Algorithms based on adjoint function ensembles for inverse modeling of transport and transformation of atmospheric pollutants

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Motivation

•The progress in the parallel computations technologies: the speedup is achieved trough the intensive parallelization (ensemble algorithms, splitting, decomposition, etc.)

•The progress in nonlinear ill-posed operator equation solution (different regularization methods, SVD, convergence theory, etc.) and **analysis** methods

•Variety of applications for the inverse and data assimilation problems for advection-diffusion-reaction models. E.g.

- •Air quality studies (environmental applications)
- •*Morphogen theory (developmental biology)*

•Unified approach to different measurement data including image-type measurement data in air quality applications (large volume of data with unknown value w.r.t. the considered inverse modelling task):

- •Time-series (*in situ*)
- •Vertical concentration profiles (aircraft sensing, lidar profiles, etc).
- •Satellite images (total column 2D images).

Advection-diffusion-reaction model

The domain $\Omega_T = \Omega \times [0, T]$ $\quad \Omega$ rectangular in (0D,)1D,2D

$$\frac{\partial \varphi_l}{\partial t} - \underbrace{\nabla \cdot \left(\mathrm{diag}\left(\mu_l\right) \nabla \varphi_l - \mathbf{u} \varphi_l\right)}_{\text{advection-diffusion}} + \underbrace{P_l(t, \boldsymbol{\varphi}, \mathbf{y}) \varphi_l = \Pi_l(t, \boldsymbol{\varphi}, \mathbf{y})}_{\text{destruction-production}} + f_l + r_l,$$

Model scale: 0D,1D,2D $\quad l = 1, \ldots, N_c$ - number of species

$$\textbf{BC:} \begin{cases} \mathbf{n} \cdot \left(\mathrm{diag}\left(\mu_l\right) \nabla \varphi_l\right) + \beta_l \varphi_l = \alpha_l^R, & (\mathbf{x}, t) \in \Gamma_{out} \subset \partial\Omega \times (0, T], \\ \varphi_l = \alpha_l^D, & (\mathbf{x}, t) \in \Gamma_{in} \subset \partial\Omega \times (0, T], \end{cases}$$

$$\textbf{IC:} \quad \varphi_l = \varphi_l^0, \quad \mathbf{x} \in \Omega, t = 0,$$

Direct problem operator

$$\varphi : \begin{cases} R \times Y \to \Phi \\ \{\mathbf{r}, \mathbf{y}\} \mapsto \boldsymbol{\varphi} \end{cases},$$

Linear measurement operators, e.g.

- Pointwise concentrations
- Total column 2D images
- Vertical profiles

Subspace $Span U_{mes}$

Inverse problem

$$\underbrace{\mathbf{I}}_{\text{Given}} = \Pr_{U_{mes}} \boldsymbol{\varphi}[\underbrace{\mathbf{r}^{(*)}, \mathbf{y}^{(*)}}_{\text{To find (or)}}] + \underbrace{\delta \mathbf{I}}_{\text{Noise}},$$

Adjoint problem

Lagrange type identity (sensitivity relation)

$$\langle \mathbf{h}, \delta\boldsymbol{\varphi}\rangle_\Phi = \langle \boldsymbol{\delta}\mathbf{r}, \boxed{\Psi[\mathbf{h}]}\rangle_R + \langle \delta\mathbf{y}, \boxed{K(t,\boldsymbol{\varphi}^{(2)},\mathbf{y}^{(2)},\boldsymbol{\varphi}^{(1)},\mathbf{y}^{(1)})''\ \Psi[\mathbf{h}]}\rangle_Y$$

Sensitivity functions

$$\boldsymbol{\varphi}^{(m)} = \boldsymbol{\varphi}[\mathbf{r}^{(m)},\mathbf{y}^{(m)}]$$

$$K(t,\boldsymbol{\varphi}^{(2)},\mathbf{y}^{(2)},\boldsymbol{\varphi}^{(1)},\mathbf{y}^{(1)})'' = \bar{\nabla}_y \Pi(t,\boldsymbol{\varphi}^{(2)};\mathbf{y}^{(2)},\mathbf{y}^{(1)})'' - \bar{\nabla}_y P(t,\boldsymbol{\varphi}^{(2)};\mathbf{y}^{(2)},\mathbf{y}^{(1)})''\ diag(\boldsymbol{\varphi}^{(1)}),$$

Adjoint problem: Given $\mathbf{h},\boldsymbol{\varphi}^{(m)},\mathbf{y}^{(m)}, m=1,2,$ find $\boldsymbol{\Psi}$:

$$-\frac{\partial \Psi_l}{\partial t} - \mathbf{u}\cdot\nabla\Psi_l - \nabla\cdot(diag(\mu)\nabla\Psi_l) + (G(t,\boldsymbol{\varphi}^{(2)},\mathbf{y}^{(2)},\boldsymbol{\varphi}^{(1)},\mathbf{y}^{(1)})\boldsymbol{\Psi})_l = h_l,$$

$$G(t,\boldsymbol{\varphi}^{(2)},\mathbf{y}^{(2)},\boldsymbol{\varphi}^{(1)},\mathbf{y}^{(1)}) = diag\left(P\left(t,\boldsymbol{\varphi}^{(2)},\mathbf{y}^{(2)}\right)\right) +$$

$$\bar{\nabla} P\left(t,\boldsymbol{\varphi}^{(2)},\boldsymbol{\varphi}^{(1)};\mathbf{y}^{(1)}\right)^* diag\left(\boldsymbol{\varphi}^{(1)}\right) - \bar{\nabla}\Pi\left(t,\boldsymbol{\varphi}^{(2)},\boldsymbol{\varphi}^{(1)};\mathbf{y}^{(1)}\right)^*,$$

$\bar{\nabla}$ -divided difference operator

+ adjoint problem boundary conditions

TC: $\boldsymbol{\Psi}(T) = 0,$

Linear parametrizations $\delta r = \sum_m \beta_m \delta r_m$ $\quad \langle \mathbf{h}, \delta\boldsymbol{\varphi}\rangle_\Phi = \sum_m \beta_m \langle \delta r_m, \Psi[\mathbf{h}]\rangle_R$

Gradient algorithms

(inverse source problem)

Given the cost function

$$J(\mathbf{r}) = \sum_{l \in L_{mes}} \left\| \varphi_l[\mathbf{r}] - I_l \right\|^2_{L_2(\Omega_T)} \rho_l .$$

if the parameters are smooth enough, then

$$\boldsymbol{\varphi}[\mathbf{r}] \Rightarrow \mathbf{h} = \left\{ \begin{cases} 2\left(\varphi_l[\mathbf{r}] - I_l\right), l \in L_{mes} \\ 0, l \notin L_{mes} \end{cases} \right\}_{l=1}^{N_c} \Rightarrow \nabla J(\mathbf{r}) = \Psi[\mathbf{r}, \mathbf{r}, \mathbf{h}],$$

uncertainty

Penenko, V. V. & Obraztsov, N. N. A variational initialization method for the fields of the meteorological elements // English translations Soviet Meteorology and Hydrology, 1976 , 11 , 3-16

Пененко, В. В. Методы численного моделирования атмосферных процессов Гидрометеоиздат, 1981

4DVAR

state

Dimet, F.-X. L. & Talagrand, O. Variational algorithms for analysis and assimilation of meteorological observations: theoretical aspects // Tellus, 1986 , 38A , 97-110

E.g. Polak-Ribiere conjugate gradient algorithm implemented in GSL

$$\mathbf{r}^{(\mathbf{k+1})} := \mathbf{r}^{(\mathbf{k})} - \alpha^{(k)} \mathbf{s}^{(\mathbf{k})}, \quad \alpha^{(k)} = \arg\min_{\alpha > 0} J\left(\mathbf{r}^{(\mathbf{k})} - \alpha \mathbf{s}^{(\mathbf{k})}\right),$$

$$\mathbf{s}^{(\mathbf{k})} = \begin{cases} \mathbf{g}^{(\mathbf{k})} + \beta^{(k)} \mathbf{s}^{(\mathbf{k\text{-}1})}, & k > 1 \\ \mathbf{g}^{(\mathbf{k})}, & k = 1 \end{cases}, \quad \beta^{(k)} = \frac{\left\langle \mathbf{g}^{(\mathbf{k})}, \mathbf{g}^{(\mathbf{k})} - \mathbf{g}^{(\mathbf{k\text{-}1})} \right\rangle}{\left\langle \mathbf{g}^{(\mathbf{k\text{-}1})}, \mathbf{g}^{(\mathbf{k\text{-}1})} \right\rangle}, \quad \mathbf{g}^{(\mathbf{k})} = -\nabla_r J(\mathbf{r}^{(\mathbf{k})}).$$

Sequential Data Assimilation at the Splitting Stages

Consider a splitting scheme on the interval $t^{j-1} \le t \le t^{j}$ ([Gordeziani,Meladze, 1974], [Samarski, Vabishevich, 2003]),

$$\phi\left(t^{j-1}\right)$$

•Transport

$$\gamma_\xi \frac{\partial \phi_\xi}{\partial t} + L_\xi \phi_\xi = \gamma_\xi \left(f + r_\xi\right),$$

$$\{x,t\} \in [0, X_\xi] \times [t^{j-1}, t^{j}],$$

$$\phi_\xi\left(t^{j-1}\right) = \phi\left(t^{j-1}\right),$$

$$\xi \in \{x, y, z\}$$

•Transformation

$$\gamma_c \frac{\partial (\varphi_c)_l}{\partial t} + P_l(t, \vec{\varphi}_c)(\varphi_c)_l$$

$$= \Pi_l(t, \vec{\varphi}_c) + \gamma_c \left(f_l + (r_c)_l\right),$$

$$\phi_c\left(t^{j-1}\right) = \phi\left(t^{j-1}\right).$$

Variational DA WRT r_l

Measurements I

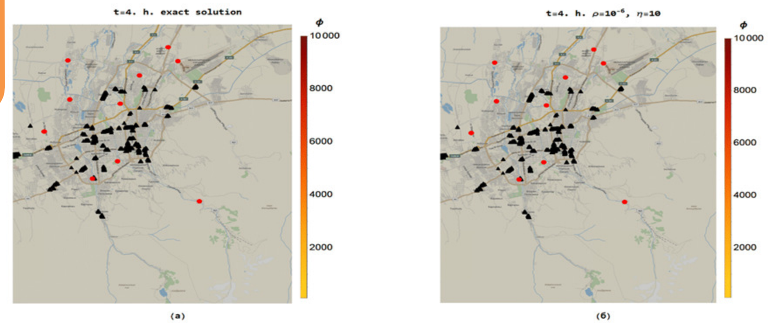
Variational DA WRT r_l

Direct Algorithm

Next step

$$\phi(t^{j}) = \sum_{\xi \in \{x,y,z,c\}} \gamma_\xi \phi_\xi(t^{j}).$$

$$\sum_{\xi \in \{x,y,z\}} \gamma_\xi + \gamma_c = 1.$$



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Adjoint problem solution ensembles in inverse problem algorithms

Cost function based

- **Cost functional gradients with adjoint problem solution** (single element ensemble for the discrepancy)
- **Gradient computation with adjoint ensemble when adjoint is independent of direct solution** [Karchevsky, A., Eurasian journal of mathematical and computer applications, 2013 , 1 , 4-20]
- **Representer method (optimality system decomposition, ensemble generated for discrepancies for each measurement data)** [Bennett, A. F. Inverse Methods in Physical Oceanography (Cambridge Monographs on Mechanics) Cambridge University Press, 1992]

Sensitivity relation based

- **Coarse-fine mesh method (Sequential solution refinement with sequential adjoint problems solving)** [Hasanov, A.; DuChateau, P. & Pektas, B. An adjoint problem approach and coarse-fine mesh method for identification of the diffusion coefficient in a linear parabolic equation// Journal of Inverse and Ill-Posed Problems, 2006 , 14 , 1-29]
- **Adjoint function for each measurement datum with the solution of the resulting operator equation** [Marchuk G. I., On the formulation of certain inverse problems, Dokl. Akad. Nauk SSSR, 156:3 (1964), 503–506], [Issartel, J.-P. Rebuilding sources of linear tracers after atmospheric concentration measurements // Atmospheric Chemistry and Physics, Copernicus GmbH, 2003 , 3 , 2111-2125]

ИВМиМГ

Sensitivity operator

(inverse source problem)

Image (model) to structure operator [Dimet et al,2015]

Given Ξ functions $U = \{\mathbf{u}^{(\xi)}\}_{\xi\in\Xi} \subset Span U_{meas}$

$$H_U\left(\boldsymbol{\varphi}[\mathbf{r}^{(2)}]-\boldsymbol{\varphi}[\mathbf{r}^{(1)}]\right)=\sum_{\xi\in\Xi}\left\langle \boldsymbol{\varphi}[\mathbf{r}^{(2)}]-\boldsymbol{\varphi}[\mathbf{r}^{(1)}],\mathbf{u}^{(\xi)}\right\rangle \mathbf{e}^{(\xi)}$$

Sensitivity relation
(Lagrange type identity)

$$\left\langle \boldsymbol{\varphi}[\mathbf{r}^{(2)}]-\boldsymbol{\varphi}[\mathbf{r}^{(1)}],\mathbf{u}^{(\xi)}\right\rangle = \left\langle \Psi[\mathbf{r}^{(2)},\mathbf{r}^{(1)};\mathbf{u}^{(\xi)}],\mathbf{r}^{(2)}-\mathbf{r}^{(1)}\right\rangle$$

Sensitivity operator

$$M_U[\mathbf{r}^{(2)},\mathbf{r}^{(1)}]:\begin{cases} R\to\mathbb{R}^{\Xi} \\ \mathbf{z}\mapsto\sum_{\xi\in\Xi}\left\langle \boldsymbol{\Psi}[\mathbf{r}^{(2)},\mathbf{r}^{(1)};\mathbf{u}^{(\xi)}],\mathbf{z}\right\rangle \mathbf{e}^{(\xi)}, \end{cases}$$

Parallel w.r.t. U

The inverse problem solution $\mathbf{r}^{(*)}$ for any $\mathbf{r}$ and U satisfy

$$H_U\left(\mathbf{I}-\Pr_{U_{mes}}\boldsymbol{\varphi}[\mathbf{r}]\right)=M_U[\mathbf{r}^{(*)},\mathbf{r}]\left(\mathbf{r}^{(*)}-\mathbf{r}\right)+H_U\delta\mathbf{I}.$$

Parametric family of quasi-linear operator equations

Adjoint ensemble construction

(inverse source problem, 2D, L_{mes} components are measured)

Defined by the adjoint problem sources sets

«*a priori*» approach – ensemble for the class of problems (smoothness)

- Fourier cos-basis $U_\Theta = \left\{ \mathbf{e}_{\eta\theta_x\theta_y\theta_t} \mid \theta_x \in [0,\Theta_x], \theta_y \in [0,\Theta_y], \theta_t \in [0,\Theta_t], \eta \in L_{mes} \right\}$,

$$e_{\eta\theta_x\theta_y\theta_t} = \left\{ \begin{cases} \frac{1}{\sqrt{\rho_\eta}} C(T,\theta_t,t^k) C(X,\theta_x,x_i) C(Y,\theta_y,y_j), l=\eta \\ 0,\ l \neq \eta \end{cases} \right\}_{l=1}^{N_c}, \quad C(T,\theta,t) = \frac{1}{\sqrt{T}} \begin{cases} \sqrt{2}\cos\left(\frac{\pi\theta t}{T}\right), \theta > 0 \\ 1, \theta = 0 \end{cases}.$$

- Wavelets, curvlets, etc. [Dimet et al.,2015]

«*a posteriori*» approach – ensemble for the considered problem

- **«Adaptive basis»**: chose elements of U_Θ with maximal projections

$$\left\langle \Pr_{U_{mes}} \boldsymbol{\varphi}[\mathbf{r}^{(0)}] - \mathbf{I}, \mathbf{e}_{\eta\theta_x\theta_y\theta_t} \right\rangle$$

Penenko, A.; Zubairova, U.; Mukatova, Z. & Nikolaev, S. Numerical algorithm for morphogen synthesis region identification with indirect image-type measurement data // Journal of Bioinformatics and Computational Biology, World Scientific Pub Co Pte Lt, 2019 , 17 , 1940002

- **«Informative basis»**: Use left singular vectors of the operator $m_{U_\Theta}[\mathbf{r}^{(0)}, \mathbf{r}^{(0)}]$

Penenko, A. V.; Nikolaev, S. V.; Golushko, S. K.; Romashenko, A. V. & Kirilova, I. A. Numerical Algorithms for Diffusion Coefficient Identification in Problems of Tissue Engineering // Math. Biol. Bioinf., 2016 , 11 , 426-444 (In Russian)

Inversion algorithm

$$H_U\left(\mathbf{I}-\Pr_{U_{mes}}\boldsymbol{\varphi}[\mathbf{q}]\right)=m_U[\mathbf{q},\mathbf{q}]\left(\mathbf{q}^{(*)}-\mathbf{q}\right)+\left(m_U[\mathbf{q}^{(*)},\mathbf{q}]-m_U[\mathbf{q},\mathbf{q}]\right)\left(\mathbf{q}^{(*)}-\mathbf{q}\right)+H_U\boldsymbol{\delta}\mathbf{I},$$

$$m\leftarrow m_U[q,q] \quad (\Xi\times N_{unknowns})$$

$$N_{unknowns}=\begin{cases}|L_{src}|\cdot N_t\cdot N_x\cdot N_y, & \text{inverse source problem}\\ N_{coeff}, & \text{inverse coefficient problem}\end{cases}$$

Newton-Kantorovich -type update

$$\boldsymbol{\delta}\mathbf{q}=\left(\begin{cases}m^T\left[mm^T\right]_\Sigma^+, & \Xi<N_{unknowns}\\ \left[m^Tm\right]_\Sigma^+m^T, & \Xi>N_{unknowns}\end{cases}\right)H_U\left(I-\Pr_{U_{mes}}\boldsymbol{\varphi}[\mathbf{q}]\right).$$

$[C]_\Sigma^+$ -truncated SVD inversion parametrized by conditional number Σ

Nonlinearity: sequential increase of the conditional number

Noise: discrepancy principle

Admissible solutions: projection regularization

Optional monotonicity: monotonic decrease of the discrepancy

Theoretical foundations: [Issartel, J.-P., 2003], [Cheverda V.A., Kostin V.I., 1995], [Kaltenbacher et al, 2008], [Vainikko, Veretennikov, 1986]

Inverse source problem (0D)

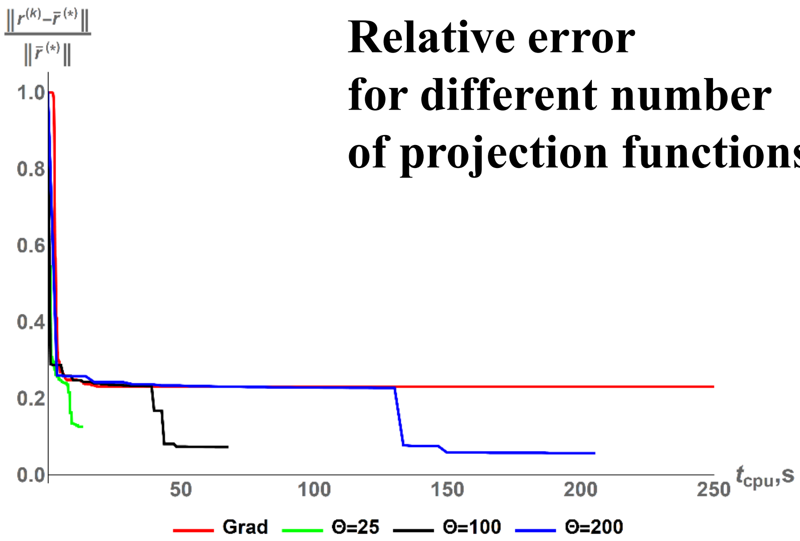
$$
\begin{array}{cc}
hv + NO_2 \to NO + O_3P & hv + O_3 \to O^1D + O_2 \\
HCHO + hv \to CO + 2HO_2 & HCHO + hv \to CO + H_2 \\
O_2 + O_3P \to O_3 & N_2 + O^1D \to N2 + O_3P \\
O^1D + O_2 \to O_2 + O_3P & H_2O + O^1D \to 2OH \\
HO_2 + NO \to NO_2 + OH & NO + O_3 \to NO_2 + O_2 \\
NO + RO_2 \to HCHO + HO_2 + NO_2 & CO + OH \to CO_2 + HO_2 \\
HC + OH \to H_2O + RO_2 & HCHO + OH \to CO + H_2O + HO_2 \\
NO_2 + OH \to HNO_3 & 2HO_2 \to H_2O_2 + O_2 \\
H_2O + 2HO_2 \to H_2O + H_2O_2 + O_2 & HO_2 + RO_2 \to O_2 + ROOH \\
2RO_2 \to HCHO + HO_2 & OH + SO_2 \to HO_2 + SULF.
\end{array}
$$

Modified [Stockwell,2002] $N_c = 22$

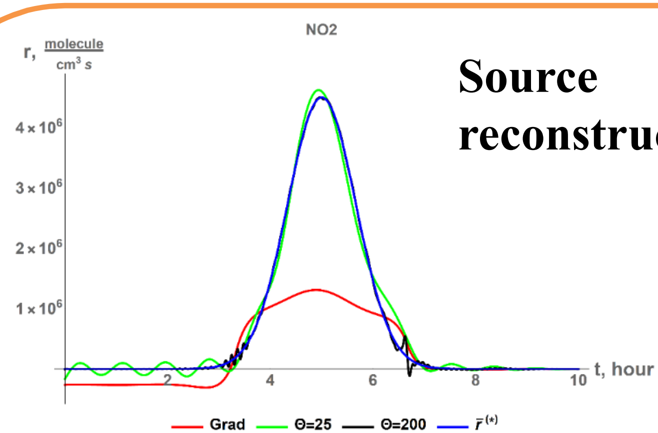
$$L_{mes} = \{CO_2, O_3\}$$
$$r^{(0)} = 0$$

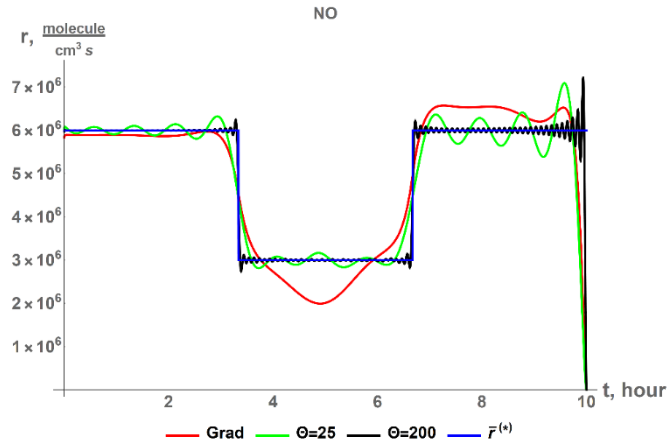
$$T = 10 \times 3600$$
$$N_t = 3000$$

Relative error for different number of projection functions



Source reconstruction

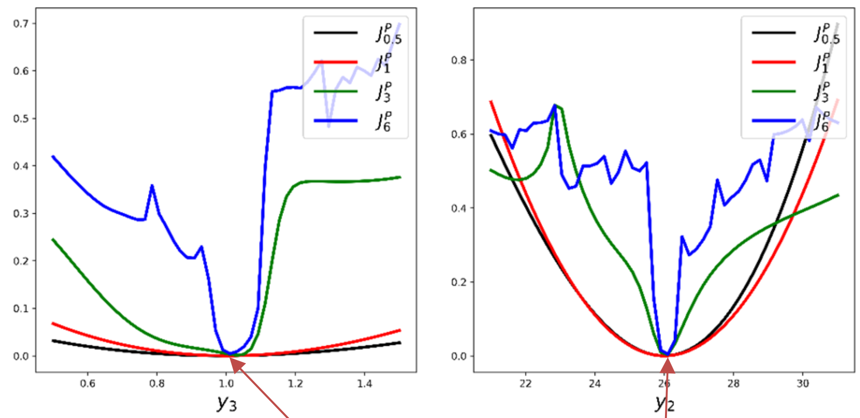




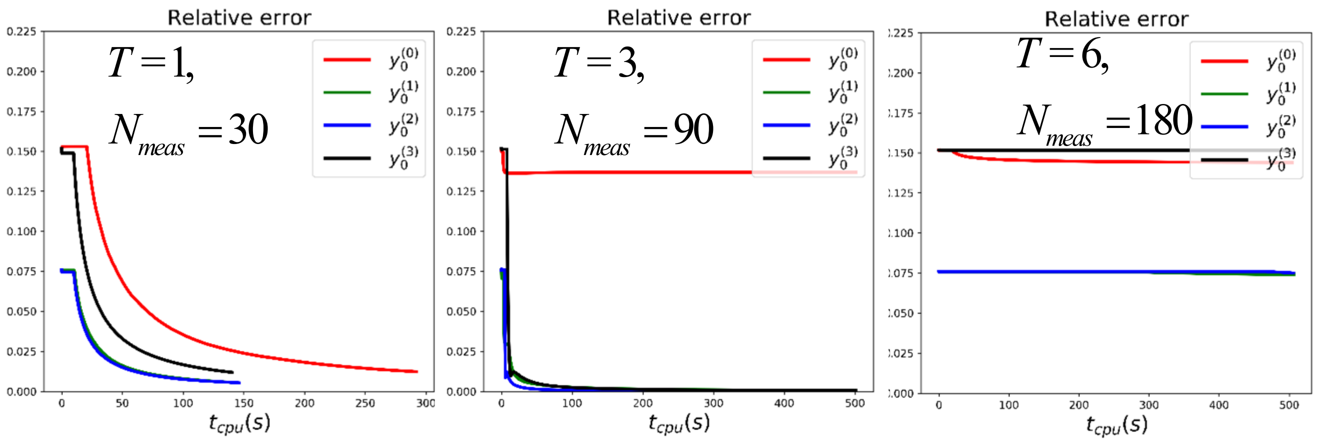
Penenko, A. V. A Newton–Kantorovich Method in Inverse Source Problems for Production-Destruction Models with Time Series-Type Measurement Data // Numerical Analysis and Applications, 2019 , 12 , 51-69

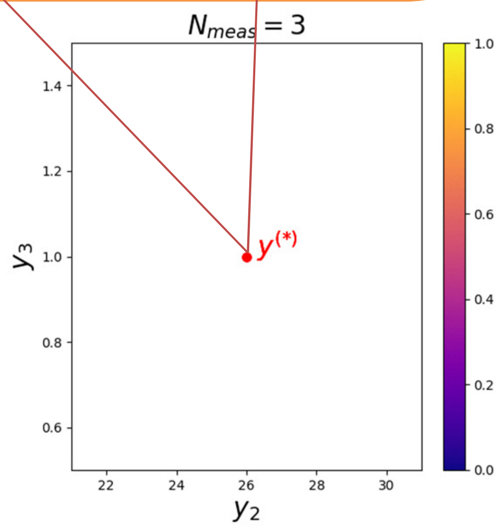
Larger ensembles and better solutions (0D)

- Lorenz’63 model,
- **Inverse coefficient problem** (2 unknown + 1 fixed coefficient)
- Regular in time state function measurements ($N_{meas} = T \times 3 \times 10$)
- **Monotonic discrepancy decrease**



Normalized cost functions cross-sections for increasing measurement datasets





Reconstruction error dynamics WRT computation time

A.V. Penenko Z.S. Mukatova, A.B. Salimova Numerical study of the coefficient identification algorithm based on ensembles of adjoint problem solutions for a production-destruction model // submitted

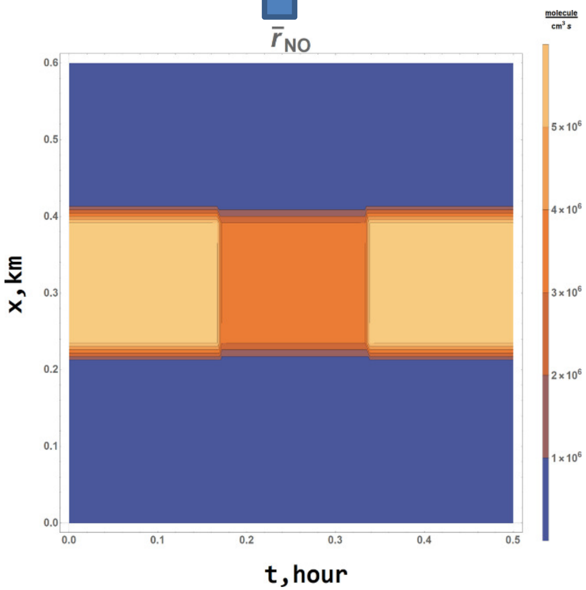
Data assimilation mode (2D)

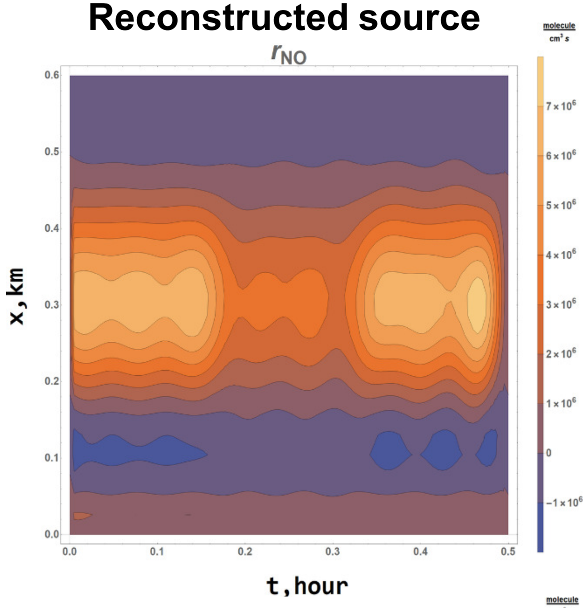
(data assimilation problem = sequence of inverse problems)

Exact source

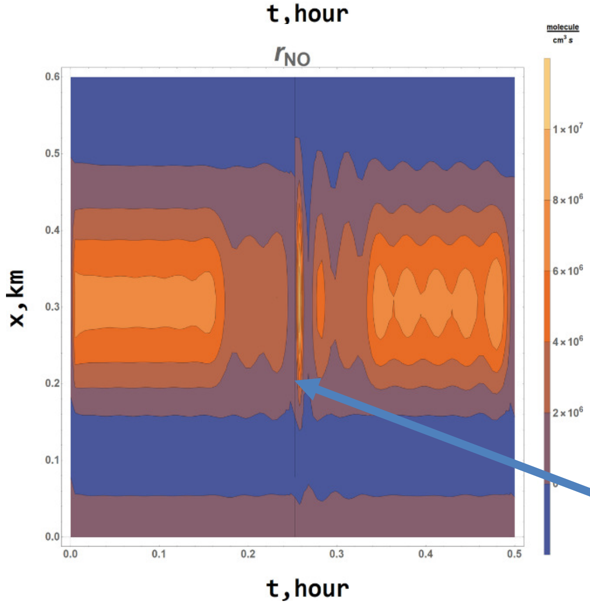
Reconstructed source

«Inverse problem mode»
(1 assimilation window)





«4DNK» algorithm



«Data assimilation mode»
(2 assimilation windows)

Source: NO

Measurements: O_3 concentration images (movies)

Initial guess: zero

$$T = 0.5 \times 3600$$
$$N_t = 100$$
$$X = Y = 600$$
$$N_x = 100$$
$$\theta_x = \theta_y = 5$$
$$\theta_t = 10$$

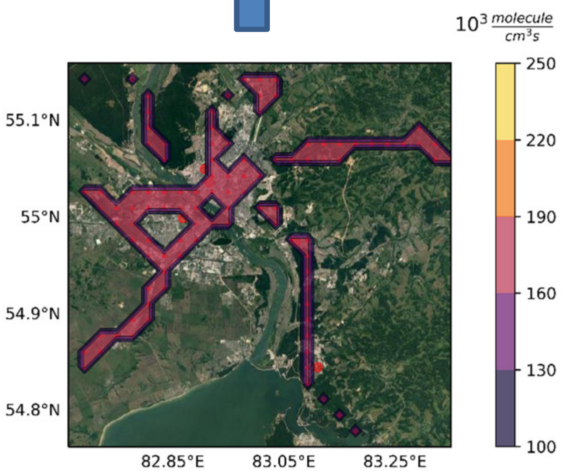
Assimilation window boundary

Penenko, A. V. Algorithms for the inverse modelling of transport and transformation of atmospheric pollutants // IOP Conference Series: Earth and Environmental Science, IOP Publishing, 2018 , 211 , 012052

Sources identification with direct and indirect *in situ* (5 sites) measurements

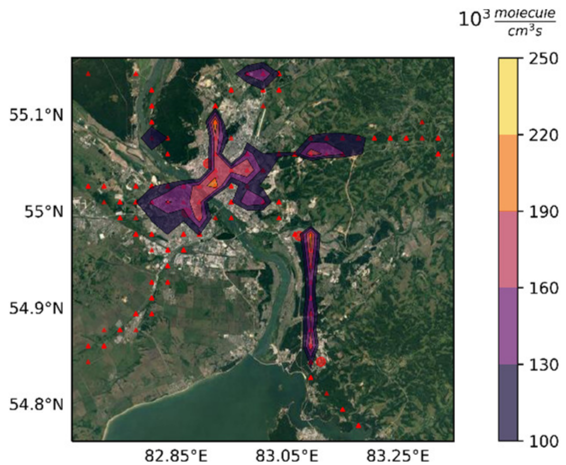
$T = 4 \times 24 \times 3600 \quad \Xi = 5 \times 10$

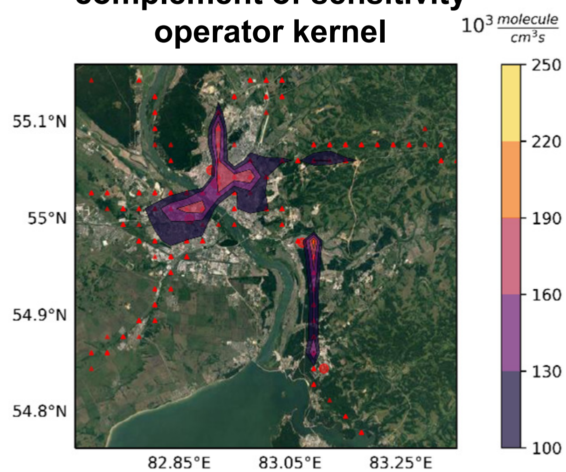
NO concentrations are measured



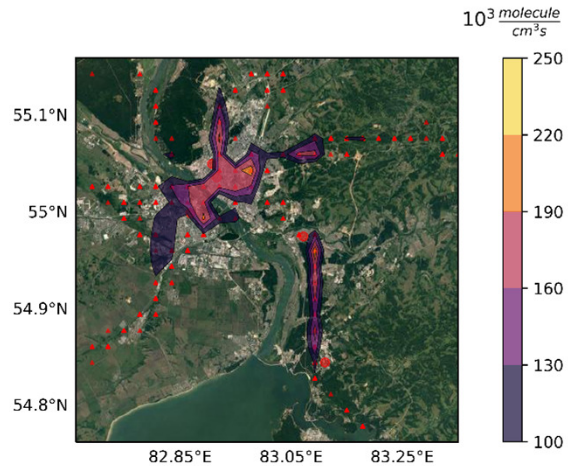
Exact **stationary** NO source function (city traffic)

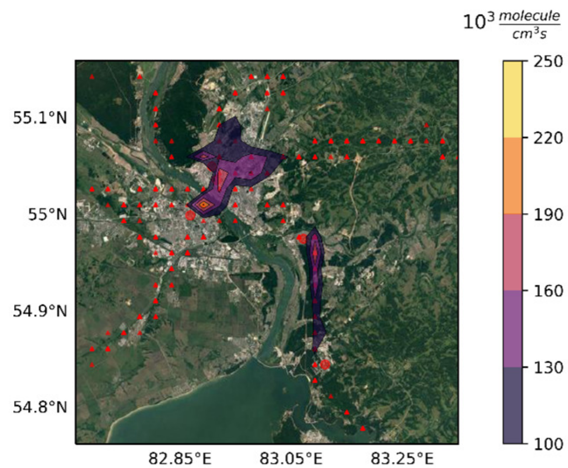
O3 concentrations are measured





Projection to orthogonal complement of sensitivity operator kernel





Reconstructed sources

V. V. Penenko A. V. Penenko, E. A. Tsvetova and A. V. Gochakov Methods for studying the sensitivity of atmospheric quality models and inverse problems of geophysical hydrothermodynamics // Journal of Applied Mechanics and Technical Physics, 2019, Vol. 60, No. 2, pp. 392–399.

Adjoint ensemble references

1. Penenko, A.; Zubairova, U.; Mukatova, Z. & Nikolaev, S. Numerical algorithm for morphogen synthesis region identification with indirect image-type measurement data // Journal of Bioinformatics and Computational Biology, 2019 , 17 , 1940002 **doi:10.1142/s021972001940002x**
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Summary

- **Given the adjoint model, the sensitivity operator allow reformulating the inverse problem stated as a PDE system to a parametric family of quasilinear operator equations**

- **Nonlinear ill-posed operator equation methods can be applied to the analysis and solution of the considered inverse problems**

- **To solve the operator equations, the Newton-Kantorovich-type inversion algorithm has been proposed using**
  - **The sequential increase of the considered spectrum in TSVD**
  - **Discrepancy principle and the iterative regularization**

- **Both ensemble size and its construction affects the efficiency of the inverse problem solution (accuracy, time, local convergence)**

- **The algorithm was tested numerically in inverse modeling (inverse and data assimilation, source and coefficient) problems for advection-diffusion-reaction-model.**

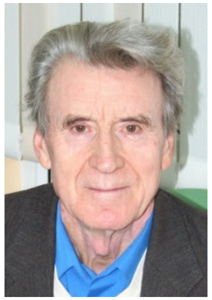
ИВМиМГ

ИНСТИТУТ ОПТИКИ АТМОСФЕРЫ им. В.Е. ЗУЕВА СО РАН

СИБНИГМИ

Thank you for your attention!

Co-authors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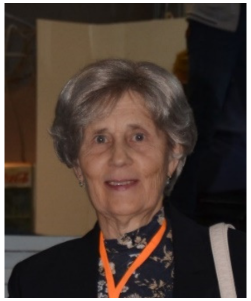
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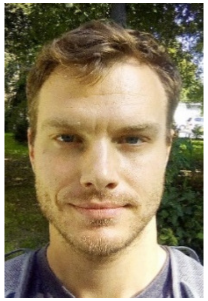
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