

Eliminating finite-amplitude non-physical oscillations in the time evolution of adjoint model solutions introduced by the leapfrog time-integration scheme

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ABSTRACT

This note provides a detailed theoretical derivation for the removal of non-physical finite-amplitude computational oscillations from the solution of the adjoint of a discretized model using the leapfrog finite-difference scheme. Numerical results are shown using a 1-dimensional shallow water equation model.

1. Introduction

Since the work of Le Dimet and Talagrand (1986), adjoint models have been applied to solve many types of problems in atmospheric science and numerical weather prediction. These include 4-dimensional variational data assimilations, parameter estimations, sensitivity studies, ensemble forecasts, Kalman filters, and stability studies that include either singular vectors or finite-time normal modes.

The adjoint model of a numerical forecast model can be derived in two ways. One, the adjoint of finite difference (AFD, Zou et al., 1997), is defined and constructed as a transpose operator of the resolvent of the discretized tangent linear model. The other, called the finite-difference of adjoint (FDA, Sirkes and Tziperman, 1997), is developed by first deriving the analytic adjoint equations by using the Euler–Lagrange method, followed by a discretization of the equations in space and time.

Traditionally, AFD is used for the development of the adjoint models of many complex primitive equation models with sophisticated physics, and FDA is used mostly for simple models. Both adjoint models provide the same values for the adjoint variables at the initial time, given the same forcing terms at the future times. For instance, given a response function (a scalar function of the model forecast at a future time)

$$J = g(\mathbf{x}(t_f)), \quad (1)$$

where $\mathbf{x}(t_f)$ is the model forecast at the time t_f from the initial time t_0 and g is a scalar function of $\mathbf{x}(t_f)$, a single backward time integration of both adjoint models (AFD and FDA) from t_f to t_0 , with

$$\hat{\mathbf{x}}^{\text{AFD,FDA}}(t_f) = \frac{\partial g}{\partial \mathbf{x}(t_f)} \quad (2)$$

as the input to the adjoint model at time t_f , will result in the same value of the adjoint variables $\hat{\mathbf{x}}$ at the initial time t_0 , which is equal to the gradient of J with respect to the model state at the initial time $\mathbf{x}(t_0)$, i.e.,

$$\hat{\mathbf{x}}^{\text{AFD}}(t_0) = \hat{\mathbf{x}}^{\text{FDA}}(t_0) = \nabla_{\mathbf{x}(t_0)} J. \quad (3)$$

In addition to eq. (3), the value of the adjoint

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variables from the FDA model, $\hat{\mathbf{x}}^{\text{FDA}}(t)$, is equal to the gradient of J with respect to the forward model state (sometimes called the basic state) at the time t , $\mathbf{x}(t)$, $t_0 < t < t_f$, i.e.,

$$\hat{\mathbf{x}}^{\text{FDA}}(t) = \nabla_{\mathbf{x}(t)} J. \quad (4)$$

However, the two-time-step computational mode that exists in the forward finite-difference model renders the time evolution of the AFD adjoint variables to be characterized by a non-physical oscillation with finite-amplitude (Sirkes and Tziperman, 1997). As a result, eq. (4) is not valid for $\hat{\mathbf{x}}^{\text{AFD}}(t)$, i.e.,

$$\hat{\mathbf{x}}^{\text{AFD}}(t) \neq \nabla_{\mathbf{x}(t)} J \quad \text{when } t_0 < t < t_f. \quad (5)$$

The fact that eq. (4) is not valid for $\hat{\mathbf{x}}^{\text{AFD}}(t)$ does not affect very many applications of AFD, such as data assimilation, parameter estimation, and singular vector calculation. However, the sensitivities of a forecast aspect, with respect to more than one model state between time t_0 and t_f , cannot be obtained by a single backward adjoint integration! AFD is used more frequently than FDA, especially for complex primitive-equation models with parameterized physical processes. The nice features of AFD include coding convenience both manually or automatically using an automatic adjoint generator, the correctness check of the adjoint model against the tangent linear model, the convenience in adding and subtracting parts of the code, the higher accuracy of $\hat{\mathbf{x}}^{\text{AFD}}$ than $\hat{\mathbf{x}}^{\text{FDA}}$ in representing the gradient of J with respect to the model initial condition, and the straightforwardness in the development of adjoint physics. It will be nice to find a way to remove the two-time-step computational oscillations from the AFD model solution (possibly the only disadvantage of its use compared to the use of FDA).

The purpose of this note is to demonstrate, both theoretically and numerically, that simple modifications to the AFD model can be made to eliminate the computational mode from the AFD model solution in time, and obtain accurate gradients distribution over the entire time period of interest. In the following section (Section 2), we briefly present the two traditional adjoint formulations, and the proposed modifications made to the AFD formulation of the adjoint model. Discussions apply to any general non-linear forecast model using the leapfrog time differencing scheme. Numerical results from the two adjoint

formulations and the modified AFD model are compared in Section 3 using a 1-dimensional (1D) shallow water equation model, and Section 4 provides a summary.

2. ADF, FDA, and modified AFD formulations for any non-linear model using the leapfrog time differencing scheme

2.1. Non-linear model

Any numerical prediction model can be symbolically written as

$$\frac{\partial \mathbf{x}(t)}{\partial t} = F(\mathbf{x}(t)), \quad (6)$$

where $\mathbf{x}(t)$ is an N -dimensional vector describing the atmospheric state at time t , and $F(\mathbf{x})$ is a non-linear function of the model state, representing all the operations consisting of dynamical terms, physical parameterizations, and model numerics such as diffusion and filtering. Given an initial condition of the model state (we assume no lateral boundary):

$$\mathbf{x}|_{t=0} = \mathbf{x}(0), \quad (7)$$

eq. (6) determines a unique solution for the model state at any time $t > t_0$; i.e., given the current state of the atmosphere (input), the forward non-linear model (6) provides the future state of the atmosphere (output).

The discretized version of the above non-linear model can be symbolically written as

$$\mathbf{x}(t) = M(\mathbf{x})\mathbf{x}(0), \quad (8)$$

where $\mathbf{x}(0)$ is the input model initial condition, and M includes all the operations in the non-linear model needed to generate the forecasting model state at a future time t , $\mathbf{x}(t)$.

2.2. Tangent linear model

The tangent linear model in an analytical form corresponding to (6) can be symbolically written as

$$\frac{\partial \mathbf{x}'}{\partial t} = \frac{\partial F}{\partial \mathbf{x}} \mathbf{x}'. \quad (9)$$

The discretized tangent linear model, corresponding to (8), is developed by a differentiation procedure carried out at the coding level. The

numerical tangent linear model can be expressed symbolically as

$$\mathbf{x}'(t) = \mathbf{M}(t, t_0)\mathbf{x}'(0), \quad (10)$$

where $\mathbf{x}'(t)$, ($t \geq 0$) represents the time evolution of the perturbation solution, and $\mathbf{M} = \partial M / \partial \mathbf{x}$ is called the resolvent of the tangent linear model (9) between times t_0 and t .

2.3. FDA model

The FDA model is defined as the adjoint of the linear differential equation (9) (Nering, 1970)

$$-\frac{\partial \hat{\mathbf{x}}}{\partial t} = \left(\frac{\partial F}{\partial \mathbf{x}} \right)^T \hat{\mathbf{x}}. \quad (11)$$

In practice, the FDA model can be obtained by a three-step procedure. First, define a constrained minimization problem

$$L(\mathbf{x}, \hat{\mathbf{x}}) = \left\langle \hat{\mathbf{x}}, \frac{\partial \mathbf{x}}{\partial t} - \frac{\partial F}{\partial \mathbf{x}} \right\rangle, \quad (12)$$

using a Lagrange multiplier method, where

$$\langle \mathbf{x}_1, \mathbf{x}_2 \rangle = \int_t \int_{\Omega} \mathbf{x}_1^T \mathbf{W} \mathbf{x}_2 \, d\Omega \, dt \quad (13)$$

represents an inner product defined in the time and space domain $t \times \Omega$, and $\mathbf{W}$ is a weighting matrix. For simplicity, the Euclidean " L_2 norm" will be used in this study. The relationship between the adjoint model in the L_2 norm and the other norm (such as an energy norm) is easy to derive (Buizza et al., 1993).

Second, derive the equation

$$\frac{\partial L(\mathbf{x}, \hat{\mathbf{x}})}{\partial \mathbf{x}} = 0, \quad (14)$$

which gives an explicit set of analytic equations of the FDA model. Finally, a numerical discretization procedure, similar to that used for the forward model (8), is applied to (13-12) to obtain a numerical FDA model.

2.4. AFD model

The AFD model is developed at the coding level as a transpose operator of the resolvent $\mathbf{M}$ of the tangent linear model (10), i.e.,

$$\hat{\mathbf{x}}(0) = \mathbf{M}^T(t, t_0)\hat{\mathbf{x}}(t), \quad (15)$$

where $\hat{\mathbf{x}}(t)$ represents values of the adjoint vari-

ables at time t and $\mathbf{M}^T(t, t_0) = \mathbf{Z}(t_0, t)$ is the resolvent of the adjoint model between times t and t_0 .

If we view the tangent linear operator $\mathbf{M}$ as a linear transformation σ , then the adjoint operator $\mathbf{M}^T$ represents a linear transformation σ^* , which is the adjoint of σ . The concept of adjoint (AFD) in meteorological data assimilation is thus the same as that in linear algebra.

The equivalence between AFD and FDA models can be obtained by verifying that the resolvent $\mathbf{Z}(t', t)$ ($t_0 \leq t' < t$) of the adjoint equation (11) is the adjoint operator $\mathbf{M}^T(t, t_0)$ of the resolvent $\mathbf{M}(t, t_0)$ of the tangent linear model (10).

2.5. Leapfrog time-integration schemes and modified AFD model

Subsections 2.3 and 2.4 describe the two ways of obtaining a discretized adjoint model for a given forward non-linear model. One is to obtain a computer program of the adjoint model without any explicit knowledge of the analytic form of the adjoint model equations. The other is to derive the analytic form of a set of adjoint model equations, discretized it, and turn it into a computer program of the adjoint model. We have adopted the names of adjoint of finite-difference (AFD) for the first type and the finite-difference of adjoint (FDA) for the second, as was used by Sirkes and Tziperman (1997).

In this section, we seek a way to modify the AFD model to enable it to produce a usable adjoint model solution at all the time steps, and thus remove the non-physical computational mode from the AFD model solution.

Differences in the AFD and FDA are due to the differences in the way the backward time integration of the adjoint model is carried out. We start by examining the time stepping procedure in both AFD and FDA models. In order to simplify the notations for the adjoint variables, we assume:

$$\begin{aligned} \xi &\equiv \hat{\mathbf{x}}^{\text{FDA}} && \text{(variables in the FDA model),} \\ \tau &\equiv \hat{\mathbf{x}}^{\text{AFD}} && \text{(variables in the AFD model),} \\ \mathbf{y} &\equiv \hat{\mathbf{x}}^{\text{MAFD}} && \text{(variables in the modified AFD model),} \\ \mathbf{P}_n &\equiv \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}(t_n)) && \text{(the matrix of the first-order derivatives of } F \text{).} \end{aligned}$$

In the FDA, we have

$$-\frac{\partial \xi}{\partial t} = \left(\frac{\partial F}{\partial \mathbf{x}} \right)^T \xi. \quad (16)$$

Its solution in time can be written as

$$\xi_n = \frac{\partial J}{\partial \mathbf{x}(t_n)}, \quad (17)$$

$$\eta_{n-1} = \xi_n + DTP_n^T \xi_n, \quad \xi_{j-1} = \xi_{j+1} + 2DTP_j^T \xi_j, \quad j = n-1, \dots, 1,$$

where DT is the time step.

The time stepping procedure in AFD can be found from the time integration of the tangent linear model (9), which is discretized in time as

$$\begin{aligned} \mathbf{x}'_1 &= \mathbf{x}'_0 + DTP_0 \mathbf{x}'_0, \\ \mathbf{x}'_2 &= \mathbf{x}'_0 + 2DTP_1 \mathbf{x}'_1, \\ \mathbf{x}'_{j+1} &= \mathbf{x}'_{j-1} + 2DTP_j \mathbf{x}'_j, \quad j = 1, \dots, n-1. \end{aligned} \quad (18)$$

The transpose of the above operations results in the following solution of the AFD model:

$$\begin{aligned} \mathbf{z}_n &= \frac{\partial J}{\partial \mathbf{x}(t_n)}, \\ \mathbf{z}_{n-1} &= 2DTP_{n-1}^T \mathbf{z}_n, \\ \mathbf{z}_{j-1} &= \mathbf{z}_{j+1} + 2DTP_j^T \mathbf{z}_j, \quad j = n-1, \dots, 2, \\ \mathbf{z}_0 &= \mathbf{z}_1 + DTP_0^T \mathbf{z}_1 + \mathbf{z}_2. \end{aligned} \quad (19)$$

Comparing (19) with (17), we find that the AFD model can be modified in the following manner so that the time evolution of the modified AFD model can then produce the same results as those of the FDA model at every time step. The modified AFD does the backward time integration in the following manner:

$$\begin{aligned} \mathbf{y}_{n+1} &= \frac{\partial J}{\partial \mathbf{x}(t_n)} \equiv \xi_n, \\ \mathbf{y}_n &= 2DTP_n^T \mathbf{y}_{n+1}, \\ \mathbf{y}_n &= 0.5\mathbf{y}_n + \mathbf{y}_{n+1} \equiv \xi_{n-1}, \\ \mathbf{y}_j &= \mathbf{y}_{j+2} + 2DTP_j^T \mathbf{y}_{j+1} \equiv \xi_{j-1}, \\ & \quad j = n-1, \dots, 2, 1. \end{aligned} \quad (20)$$

The three steps to obtain a time evolution of sensitivity of any forecast aspect are summarized as follows:

1. Add one more time step to the original time window of interest;

2. Add a simple algebraic operation $\mathbf{y}_n = 0.5\mathbf{y}_n + \mathbf{y}_{n+1}$ after the first time step of the AFD adjoint model integration;

3. Shift one-time step forward: $\xi_{j-1} = \mathbf{y}_j$, where $j = n, n-1, \dots, 1$. In other words, the values of the modified adjoint-model solution ($\mathbf{y}_j$, $j = n+1, n-1, \dots, 1$), initialized by $\partial J / \partial \mathbf{x}_n$ at the time t_{n+1} , contain no computational mode and represent the sensitivities of J with respect to the model state at the times t_{j-1} .

We notice that the modified AFD is not the adjoint of the tangent linear model (eq. (15)). It is the adjoint of the tangent linear model (eq. (9)) with some modified time-integration schemes. The modified AFD is recommended only for obtaining the time evolution of sensitivity. For 4D-Var data assimilation and parameter estimation, the use of AFD is not a problem.

3. Numerical results using a 1D shallow-water equation model

In order to compare the results of the three adjoint formulations, we used a one-dimensional, homogeneous, inviscid, one-layer fluid including rotation and topography shallow-water equations (Parrett and Cullen, 1984)

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{\partial \phi}{\partial x} &= fv - g \frac{\partial H}{\partial x}, \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} &= -fu, \end{aligned} \quad (21)$$

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} + \phi \frac{\partial u}{\partial x} = 0,$$

where $\phi = gh$, geopotential height; h , the depth of fluid; f , Coriolis parameter; H , height of bottom topography; u, v , zonal and meridional wind components.

The initial fields for the experiment can be given by

$$\begin{aligned} u(x, 0) &= U \cos \frac{x}{L}, \\ v(x, 0) &= 0, \end{aligned} \quad (22)$$

$$\begin{aligned} \phi(x, 0) &= \phi_m + U \left(\frac{U}{8} \cos \frac{2x}{L} \right. \\ & \quad \left. + \left(\phi_m - \frac{U^2}{8} \right)^{1/2} \cos \frac{x}{L} \right), \end{aligned} \quad (22)$$

where the length of the domain $= 2\pi L$, $\phi_m = gh_m$, h_m is the mean height of the fluid, and U is constant. Periodic boundary conditions are enforced. Parameter values of U , L , ϕ_m , Δx and Δt are taken as follows:

$$L = 2 \times 10^6, \quad f = 10^{-4}, \quad U = fL, \\ \phi_m = U^2, \quad \Delta x = \frac{2\pi L}{N}, \quad N = 61, \quad (23)$$

$$KTT = \frac{2.8 \times N}{2\pi \times 0.210}, \quad \Delta T = \frac{2.8 \times L/U}{KTT},$$

$$K = 2.5 \times 10^4 \text{ m}^2 \text{ s}^{-1},$$

where KTT is chosen so that $U\Delta t/\Delta x < 0.210$ to ensure the computational stability. A total of 63 grid points is used in the x coordinate.

The AFD model of the above 1D shallow water model is developed by first writing the tangent linear model and then its transpose. All these procedures are carried out at the coding level as described in Subsection 2.2.

The FDA of the above 1D shallow water model is developed by first deriving its analytic adjoint equations and then discretizing them in space and time. The adjoint model equations in analytic form can be derived by defining an inner product as

$$\langle \mathbf{x}_1, \mathbf{x}_2 \rangle = \int_t \int_x \mathbf{x}_1^T \mathbf{x}_2 \, dx \, dt, \quad (24)$$

and substituting the 1D shallow water equation (21) into (12), carrying out the integration by parts, neglecting all the boundary terms (set them to zero), and taking the derivative of L with respect to $\mathbf{x}$. Thus, we obtain the explicit form of (14). The result of the analytic form of the adjoint model of the 1D shallow water equation model is:

$$\begin{aligned} -\frac{\partial \hat{u}}{\partial t} - 2u \frac{\partial \hat{u}}{\partial x} - v \frac{\partial \hat{v}}{\partial x} + f\hat{v} &= \frac{\partial \hat{\phi}}{\partial x} + k \frac{\partial^2 \hat{u}}{\partial x^2}, \\ -\frac{\partial \hat{v}}{\partial t} - u \frac{\partial \hat{v}}{\partial x} - f\hat{u} &= k \frac{\partial^2 \hat{v}}{\partial x^2}, \\ -\frac{\partial \hat{\phi}}{\partial t} - \phi \frac{\partial \hat{u}}{\partial x} + u^2 \frac{\partial \hat{u}}{\partial x} + uv \frac{\partial \hat{v}}{\partial x} &= k \frac{\partial^2 \hat{\phi}}{\partial x^2}. \end{aligned} \quad (25)$$

Discretization of the above analytic adjoint equations (11) in both time and space is carried out in a fashion similar to what was performed for the original discretized non-linear model. A one-step-forward time differencing scheme is done

from the end of the time window t_n to t_{n-1} , followed by the two-time-step-leapfrog time differencing scheme. The finite-difference schemes for spatial derivatives are identical to the schemes used in the original forward model. A cyclic boundary condition is employed as was done in the original model.

Numerical results of the adjoint model integrations are shown in Figs. 1, 2 for the following two response functions:

$$J_1 = \phi(I, t_n)|_{I=15, n=20}, \quad (26)$$

and

$$J_2 = u(I, t_n)|_{I=15, n=20}, \quad (27)$$

respectively. Fig. 1 shows the time evolution of the adjoint geopotential height $\hat{\phi}$ at the point $I = 15$ with a unit forcing of $\hat{\phi}$ at the point $I = 15$ and zero everywhere else at time t_n , $n = 20$. The AFD model produces an oscillating curve (dashed line), the FDA model produces a smooth evolution (thick solid line), and the modified AFD model generates a solution (thin line with circles) close to that of the FDA model. The finite-amplitude non-physical oscillations are removed from the modified AFD model solution with the simple fix applied to the AFD model (Subsection 2.4). From

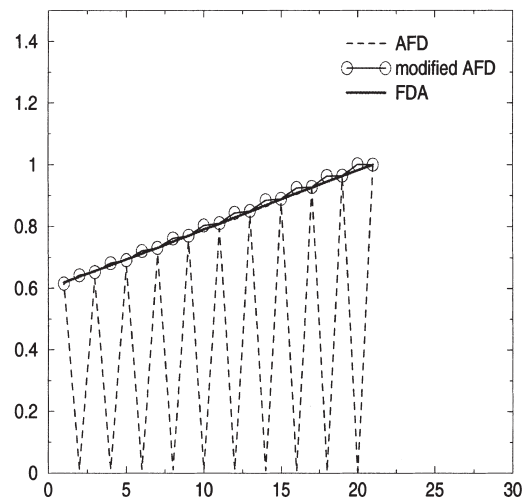


Fig. 1. The time evolution of the adjoint variable $\hat{\phi}$ at $I = 15$ with $\hat{\phi} = 1$ at $I = 15$ and t_n and zero elsewhere. Thick solid line: the FDA model, dashed line: the AFD model, and thin solid line with circles: the modified AFD model.

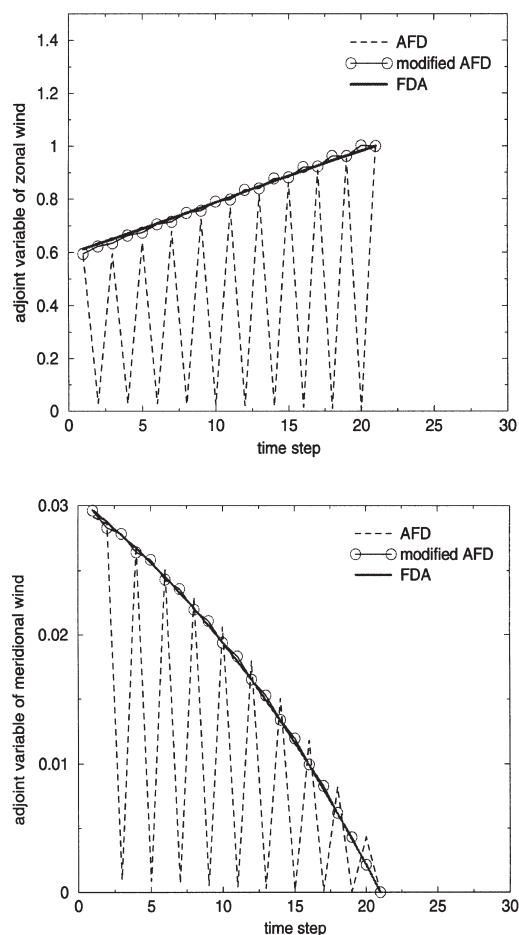


Fig. 2. The time evolution of the adjoint variables $\hat{u}$ and $\hat{v}$ with $u = 1$ at $I = 15$ and t_n and zero elsewhere. Thick solid line: the FDA model, dashed line: the AFD model, and thin solid line with circles: the modified AFD model.

Fig. 1 we find that the sensitivity of J_1 with respect to the model state of the geopotential height at the same point decreases linearly with increasing time intervals.

Fig. 2 is similar to Fig. 1 except for the adjoint wind fields using J_2 . Again, the finite-amplitude computational oscillations are found in both the u and v solutions of the AFD model. These oscillations are removed in the modified AFD model solutions. While a linear decrease in the sensitivity of J_2 with respect to the u field is observed, the sensitivity of J_2 with respect to the v field shows a parabolic increase with the

increased time interval between the forecasting time (t_n) and the time of the model state to which J_2 is sensitive.

4. Summary

The adjoint of a finite-difference model is superior to the finite-difference of an adjoint model in many respects, especially for complex primitive equation models with parameterized physical processes. However, it is well-known that the time evolution of adjoint model states generated by a numerical adjoint model may contain a non-physical, finite-amplitude computational mode. This is true if the adjoint model is obtained by transposing the resolvent of a linearized forward numerical forecasting model, which employs the leapfrog time-difference scheme. Although this does not present a problem for those adjoint applications in which only the values of the adjoint variables at the beginning of the time period of interest are used, it is an undesirable feature and may be prevented from being used for other adjoint applications, such as a time-continuous sensitivity study. It was shown here that the non-physical computational mode can be removed from the time evolution of the adjoint model state through a simple procedure applied to the original adjoint model. Therefore, the gradients of any forecast aspect, with respect to forward model states at all the previous times, can be obtained by a single backward time integration of the adjoint model derived directly from the finite-difference forecasting model.

Although we showed numerical results using a 1D shallow-water equation model, the derivation for the removal of non-physical finite-amplitude computational oscillations from the time evolution of the adjoint model solution in Subsection 2.4 can be applied to any numerical weather prediction model which uses the leapfrog scheme. If the FDA model is not available or is difficult to develop, the results of the modified AFD model can be tested against multiple runs of the AFD model, i.e., using the model state at every time step (t_j) as the model initial condition for the sensitivity calculation between t_i and t_n , where $j = 0, 1, 2, \dots, n-1$.

The proposed method solves the problem in the AFD model solution assuming the forward model

uses a leapfrog time integration scheme and is not to be changed. However, the adjoint problem can also be solved by overcoming the instability problem in the forward model. For examples, using a Roberts filter in the forward model eliminates the non-physical oscillations in the AFD model solution, and using an Euler-forward time step at a selected time step allows one to calculate the adjoint sensitivity at that time.

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