

On the guess consistency in multi-incremental multi-resolution variational data assimilation

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Abstract. Variational Data Assimilation (DA) schemes are often used to adress high dimensional non-linear problems in operational applications in the Numerical Wheather Prediction (NWP) domain. Because of the high computational cost of such minimization problems, various methods can be applied to improve the convergence at a reasonable numerical cost. One of these methods currently applied in operational DA schemes is the multi-incremental approach that consists in solving a succession of linearized versions of the original non-linear problem in several outer loops, by using well known algorithms to ensure the convergence of the linear problem at the inner loop level, and using the solution of the inner loops to update the problem at each outer loop. In order to save computational cost, the multi-incremental multi-resolution method consists in starting the minimization at a lower resolution than the original one, and increasing it at the outer loop level until the full resolution of the problem. In such a scheme, the way to compute the new guess at each outer loop from the previous iterations is crucial. We adress the question of the guess consistency in the standard method currently used in operational systems, and also present a new method which ensures the guess consistency and need simpler calculations.

1 Introduction

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2 Data Assimilation Problem

In Data Assimilation (DA), one wants to minimize the following non linear cost function representing the ability of a model state to be compatible with observations:

$$\mathcal{J}(\mathbf{x}) = \frac{1}{2} (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + \frac{1}{2} (\mathbf{y}^o - \mathcal{H}(\mathbf{x}))^T \mathbf{R}^{-1} (\mathbf{y}^o - \mathcal{H}(\mathbf{x})), \quad (1)$$

where $\mathbf{x} \in \mathbb{R}^n$ is the state in model space of size n , $\mathbf{x}^b \in \mathbb{R}^n$ is the background state, $\mathbf{B} \in \mathbb{R}^{n \times n}$ is the background error covariance matrix, $\mathbf{y}^o \in \mathbb{R}^p$ is the observation vector in observation space of size p (note that in general $p < n$), $\mathbf{R} \in \mathbb{R}^{p \times p}$ is the observation error covariance matrix, and $\mathcal{H} : \mathbb{R}^n \rightarrow \mathbb{R}^p$ is the observation operator which maps the model space to the observation space.

2.1 Problem linearization

In general the observation operator is nonlinear and can be linearized around a guess state $\mathbf{x}_k^g \in \mathbb{R}^n$ so that: $\mathcal{H}(\mathbf{x}) \approx \mathcal{H}(\mathbf{x}_k^g) + \mathbf{H}_k \delta \mathbf{x}_k$ for $\mathbf{x} \approx \mathbf{x}_k^g$, defining the increment $\delta \mathbf{x}_k = \mathbf{x} - \mathbf{x}_k^g$, and where $\mathbf{H}_k \in \mathbb{R}^{p \times m}$ is the observation operator linearized around the guess state: $H_{k,ij} = \left. \frac{\partial \mathcal{H}_i}{\partial x_j} \right|_{\mathbf{x}=\mathbf{x}_k^g}$. Instead of minimizing the full cost function $\mathcal{J}(\mathbf{x})$, it is now possible to minimize successive quadratic approximations around successive guess states:

$$J(\delta \mathbf{x}_k) = \frac{1}{2} (\delta \mathbf{x}_k - \delta \mathbf{x}_k^b)^T \mathbf{B}^{-1} (\delta \mathbf{x}_k - \delta \mathbf{x}_k^b) + \frac{1}{2} (\mathbf{d}_k - \mathbf{H}_k \delta \mathbf{x}_k)^T \mathbf{R}^{-1} (\mathbf{d}_k - \mathbf{H}_k \delta \mathbf{x}_k) \quad (2)$$

where k indicates the k^{th} iteration (hereafter these iterations are called "outer loops" since the minimization of the successive approximations are realized using well known iterative solvers such as lanczos algorithms. We call "inner loops" the iterations of these algorithms), $\delta \mathbf{x}_k^b = \mathbf{x}^b - \mathbf{x}_k^g$ is the background increment and $\mathbf{d}_k = \mathbf{y}^o - \mathcal{H}(\mathbf{x}_k^g)$ is the innovation vector.

Setting the gradient of $J(\delta \mathbf{x}_k)$ to zero gives the analysis increment $\delta \mathbf{x}_k^a$:

$$\begin{aligned} & \mathbf{B}^{-1} (\delta \mathbf{x}_k^a - \delta \mathbf{x}_k^b) - \mathbf{H}_k^T \mathbf{R}^{-1} (\mathbf{d}_k - \mathbf{H}_k \delta \mathbf{x}_k^a) = 0 \\ \Leftrightarrow & (\mathbf{B}^{-1} + \mathbf{H}_k^T \mathbf{R}^{-1} \mathbf{H}_k) \delta \mathbf{x}_k^a = \mathbf{B}^{-1} \delta \mathbf{x}_k^b + \mathbf{H}_k^T \mathbf{R}^{-1} \mathbf{d}_k \\ 35 \quad \Leftrightarrow & \boxed{\mathbf{A}_k^{\mathbf{x}} \delta \mathbf{x}_k^a = \mathbf{b}_k^{\mathbf{x}}} \end{aligned} \quad (3)$$

with $\mathbf{A}_k^{\mathbf{x}} \in \mathbb{R}^{n \times n}$ and the right hand side $\mathbf{b}_k^{\mathbf{x}} \in \mathbb{R}^n$ defined as:

$$\mathbf{A}_k^{\mathbf{x}} = \mathbf{B}^{-1} + \mathbf{H}_k^T \mathbf{R}^{-1} \mathbf{H}_k, \quad (4)$$

$$\mathbf{b}_k^{\mathbf{x}} = \mathbf{B}^{-1} \delta \mathbf{x}_k^b + \mathbf{H}_k^T \mathbf{R}^{-1} \mathbf{d}_k. \quad (5)$$

The problem can now be solved using Gauss-Newton algorithm. It is very common to use the background state as a guess for the first iteration $k = 1$ ($\mathbf{x}_1^g = \mathbf{x}^b$), and then for $k > 1$, the analysis of the previous iteration is used to define the guess ($\mathbf{x}_k^g = \mathbf{x}_{k-1}^a$). Thus, the first background increment is $\delta \mathbf{x}_1^b = \mathbf{x}_1^g - \mathbf{x}^b = 0$, and the following ones can be computed as:

$$\begin{aligned} \delta \mathbf{x}_k^b &= \mathbf{x}^b - \mathbf{x}_k^g, \\ &= \mathbf{x}^b - \mathbf{x}_{k-1}^a, \\ &= \mathbf{x}^b - (\mathbf{x}_{k-1}^g + \delta \mathbf{x}_{k-1}^a), \\ 45 \quad &= \delta \mathbf{x}_{k-1}^b - \delta \mathbf{x}_{k-1}^a, \end{aligned} \quad (6)$$

which can be combined recursively to yield:

$$\delta \mathbf{x}_k^b = - \sum_{i=1}^{k-1} \delta \mathbf{x}_i^a. \quad (7)$$

In general, the condition number of this problem is poor, and one has to use preconditionning techniques to improve it.

2.2 Preconditionning

50 In this section we describe the square root \mathbf{B} preconditionning, which is widely used in DA. The \mathbf{B} matrix have the important property of being positive definite, so that there is an infinity of square-roots \mathbf{U} verifying $\mathbf{B} = \mathbf{U}\mathbf{U}^T$. The square root \mathbf{B} preconditionning consists in defining a new control variable $\delta\mathbf{v}_k = \mathbf{U}^T\mathbf{B}^{-1}\delta\mathbf{x}_k$, so that the linear system (3) can now be written in control space as $\mathbf{A}_k^\mathbf{v}\delta\mathbf{v}_k^a = \mathbf{b}_k^\mathbf{v}$ with:

$$\mathbf{A}_k^\mathbf{v} = \mathbf{I}_m + \mathbf{U}^T\mathbf{H}_k^T\mathbf{R}^{-1}\mathbf{H}_k\mathbf{U}, \quad (8)$$

$$55 \quad \mathbf{b}_k^\mathbf{v} = \delta\mathbf{v}_k^b + \mathbf{U}^T\mathbf{H}_k^T\mathbf{R}^{-1}\mathbf{d}_k. \quad (9)$$

Using this technique allows to recursively solve the system without using \mathbf{B}^{-1} which is, in general, not available due to its high dimension, even if it is needed in general to compute the right-hand side $\mathbf{b}_k^\mathbf{v}$; $\mathbf{U}^T\mathbf{B}^{-1}$ can be applied on both side of equation (7), leading to:

$$\delta\mathbf{v}_k^b = -\sum_{i=1}^{k-1} \delta\mathbf{v}_i^a, \quad (10)$$

60 which can be used to compute the right hand side $\mathbf{b}_k^\mathbf{v}$ without requiring \mathbf{B}^{-1} .

2.3 Changing the resolution between the outer loops

In special cases, the background error covariance matrix can be updated between outer iterations defining \mathbf{B}_k , and its square-root \mathbf{U}_k . In this case, it is not systematically possible to compute the background increment without using \mathbf{B}^{-1} . One example of such a scheme is the multi-incremental multi-resolution approach, in which the resolution increases at each outer loop for computational efficiency, and therefore, the \mathbf{B} matrix depends on k . In this case, Equation (10) is valid and one can obtain the background increment as follows:

$$\begin{aligned} \delta\mathbf{v}_k^b &= -\mathbf{U}_k^T\mathbf{B}_k^{-1}\sum_{i=1}^{k-1} \delta\mathbf{x}_i^a, \\ &= -\sum_{i=1}^{k-1} \mathbf{U}_k^T\mathbf{B}_k^{-1}\mathbf{U}_i\delta\mathbf{v}_i^a. \end{aligned} \quad (11)$$

It should be emphasized that if $\mathbf{U}_k^T\mathbf{B}_k^{-1}\mathbf{U}_i\delta\mathbf{v}_i^a \neq \delta\mathbf{v}_i^a$, equation (10) cannot be used consistently. To realize the change of resolution, one needs to use interpolators in model space $\mathbf{T}_{i \rightarrow k}^\mathbf{x} \in \mathbb{R}^{n_k \times n_i}$ and in control space $\mathbf{T}_{i \rightarrow k}^\mathbf{v} \in \mathbb{R}^{m_k \times m_i}$ from the resolution \mathcal{R}_i to \mathcal{R}_k , where n_k and m_k respectively denotes the size of the model space and the control space. For clarity, we now assume that the resolutions are stricly increasing: for $i < k$, $n_i < n_k$ and $m_i < m_k$, and that the full resolution is obtained at the last iteration K . We define two interpolators from resolution \mathcal{R}_i to resolution \mathcal{R}_k :

- $\mathbf{T}_{i \rightarrow k}^\mathbf{x} \in \mathbb{R}^{n_k \times n_i}$ in model space,
- 75 - $\mathbf{T}_{i \rightarrow k}^\mathbf{v} \in \mathbb{R}^{m_k \times m_i}$ in control space,

A special class of interpolators called "transitive interpolators" have three extra properties:

- Upscaling transitivity: for $n_i < n_j$ and $n_i < n_k$:

$$\mathbf{T}_{j \rightarrow k}^{\mathbf{x}} \mathbf{T}_{i \rightarrow j}^{\mathbf{x}} = \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \quad (12)$$

- 80 – Downscaling transitivity: for $n_i < n_j < n_k$:

$$\mathbf{T}_{j \rightarrow i}^{\mathbf{x}} \mathbf{T}_{k \rightarrow j}^{\mathbf{x}} = \mathbf{T}_{k \rightarrow i}^{\mathbf{x}} \quad (13)$$

- Right-inverse: for $n_i < n_k$

$$\mathbf{T}_{k \rightarrow i}^{\mathbf{x}} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} = \mathbf{I}_{n_i} \quad (14)$$

and similarly for $\mathbf{T}_{i \rightarrow k}^{\mathbf{y}}$ in control space, replacing n with m .

- 85 A generic family of transitive interpolators is based on a zero-padding operator surrounded by an orthogonal transform. For instance in model space:

$$\mathbf{T}_{i \rightarrow k}^{\mathbf{x}} = \mathbf{S}_k^{\mathbf{T}} \mathbf{\Delta}_{i \rightarrow k} \mathbf{S}_i, \quad (15)$$

where

- $\mathbf{\Delta}_{i \rightarrow k} \in \mathbb{R}^{n_k \times n_i}$ is a zero-padding operator:

$$90 \quad \Delta_{i \rightarrow k, \alpha \beta} = \begin{cases} 1 & \text{if } \alpha = \beta \\ 0 & \text{if } \alpha \neq \beta \end{cases} \quad (16)$$

- $\mathbf{S}_k \in \mathbb{R}^{n_k \times n_k}$ is any orthogonal transform:

$$\mathbf{S}_k \mathbf{S}_k^{\mathbf{T}} = \mathbf{S}_k^{\mathbf{T}} \mathbf{S}_k = \mathbf{I}_{n_k}. \quad (17)$$

It is easy to check the three required properties:

- Upscaling transitivity: for $n_i \leq n_j$ and $n_i \leq n_k$:

$$95 \quad \begin{aligned} \mathbf{T}_{j \rightarrow k}^{\mathbf{x}} \mathbf{T}_{i \rightarrow j}^{\mathbf{x}} &= \mathbf{S}_k^{\mathbf{T}} \mathbf{\Delta}_{j \rightarrow k} \mathbf{S}_j \mathbf{S}_j^{\mathbf{T}} \mathbf{\Delta}_{i \rightarrow j} \mathbf{S}_i \\ &= \mathbf{S}_k^{\mathbf{T}} \mathbf{\Delta}_{j \rightarrow k} \mathbf{\Delta}_{i \rightarrow j} \mathbf{S}_i \\ &= \mathbf{S}_k^{\mathbf{T}} \mathbf{\Delta}_{i \rightarrow k} \mathbf{S}_i \\ &= \mathbf{T}_{i \rightarrow k}^{\mathbf{x}}. \end{aligned} \quad (18)$$

- Downscaling transitivity: for $n_i \leq n_j \leq n_k$:

$$\begin{aligned}
100 \quad \mathbf{T}_{j \rightarrow i}^{\mathbf{x}} \mathbf{T}_{k \rightarrow j}^{\mathbf{x}} &= \mathbf{S}_i^{\mathbf{T}} \Delta_{j \rightarrow i} \mathbf{S}_j \mathbf{S}_j^{\mathbf{T}} \Delta_{k \rightarrow j} \mathbf{S}_k \\
&= \mathbf{S}_i^{\mathbf{T}} \Delta_{j \rightarrow i} \Delta_{k \rightarrow j} \mathbf{S}_k \\
&= \mathbf{S}_i^{\mathbf{T}} \Delta_{k \rightarrow i} \mathbf{S}_k \\
&= \mathbf{T}_{k \rightarrow i}^{\mathbf{x}}.
\end{aligned} \tag{19}$$

- Right-inverse: for $n_i \leq n_k$

$$\begin{aligned}
105 \quad \mathbf{T}_{k \rightarrow i}^{\mathbf{x}} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} &= \mathbf{S}_i^{\mathbf{T}} \Delta_{k \rightarrow i} \mathbf{S}_k \mathbf{S}_k^{\mathbf{T}} \Delta_{i \rightarrow k} \mathbf{S}_i \\
&= \mathbf{S}_i^{\mathbf{T}} \Delta_{k \rightarrow i} \Delta_{i \rightarrow k} \mathbf{S}_i \\
&= \mathbf{S}_i^{\mathbf{T}} \mathbf{S}_i \\
&= \mathbf{I}_{n_i}.
\end{aligned} \tag{20}$$

Associated to the various resolution, we qualify a \mathbf{B} family as "projective" if the low-resolution members can be defined as
110 a projection of the high-resolution one, using transitive interpolators. For $n_i < n_k$, that would mean:

$$\mathbf{U}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} = \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \mathbf{U}_i. \tag{21}$$

Finally, the multi-resolution problem should be solved with the following requirements in mind:

- The background \mathbf{x}^b is provided at full resolution, but it can be simplified at resolution \mathcal{R}_k :

$$\mathbf{x}_k^b = \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \mathbf{x}^b \tag{22}$$

- 115 – A full resolution guess denoted \mathbf{x}_k^{g+} has to be computed at each outer iteration to run model trajectories used in the operators linearization. This full resolution guess can be simplified at resolution \mathcal{R}_k to give the actual guess of the outer iteration k :

$$\mathbf{x}_k^g = \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \mathbf{x}_k^{g+} \tag{23}$$

- Only δ -quantities should be interpolated to higher resolution, and then possibly added to full quantities at full resolution.

120 3 Guess consistency

In the linear systems solved at each outer iteration, the the full resolution guess \mathbf{x}_k^{g+} appears for two distinct purposes:

- First, it is explicitly defined to be used as the linearization state for the observation operator at each outer loops and to compute the innovation \mathbf{d}_k . The first guess for $k = 1$ is taken as the background state, also provided at full resolution

125 $\mathbf{x}_1^{g+} = \mathbf{x}^b$. At the end of iteration k , without any loss of generality, we can define the analysis increment at full resolution $\delta\mathbf{x}_{k-1}^{a+}$ that updates the full resolution guess:

$$\mathbf{x}_k^{g+} = \mathbf{x}_{k-1}^{g+} + \delta\mathbf{x}_{k-1}^{a+} \quad (24)$$

The way the analysis increment at full resolution $\delta\mathbf{x}_{k-1}^{a+}$ is obtained from the products of previous outer iterations does not matter at this point.

– Second, it is implicitly present in the first term of the right-hand side:

$$\begin{aligned} 130 \quad \delta\mathbf{v}_k^b &= \mathbf{U}_k^T \mathbf{B}_k^{-1} \delta\mathbf{x}_k^b \\ &= \mathbf{U}_k^T \mathbf{B}_k^{-1} (\mathbf{x}_k^b - \mathbf{x}_k^g) \\ &= \mathbf{U}_k^T \mathbf{B}_k^{-1} \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} (\mathbf{x}^b - \mathbf{x}_k^{g+}) \end{aligned} \quad (25)$$

The question of the consistency between these two occurrences of the guess state in the minimization is crucial and is detailed in the following sections.

135 3.1 Theoretical method

In the "theoretical" method, one assumes that \mathbf{B}_k^{-1} is available and can be used to compute the increment $\delta\mathbf{v}_k^b$ explicitly from \mathbf{x}_k^{g+} using equations (25). There is no requirement on the expression of the analysis increment at full resolution $\delta\mathbf{x}_{k-1}^{a+}$.

3.2 Standard method

140 In the "standard" method, which is currently used in operational multi-incremental multi-resolution schemes, \mathbf{B}_k^{-1} is not available and the first term of the right-hand side is computed separately, using transformed versions of equation (10) with appropriate interpolations:

$$\delta\mathbf{v}_k^b = - \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta\mathbf{v}_i^a. \quad (26)$$

This additional constraint imposes a unique expression for the analysis increment at full resolution $\delta\mathbf{x}_{k-1}^{a+}$, if the guess consistency has to be maintained.

145 3.2.1 General case

Using equation (24) and the fact that the first full resolution guess is taken as the background state, the full resolution guess at iteration k can be expressed as:

$$\mathbf{x}_k^{g+} = \mathbf{x}^b + \sum_{i=1}^{k-1} \delta\mathbf{x}_i^{a+} \quad (27)$$

which is equivalent to:

$$150 \quad \mathbf{x}^b - \mathbf{x}_k^{g+} = - \sum_{i=1}^{k-1} \delta \mathbf{x}_i^{a+} \quad (28)$$

This result can be introduced into equation (25) to get the background increment as a function of the analysis increment at full resolution $\delta \mathbf{x}_i^{a+}$:

$$\delta \mathbf{v}_k^b = -\mathbf{U}_k^T \mathbf{B}_k^{-1} \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-1} \delta \mathbf{x}_i^{a+} \quad (29)$$

Comparing equations (26) and (29), the guess consistency is maintained if:

$$155 \quad \begin{aligned} & \mathbf{U}_k^T \mathbf{B}_k^{-1} \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-1} \delta \mathbf{x}_i^{a+} = \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a, \\ \Leftrightarrow & \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-1} \delta \mathbf{x}_i^{a+} = \mathbf{U}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a, \\ \Leftrightarrow & \boxed{\mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \delta \mathbf{x}_{k-1}^{a+} = \mathbf{U}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-2} \delta \mathbf{x}_i^{a+}}. \end{aligned} \quad (30)$$

To understand this result, one needs to distinguish between two cases according to the number of outer loops to be realized: if $K = 2$, equation (30) corresponding to the last iteration $k = K = 2$ becomes $\delta \mathbf{x}_1^{a+} = \mathbf{U}_2 \mathbf{T}_{1 \rightarrow 2}^{\mathbf{v}} \delta \mathbf{v}_1^a$ leading to an explicit
 160 expression of $\delta \mathbf{x}_1^{a+}$. In the case where $K > 2$, equation (30) can be solved explicitly if $\mathbf{T}_{K \rightarrow k}^{\mathbf{x}}$ has a known right-inverse denoted $(\mathbf{T}_{K \rightarrow k}^{\mathbf{x}})^{-1}_{\text{right}}$, such that $\mathbf{T}_{K \rightarrow k}^{\mathbf{x}} (\mathbf{T}_{K \rightarrow k}^{\mathbf{x}})^{-1}_{\text{right}} = \mathbf{I}_{n_k}$. In this case, equation (30) becomes:

$$\delta \mathbf{x}_{k-1}^{a+} = (\mathbf{T}_{K \rightarrow k}^{\mathbf{x}})^{-1}_{\text{right}} \left(\mathbf{U}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-2} \delta \mathbf{x}_i^{a+} \right) \quad (31)$$

Not that if this right-inverse exists, its unicity depends on the rank of the kernel of $\mathbf{T}_{K \rightarrow k}^{\mathbf{x}}$: if $\delta \mathbf{x}_{k-1}^{a+}$ is a solution of equation (30) and $\mathbf{u} \in \text{Ker}(\mathbf{T}_{K \rightarrow k}^{\mathbf{x}})$, then $(\delta \mathbf{x}_{k-1}^{a+} + \mathbf{u})$ is also a solution.

165 3.2.2 Simplified standard method

The right-hand side of equation (36) can be split in order to extract the term coming from outer iteration $k - 1$:

$$\delta \mathbf{x}_{k-1}^{a+} = \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \mathbf{U}_k \mathbf{T}_{k-1 \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_{k-1}^a + \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \sum_{i=1}^{k-2} (\mathbf{U}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \delta \mathbf{x}_i^{a+}) \quad (32)$$

If the \mathbf{B} family is projective, then:

$$\mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \mathbf{U}_k \mathbf{T}_{k-1 \rightarrow k}^{\mathbf{v}} = \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \mathbf{T}_{k-1 \rightarrow k}^{\mathbf{x}} \mathbf{U}_{k-1} = \mathbf{T}_{k-1 \rightarrow K}^{\mathbf{x}} \mathbf{U}_{k-1} \quad (33)$$

170 so a simplified expression of $\delta \mathbf{x}_{k-1}^{a+}$ is:

$$\boxed{\delta \mathbf{x}_{k-1}^{a+} = \mathbf{T}_{k-1 \rightarrow K}^{\mathbf{x}} \mathbf{U}_{k-1} \delta \mathbf{v}_{k-1}^a} \quad (34)$$

that verifies (36) since both terms inside the summation cancel each other:

$$\begin{aligned} \mathbf{U}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \delta \mathbf{x}_i^{a+} &= \mathbf{U}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \mathbf{T}_{i \rightarrow K}^{\mathbf{x}} \mathbf{U}_i \delta \mathbf{v}_i^a \\ &= (\mathbf{U}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} - \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \mathbf{U}_i) \delta \mathbf{v}_i^a \\ 175 \quad &= 0 \end{aligned} \quad (35)$$

Equation (34) now estimates $\delta \mathbf{x}_{k-1}^{a+}$ using results from outer iterations $k-1$ only and this expression is referred to as "simplified expression" in the following.

3.2.3 Corrected standard method

If one uses transitive interpolators, the right inverse of $\mathbf{T}_{K \rightarrow k}^{\mathbf{x}}$ exists and is defined as $\mathbf{T}_{k \rightarrow K}^{\mathbf{x}}$, so that:

$$180 \quad \boxed{\delta \mathbf{x}_{k-1}^{a+} = \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \left(\mathbf{U}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{v}} \delta \mathbf{v}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-2} \delta \mathbf{x}_i^{a+} \right)} \quad (36)$$

Equation (36) estimates $\delta \mathbf{x}_{k-1}^{a+}$ using results from outer iterations 1 to $k-1$, not outer iteration $k-1$ only. Hereafter, this expression is referred to as "corrected expression".

3.3 Consistent method

185 An new alternative method in which the guess consistency is guaranteed can be defined. This method also have the advantage of requiring much more simpler calculations than the "standard" method and gives the same results. The basic idea is to reverse the order of computations: the first term of the right-hand side is computed first from equation (26), and then the background increment is given by:

$$\delta \mathbf{x}_k^b = \mathbf{U}_k \delta \mathbf{v}_k^b \quad (37)$$

Finally, the full resolution guess is deduced as:

$$190 \quad \mathbf{x}_k^{g+} = \mathbf{x}^b - \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \delta \mathbf{x}_k^b, \quad (38)$$

ensuring its consistency.

3.4 Methods comparision

Guess consistency is always ensured for the "theoretical" and "consistent" methods. For the "standard" method, it is only ensured if one uses transitive interpolators, and the correct formula for the analysis increment at full resolution $\delta \mathbf{x}_{k-1}^{a+}$. In the

195 general case, it depends whether equation (30) can be solved or not. In the general case, if a solution exists for the "standard" method, the same $\delta \mathbf{x}_{k-1}^{a+}$ can be used for the "theoretical" method and all methods give the same results. In the case where no solution can be found for the "standard" method, another expression is used for the "theoretical" one, which leads to different results from the "alternative" method. In the case of transitive interpolators, "standard" and "consistent" methods always give the same results and are in agreement with the "theoretical" method if the same expression is used for $\delta \mathbf{x}_{k-1}^{a+}$. The case of a
200 projective \mathbf{B} family is just a subcase of the transitive interpolators one, where the expression of $\delta \mathbf{x}_{k-1}^{a+}$ can be simplified for the "theoretical" and "standard" methods.

The figure (1), (2) and (3) respectively illustrate the workflow of the three methods.

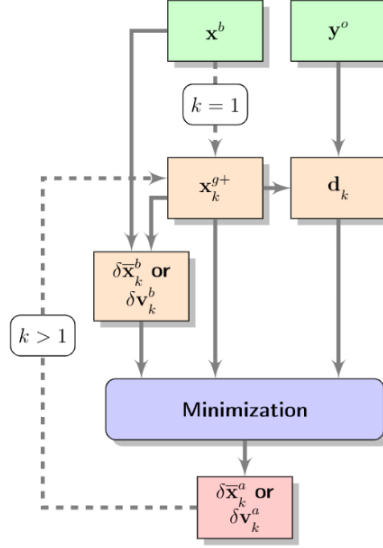


Figure 1. Illustrative workflow of the theoretical method. The full resolution background and guess are used at each outer iteration to compute the $\delta \bar{\mathbf{x}}_k^b$ or $\delta \mathbf{v}_k^b$, using \mathbf{B}_k^{-1} :

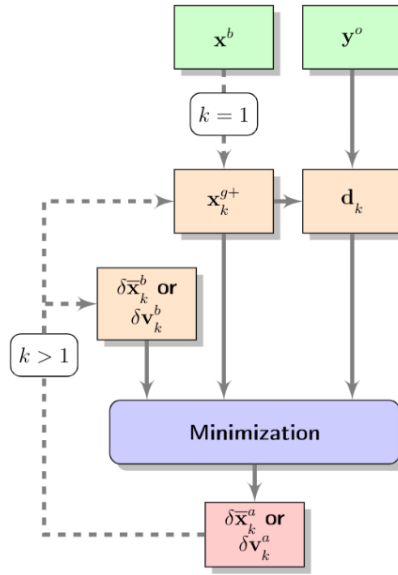


Figure 2. Illustrative workflow of the standard method. The potential guess inconsistency of the "standard" method comes from the fork in the use of the minimization output, to compute the full resolution guess and the first term of the right-hand side independently. If the correct formula is not used, then a guess inconsistency can arise.

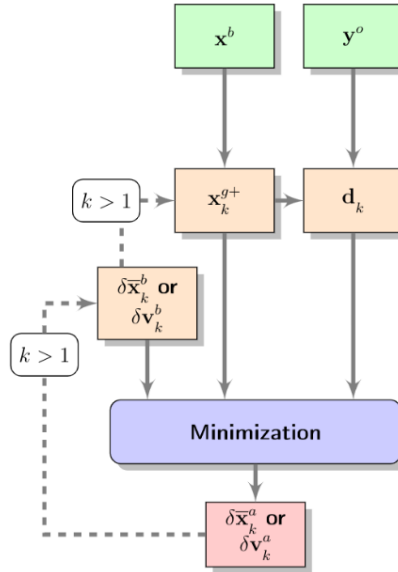


Figure 3. Illustrative workflow of the consistent method. Because of its closed cycle form (no fork), the "consistent" method ensures the guess consistency, without requiring \mathbf{B}_k^{-1} .

The fork in the "standard" method using the analysis of iteration k to compute separately the background increment and the guess of iteration $k + 1$ is responsible of the potential inconsistency of the guess.

205 The differences between the three methods coming from this guess inconsistency are illustraed using a toy problem which is describe in section ??.

Another important problem is the equivalence between the square root \mathbf{B} preconditionning and the full \mathbf{B} preconditionning which may also be used for computationnal efficiency. This equivalence in the case of a multi-incremental multi-resolution framework is discussed in the following section.

210 4 Equivalence between preconditionners

Another preconding technique consists in defining a new variable $\delta\bar{\mathbf{x}}_k = \mathbf{B}_k^{-1}\delta\mathbf{x}_k$ so that the linear system to solve can be written as:

$$\mathbf{A}_k^{\bar{}}\delta\bar{\mathbf{x}}_k^a = \mathbf{b}_k^{\bar{}}, \quad (39)$$

$\delta\bar{\mathbf{x}}_k^a$ being the preconditionned analysis increment, and with:

$$215 \quad \mathbf{A}_k^{\bar{}} = \mathbf{I}_n + \mathbf{H}_k^T \mathbf{R}^{-1} \mathbf{H}_k \mathbf{B}_k, \quad (40)$$

and the right hand side now written as:

$$\mathbf{b}_k^{\bar{}} = \delta\bar{\mathbf{x}}_k^b + \mathbf{H}_k^T \mathbf{R}^{-1} \mathbf{d}_k. \quad (41)$$

An equivalent form of equation (42) can be found by applying \mathbf{B}^{-1} on both side of equation (7) to express the so preconditionned background increment as:

$$220 \quad \delta\bar{\mathbf{x}}_k^b = - \sum_{i=1}^{k-1} \delta\bar{\mathbf{x}}_i^a. \quad (42)$$

In the same way as for the square root \mathbf{B} preconditionning, if the \mathbf{B} matrix changes between the outer loops and so depends on k , one can write:

$$\begin{aligned} \delta\bar{\mathbf{x}}_k^b &= -\mathbf{B}_k^{-1} \sum_{i=1}^{k-1} \delta\mathbf{x}_i^a \\ &= - \sum_{i=1}^{k-1} \mathbf{B}_k^{-1} \mathbf{B}_i \delta\bar{\mathbf{x}}_i^a \end{aligned} \quad (43)$$

225 and similarly if $\mathbf{B}_k^{-1} \mathbf{B}_i \delta\bar{\mathbf{x}}_i^a \neq \delta\bar{\mathbf{x}}_i^a$, equation (42) cannot be used consistently.

In the "standard" method using this preconditionner, one can write equivalent forms of equations (26) and (45):

$$\delta\bar{\mathbf{x}}_k^b = - \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta\bar{\mathbf{x}}_i^a, \quad (44)$$

$$\delta \bar{\mathbf{x}}_k^b = -\mathbf{B}_k^{-1} \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-1} \delta \mathbf{x}_i^{a+}. \quad (45)$$

230 Now comparing equations (44) and (45), the guess consistency is maintained if:

$$\begin{aligned} \mathbf{B}_k^{-1} \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-1} \delta \mathbf{x}_i^{a+} &= \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a, \\ \Leftrightarrow \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-1} \delta \mathbf{x}_i^{a+} &= \mathbf{B}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a, \\ \Leftrightarrow \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \delta \mathbf{x}_{k-1}^{a+} &= \mathbf{B}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-2} \delta \mathbf{x}_i^{a+}. \end{aligned} \quad (46)$$

$$\delta \mathbf{x}_1^{a+} = \mathbf{B}_2 \mathbf{T}_{1 \rightarrow 2}^{\mathbf{x}} \delta \bar{\mathbf{x}}_1^a \quad (47)$$

235 and

$$\delta \mathbf{x}_{k-1}^{a+} = (\mathbf{T}_{K \rightarrow k}^{\mathbf{x}})_{\text{right}}^{-1} \left(\mathbf{B}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-2} \delta \mathbf{x}_i^{a+} \right) \quad (48)$$

and

$$\delta \mathbf{x}_{k-1}^{a+} = \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \left(\mathbf{B}_k \sum_{i=1}^{k-1} \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \sum_{i=1}^{k-2} \delta \mathbf{x}_i^{a+} \right) \quad (49)$$

Similarly in control space:

$$240 \quad \delta \mathbf{x}_{k-1}^{a+} = \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \mathbf{B}_k \mathbf{T}_{k-1 \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_{k-1}^a + \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \sum_{i=1}^{k-2} (\mathbf{B}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \delta \mathbf{x}_i^{a+}) \quad (50)$$

If the \mathbf{B} family is projective, then:

$$\mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \mathbf{B}_k \mathbf{T}_{k-1 \rightarrow k}^{\mathbf{x}} = \mathbf{T}_{k \rightarrow K}^{\mathbf{x}} \mathbf{T}_{k-1 \rightarrow k}^{\mathbf{x}} \mathbf{B}_{k-1} = \mathbf{T}_{k-1 \rightarrow K}^{\mathbf{x}} \mathbf{B}_{k-1} \quad (51)$$

so a simplified expression of $\delta \mathbf{x}_{k-1}^{a+}$ is:

$$\delta \mathbf{x}_{k-1}^{a+} = \mathbf{T}_{k-1 \rightarrow K}^{\mathbf{x}} \mathbf{B}_{k-1} \delta \bar{\mathbf{x}}_{k-1}^a \quad (52)$$

245 that verifies (49) since both terms inside the summation cancel each other:

$$\begin{aligned}
\mathbf{B}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \delta \mathbf{x}_i^{a+} &= \mathbf{B}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \delta \bar{\mathbf{x}}_i^a - \mathbf{T}_{K \rightarrow k}^{\mathbf{x}} \mathbf{T}_{i \rightarrow K}^{\mathbf{x}} \mathbf{B}_i \delta \bar{\mathbf{x}}_i^a \\
&= (\mathbf{B}_k \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} - \mathbf{T}_{i \rightarrow k}^{\mathbf{x}} \mathbf{B}_i) \delta \bar{\mathbf{x}}_i^a \\
&= 0
\end{aligned} \tag{53}$$

$$\delta \mathbf{x}_k^b = \mathbf{B}_k \delta \bar{\mathbf{x}}_k^b \tag{54}$$

250 5 Methodology and results

In order to illustrate the differences arising between the three methods due to the guess consistency, we have compared the results obtained with all the methods on a toy problem detailed in the present section.

5.1 Methodology

255 In this section we illustrate the differences arising between the three above-mentionned methods related to the guess consistency. To do so, we have built a bidimensional toy problem as follows:

- We consider periodic domain composed of bidimensional square grids with $N_x = 101$ x-coordinates and $N_y = 101$ y-coordinates (leading to a total of $m = N_x \times N_y$ points) and assume that this resolution corresponds to the full resolution of our problem (e.g. this resolution corresponds to the last iteration $k = K$ of our multi-incremental multi-resolution scheme).

260 – A \mathbf{B} matrix is introduced with gaussian spectral variances defined as:

$$\mathbf{B}_{\mathbf{k},\mathbf{l}} = e^{-2((k^2+l^2)\pi L_b)^2}, \tag{55}$$

where $k \in [0 : N_x/2]$, $l \in [-N_y/2 : N_y/2]$ are the accessible wave numbers and L_b is a correlation lengthscale. We also define its grid point variance as:

$$\mathbf{B}_{\mathbf{i},\mathbf{j}} = 1 + \sigma^b \sin(2\pi x_i) \sin(2\pi y_j), \tag{56}$$

265 where σ^b can be modified, x_i is the i^{th} x-coordinate of the grid, and y_j is the j^{th} y-coordinate of the grid.

- A full resolution truth state \mathbf{x}^t is defined on this grid by applying the square root of \mathbf{B} (denoted \mathbf{U}) on a random field ν^t with normal distribution: (NB: I do not remember why is there $x^t = 1 + x^t$ in the code? - Find a way to write the identity operator):

$$\mathbf{x}^t = \mathbf{1}_m + \mathbf{U} \nu^t. \tag{57}$$

270 – A full resolution background state is defined in same manner with a different random field ν^b (NB: idem for this):

$$\mathbf{x}_b = \mathbf{x}^t + \mathbf{U}\nu^b. \quad (58)$$

– In order to have the simpler problem, the observation operator is taken to be the identity. We also introduce p observation points that are not necessarily on a grid point: (NB: we do not discuss about the cubic version ?)

$$\mathcal{H}\mathbf{x} = \mathbf{x}. \quad (59)$$

275 – And finally the observation error covariance matrix $\mathbf{R} \in \mathbb{R}^{p \times p}$ is simply defined as:

$$\mathbf{R}_{i,j} = \sigma^o. \quad (60)$$

In order to illustrate the differences between the different cases we have mentioned, we applied a multi-incremental multi-resolution scheme using the three methods as well as different interpolators. The spectral decomposition is an orthogonal operator, which can be associated with a zero padding operator to build a transitive interpolator. It should be noted that usual
 280 grid-points interpolators like (bi-)linear and nearest-neighbor interpolators are not transitive in general. An important exception is the (bi-)linear interpolator when coarse grid points are colocated with fine grid points.

5.2 Results

As an illustrative case, we have choosen NB:Show the quadratic cost function (obs and background) + tables

6 Conclusions

285 TEXT

Code availability. TEXT

Data availability. TEXT

Code and data availability. TEXT

Sample availability. TEXT

290 *Video supplement.* TEXT

Author contributions. TEXT

Competing interests. TEXT

Disclaimer. TEXT

Acknowledgements. TEXT

295 **References**

REFERENCE 1
REFERENCE 2