Multidimensional variational data assimilation algorithm for convection-diffusion models

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Emission tracking scenario (X,Y,T)

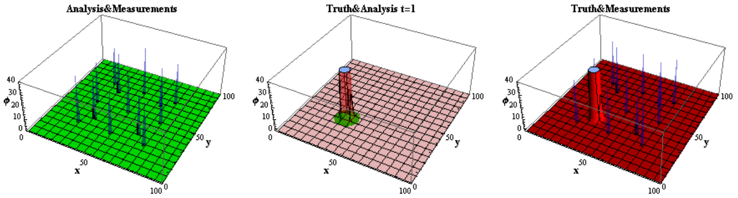

Fig. 1: Data assimilation scenario with 12 regularly placed measurement devices for the model with zero sources. Analysis is marked with green and measurement locations are marked with blue spikes (left). "Truth" is red with blue spikes in measurement locations (right) and superposition of Truth and Analysis in the middle.

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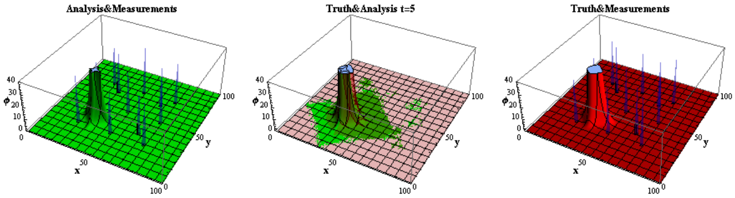

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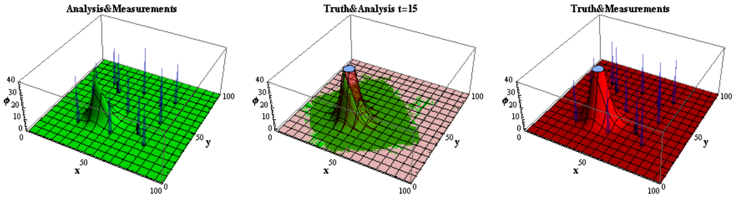

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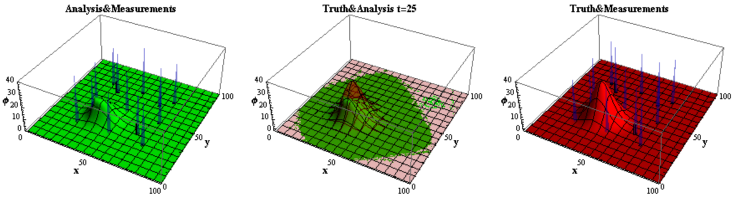

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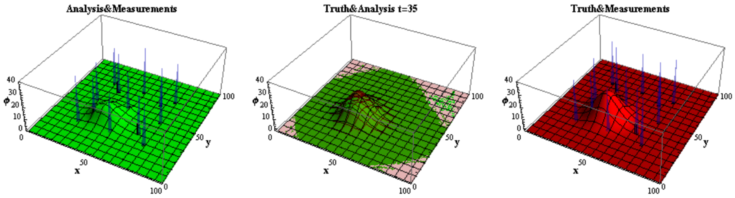

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Data assimilation features

Data assimilation algorithms are used to improve a model-based forecast with the use of measurement data.

- Measurement data is not enough to reconstruct the whole field (How to define the solution?)
- Model state is of interest (e.g. atmosphere parameters are rapidly changing).
- Solution should be obtained in "real-time" for the situation goes out of date very fast.

Convection diffusion reaction model

- Multidimensional mathematical models describing heat, moisture, radiation and substances transport has the following general structure:

$$L(\vec{\phi}, \vec{Y}) \equiv \frac{\partial \rho \vec{\phi}}{\partial t} + \operatorname{div} \rho(\vec{\phi}\vec{u} - \mu \operatorname{grad} \vec{\phi}) + \rho((S\vec{\phi}) - \vec{f}_a - \vec{r}) = 0,$$

$$\vec{\phi}^0 = \vec{\phi}_a^0 + \vec{\xi}, \quad R_{bound}(\vec{\phi}) = \vec{g}_a + \vec{\varepsilon}, \quad \vec{Y} = \vec{Y}_a + \vec{\zeta}.$$

  Here $\vec{\phi}$ is model statefunction, $\{\rho, \vec{u}, \mu\} = \vec{Y}$ are parameters of the model, S is transformation operator, $\vec{f}_a$, $\vec{g}_a$, $\vec{\phi}_a^0$ are *a priori* sources and initial condition.
- Incoming measurement data $\vec{\Psi}_m$ are connected with model statefunction with the measurement operator **H**

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

- $\vec{r}$, $\vec{\xi}$, $\vec{\varepsilon}$, $\vec{\zeta}$, $\vec{\eta}$ are control functions introduced to the model rigid structure to provide flexibility for data assimilation.

Data assimilation and Tikhonov regularization

Consider the following constrained optimization problem

$$J(\phi^{j+1}, r^{j+1}) = \left\| H\phi^{j+1} - \Psi \right\|^2 + \alpha \left\| r^{j+1} \right\|^2 .$$

WRT the model approximated with implicit finite-difference scheme

$$L\phi^{j+1} = \phi^j + \tau f^{j+1} + r^{j+1}.$$

Stationary point of the augmented functional is the solution of

$$\begin{pmatrix} L & -\frac{1}{2\alpha} \\ 2H^*H & L^* \end{pmatrix} \begin{pmatrix} \phi^{j+1} \\ \phi^{j+1*} \end{pmatrix} = \begin{pmatrix} \phi^j + \tau f^{j+1} \\ 2H^*\Psi \end{pmatrix}.$$

Solution ϕ^{j+1} of the system is also the solution of

$$\left(H^*H + \alpha L^*L\right)\phi^{j+1} = H^*\Psi + \alpha L^*(\phi^j + \tau f^{j+1})$$

and a minimum of

$$J\left(\phi^{j+1}\right) = \left\| H\phi^{j+1} - \Psi \right\|^2 + \alpha \left\| L\phi^{j+1} - (\phi^j + \tau f^{j+1}) \right\|^2 .$$

Assimilation schemes

- "Explicit" scheme (Strong constrained)

$$L\tilde{\phi}^{j+1} = \phi^j + \tau f^{j+1},$$
$$\phi^{j+1} = \tilde{\phi}^{j+1} + K\left(H\tilde{\phi}^{j+1} - \Psi\right),$$

  with the corresponding Tikhonov functional [Perianez,Reich,Potthast, 2013]

$$J(\phi^{j+1}) = \left\|H\phi^{j+1} - \Psi\right\|^2 + \alpha\left\|\phi^{j+1} - \tilde{\phi}^{j+1}\right\|_K^2.$$

- "Implicit" scheme (Weak constrained)

$$L\phi^{j+1} = \phi^j + \tau f^{j+1} + \frac{1}{2\alpha}\phi^*,$$
$$L^*\phi^* = H^*\left(H\phi^{j+1} - \Psi\right),$$

  corresponding Tikhonov functional

$$J(\phi^{j+1}) = \left\|H\phi^{j+1} - \Psi\right\|^2 + \alpha\left\|L\phi^{j+1} - (\phi^j + \tau f^{j+1})\right\|^2.$$

Variational data assimilation and Tikhonov regularization

Denote functional

$$J(\phi^{j+1}) = \left\|H\phi^{j+1} - \Psi\right\|^2 + \alpha \left\|L\phi^{j+1} - (\phi^j + \tau f^{j+1})\right\|^2.$$

minimum with $\phi^{j+1}(\alpha)$. Consider the following notations

$$\Phi(\alpha) = J(\phi^{j+1}(\alpha)), \quad \xi(\alpha) = \left\|L\phi^{j+1}(\alpha) - (\phi^j + \tau f^{j+1})\right\|^2,$$
$$\beta(\alpha) = \left\|H\phi^{j+1}(\alpha) - \Psi\right\|^2.$$

Theorem (Analogous to [Tikhonov,Goncharsky,Stepanov,Yagola,1990])Let H, L be matrices, and L is invertible one, then

- Functions are continuous with $\alpha > 0$
- Function $\Phi(\alpha)$ is convex and differentiable $\Phi'(\alpha) = \xi(\alpha)$.
- Function $\xi(\alpha)$ is monotonically nonincreasing and functions $\Phi(\alpha), \beta(\alpha)$ are monotonically nondecreasing with $\alpha > 0$. On the interval $(0, \alpha_0)$ with $L\phi^{j+1}(\alpha) \neq (\phi^j + \tau f^{j+1})$ functions $\Phi(\alpha)$ are strictly monotone.

Variational data assimilation and Tikhonov regularization

$$\Phi(\alpha) = J(\phi^{j+1}(\alpha)), \quad \xi(\alpha) = \left\| L\phi^{j+1}(\alpha) - (\phi^j + \tau f^{j+1}) \right\|^2,$$
$$\beta(\alpha) = \left\| H\phi^{j+1}(\alpha) - \Psi \right\|^2.$$

The following holds:

- With increasing model "weight":

$$\lim_{\alpha\to+\infty} \xi(\alpha) = 0,$$
$$\lim_{\alpha\to+\infty} \Phi(\alpha) = \lim_{\alpha\to+\infty} \beta(\alpha) = \left\| HL^{-1}(\phi^j + \tau f^{j+1}) - \Psi \right\|^2.$$

- With increasing data "weight":

$$\lim_{\alpha\to 0+0} \alpha\xi(\alpha) = 0, \quad \lim_{\alpha\to 0+0} \Phi(\alpha) = \lim_{\alpha\to 0+0} \beta(\alpha) = 0.$$

Assimilation parameter

- Let the discrepancy level be δ_*.

$$\left\|\phi^{j+1} - \Psi^{j+1}\right\|_\sigma = \sqrt{\sum_{m=1}^{M} \left(\frac{\phi_{i(m)}^{j+1} - \Psi_m^{j+1}}{\sigma_m} \right)^2} = \delta_*.$$

- Due to monotonicity the assimilation parameter can be calculated with the following algorithm

$$\alpha_1 = 1,$$
$$\alpha_{k+1} := \frac{\delta_*}{\left\|\phi^{j+1} - \Psi^{j+1}\right\|_\sigma} \alpha_k.$$

Assimilation parameter based on statistical considerations

- Let data consist of "exact" solution with additive Gaussian noise

$$\Psi^j_m = \phi^j_{i(m)} + \sigma_m \xi_m, \;\; \xi_m \sim N(0,1).$$

- With probability p

$$\delta_* = \sqrt{\sum_{m=1}^{M} \left(\frac{\Psi^j_m - \phi^j_{i(m)}}{\sigma_m} \right)^2} < \sqrt{\chi^2_{inv}(M,p)},$$

where $\chi^2_{inv}(M,p)$ is solution of

$$P(\chi^2_N < \chi^2_{inv}(M,p)) = p.$$

- I.e. the probability p serves as an assimilation parameter.

Splitting method

In 2D case the problem can be approximated with the following equation

$$\phi^0 = 0,$$
$$\frac{\bar{\phi}^{j+1} - \bar{\phi}^j}{\tau} + A_x\bar{\phi}^{j+1} + A_y\bar{\phi}^{j+1} = f^{j+1}.$$

From the point of view of parallel computations an additive-averaged splitting scheme is of special interest [Samarsky,Vabishevich,2003].

$$\frac{\phi_x^{j+1} - \phi^j}{2\tau} + A_x\phi_x^{j+1} = f_x^{j+1}, \quad \frac{\phi_y^{j+1} - \phi^j}{2\tau} + A_y\phi_y^{j+1} = f_y^{j+1},$$
$$f^{j+1} = f_x^{j+1} + f_y^{j+1},$$
$$\phi^{j+1} = \frac{1}{2}\left(\phi_x^{j+1} + \phi_y^{j+1}\right).$$

"Implicit" data assimilation algorithm for 1D convection-diffusion model

Nonstationary 1D model can be approximated with matrix equation on a space-time domain:

$$\phi^0 = 0,$$
$$L\phi^{j+1} = (E + \tau A)\,\phi^{j+1} = \phi^j + \tau f^{j+1} + \tau r^{j+1}.$$

Convection-diffusion operators are approximated with tridiagonal systems.

$$-a_i\phi_{i+1}^{j+1} + b_i\phi_i^{j+1} = \phi_i^j + \tau f_i^{j+1} + \tau r_i^{j+1}, i = 0,$$
$$-a_i\phi_{i+1}^{j+1} + b_i\phi_i^{j+1} - c_i\phi_{i-1}^{j+1} = \phi_i^j + \tau f_i^{j+1} + \tau r_i^{j+1},\ i = 1, \ldots, N-2,$$
$$b_i\phi_i^{j+1} - c_i\phi_{i-1}^{j+1} = \phi_i^j + \tau f_i^{j+1} + \tau r_i^{j+1},\ i = N-1,$$

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Data assimilation problem solution

Data assimilation problem solution is minimum of the functional

$$\Phi(\phi^{j+1}, r^{j+1}) = \left(\sum_{i=1}^{N-1} \left(\frac{\phi_i^{j+1} - \Psi_i^{j+1}}{\sigma_i} \right)^2 M_i^{j+1} + \alpha \sum_{i=1}^{N-1} \left(r_i^{j+1} \right)^2 \right) \frac{\tau}{2},$$

WRT numerical scheme for direct problem. Here σ_i are standard deviations of measurement device errors. Mask M_i^{j+1} is equal to 1 in a measurement point and 0 otherwise.

Introducing Lagrange multipliers (adjoint functions) ϕ^*:

$$\bar{\Phi}(\phi^{j+1}, r^{j+1}, \phi^{*j+1}) = \left(\sum_{i=0}^{N-1} \left(\frac{\phi_i^{j+1} - \Psi_i^{j+1}}{\sigma_i} \right)^2 M_i^{j+1} + \alpha \sum_{i=0}^{N-1} \left(r_i^{j+1} \right)^2 \right) \frac{\tau}{2}$$

$$+ \sum_{i=0}^{N-1} \left(-a_i \phi_{i+1}^{j+1} + b_i \phi_i^{j+1} - c_i \phi_{i-1}^{j+1} - \phi_i^j - \tau f_i^{j+1} - \tau r_i^{j+1} \right) \phi_i^{*j+1}.$$

Assimilation system

Equating first variations of target functional to 0, we obtain the following algorithm:

$$\partial_{\phi_i^*}\Phi(\phi^{j+1}, r^{j+1}, \phi^{*j+1}) = 0$$

is equivalent to the direct problem scheme.

$$\partial_{r_i^{j+1}}\Phi(\phi^{j+1}, r^{j+1}, \phi^{*j+1}) = 0$$

is equivalent to

$$\alpha r_i^{j+1} - \phi_i^{*j+1} = 0,\ \ i = 0, \ldots, N-1.$$

Data assimilation system

$$\partial_{\phi_i^{j+1}} \Phi(\phi^{j+1}, r^{j+1}, \phi^{*j+1}) = 0,$$

is equivalent to

$$-c_{i+1}\phi^{*j+1}_{i+1} + b_i\phi^{*j+1}_{i} = -\frac{M_i}{\alpha\sigma_i^2}\left(\phi_i^{j+1} - \Psi_i^{j+1}\right)\tau, \; i = 0,$$

$$-c_{i+1}\phi^{*j+1}_{i+1} + b_i\phi^{*j+1}_{i} - a_{i-1}\phi^{*j+1}_{i-1} = -\frac{M_i}{\alpha\sigma_i^2}\left(\phi_i^{j+1} - \Psi_i^{j+1}\right)\tau,$$

$$i = 1, \ldots, N-2,$$

$$b_i\phi^{*j+1}_{i} - a_{i-1}\phi^{*j+1}_{i-1} = -\frac{M_i}{\alpha\sigma_i^2}\left(\phi_i^{j+1} - \Psi_i^{j+1}\right)\tau, \; i = N-1.$$

Matrix Data Assimilation System in 1D Case

The system can be aggregated to matrix equation [Penenko,2009, PenenkoAV,2006]

$$-A_i\Phi_{i+1}^{j+1} + B_i\Phi_i^{j+1} = F_i^{j+1},$$
$$-A_i\Phi_{i+1}^{j+1} + B_i\Phi_i^{j+1} - C_i\Phi_{i-1}^{j+1} = F_i^{j+1},$$
$$B_i\Phi_i^{j+1} - C_i\Phi_{i-1}^{j+1} = F_i^{j+1},$$

where

$$A_i = \begin{pmatrix} a_i & 0 \\ 0 & c_{i+1} \end{pmatrix},\ B_i = \begin{pmatrix} b_i & -\tau \\ \frac{M_i\tau}{\alpha\sigma_i^2} & b_i \end{pmatrix},\ C_i = \begin{pmatrix} c_i & 0 \\ 0 & a_{i-1} \end{pmatrix},$$

$$\Phi_i^{j+1} = \begin{pmatrix} \phi_i^{j+1} \\ \phi_i^{*j+1} \end{pmatrix},\ F^{j+1} = \begin{pmatrix} \phi_i^j \\ \frac{M_i\tau}{\alpha\sigma_i^2}\Psi_i^{j+1} \end{pmatrix},$$

that is solved with matrix sweep method.

Fine-grained data assimilation in multidimensional case

Splitting steps corresponding to spatial grid lines containing (projected) measurement data are substituted with minimum of the augmented functional

$$\bar{\Phi}_x(\phi_x^{j+1}, r_x^{j+1}, \phi_x^*) = \sum_{i=0}^{N_x-1} \left(\frac{\left(\phi_x^{j+1}\right)_i - \Psi_i^{j+1}}{\sigma_i} \right)^2 M_i^{j+1}\tau + \alpha_l \sum_{i=0}^{N_x-1} \left({r_x}_i^{j+1} \right)^2 \tau$$
$$+ \left\langle \left((I + 2\tau A_x)\, \phi_x^{j+1} - \phi^j - \tau f_x^{j+1} - \tau r_x^{j+1} \right)_l, \phi_x^* \right\rangle .$$

$$\bar{\Phi}_y(\phi_y^{j+1}, r_y^{j+1}, \phi_y^*) = \sum_{l=0}^{N_y-1} \left(\frac{\left(\phi_y^{j+1}\right)_l - \Psi_l^{j+1}}{\sigma_l} \right)^2 M_l^{j+1}\tau + \alpha_i \sum_{l=0}^{N_y-1} \left({r_y}_l^{j+1} \right)^2 \tau$$
$$+ \left\langle \left((I + 2\tau A_y)\, \phi_y^{j+1} - \phi^j - \tau f_y^{j+1} - \tau r_y^{j+1} \right)_l, \phi_y^* \right\rangle .$$

Data assimilation scenario (X,T) with stationary measurement devices

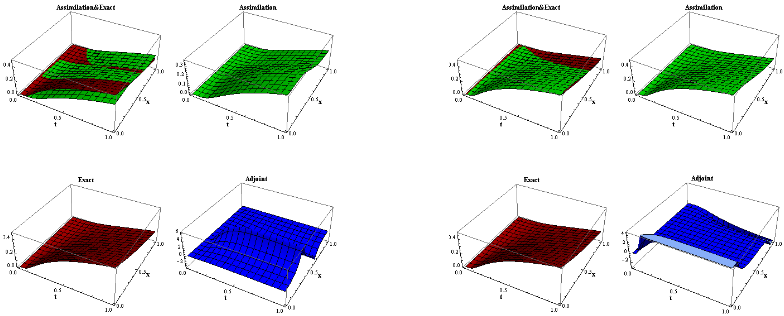

Fig. 2: Data assimilation of data collected in two points on each time step. Points are chosen inside the domain (left) and on the boundary (right).

Data assimilation scenario (X,T) with mobile measurement device

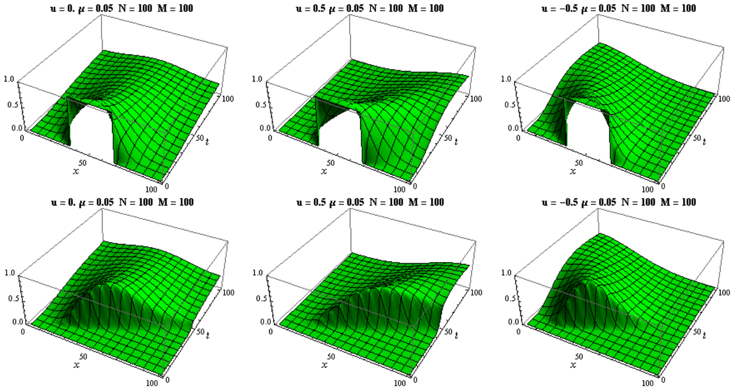

Fig. 3: Data assimilation of data collected with mobile measurement device. "Truth" (upper) and analysis(inner) with the model for zero *a priori* data [Ajnur Kussainova NSU master thesis,2013].

Data assimilation scenario (X,T) with stationary measurement devices

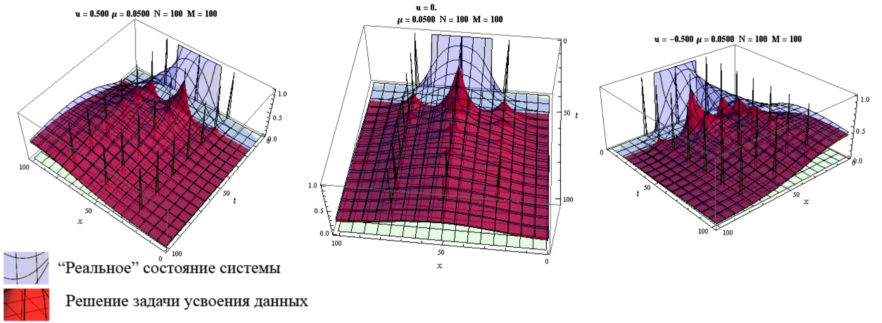

Fig. 4: Data assimilation with stationary measurement devices [Ajnur Kussainova NSU master thesis,2013].

Assimilation parameter with "small errors"

Conditions

Measurement system

m	1	2	3	4	5	6	7	8	9	10	11	12
iX_m	33	33	67	67	25	25	75	75	40	60	40	60
iY_m	33	67	33	67	25	75	25	75	60	40	40	60
σ_m	0.1	1.	0.5	1.	1.	2.	1.	0.5	1.	0.5	3.	0.1

Meteorology

$$u = 0.1 \quad v = 0.1 \quad \mu = 0.1$$

Grid domain

$$\begin{aligned} \mathrm{nT} &= 100 \quad T = 1. \\ \mathrm{nX} &= 100 \quad X = 1. \\ \mathrm{nY} &= 100 \quad Y = 1. \end{aligned}$$

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Assimilation parameter with "small errors"

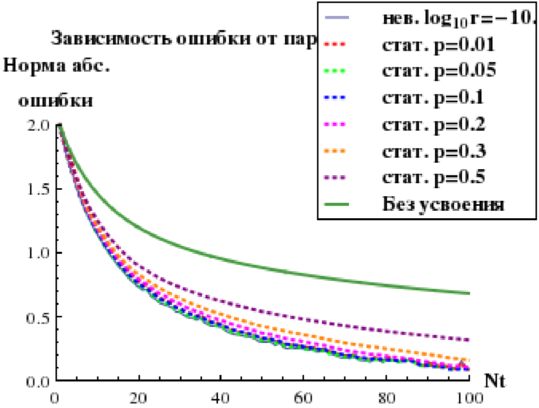

Fig. 6: Solution error WRT assimilation parameter on "small errors"

Assimilation parameter with "big errors"

Conditions

Measurement system

m	1	2	3	4	5	6	7	8	9	10	11	12
iX_m	33	33	67	67	25	25	75	75	40	60	40	60
iY_m	33	67	33	67	25	75	25	75	60	40	40	60
σ_m	0.5	5.	2.5	5.	5.	10.	5.	2.5	5.	2.5	15.	0.5

Meteorology

$$u = 0.1 \quad v = 0.1 \quad \mu = 0.1$$

Grid domain

$$\begin{aligned} nT &= 100 \quad & T &= 1. \\ nX &= 100 \quad & X &= 1. \\ nY &= 100 \quad & Y &= 1. \end{aligned}$$

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Assimilation parameter with "big errors"

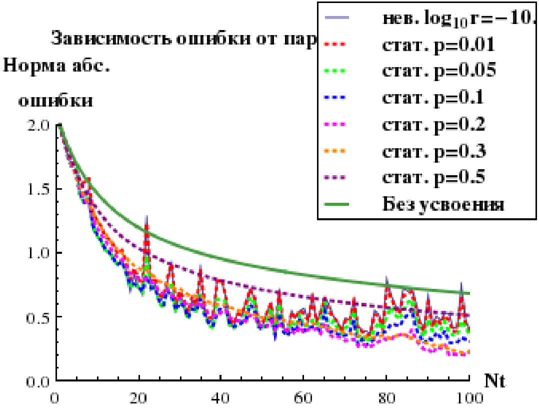

Fig. 7: Solution error WRT assimilation parameter on "big errors".

Measurement system with "small errors"

Conditions

Measurement system

m	1	2	3	4	5	6	7	8	9	10	11	12
iX_m	33	33	67	67	25	25	75	75	40	60	40	60
iY_m	33	67	33	67	25	75	25	75	60	40	40	60
σ_m	0.1	1.	0.5	1.	1.	2.	1.	0.5	1.	0.5	3.	0.1

Assimilation parameter

$$\log_{10} r = -10. \quad p = 0.3$$

Meteorology

$$u = 0.1 \quad v = 0.1 \quad \mu = 0.1$$

Grid domain

$$\mathrm{nT} = 100 \quad T = 1.$$
$$\mathrm{nX} = 100 \quad X = 1.$$
$$\mathrm{nY} = 100 \quad Y = 1.$$

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Measurement system with "small errors"

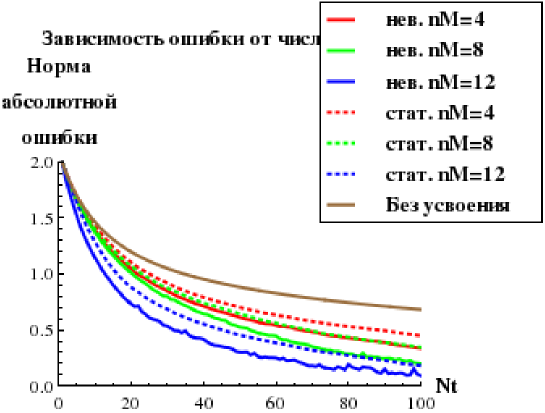

Fig. 8: Solution error WRT measurement device number with "small errors". The more data the better.

Measurement system with "big errors"

Conditions

Measurement system

m	1	2	3	4	5	6	7	8	9	10	11	12
iX_m	33	33	67	67	25	25	75	75	40	60	40	60
iY_m	33	67	33	67	25	75	25	75	60	40	40	60
σ_m	0.7	7.	3.5	7.	7.	14.	7.	3.5	7.	3.5	21.	0.7

Assimilation parameter

$$\log_{10} r = -10. \quad p = 0.3$$

Meteorology

$$u = 0.1 \quad v = 0.1 \quad \mu = 0.1$$

Grid domain

$$\mathrm{nT} = 100 \quad T = 1.$$
$$\mathrm{nX} = 100 \quad X = 1.$$
$$\mathrm{nY} = 100 \quad Y = 1.$$

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Measurement system with "big errors"

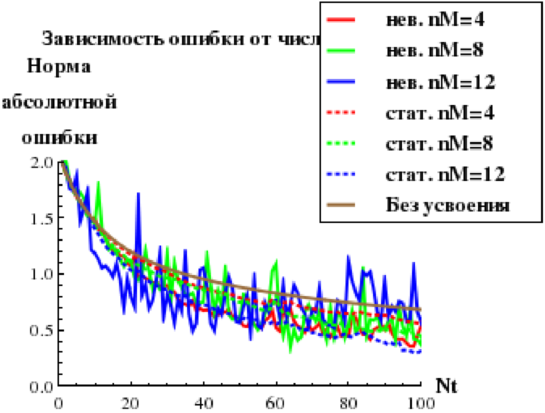

Fig. 9: Solution error WRT measurement device number with "big errors". The more data the better.

Conclusions

- Data assimilation problems are solved with incomplete data and solution interpretation is not obvoius.
- Variational data assimilation algorithms can be categorized as Tikhonov regularization for measurement data inversion problem with models as regularizers.
- Combination of splitting schemes with data assimilation allows to obtain computationally efficient algorithms. Their performance is confirmed with numerical experiments.

Acknowledgements

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Main data assimilation approaches

- Stochastic-dynamics approach (statistical parameter estimation) [Ghil, Malanotte-Rizzoli,1991] et.al.
  - Kalman-type filters (Gussian distributions parameters are evaluated with measurement data).
  - Particle filters (measurement data are used to weight ensemble members) [review by van Leeuwen,2009].
- Variational (data assimilation problem solution is sought as the minimum of a functional) [В.В.Пененко, Образцов, 1976], [Le Dimet, Talagrand, 1986], [Talagrand, Courtirer, 1987], [Rabier et al., 2001], [Shutyaev,2001], [Agoshkov,Ipatova,2006] et al.
  - 3D-4DVAR (data assimilation window).
  - Trajectory tracking (strong/weak-constrained).
  - ...
- Hybrid approaches EnVar и т.д.

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