



A note on domain decomposition approaches for solving 3D variational data assimilation models

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Abstract

Data assimilation (DA) is a methodology for combining mathematical models simulating complex systems (the background knowledge) and measurements (the reality or observational data) in order to improve the estimate of the system state (the forecast). The DA is an inverse and ill posed problem usually used to handle a huge amount of data, so, it is a big and computationally expensive problem. In the present work we prove that the functional decomposition of the 3D variational data assimilation (3D Var DA) operator, previously introduced by the authors, is equivalent to apply multiplicative parallel Schwarz (MPS) method, to the Euler–Lagrange equations arising from the minimization of the data assimilation functional. It results that convergence issues as well as mesh refinement techniques and coarse grid correction—issues of the functional decomposition not previously addressed—could be employed to improve performance and scalability of the 3D Var DA functional decomposition in real cases.

Keywords 3D VarDA · DD methods · Multiplicative Schwarz method

Mathematics Subject Classification 65F22 · 65K15 · 65M55 · 65N55 · 8608

1 Introduction and motivations

Data assimilation (DA) has long been playing a crucial role in numerical weather prediction (NWP) and oceanography [1–3] and more in general, in climate science; recently, DA started to be applied more widely to numerical simulations beyond

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geophysical applications [4], medicine and biological science [5] for improving the accuracy and reliability of the computational approach.

DA is an ill posed inverse problem [6] and, today, there is a variety of DA algorithms. In the last decennium variational approach [7]—where DA is performed by minimizing a functional estimating the discrepancy between numerical results and measures—and the Kalman Filter [8]—where DA is performed by recursive filtering—have gained acceptance as powerful methods for data assimilation. Finally a more recent algorithm is proposed in [4] that is an intermediate between the two approaches, i.e. the back and forth nudging algorithm, consisting in adding to the equation of the model a relaxation term that fits the model to the observations. However, most significant feature of such approaches is the very large computational burden required in concrete scenarios. Solution of this computationally difficult large-scale problem requires designing of numerical approaches capable to exploit the performance of the emerging computing architectures in order to get a solution in a real time, as well as, capable to ensure the maximum attainable accuracy on the computed solution from data [9,10].

1.1 Motivations

Our work was inspired by the papers in [11]. In [11] the authors proposed a parallel algorithm to extend three dimensional variational DA problems for coupled models, using a domain decomposition approach. More precisely, they assume that, on each sub domain, different models interact, for instance, ocean-atmosphere where there is a physical interface, or chemistry-atmosphere, where the models being coupled through radiative transfers. The parallel algorithm consists in performing the data assimilation process on each subdomain with an exchange of boundary conditions. On each subdomain, the cost function, measuring the distance between the observations and the solution of the model running on that subdomain, was modified adding a new term to enforce coupling between the domains. The DA functional was in the form:

$$J_i(U) = \frac{1}{2} \left[\int_0^T \|C^i X^i(t) - X_{obs}^i(t)\|^2 dt + \frac{1}{\epsilon} \int_0^T \|C^i X^i(t) - C^j X^j(t)\|^2 dt \right]$$

where X^i is the solution of the physical model on the i -th subdomain, X_{obs}^i are the observations on $[0, T]$ on the i -th subdomain, U is the solution of the DA problem, $\epsilon > 0$ and $\|\cdot\|$ denotes a suitable norm. In this paper, we present a domain decomposition-based framework for solution of variational DA problems, involving decomposition of the physical domain, partitioning of the solution and modification of the regularization functional describing the variational DA problem. We prove that the functional decomposition of the 3D variational data assimilation (3D Var DA) operator, previously introduced by the authors in [12–14], is equivalent to apply multiplicative parallel Schwarz (MPS) method, to the resulting Euler–Lagrange equations. It results that MPS convergence issues (such as convergence rate and its dependence on discretization parameters and on decomposition parameters, i.e. the number of levels and of subregions) as well as coarse grid correction and mesh refinement techniques—issues of the functional decomposition that were not previously addressed—could be

even employed in this case to improve the performance of the 3D Var DA functional decomposition in real applications [15].

1.2 Related works

DD methods were introduced as techniques for solving partial differential equations based on a decomposition of the spatial domain of the problem into several subdomains [16,17]. In the past three decades, domain decomposition methods have been intensively studied for linear and nonlinear partial differential equations. We refer to [18] and the references therein. Moreover, there have been some literatures in which the DD were constructed from an optimization point of view [19]. Finally, DD methods have also been considered as special subspace correction methods such as many iterative methods, including Jacobi method, Gauss–Seidel method and multigrid [20,21]. Taking into account that many partial differential equations can be formulated as a variational problem in some way, and that the Schwarz alternating method for the overlapping domain decomposition is a Gauss–Seidel iterative method, similar results were extended to convex [22] and non convex minimization problems [23].

The key point of all DD methods is the divide et conquer approach to the original problem solving, giving rise to an iterative numerical scheme. They differ on the way to proceed for the operator decomposition, for the space decomposition, and for the local solution within each subdomain [24,25].

2 The DA inverse problem

In the following we review the mathematical setting for space and function decomposition then we state some notations used later. In particular, we first introduce the function and domain decomposition then by using the restriction and the extension operators, we associate to the domain decomposition a functional decomposition (see [14,26] and the references therein).

Definition 1 (*Function and domain decomposition*) Let $t \in [0, T]$ and $x \in \mathbb{R}^N$. Let f be a function belonging to the Hilbert space $\mathcal{K}([0, T] \times \Omega)$, that is:

$$f(t, x) : [0, T] \times \Omega \mapsto \mathcal{K}$$

Let $\Omega \subset \mathbb{R}^N$ be decomposed into a sequence of overlapping subdomains $\Omega_i \subset \mathbb{R}^{M_i}$, $M_i \leq N$, $i = 1, \dots, n$ such that

$$\Omega = \bigcup_{i=1}^n \Omega_i \quad (1)$$

where

$$\Omega_i \cap \Omega_j = \Omega_{ij} \neq \emptyset$$

if $i = j \pm 1$ or $i = j \pm 1$ (i.e. when the subdomains are adjacent).

Associated with such a decomposition we define the so-called **Restriction Operator**:

Definition 2 (*Restriction operator*) Let us define:

$$RO_i : \mathcal{K}([0, T] \times \Omega) \mapsto \mathcal{K}([0, T] \times \Omega_i)$$

such that:

$$RO_i(f(t, x)) \equiv f(t, x), (t, x) \in [0, T] \times \Omega_i$$

Moreover, for simplicity of notations, we pose:

$$f_i^{RO}(t, x) \equiv RO_i[f(t, x)]$$

By the same way, given a set of n function $g_i, i = 1, \dots, n$, each belonging to the Hilbert space $\mathcal{K}([0, T] \times \Omega_i)$, we define the adjoint **Extension Operator**:

Definition 3 (*Extension operator*) Let us define:

$$EO_i : \mathcal{K}([0, T] \times \Omega_i) \mapsto \mathcal{K}([0, T] \times \Omega)$$

such that:

$$EO_i(g_i(t, x)) = \begin{cases} g_i(t, x) & x \in \Omega_i \\ 0 & \text{elsewhere} \end{cases}$$

Moreover, for simplicity of notations, we define:

$$g_i^{EO}(t, x) \equiv EO_i[g_i(t, x)]$$

Remark 1 We observe that, associated to the domain decomposition (1) for any function $f \in \mathcal{K}([0, T] \times \Omega)$ it holds that:

$$f(t, x) = \sum_{i=1, n} EO_i \left[f_i^{RO}(t, x) \right]. \quad (2)$$

Remark 2 Given n functions $g_i(t, x) \in \mathcal{K}([0, T] \times \Omega_i)$, the summation

$$\sum_{i=1, n} g_i^{EO}(t, x) \quad (3)$$

defines a function $g \in \mathcal{K}([0, T] \times \Omega)$ such that:

$$RO_j[g(t, x)] = RO_j \left[\sum_{i=1, n} g_i^{EO}(t, x) \right] = g_j(t, x)$$

Remark 3 We observe that the definition of the restriction operator RO_i , as well as the extension operator EO_i , can be generalized to operators acting onto vectors instead of functions. Hence, for any vector $w = (w_1, w_2, \dots, w_N) \in \mathfrak{R}^N$ we may use the same notation in order to denote the restriction/extension operators, i.e. we get:

$$RO_i(w) \equiv w_{RO_i} = (w_1, w_2, \dots, w_{M_i}) \in \mathfrak{R}^{M_i}, \quad M_i \leq N$$

By the same way, if $z = (z_1, z_2, \dots, z_{M_i}) \in \mathfrak{R}^{M_i}$, where $M_i \leq N$, we get:

$$EO_i(z) = \begin{cases} z_k & k \leq M_i \\ 0 & elsewhere \end{cases}$$

and

$$EO_i(z) \equiv z^{EO_i} = (z_1, z_2, z_{M_i}, 0, \dots, 0) \in \mathfrak{R}^N$$

Let $w \in \mathfrak{R}^N$ be a vector, and let us denote by $C(w)$ the covariance matrix related to w , such that:

$$C(w) = ww^T$$

Associated to the domain decomposition (1), we define:

Definition 4 (Covariance matrix decomposition) Let $C(w) \in \mathfrak{R}^{N \times N}$ be the covariance matrix of a random vector $w = (w_1, w_2, \dots, w_N) \in \mathfrak{R}^N$, that is the coefficient $c_{i,j}$ of C is $c_{i,j} = \sigma_{ij} = \text{Cov}(w_i, w_j)$. Let $s < N$, we define the restriction operator RO_s onto $C(w)$ acting as follows:

$$RO_s : C(w) \in \mathfrak{R}^{N \times N} \mapsto RO_s[C(w)] \stackrel{\text{def}}{=} C(w_{RO_s}) \in \mathfrak{R}^{s \times s}$$

i.e., the covariance matrix defined on the restriction w_{RO_s} of the vector w .

Let $x \in \Omega \subset \mathbb{R}^N$, $t \in [0, T]$ and let $u(t, x)$ be the state evolution of a predictive system from time $t - \Delta t$ to time t , governed by the mathematical model $\mathcal{M}_t[u(t, x)]$. So, it is

$$\mathcal{M}_{t-\Delta t, t} : u(t - \Delta t, x) \rightarrow u(t, x).$$

Let $\{t_k\}_{k=0,1,\dots,M}$ be a discretization of interval of time $[0, T]$, where $t_k = t_0 + k\Delta t$, and let $D_{NP}(\Omega) = \{(x_j)\}_{j=1,\dots,NP} \in \mathbb{R}^{NP \times N}$, be a discretization of $\Omega \subset \mathbb{R}^N$, where $x_j \in \Omega$.

Let:

$$v(t, y) = \mathcal{H}(u(t, y)), \quad y \in \Omega$$

denote the observations mapping, where \mathcal{H} is a given nonlinear operator.

For each $k = 0, \dots, M$, we consider

- $\mathbf{u}_k^b = \{u_k^j\}_{j=1,\dots,NP}^b \equiv \{u(t_k, x_j)^b\}_{j=1,\dots,NP} \in \mathbb{R}^{NP}$: (background) numerical solution of the model $\mathcal{M}_t[u(t, x)]$ on $\{t_k\} \times D_{NP}(\Omega)$;
- $\mathbf{v}_k = \{v(t_k, y_j)\}_{j=1,\dots,nobs}$: the vector values of the observations on $y_j \in \Omega$ at time t_k ;
- $\mathcal{H}(x) \simeq \mathcal{H}(y) + \mathbf{H}(x - y)$: a linearization of \mathcal{H} , where $\mathbf{H} \in \mathbb{R}^{NP \times nobs}$ is the matrix obtained by the first order approximation of the Jacobian of \mathcal{H} and $nobs \ll NP$;
- \mathbf{R} and \mathbf{B} the covariance matrices of the errors on the observations and on the background, respectively. These matrices are symmetric and positive definite.

Definition 5 (*The DA inverse problem*) The DA inverse problem is to compute the vector $\mathbf{u}_k^{DA} = \{u_k^j\}_{j=1,\dots,NP}^{DA}$ such that:

$$\mathbf{v}_k = \mathbf{H}[\mathbf{u}_k^{DA}]. \quad (4)$$

Since \mathbf{H} is typically rank deficient and highly ill conditioned, DA is an ill posed inverse problem [14]. The objective is determine the solution in least squares sense.

Definition 6 The solution in least squares sense for the problem in (4) is a vector \mathbf{u}^{DA} such that:

$$\mathbf{u}^{DA} = \operatorname{argmin}_{\mathbf{u} \in \mathbb{R}^{NP}} \mathbf{J}(\mathbf{u}) = \operatorname{argmin}_{\mathbf{u}} \left\{ \|\mathbf{H}\mathbf{u} - \mathbf{v}\|_{\mathbf{R}}^2 \right\}. \quad (5)$$

The problem in (5) ignores the background, so we consider the following Tikhonov-regularized formulation. In the following we let time t_k be fixed, i.e. we consider the so-called 3D-Var DA problem [14], then for simplicity of notations, we refer to \mathbf{u}_k^b and \mathbf{u}_k^{DA} omitting index k .

Definition 7 (*The 3D-Var DA problem*) 3D variational DA problem is to compute the vector \mathbf{u}^{DA} such that

$$\mathbf{u}^{DA} = \operatorname{argmin}_{\mathbf{u} \in \mathbb{R}^{NP}} \mathbf{J}(\mathbf{u}) = \operatorname{argmin}_{\mathbf{u}} \left\{ \|\mathbf{H}\mathbf{u} - \mathbf{v}\|_{\mathbf{R}}^2 + \lambda \|\mathbf{u} - \mathbf{u}^b\|_{\mathbf{B}}^2 \right\} \quad (6)$$

where λ is the regularization parameter.

When the regularization parameter λ approaches to zero the regularized problem tends to the DA (ill posed) inverse problem, while the increase the regularization parameter has the effect of decreasing the uncertainty in the background [27]. The 3D-Var operator is:

$$\mathbf{J}(\mathbf{u}) \equiv \mathbf{J}(\mathbf{u}, \mathbf{R}, \mathbf{B}, D_{NP}(\Omega)) = (\mathbf{H}\mathbf{u} - \mathbf{v})^T \mathbf{R}(\mathbf{H}\mathbf{u} - \mathbf{v}) + \lambda (\mathbf{u} - \mathbf{u}^b)^T \mathbf{B}(\mathbf{u} - \mathbf{u}^b). \quad (7)$$

The matrix \mathbf{H} is ill conditioned so we consider the preconditioner matrix \mathbf{V} such that $\mathbf{B} = \mathbf{V}\mathbf{V}^T$. Let $\partial \mathbf{u}^{DA} = \mathbf{u}^{DA} - \mathbf{u}^b$ and $\mathbf{w} = \mathbf{V}^T \partial \mathbf{u}^{DA}$, the operator \mathbf{J} in (7) can be rewritten as follows:

$$\mathbf{J}(\mathbf{w}) = \frac{1}{2} \lambda \mathbf{w}^T \mathbf{w} + \frac{1}{2} (\mathbf{H}\mathbf{V}\mathbf{w} - \mathbf{d})^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{V}\mathbf{w} - \mathbf{d}), \quad (8)$$

where $\mathbf{d} = [\mathbf{v} - \mathbf{H}(\mathbf{u})]$.

3 The DD approaches

The class of MPS originated from the classical Schwarz alternating method. The basic idea is to divide the region into several overlapping subregions and then to solve the subproblems in the subregions alternatively with boundary information from the neighboring subregions. Let us review the main steps of MPS method applied to 3D VAR DA problem [16]. It is composed of the following steps:

1. decomposition of domain Ω into a sequence of subdomains Ω_i such that:

$$\Omega = \bigcup_{i=1}^N \Omega_i.$$

2. definition of interfaces of subdomains Ω_i :

$$\Gamma_{ij} := \partial\Omega_i \cap \Omega_j \quad \text{for } i, j = 1, \dots, J. \quad (9)$$

3. definition of restriction matrices R_i and extension matrices R_i^T , for $i = 1, \dots, J$ as follows:

$$R_i = \begin{pmatrix} & & & s_{i-1}+1 & \cdots & s_{i-1}+r_i & & & \\ & 0 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ & \vdots & & \vdots & & \vdots & \vdots & & \vdots \\ & 0 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ s_{i-1}+1 & 0 & \cdots & 0 & 1 & & 0 & \cdots & 0 \\ & \vdots & & \vdots & & \ddots & & & \\ s_{i-1}+r_i & 0 & \cdots & 0 & 0 & & 1 & 0 & \cdots & 0 \\ & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ & \vdots & & \vdots & & \vdots & \vdots & & \vdots \\ & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad (10)$$

$$R_i^T = \begin{pmatrix} & & & \bar{s}_{i-1,i}+1 & \cdots & \bar{s}_{i-1,i}+r_i & & & \\ & 0 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ & \vdots & & \vdots & & \vdots & \vdots & & \vdots \\ & 0 & \cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \bar{s}_{i-1,i}+1 & 0 & \cdots & 0 & 1 & & 0 & \cdots & 0 \\ & \vdots & & \vdots & & \ddots & & & \\ \bar{s}_{i-1,i}+r_i & 0 & \cdots & 0 & 0 & & 1 & 0 & \cdots & 0 \\ & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ & \vdots & & \vdots & & \vdots & \vdots & & \vdots \\ & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{pmatrix} \quad (11)$$

where $s_{i,j} = r_i - C_{i,j}$, $\bar{s}_{i,j} = s_{i,j} + t_{ij}$, and $r_i, t_{i,j}, C_{i,j}$ points of sub domain Ω_i , interfaces Γ_{ij} and sub domain $\Omega_{ij} = \Omega_i \cap \Omega_j$, respectively.

4. solution of J subproblems, let us say P_i^{n+1} , for $n = 0, 1, 2, \dots$ until convergence is reached, where P_i^{n+1} is defined as follows:

$$\begin{aligned} \operatorname{argmin}_{\mathbf{u}_i^{n+1} \in \mathbb{R}^{r_i}} \mathbf{J}_i(\mathbf{u}_i^{n+1}) = \operatorname{argmin}_{\mathbf{u}_i^{n+1} \in \mathbb{R}^{r_i}} (& \|\mathbf{H}_i \mathbf{u}_i^{n+1} - \mathbf{v}_i\|_{\mathbf{R}_i}^2 \\ & + \lambda \|\mathbf{u}_i^{n+1} - (\mathbf{u}_i^b)\|_{\mathbf{B}_i}^2 \\ & + \|\mathbf{u}_i^{n+1}/\Gamma_{ij} - \mathbf{u}_k^n/\Gamma_{ij}\|_{\mathbf{B}/\Gamma_{ij}}^2); \end{aligned} \quad (12)$$

$\mathbf{B}_i = R_i \mathbf{B} R_i^T$ is a covariance matrix, $\mathbf{B}/\Gamma_{ij} = R_i \mathbf{B} R_{ij}^T$ is restriction of matrix \mathbf{B} to Γ_{ij} ; $\mathbf{H}_i = R_i \mathbf{H} R_i^T$, $\mathbf{R}_i = R_i \mathbf{R} R_i^T$ are restriction of matrices \mathbf{H} and \mathbf{R} to sub domain Ω_i , $\mathbf{u}_i^b = R_i \mathbf{u}^b$ while $\mathbf{u}_i^{n+1}/\Gamma_{ij} = R_{ij} \mathbf{u}_i^{n+1}$, $\mathbf{u}_j^n/\Gamma_{ij} = R_{ij} \mathbf{u}_j^n$ are restriction of vectors \mathbf{u}^b , \mathbf{u}_i^{n+1} , \mathbf{u}_j^n to sub domain Ω_i and interface Γ_{ij} for $i, j = 1, 2, \dots, J$. The gradient of \mathbf{J}_i :

$$\nabla \mathbf{J}_i(\mathbf{w}_i^{n+1}) = \mathbf{w}_i^{n+1} + \mathbf{V}_i^T \mathbf{H}_i^T \mathbf{R}_i^{-1} (\mathbf{H}_i \mathbf{V}_i \mathbf{w}_i^{n+1} - \mathbf{d}_i) + \mathbf{V}_{ij}^T (\mathbf{V}_{ij} \mathbf{w}_i^{n+1} - \mathbf{V}_{ij} \mathbf{w}_j^n) \quad (13)$$

can be written as follows

$$\nabla \mathbf{J}_i(\mathbf{w}_i^{n+1}) = (\mathbf{V}_i^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{V}_i + I_i + \mathbf{B}/\Gamma_{ij}) \mathbf{w}_i^{n+1} - \mathbf{c}_i + \mathbf{B}/\Gamma_{ij} \mathbf{w}_j^n, \quad (14)$$

where

$$\mathbf{c}_i = (\mathbf{V}_i^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{V}_i \mathbf{d}_i), \quad (15)$$

and $I_i \in \mathbb{R}^{r_i \times r_i}$ is the identity matrix.

From (14), according to MPS method and considering the Euler–Lagrange equations corresponding to (12), for $i, j = 1, \dots, J$ and for $n = 0, 1, \dots$, the systems $(S_i^{MPS})^{n+1}$ defined as:

$$(S_i^{MPS})^{n+1} : A_i^{MPS} \mathbf{w}_i^{n+1} = \mathbf{c}_i - \sum_{j \neq i} A_{i,j} \mathbf{w}_j^n, \quad (16)$$

and:

$$A_i^{MPS} = (\mathbf{V}_i^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{V}_i + I_i + \mathbf{B}/\Gamma_{ij}), \quad (17)$$

where $A_{ij} = \mathbf{B}/\Gamma_{ij}$, are solved.

5. computation of \mathbf{u}_i^{n+1} , related to sub domain Ω_i as:

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^b + \mathbf{B}_i^{-1} \mathbf{V}_i \mathbf{w}_i^{n+1}, \quad \text{for } i = 1, \dots, J. \quad (18)$$

6. computation of \mathbf{u}^{DA} , solution of 3D-Var DA problem in (6), by patching together vectors \mathbf{u}_i^{n+1} , i.e.:

$$\mathbf{u}^{DA}(x_j) = \begin{cases} \mathbf{u}_i^n(x_j) & \text{if } x_j \in \Omega_i \\ \mathbf{u}_k^n(x_j) & \text{if } x_j \in \Omega_k \text{ or } x_j \in \Omega_i \cap \Omega_k, \end{cases} \quad (19)$$

for $i, k = 1, \dots, J$, and m corresponding iterations needed to stop of the iterative procedure.

The DD approach in [14] provides the minimum of functional \mathbf{J} in (7) (defined on the entire domain) as a piecewise function by collecting the minimum of each local functional \mathbf{J}_i^{DD-DA} defined on sub domain Ω_i by adding a local constraint about the entire overlap region. The functional DD method introduced in [14] is composed of the following steps:

1. Decomposition of domain Ω into a sequence of subdomains Ω_i such that:

$$\Omega = \bigcup_{i=1}^N \Omega_i.$$

2. Definition of the overlap regions of the subdomains Ω_i , as follows:

$$\Omega_{ij} = \Omega_i \cap \Omega_j \quad \text{for } i, j = 1, \dots, J.$$

3. Definition of operators RO_i and EO_i , as follows.

Definition 8 (*Restriction operator*) Let f be a function belonging to the Hilbert space $\mathcal{K}([0, T] \times \Omega)$, that is:

$$f(t, x) : [0, T] \times \Omega \mapsto \mathbb{R},$$

then

$$RO_i : \mathcal{K}([0, T] \times \Omega) \mapsto ([0, T] \times \Omega_i)$$

is the Restriction Operator such that

$$RO_i(f(t, x)) \equiv f(t, x), \quad (t, x) \in [0, T] \times \Omega_i,$$

where $i = 1, \dots, J$.

Moreover, for simplicity of notations, we let:

$$f_i(t, x) \equiv RO_i[f(t, x)].$$

Definition 9 (*Extension operator*) Let g_i con $i = 1, \dots, J$ be a functions belonging to the Hilbert space $\mathcal{K}([0, T] \times \Omega_i)$, then

$$EO_i : \mathcal{K}([0, T] \times \Omega_i) \mapsto ([0, T] \times \Omega)$$

is the Extension Operator such that

$$EO_i(g_i(t, x)) = \begin{cases} g_i(t, x) & x \in \Omega_i \\ 0 & \text{elsewhere} \end{cases}$$

4. Solution of J subproblems $(P_i^{DD-DA})^{n+1}$ for $n = 0, 1, 2, \dots$ where

$$\begin{aligned} & (P_i^{DD-DA})^{n+1} \operatorname{argmin}_{\mathbf{u}_i^{n+1} \in \mathbb{R}^{r_i}} \mathbf{J}_i^{DD-DA}(\mathbf{u}_i^{n+1}) \\ &= \operatorname{argmin}_{\mathbf{u}_i^{n+1} \in \mathbb{R}^{r_i}} (\|\mathbf{H}_i \mathbf{u}^{RO_i} - \mathbf{v}^{RO_i}\|_{\mathbf{R}_i}^2 + \lambda \|\mathbf{u}^{RO_i} - (\mathbf{u}^b)^{RO_i}\|_{\mathbf{B}_i}^2 \\ &+ \mu \|\mathbf{u}^{RO_i} / \Omega_{ij} - \mathbf{u}^{RO_j} / \Omega_{ij}\|_{\mathbf{B}_{ij}}^2), \end{aligned} \quad (20)$$

where \mathbf{B}_{ij} is restriction of matrix \mathbf{B} to overlap region Ω_{ij} , and $\mathbf{H}_i, \mathbf{B}_i$ restriction of matrices \mathbf{H}, \mathbf{B} to sub domain Ω_i for $i = 1, \dots, J$, according the description in [14]. Finally μ is non negative parameter.

From (20) the Euler–Lagrange equations give rise to the following systems $(S_i^{DD-DA})^{n+1}$ [14]:

$$(S_i^{DD-DA})^{n+1} : A_i^{DD-DA} \mathbf{w}_i^{n+1} = c_i^{DD-DA}, \quad (21)$$

to solve for $n = 0, 1, \dots$, while the vectors c_i^{DD-DA} and matrices A_i^{DD-DA} are defined as follows:

$$c_i^{DD-DA} = (\mathbf{V}_i^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{V}_i \mathbf{d}_i), \quad (22)$$

$$A_i^{DD-DA} = (\mathbf{V}_i^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{V}_i + I_i) \quad (23)$$

and I_i is the identity matrix, for $i = 1, \dots, J$.

5. Computation of \mathbf{u}_i^{n+1} , as in (18), for $i = 1, \dots, J$.

6. Computation of \mathbf{u}^{DA} , solution of problem 3D-Var DA in (6) obtained as in (19).

In order to prove equivalence between the DD method in [14] and MPS for solving the DA problem, firstly we note that the following equivalence holds on:

$$EO_i \equiv R_i, \quad RO_i \equiv R_i^T,$$

so that if we let $A \in \mathbb{R}^{NP \times NP}$ and consider r_i points of Ω_i , it is

$$RO_i(A) \equiv R_i A R_i^T,$$

for $i = 1, \dots, J$. We now prove the following result.

Proposition 1 Let \mathbf{u}^{DA} in (19) be the solution 3D-Var DA problem in (6) obtained applying the DD method in [26], that is, by solving for $n = 0, 1, \dots$ systems $(S_i^{DD-DA})^{n+1}$ in (21). Similarly, the MPS, provides \mathbf{u}^{DA} by solving for $n = 0, 1, \dots$ systems $(S_i^{MPS})^{n+1}$ in (16). We prove that systems in (16) and (21) are equivalent.

Proof Let us assume that $J = 2$. We consider subdomains Ω_1, Ω_2 and interfaces $\Gamma_{12} := \partial\Omega_1 \cap \Omega_2, \Gamma_{21} := \partial\Omega_2 \cap \Omega_1$.

By using the DD method in [26] it follows that:

$$(S_1^{DD-DA})^{n+1} : A_1^{DD-DA} \mathbf{w}_1^{n+1} = c_1^{DD-DA} \longrightarrow \mathbf{w}_1^{n+1} = (A_1^{DD-DA})^{-1} c_1^{DD-DA} \quad (24)$$

and

$$(S_2^{DD-DA})^n : A_2^{DD-DA} \mathbf{w}_1^n = c_1^{DD-DA} \longrightarrow \mathbf{w}_2^n = (A_2^{DD-DA})^{-1} c_2^{DD-DA}$$

by using MPS we get

$$\begin{aligned} (S_1^{MPS})^{n+1} : A_1^{MPS} \mathbf{w}_1^{n+1} &= c_1 + A_{12} \mathbf{w}_2^n \\ (S_2^{MPS})^{n+1} : A_2^{MPS} \mathbf{w}_2^{n+1} &= c_2 + A_{21} \mathbf{w}_1^n. \end{aligned} \quad (25)$$

We prove the equivalence between $(S_1^{DD-DA})^{n+1}$ in (24) and $(S_1^{MPS})^{n+1}$ in (25), i.e. we prove that solutions obtained from $(S_1^{DD-DA})^{n+1}$ and $(S_2^{DD-DA})^n$ in (24) satisfy $(S_1^{MPS})^{n+1}$ in (25).

Replacing \mathbf{w}_1^{n+1} by $(A_1^{DD-DA})^{-1} c_1^{DD-DA}$ in (25), it follows that:

$$A_1^{MPS} (A_1^{DD-DA})^{-1} c_1^{DD-DA} = c_1 + A_{12} \mathbf{w}_2^n; \quad (26)$$

matrix A_1^{MPS} in (17) can be rewritten as

$$A_1^{MPS} := (\mathbf{V}_1^T \mathbf{H}_1^T \mathbf{R}_1^{-1} \mathbf{H}_1 \mathbf{V}_1 + I_1 + \mathbf{B}/\Gamma_{12}) = A_1^{DD-DA} + A_{12}, \quad (27)$$

where A_1^{DD-DA} is defined in (23). Then, the (26) becomes:

$$(A_1^{DD-DA} + A_{12})(A_1^{DD-DA})^{-1} c_1^{DD-DA} = c_1 + A_{12} \mathbf{w}_2^n. \quad (28)$$

Replacing \mathbf{w}_2^n with $(A_2^{DD-DA})^{-1} c_2^{DD-DA}$ in (28), it follows that:

$$c_1^{DD-DA} + A_{12}((A_1^{DD-DA})^{-1} c_1^{DD-DA})|_{\Gamma_{12}} = c_1 + A_{12}((A_2^{DD-DA})^{-1} c_2^{DD-DA})|_{\Gamma_{12}}$$

then, we obtain

$$c_1^{DD-DA} = c_1. \quad (29)$$

From (15) and (22) we have

$$c_1^{DD-DA} = (\mathbf{V}_i^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \mathbf{H}_i \mathbf{V}_i \mathbf{d}_i) = c_1,$$

and the proof is complete. \square

4 Conclusions

Domain decomposition has been continually reinvented for several reasons: it is natural for task-based divide-and-conquer algorithms on problems with multi-physics and/or multi-discretizations, it provides a framework for combination and reuse of legacy software, and it organizes access to massive amounts of memory. However, the main motivation for the focus on domain decomposition methods in the past two decades is scalable performance through data parallelism [28]. Besides concurrency features, the memory locality of domain decomposition methods makes them highly suitable for advanced architectures, and many avenues remain open for conquering practical difficulties arising from complex applications and architecture, with correspondingly complex algorithmic adaptations. We present a domain decomposition-based framework for solution of Variational Data Assimilation methods, involving decomposition of the physical domain, partitioning of the solution and modification of the regularization functional describing the Data Assimilation model. We provide a mathematical justification for this framework in agreement with the Multiplicative Parallel Schwarz approach. In this way, convergence issues as well as mesh refinement techniques can be assessed to improve performance and scalability of the 3D Var DA functional decomposition in real applications.

References

1. Ghil, M., Malanotte-Rizzoli, P.: Data Assimilation in Meteorology and Oceanography, Advances in Geophysics, vol. 33. Academic Press, New York (1991)
2. Kalnay, E.: Atmospheric Modeling, Data Assimilation and Predictability. Cambridge University Press, Cambridge (2003)
3. Navon, I.M.: Data assimilation for numerical weather prediction: a review. In: Park, S.K., Xu, L. (eds.) Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications. Springer, Berlin (2009)
4. Blum, J., Le Dimet, F.X., Navon, I.M.: Data Assimilation for Geophysical Fluids, Volume XIV of Handbook of Numerical Analysis, vol. 9. Elsevier, Amsterdam (2005)
5. D'Elia, M., Perego, M., Veneziani, A.: A variational data assimilation procedure for the incompressible Navier-Stokes equations in hemodynamics. *J. Sci. Comput.* **52**(2), 340–359 (2011)
6. Murli, A., Cuomo, S., D'Amore, L., Galletti, A.: Numerical regularization of a real inversion formula based on the Laplace transform's eigenfunction expansion of the inverse function. *Inverse Probl.* **23**(2), 713–731 (2007)
7. Le Dimet, F.X., Talagrand, O.: Variational algorithms for analysis and assimilation of meteorological observations: theoretical aspects. *Tellus* **38A**, 97–110 (1986)
8. Kalman, R.E.: A new approach to linear filtering and prediction problems. *Trans. ASME J. Basic Eng.* **82**(Series D), 35–45 (1960)
9. D'Amore, L., Casaburi, D., Galletti, A., Marcellino, L., Murli, A.: Integration of emerging computer technologies for an efficient image sequences analysis. *Integr. Comput. Aided Eng.* **18**(4), 365–378 (2011)
10. Miyoshi, T.: Computational Challenges in Big Data Assimilation with Extreme-Scale Simulations, Talk at BDEC Workshop. Charleston, SC (2013)
11. Tremolet, Y., Le Dimet, F.X.: Parallel algorithms for variational data assimilation and coupling models. *Parallel Comput.* **22**, 657–674 (1986)
12. Arcucci, R., D'Amore, L., Celestino, S., Laccetti, G., Murli, A.: A scalable numerical algorithm for solving Tikhonov regularization problems. In: Wiatr, K., Karczewski, K., Wyrzykowski, R., Deelman, E., Kitowski, J., Dongarra, J. (eds.) 11th International Conference on Parallel Processing and Applied Mathematics, PPAM 2015. Lecture Notes in Computer Science, vol. 9574, pp. 45–54. Springer (2016). <https://doi.org/10.1007/978-3-319-32152-3-5>

13. Arcucci, R., D'Amore, L., Carracciolo, L., Scotti, G., Laccetti, G.: A decomposition of the tikhonov regularization functional oriented to exploit hybrid multilevel parallelism. *Int. J. Parallel Program.* **45**(5), 1214–1235 (2017). <https://doi.org/10.1007/s10766-016-0460-3>
14. D'Amore, L., Arcucci, R., Carracciolo, L., Murli, A.: A scalable approach for variational data assimilation. *J. Sci. Comput.* **61**, 239–257 (2014)
15. D'Amore, L., Arcucci, R., Carracciolo, L., Murli, A.: DD-ocean var: a domain decomposition fully parallel data assimilation software for the mediterranean forecasting system. In: *Procedia Computer Science*, 13th Annual International Conference on Computational Science, ICCS, vol. 8, pp. 1235–1244. Elsevier (2013). <https://doi.org/10.1016/j.procs.2013.05.290>
16. Chan, T., Mathew, T.P.: Domain decomposition algorithms. *Acta Numer.* **3**, 64–143 (1994)
17. Dolean V., Jolivet P., Nataf, F.: An Introduction to Domain Decomposition Methods: Algorithms, Theory and Parallel Implementation, HAL Id: cel-01100932 (2016)
18. Toselli, A., Widlund, O.: *Domain Decomposition Methods. Algorithms and Theory*. Springer, New York (2005)
19. Gunzburger, M.D., Lee, J.: A domain decomposition method for optimization problems for partial differential equations. *Comput. Math. Appl.* **40**, 177–192 (2000)
20. Tai, X.-C., Tseng, P.: Convergence rate analysis of an asynchronous space decomposition method for convex minimization. *Math. Comput.* **71**(239), 1105–1135 (2001)
21. Xu, J.: Iterative methods by space decomposition and subspace correction. *SIAM Rev.* **34**(4), 581–613 (1992)
22. Tai, X.-C., Xu, J.: Global convergence of subspace correction methods for convex optimization problems. *Math. Comput.* **71**(237), 105–124 (2002)
23. Fornasier, M., Schonlieb, C.B.: Subspace correction methods for total variation and l_1 minimization. *SIAM J. Numer. Anal.* **47**(5), 3397–3428 (2009)
24. Cardin, F., Favretti, M., Lovison, A., Masci, L.: Stochastic and geometric aspects of reduced reaction-diffusion dynamics. *Ricerche Matematica* **8**, 1–16 (2018). <https://doi.org/10.1007/s11587-018-0387-7>
25. Zayed, E.M.E., Rahman, H.M.A.: On using the modified variational iteration method for solving the nonlinear coupled equations in the mathematical physics. *Ricerche di Matematica* **59**, 137–159 (2010)
26. D'Amore, L., Arcucci, R., Pistoia, J., Toumi, R., Murli, A.: On the variational data assimilation problem solving and sensitivity analysis. *J. Comput. Phys.* **335**, 311–326 (2017)
27. D'Amore, L., Murli, A.: Regularization of a Fourier series method for the Laplace transform inversion with real data. *Inverse Prob.* **18**(4), 1185–1205 (2002)
28. Arcucci, R. D'Amore, L., Carracciolo, L.: On the problem-decomposition of scalable 4D-Var Data Assimilation models. In: *Proceedings of the 2015 International Conference on High Performance Computing and Simulation, HPCS 2015*, 2 September 2015, Article number 7237097, pp. 589–594 (2015)