Optimal solution error analysis in variational data assimilation

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Statement of the problem

Consider the *mathematical model* of a physical process that is described by the evolution problem

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi) + f, & t \in (0, T) \\ \varphi\big|_{t=0} = u, \end{cases} \tag{1.1}$$

where $\varphi = \varphi(t)$ is the unknown function belonging for any t to a Hilbert space X, $u \in X$, F is a nonlinear operator mapping Y into Y, with $Y = L_2(0, T; X)$, $\| \cdot \|_Y = (\cdot, \cdot)_Y^{1/2}$, $f \in Y$.

Let us introduce the *functional*

$$S(u) = \frac{1}{2}(V_1(u - u_0), u - u_0)_X + \frac{1}{2}(V_2(C\varphi - \varphi_{obs}), C\varphi - \varphi_{obs})_{Y_{obs}}, \tag{1.2}$$

where $u_0 \in X$ is a prior initial-value function (background state), $\varphi_{obs} \in Y_{obs}$ is a prescribed function (observational data), Y_{obs} is a Hilbert space (observation space), $C : Y \longrightarrow Y_{obs}$ is a linear bounded operator, $V_1 : X \longrightarrow X$ and $V_2 : Y_{obs} \longrightarrow Y_{obs}$ are symmetric positive definite operators.

Data assimilation problem

Data assimilation problem: find $u \in X$ and $\varphi \in Y$ such that

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi) + f, \quad t \in (0,T) \\ \varphi\big|_{t=0} = u, \\ S(u) = \inf_v S(v). \end{cases} \tag{1.3}$$

The necessary optimality condition reduces the problem (1.3) to the following system :

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = F(\varphi) + f, \quad t \in (0,T) \\ \varphi\big|_{t=0} = u, \end{cases} \tag{1.4}$$

$$\begin{cases} -\dfrac{\partial \varphi^*}{\partial t} - (F'(\varphi))^* \varphi^* = -C^* V_2 (C\varphi - \varphi_{obs}), \quad t \in (0,T) \\ \varphi^*\big|_{t=T} = 0, \end{cases} \tag{1.5}$$

$$V_1(u - u_0) - \varphi^*\big|_{t=0} = 0 \tag{1.6}$$

with the unknowns φ, φ^*, u, where $(F'(\varphi))^*$ is the adjoint to the Frechet derivative of F.

Errors

Suppose that $u_0 = \bar{u} + \xi_1,\ \varphi_{obs} = C\bar{\varphi} + \xi_2$, where $\xi_1 \in X,\ \xi_2 \in Y_{obs}$, and $\bar{\varphi}$ is the ("true") solution to the problem (1.1) with $u = \bar{u}$:

$$\begin{cases} \dfrac{\partial \bar{\varphi}}{\partial t} & = & F(\bar{\varphi}) + f, \quad t \in (0, T) \\ \bar{\varphi}\big|_{t=0} & = & \bar{u}. \end{cases} \tag{1.7}$$

The functions ξ_1, ξ_2 may be treated as the errors of the input data u_0, φ_{obs} (background and observation errors, respectively). For V_1 and V_2 in (1.2), we consider

$$V_1 = V_{\xi_1}^{-1}, \quad V_2 = V_{\xi_2}^{-1},$$

where V_{ξ_i} is the covariance operator of the corresponding error ξ_i, i.e.

$$V_{\xi_1} \cdot = E[(\cdot, \xi_1)_X \xi_1], \quad V_{\xi_2} \cdot = E[(\cdot, \xi_2)_{Y_{obs}} \xi_2],$$

where E is the expectation. If ξ is a vector, then the covariance matrix is defined by $V_\xi = E[\xi \xi^T]$.

Error analysis via Hessian

The system (1.4)–(1.6) with the three unknowns φ, φ^*, u may be treated as an operator equation of the form

$$\mathcal{F}(U, U_d) = 0, \tag{2.1}$$

where $U = (\varphi, \varphi^*, u),\ U_d = (u_0, \varphi_{obs}, f)$.
The following equality holds for the "exact solution" ("true state"):

$$\mathcal{F}(\bar{U}, \bar{U}_d) = 0, \tag{2.2}$$

with $\bar{U} = (\bar{\varphi}, \bar{\varphi}^*, u),\ \bar{U}_d = (\bar{u}, C\bar{\varphi}, f),\ \bar{\varphi}^* = 0$. The system (2.2) is the necessary optimality condition of the following minimization problem: find u and φ such that

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} & = & F(\varphi) + f, \quad t \in (0, T) \\ \varphi\big|_{t=0} & = & u, \\ \bar{S}(u) & = & \inf\limits_{v} \bar{S}(v), \end{cases}$$

where

$$\bar{S}(u) = \frac{1}{2}(V_1(u - \bar{u}), u - \bar{u})_X + \frac{1}{2}(V_2(C\varphi - C\bar{\varphi}), C\varphi - C\bar{\varphi})_{Y_{obs}}.$$

System for errors

From (2.1)–(2.2), we get

$$\mathcal{F}(U, U_d) - \mathcal{F}(\bar{U}, \bar{U}_d) = 0. \tag{2.3}$$

Let $\delta U = U - \bar{U}, \; \delta U_d = U_d - \bar{U}_d$. Then (2.3) gives

$$\mathcal{F}(\bar{U} + \delta U, \bar{U}_d + \delta U_d) - \mathcal{F}(\bar{U}, \bar{U}_d) = 0. \tag{2.4}$$

Let $\delta\varphi = \varphi - \bar{\varphi}, \; \delta u = u - \bar{u}$; then $\delta U = (\delta\varphi, \varphi^*, \delta u), \; \delta U_d = (\xi_1, \xi_2, 0)$. From (2.4), for regular F, there exists $\tilde{\varphi} = \bar{\varphi} + \tau(\varphi - \bar{\varphi}), \; \tau \in [0, 1]$, such that equation (2.4) is equivalent to the system:

$$\left\{ \begin{array}{rcl} \dfrac{\partial \delta\varphi}{\partial t} - F'(\tilde{\varphi})\delta\varphi & = & 0, \quad t \in (0, T), \\ \delta\varphi|_{t=0} & = & \delta u, \end{array} \right. \tag{2.5}$$

$$\left\{ \begin{array}{rcl} -\dfrac{\partial \varphi^*}{\partial t} - (F'(\varphi))^* \varphi^* & = & -C^* V_2 (C\delta\varphi - \xi_2), \\ \varphi^* \big|_{t=T} & = & 0, \end{array} \right. \tag{2.6}$$

$$V_1(\delta u - \xi_1) - \varphi^*|_{t=0} = 0. \tag{2.7}$$

Equivalent system

The system (2.5)–(2.7) may be written in the form:

$$\begin{cases} \dfrac{\partial \delta\varphi}{\partial t} - F'(\bar{\varphi})\delta\varphi = \xi_3, \quad t \in (0,T), \\ \delta\varphi|_{t=0} = \delta u, \end{cases} \tag{2.8}$$

$$\begin{cases} -\dfrac{\partial \varphi^*}{\partial t} - (F'(\bar{\varphi}))^*\varphi^* = -C^* V_2 (C\delta\varphi - \xi_2) + \xi_4, \\ \varphi^*\big|_{t=T} = 0, \end{cases} \tag{2.9}$$

$$V_1(\delta u - \xi_1) - \varphi^*|_{t=0} = 0, \tag{2.10}$$

where

$$\xi_3 = [F'(\tilde{\varphi}) - F'(\bar{\varphi})]\delta\varphi, \;\; \xi_4 = [(F'(\varphi))^* - (F'(\bar{\varphi}))^*]\varphi^*.$$

Hessian

$$\begin{cases} \dfrac{\partial \delta\varphi}{\partial t} - F'(\bar{\varphi})\delta\varphi = 0, \quad t \in (0,T) \\ \delta\varphi\big|_{t=0} = \delta u \\ S_1(\delta u) = \inf\limits_{v} S_1(v), \end{cases} \tag{2.11}$$

$$S_1(\delta u) = \frac{1}{2}(V_1(\delta u - \xi_1), \delta u - \xi_1)_X + \frac{1}{2}(V_2(C\delta\varphi - \xi_2), C\delta\varphi - \xi_2)_{Y_{obs}}. \tag{2.12}$$

Consider the Hessian H of the functional (2.12); it is defined by the formulas:

$$\begin{cases} \dfrac{\partial \psi}{\partial t} - F'(\bar{\varphi})\psi = 0, \; t \in (0,T), \\ \psi|_{t=0} = v, \end{cases} \tag{2.13}$$

$$\begin{cases} -\dfrac{\partial \psi^*}{\partial t} - (F'(\bar{\varphi}))^*\psi^* = -C^*V_2C\psi, \quad t \in (0,T) \\ \psi^*\big|_{t=T} = 0, \end{cases} \tag{2.14}$$

$$Hv = V_1 v - \psi^*|_{t=0}. \tag{2.15}$$

Error equation

Below we introduce four auxiliary operators R_1, R_2, R_3, R_4. Let $R_1 = V_1$. For example, the operator $R_2 : Y_{obs} \longrightarrow X$ acts on the functions $g \in Y_{obs}$ according to the formula $R_2 g = \theta^*|_{t=0}$, where θ^* is the solution to the adjoint problem

$$\left\{ \begin{array}{rcl} -\dfrac{\partial\theta^*}{\partial t} - (F'(\bar{\varphi}))^*\theta^* & = & C^* V_2 g, \quad t \in (0,T) \\ \theta^*\big|_{t=T} & = & 0. \end{array} \right. \tag{2.16}$$

From (2.13)–(2.15) we conclude that the system (2.19)–(2.21) is equivalent to the single equation for δu:

$$H\delta u = R_1\xi_1 + R_2\xi_2 + R_3\xi_3 + R_4\xi_4. \tag{2.17}$$

The Hessian H acts in X as a self-adjoint operator with domain of definition $D(H){=}X$. Moreover, due to V_1, V_2, the operator H is positive definite. Hence,

$$\delta u = T_1\xi_1 + T_2\xi_2 + T_3\xi_3 + T_4\xi_4,$$

where $T_i = H^{-1}R_i, i = 1, 2, 3, 4.$

Approximation

Since $\tilde{\varphi} = \bar{\varphi} + \tau\delta\varphi,\ \varphi = \bar{\varphi} + \delta\varphi$, we assume that $T_3\xi_3 \approx 0,\ T_4\xi_4 \approx 0$. Then

$$\delta u = T_1\xi_1 + T_2\xi_2, \tag{2.18}$$

and (2.5)–(2.7) reduces to the auxiliary DA problem:

$$\begin{cases} \dfrac{\partial\delta\varphi}{\partial t} - F'(\bar{\varphi})\delta\varphi &= 0, \quad t \in (0,T), \\ \delta\varphi|_{t=0} &= \delta u, \end{cases} \tag{2.19}$$

$$\begin{cases} -\dfrac{\partial\varphi^*}{\partial t} - (F'(\bar{\varphi}))^*\varphi^* &= -C^*V_2(C\delta\varphi - \xi_2), \\ \varphi^*\big|_{t=T} &= 0, \end{cases} \tag{2.20}$$

$$V_1(\delta u - \xi_1) - \varphi^*|_{t=0} = 0. \tag{2.21}$$

The problem (2.19)–(2.21) is a linear data assimilation problem; with the fixed $\bar{\varphi}$ it is the necessary optimality condition to the following minimization problem: find u and φ such that (2.11) is satisfied.

Sensitivity coefficients

Since $\delta u = T_1\xi_1 + T_2\xi_2$ for $T_i = H^{-1}R_i$, the *sensitivity coefficients* are defined by

$$r_i = \sqrt{\|T_i^* T_i\|}.$$

For $V_1 = \alpha E,\ V_2 = E$ we have for r_1:

$$r_1 = \sqrt{\|T_1^* T_1\|} = \frac{\alpha}{\mu_{\min}}. \tag{2.22}$$

The singular values σ_k^2 and the corresponding orthonormal (right) singular vectors $w_k \in Y_{obs}$ of the operator T_2 are defined by the formulas (Le Dimet, Shutyaev, 2005):

$$\sigma_k^2 = \frac{\mu_k - \alpha}{\mu_k^2}, \quad w_k = \frac{1}{\sqrt{\mu_k - \alpha}} C^h \varphi_k, \tag{2.23}$$

where μ_k are the eigenvalues of the Hessian H, and φ_k are the fundamental control functions, and

$$r_2 = \max_k \frac{\sqrt{\mu_k - \alpha}}{\mu_k}. \tag{2.24}$$

Covariance operators

Consider the error equation (2.18). Since H is invertible, we get

$$\delta u = T_1 \xi_1 + T_2 \xi_2, \tag{3.1}$$

where $T_i{=}H^{-1}R_i,\ T_1 : X{\rightarrow}X,\ T_2 : Y_{obs}{\rightarrow}X$. We suppose that the errors ξ_1, ξ_2 are normally distributed, unbiased, and mutually uncorrelated. By V_{ξ_i} we denote the covariance operator of the corresponding error $\xi_i,\ i = 1, 2$, i.e. $V_{\xi_1}\cdot = E[(\cdot, \xi_1)_X \xi_1]$, $V_{\xi_2}\cdot = E[(\cdot, \xi_2)_{Y_{obs}} \xi_2]$, where E is the expectation. By $V_{\delta u}$ we denote the covariance operator of the optimal solution (analysis) error: $V_{\delta u}\cdot = E[(\cdot, \delta u)_X \delta u]$. From (3.1) we get

$$V_{\delta u} = T_1 V_{\xi_1} T_1^* + T_2 V_{\xi_2} T_2^*. \tag{3.2}$$

To find the covariance operator $V_{\delta u}$, we need to construct the operators $T_i V_{\xi_i} T_i^*,\ i = 1, 2$. Consider the operator $T_1 V_{\xi_1} T_1^*$. Since $T_1 = H^{-1}R_1 = H^{-1}V_1 = T_1^*$, we have $T_1 V_{\xi_1} T_1^* = H^{-1}V_1 V_{\xi_1} V_1 H^{-1}$. Moreover, if $V_1 = V_{\xi_1}^{-1}$, then

$$T_1 V_{\xi_1} T_1^* = H^{-1} V_1 H^{-1} = H^{-1} V_{\xi_1}^{-1} H^{-1}. \tag{3.3}$$

Operator R_2^*

Consider the operator $T_2 V_{\xi_2} T_2^*$. Since $T_2 = H^{-1} R_2$, then

$$T_2 V_{\xi_2} T_2^* = H^{-1} R_2 V_{\xi_2} R_2^* H^{-1}.$$

To determine R_2^*, consider the inner product $(R_2 g, p)_X,\ g \in Y_{obs}, p \in X$. From (**??**)–(2.16),

$$(R_2 g, p)_X = (\theta^*|_{t=0}, p)_X = (C^* V_2 g, \phi)_Y = (g, R_2^* p)_{Y_{obs}},$$

where $R_2^* p = V_2 C\phi$, and ϕ is the solution to the problem

$$\begin{cases} \dfrac{\partial \phi}{\partial t} - F'(\bar{\varphi})\phi = 0, \ t \in (0, T), \\ \phi|_{t=0} = p. \end{cases} \tag{3.4}$$

Operator $T_2 V_{\xi_2} T_2^*$

The operator $T_2 V_{\xi_2} T_2^* = H^{-1} R_2 V_{\xi_2} R_2^* H^{-1}$ is defined by successive solutions of the following problems (for a given $v \in X$):

$$Hp = v, \tag{3.5}$$

$$\left\{ \begin{array}{rcl} \dfrac{\partial \phi}{\partial t} - F'(\bar{\varphi})\phi & = & 0,\ t \in (0,T), \\ \phi|_{t=0} & = & p, \end{array} \right. \tag{3.6}$$

$$\left\{ \begin{array}{rcl} -\dfrac{\partial \theta^*}{\partial t} - (F'(\bar{\varphi}))^* \theta^* & = & C^* V_2 V_{\xi_2} V_2 C \phi,\ \ t \in (0,T) \\ \theta^* \big|_{t=T} & = & 0, \end{array} \right. \tag{3.7}$$

$$Hw = \theta^* \big|_{t=0}, \tag{3.8}$$

then

$$T_2 V_{\xi_2} T_2^* v = w. \tag{3.9}$$

If $V_2 = V_{\xi_2}^{-1}$, then $C^* V_2 V_{\xi_2} V_2 C = C^* V_2 C$ and $\theta^* \big|_{t=0} = Hp - V_1 p$.

Optimal solution error covariance

We get

$$R_2 V_{\xi_2} R_2^* = H - V_1$$

and

$$T_2 V_{\xi_2} T_2^* = H^{-1} R_2 V_{\xi_2} R_2^* H^{-1} = H^{-1}(H - V_1)H^{-1}. \tag{3.10}$$

From (3.3), (3.10) it follows the result for $V_{\delta u}$:

$$V_{\delta u} = T_1 V_{\xi_1} T_1^* + T_2 V_{\xi_2} T_2^* = H^{-1} V_1 H^{-1} + H^{-1}(H - V_1)H^{-1}.$$

Therefore

$$V_{\delta u} = H^{-1} H H^{-1} = H^{-1}. \tag{3.11}$$

The last formula gives the analysis-error covariance operator through the Hessian H.

Gejadze, I., Le Dimet, F.-X., Shutyaev, V.P. On analysis error covariances in variational data assimilation. SIAM J. Sci. Comput. (2008), v.30, no.4, 1847-1874.

Numerical algorithm to compute covariances

Consider the covariance operator $V = V_{\delta u}$ defined by (3.11):

$$V = H^{-1}. \tag{4.1}$$

To find the inverse Hessian H^{-1}, the quasi-Newton BFGS method may be used, because it generates an approximation of H^{-1} directly in the course of a minimization process.
Since the Hessian H of the functional S_1 does not depend on functions ξ_1, ξ_2 entering (2.12), we suggest using as follows:

$$\xi_1 = \tilde{u}, \quad \xi_2 = C\delta\tilde{\varphi}, \tag{4.2}$$

where $\delta\tilde{\varphi}$ satisfies the problem

$$\begin{cases} \dfrac{\partial\delta\tilde{\varphi}}{\partial t} - F'(\bar{\varphi})\delta\tilde{\varphi} & = & 0, \; t \in (0,T), \\ \delta\tilde{\varphi}|_{t=0} & = & \tilde{u}. \end{cases} \tag{4.3}$$

In this case, the solution of (2.11) is $\delta u = \tilde{u}$, and $S_1(\tilde{u}) = 0$. The initial guess to start the iterations is $u^0 = 0$.

BFGS method

Applied for solving the auxiliary DA problem (2.11)-(2.12), the BFGS method has the form:

$$d^k = H_k^{-1} S_1'(\delta u^k), \tag{4.4}$$

$$\delta u^{k+1} = \delta u^k - \alpha^k d^k, \tag{4.5}$$

$$H_{k+1}^{-1} = \left(I - \frac{sy^T}{y^T s}\right) H_k^{-1} \left(I - \frac{ys^T}{y^T s}\right) + \frac{ss^T}{y^T s}, \tag{4.6}$$

where $s = \delta u^{k+1} - \delta u^k,\ y = S_1'(\delta u^{k+1}) - S_1'(\delta u^k)$, H_k^{-1} is the approximation to H^{-1} on the k-th iteration, $S_1'(\delta u^k)$ is the value of the gradient of S_1 in δu at the point δu^k, α^k are iterative parameters, I is the identity operator.

Optimal minimization step

Another key point is a need for the exact minimum along the direction of descent to be achieved. Let us denote k the iteration index and d^k the direction of descent built by the minimization algorithm, then the optimal step β^k can be derived from the condition

$$\frac{\partial S_1(\delta u^k + \beta d^k)}{\partial \beta} = 0. \tag{4.7}$$

Applying this condition to (2.12) we obtain as follows

$$\beta = -\frac{(V_1(\delta u^k - \xi_1), d^k)_X + (V_2(C\delta\varphi^k - \xi_2), C\varphi_d)_{Y_{obs}}}{(V_1 d^k, d^k)_X + (V_2 C\varphi_d, C\varphi_d)_{Y_{obs}}}, \tag{4.8}$$

where φ_d and $\delta\varphi^k$ are the solutions of the problem (2.11) for $\delta u = d^k$ and $\delta u = \delta u^k$, respectively.

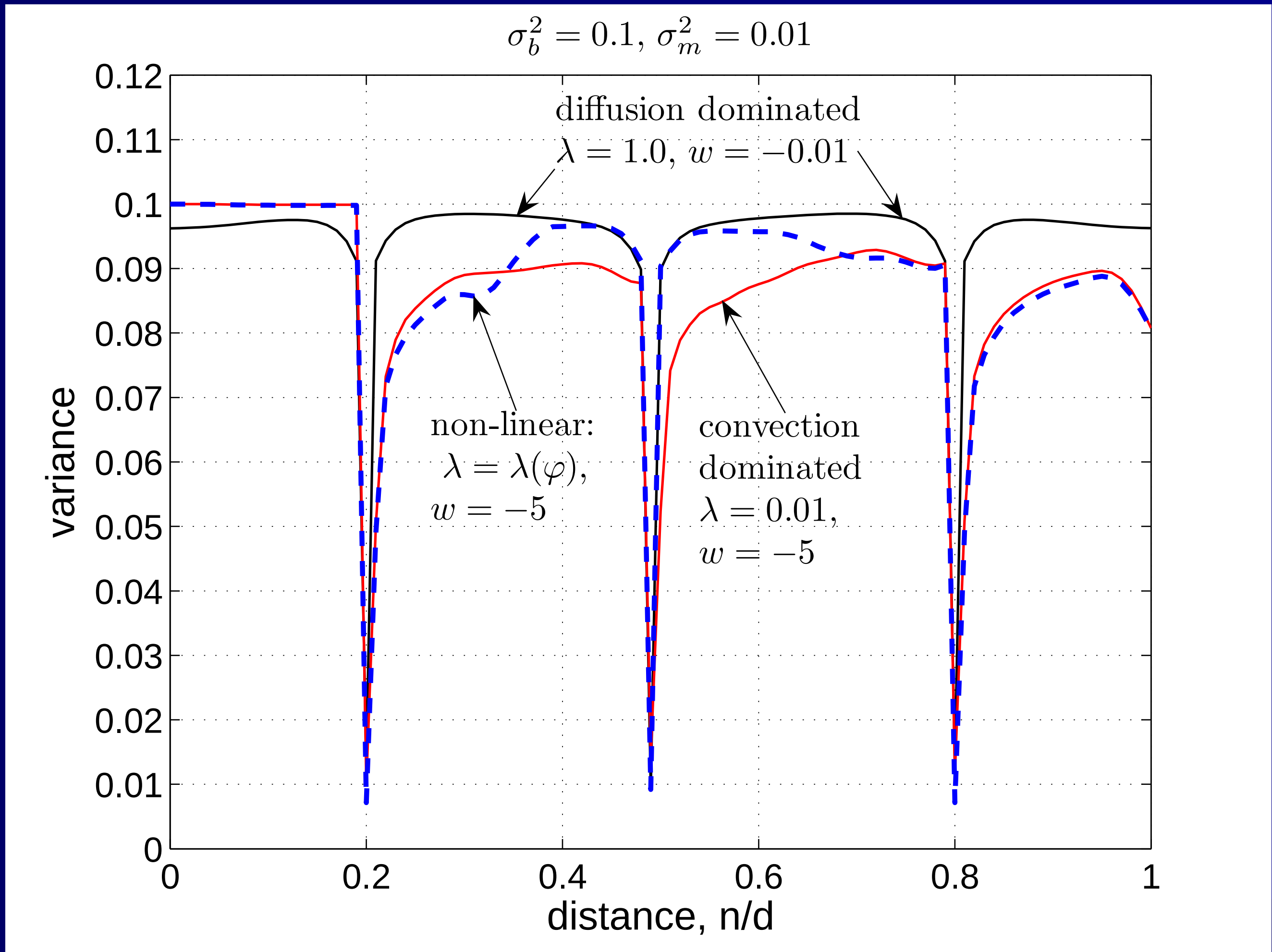
Numerical examples for convection-diffusion model

We assume that the time-continuous measurements of φ are available at the following locations $x_1 = 0.2$, $x_2 = 0.5$, $x_3 = 0.8$. We assume that $\sigma_b^2(x) = diag\left\{V_{\xi_1}\right\} \neq 0$, $\sigma_m^2(x) = diag\left\{V_{\xi_2}\right\} \neq 0$. In Figs. we show the variances $\sigma_a^2(x) = diag\left\{V\right\}$ which correspond to the three cases. We note that the variance basically changes from the background error value $\sigma_b^2(x)$ in the areas where no information is available to the measurement error value $\sigma_m^2(x)$ at the sensor location points. The transition between two levels depends on the transport phenomena supported by the model. In the diffusion dominated case the transition function is quite sharp, since diffusion is a process of dissipation, both applied to the forward and adjoint variables (information). In the convection dominated case one can see that the transition function is less steep in the upwind direction. This shows that the information is delivered to the sensor by convection not being dissipated by diffusion. In the non-linear case we observe a mixed behaviour, where in the areas with weak diffusion it follows the convection dominated pattern, while in the area with strong diffision it follows the diffusion dominated pattern.

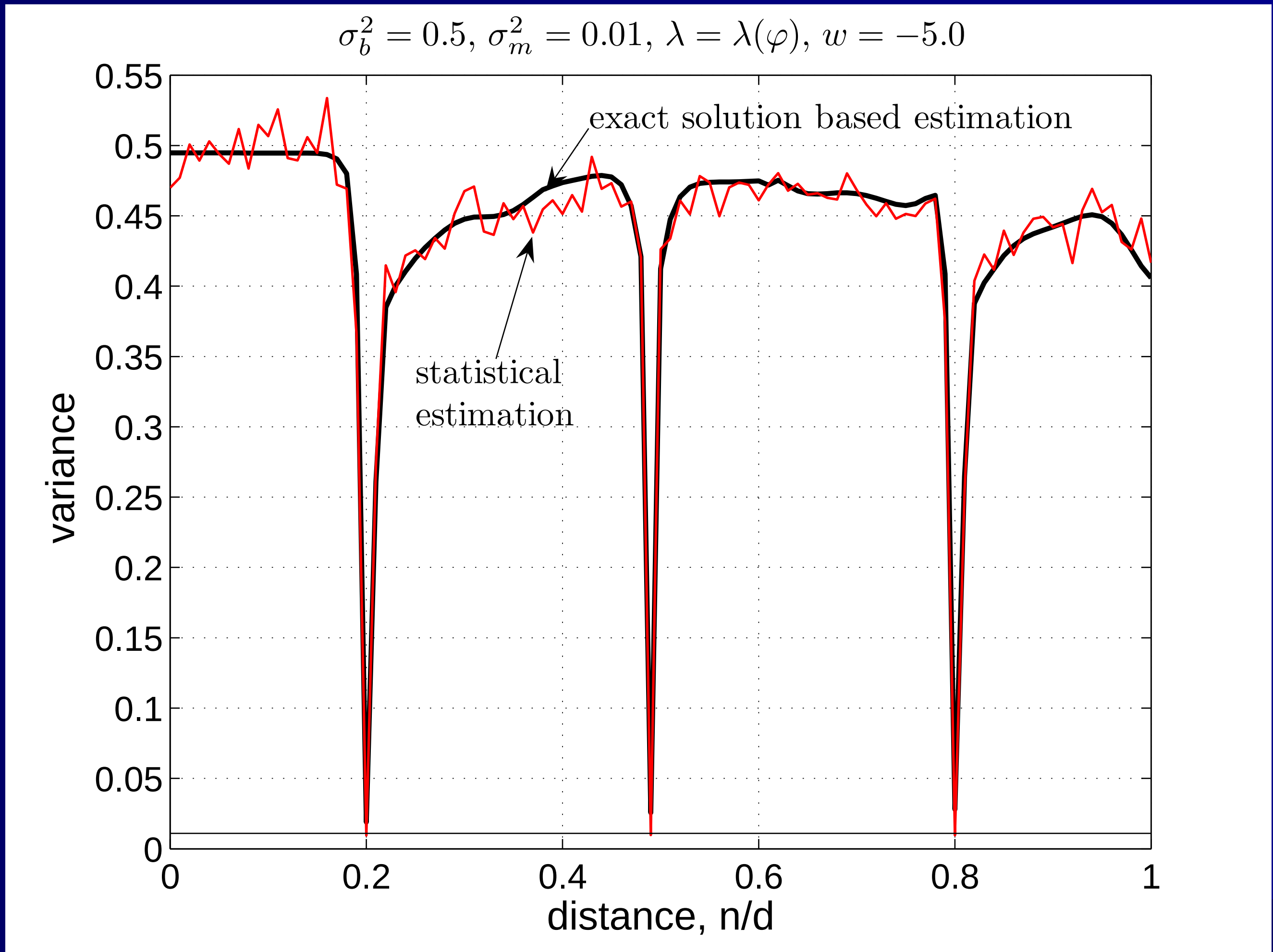
Numerical results

An important result is that H^{-1} built on the exact solution $\tilde{\varphi} = \bar{\varphi}$ by the formulas (2.13)–(2.15) gives the covariance V of the original non-linear problem. In order to validate the latest statement we estimate V using the statistical (ensemble) approach. For a given 'exact solution' $\bar{u}$ we compute $\hat{\varphi} = C\bar{\varphi} + \xi_1$ and $u_b = \bar{u} + \xi_2$, where ξ_1, ξ_2 are normally distributed (Gaussian) random perturbations such that $E[\,\xi_1\xi_1^T\,] = V_{\xi_1}$ and $E[\,\xi_2\xi_2^T\,] = V_{\xi_2}$.
For these data we solve the DA problem and find $\delta u = u - \bar{u}$. The procedure is repeated k times for new values ξ_1, ξ_2 each time to get an ensemble of δu, then the covariance is finally estimated as $V_* = E[\,\delta u \delta u^T\,]$. The results of numerical experiments show that H^{-1} build on the exact solution $\bar{\varphi}$ via the formulas (2.13)–(2.15) matches to the covariance V_* obtained by the statistical method being in satisfactory agreement with the χ^2 distribution. Here the analysis error variances obtained by two methods are presented, while the ensemble size used in the statistical method is $k = 2500$.

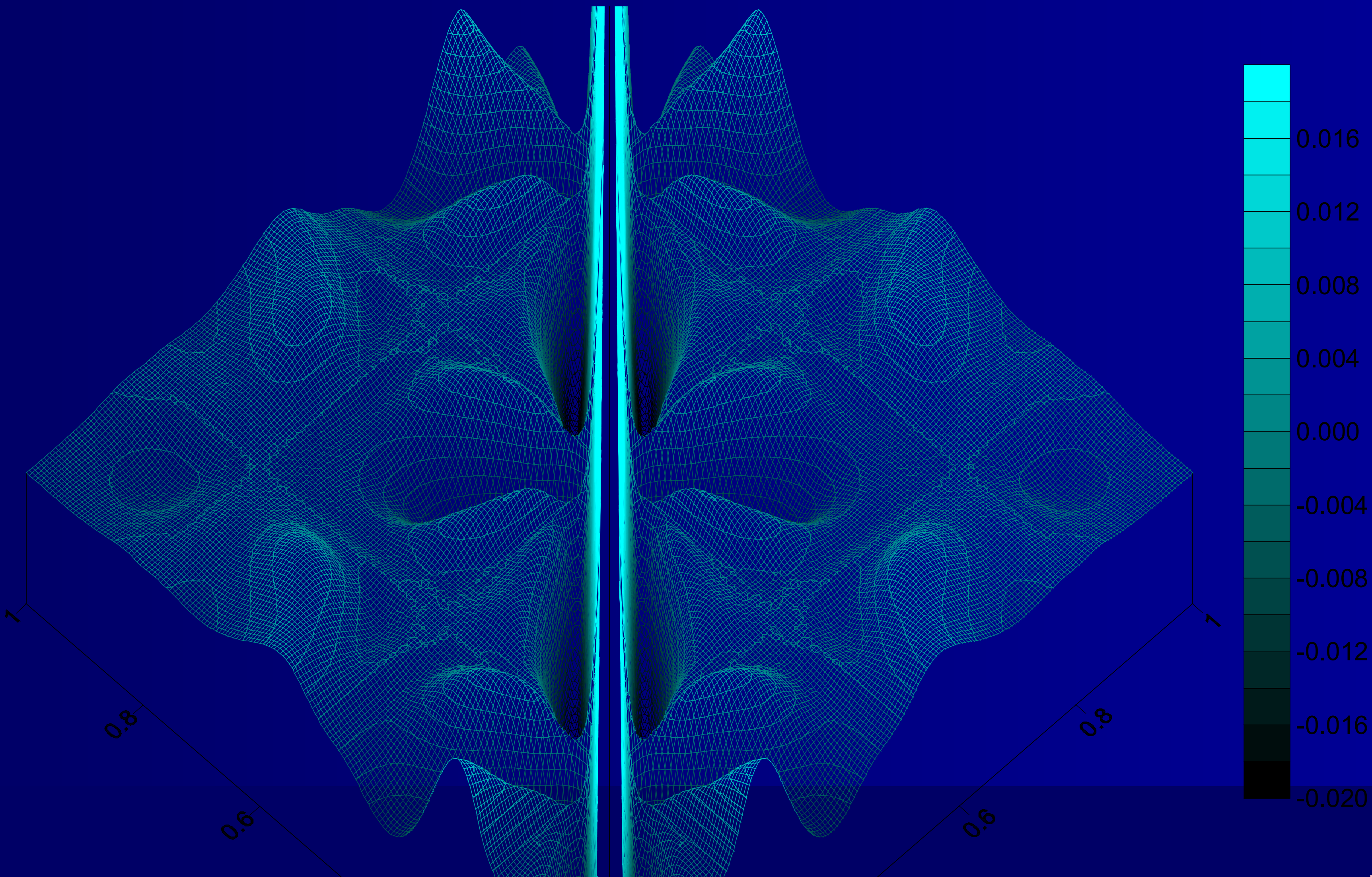
Variance via H^{-1} built on the 'exact' solution



Statistical variance $\sigma_a^2 = diag\{V_*\}$ and variance via H^{-1}



Covariance



0.016
0.012
0.008
0.004
0.000
-0.004
-0.008
-0.012
-0.016
-0.020
1
0.8
0.6
1
0.8
0.6

Conclusions

The error of the optimal initial-value function in variational data assimilation for a nonlinear evolution model may be expressed by an equation through the errors of the input data without the tangent linear hypothesis. The approximation of the error equation allows to derive the analysis error covariance operator which turnes to be the inverse Hessian of the auxiliary (linearized) error assimilation problem. This Hessian does not coincide in general with the Hessian of the original cost functional. With the use of the quasi-Newton BFGS method, a numerical algorithm is developed to compute the analysis error covariance operator as the inverse Hessian. The algorithm is based on a special choice of input functions in the auxiliary data assimilation problem and the analytical step search for the minimization along the direction of descent. This leads to obtain the covariance operator which perfectly matches the one obtained by the statistical (ensemble) method.

Shutyaev, V., Le Dimet, F.-X., Gejadze, I. On optimal solution error covariances in variational data assimilation. Russ. J. Numer. Anal. Math. Modelling (2008), v.23, no.2, 197-206.

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On optimal solution error in variational data assimilation for the sea thermodynamics model

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Thermodynamics equations

$$T_t + (U, Grad)T - Div(\hat{a}_T \cdot Grad\ T) = f_T \ in\ D \times (t_0, t_1),$$

$$T = T_0 \text{ for } t = t_0 \ on\ D,$$

$$-\nu_T \frac{\partial T}{\partial z} = Q \text{ on } \Gamma_S \times (t_0, t_1),$$

$$\frac{\partial T}{\partial N_T} = 0 \text{ on } \Gamma_{w,c} \times (t_0, t_1),$$

$$U_n^{(-)} T + \frac{\partial T}{\partial N_T} = U_n^{(-)} d_T + Q_T \text{ on } \Gamma_{w,op} \times (t_0, t_1),$$

$$\frac{\partial T}{\partial N_T} = 0 \text{ on } \Gamma_H \times (t_0, t_1).$$

Operator formulation of the forward problem

$$T_t + LT = F + BQ, \quad t \in (t_0, t_1),$$
$$T = T_0, \quad \text{for} \quad t = t_0,$$

in a week sense:

$$(T_t, \hat{T}) + (LT, \hat{T}) = F(\hat{T}) + (BQ, \hat{T}) \quad \forall \hat{T} \in W_2^1(D),$$

and *L, F, B,* are defined by

$$(LT, \hat{T}) \equiv \int_D (-TDiv(\overline{U}\hat{T})) + \int_{\Gamma_{w,op}} \overline{U}_n^{(+)} T\hat{T} d\Gamma + \int_D \hat{a}_T Grad(T) \cdot Grad(\hat{T}) dD,$$

$$F(\hat{T}) = \int_{\Gamma_{w,op}} (Q_T + \overline{U}_n^{(-)} d_T)\hat{T} dT + \int_D f_T \hat{T} dD, \;\; (T_t, \hat{T}) = \int_D T_t \hat{T} dD, \;\; (BQ, \hat{T}) = \int_\Omega Q\hat{T}\,|_{z=0}\, d\Omega.$$

SST data assimilation problem

$$\begin{cases} T_t + LT & = & F + BQ \quad \text{in } D \times (t_0, t_1), \\ T & = & T_0 \quad \text{for } t = t_0, \\ J(Q) & = & \inf_Q J(Q), \end{cases}$$

$$J(Q) = \frac{1}{2}\int_{t_0}^{t_1}\int_{\Omega} \alpha \,|\, Q - Q^{(0)} \,|^2 \, d\Omega dt + \frac{1}{2}\int_{t_0}^{t_1}\int_{\Omega} m_0 \,|\, T|_{z=0} - T_{\text{obs}} \,|^2 \, d\Omega dt.$$

The optimality system:

$$T_t + LT = F + BQ \quad \text{in} \quad D \times (t_0, t_1),$$

$$T = T_0 \quad \text{for} \quad t = t_0,$$

$$-(T^*)_t + L^* T^* = B^* m_0 (T - T_{\text{obs}}) \quad \text{in} \quad D \times (t_0, t_1),$$

$$T^* = 0 \quad \text{for} \quad t = t_1,$$

$$\alpha (Q - Q^{(0)}) + T^* = 0 \quad \text{on} \quad \Omega \times (t_0, t_1),$$

Input errors

$$Q^{(0)} = \overline{Q} + \xi_1, \quad T_{obs} = \overline{T}|_{z=0} + \xi_2,$$

where $\delta T = T - \overline{T}, \delta Q = Q - \overline{Q}$ and

$$\overline{T}_t + L\overline{T} = F + B\overline{Q} \quad \text{in} \quad D \times (t_0, t_1),$$

$$\overline{T} = T_0 \quad \text{for} \quad t = t_0.$$

System for the errors

$$\delta T_t + L'(\bar{T})\delta T = B\delta Q \quad \text{in} \;\; D\times(t_0, t_1),$$

$$\delta T = 0 \quad \text{for} \;\; t = t_0,$$

$$-(T^*)_t + (L'(\bar{T}))^* T^* = B^* m_0(\delta T - \xi_2) \;\; \text{in} \;\; D\times(t_0, t_1),$$

$$T^* = 0 \quad \text{for} \;\; t = t_1,$$

$$\alpha(\delta Q - \xi_1) + T^* = 0 \quad \text{on} \;\; \Omega\times(t_0, t_1).$$

Auxiliary minimization problem

$$\begin{cases} \delta T_t + L'(\bar{T})\delta T & = & B\delta Q \quad \text{in } D \times (t_0, t_1), \\ \delta T & = & 0 \quad \text{for } t = t_0, \\ S(\delta Q) & = & \inf\limits_{Q} S(Q), \end{cases}$$

$$S(\delta Q) = \frac{1}{2}\int_{t_0}^{t_1}\int_{\Omega} \alpha \,|\, \delta Q - \xi_1 |^2 \, d\Omega dt + \frac{1}{2}\int_{t_0}^{t_1}\int_{\Omega} m_0 \,|\, \delta T|_{z=0} - \xi_2 |^2 \, d\Omega dt.$$

Hessian of the functional S

$$\psi_t + L'(\bar{T})\psi = Bv \quad \text{in} \quad D \times (t_0, t_1),$$

$$\psi = 0 \quad \text{for} \quad t = t_0,$$

$$-(\psi^*)_t + (L'(\bar{T}))^* \psi^* = B^* m_0 \psi \quad \text{in} \quad D \times (t_0, t_1),$$

$$\psi^* = 0 \quad \text{for} \quad t = t_1,$$

$$Hv = \alpha v + \psi^* \quad \text{on} \quad \Omega \times (t_0, t_1).$$

Error control equation

$$H\,\delta Q = R_1\xi_1 + R_2\xi_2\,.$$

$$R_1 = \alpha E,\; R_2\xi_2 = \theta^*\big|_{z=0},$$

$$-(\theta^*)_t + (L'(\bar{T}))^*\theta^* = B^* m_0 \xi_2 \quad \text{in } D\times(t_0,t_1),$$
$$\theta^* = 0 \quad \text{for } t = t_1.$$

The optimal solution error:

$$\delta Q = T_1\xi_1 + T_2\xi_2, \qquad T_1 = H^{-1}R_1,\, T_2 = H^{-1}R_2\,.$$

Sensitivity coefficients

$$r_1 = \sqrt{\left\| T_1^{*} T_1 \right\|}, \quad r_2 = \sqrt{\left\| T_2^{*} T_2 \right\|}$$

$$r_1 = \frac{\alpha}{\mu_{\min}}, \qquad r_2 = \sqrt{\left\| (H - \alpha E) H^{-2} \right\|}.$$

Fundamental control functions

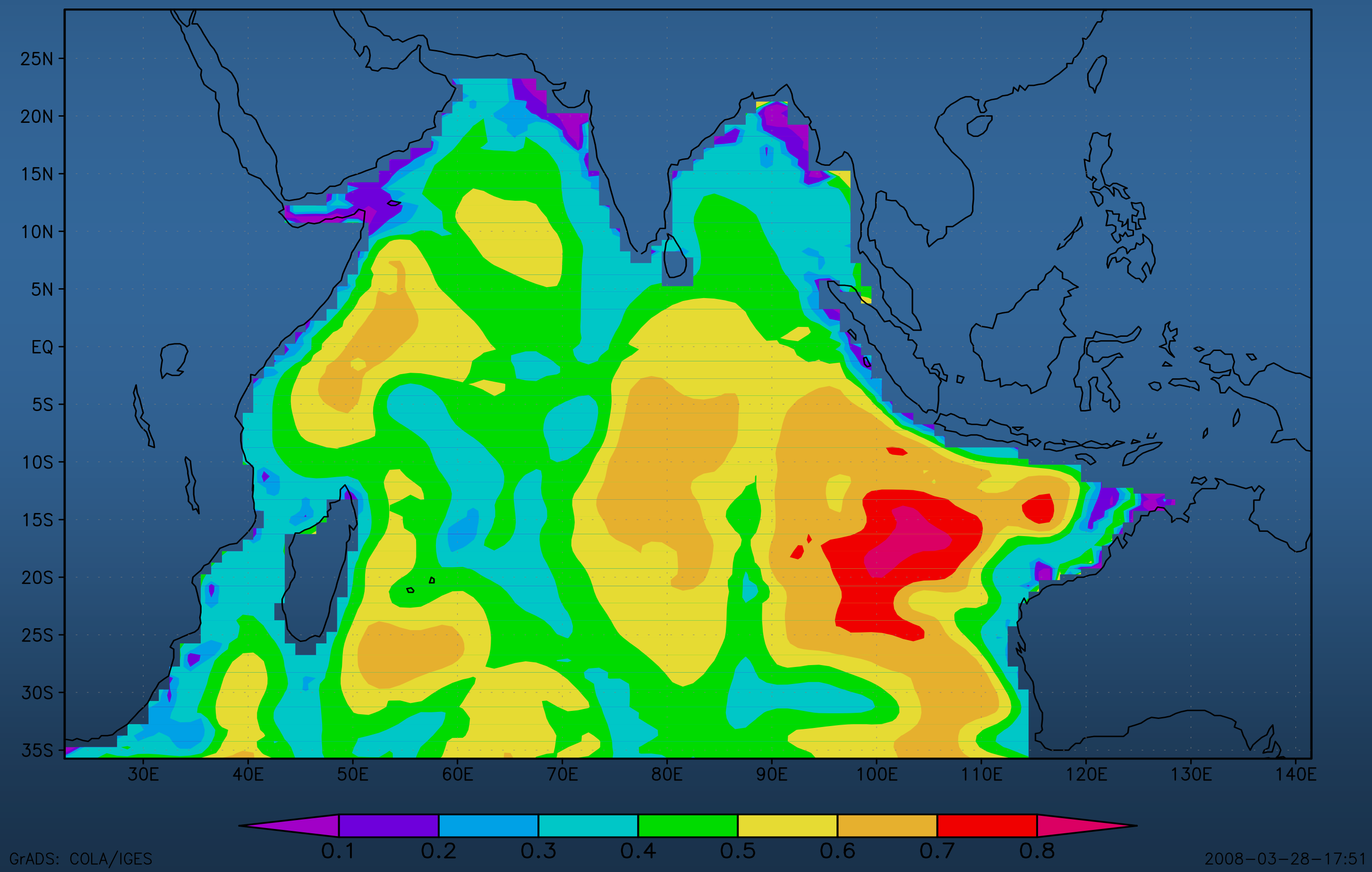
$$(\varphi_k)_t + L\varphi_k = Bv_k \quad \text{in} \quad D\times(t_0,t_1),$$
$$\varphi_k = 0 \quad \text{for} \quad t = t_0,$$

$$-(\varphi_k^*)_t + L^*\varphi_k^* = B^* m_0 \varphi_k \quad \text{in} \quad D\times(t_0,t_1),$$
$$\varphi_k^* = 0 \quad \text{for} \quad t = t_1,$$
$$\alpha v_k + \varphi_k^* = \mu_k v_k \quad \text{on} \quad \Omega\times(t_0,t_1).$$

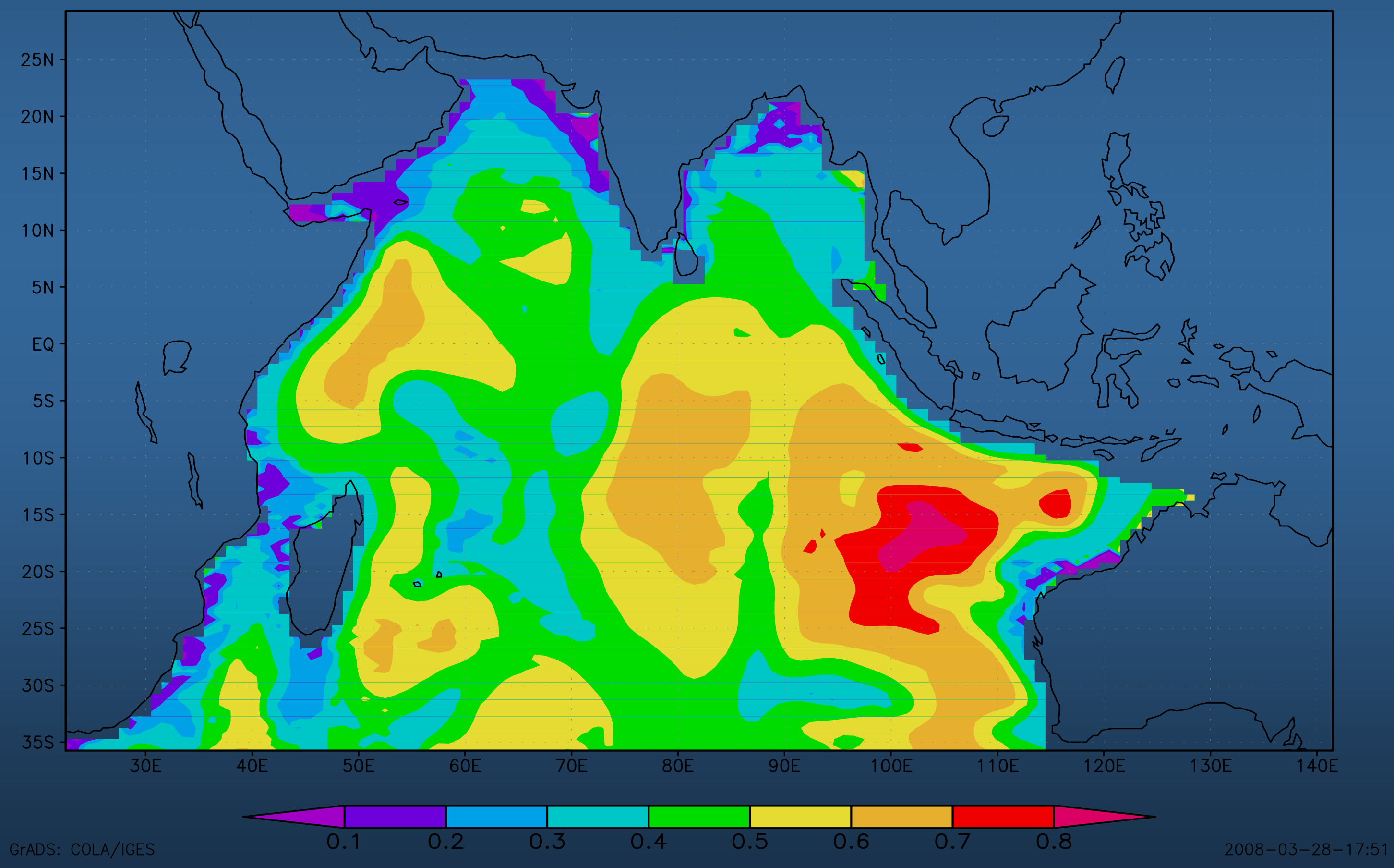
Singular vectors:

$$T_2^* T_2 w_k = \sigma_k^2 w_k, \quad w_k = \frac{1}{\sqrt{\mu_k - \alpha}} \varphi_k \big|_{z=0}, \qquad k = 1,2,\ldots \; \sigma_k^2 = \frac{\mu_k - \alpha}{\mu_k^2}.$$

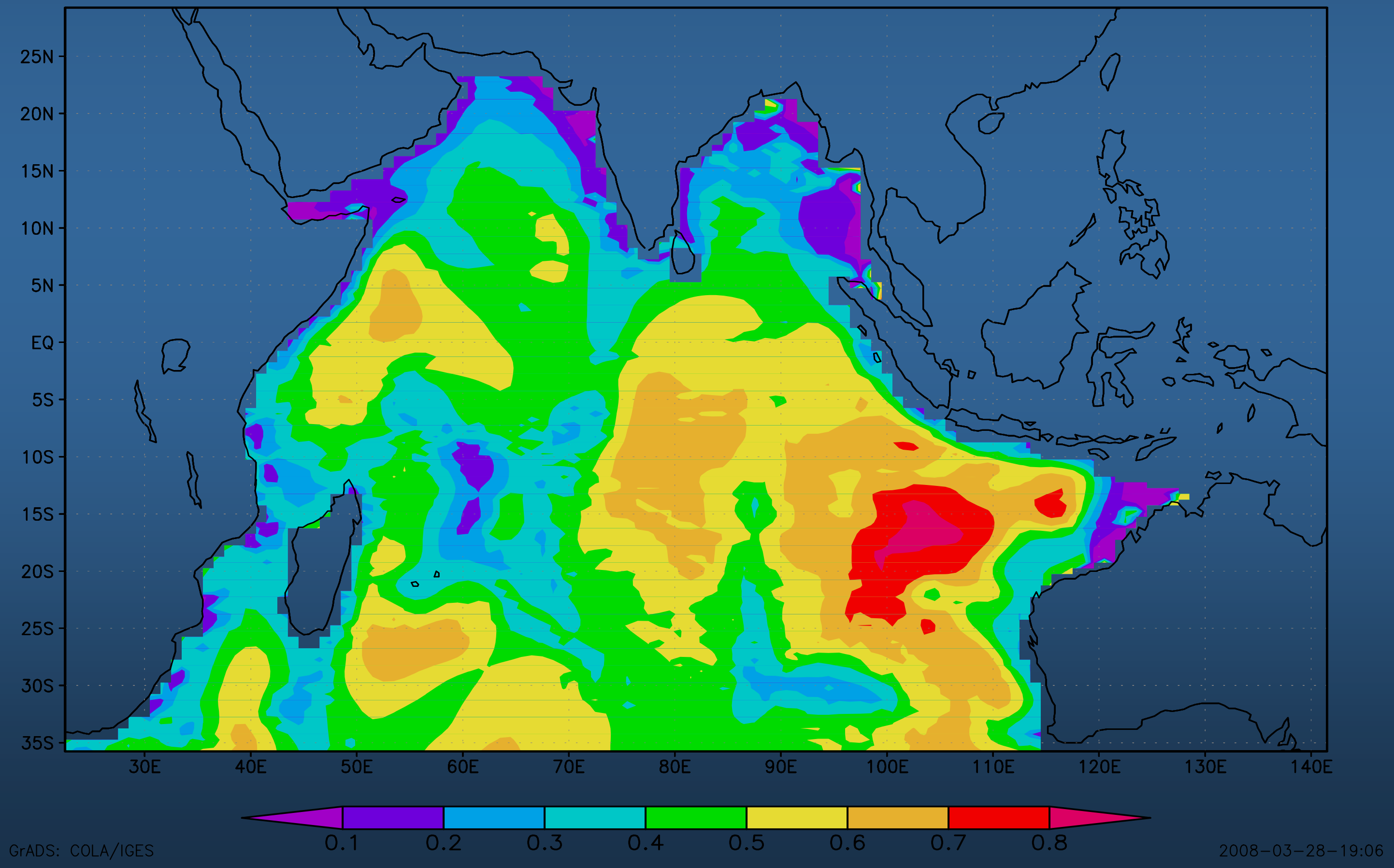
Numerical examples (Indian Ocean, t=24h)



Numerical examples (Indian Ocean, t=240h)



Numerical examples (Indian Ocean, t=1month)



Thank you for your attention!