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Sensitivity Analysis of the Data Assimilation-Driven Decomposition in Space and Time to Solve PDE-Constrained Optimization Problems

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Abstract: This paper is presented in the context of sensitivity analysis (SA) of large-scale data assimilation (DA) models. We studied consistency, convergence, stability and roundoff error propagation of the reduced-space optimization technique arising in parallel 4D Variational DA problems. The results are helpful to understand the reliability of DA, to assess what confidence one can have that the simulation results are correct and to determine its configuration in any application. The main contributions of the present work are as follows. By using forward error analysis, we derived the number of conditions of the parallel approach. We found that the parallel approach reduces the number of conditions, revealing that it is more appropriate than the standard approach usually implemented in most operative software. As the background values are used as initial conditions of local PDE models, we analyzed stability with respect to time direction. Finally, we proved consistency of the proposed approach by analyzing local truncation errors of each computational kernel.

Keywords: sensitivity analysis; data assimilation; domain decomposition; stability; consistency; convergence



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1. Introduction

Data assimilation (DA) has long played a crucial role in the quantification of uncertainties in numerical weather prediction (NWP), oceanography [1,2] and, more generally, in data science. Recently, DA has been applied more widely to numerical simulations beyond geophysical applications [3], medicine and biological science [4] to improve the accuracy and reliability of computational approaches. DA encompasses the entire sequence of operations that, starting from observations/measurements of physical quantities and with additional information, such as mathematical models governing the evolution of these quantities, improve their estimation of a suitable function. In order to understand how such a function is obtained, we suggest that, from a mathematical perspective, DA is an inverse and ill-posed problem [5]. Hence, regularization methods are used to obtain a well-posed problem. A popular approach to obtain a unique solution to DA inverse problems in such circumstances is to formulate them as variational problems, minimizing the sum of two terms, the first of which is a combination of the residual between the observed and predicted outputs (the so-called misfit) in an appropriate norm and the second of which is a regularization term that penalizes unwanted features of the parameters. The inverse problem leads to a nonlinear variational problem in which the forward simulation model is embedded in the residual term. When the forward model takes the form of partial differential equations (PDEs) or some other expensive model, the result is a PDE-based variational problem [6–10]. In this way, DA provides mathematical methods to identify an optimal trade-off between the current estimate of the model state and the observations, accounting for uncertainties. This poses a formidable computational challenge, making DA an example an ill-posed inverse big data problem.

In [11–14], we proposed a design for an innovative mathematical model and the development and analysis of related numerical algorithms based on the simultaneous introduction of space-time decomposition in the overlapping case of PDE equations governing the physical model and the DA model. The proposed method is a so-called reduced-space optimization technique. In such an approach, the DA model acts as a coarse/predictor operator of local PDE models by providing the background values as initial conditions of the local PDE models. Hereafter, we refer to such an approach as a DD-DA (domain decomposition data assimilation) method.

In this paper, we present a sensitivity analysis (SA) and DD-DA study of consistency, convergence, and stability, as well as a roundoff error analysis. SA refers the contributions of uncertain data to the uncertainty of the solution. The aim of SA is to understand the errors that arise at the different stages of the solution process, namely the uncertainty in the mathematical model, in the model solution and in the measurements. Moreover, approximation errors are introduced by linearization, discretization and the local model. SA is helpful in understanding how all these errors impact the solution of a DD-DA model and in assessing its practical configuration [15]. The main contributions of the present work are as follows.

- By using the forward error analysis (FEA), we derive the number of conditions of DD-DA. We find that DD-DA actually reduces the number of conditions of DA, revealing that it is much more appropriate than the standard approach that is usually implemented in most operative software;
- As the background values are used as initial conditions of local PDE models, we prove that small changes in initial values must not cause large changes in the final result. Then, we analyze the stability with respect to the time direction;
- We analyze the consistency of DD-DA in terms of local truncation errors;
- Overall, the present work complements the study reported in [16], in which the authors performed SA of DD in 3D space in the context of a variational data assimilation problem.

The remainder of this article is structured as follows. Section 2 provides a brief introduction to DA, 4D variational models and DD-DA following the discretize-then-optimize approach. The main results are presented in Section 3. Validation analysis is addressed in Section 4 with respect to one-dimensional shallow water equations.

2. 4D Variational DA Formulation

Before presenting our results, we briefly review the main concepts of 4D variational DA formulation. If $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$ is a spatial domain with a Lipschitz boundary, let

$$\begin{cases} u^{\mathcal{M}}(t+h, x) = \mathcal{M}_{t,t+h}[u(t, x)] & \forall x \in \Omega, t, t+h \in [0, T], (h > 0) \\ u^{\mathcal{M}}(t_0, x) = u_0(x) & t_0 \equiv 0, x \in \Omega \\ u^{\mathcal{M}}(t, x) = f(x) & x \in \partial\Omega, \forall t \in [0, T] \end{cases}, \quad (1)$$

be a symbolic description of the model of interest, where

$$u^{\mathcal{M}} : (t, x) \in [0, T] \times \Omega \mapsto u^{\mathcal{M}}(t, x) = [u^{\mathcal{M}}[1](t, x), u^{\mathcal{M}}[2](t, x), \dots, u^{\mathcal{M}}[s](t, x)] \quad (2)$$

is the state function of \mathcal{M} , $s \in \mathbb{N}$ is the number of physical variables and f is a known function defined based on the boundary $\partial\Omega$. Let

$$v : (t, x) \in \Delta \times \Omega \mapsto v(t, x), \quad (3)$$

be the observations function, and let

$$\mathcal{H} : u^{\mathcal{M}}(t, x) \mapsto v(t, x), \quad \forall (t, x) \in \Delta \times \Omega, \quad (4)$$

denote non-linear observation mapping. To simplify future treatments, we assume $s \equiv 1$.

Definition 1 (Discretization of $\Omega \times \Delta$ or Mesh Generation). Let

$$\Omega_I \equiv \{x_i\}_{i \in I} \subset \Omega$$

be the discretization of Ω , if $|I|$ is the cardinality of set I , then

$$I = \{1, \dots, N_p\}, N_p = |I|, \tag{5}$$

are, respectively, the set of indices of nodes in Ω and its cardinality, i.e., the number of inner nodes in Ω . Let

$$\Delta_K \equiv \{t_{\bar{k}}\}_{\bar{k} \in K} \subset \Delta$$

be the discretization of Δ where

$$K = \{1, \dots, N\}, N = |K| \tag{6}$$

are, respectively, the set of indices of the time variable in Δ and its cardinality, i.e., number of time instants in Δ . Consequently, we refer to

$$\Omega_I \times \Delta_K \equiv \{(x_i, t_{\bar{k}})\}_{i \in I; \bar{k} \in K} \subset \Omega \times \Delta \tag{7}$$

as the discrete domain/mesh.

We introduce the 4D variational problem (see Figure 1).

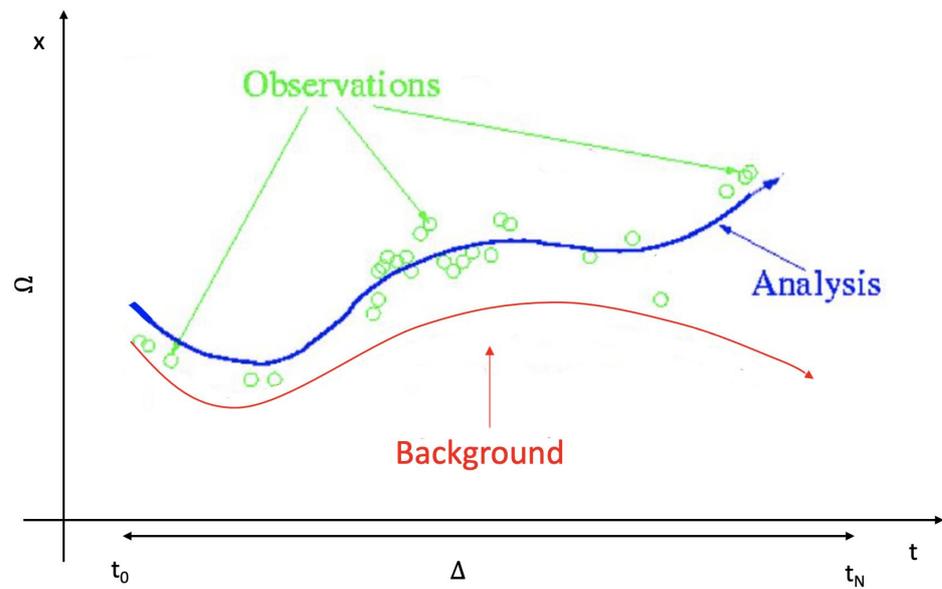


Figure 1. The 4D variational problem.

Definition 2. Let $\Omega \subset \mathbb{R}^n$ and $\Delta \subset \mathbb{R}$ be the spatial domain and the time interval, respectively. The 4DVAR DA problem consists of computing the so-called analysis:

$$\mathbf{u}^{DA} = \operatorname{argmin}_{u \in \mathbb{R}^{N_p \times N}} J(u), \tag{8}$$

in $\Omega \times \Delta$ with

$$J(u) = \alpha \|u - u^M\|_{B^{-1}}^2 + \|Gu - y\|_{R^{-1}}^2, \tag{9}$$

where N_p is the number of nodes in $\Omega \subset \mathbb{R}^n$; n_{obs} , with $n_{obs} \ll N_p$, is the number of observations in Ω ; N is the number of time instants in Δ ; α is the regularization parameter; $u_0 = \{u_{0,j}\}_{j=1,\dots,N_p} \equiv \{u_0(x_j)\}_{j=1,\dots,N_p} \in \mathbb{R}^{N_p}$ is the state at time t_0 ; the operator

$$M_{l-1,l} \in \mathbb{R}^{N_p \times N_p}, \quad l = 1, \dots, N, \tag{10}$$

is the discretization of the linear approximation of $\mathcal{M}_{t_{l-1},t_l}$ from t_{l-1} to t_l ; the operator

$$M \in \mathbb{R}^{N_p \times N_p} \tag{11}$$

is the discretization of the linear approximation of \mathcal{M} , running from t_0 to t_N ; the matrix

$$u^M := \{u_{j,l}^M\}_{j=1,\dots,N_p;l=1,\dots,N} \equiv \{u^M(x_j, t_l)\}_{j=1,\dots,N_p;l=0,1,\dots,N-1} \in \mathbb{R}^{N_p \times N} \tag{12}$$

is the solution of M , i.e., the background; $y := \{y(z_j, t_l)\}_{j=1,\dots,n_{obs};l=0,1,\dots,N-1} \in \mathbb{R}^{n_{obs} \times N}$: are the observations; $H_l \in \mathbb{R}^{n_{obs} \times N_p}$, $l = 0, \dots, N - 1$: is the linear approximation of the observation mapping \mathcal{H} ; $G \equiv G_{N-1} \in \mathbb{R}^{(N \times n_{obs}) \times N_p}$ is a block diagonal matrix $G \in \mathfrak{R}^{(N \times n_{obs}) \times (N_p \times N)}$ such that

$$G = \begin{cases} \text{diag} [H_0, H_1 M_{0,1}, \dots, H_{N-1} M_{N-2,N-1}] & N > 1; \\ H_0 & N = 1. \end{cases} \tag{13}$$

$R = \text{diag}(R_0, R_1, \dots, R_{N-1})$ and $B = VV^T$ are the covariance matrices of the errors on observations and on the background, respectively.

The Space and Time DA—Driven Domain Decomposition Method

The strength of the DD-DA approach is the exploitation of the coupling between the DA functional and the underlying PDE model. The idea goes back to the work of Schwarz [17] on overlapping domains and to Parallel in Time (PinT) methods, introduced by Lions [18]. Briefly, in DD-DA, DA acts as a predictor for the PDE-based local model, providing the approximations needed to locally solve the initial value problems on each subdomain, concurrently. Leveraging Schwarz and PinT methods’ consistency constraints for PDEs-based models, the DD-DA framework iteratively adjusts local solutions by adding the contribution of adjacent subdomains to the local filter, along overlapping regions. As a consequence, this approach increases the accuracy of local solutions and it allows us to apply in parallel both the fine and coarse solvers.

In the following, we briefly resume the method, according to its schematic description reported in Figure 2.

We describe the DD of $\Omega \times \Delta$ and of $\Omega_I \times \Delta_k$. The DD of $\Omega \times \Delta$ consists in decomposing $\Omega \subset \mathbb{R}^n$ into a set of subdomains Ω_i such that:

$$\Omega = \bigcup_{i=1}^{N_{sub}} \Omega_i \tag{14}$$

and consequently we define the set J_i , with cardinality ad_i , made of indices of subdomains adjacent to Ω_i :

$$J_i \subset \{1, \dots, N_{sub}\} \quad \text{and} \quad ad_i = |J_i|. \tag{15}$$

For $i = 1, \dots, N_{sub}$, we define the overlap regions Ω_{ij} :

$$\Omega_{ij} := \Omega_i \cap \Omega_j \neq \emptyset \quad \forall j \in J_i. \tag{16}$$

We define interfaces Γ_{ij} , for $i = 1, \dots, N_{sub}$:

$$\Gamma_{ij} := \partial\Omega_i \cap \Omega_j \quad j \in J_i. \tag{17}$$

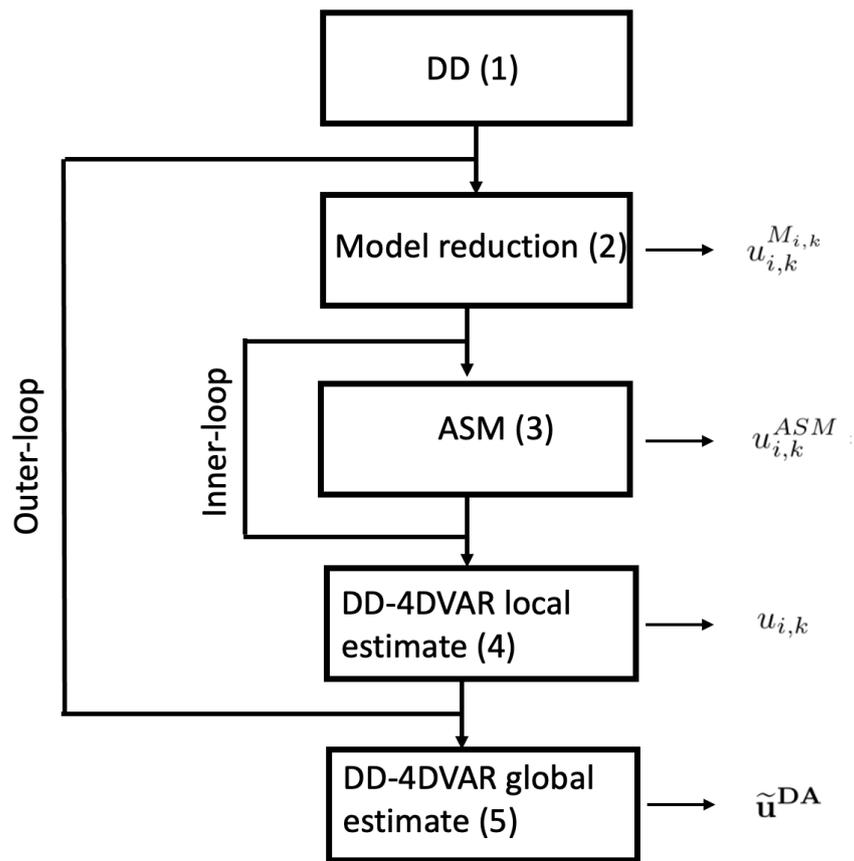


Figure 2. Schematic description of DD-DA algorithm. DD, local model, ASM (Additive Schwarz Method), DD-DA local solutions and global solution are identified. The Arabic numbers in parentheses refer to the corresponding module described in Section 2. For each module, we report its solution.

In the same way, time interval $\Delta \subset \mathbb{R}$ is decomposed into a sequence of intervals Δ_k such that:

$$\Delta = \bigcup_{k=1}^{N_t} \Delta_k.$$

Consequently, we define

$$\{\Omega_i \times \Delta_k\}_{i=1, \dots, N_{sub}; k=1, \dots, N_t} \tag{18}$$

as local domains.

DD of $\Omega_I \times \Delta_K$ defined in (7): for $i = 1, \dots, N_{sub}$, the set

$$\{x_{\tilde{i}}\}_{\tilde{i} \in I_i} \subset \Omega_i$$

is made of inner nodes of Ω_i where I_i is

$$I_i := \left\{ (i-1) \frac{N_p}{N_{sub}} + 1, \dots, i \frac{N_p}{N_{sub}} + \frac{\delta}{2} \right\}$$

such that

$$I = \bigcup_{i=1}^{N_{sub}} I_i. \tag{19}$$

I is the set of indices of inner nodes in Ω defined in (5) and

$$\delta := |I_{ij}| \tag{20}$$

where

$$I_{ij} := I_i \cap I_j \neq \emptyset, \quad \forall j \in J_i. \tag{21}$$

Selection of inner nodes belonging to the overlap regions $\{\Omega_{ij}\}_{i=1, \dots, N_{sub}, j \in J_i}$ proceeds in the same way. For $i = 1, \dots, N_{sub}$

$$\Omega_{I_i} \equiv \{x_{\tilde{j}}\}_{\tilde{j} \in I_{ij}} \subset \Omega_{ij}, \quad \forall j \in J_i$$

are the inner nodes of Ω_{ij} . Consequently, for $i = 1, \dots, N_{sub}$, we define the cardinality of I_i as the number of inner nodes of Ω_i and we denote it as

$$N_{loc} := |I_i| = \frac{N_p}{N_{sub}} + \frac{\delta}{2}. \tag{22}$$

Finally, the selection of time values in $\{\Delta_k\}_{k=1, \dots, N_t}$ proceeds as follows. For $k = 1, \dots, N_t$

$$\Delta_{K_k} \equiv \{t_{\tilde{k}}\}_{\tilde{k} \in K_k} \subset \Delta$$

are time values in Δ_k where K_k is defined as:

$$K_k := \left\{ (k-1) \frac{N}{N_t}, k \frac{N}{N_t} \right\},$$

where

$$K_k \cap K_{k+1} = \left\{ k \frac{N}{N_t} \right\} \neq \emptyset, \quad \forall k = 1, \dots, N_t - 1$$

and

$$N_k := |K_k| = \frac{N}{N_t}$$

is the cardinality of K_k , i.e., the number of time values belonging to K_k , such that

$$K = \bigcup_{k=1}^{N_t} K_k, \tag{23}$$

where K is defined in (6).

Consistently with Definition 1, for $i = 1, \dots, N_{sub}$ and $k = 1, \dots, N_t$

$$\Omega_{I_i} \times \Delta_{K_k} := \{(x_{\tilde{i}}, t_{\tilde{k}})\}_{\tilde{i} \in I_i, \tilde{k} \in K_k} \subset \Omega_i \times \Delta_k$$

is the local discrete domain/mesh.

For $i = 1, \dots, N_{sub}$ and $k = 1, \dots, N_t$, we pose

$$z_{i,k} = \{z(\tilde{i}, \tilde{k})\}_{\tilde{i} \in I_i, \tilde{k} \in K_k} \in \mathbb{R}^{N_{loc} \times N_k}$$

i.e., this is a vector defined on local domain $\Omega_i \times \Delta_k$.

We define the restriction and extension operators underlying the DD method.

Definition 3 (Restriction Operator). *Given $x \in \mathbb{R}^{N_p \times N}$ and $z \in \mathbb{R}^{N_p \times 1}$, for $i = 1, \dots, N_{sub}$ we define restriction of x to Ω_i by*

$$x/\Omega_i := R_i x = \{x(\tilde{i}, \tilde{k})\}_{\tilde{i} \in I_i, \tilde{k} \in K_k} \in \mathbb{R}^{N_{loc} \times 1} \tag{24}$$

$$x/\Omega_{ij} := R_{ij} x = \{x(\tilde{j}, \tilde{k})\}_{\tilde{j} \in I_{ij}, \tilde{k} \in K_k} \in \mathbb{R}^{\delta \times 1}$$

and restriction of y to $\Omega_i \times \Delta_k$ by

$$z/(\Omega_i \times \Delta_k) := \{z(\cdot, \tilde{k})\}_{\tilde{k} \in K_k} / \Omega_i = R_i \{z(\cdot, \tilde{k})\}_{\tilde{k} \in K_k} = \{z(\tilde{i}, \tilde{k})\}_{\tilde{i} \in I_i, \tilde{k} \in K_k} \in \mathbb{R}^{N_{loc} \times N_k}$$

$$z/(\Omega_{ij} \times \Delta_k) := \{z(\cdot, \tilde{k})\}_{\tilde{k} \in K_k} / \Omega_{ij} = R_{ij} \{z(\cdot, \tilde{k})\}_{\tilde{k} \in K_k} = \{z(\tilde{i}, \tilde{k})\}_{\tilde{i} \in I_{ij}, \tilde{k} \in K_k} \in \mathbb{R}^{N_{loc} \times N_k}$$

where I_i and I_{ij} are, respectively, set of indices of inner nodes in Ω_i and Ω_{ij} , $\forall j \in J_i$.

Definition 4 (Extension operator). If $x \in \mathbb{R}^{N_{loc} \times N_k}$, the Extension Operator (EO) is defined by

$$EO(x) := R_i^T x = \begin{cases} x(\tilde{i}, \tilde{k}) & \text{if } (\tilde{i}, \tilde{k}) \in I_i \times K_k \\ 0 & \text{elsewhere} \end{cases}$$

where R_i^T is the transpose of R_i in (24) and $EO(x) \equiv x^{EO}$.

For $n = 0, 1, \dots$ fixed, we now define the local model in each subdomain $\Omega_i \times \Delta_k$, where $i = 1, \dots, N_{sub}$ and $k = 1, \dots, N_t$. If $u_{i,k}^0 := \{u^M(x_i, t_k)\}_{\tilde{i} \in I_i, \tilde{k} \in K_k}$ is the background used as the initial value of the local model (see Figure 3), let $u_{i,k}^{M_{i,k}, n+1}$ be the solution of the problem $(P_{i,k}^{M_{i,k}, n})_{i=1, \dots, N_{sub}, k=1, \dots, N_t}$ where:

$$(P_{i,k}^{M_{i,k}, n})_{i=1, \dots, N_{sub}, k=1, \dots, N_t} : \begin{cases} u_{i,k}^{M_{i,k}, n} = M_{i,k} u_{i,k-1}^n + b_{i,k}^n, \\ u_{i,k-1}^n = u_{i,k-1}^{M_{i,k}, n} \\ u_{i,k}^n / \Gamma_{ij} = u_{j,k}^n / \Gamma_{ij}, \quad j \in J_i \end{cases} \quad (25)$$

In (25) $u_{i,k}^M$ and $b_{i,k}^n$ are, respectively, the background in $\Omega_i \times \Delta_k$ and the vector accounting boundary conditions of Ω_i and

$$M_{i,k} := M_k / \Omega_i \quad (26)$$

is the restriction to Ω_i of the matrix

$$M_k \equiv M_{\bar{s}_{k-1}, \bar{s}_k} := M_{\bar{s}_{k-1}, \bar{s}_{k-1}+1} \cdots M_{\bar{s}_{k-1}, \bar{s}_k}. \quad (27)$$

where

$$\bar{s}_k := \sum_{j=1}^{k-1} N_j - (N - 1) \quad \text{and} \quad \bar{s}_0 := 0 \quad (28)$$

are the first index of Δ_{K_k} and Δ_{K_1} , respectively.

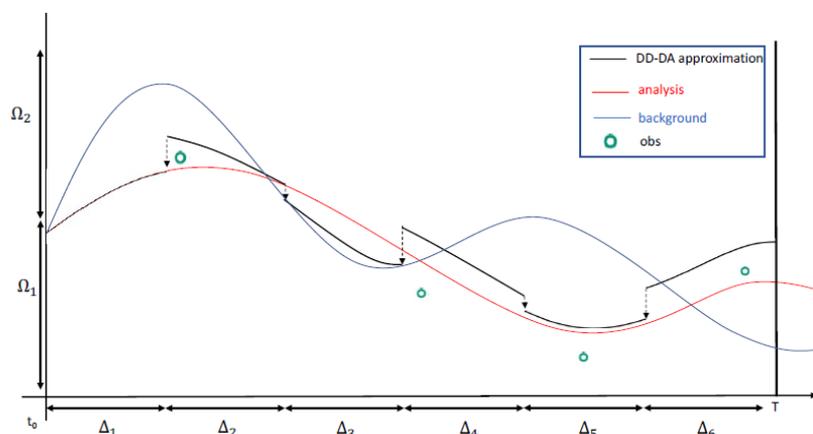


Figure 3. Initial conditions of local models in $\Omega_i \times \Delta_k$.

Let:

$$(P_{i,k}^n)_{i=1,\dots,N_{sub},k=1,\dots,N_t} : u_{i,k}^{ASM,n} = \arg \min_{u_{i,k}^n} J_{i,k}(u_{i,k}^n) \tag{29}$$

be the local 4DVAR DA model with

$$J_{i,k}(u_{i,k}^n) := J(u_{i,k}^n)/(\Omega_i \times \Delta_k) + \mathcal{O}_{ij}. \tag{30}$$

We let

$$\mathcal{O}_{ij} := \sum_{j \in J_i} \beta_j \|u_{i,k}^n/\Omega_{ij} - u_{j,k}^n/\Omega_{ij}\|_{\mathbf{B}_{ij}^{-1}}^2 \tag{31}$$

denote the overlapping operator in Γ_{ij} , and

$$J_{i,k}(u_{i,k}^n)/(\Omega_i \times \Delta_k) := \alpha_{i,k} \|u_{i,k}^n - u_{i,k}^{M_{i,k},n}\|_{\mathbf{B}_i^{-1}} + \|G_{i,k}u_{i,k}^n - y_{i,k}\|_{\mathbf{R}_i^{-1}}^2$$

denote the restriction of \mathbf{J} to $\Omega_i \times \Delta_k$ where $G_{i,k}$ is the restriction of G to $\Delta_i \times \Omega_k$. Parameters $\alpha_{i,k}$ and β_j in (31) are the regularization parameters. For simplicity, we assume that $\alpha_{i,k} = \beta_j = 1$, for $j \in J_i$.

The gradient of $J_{i,k}$ is [16]:

$$\nabla J_{i,k}(\mathbf{w}_{i,k}^n) = (\mathbf{V}_i^T(G_{i,k})^T(\mathbf{R}_{i,k})^{-1}G_{i,k}\mathbf{V}_i + I_i + ad_i \times \mathbf{B}_{ij})\mathbf{w}_{i,k}^n - \mathbf{c}_i + \sum_{j \in J_i} \mathbf{B}_{ij}\mathbf{w}_{j,k}^n, \tag{32}$$

where

$$\mathbf{w}_{i,k}^n = \mathbf{V}_i^{-1}(u_{i,k}^n - u_{i,k}^{M_{i,k},n}), \tag{33}$$

$$\mathbf{d}_i = (\mathbf{v}_i - G_{i,k}u_{i,k}^{M_{i,k},n}), \quad \mathbf{c}_i = (\mathbf{V}_i^T(G_{i,k})^T(\mathbf{R}_{i,k})^{-1}\mathbf{d}_i)$$

where $B_i = V_i V_i^T$ and I_i is the identity matrix. The solution of $(P_{i,k}^n)_{i=1,\dots,N_{sub},k=1,\dots,N_t}$ is obtained by requiring that $\nabla J_{i,k}(\mathbf{w}_{i,k}^n) = 0$. This requirement leads to the linear system:

$$A_{i,k}\mathbf{w}_{i,k}^n = c_i - \sum_{j \in J_i} \mathbf{B}_{ij}\mathbf{w}_{j,k}^n, \tag{34}$$

where

$$A_{i,k} = (\mathbf{V}_i^T(G_{i,k})^T\mathbf{R}_{i,k}^{-1}G_{i,k}\mathbf{V}_i + I_i + ad_i \times \mathbf{B}_{ij}). \tag{35}$$

where ad_i are the number of subdomains adjacent to Ω_i .

For each n , the r.h.s. of (34) depends on unknown value $\mathbf{w}_{j,k}^n$ defined on those Ω_{ij} , where $j \in J_i$, which are adjacent to Ω_i . According to the Additive Schwarz Method (ASM) [19] for $r = 0, 1, \dots, \bar{r}$ we solve

$$A_{i,k}\mathbf{w}_{i,k}^{r+1,n} = c_i - \sum_{j \in J_i} \mathbf{B}_{ij}\mathbf{w}_{j,k}^r, \tag{36}$$

by using Conjugate Gradient (CG) method where at step $r + 1$, then Ω_i receives $\mathbf{w}_{i,k}^{r,n}$ from Ω_{ij} , where $j \in J_i$, for computing the r.h.s. of (36) and finally it sends $\mathbf{w}_{i,k}^{r+1,n}$ to Ω_{ij} , where $j \in J_i$, for updating the r.h.s. of (36) is needed for the next iteration. At step 0, $\mathbf{w}_{i,k}^{0,n}$ is an arbitrary initial value.

Finally, we pose

$$\mathbf{w}_{i,k}^n \equiv \mathbf{w}_{i,k}^{\bar{r},n},$$

and consequently we have that

$$u_{i,k}^{ASM,n} := u_{i,k}^{ASM,\bar{r}}. \tag{37}$$

The local solution update is performed by using (25) and (33):

$$u_{i,k}^{n+1} = u_{i,k}^{M_{i,k}^{n+1}} + \mathbf{V}_i \mathbf{w}_{i,k}^n = u_{i,k}^{M_{i,k}^{n+1}} + [u_{i,k}^{ASM,n} - u_{i,k}^{M_{i,k}^n}]. \tag{38}$$

The global solution in $\Omega \times \Delta$ is

$$\tilde{\mathbf{u}}^{DD-DA,n} := \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} (u_{i,k}^n)^{EO}. \tag{39}$$

where $(u_{i,k}^n)^{EO}$ is the extension to $\Omega \times \Delta$ of local approximations computed in $\Omega_i \times \Delta_k$. For simplicity, we let

$$\tilde{\mathbf{u}}^{DD-DA} := \tilde{\mathbf{u}}^{DD-DA,\bar{n}} \tag{40}$$

be the solution in $\Omega \times \Delta$.

Note that $\mathbf{B}_i = R_i \mathbf{B} R_i^T$ and $\mathbf{B}_{ij} := \mathbf{B} / \Gamma_{ij} = R_i \mathbf{B} R_{ij}^T$ are the restrictions of the covariance matrix \mathbf{B} , respectively, to subdomain Ω_i and interface Γ_{ij} defined in (17), while $G_{i,k}$, and $\mathbf{R}_{i,k}$ are the restriction of $G_k := G_{\bar{s}_k}$ and of $\mathbf{R}_k := \text{diag}(\mathbf{R}_0, \mathbf{R}_1, \dots, \mathbf{R}_{\bar{s}_k})$ to Ω_i and, finally, $u_{i,k}^M = R_i u_k^M$, $u_{i,k}^{n+1} / \Gamma_{ij} = R_{ij} u_{i,k}^{n+1}$, $u_{j,k}^n / \Gamma_{ij} = R_{ij} u_k^n$ are the restriction of vectors u_k^b , $u_{i,k}^{n+1}$, $u_{j,k}^n$ to Ω_i and to Γ_{ij} , for $i = 1, 2, \dots, N_{sub}$ and $j \in J_i$.

In [11,12], the authors proved that the minimum of \mathbf{J} can be obtained by patching together local solutions obtained as the minimum of local functions $\mathbf{J}_{i,k}$. In this way, the global minimum can be searched for among the global minima of the local functional.

3. Sensitivity Analysis

As already said, the core of the DD-DA approach is that the DA model acts as coarse/predictor operator to solve the local PDE model by providing the background values as initial conditions of the local PDE models. Then, we analyze the propagation of the errors with respect to the time direction. In the following, we use $\|\cdot\| = \|\cdot\|_2$. We refer to $\|z_{i,k}\|_2 = \|\{z_{i,k}(\bar{i}, \bar{k})\}_{\bar{i} \in I_i, \bar{k} \in K_k}\|_2$ where $z \in R^{N_p \times N}$ and $z_{i,k} := z / (\Omega_i \times \Delta_k)$ and I_i and K_k are defined in (19) and (23), respectively.

Lemma 1. [20] *Let $R > 0$ and $T \geq 0$ be two positive constant quantities. If we have a sequence E_k which is such that for $k = 1, \dots, N_t$:*

$$|E_k| \leq (1 + R)|E_{k-1}| + T$$

then it holds:

$$|E_k| \leq e^{N_t R} |E_1| + \frac{e^{N_t R} - 1}{R} T.$$

Definition 5. *Let $u_{i,k}^{n+1}$ and $\tilde{u}_{i,k}^{n+1}$ be, respectively, the numerical solution at step $(n + 1)$ in (38) and the corresponding floating point representation. Fixed n , for $i = 1, \dots, N_{sub}$, $k = 1, \dots, N_t$ let*

$$R_{i,k}^{n+1} := u_{i,k}^{n+1} - \tilde{u}_{i,k}^{n+1} \tag{41}$$

denote the round-off error in $\Omega_i \times \Delta_k$.

From (25), the numerical solution at step $(n + 1)$ can be written as follows:

$$\begin{aligned} u_{i,k}^{n+1} &= (M_{i,k} u_{i,k-1}^{n+1} + b_{i,k}^{n+1}) + [u_{i,k}^{ASM,n} - (M_{i,k} u_{i,k-1}^n + b_{i,k}^n)] \\ &= M_{i,k} u_{i,k-1}^{n+1} + \delta(u_{i,k}^n) \end{aligned}$$

consequently, the corresponding floating point representation is

$$\tilde{u}_{i,k}^{n+1} = M_{i,k} \tilde{u}_{i,k-1}^{n+1} + \delta(\tilde{u}_{i,k}^n) + \rho_k^{n+1}$$

where $\delta(u_{i,k}^n) := (u_{i,k}^{ASM,n} - M_{i,k}u_{i,k-1}^n) + (b_{i,k}^{n+1} - b_{i,k}^n)$ and ρ_k^{n+1} is the local round-off error. Fixed $n + 1$, we have that

$$\begin{aligned} \|R_{i,k}^{n+1}\| &= \|u_{i,k}^{n+1} - \tilde{u}_{i,k}^{n+1}\| = \|M_{i,k}u_{i,k-1}^{n+1} + \delta(u_{i,k}^n) - M_{i,k}\tilde{u}_{i,k-1}^{n+1} - \delta(\tilde{u}_{i,k}^n) - \rho_k^{n+1}\| \\ &\leq \|M_{i,k}u_{i,k-1}^{n+1} - M_{i,k}\tilde{u}_{i,k-1}^{n+1}\| + \|\delta(u_{i,k}^n) - \delta(\tilde{u}_{i,k}^n)\| + |\rho_k^{n+1}| \\ &\leq \|M_{i,k}\| \|u_{i,k-1}^{n+1} - \tilde{u}_{i,k-1}^{n+1}\| + \|u_k^{ASM,n} - \tilde{u}_k^{ASM,n}\| \\ &\quad + \|M_{i,k}u_{i,k-1}^n + b_{i,k}^n - (M_{i,k}\tilde{u}_{i,k-1}^n + \tilde{b}_{i,k}^n)\| + \|b_k^{n+1} - \tilde{b}_{i,k}^{n+1}\| \\ &\quad + |\rho_k^{n+1}|; \end{aligned}$$

from (25) it is

$$\|b_{i,k}^{n+1} - \tilde{b}_{i,k}^{n+1}\| = \|M_{i,k}u_{i,k-1}^{n+1} - M_{i,k}\tilde{u}_{i,k-1}^{n+1}\|$$

and according to [16] we let $\mu(M_{i,k}) \geq \|M_{i,k}\|$, where $\mu(M_{i,k})$ denotes the condition number of $M_{i,k}$, then

$$\begin{aligned} \|R_{i,k}^{n+1}\| &\leq \mu(M_i^k) \|u_{i,k-1}^{n+1} - \tilde{u}_{i,k-1}^{n+1}\| + \|u_k^{ASM,n} - \tilde{u}_k^{ASM,n}\| + \|u_{i,k}^{M_{i,k},n} - \tilde{u}_{i,k}^{M_{i,k},n}\| \\ &\quad + \mu(M_{i,k}) \|u_{i,k-1}^{n+1} - \tilde{u}_{i,k-1}^{n+1}\| + \mu(M_{i,k}) \|u_{i,k-1}^n - \tilde{u}_{i,k-1}^n\| + |\rho_i^k| \end{aligned}$$

and in compact form

$$\|R_k^{n+1}\| \leq 2\mu(M_{i,k}) \|R_{i,k-1}^{n+1}\| + \|R_{i,k}^{ASM,n}\| + \|R_{i,k}^{M_{i,k},n}\| + \mu(M_{i,k}) \|R_{i,k-1}^n\| + |\rho_i^k|$$

where

$$R_{i,k}^{ASM,n} := u_{i,k}^{ASM,n} - \tilde{u}_{i,k}^{ASM,n} \quad R_{i,k}^{M_{i,k},n} := u_{i,k}^{M_{i,k},n} - \tilde{u}_{i,k}^{M_{i,k},n}. \tag{42}$$

Using Lemma 1, with $R = 2\mu(M_{i,k}) - 1$ and $H = R_{i,k}^{ASM,n} + R_{i,k}^{M_{i,k},n+1} + \mu(M_{i,k})R_{i,k-1}^n + \rho_i^k$, it follows that:

$$\|R_k^{n+1}\| \leq e^{N_i R} \|R_{i,1}^{n+1}\| + \frac{e^{N_i R} - 1}{R_{\mu(M_{i,k})}} \left[\|R_{i,k}^{ASM,n}\| + \|R_{i,k}^{M_{i,k},n}\| + \mu(M_{i,k}) \|R_{i,k-1}^n\| + \rho_i^k \right].$$

then, it is

$$\|R_k^{n+1}\| \leq e^{N_i R} \|R_{i,1}^{n+1}\| + \frac{e^{N_i R} - 1}{R} \left[\|R_{i,k}^{ASM,n}\| + \|R_{i,k}^{M_{i,k},n}\| + \|R_{i,k-1}^n\| \right] + \frac{e^{N_i R} - 1}{R} \rho_i^k. \tag{43}$$

The upper bound in (43) is made of three terms: the first one represents the propagation of the error introduced on the first time interval, the second one represents the propagation of the error introduced at the previous step and the last term depends on the local round-off error. In particular, we note that, as expected, round-off error propagation grows with N_t , i.e., the number of subdomains of Δ .

3.1. Convergence, Consistence and Stability of DD-DA Method

In [12], we proved the convergence of the outer loop, i.e.:

$$\lim_{n \rightarrow \infty} \|\tilde{\mathbf{u}}^{DD-DA,n+1} - \tilde{\mathbf{u}}^{DD-DA,n}\| = 0 \tag{44}$$

where $\mathbf{u}^{DA,n}$ is defined in (39). The convergence of ASM is proved in [19].

3.1.1. Consistence

We analyze the consistence in terms of the local truncation errors $E_{i,k}^{M_{i,k}}$, $E_{i,k}^{ASM}$, $E_{i,k}$ and E_g , which are reported in Figure 4.

Similar to [21], local truncation errors $E_{i,k}^{M_{i,k}}$, $E_{i,k}^{ASM}$, $E_{i,k}$ in $\Omega_i \times \Delta_k$ and E^{glob} in $\Omega \times \Delta$ are defined as the remainder after the solutions u^M of the model (1) and the solution \mathbf{u}^{DA}

of the 4D-DA problem (8) are substituted into the discrete models. To this aim, we give the following definitions.

Definition 6. We define

$$u^{\mathcal{M} \rightarrow M} := M \cdot \{u^{\mathcal{M}}(x_i, t_k)\}_{\tilde{i} \in I; \tilde{k} \in K} \tag{45}$$

as the approximation in $\Omega \times \Delta$ of $u^{\mathcal{M}}$, defined in (1), obtained by replacing $u^{\mathcal{M}}$ evaluated in $\Omega_I \times \Delta_K$ and defined in (1), into M , which is defined in (11).

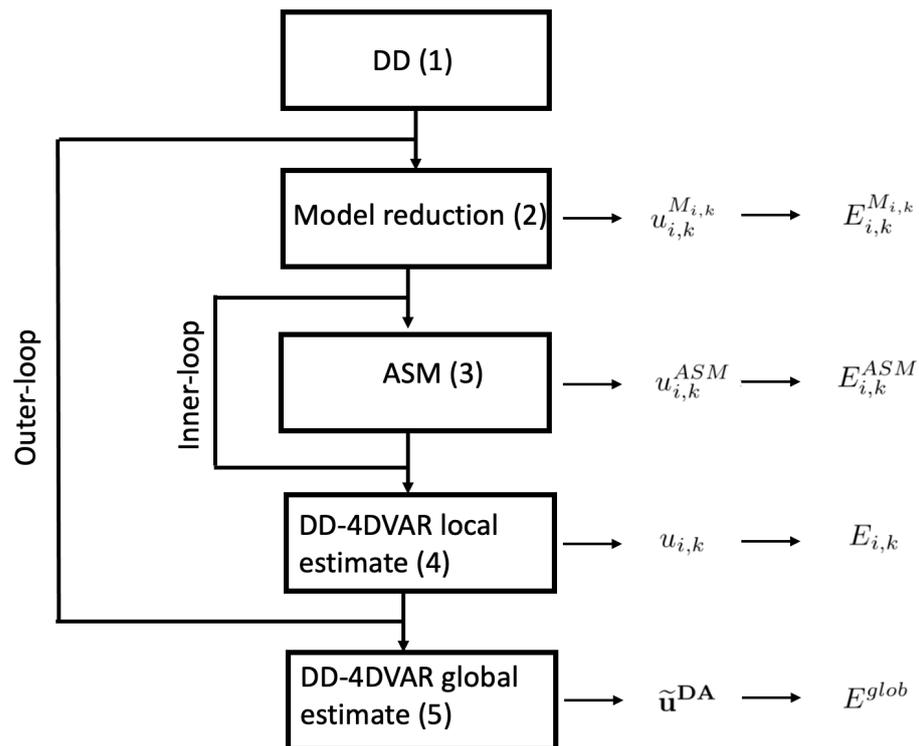


Figure 4. Local truncation errors related to each module of DD-DA.

Definition 7 (Local truncation errors in $\Omega_i \times \Delta_k$). $\forall i = 1, \dots, N_{sub}$ and $k = 1, \dots, N_t$, at iteration \bar{n} , we define

$$E_{i,k}^{M_{i,k},\bar{n}} := \left\| u^{\mathcal{M} \rightarrow M} / (\Omega_i \times \Delta_k) - u_{i,k}^{M_{i,k},\bar{n}} \right\| \tag{46}$$

as the local truncation error of $M_{i,k}$ restricted to $\Omega_i \times \Delta_k$;

$$E_{i,k}^{ASM,\bar{n}} := \left\| \mathbf{u}^{DA} / (\Omega_i \times \Delta_k) - u_{i,k}^{ASM,\bar{n}} \right\| \tag{47}$$

as the local truncation error of ASM restricted to $\Omega_i \times \Delta_k$;

$$E_{i,k}^{\bar{n}} := \left\| \mathbf{u}^{DA} / (\Omega_i \times \Delta_k) - u_{i,k}^{\bar{n}} \right\| \tag{48}$$

as the local truncation error of DD-DA restricted to $\Omega_i \times \Delta_k$;

$$E^{glob} := \left\| \mathbf{u}^{DA} - \tilde{\mathbf{u}}^{DD-DA} \right\| \tag{49}$$

as the local truncation error of DD-DA in $\Omega \times \Delta$.

The DD-4DVAR method needs few iterations of the outer loop over n to update the approximation in (38). Consequently, in the following analysis, we neglect the dependency on \bar{n} of $u_{i,k}^{M_{i,k},\bar{n}}$, $u_{i,k}^{ASM,\bar{n}}$ and $u_{i,k}^n$, defined, respectively, in (25), (29) and (38) and $E_{i,k}^{M_{i,k},\bar{n}}$, $E_{i,k}^{ASM,\bar{n}}$ and $E_{i,k}^{\bar{n}}$ in $\Omega_i \times \Delta_k$, defined, respectively, in (46), (47) and (48).

For $i = 1, \dots, N_{sub}$ and $k = 1, \dots, N_t$, we pose

$$\tilde{u}_{i,k} := u_{i,k}^{\bar{n}}. \tag{50}$$

From (50), the approximation in $\Omega \times \Delta$ defined in (40) becomes

$$\tilde{u}^{DD-DA} = \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} \tilde{u}_{i,k}^{EO}. \tag{51}$$

For $i = 1, \dots, N_{sub}$ and $k = 1, \dots, N_t$, we pose

$$u_{i,k}^{ASM} = u_{i,k}^{ASM,\bar{n}}; u_{i,k}^{M_{i,k}} = u_{i,k}^{M_{i,k},\bar{n}}; u_{i,k} = u_{i,k}^{\bar{n}}. \tag{52}$$

Consequently, from (52) we pose

$$E_{i,k}^{M_{i,k}} = E_{i,k}^{M_{i,k},\bar{n}}, \tag{53}$$

as the local model truncation error in $\Omega_i \times \Delta_k$;

$$E_{i,k}^{ASM} = E_{i,k}^{ASM,\bar{n}}, \tag{54}$$

as the local ASM truncation error in $\Omega_i \times \Delta_k$ in (47);

$$E_{i,k} = E_{i,k}^{\bar{n}}. \tag{55}$$

as the local truncation error $\Omega_i \times \Delta_k$ in (48).

We introduce the definition of consistency of the DD-DA method. We pose $\|\cdot\| = \|\cdot\|_2$. (We refer to $\|z_{i,k}\|_2 = \|\{z_{i,k}(\bar{i}, \bar{k})\}_{\bar{i} \in I_i, \bar{k} \in K_k}\|_2$ where $z \in R^{N_p \times N}$ and $z_{i,k} := z / (\Omega_i \times \Delta_k)$ and I_i and K_k are defined in (19) and (23), respectively).

Definition 8 (Consistency of DD-DA method). *The DD-DA method is said to be consistent if*

$$\lim_{\Delta x, \Delta t \rightarrow 0} E_g = 0$$

where

$$\Delta x := \max_{i=1, \dots, N_{sub}} (\Delta x)_i$$

and $\{(\Delta x)_i\}_{i=1, \dots, N_{sub}}$ are spatial-step sizes of $M_{i,k}$;

$$\Delta t := \max_{k=1, \dots, N_t} (\Delta t)_k$$

and $\{(\Delta t)_k\}_{k=1, \dots, N_t}$ are time-step sizes of $M_{i,k}$.

In order to prove the consistency, we perform the analysis of local truncation errors $E_{i,k}^{M_{i,k}}$, $E_{i,k}^{ASM}$, $E_{i,k}$ and E^{glob} , defined, respectively, in (53), (54), (55) and (49).

Assumption 1. (Local truncation error of Model in $\Omega_i \times \Delta_k$) Let

$$E_{i,k}^{M_{i,k}} = \mathcal{O}((\Delta x)_i^p + (\Delta t)_k^q), \quad \forall (i,k) \in \{1, \dots, N_{sub}\} \times \{1, \dots, N_t\} \tag{56}$$

be the local truncation error defined in (53) where $(\Delta x)_i$ and $(\Delta t)_k$ are spatial and temporal step sizes of $M_{i,k}$, defined in (26), and p and q are the order of convergence in space and in time. In the

experimental results (see Section 4), in order to discretize the Shallow Water Equations (SWEs) model, we consider Lax–Wendroff scheme [22]. Hence, in that case, $p = q = 2$.

Lemma 2 (Local truncation error of ASM in $\Omega_i \times \Delta_k$). *Let us consider the following quantities: σ_0^2 , observational error variance; $\mathbf{B}_i = \mathbf{V}_i \mathbf{V}_i^T$, restriction to Ω_i of covariance matrices of the error on background; $G_{i,k}$, restriction to $\Omega_i \times \Delta_k$ of matrix G defined in (13); ad_i , number of subdomains adjacent to Ω_i , defined in (15); $\mathbf{B}_{ij} = \mathbf{V}_{ij} \mathbf{V}_{ij}^T$, restriction to Ω_{ij} of the covariance matrix of the error on the background; $\mu(\mathbf{V}_i)$, $\mu(G_{i,k})$, $\mu(M_{i,k})$ and $\mu(\mathbf{V}_{ij})$, condition number of \mathbf{V}_i , $G_{i,k}$, $M_{i,k}$ and \mathbf{V}_{ij} , respectively. Then, $\forall i = 1, \dots, N_{sub}$ and $k = 1, \dots, N_t$, it holds that:*

$$E_{i,k}^{ASM} \leq \mu_{i,k}^{DD-DA} \times E_{i,1}^{ASM} \tag{57}$$

where

$$\mu_{i,k}^{DD-DA} := \left[1 + \frac{1}{\sigma_0^2} \mu^2(\mathbf{V}_i) \mu^2(G_{i,k}) + ad_i \times \mu^2(\mathbf{V}_{ij}) \right] \mu(M_{i,k}). \tag{58}$$

Proof. As in [16], it is

$$\|\mathbf{u}^{DA}/(\Omega_i \times \Delta_k) - u_{i,k}^{ASM}\| \leq \mu(\mathbf{J}_{i,k}) \mu(M_{i,k}) \times \|\mathbf{u}^{DA}/(\Omega_i \times \Delta_1) - u_{i,1}^{ASM}\| \tag{59}$$

where $\|\mathbf{u}^{DA}/(\Omega_i \times \Delta_1) - u_{i,1}^{ASM}\|$ is the error in $\Omega_i \times \Delta_1$. As proved in [16], it is

$$\mu(\mathbf{J}_{i,k}) = \mu(A_{i,k}) \tag{60}$$

where $\mathbf{J}_{i,k}$ and $A_{i,k}$ are, respectively, defined in (30) and (35), and by using triangle inequality, it is

$$\mu(A_{i,k}) \leq 1 + \frac{1}{\sigma_0^2} \mu^2(\mathbf{V}_i) \mu^2(G_{i,k}) + ad_i \times \mu(\mathbf{B}_{ij}) \tag{61}$$

$$\leq 1 + \frac{1}{\sigma_0^2} \mu^2(\mathbf{V}_i) \mu^2(G_{i,k}) + ad_i \times \mu^2(\mathbf{V}_{ij}), \tag{62}$$

From (59) and (61), the (57) follows. \square

Theorem 1. (Local truncation error in $\Omega_i \times \Delta_k$) $\forall i = 1, \dots, N_{sub}; k = 1, \dots, N_t$, it holds that:

$$E_{i,k} \leq \mu_{i,k}^{DD-DA} \times E_{i,1}^{ASM} + 2 \times E_{i,k}^{M_{i,k}} \tag{63}$$

where $\mu_{i,k}^{DD-DA}$ is defined in (58).

Proof. From (52) and (38), $E_{i,k}$ defined in (55) can be rewritten as follows:

$$E_{i,k} := \|\mathbf{u}^{DA}/(\Omega_i \times \Delta_k) - u_{i,k}\| = \|\mathbf{u}^{DA}/(\Omega_i \times \Delta_k) - u_{i,k}^{M_{i,k},\bar{n}} - (u_{i,k}^{ASM,\bar{n}-1} - u_{i,k}^{M_{i,k},\bar{n}-1})\|;$$

by using the triangle inequality, it is

$$E_{i,k} \leq \|\mathbf{u}^{DA}/(\Omega_i \times \Delta_k) - u_{i,k}^{ASM,\bar{n}}\| + \|u_{i,k}^{M_{i,k},\bar{n}-1} - u_{i,k}^{M_{i,k},\bar{n}}\|; \tag{64}$$

as consequence of Lemma 2 and (54), we have that

$$E_{i,k} \leq \mu_{i,k}^{DD-DA} \times E_{i,1}^{ASM} + \|u_{i,k}^{M_{i,k},\bar{n}-1} - u_{i,k}^{M_{i,k},\bar{n}}\| \tag{65}$$

where $E_{i,1}^{ASM}$ is defined in (54) and $\mu_{i,k}^{DD-DA}$ is defined in (58). In particular, by adding and subtracting $u^{M \rightarrow M} / (\Omega_i \times \Delta_k)$ in $\|u_{i,k}^{M_{i,k,\bar{n}-1}} - u_{i,k}^{M_{i,k,\bar{n}}}\|$, we obtain:

$$\begin{aligned} \|u_{i,k}^{M_{i,k,\bar{n}-1}} - u_{i,k}^{M_{i,k,\bar{n}}}\| &= \|(u_{i,k}^{M_{i,k,\bar{n}-1}} - u^{M \rightarrow M} / (\Omega_i \times \Delta_k)) \\ &\quad + (u^{M \rightarrow M} / (\Omega_i \times \Delta_k) - u_{i,k}^{M_{i,k,\bar{n}}})\| \end{aligned}$$

and by using the triangle inequality

$$\begin{aligned} \|u_{i,k}^{M_{i,k,\bar{n}-1}} - u_{i,k}^{M_{i,k,\bar{n}}}\| &\leq \|u_{i,k}^{M_{i,k,\bar{n}-1}} - u^{M \rightarrow M} / (\Omega_i \times \Delta_k)\| \\ &\quad + \|u^{M \rightarrow M} / (\Omega_i \times \Delta_k) - u_{i,k}^{M_{i,k,\bar{n}}}\| \\ &= E_{i,k}^{M_{i,k,\bar{n}}} + E_{i,k}^{M_{i,k,\bar{n}-1}}. \end{aligned} \tag{66}$$

$\{\tilde{\mathbf{u}}^{DD-DA,n}\}_{n \in \mathbb{N}}$ is a convergent sequence, then it is a Cauchy sequence. From (39), we find that $\{u_{i,k}^{M_{i,k,n}}\}_{n \in \mathbb{N}}$ is also a Cauchy sequence, i.e.,

$$\forall \epsilon > 0 \exists \mathbf{N} > 0 : \|u_{i,k}^{M_{i,k,n}} - u_{i,k}^{M_{i,k,m}}\| \leq \epsilon \quad \forall n, m > \mathbf{N}. \tag{67}$$

In particular, the equation (67) is true for $n = \bar{n}$ and $m = \bar{n} - 1$, assuming that \bar{n} is large enough. Consequently, we can neglect the dependency on the outer loop in $E_{i,k}^{M_{i,k,\bar{n}}}$ and $E_{i,k}^{M_{i,k,\bar{n}-1}}$ in (66), i.e.,

$$\|u_{i,k}^{M_{i,k,\bar{n}-1}} - u_{i,k}^{M_{i,k,\bar{n}}}\| \leq 2E_{i,k}^{M_{i,k}} \tag{68}$$

where $E_{i,k}^{M_{i,k}}$ is defined in (53). From (65), (66) and (68), we obtain the thesis in (63). \square

Lemma 3. *If e_0 , the error on initial condition of M in (11) is equal to zero, i.e.,*

$$e_0 = 0 \tag{69}$$

then

$$E_{i,k} \leq c((\Delta x)_i^p + (\Delta t)_k^q) \tag{70}$$

where $E_{i,k}$ is the local truncation error defined in (55) and c is positive constant independent on DD .

Proof. By applying Theorem 1 to $E_{i,1}^{ASM}$ on $\Omega_i \times \Delta_1$, we obtain

$$E_{i,1}^{ASM} \leq F_{i,1}e_0 / \Omega_i. \tag{71}$$

where $F_{i,1}$ is defined in (58) and e_0 / Ω_i is the restriction of e_0 to Ω_i . As it is $e_0 / \Omega_i = 0$, then by replacing $e_0 / \Omega_i = 0$ in (71), it results that

$$E_{i,1}^{ASM} = 0 \tag{72}$$

consequently, we have that

$$E_{i,k}^{ASM} = 0. \tag{73}$$

From (73), (56) and (63), we obtain the thesis in (70). \square

Theorem 2. *(Truncation error in $\Omega \times \Delta$) Under the assumption of Lemma 3 in (69), the truncation error in $\Omega \times \Delta$ is such that*

$$E^{glob} \leq c(N_{sub}N_t)[(\Delta x)^p + (\Delta t)^q], \tag{74}$$

where $c > 0$ is a positive constant independent on DD .

Proof. From (51), it results that E^{glob} , which is defined in (49), can be rewritten as follows:

$$E^{glob} := \left\| \mathbf{u}^{DA} - \tilde{\mathbf{u}}^{DD-DA} \right\| = \left\| \mathbf{u}^{DA} - \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} \tilde{\mathbf{u}}_{i,k} \right\|$$

by applying the restriction and extension operator (Definitions 3 and 4) to \mathbf{u}^{DA} , we obtain

$$E^{glob} = \left\| \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} \left[(\mathbf{u}^{DA} / (\Omega_i \times \Delta_k))^{EO} - \tilde{\mathbf{u}}_{i,k} \right] \right\|$$

by using the triangle inequality, it is

$$\begin{aligned} E_g &= \left\| \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} \left[(\mathbf{u}^{DA} / (\Omega_i \times \Delta_k))^{EO} - \tilde{\mathbf{u}}_{i,k} \right] \right\| \\ &\leq \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} \left\| (\mathbf{u}_{i,k}^{DA})^{EO} - \tilde{\mathbf{u}}_{i,k} \right\| = \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} E_{i,k} \end{aligned} \tag{75}$$

where $E_{i,k}$ is defined in (55). From Lemma 3, we have

$$\begin{aligned} \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} E_{i,k} &\leq c \sum_{i=1}^{N_{sub}} \sum_{k=1}^{N_t} ((\Delta x)_i^p + (\Delta t)_k^q) \\ &= c \left[N_t \sum_{i=1}^{N_{sub}} (\Delta x)_i^p + N_{sub} \sum_{k=1}^{N_t} (\Delta t)_k^q \right], \end{aligned} \tag{76}$$

and consequently

$$E^{glob} \leq c \left[N_t \sum_{i=1}^{N_{sub}} (\Delta x)_i^p + N_{sub} \sum_{k=1}^{N_t} (\Delta t)_k^q \right].$$

By defining

$$\begin{aligned} \Delta x &:= \max_{i=1, \dots, N_{sub}} (\Delta x)_i \\ \Delta t &:= \max_{k=1, \dots, N_t} (\Delta t)_k \end{aligned}$$

we obtain

$$\begin{aligned} E^{glob} &\leq c \left[N_t \sum_{i=1}^{N_{sub}} (\Delta x)_i^p + N_{sub} \sum_{k=1}^{N_t} (\Delta t)_k^q \right] \\ &\leq c \left[N_t \sum_{i=1}^{N_{sub}} (\Delta x)^p + N_{sub} \sum_{k=1}^{N_t} (\Delta t)^q \right] \\ &\leq c(N_{sub} N_t) [(\Delta x)^p + (\Delta t)^q]. \end{aligned}$$

Hence, the (74) is proved. \square

3.1.2. Stability

Now, we prove the stability of the method with respect to the time direction, and assuming that the predictive model is stable. We will perform SA by obtaining worst-case error bounds with the aid of the condition number.

We assume that the discrete scheme applied to the model \mathcal{M} in (1) is stable, i.e., $\exists D > 0$ such that

$$\|u^M - v^M\| \leq D e_0, \tag{77}$$

where u^M is the computed solution of M in (11) and v^M is the solution of \bar{M} , where \bar{M} is obtained by adding error e_0 to initial condition of M . For simplicity of notations in the sequel, we omit any subscripts of \mathcal{M} .

Definition 9 (Propagation error from Δ_{k-1} to Δ_k). Let $\tilde{v}^{\text{DD-DA}}$ be the solution in $\Omega \times \Delta$ computed by adding the perturbation e_k to the initial condition of $P_{i,k}^{M_{i,k}^n}$, defined in (25). We define

$$\bar{E}_k := \|\tilde{\mathbf{u}}^{\text{DD-DA}} / \Delta_k - \tilde{\mathbf{v}}^{\text{DD-DA}} / \Delta_k\| \tag{78}$$

as the propagation error from Δ_{k-1} to Δ_k .

Theorem 3 (Stability). If the error on initial condition of M in (11), is equal to zero, i.e.,

$$e_0 = 0 \tag{79}$$

then, $\forall k = 1, \dots, N_t \exists C_k > 0$ such that

$$\bar{E}_k \leq C_k \bar{e}_k$$

where C_k is a constant depending on the model and on the ASM; \bar{e}_k is the perturbation on the initial condition of $P_{i,k}^{M_{i,k}}$, defined in (25).

Proof. To simplify the notations in the proof, we consider $\bar{e}_k = \bar{e}$, $\forall k = 1, \dots, N_t$. From (38), (52) and using the triangle inequality, we obtain

$$\begin{aligned} \bar{E}_k := \|\tilde{\mathbf{u}}^{\text{DD-DA}} / \Delta_k - \tilde{\mathbf{v}}^{\text{DD-DA}} / \Delta_k\| &\leq \|(u_{i,k}^{M_{i,k},\bar{n}})^{EO} / \Delta_k - (v_{i,k}^{M_{i,k},\bar{n}})^{EO} / \Delta_k\| \\ &\quad + \|(u_{i,k}^{M_{i,k},\bar{n}-1})^{EO} / \Delta_k - (v_{i,k}^{M_{i,k},\bar{n}-1})^{EO} / \Delta_k\| \\ &\quad + \|(u_{i,k}^{\text{ASM},\bar{n}})^{EO} / \Delta_k - (v_{i,k}^{\text{ASM},\bar{n}})^{EO} / \Delta_k\|. \end{aligned} \tag{80}$$

From (67) and (54), we can neglect the dependency on \bar{n} , i.e.,

$$\bar{E}_k \leq 2 \|(u_{i,k}^{M_{i,k}})^{EO} / \Delta_k - (v_{i,k}^{M_{i,k}})^{EO} / \Delta_k\| + \|(u_{i,k}^{\text{ASM}})^{EO} / \Delta_k - (v_{i,k}^{\text{ASM}})^{EO} / \Delta_k\|. \tag{81}$$

From the assumption on the model, we may say that $\exists \bar{D} > 0$ such that

$$\|(u_{i,k}^{M_{i,k}})^{EO} / \Delta_k - (v_{i,k}^{M_{i,k}})^{EO} / \Delta_k\| \leq \bar{D} e_0. \tag{82}$$

where e_0 is the error on the initial condition of M in (11). By adding and subtracting $\mathbf{u}^{\text{DA}} / \Delta_k$ to $[(u_{i,k}^{\text{ASM}})^{EO} / \Delta_k - (v_{i,k}^{\text{ASM}})^{EO} / \Delta_k]$ and using the triangle inequality, it is

$$\begin{aligned} \|(u_{i,k}^{\text{ASM}})^{EO} / \Delta_k - (v_{i,k}^{\text{ASM}})^{EO} / \Delta_k\| &\leq \|\mathbf{u}^{\text{DA}} / \Delta_k - (u_{i,k}^{\text{ASM}})^{EO} / \Delta_k\| \\ &\quad + \|\mathbf{u}^{\text{DA}} / \Delta_k - (v_{i,k}^{\text{ASM}})^{EO} / \Delta_k\|. \end{aligned} \tag{83}$$

From (83) and (57), we obtain

$$\|(u_{i,k}^{\text{ASM}})^{EO} / \Delta_k - (v_{i,k}^{\text{ASM}})^{EO} / \Delta_k\| \leq \mu_k^{\text{DD-DA}} E_1^{\text{ASM}} + \bar{\mu}_k^{\text{DD-DA}} \bar{E}_1^{\text{ASM}} \tag{84}$$

where

$$\begin{aligned} E_1^{ASM} &= \|\mathbf{u}^{DA}/\Delta_1 - (u_{i,1}^{ASM})^{EO}/\Delta_1\| \\ \bar{E}_1^{ASM} &= \|\mathbf{u}^{DA}/\Delta_1 - (v_{i,1}^{ASM})^{EO}/\Delta_1\|. \end{aligned} \tag{85}$$

and

$$\begin{aligned} \mu_k^{DD-DA} &:= \left[1 + \frac{1}{\sigma_0^2} \mu^2(\mathbf{V}) \mu^2(G/\Delta_k) \right] \mu(M/\Delta_k) \\ \bar{\mu}_k^{DD-DA} &:= \left[1 + \frac{1}{\sigma_0^2} \mu^2(\mathbf{V}) \mu^2(G/\Delta_k) \right] \mu(\bar{M}/\Delta_k) \end{aligned} \tag{86}$$

with σ_0 denoting the observational error variance, $\mathbf{B} = \mathbf{V}\mathbf{V}^T$ the covariance matrix of the error on the background to Ω , G the matrix defined in (13), M defined in (11) and \bar{M} the discrete model obtained by considering initial error e_0 on the initial condition of M . By applying (57) to E_1^{ASM} and \bar{E}_1^{ASM} in (85), we obtain

$$\|(u_{i,k}^{ASM})^{EO}/\Delta_k - (v_{i,k}^{ASM})^{EO}/\Delta_k\| \leq \mu_k^{DD-DA} \mu_1^{DD-DA} e_0 + \bar{\mu}_k^{DD-DA} \bar{\mu}_1^{DD-DA} \bar{e}. \tag{87}$$

From (81), (82) and (84), it is

$$\bar{E}_k \leq 2\bar{D} \times e_0 + \mu_k^{DD-DA} \mu_1^{DD-DA} e_0 + \bar{\mu}_k^{DD-DA} \bar{\mu}_1^{DD-DA} \bar{e}$$

and from the hypothesis in (79), we obtain

$$\bar{E}_k \leq \bar{\mu}_k^{DD-DA} \bar{\mu}_1^{DD-DA} \bar{e} \tag{88}$$

Consequently, for $k = 1, \dots, N_t$, we find that $\exists C_k > 0$ such that

$$\bar{E}_k \leq C_k \bar{e} \tag{89}$$

where

$$C_k := \bar{\mu}_k^{DD-DA} \bar{\mu}_1^{DD-DA}. \tag{90}$$

The thesis is proved. \square

From Theorem 3, we obtain the stability of DD-DA.

Remark from Lemma 2 it follows that the quantity $\mu_{i,k}^{DD-DA}$ can be regarded as the condition number of local problems restricted to the space-time directions. Further, in Theorem 3, we study the propagation error along the time direction according to the forward error analysis. As a consequence, we may say that μ_k^{DD-DA} can be regarded as the condition number of local problems restricted to the time direction. In [16], the authors apply the SA to the reduced DA functional obtained by applying domain decomposition across space. The results in [16] proved that Tikhonov regularization revealed to be more appropriate than truncation of EOFs to improve the conditioning of the covariance matrix. The results obtained in the present study complement the study in [16].

4. Validation Analysis

The validation is performed mapping the space-time domain (Figure 5) on the high performance hybrid computing architecture of the SCoPE (Sistema Cooperativo Per Elaborazioni scientifiche multidisciplinari) data center, which is located in the University of Naples Federico II. Specifically, the architecture is composed of eight nodes that consist of distributed memory DELL M600 blades. The blades are connected by a 10 Gigabit Ethernet technology and each of them is composed of 2 Intel Xeon@2.33 GHz quadcore processors sharing the same local 16 GB RAM memory for a number of 8 cores per blade and of 64 total cores. Experimental results allow us to verify that the experimental order of consistency

corresponds to the theoretical one obtained in Theorem 2 and that the local problems are well-conditioned. We consider the following experimental setup .

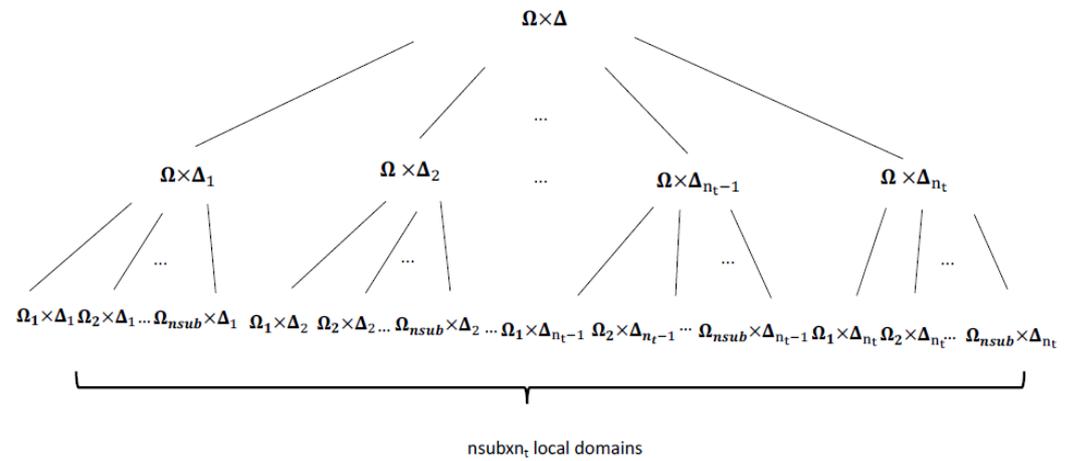


Figure 5. Space-time domain decomposition.

4DVAR DA setup.

- $\Omega = (0, 1) \subset \mathbb{R}$: spatial domain;
- $\Delta = [0, 1.5] \subset \mathbb{R}$: time interval;
- $N_p = 640$: numbers of inner nodes of Ω defined in (5);
- $N = 9, 20$: numbers of occurrences of time in Δ ;
- $n_{obs} = 64$: number of observations considered at each step $l = 0, 1, \dots, N$;
- $y \in \mathbb{R}^{N \times n_{obs}}$: observations vector at each step $l = 0, 1, \dots, N$. Observations are obtained choosing (randomly) these values among the values of the state function (the so called background) and perturbing (randomly) them. (We choice the observation in this way because the experimental set up is aimed to validate the sensitivity analysis of DD-DA instead of the reliability of DD-DA method);
- $H_l \in \mathbb{R}^{n_{obs} \times N_p}$: piecewise linear interpolation operator whose coefficients are computed using the nodes of Ω nearest to the observation values;
- $G \in \mathbb{R}^{N \times n_{obs} \times N_p}$: obtained as in (13) from the matrix $H_l, l = 0, 1, \dots, N$;
- $\sigma_m^2 = 0.5, \sigma_0^2 = 0.5$: model and observational error variances;
- $\mathbf{B} \equiv B_l = \sigma_m^2 C$: covariance matrix of the error of the model at each step $l = 0, 1, \dots, N$, where $C \in \mathbb{R}^{N_p \times N_p}$ denotes the Gaussian correlation structure of the model errors in (91);
- $R_l = \sigma_0^2 I_{n_{obs}, n_{obs}} \in \mathbb{R}^{n_{obs} \times n_{obs}}$: covariance matrix of the errors of the observations at each step $l = 0, 1, \dots, N - 1$.
- $\mathbf{R} \in \mathbb{R}^{N \times n_{obs} \times N \times n_{obs}}$: a diagonal matrix obtained from the matrices $R_l, l = 0, 1, \dots, N - 1$.

DD-DA setup: we consider the following setup:

- $p = N_{sub} \times N_t$: number of cores;
- N_{sub} : number of spatial subdomains;
- $N_t = 4$: number of time intervals;
- δ : number of inner nodes of overlap regions defined in (20);
- N_{loc} : inner nodes of subdomains defined in (22);
- Δx and Δt : spatial and temporal step sizes of $M_{i,k}$ defined in (26);
- $C := \{c_{i,j}\}_{i,j=1,\dots,N_p} \in \mathbb{R}^{N_p \times N_p}$: the Gaussian correlation structure of the model error where

$$c_{i,j} = \rho^{|i-j|^2}, \quad \rho = \exp\left(\frac{-\Delta x^2}{2}\right), \quad |i-j| < N_p/2 \quad \text{for } i, j = 1, \dots, N_p. \quad (91)$$

Given δ, N_{sub}, N_t , we introduce

$$e_{\Delta x, \Delta t}^p := \|\mathbf{u}^{DA} - \tilde{\mathbf{u}}^{DD-DA}\|_2, \tag{92}$$

where \mathbf{u}^{DA} denotes the minimum of the 4DVAR (global) functional \mathbf{J} in (9) while $\tilde{\mathbf{u}}^{DD-DA}$ is obtained by gathering all minima of the local 4DVar functionals $J_{i,k}$, in (30), by considering different values of δ defined in (20). $\mathbf{u}^{DA} \in \mathbb{R}^{N_p \times N}$ is computed by running the DD-DA algorithm for $N_{sub} = 1$, while $\tilde{\mathbf{u}}^{DD-DA} \in \mathbb{R}^{N_p \times N}$ is computed by gathering local solutions obtained by running the DD-DA algorithm for different values of $N_{sub} > 1$ and with $\delta \geq 0$, as shown in Figure 6.

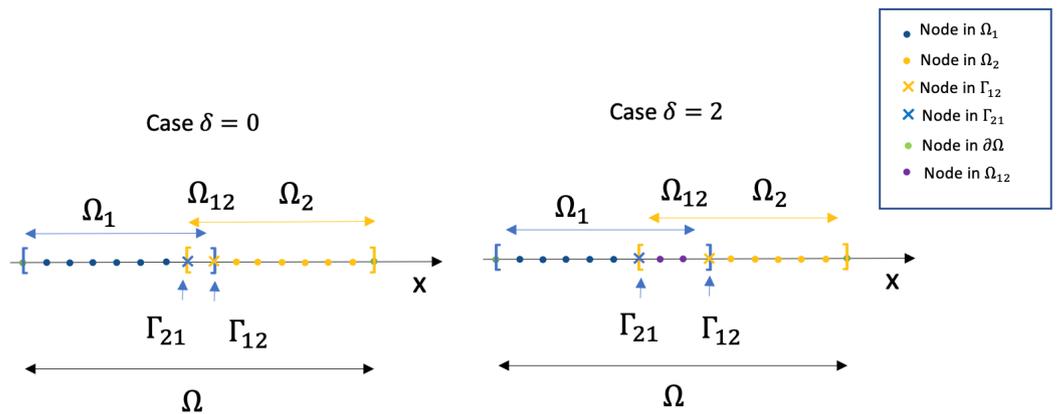


Figure 6. Decomposition of the spatial domain $\Omega \subset \mathbb{R}$ in two subdomains $\{\Omega_i\}_{i=1,2}$ by identifying overlap region Ω_{12} defined in (16) and interfaces Γ_{12} and Γ_{21} defined in (17). On the left case $\delta = 0$, i.e., no inner nodes in Ω_{12} , on the right case $\delta = 2$, i.e., two inner nodes in overlap region Ω_{12} .

In the following, we present the experimental results of the consistency and the stability analysis by considering the initial boundary problem of the Shallow Water Equations (SWEs) in 1D. The discrete model is obtained using the Lax–Wendroff scheme [22] on $\Omega \times \Delta$ where the orders of convergence in space and time are equal to 2.

- Consistency. From Table 1, we obtain

$$e_{\frac{\Delta x}{d}, \frac{\Delta t}{d}}^p \approx \frac{e_{\Delta x, \Delta t}^p}{d^2} \quad d = 1, 2, 4, 6, 8, 10. \tag{93}$$

As shown in Table 1 and Figure 7, the experimental order of consistency corresponds to the theoretical one obtained in Theorem 2.

- Stability. In Table 2 and Figure 8, we report values of \bar{E}_k for different values of the perturbation \bar{e}_k on the initial condition of $P_{i,k}^{M_{i,k}}$ defined in (25). Then, we may estimate C_k in (90). In particular, we found that

$$C_k \approx 2.00 \times 10^1 \quad \forall k = 1, \dots, N_t.$$

Consequently, the local problems with initial boundary problem of SWEs 1D, are well-conditioned with respect to the time direction.

Table 1. We fix $N_p = 640$, the number of inner nodes in Ω , $N = 9$ the number of time values in Δ , $N_{sub} = 4$ the number of spatial subdomain and $N_t = 4$ time intervals. We report the values of e^p , which is defined in (92), for different values of Δx and Δt , the spatial and temporal step sizes of $M_{i,k}$ defined in (26).

d	$\frac{\Delta x}{d}$	$\frac{\Delta t}{d}$	$e^p_{\frac{\Delta x}{d}, \frac{\Delta t}{d}}$	$\frac{e^p_{\Delta x, \Delta t}}{d^2}$
1	7.87×10^{-3}	1.09×10^{-1}	1.53×10^{-2}	1.53×10^{-2}
2	3.92×10^{-3}	5.47×10^{-2}	9.01×10^{-4}	3.83×10^{-3}
4	1.96×10^{-3}	2.74×10^{-2}	6.45×10^{-4}	9.56×10^{-4}
6	1.30×10^{-3}	1.83×10^{-2}	3.65×10^{-4}	2.39×10^{-4}
8	9.78×10^{-4}	1.37×10^{-2}	3.99×10^{-4}	4.25×10^{-4}
10	7.81×10^{-4}	1.10×10^{-2}	3.77×10^{-4}	1.53×10^{-4}

Table 2. We fix $N_p = 640$, the number of inner nodes in Ω , $N = 20$ the number of instants of time in Δ , $N_{sub} = 4$ the number of spatial subdomains and $N_t = 4$ time intervals. For $k = 1, 2, 3, 4$, we report the values of \bar{E}_k defined in (78) for different perturbations \bar{e}_k to the initial condition of $P_{i,k}^{M_{i,k}}$, defined in (25).

\bar{e}_k	\bar{E}_k
3.03×10^{-6}	6.05×10^{-5}
3.02×10^{-5}	6.06×10^{-4}
3.01×10^{-4}	6.08×10^{-3}
3.05×10^{-3}	6.04×10^{-2}

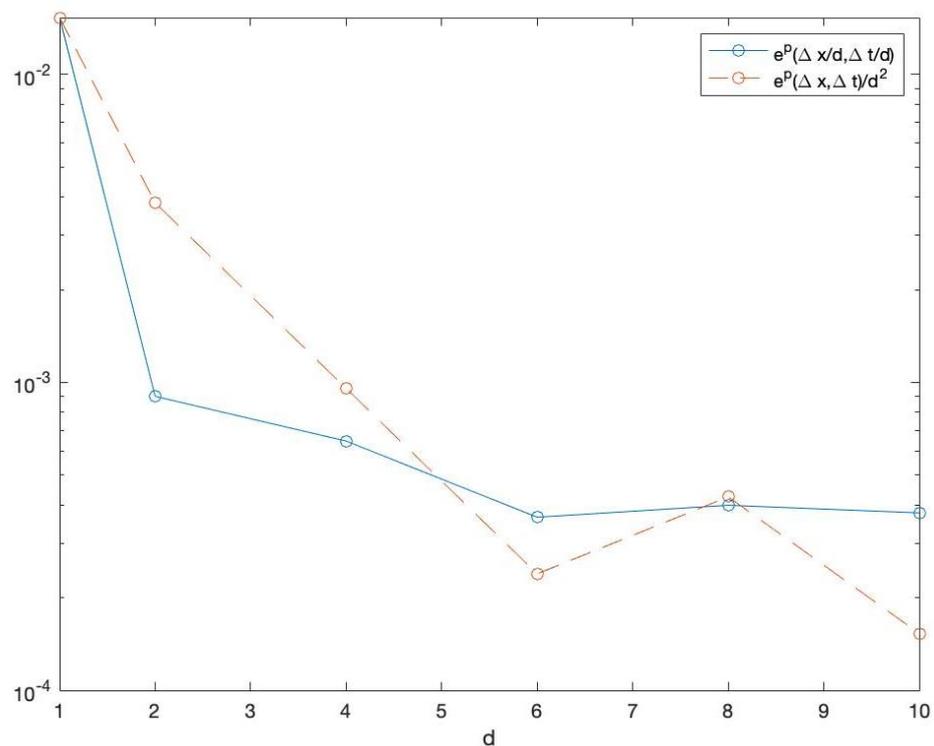


Figure 7. Values of $e^p_{\frac{\Delta x}{d}, \frac{\Delta t}{d}}$ (orange dashed line) and $\frac{e^p_{\Delta x, \Delta t}}{d^2}$ (blue full line) for $d = 1, 2, 4, 6, 8, 10$ reported in Table 1.

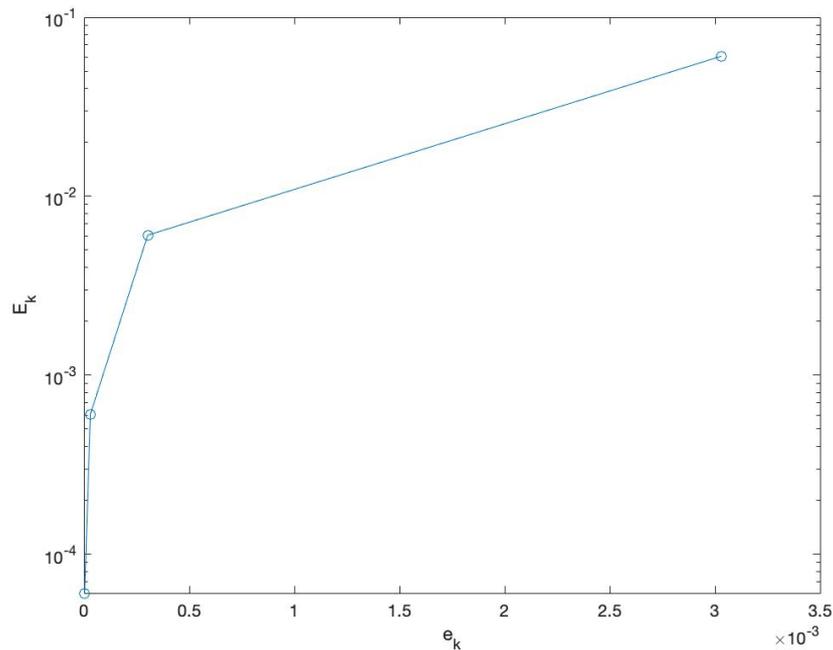


Figure 8. Values (\bar{e}_k, \bar{E}_k) as reported in Table 2.

5. Conclusions

This work concerns the sensitivity analysis for large scale DA problems that need parallel solutions. We feel that the whole analysis of uncertainties becomes crucial for the emerging approaches integrating DA with deep learning approaches. We derived and discussed the main sources of errors of the parallel DD-DA framework. We prove that the order of consistence depends on the order of local models and introduce the condition number of local problems. As the core of such a parallel approach is that the DA model acts as coarse/predictor operator solving the local PDE model, we analyze error propagation with respect to time direction. Validation analysis confirms that the experimental order of consistency corresponds to the theoretical one. Finally, we note that the SA results in [16] proved that Tikhonov regularization revealed to be more appropriate than truncation of EOFs to improve the conditioning of the covariance matrix. Our results here complement the study in [16] and we may conclude that the same findings hold true for DD-DA, too.

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