Validation of a PETSc based software implementing a 4DVAR Data Assimilation algorithm: a case study related with an Oceanic Model based on Shallow Water equation

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1 Definition of the DA problem and description of the PETSc based software implementation

The considered software intends to solve the problem defined on a suitable domain decomposition

\[ DD(\Delta \times \Omega) = \{\Delta_j \times \Omega_h\}_{j,h} \]

of time-space domain \( \Delta \times \Omega \) as described in Definition 1 (all the needed notations can be founded in [2]).

Definition 1 (The 4D-VAR DA problem defined on the domain decomposition \( DD(\Delta \times \Omega) \) - the 4D-VAR DD-DA problem). The 4D Variational DD-DA problem consists in computing the vector \( \tilde{x}_j^{DA} \) such that

\[ \tilde{x}_j^{DA} = \sum_{j,h} EO_{jh}(x_j^{DA}) \]  

where

\[ x_j^{DA} = \arg\min_{x_j} J_{jh}(u_{jh}), \]  

where the operator \( J_{jh} \) (the local 4D-VAR regularization functional) is defined as follows:

\[ J_{jh}(x_{jh}) = RO_{jh}[J] + \mu O_{ijk}(x_{ijk}), \]  

and where \( O_{ijk}(x_{ijk}) \) is a suitably defined operator on the overlapped domain \( \Delta_{ij} \times \Omega_{ik} \). Parameter \( \mu \) is a regularization parameter. The 4-D-VAR regularization functional \( J \) is defined as:

\[ J(x) = \| x - x_b \|_B^{-1} + \lambda \sum_{k=0}^{nt_{obs}-1} \| H_{tk}(M_{i0\rightarrow tk}[x]) - v_k \|_R^{-1} \]  

where \( \lambda \) is a regularization parameter, \( B \) and \( R_k \) (\( k = 0, \ldots, nt_{obs} - 1 \)) are the covariance matrices of the errors on the background and the observations respectively, while \( \| \cdot \|_B^{-1} \) and \( \| \cdot \|_R^{-1} \) denote the weighted euclidean norm.

The 4D-VAR DD-DA problem solution is computed performing the following steps on each subdomains \( \Delta_j \times \Omega_h \) (the so called 4D-VAR DD-DA algorithm):

- **Locally** compute all the parameters that define the local 4D-VAR regularization functional \( J_{jh} \)
- **Locally** compute the minimum \( x_j^{DA} \) (needed values for overlapping regions are obtained when necessary - i.e., for the model local evolution)
- **Globally** contribute to computation of \( x_j^{DA} \)

In order to compute the minimum of all the functionals \( J_{jh} \), the DD-DA algorithm has to face with some issues. In more details, we have to address:
the linearization of the operator \( M_{t-\Delta t \rightarrow t} \), let us say \( M_{t-\Delta t} \), used for the evaluations of \( J_{jh} \) required by the minimisation algorithm;

- the evaluation of the adjoint operator of \( M_{t-\Delta t} \), let us say \( M_{t-\Delta t}^* \), used for the evaluation of \( \nabla J_{jh} \) required by the minimisation algorithm;

Both the points above should require the computation of the discretization of the Jacobian of \( M_{t-\Delta t \rightarrow t} \):

\[ \nabla M_{t-\Delta t \rightarrow t} \]

Following some details about software implementation in PETSc (Portable, Extensible Toolkit for Scientific Computation) environment. To implement the entire algorithm we plan to use:

1. the PETSc time steppers \texttt{TS} module for solving time-dependent (nonlinear) PDEs, including the computation of adjoint;

2. the PETSc \texttt{DM} module which is a powerful tool for the management of all mesh data related with domain decomposition;

3. The TAO software library [8] for the computation of [2]. The Toolkit for Advanced Optimization (TAO) is aimed at the solution of large-scale optimization problems on high-performance architectures. TAO is suitable for both single-processor and massively-parallel architectures. The current version of TAO has algorithms for unconstrained and bound-constrained optimization.

4. The SLEPc software library [9] for the computation of spectral decomposition useful to compute a preconditioner of the error covariance matrices (i.e., see approach used in [2]). The Scalable Library for Eigenvalue Problem Computations (SLEPc) is a software library for the solution of large scale sparse eigenvalue problems on parallel computers. It can also be used for computing a partial SVD of a large, sparse, rectangular matrix, and to solve nonlinear eigenvalue problems.

All the above mentioned software are integrated or based on PETSc (see figure 1 for a representation of the Software stack and algorithm implementation).

To represent the Jacobian of \( M_{t-\Delta t \rightarrow t} \) in PETSc we decided to follow a “matrix-free approach”: we used a \texttt{MATHSHELL} type for PETSc \texttt{Mat} object to represent \( \nabla M_{t-\Delta t \rightarrow t} \) just defining its way of operating.

2 **Case study description**

The case study is based on the Shallow Water Equations (SWEs) on the sphere. The SWE have been used extensively as a simple model of the atmosphere or ocean circulation since they contain the essential wave propagation mechanisms found in general circulation models [1]. The SWEs in spherical coordinates are:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= -\frac{1}{a \cos \theta} \left( \frac{u}{\partial \lambda} + v \cos \theta \frac{\partial u}{\partial \theta} \right) + \left( f + \frac{u \tan \theta}{a} \right) v - \frac{g}{a \cos \theta} \frac{\partial h}{\partial \lambda} \quad \text{(5)} \\
\frac{\partial v}{\partial t} &= -\frac{1}{a \cos \theta} \left( \frac{u}{\partial \lambda} + v \cos \theta \frac{\partial v}{\partial \theta} \right) + \left( f + \frac{u \tan \theta}{a} \right) u - \frac{g}{a \cos \theta} \frac{\partial h}{\partial \theta} \quad \text{(6)} \\
\frac{\partial h}{\partial t} &= -\frac{1}{a \cos \theta} \left( \frac{\partial (hu)}{\partial \lambda} + \frac{\partial (hu \cos \theta)}{\partial \theta} \right) \quad \text{(7)}
\end{align*}
\]

Here \( f \) is the Coriolis parameter given by \( f = 2 \Omega \sin \theta \), where \( \Omega \) is the angular speed of the rotation of the Earth, \( h \) is the height of the homogeneous atmosphere (or of the free ocean surface), \( u \) and \( v \) are the zonal and meridional wind (or the ocean velocity) components, respectively, \( \theta \) and \( \lambda \) are the latitudinal and longitudinal directions, respectively, \( a \) is the radius of the earth and \( g \) is the gravitational constant.

We express the system of equations (5-7) using a compact form, i.e.:

\[
\frac{\partial Z}{\partial t} = M_{t-\Delta t \rightarrow t}(Z) \quad \text{(8)}
\]

where

\[
Z = \begin{pmatrix} u \\ v \\ h \end{pmatrix} \quad \text{(9)}
\]
Figure 1: Representation of the Software stack and algorithm implementation
and

\[ M_{t-\Delta t} (Z) = \left( \begin{array}{c} -\frac{1}{a \cos \theta} \left( \frac{\partial U_i}{\partial x} + v \cos \theta \frac{\partial h}{\partial y} \right) + \left( f + \frac{u \tan \theta}{a} \right) v - \frac{g}{a \cos \theta} \frac{\partial h}{\partial x} \\ -\frac{1}{a \cos \theta} \left( \frac{\partial U_i}{\partial y} + v \cos \theta \frac{\partial h}{\partial x} \right) + \left( f + \frac{u \tan \theta}{a} \right) u - \frac{g}{a \cos \theta} \frac{\partial h}{\partial y} \\ -\frac{1}{a \cos \theta} \left( \left( \partial h u \right) + \left( \partial (hu \cos \theta) \right) \right) \end{array} \right) \]

= \left( \begin{array}{c} F_1 \\ F_2 \\ F_3 \end{array} \right) = (10) \]

We discretize (8) just in space using an un-staggered Turkel-Zwas scheme [5, 6], and we obtain:

\[ \frac{\partial Z_{\text{disc}}}{\partial t} = M_{t-\Delta t}^{-1} (Z_{\text{disc}}) \]

where

\[ Z_{\text{disc}} = \left( \begin{array}{c} (u_{i,j})_{i=0,...,nlon-1;j=0,...,nlat-1} \\ (v_{i,j})_{i=0,...,nlon-1;j=0,...,nlat-1} \\ (h_{i,j})_{i=0,...,nlon-1;j=0,...,nlat-1} \end{array} \right) \]

and

\[ M_{t-\Delta t}^{-1} (Z_{\text{disc}}) = \left( \begin{array}{c} (U_{i,j})_{i=0,...,nlon-1;j=0,...,nlat-1} \\ (V_{i,j})_{i=0,...,nlon-1;j=0,...,nlat-1} \\ (H_{i,j})_{i=0,...,nlon-1;j=0,...,nlat-1} \end{array} \right) \]

\[ U_{i,j} = -\sigma_{\text{lon}} \frac{u_{i,j}}{\cos \theta_j} (u_{i+1,j} - u_{i-1,j}) 
-\sigma_{\text{lat}} v_{i,j} (u_{i,j+1} - u_{i,j-1}) 
-\sigma_{\text{lon}} \frac{g}{q} (h_{i+p,j} - h_{i-p,j}) 
+ \frac{1}{2} \left( 1 - \alpha \right) \left( 2 \Omega \sin \theta_j + \frac{u_{i,j}}{a} \right) v_{i,j} 
+ \frac{1}{2} (2 \Omega \sin \theta_j + \frac{u_{i+p,j}}{a} \tan \theta_j) v_{i+p,j} 
+ \frac{1}{2} (2 \Omega \sin \theta_j + \frac{u_{i-p,j}}{a} \tan \theta_j) v_{i-p,j} \]

\[ V_{i,j} = -\sigma_{\text{lon}} \frac{u_{i,j}}{\cos \theta_j} (v_{i+1,j} - v_{i-1,j}) 
-\sigma_{\text{lat}} v_{i,j} (u_{i,j+1} - u_{i,j-1}) 
-\sigma_{\text{lat}} \frac{g}{q} (h_{i,j+q} - h_{i,j-q}) 
-2 \left( 1 - \alpha \right) \left( 2 \Omega \sin \theta_j + \frac{u_{i,j}}{a} \right) u_{i,j} 
+ \frac{1}{2} \left( 2 \Omega \sin \theta_j+q + \frac{u_{i,j+q}}{a} \tan \theta_j+q \right) u_{i,j+q} 
+ \frac{1}{2} \left( 2 \Omega \sin \theta_j-q + \frac{u_{i,j-q}}{a} \tan \theta_j-q \right) u_{i,j-q} \]

\[ H_{i,j} = -\alpha \frac{u_{i,j}}{\cos \theta_j} (h_{i+1,j} - h_{i-1,j}) 
+ v_{i,j} (h_{i,j+1} - h_{i,j-1}) 
+ h_{i,j} \left( 1 - \alpha \right) (u_{i+p,j} - u_{i-p,j}) 
+ \frac{1}{2} (u_{i+p,j+q} - u_{i-p,j+q} + u_{i+p,j-q} - u_{i-p,j-q}) \left( \frac{1}{p} \right) 
+ \left( 1 - \alpha \right) (v_{i,j+q} \cos \theta_j+q - v_{i,j-q} \cos \theta_j-q) 
+ \frac{1}{2} (v_{i+p,j+q} \cos \theta_j+q - v_{i+p,j-q} \cos \theta_j-q) 
+ \frac{1}{2} (v_{i-p,j+q} \cos \theta_j+q - v_{i-p,j-q} \cos \theta_j-q) \left( \frac{1}{q} \right) \]
If we define $M_{0,\text{steps}}^{\Delta t}(\cdot)$ as follows:

$$M_{0,\text{steps}}^{\Delta t}(\cdot) = M_{\text{disc}}^{-\Delta t \to t} \left( M_{\text{disc}}^{t\to t} \left( \cdots M_{\text{disc}}^{t\to t}(\cdot) \right) \right),$$

(14)

we note that the symbol $M_{0,\text{steps}}^{\Delta t}(\cdot)$ represents the model $M_{\text{disc}}^{t\to t}(\cdot)$ “applied” $M_{\text{steps}}$ times. We also note that the numerical model is defined by the following parameters:

- $\Delta t$ discretization step in time domain,
- $\Delta \lambda$, $\Delta \theta$ discretization step in space domain,
- $\alpha$ parameter of the Turkel-Zwas schema,
- $p$, $q$ parameters of the Turkel-Zwas schema.

To verify the correct operation of the software module which implements the model, we tested the computed values of $M_{0,\text{steps}}^{\Delta t}(x_0)$, when $|DD(\Delta \times \Omega)| = 1$ (i.e., when domain $\Delta \times \Omega$ is not decomposed), where:

1. $\Delta t = 50.0, 100.0, 150.0, 200.0$,
2. $\alpha = \frac{1}{3}$,
3. $p = 4$ and $q = 2$,
4. $x_0$ is a syntetic vector containing all the considered fields: the sea-level field $h$ is generated by a Gaussian stochastic process; both velocity fields $v$ and $u$ are set to zero,
5. $\Delta \lambda$ e $\Delta \theta$ defined on the basis of discretization grid used by data available at repository Ocean Synthesis/Reanalysis Directory of Hamburg University (see \cite{3}).

We note that the values for parameters at above mentioned points\cite{1,2} and \cite{3} were chosen on the basis of the considerations and results described in \cite{4}.

In figure 2-(a) $x_0$ is represented. In figure 2-(b)-(d) are represented respectively $M_{0,\text{steps}}^{\Delta t}(x_0)$ where $\Delta t = 50.0, 100.0, 150.0, 200.0$. We used different values for $\Delta t$ with the aim to empirically determine the “best value” for $\Delta t$. The considered values for $\Delta t$ were chosen taking into account the considerations about CFL condition for Turkel-Zwas methods described in \cite{4}.

To give a measure of how $M_{0,\text{steps}}^{\Delta t}(x_0)$ differs from $x_0$ depending from $\Delta t$, in table 1 we show

$$\frac{\|M_{0,\text{steps}}^{\Delta t}(x_0) - x_0\|_2}{\|x_0\|_2}$$

for the considered values of $\Delta t$.

### 3 Test results related with the DA software module operation

To verify the correct operation of the software module which implements the DA process we tested the computed values of $x_{DA}^{\Delta t}$, when $|DD(\Delta \times \Omega)| = 1$ (i.e., when domain $\Delta \times \Omega$ is not decomposed), starting:

- from the $R_k = R$ ($\forall k = 0, \ldots, n_{l,\text{obs}} - 1$) diagonal matrix representing the covariance matrix of the errors on all the observations vectors
- from the $H$ diagonal matrix representing the observational operator and

| $\Delta t$ | $\frac{\|M_{0,\text{steps}}^{\Delta t}(x_0) - x_0\|_2}{\|x_0\|_2}$ |
|-----------|--------------------------------------------------|
| 50.0      | 2.493588e-03                                    |
| 100.0     | 4.846299e-03                                    |
| 150.0     | 6.949851e-03                                    |
| 200.0     | 8.737334e-03                                    |

Table 1: The values of $\frac{\|M_{0,\text{steps}}^{\Delta t}(x_0) - x_0\|_2}{\|x_0\|_2}$ as function of $\Delta t$. 

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- from the $H$ diagonal matrix representing the observational operator and
Figure 2: $M^0_{\Delta t} (x_0)$ ($\Delta t = 200.0, 150.0, 100.0, 50.0$)
• from the background $x_b^{\Delta t}$ and
• from the set of $n_{\text{obs}}$ observations vectors \( \{ \Delta t x_{\text{obs}}^n \}_{n=1, \ldots, n_{\text{obs}}} \),
• and by using, as preconditioner $B^{\Delta t\text{nt}}_{\text{obs}},$ of covariance matrix $B^{\Delta t},$ its Truncated SVD (the first $n_{\text{SVs}}$ singular values (\( S_i \)) = 0, ..., $n_{\text{SVs}}-1$ of $B^{\Delta t}$ are considered),

where

1. $x_b^{\Delta t} = M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+1(x_0),$

**Problem 1** For each $n = 1, \ldots, n_{\text{obs}},$

\[
\Delta t x_{\text{obs}}^n = \frac{1}{10^2} \begin{bmatrix} 102 \times M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0) \end{bmatrix},
\]

(each elements of $\Delta t x_{\text{obs}}^n$ were obtained by rounding, on the third significant digit, the respective elements of $M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0)).$ $H$ is the identity matrix.

**Problem 2** For each $n = 1, \ldots, n_{\text{obs}},$ if $i$ is a multiple of $\text{STEP} = 5$

\[
(\Delta t x_{\text{obs}}^n)_i = \left( M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0) \right)_i + 0.01 \times \text{randn},
\]

\[
diag(H)_i = 1,
\]

else

\[
(\Delta t x_{\text{obs}}^n)_i = 0,
\]

\[
diag(H)_i = 0,
\]

($\Delta t x_{\text{obs}}^n$ are sparse vectors whose length is $3 \times n_{\text{lat}} \times n_{\text{lon}}$ and whose non-zero elements (the 20% of the total) were obtained by adding a scaled number $0.01 \times \text{randn}$ from normal distribution to the respective elements of $M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0)).$

**Problem 3** For each $n = 1, \ldots, n_{\text{obs}},$

\[
\Delta t x_{\text{obs}}^n = \frac{1}{10^1} \begin{bmatrix} 101 \times M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0) \end{bmatrix},
\]

(each elements of $\Delta t x_{\text{obs}}^n$ were obtained by rounding, on the second significant digit, the respective elements of $M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0).$ $H$ is the identity matrix.

**Problem 4** For each $n = 1, \ldots, n_{\text{obs}},$ if $i$ is a multiple of $\text{STEP} = 5$

\[
(\Delta t x_{\text{obs}}^n)_i = \left( M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0) \right)_i + 0.01 \times O \left( \left( M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0) \right)_i \right) \times \text{randn},
\]

\[
diag(H)_i = 1,
\]

else

\[
(\Delta t x_{\text{obs}}^n)_i = 0,
\]

\[
diag(H)_i = 0,
\]

($\Delta t x_{\text{obs}}^n$ are sparse vectors whose length is $3 \times n_{\text{lat}} \times n_{\text{lon}}$ and whose non-zero elements (the 20% of the total) were obtained by adding, to the respective elements of $M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0),$ a number from normal distribution scaled by a factor related with order of magnitude of each elements $O \left( \left( M_0^{\Delta t, \text{steps}=30} - n_{\text{obs}}+n(x_0) \right)_i \right).$

3. $n_{\text{obs}} = 1, 2, 4, 6, 8, 10,$
4. $n_{\text{SVs}} = 4, 6, 8, 10, 12,$
5. \((R^{-1})_i = \begin{cases} \frac{1}{14+6} & \text{if } i = 0, \ldots, n_{\text{lat}} \times n_{\text{lon}} - 1 \\ 1 & \text{if } i = n_{\text{lat}} \times n_{\text{lon}}, \ldots, 3 \times n_{\text{lat}} \times n_{\text{lon}} \end{cases} \)
Figure 3: How \( x_b^{\Delta t} \) and \( \Delta t x_{\text{obs}}^m \) were chosen/built from \( M_{\Delta t}^{0, M_{\text{steps}}=m}(x_0) \) data.

6. \( B^{\Delta t} = (x_{\text{err}}^{\Delta t})^T \), where

\[
(x_{\text{err}}^{\Delta t})_i = (x_b^{\Delta t})_i - \nu^{\Delta t}
\]

and where

\[
\nu^{\Delta t} = \frac{\sum_{j=0}^{1 \ldots 3 \times \text{nlat} \times \text{nlon} - 1} (x_b^{\Delta t})_j}{3 \times \text{nlat} \times \text{nlon}}
\]

Figure 3 shows how the background \( x_b^{\Delta t} \) (the red circle in the image) and observations \( \Delta t x_{\text{obs}}^m \) (the blue circle in the image) were chosen/built from \( x_m^{\Delta t} = M_{\Delta t}^{0, M_{\text{steps}}=m}(x_0) \) data: in particular, for each value of \( n_{\text{obs}} = 1, 2, 4, 6, 8, 10 \), the image intends to show which subset of \( \{x_m^{\Delta t}\}_{m=0 \ldots 30} \) is considered to generate background and observations. In particular, the procedure used to build the input data for DA problem performs the following steps:

1. “application” of the model \( M_{\Delta t}^{0, M_{\text{steps}}=m}(\cdot) \) to the starting point \( x_0 \) to obtain the vector \( x_m^{\Delta t} \) where \( m = 30 - n_{\text{obs}} + 1 \);

2. from the vector \( x_m^{\Delta t} \) computed at above point 1 we obtain both the background vector \( x_b^{\Delta t} \) and, by using one of the definitions for Problem 1 or Problem 2, the first observation vector \( \Delta t x_{\text{obs}}^1 \);

3. further “application” of the model to compute the set of vectors \( \{x_m^{\Delta t}\}_{m=30 - n_{\text{obs}} + 2 \ldots 30} \) from which obtain, by using one of the definitions for Problem 1 or Problem 2, the remaining \( n_{\text{obs}} - 1 \) observation vectors \( \Delta t x_{\text{obs}}^i, i = 2, \ldots, n_{\text{obs}} \).

Then, the “assimilation window” \( AW_{\Delta t}^{n_{\text{steps}}=m} \) in time domain, when the value of \( \Delta t \) is fixed, is the interval defined as:

\[
AW_{\Delta t}^{n_{\text{obs}}} = [(30 - n_{\text{obs}} + 1) \Delta t, 30\Delta t].
\]
Table 2: The first $nSVs$ singular values $(S_i)_{i=0,...,nSVs-1}$ of matrix $B^{Δt}$ when $n_{tobs} = 2$ ($Δt = 50.0, 100.0, 150.0, 200.0$).

Three sets of tests are performed: the first set intends to evaluate how different values for $n_{tobs}$ and $nSVs$ influence the behavior of DA software module; the second and third sets of tests intend to give elements to evaluate how Data Assimilation used during model application (i.e., $M^{0,Δt}_{Msteps=m}(x^{Δt}_{DA})$) improve the quality of the model computed values without DA (i.e., $M^{0,Δt}_{Msteps=m}(x^{Δt}_{DA})$) with respect to observations.

Tests Set 1 In order to evaluate how different values for $n_{tobs}$ and $nSVs$ influence the behavior of DA software module, in tables 3 (for Problem 1), 4 (for Problem 2), 5 (for Problem 3) and 6 (for Problem 4) the values of $err_{DA}^{Δt}$ and $err_{DA}^{obs}$ are showed for the above listed values of $n_{tobs}$ and $nSVs$ and for the four considered problems where

$$ err_{DA}^{Δt} = \| H x^{Δt}_{DA} - \Delta t x^{n_{tobs}+1}_{obs} \|_2 / \| \Delta t x^{n_{tobs}+1}_{obs} \|_2 $$

and $Δt = 50.0, 100.0, 150.0, 200.0$. We note that values of $err_{DA}^{Δt}$ are not reported when the algorithm failed (i.e., when the Truncated SVD computation failed). The table 2 show, as examples, the values of $(S_i)_{i=0,...,nSVs-1}$ when $n_{tobs} = 2$ and $Δt = 50.0, 100.0, 150.0, 200.0$.

We also note that:

1. the smaller values for $nSVs$ is (i.e., where $nSVs = 4$), more the DA software module is able to effectively compute the solution of the DA problem;
2. the larger values for $nSVs$ is, more accurate is the solution of the DA problem computed by DA software module (if it is successful).

This behavior could be explained considering that:

1. the smaller the value of $nSVs$ is, better conditioned is the matrix $\bar{B}_{n_{SVs}}$, but also
2. the larger values for $nSVs$ is, “closer” the matrices $\bar{B}_{n_{SVs}}$ and $B$ are.

Tests Set 2 In order to evaluate how the use of the Data Assimilation influences the model’s performance, in figures 4, 5, 6 and 7 trends of

$$ \| H M^{0,Δt}_{Msteps=m}(x^{Δt}_{DA}) - \Delta t x^{n_{tobs}+1}_{obs} \|_2 / \| \Delta t x^{n_{tobs}+1}_{obs} \|_2 $$

and

$$ \| H M^{0,Δt}_{Msteps=m}(x^{Δt}_{b}) - \Delta t x^{n_{tobs}+1}_{obs} \|_2 / \| \Delta t x^{n_{tobs}+1}_{obs} \|_2 $$

We note that the symbols $M^{0,Δt}_{Msteps=m}(x^{Δt}_{b})$ and $M^{0,Δt}_{Msteps=m}(x^{Δt}_{DA})$ represent the model “applied” $n$ times to the background $x^{Δt}_{b}$ and to the solution of DA problem $x^{Δt}_{DA}$ respectively.
| $\Delta t$ | 1  | 2  | 4  | 6  | 8  | 10 |
|-----------|----|----|----|----|----|----|
| $n_{SVs}$ | 4  | 5.92300468033734e-03 | 5.91823049175874e-03 | 5.90974436752090e-03 | 5.90130686007113e-03 | 5.89309464551773e-03 | 5.88475274176764e-03 |
| $n_{SVs}$ | 6  | 5.92300468033734e-03 | 5.91823049175874e-03 | 5.90974436752090e-03 | 5.90130686007113e-03 | 5.89309464551773e-03 | 5.88475274176764e-03 |
| $n_{SVs}$ | 8  | 5.92300468033734e-03 | 5.91823049175874e-03 | 5.90974436752090e-03 | 5.90130686007113e-03 | 5.89309464551773e-03 | 5.88475274176764e-03 |
| $n_{SVs}$ | 10 | 5.92300468033734e-03 | 5.91823049175874e-03 | 5.90974436752090e-03 | 5.90130686007113e-03 | 5.89309464551773e-03 | 5.88475274176764e-03 |
| $n_{SVs}$ | 12 | 5.92300468033734e-03 | 5.91823049175874e-03 | 5.90974436752090e-03 | 5.90130686007113e-03 | 5.89309464551773e-03 | 5.88475274176764e-03 |

Table 3: $err_h^\Delta t$ and $err_{DA}^\Delta t$ as function of $n_{t_{obs}}$ and $n_{SVs}$ ($\Delta t = 50.0, 100.0, 150.0, 200.0$) - Problem 1
| $\Delta t = 50.0$ | $n_{t_{\text{obs}}}$ | $nSVs$ |
|----------------|----------------|-------|
| $err_{b}^{n}$  | 3.45346703333335884e-02 | 50 |
| 4               | 3.496046426389585e-02 | 3.461814248729758e-02 | 3.4960474070997717e-02 | 3.461815048663301e-02 | 3.496048249133106e-02 |
| 6               | 3.45346703333335884e-02 | 50 |
| 8               | 3.496046426389585e-02 | 3.461814248729756e-02 | 3.496047407097716e-02 | 3.461815048663301e-02 | 3.496048237755320e-02 |
| 10              | 3.45346703333335884e-02 | 50 |
| 12              | 3.496046426389585e-02 | 3.461814248729758e-02 | 3.496047407097717e-02 | 3.461815029375775e-02 | 3.496048249133106e-02 |

| $\Delta t = 100.0$ | $n_{t_{\text{obs}}}$ | $nSVs$ |
|----------------|----------------|-------|
| $err_{b}^{n}$  | 3.4534572381516390e-02 | 100 |
| 4               | 3.4960352646338818e-02 | 3.461805630410621e-02 | 3.496039039880471e-02 | 3.46180870666546e-02 | 3.496042291663454e-02 |
| 6               | 3.4534572381516390e-02 | 100 |
| 8               | 3.4960352646338818e-02 | 3.461805630410621e-02 | 3.496039039880471e-02 | 3.46180870666546e-02 | 3.496042291663452e-02 |
| 10              | 3.4534572381516390e-02 | 100 |
| 12              | 3.4960352646338818e-02 | 3.461805630410621e-02 | 3.496039039880471e-02 | 3.46180870666546e-02 | 3.496042291663452e-02 |

| $\Delta t = 150.0$ | $n_{t_{\text{obs}}}$ | $nSVs$ |
|----------------|----------------|-------|
| $err_{b}^{n}$  | 3.453440979970871e-02 | 150 |
| 4               | 3.4960175062418329e-02 | 3.4884297301934e-02 | 3.48360615320147e-02 | 3.461798505601022e-02 | 3.496032646744604e-02 |
| 6               | 3.453440979970871e-02 | 150 |
| 8               | 3.4960175062418329e-02 | 3.4884297301934e-02 | 3.48360615320147e-02 | 3.461798505601022e-02 | 3.496032646744605e-02 |
| 10              | 3.453440979970871e-02 | 150 |
| 12              | 3.4960175062418329e-02 | 3.4884297301934e-02 | 3.48360615320147e-02 | 3.461798505601022e-02 | 3.496032646744606e-02 |

| $\Delta t = 200.0$ | $n_{t_{\text{obs}}}$ | $nSVs$ |
|----------------|----------------|-------|
| $err_{b}^{n}$  | 3.453419617204346e-02 | 200 |
| 4               | 3.495994493035877e-02 | 3.481773213566689e-02 | 3.49600771746858e-02 | 3.496013682728978e-02 | 3.496019616952864e-02 |
| 6               | 3.453419617204346e-02 | 200 |
| 8               | 3.495994493035877e-02 | 3.481773213566689e-02 | 3.49600771746858e-02 | 3.496013682728978e-02 | 3.496019616952863e-02 |
| 10              | 3.453419617204346e-02 | 200 |
| 12              | 3.495994493035877e-02 | 3.481773213566689e-02 | 3.49600771746858e-02 | 3.496013682728978e-02 | 3.496019616952864e-02 |

Table 4: $err_{b}^{n}$ and $err_{DA}^{n}$ as function of $n_{t_{\text{obs}}}$ and $nSVs$ ($\Delta t = 50.0, 100.0, 150.0, 200.0$) - Problem 2
| $\Delta t$ | $n_{t_{obs}}$ | $n_{SVs}$ |
|-----------|-------------|-----------|
| 50.0      | 1           | err $\Delta t$ |
|           | 2           | 5.773468954018757e-02 |
|           | 4           | 5.773118330947371e-02 |
|           | 6           | 5.772450392218931e-02 |
|           | 8           | 5.771827398570289e-02 |
|           | 10          | 5.771249955261612e-02 |
|           | 12          | 5.770718624999813e-02 |
| 100.0     | 1           | err $\Delta t$ |
|           | 2           | 5.773468954018758e-02 |
|           | 4           | 5.773118330947371e-02 |
|           | 6           | 5.772450392218931e-02 |
|           | 8           | 5.771827398570289e-02 |
|           | 10          | 5.771249955261612e-02 |
|           | 12          | 5.770718624999811e-02 |
| 150.0     | 1           | err $\Delta t$ |
|           | 2           | 5.773468954018759e-02 |
|           | 4           | 5.773118330947371e-02 |
|           | 6           | 5.772450392218931e-02 |
|           | 8           | 5.771827398570289e-02 |
|           | 10          | 5.771249955261612e-02 |
|           | 12          | 5.770718624999811e-02 |
| 200.0     | 1           | err $\Delta t$ |
|           | 2           | 5.773468954018760e-02 |
|           | 4           | 5.773118330947371e-02 |
|           | 6           | 5.772450392218931e-02 |
|           | 8           | 5.771827398570289e-02 |
|           | 10          | 5.771249955261612e-02 |
|           | 12          | 5.770718624999811e-02 |

Table 5: $err_{DA}$ and $err_{DA}$ as function of $nt_{obs}$ and $nSV$s ($\Delta t = 50.0, 100.0, 150.0, 200.0$) - Problem 3
| \(\Delta t\)  | \(n_{\text{obs}}\) | \(n_{SVs}\) |
|---|---|---|
| 50.0 | 3.212944523284356e-02 | 3.146374761827107e-02 |
| 100.0 | 3.212934767372494e-02 | 3.146365882582471e-02 |
| 150.0 | 2.983871447550081e-02 | 3.146357791255923e-02 |
| 200.0 | 3.212928155458578e-02 | 3.146357791255923e-02 |

Table 6: \(err_t^A\) and \(err_D^A\) as function of \(n_{\text{obs}}\) and \(n_{SVs}\) (\(\Delta t = 50.0, 100.0, 150.0, 200.0\)) - Problem 4
Figure 4: $\|HM_{\Delta t}^{M_{\text{steps}}=n}(x_{DA}^{\Delta t}) - \Delta t x_{\text{obs}}^{n+1}\|_2/\|\Delta t x_{\text{obs}}^{n+1}\|_2$ and $\|HM_{\Delta t}^{M_{\text{steps}}=n}(x_{b}^{\Delta t}) - \Delta t x_{\text{obs}}^{n+1}\|_2/\|\Delta t x_{\text{obs}}^{n+1}\|_2$ as functions of $n$ ($\Delta t = 50.0$, $n_{\text{obs}} = 10, nSVs = 4$, (a)-(d)-labeled plots are related with Problem 1-4 respectively)

Tests Set 3 In order to evaluate how the use of 4DVAR approach (which use a number of observations vectors $n_{\text{obs}}$ greater than 1) influences the model’s performance, in figures 8, 9, 10 and 11, trends of $\|HM_{\Delta t}^{M_{\text{steps}}=n}(x_{DA}^{\Delta t}) - \Delta t x_{\text{obs}}^{n+1}\|_2/\|\Delta t x_{\text{obs}}^{n+1}\|_2$ and $\|HM_{\Delta t}^{M_{\text{steps}}=n}(x_{b}^{\Delta t}) - \Delta t x_{\text{obs}}^{n+1}\|_2/\|\Delta t x_{\text{obs}}^{n+1}\|_2$ as functions of $n = 0, \ldots, n_{\text{obs}} - 1$ are compared when $n_{\text{obs}} = 2, 6, 10$ (the value of $nSVs$ is fixed and its value is $nSVs = 4$, (a)-(b)-labeled plots are related with Problem 1-4 respectively). It seems that the use of a number of observations greater than 1 doesn’t significantly influence the model performance so it may not be convenient to use multiple observations (indeed, the computational cost of the DA algorithm increases with $n_{\text{obs}}$).

In figures 12, 13, 14 and 15 $M_{\Delta t}^{M_{\text{steps}}=n_{\text{obs}}-1}(x_{DA}^{\Delta t})$ are showed where $\Delta t = 50.0, 100.0, 150.0, 200.0$ (values of $n_{\text{obs}}$ and $nSVs$ are fixed and their values are $n_{\text{obs}} = 10 e nSVs = 4$, (a)-(b)-labeled plots are related with Problem 1-4 respectively).
Figure 5: $\|H_{M_{\Delta t}}^{n,M_{\text{steps}}=n}(x_{D,A}^{n+1}) - \Delta t x_{\text{obs}}^{n+1}\|_2 / \|\Delta t x_{\text{obs}}^{n+1}\|_2$ and $\|H_{M_{\Delta t}}^{n,M_{\text{steps}}=n}(x_{b}^{n+1}) - \Delta t x_{\text{obs}}^{n+1}\|_2 / \|\Delta t x_{\text{obs}}^{n+1}\|_2$ as function of $n$ ($\Delta t = 100.0$, $n_{\text{obs}} = 10$, $nSVs = 4$, (a)-(d)-labeled plots are related with Problem 1-4 respectively)
\[ \| H_{M, n=t=0}^{M, t=p=0} (x_{DA}^{n=0}) - \Delta t x_{obs}^{n+1} \|_2 / \| \Delta t x_{obs}^{n+1} \|_2 \] and

\[ \| H_{M, n=t=0}^{M, t=p=0} (x_{b}^{n=0}) - \Delta t x_{obs}^{n+1} \|_2 / \| \Delta t x_{obs}^{n+1} \|_2 \] as function of \( n \) (\( \Delta t = 150.0, n_{t, obs} = 10, nSVs = 4 \)). (a)-(d)-labeled plots are related with Problem 1-4 respectively.

Figure 6: \( nSVs = 4, n_{t, obs} = 10, p = 4, q = 2, \alpha = 0.33 \)
Figure 7: $\|H_{M,0,M_{t=0}=0}(x^{\Delta t}_{b}) - \Delta t x_{obs}^{n+1}\|_2/\|\Delta t x_{obs}^{n+1}\|_2$ and $\|H_{M,0,M_{t=0}=0}(x^{\Delta t}_{b}) - \Delta t x_{obs}^{n+1}\|_2/\|\Delta t x_{obs}^{n+1}\|_2$ as function of $n$ ($\Delta t = 200.0$, $n_{t_{obs}} = 10$, $nSVs = 4$, (a)-(d)-labeled plots are related with Problem 1-4 respectively)
Figure 8: \( \| \mathbf{H}_{M, \text{steps}=n} (x^{n+1}_{\Delta t} - x^{n+1}_{\Delta t}) \|_2 / \| \Delta t x^{n+1}_{\Delta t} \|_2 \) and \( \| \mathbf{H}_{M, \text{steps}=n} (x^{n+1}_{\Delta t} - x^{n+1}_{\Delta t}) \|_2 / \| \Delta t x^{n+1}_{\Delta t} \|_2 \) as function of \( n = 0, \ldots, n_{\text{obs}} - 1 \) (\( \Delta t = 50.0 \), \( n_{\text{obs}} = 2, 6, 10 \), \( nSVs = 4 \), (a)-(b)-labeled plots are related with Problem 1-4 respectively)
Figure 9: $\|HM_{\Delta t}^{0,M_{\text{steps}}=n}(x_{\Delta t}^{n}) - \Delta t x_{\text{obs}}^{n+1}\|_2/\|\Delta t x_{\text{obs}}^{n+1}\|_2$ and $\|HM_{\Delta t}^{0,M_{\text{steps}}=n}(x_{\Delta t}^{n}) - \Delta t x_{\text{obs}}^{n+1}\|_2/\|\Delta t x_{\text{obs}}^{n+1}\|_2$ as function of $n = 0, \ldots, n_{\text{obs}} - 1$ ($\Delta t = 100.0$, $n_{\text{obs}} = 2, 6, 10$, $nSVs = 4$, (a)-(b)-labeled plots are related with Problem 1-4 respectively)
Figure 10: \(\|HM_{M,steps}^n(x^Dk) - \Delta t x_{obs}^{n+1}\|_2 / \|\Delta t x_{obs}^{n+1}\|_2\) and \(\|HM_{M,steps}^n(x^Dk) - \Delta t x_{obs}^{n+1}\|_2 / \|\Delta t x_{obs}^{n+1}\|_2\) as function of \(n = 0, \ldots, nt_{obs} - 1\) (\(\Delta t = 150.0\), \(nt_{obs} = 2, 6, 10\), \(nSVs = 4\), (a)-(b)-labeled plots are related with Problem 1-4 respectively)
Figure 11: \( \| H^{0,M_{\text{steps}=n}}_M(x^{\Delta t}_{k+1}) - \Delta t x^{n+1}_{\text{obs}} \|_2 / \| \Delta t x^{n+1}_{\text{obs}} \|_2 \) and \( \| H^{2,M_{\text{steps}=n}}_M(x^{\Delta t}_{k+1}) - \Delta t x^{n+1}_{\text{obs}} \|_2 / \| \Delta t x^{n+1}_{\text{obs}} \|_2 \) as function of \( n = 0, \ldots, n_{\text{obs}} - 1 \) (\( \Delta t = 200.0 \), \( n_{\text{obs}} = 2, 6, 10 \), \( nSVs = 4 \), (a)-(b)-labeled plots are related with Problem 1-4 respectively)
Figure 12: $M_{\Delta t = 50.0, nt_{obs} = 10, (a)-(b)-labeled}$ plots are related with Problem 1-4 respectively.

Figure 13: $M_{\Delta t = 100.0, nt_{obs} = 10, (a)-(b)-labeled}$ plots are related with Problem 1-4 respectively.
Figure 14: $M^{0, M_{steps} = n_{tobs} - 1}_{\Delta t} \left( x_{DA}^\Delta t \right)$ ($\Delta t = 150.0$, $n_{tobs} = 10$, (a)-(b)-labeled plots are related with Problem 1-4 respectively)

Figure 15: $M^{0, M_{steps} = n_{tobs} - 1}_{\Delta t} \left( x_{DA}^\Delta t \right)$ ($\Delta t = 200.0$, $n_{tobs} = 10$, (a)-(b)-labeled plots are related with Problem 1-4 respectively)
4 Conclusions

In this work are presented and discussed some results of tests performed to validate a software module which implements a DA process.

Such module depends from some parameters such as the number $nt_{obs}$ of observations vectors and the number $nSVs$ of singular values considered for the Truncated SVD of matrix $B$.

The parameter $nSVs$ influences the behavior of DA software module: in particular, the smaller values for $nSVs$ is (i.e., where $nSVs = 4$), more the DA software module is able to effectively compute the solution of the DA problem. Also the value of $\Delta t$, the discretization step in time domain used by numerical model, seems to have some influences on the behavior of DA software module: when the bigger values for $\Delta t$ are used (i.e., when $\Delta t = 200$), the DA software module often fails to compute the solution of the DA problem.

About the $nt_{obs}$ parameter, the use of larger values doesn’t have significant effects both on the behavior of DA software module and on use of DA solution in model’s application. Furthermore, the use of larger values for $nt_{obs}$ has a bigger computational cost. All that said, the use of small values for $nt_{obs}$ (i.e., where $nt_{obs} = 1$) seems to be more desirable.

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