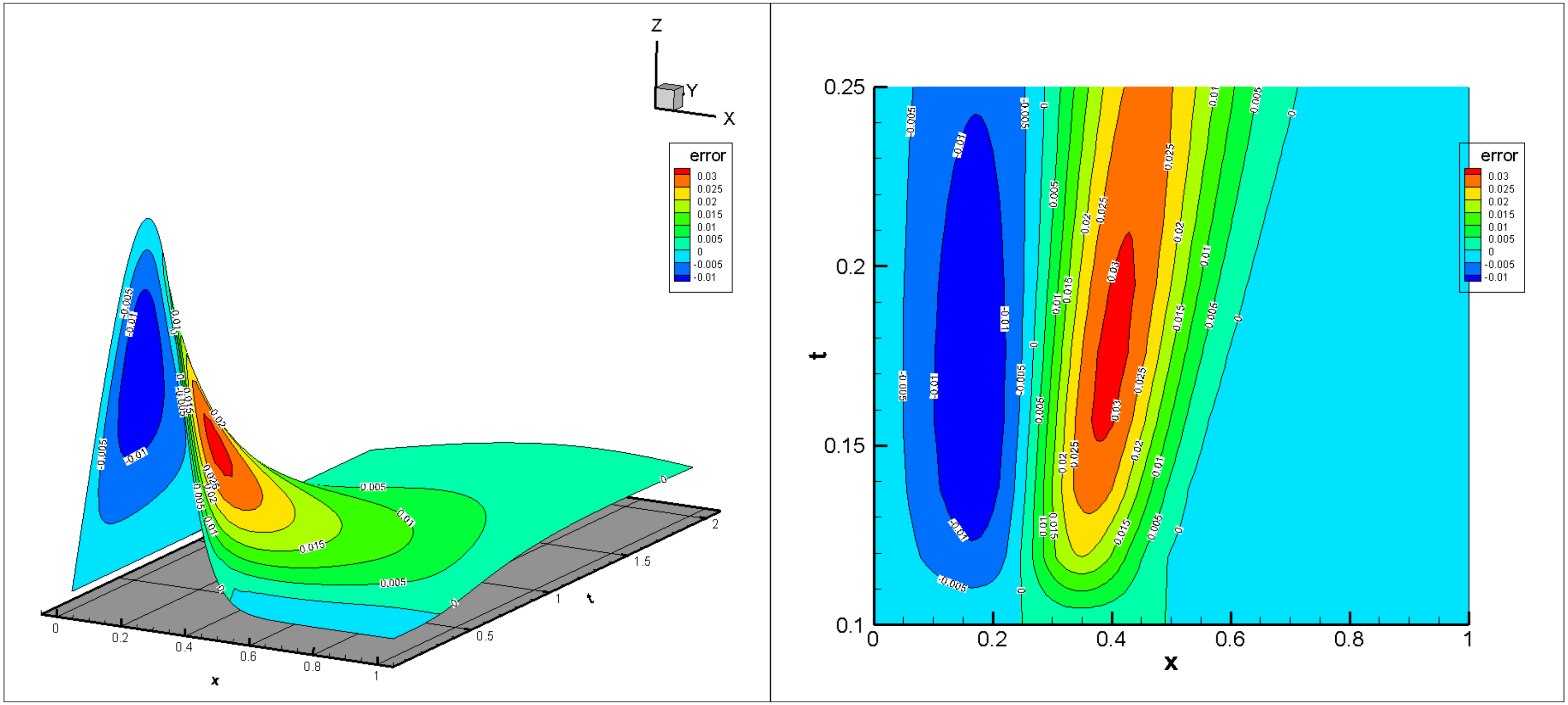
•Nonlinear term is approximated from the previous time step

Hopf equation test



Exact solution on left and DiAn scheme on the right

Hopf equation test



Absolute error

Chemical kinetics equations test

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

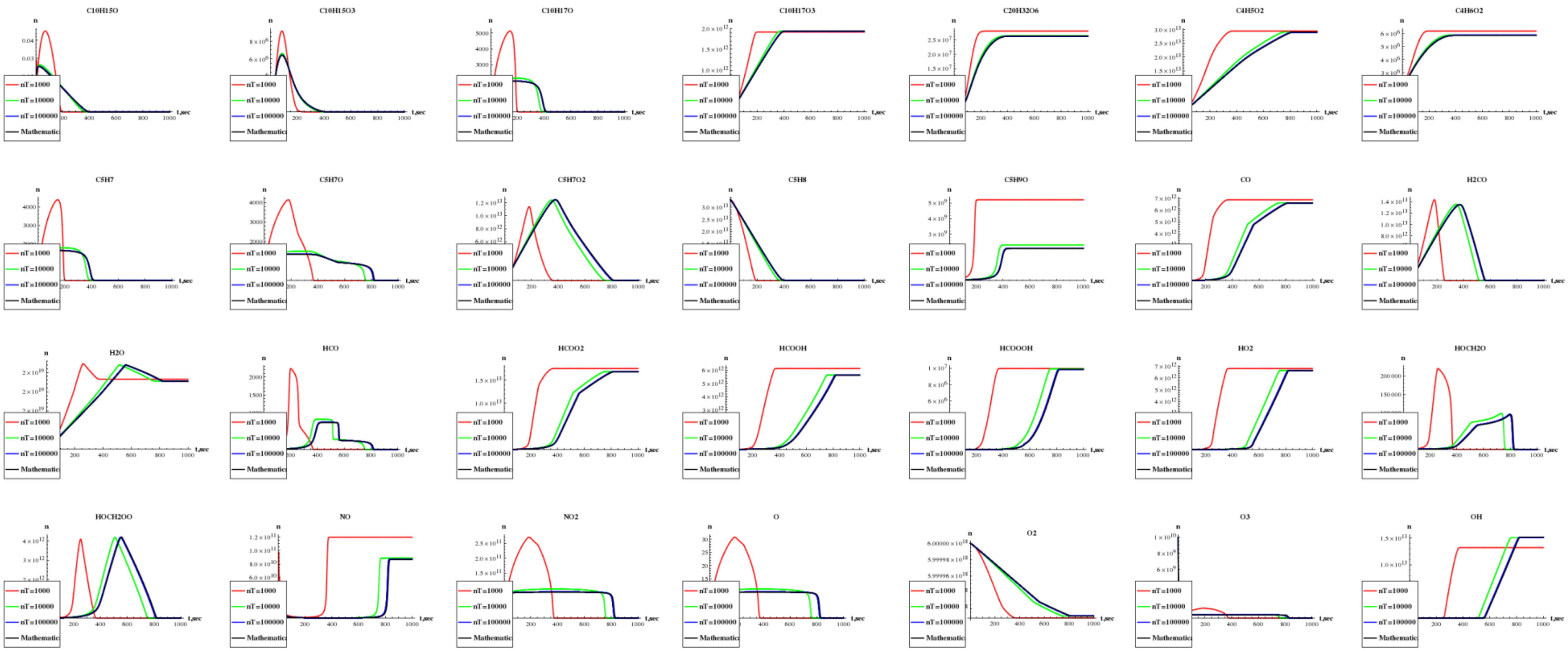
$\mathrm{C5H8}(0) = 3.3\times 10^{13}$

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

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

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).