Theoretical Aspect of Suitable Spatial Boundary Condition Specified for Adjoint Model on Limited Area①

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ABSTRACT

Theoretical argumentation for so-called suitable spatial condition is conducted by the aid of homotopy framework to demonstrate that the proposed boundary condition does guarantee that the over-specification boundary condition resulting from an adjoint model on a limited-area is no longer an issue, and yet preserve its well-poseness and optimal character in the boundary setting. The ill-poseness of over-specified spatial boundary condition is in a sense, inevitable from an adjoint model since data assimilation processes have to adapt prescribed observations that used to be over-specified at the spatial boundaries of the modeling domain.

In the view of pragmatic implement, the theoretical framework of our proposed condition for spatial boundaries indeed can be reduced to the hybrid formulation of nudging filter, radiation condition taking account of ambient forcing, together with Dirichlet kind of compatible boundary condition to the observations prescribed in data assimilation procedure. All of these treatments, no doubt, are very familiar to mesoscale modelers.

Key words: Variational data assimilation, Adjoint model, Over-specified partial boundary condition

1. Introduction

Many devastating weather events occurring in the regions are of mesoscale characters. The numerical weather prediction (NWP) on limited-area domain is essentially required in order to simulate such complex local weather and climate systems. The accuracy of NWP depends not only on the exact representation of dynamic and physical processes in the atmosphere but also critically on the initial-boundary conditions employed for integrating the model. Just at this point, quarter-space variational data assimilation (4dVAR) has been introduced in order to determine the initial state of NWP model, so that the corresponding solution is closer, in a sense, to the observations available over the assimilation period. The measurement of difference between observations and model solutions leads to solving the optimization problem, intended at determining the initial values of the model that optimize some property of NWP output. It turns out that, with the present NWP models and computers, the only practical way to conduct variational assimilation is dependent on appropriate

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using of the so–called adjoint model (Lewis and Derber, 1985; Rostating et al., 1993).

The implementation of the adjoint model over the global domain has been so far very successful (Talagrand, 1997). The success is simply because the periodic boundary condition used here is well–posed condition in any sense (Couraut and Hilbert, 1962). However, such periodic condition in real simulations and / or predictions over the limited–area of interest is just out of our consideration, since the condition closes the modeling domain off its ambient. On the other hand, the adjoint model defined over limited–area, in fact, still meets many difficulties; among others, how to set well–posed spatial boundary conditions has been rarely discussed in detail. Most of the researchers ignored the additional problems related to the necessity of specifying appropriate spatial boundary conditions, particularly the setting of lateral boundary conditions for limited–area model, which were either high arbitrarily designed or totally by pragmatic approach.

Inevitably, the prescribed observation has to be introduced into the adjoint model. The obvious solution for the boundary condition of adjoint model is directly to define the ambient variables from observations on the boundaries. However, such boundary definition nevertheless lead to the so–called over–specification problem (Hill, 1968, Chen, 1973, Kar and Turco, 1995) at the boundaries. The problem of over–specified boundary conditions is simply created by the over–definition of values of ambient variables at the boundaries so that the numbers of boundary conditions is exceeding the right numbers of well–posed boundary conditions required for the model. The problem becomes further complicated by the requirement of additional boundary conditions in numerical calculation using a finite difference method i.e., computational boundary conditions, due to the order–inconsistency between the difference equations and the corresponding differential equations. The over–specified conditions therefore result in the extraneous solution.

On the other hand, the over–specification is not totally of the negative impact; at least it reduces the complicacy of boundary treatment so that all of possibly ill–posed boundary conditions, such as the down–specification conditions (numbers of boundary conditions is less than the right numbers required for well–posed boundary conditions; (Chen, 1973)) are all simplified to the single —over–specified problem at the boundaries. Such simplification may have profound importance because any kind of well–posed conditions in primitive equations model of NWP is nearly impossible to conduct. That is either due to the introduction of hydrostatic approximation (Oliger and Sundström, 1978), or that even for some end–to–end non–hydrostatic model of NWP, the possible well–posed conditions are indeed too complex and too expensive to specify in practice.

Clearly, the task now is to seek a suitable boundary condition under the circumstances of prescribed observations so that the over–specified conditions or any ill–posed condition resulting from computational and theoretical aspects of the primitive equations of NWP are no longer an issue for an adjoint model.

2. Theoretical background

Consider that a limited–area NWP model is defined as a four dimensional domain $D = \bar{\Omega} \times I \times T$, where $\bar{\Omega} = \Omega \bigcup \partial\Omega$, $\bar{\Omega} = \{r: r \leqslant r_b\}$ is the horizontal domain and its lateral boundary is denoted by $\partial\Omega$. Its temporal domain is $T = [t_0, t_n]$, that is integrated from initial state to the required step; the vertical coordinate is expressed by $I = [0,1]$, which presents a normalized coordinate, like sigma coordinate or other terrain–following coordinates familiar to meteorologists. For futher convenience, we denote $\Gamma = \partial\Omega \times I \times T$, that is a general expression of time–dependent spatial boundary condition.

Generally, NWP over a limited–area is expressed as:

$$\frac{DY}{Dt} = F(Y) \quad \text{in} \quad D = \bar{\Omega} \times I \times T, \tag{1}$$

where $F(Y)$ represents local forces tending to change Y and $\frac{D}{Dt}$ is the Lagrangian derivative. Obviously, the initial condition is

$$Y|_{t=t_0} = Y(r,t_0) \quad \text{at} \quad \bar{\Omega} \times I. \tag{2}$$

The appropriate solutions of Eq.(1) can be obtained under the condition of Eq.(2), as well as by imposing suitable spatial boundary conditions for the limited–area domain. For the computational model of quarter–space assimilation problem, the time–dependent boundary condition is readily prescribed from valid four–dimensional data source, e.g., radar, satellite, etc., therefore

$$Y|_{\partial\Omega} = \hat{Y}(r_b,t) \quad \text{at} \quad \Gamma = \partial\Omega \times I \times T, \tag{3}$$

where r_b is the position just at the boundaries of $\partial\ \Omega$, and $\hat{Y}$ is the prescribed observation as the analogy of Y and it is to be specified in the whole domain of $D = \bar{\Omega} \times I \times T$. The well–poseness of such prescribed spatial boundary condition to tangent equation and its corresponding adjoint equation appearing in typical 4dVAR problem is still at this stage totally unknown. What we know is that Eq.(3) is the over–specified boundary condition to Eq.(1) (Chen, 1973 and Oliger and Sundstrôm, 1978); and what we now understand the situation is that we do not have any choice but just face such over–specification resulting from general 4DVAR process. Those boundary problems will be discussed in the following section.

For the initial condition of Eq.(2), based on the optimizing principle of functional, the updated and indeed the optimal initial condition Y_0^* should be given by

$$Y_0^* = Y^{v+1}(t_0) = Y^v(t_0) - \rho^v \nabla^v J, \tag{4}$$

where $t_0 = 0$ is at initial time, v is iteration step and ρ is convergent speed. ∇J represents the gradient of J with respect to the initial condition $Y(t_0)$. Eq. (4) is derived from the following functional:

$$J = \frac{1}{2}\int_D W(r,t)[Y(r,t) - \hat{Y}(r,t)]^2\, dr dt, \tag{5}$$

by seeking an approximate solution of Y_0^* in Eq.(4) so that the gradient of J approaches to zero subjected to the initial condition $Y(t_0)$. J presents the cost function which measures the misfit between the prescribed observations $\hat{Y}(r,t)$ and model solutions $Y(r,t)$. $W(r,t)$ is the weighting coefficient and might be expanded by $W(r,t) = \sum \Psi_t(t)\Lambda_r(r)$. For the sake of simplification, assume that $\Psi_t(t) = 1$ here, then $W(x,t)$ is renamed as $\Lambda(r) = \sum \Lambda_r(r)$.

In order to search the gradient of J, the optimal value Y_0^* can be obtained by Eq. (4), the first–order variation δJ resulting from the variation $\delta Y(t_0)$ of $Y(t_0)$ is firstly required,

$$\delta J = \int_D \Lambda(r)[Y(r,t) - \hat{Y}(r,t)]\delta Y\, dr dt, \tag{6}$$

Given the initial condition $Y(t_0)$ and its perturbation $\delta Y(t_0)$, we have the perturbation

δJ. On the other hand, the first-order perturbation δY can be derived from the integration of linearized perturbation of equation (1), starting from the initial condition $\delta Y(t_0)$. That is:

$$\frac{D\delta Y}{Dt} = F'(t)\delta Y, \tag{7}$$

where $F'(t)$ is the linear Jacobian operator obtained by differentiating $F(t)$ with respect to Y. The perturbation δJ in Eq.(6) is thus constrained by Eq.(7). Since the equation (7) (namely TLM, i.e. tangent linear model) is linear, its solution at a given time t_i depends linearly on the initial condition at time t_0, which can be expressed as

$$\delta Y(t_i) = L(t_i, t_0)\delta Y(t_0), \tag{8}$$

where $L(t_i, t_0)$ is called the resolvent of Eq.(7) between time t_i and t_0. Substituting Eq. (8) into the corresponding time-discrete form of equation (6), we get

$$\begin{aligned}\delta J(Y(t_0)) &= \sum_{i=0}^{n} < \Lambda(Y(t_i) - \hat{Y}(t_i)), L(t_i, t_0)\delta Y(t_0) > \\ &= \sum_{i=0}^{n} < L^*(t_i, t_0)\Lambda[Y(t_i), \hat{Y}(t_i)], \delta Y(t_0) > .\end{aligned} \tag{9}$$

Since we have the relation $\delta J = < \nabla J, \delta Y >$, thus

$$\nabla J(Y(t_0)) = \sum_{i=0}^{n} L^*(t_i, t_0)\Lambda[Y(t_i) - \hat{Y}(t_i)]. \tag{10}$$

Clearly $L^*(t_i, t_0)$ is the adjoint of $L(t_i, t_0)$ and it should be written in

$$\delta Y_i^*(t_0) = L^*(t_i, t_0)\delta Y^*(t_i), \tag{11}$$

where $\delta Y^*(t_i) = \Lambda[Y(t_i) - \hat{Y}(t_i)]$, and Eq. (11) indeed represents the resolvent form of following equation:

$$-\frac{D\delta Y^*}{Dt} = F'^*(t)\delta Y^*. \tag{12}$$

Obviously Eq. (12) is the adjoint equation of Eq. (7), therefore δY^* is the adjoint of δY, and $F'^*(t)$ represents the adjoint of $F'(t)$. By using Eq.(11), now Eq. (10) can be expressed as

$$\nabla J(Y(t_0)) = \sum_{i=0}^{n} L^*(t_i, t_0)\Lambda(Y(t_i) - \hat{Y}(t_i)) = \sum_{i=0}^{n} \delta Y_i^*(t_0). \tag{13}$$

Eq. (13) implies $\nabla J(Y(t_0))$, obtained through a single backward integration of adjoint Eq. (12) in the reverse period of $[t_n, t_0]$; and at each time step, the misfit, i.e., $\delta Y^*(t_i) = \Lambda[Y(t_i) - \hat{Y}(t_i)]$ is inserted.

3. Boundary condition specification

To find a suitable boundary conditions for adjoint model, we firstly seek a suitable weak form of Eq. (1). Taking the prescribed observation $\hat{Y}$ into account, it follows that

$$\frac{DY}{Dt} = (I - \Lambda)F(Y) + \Lambda G(\delta Y) \quad \text{in} \quad D = \bar{\Omega} \times I \times T. \tag{14}$$

Such re–formulation of Eq.(1) is clearly based on homotopy framework (Moore et al., 1994). $G(\delta Y)$ is in arbitrary function form and represents the ambient forcing due to the existence of the prescribed observations, and I is unit matrix. Obviously, Λ is the blending coefficient in homotopy framework. More clearly, see Eq.(14) in another way

$$\frac{DY}{Dt}=F(Y)-\Lambda[F(Y)-G(\delta Y)] \quad \text{in} \quad D=\overline{\Omega}\times I\times T. \tag{15}$$

This familiar formulation tells us that the rhs of last term in Eq. (15) actually represents the Newtonian cooling and generally represents non–linear nudging in mathematical form. This understanding of $\Lambda(r)$ leads to the following definition

$$\begin{cases} \Lambda(r)=\dfrac{\|r-r_c\|^n}{\|r_b-r_c\|^n}; & r_c\leqslant r\leqslant r_b \\ \Lambda(r)=I\ ; & r>r_b \\ \Lambda(r)=0\ ; & \text{otherwise} \end{cases}, \tag{16}$$

where r_b is the position just at the boundaries of $\partial\Omega$, r_c is located in the interior domain of Ω. Clearly, $\|r_b-r_c\|$ represents the distance from the boundary point to a certain interior point. The superscript of n in Eq.(16) represents the order of smoothness, higher order of n it takes, the smoother variations in $\Lambda(r)$ is from the boundaries to the interior. In the simplest situation as we discussed here, it might take $n\equiv 1$.

Clearly from the expression of Λ, Eq.(15) has no difference with its original form of $\frac{DY}{Dt}=F(Y)$ in the interior, since $\Lambda=0$ can be ordered by taking $\|r_b-r_c\|$ as a narrow zone (actually, the buffering zone). On the other hand, $\Lambda=I$ held at the boundary $r=r_b$, then $\frac{DY}{Dt}=G(\delta Y)$; therefore its corresponding TLM is of the form $\frac{D\delta Y}{Dt}=G'\delta Y$ at the boundary. Furthermore, because of the existence of prescribed boundary condition of Eq.(3), i.e., $Y|_{\partial\Omega}=\hat{Y}(r_b,t)$ at $\Gamma=\partial\Omega\times I\times T$, therefore $\delta Y|_\Gamma=(Y-\hat{Y})|_\Gamma=0$ must hold at the boundary. It thus leads $\left.\frac{D\delta Y}{Dt}\right|_\Gamma=0$. In order to suit such boundary setting for TLM, the arbitrary function of $G(\delta Y)$ is simply chosen to be $G=-(Y-\hat{Y})$, a linear form that satisfies the aforementioned boundary condition. Then $\left.\frac{DY}{Dt}\right|_\Gamma=0$ is required. The mathematic expression for those argumentations is straightly addressed in the following two groups of equations

$$\begin{aligned} &\frac{DY}{Dt}=(I-\Lambda)F(Y)-\Lambda(Y-\hat{Y}) \ \text{in}\ D, \\ &\frac{DY}{Dt}=0 \ \text{at}\ \Gamma, \end{aligned} \tag{17}$$

and

$$\begin{aligned} &\frac{D\delta Y}{Dt}=(I-\Lambda)F'\delta Y-\Lambda\delta Y \ \text{in}\ D, \\ &\frac{D\delta Y}{Dt}=0 \ \text{at}\ \Gamma. \end{aligned} \tag{18}$$

The formulae of Eq.(18) can be directly derived through making the linear perturbations of Eq.(17). It is worth noting while the physical interpretation for Eq.(17) and Eq.(18) is that they are weak form of Eq.(1) and Eq.(7), so that the ambient forcing defined on the whole domain D from the observation in typical 4DVAR problem can be taken into account, then the forcing in the spatial scale is escalated (cf. Eq.(16)) from the interior domain to the boundary where the model variable Y is needed to equal the observation $\hat{Y}$ (cf. Eq.(3)). An important advantage can be found in Eq.(17) and Eq.(18), the over-specified boundary condition is relaxed to be no longer an issue because that $\left.\frac{DY}{Dt}\right|_{\Gamma} = 0$ and $\left.\frac{D\delta Y}{Dt}\right|_{\Gamma} = 0$, together with $Y|_{\partial\Omega} = \hat{Y}(r_b, t)$, is the exact boundary condition in well-poseness to respectively satisfy $\frac{DY}{Dt} = (I - \Lambda)F(Y) - \Lambda(Y - \hat{Y})$ and $\frac{D\delta Y}{Dt} = (I - \Lambda)F'\delta Y - \Lambda\delta Y$, provided that $\Lambda = I$ always holds well at the boundary.

We now consider the adjoint variable δY^* defined over the entire domain D, but its boundary condition has been not yet specified at this stage. In order to derive the suitable boundary condition for adjoint equation in the boundary over-specification circumstances, we firstly specify the first-order boundary variation of cost function as $\delta J|_{\Gamma} = \int_{\Gamma} \Lambda(r)[Y(r,t) - \hat{Y}(r,t)]\delta Y drdt$; secondly we multiply Eq.(18) by δY^*, integrating over the boundary Γ, and subtracting the result from $\delta J|_{\Gamma}$. This leads to the following expression for δJ at the boundary

$$\delta J|_{\Gamma} = \int_{\Gamma} \Lambda(r)[Y(r,t) - \hat{Y}(r,t)]\delta Y drdt - \int_{\Gamma} [\frac{\partial \delta Y}{\partial t} + \frac{\partial(\dot{r}\delta Y)}{\partial r}]\delta Y^* drdt, \tag{19}$$

where $\frac{\partial \delta Y}{\partial t} + \frac{\partial(\dot{r}\delta Y)}{\partial r} = \frac{D\delta Y}{Dt}$ and performing the integration by parts and rearranging terms lead to

$$\delta J|_{\Gamma} = \int_{\Gamma} [\frac{D\delta Y^*}{Dt} + \Lambda(r)(Y(r,t) - \hat{Y}(r,t))]\delta Y drdt$$
$$- \int_{\partial\Omega \times I} (\delta Y \delta Y^*)|_{t=t_0}^{t=t_n} dr - \int_{\Gamma} (\dot{r}\delta Y \delta Y^*)|_{\partial\Omega \times I} dt. \tag{20}$$

We can first observe that the first term on the rhs. of Eq.(20), which is an integral over $\Gamma = \partial\Omega \times I \times T$, becomes zero if δY^* is chosen as to verify the following inhomogeneous partial differential equation

$$\frac{D\delta Y^*}{Dt} + \Lambda(r)[Y(r,t) - \hat{Y}(r,t)] = 0, \quad \text{along} \quad \Gamma = \partial\Omega \times I \times T. \tag{21}$$

The other two terms on rhs of Eq.(20) can be eliminated by imposing δY^* to zero along Γ, i.e.,

$$\delta Y^* \equiv 0 \quad \text{along} \quad \Gamma = \partial\Omega \times I \times T, \tag{22}$$

the condition Eq. (22) together with the condition of Eq. (21) ensure that $\delta J|_{\Gamma} = 0$, so that the optimal character during the forward and backward integration is properly retained. Furthermore, both Eq.(21) and Eq.(22) can be consolidated in the form

$$\frac{D\delta Y^*}{Dt}=0,\quad \text{along}\quad \Gamma=\partial\Omega\times I\times T. \tag{23}$$

In fact, since $\delta Y^* \equiv \Lambda[Y(r,t)-\hat{Y}(r,t)]$ and $\delta Y^*|_\Gamma \equiv 0$ along the boundary are always held in the backward integrating process, the second term on the left side of Eq.(21) is thus reduced to be zero. To test whether Eq.(23) is a suitable boundary condition in well–poseness for the adjoint model, the original form of the adjoint equation Eq.(12) is written in the homotopy framework, a similar way that we did for TLM

$$-\frac{D\delta Y^*}{Dt}=(I-\Lambda)F'^*\delta Y^*-\Lambda\delta Y^*\quad \text{in}\quad D. \tag{24}$$

It is important to note while $\Lambda=0$ in the interior domain or $\Lambda=I$ at the boundary, then Eq.(24) has no difference with the original adjoint equation of Eq.(12), and has no difference with the boundary condition Eq.(23), respectively. Therefore, the condition Eq. (23) satisfies Eq.(24). In other words, it is one kind of well–posed condition being sought.

4. Numerical representation of boundary condition

Consider that the aforementioned boundary conditions $\frac{D\delta Y}{Dt}=0$ (cf. Eq. (18)), $\frac{D\delta Y^*}{Dt}=0$ (cf. Eq. (23)) for TLM and adjoint model, respectively. Without loss of generality, it can be recast and therefore mapped in its one–dimensional characteristic scalar form

$$\frac{\partial\delta\varphi}{\partial t}+\tilde{C}\frac{\partial\delta\varphi}{\partial x}=0, \tag{25}$$

where $\delta\varphi$ represents the perturbation of arbitrary scale variable φ and $\tilde{C}$ is the phase speed of $\delta\varphi$. Clearly, it is one kind of Sommerfeld's radiation boundary condition (Sommerfeld, 1964). The value of $\tilde{C}$ is numerically determined. The numerical scheme of Miller and Thorpe (1981) is suggested. It is worth noting while the numerical expression of $\tilde{C}$ in Miller and Thorpe's method is based on the idea of "floating wave speed" (Orlanski, 1976), therefore the fix value of $\tilde{C}$ is step by step in iteration relaxed to non–constant value. The necessary non–linear feature is thus retained, of course in the view of numerical method.

The above equation can be arranged by using $\delta\varphi=\varphi-\hat{\varphi}$, so that

$$\frac{\partial\varphi}{\partial t}=\frac{\partial\hat{\varphi}}{\partial t}-\tilde{C}\left(\frac{\partial\varphi}{\partial x}-\frac{\partial\hat{\varphi}}{\partial x}\right), \tag{26}$$

where $\hat{\varphi}$ represents the prescribed observation. The boundary condition is thus rewritten in the special circumstances under ambient forcing in order to validate it through comparing with Carpenter's 1981's well–recognized boundary condition. We should note that Carpenter's modification has extended the original Sommerfeld's radiation boundary condition in which it fundamentally restrains the prescribed information transmitted into the interior of domain. He was probably the first author who made a clear–cut verdict for using the radiation condition under ambient forcing. The boundary condition equation Eq.(26) is actually of the same form with his definition.

5. Conclusion

This paper discusses the over–specified boundary problems in adjoint model. In fact, the over–specified boundary conditions are always employed in the current adjoint and its accompanied TLM equations since the observation data has been prescribed readily over the outer and / or interior of model domain of interest.

To alleviate the ill–poseness of over–specification, the basic treatment of boundary conditions is actually designed following a homotopy approach. We first seek homotopy form of original NWP, TLM and adjoint model, so that the suitable boundary conditions in well–poseness can be derived from and viz. the homotopy solutions. Furthermore, Such solutions can return back to the original formulation of the corresponding models in the interior domain. This treatment of boundary conditions become available simply because the existence of model analogue $\hat{Y}$ for the model solution Y.

The proposed spatial boundary conditions can be indeed reduced to the modified radiation boundary conditions considering outer forcing came from the observations. Such boundary conditions guarantee the possible over–specified conditions is no longer an issue in the adjoint model as well as TLM model in a limited–area domain.

In practice, the proposed treatment of the boundary setting is quite familiar to atmospheric modelers. It can be schemed into three steps: (1) specify the prescribed observation at *the boundaries that is just one kind of Dirichlet boundary condition*, as well as *specify the prescribed* observation over the whole interior domain of interest in addition; it implies that it forbids to extrapolate the prognostic variable value from interior to the boundaries; (2) specify the radiation boundary condition i.e. Eq. (26) taking account for prescribed observations — one kind of Neumann condition; (3) take one kind of non–linear nudging filter, such as Eq.(16). All of these boundary settings, and the corresponding numerical schemes perhaps in different extensions or variabilities are well documented for long time in some famous mesoscale models, like MM5 (Penn State / NCAR Mesoscale Modeling System), ARPS (Advanced Regional Prediction System, University of Oklahoma), etc. But those existing codes are necessarily reordered to suit the boundary formulation proposed in this paper.

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有限区域伴随模式中适定空间边界条件的理论研究

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摘 要

从理论上论证了借助于同伦方法构造的适定空间边界条件确保有限区域上伴随模式产生的超定边界条件问题得到解决，同时又能维持伴随模式中边界处理的优化特征。从某种意义上讲，伴随模式超定空间边界条件的存在是不可避免的，这是因为数据同化过程必须引进和采用给定的观测资料，而它们在模式空间边界上的定义往往是超定的。我们提出的空间边界条件的算法构架事实上是在数据同化过程中综合运用了张弛滤波、考虑外部强迫的辐射边界条件以及与观测相容的狄里希利边界条件。显然，对于该理论构架所涉及到的具体数值处理方法在中尺度模式中都十分成熟易行。

关键词：变分数据同化，伴随模式，超定局地边界条件