Mesoscale adjoint analysis and data assimilation: Development of RAMS adjoint

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1 Introduction

Accurate mesoscale forecast and analysis are among most challenging tasks in modern Numerical Weather Prediction. The analysis of mesoscale weather includes both the diagnosing of processes with high spatial and temporal variability and the proper representation of the associated physical fields in the atmospheric data sets. The advances in understanding of the physical processes, atmospheric data analysis and NWP are mutually dependent. Thus, it is necessary to include all three components in comprehensive research of methodology for better mesoscale weather analysis and forecast. This methodology includes: mesoscale numerical modeling, analysis of model solution dependencies on control parameters, optimal data assimilation for mesoscales and improving direct observations of mesoscale fields.

In the last decade new adjoin method has been developed in numerical weather forecast, ocean and chemistry transport research to analyze model solutions and physical processes represented by the model. The adjoint analysis method has been used in a number of studies in meteorology to assess the impact of various processes on the model solution. These studies include an examination of the effect of selected processes on atmospheric blocking (Zou et al., 1993), cyclogenesis (Rabier et al., 1992; Vukićević and Raeder, 1995; Vukićević, 1998), and global tropospheric transport (Robertson, 1992; Marchuk, 1995; Pudykiewicz, 1998; Vukićević and Hess, 2000). The adjoint method has also been used in global climate studies using simplified models (e.g., Hall et al., 1982), and to examine the seasonal cycle of CO_2 as a function of surface fluxes (Kaminski et al., 1997).

The adjoint method is also applied in modern optimal data assimilation schemes in meteorology and oceanography as part of a variational data assimilation algorithm (see for example Programme of WMO Symposium on Data Assimilation, 1999 and references therein). In this paper we briefly describe the mesoscale model (section 2), theory of adjoint analysis (section 3), application of the adjoint method in the theory of four-dimensional variational data assimilation (4DVAR) (section 4), progress on the RAMS adjoint model development (section 5) and plans for applications of the RAMS adjoint model in the research of cloud formation and satellite data assimilation.

2 Model

In this study we use the Regional Atmospheric Modeling System (RAMS). Detailed description of the RAMS is beyond the scope of this paper. This modeling system is well documented in a number of peer reviewed papers (Pielke et al, 1992; Nichols et al., 1995) A few main characteristics of the model that are of interest for the current application are listed in this section.

The Regional Atmospheric Modeling System (RAMS) was developed at Colorado State University. It is a fully three-dimensional, nonhydrostatic, general-purpose atmospheric simulation modeling system consisting of equations of motion, heat, moisture, and continuity in a terrain-following coordinate system (Pielke et al. 1992). The model has flexible vertical and horizontal resolution and a large range of options that permit the selection of which processes are to be included in a simulation (such as cloud physics, radiative transfer, subgrid diffusion, and convective parameterization). The model's two-way interactive grid nesting (Clark and Farley 1984; Nicholls et al. 1995; Walko et al. 1995a) allows for a wide range of motion scales to be modeled simultaneously and interactively. For example, with nesting, RAMS can feasibly model mesoscale circulations in a large domain where low resolution is adequate, while at the same time resolve the eddy fluxes caused by juxtaposition of different land cover types, such as occur when irrigated crop land lies adjacent to dry-lands (Pielke et al. 1992). Typically the coarsest RAMS grid is nested within the outputs from a global analysis or weather prediction model, and it is these data that provide the lateral boundary and initial conditions for the simulation.

RAMS supports various turbulence closure (Deardorf 1980; McNider and Pielke 1981; Tripoli and Cotton 1986), short and long wave radiation (Mahrer and Pielke 1977; Chen and Cotton 1983, 1987; Harrington and Cotton 1996), initialization (Tremback 1990), and boundary condition schemes (see Pielke et al. 1992); includes a land-surface energy balance submodel which accounts for vegetation-, open water-, and snow-related surface fluxes (Mahrer and Pielke 1977; McCumber and Pielke 1981; Tremback and Kessler 1985;

Avissar and Mahrer 1988; Lee 1992; Liston et al. 1997; Walko et al. 1997); and includes explicit cloud microphysical submodels describing liquid and ice processes related to clouds and precipitation (Meyers et al. 1992; Meyers 1995; Walko et al. 1995a). In over 100 refereed publications, RAMS has been shown to successfully simulate mesoscale weather and earth-atmosphere interactions and processes over a wide range of spatial and temporal scales.

3 Adjoint analysis theory

To evaluate the sensitivity of the basic state solution for the model (RAMS) solution (χ), a general function of χ is used to characterize the solution over a particular area and time:

$$\mathrm{J}(\chi) = \int_{\tau_1}^{\tau_2} \int_{\Omega} g(\chi) d\omega \mathrm{dt} \tag{1}$$

where $[\tau_1, \tau_2]$ is the time interval examined, Ω is the spatial domain, $d\omega$ is the area differential, and $g(\chi)$ is a diagnostic operator. For example, the operator $g(\chi)$ might be the simulated temperature, water vapor mixing ratio or vind at a particular location ($\mathbf{x_o}$) and time (t_o) (e.g., $g(\chi) = \chi(\mathbf{x}, \mathrm{t}) \cdot \delta(\mathbf{x} - \mathbf{x_o}) \cdot \delta(t - t_o)$, where δ represents the delta function). It might also be the weighted sum of any of the forecast quantities over a specific area and time period, as well as more complex diagnostic such as energy, liquid water content or equivalent model radiance at the top of the atmosphere.

The sensitivity of the solution to variations in the controlling parameters (boundary conditions, initial conditions or free parameters) is measured through changes in J. Using expression (1), this change is expressed as

$$\Delta \mathrm{J} = \int_{\tau_1}^{\tau_2} \int_{\Omega} (\frac{\partial g}{\partial \chi}) \Delta \chi d\omega \mathrm{dt} \tag{2}$$

where $\Delta\chi$ is the perturbation of the model solution due to variations in the controlling parameters. It is assumed in (2) that g is either a linear function of χ or that the variation of g and J are evaluated in the neighborhood of the unperturbed solution from the model (e.g., RAMS).

The perturbation $\Delta\chi$ is related to the variations in controlling parameters via a perturbation model. We define the model as to be linearized about the basic state. The resulting tangent linear model derived from the original model equations is:

$$\left(\frac{\partial}{\partial t} - \mathrm{T}_\chi - \mathrm{D}_\chi\right)\Delta\chi = \left(\mathrm{T}_\alpha + \mathrm{D}_\alpha\right)\Delta\alpha \tag{3}$$

where T_χ and D_χ are Jacobians of dynamical and physical parts of the original model, respectively and T_α and D_α are derivatives of the same operators with respect to a vector of physical parameters α in the model. The equation (3) can be written succinctly as:

$$\mathrm{L}\Delta\chi = \mathrm{H}_\alpha\Delta\alpha$$

where

$$\mathrm{L} \equiv \frac{\partial}{\partial t} - (\mathrm{H}_\chi)$$

and

$$\mathrm{H}_\chi \equiv (\mathrm{T}_\chi + \mathrm{D}_\chi)$$

$$\mathrm{H}_\alpha \equiv (\mathrm{T}_\alpha + \mathrm{D}_\alpha)$$

These Jacobian operators measure the linear local sensitivity of the basic state solution to perturbations, either in the state vector χ ratio or the free parameters (α). L is the linear operator for the homogeneous perturbation model. The initial and boundary conditions for the perturbation model solution are defined as perturbations of the original initial and boundary conditions. Equation (3) describes the evolution of $\Delta\chi$, forced by a perturbation in the controlling parameters.

In practice we could evaluate $\Delta\mathrm{J}$ by perturbing the model controlling parameters and solving for $\Delta\chi$. This procedure is typically referred to as a forward sensitivity analysis. For each perturbation this method requires one model run. To characterize the actual sensitivity fields over the model phase space would require an integration of the original model for each model grid point (the total number of grid points in the domain of integration of the mesoscale model is typically of the order 10^9 points) and for each time interval $[\tau, \tau_2]$.

The adjoint method offers a far more practical alternative to solve for $\Delta\mathrm{J}$. This method involves finding the adjoint function χ^*, which transfers a change in a controlling parameter at position $\mathbf{x_1}$ and time τ_1 into $\Delta\mathrm{J}$. We also refer to the adjoint function χ^*, as the transfer function. This function is defined for over all model points and times. It is not necessary to recalculate $\Delta\chi$ through an additional integration for each desired perturbation. As we show below, the adjoint solution necessitates solving a differential equation to find the adjoint function χ^*. However, once this function is found the adjoint model produces the required sensitivity results in one integration. Its accuracy with respect to the forward sensitivity results is limited only by the linear assumption.

In the remainder of this section we briefly describe the adjoint function. Whereas, the forward sensitivity model is forced through a perturbation on the right hand side of equation (3) (a perturbation in the model controlling parameters), the adjoint equation is forced by $\partial g/\partial\chi$ as described below. Note that $\partial g/\partial\chi$ can be interpreted as the weight by which forward model solution ($\Delta\chi$) must be multiplied to give the model sensitivity (ΔJ). The adjoint function describes how the solution sensitivity to varying the model controlling parameters, as measured by ΔJ, propagates backward in time through the model domain away from the region in which the solution sensitivity is measured (defined by g).

The adjoint to the differential operator L over the considered domain is defined as:

$$\int_{\tau_1}^{\tau_2}\int_{\Omega} uLv\,d\omega\mathrm{dt} = \int_{\tau_1}^{\tau_2}\int_{\Omega} vL^*u\,d\omega\mathrm{dt} + BT \tag{4}$$

where u and v are bounded differentiable functions of the state variables, BT depends on the boundary and initial conditions and L* is the adjoint operator to L. Equation (6) is derived through integration by parts.

Integration by parts shows the form of L* is:

$$\mathrm{L}^* \equiv -\frac{\partial}{\partial t} - (\mathrm{T^*}_\chi + \mathrm{D^*}_\chi) \tag{5}$$

where D_χ^* and T_χ^* are adjoint operators for D_χ and T_χ.

The adjoint operator defines an adjoint equation for χ^*. As discussed above, it is appropriate to force this equation with the weight through which the solution sensitivity is defined:

$$\mathrm{L}^*\chi^* = \frac{\partial g}{\partial\chi} \tag{6}$$

The utility of this procedure is seen by multiplying equation (3) by χ^* and equation (6) by $\Delta\chi$, subtracting and integrating over time and over the spatial domain (Ω) to give, after integration by parts:

$$\Delta \mathrm{J} = \int_{\tau_1}^{\tau_2} \int_{\Omega} (\mathrm{H}_\alpha \Delta\alpha)\chi^* d\omega \mathrm{dt} - \int_{\Omega} [\chi^* \Delta\chi]_{\tau_1}^{\tau_2} d\omega - \int_{\tau_1}^{\tau_2} [\chi^* \Delta\chi]_{\mathcal{O}(\omega)} dt \tag{7}$$

where, $\mathcal{O}(\omega)$ denotes the boundary of the integration domain. Equation (9) gives an alternative expression to (4) for ΔJ.

Adjoint analysis consists of determining the function (χ^*) from (6) at time t$< \tau_2$, and then using this function to analyze the relationship between the response of the system, as defined by ΔJ, and changes in the model solution parameters. The adjoint model equation (6) is integrated backward in time to solve for χ^*, as the partial time derivative in the adjoint equation has a negative sign (equation 5). The adjoint "initial" condition must therefore be specified at t$= \tau_2$. Specifying $\chi^*(\mathbf{x}, \tau_2) = 0$, allows the second term on the right hand side of (7) to be expressed as:

$$\int_{\Omega} \chi^*(\tau_1)\Delta\chi(\tau_1) d\omega \tag{8}$$

This term transfers a perturbation in the model solution field at any position $\mathbf{x}$ within the model domain at any time $\tau_1 < \tau_2$ into the change in ΔJ through χ^*. For example, if $\chi(\mathbf{x_1}, \tau_1)$ is changed by $\Delta\chi \cdot \delta(\mathbf{x} - \mathbf{x_1})$, the associated change in J would be $\Delta\chi \cdot \chi^*(\mathbf{x_1},\tau_1)$. The adjoint solution also gives the sensitivity of the model solution to variations in the boundary conditions ($\Delta\chi|_{\mathcal{O}(\omega)}$) through term 3. Similarly, the first term in (7) relates the change in J to the change in the model parameters ($\mathrm{H}_\alpha\Delta\alpha$) through the model adjoint function.

4DVAR data assimilation method

In short, the variational data assimilation consists of minimizing a cost function (J). This function is a quadratic measure of model discrepancy with respect to data and prior information on the control parameters. J is written :

$$\mathrm{J} = \frac{1}{2}\int_0^{\tau}[\mathrm{K}(\chi) - Y]^{*}\mathrm{O}^{-1}[\mathrm{K}(\chi) - Y]\mathrm{dt} + \frac{1}{2}[\chi_{\mathrm{c}} - \chi_{\mathrm{b}}]^{*}\mathrm{B}^{-1}[\chi_{\mathrm{c}} - \chi_{\mathrm{b}}] \tag{9}$$

where, t is time in the interval $(0, \tau)$, $\mathrm{K}(\chi)$ is model equivalent of observations Y, O^{-1} is inverse of observation plus error covariance matrix, χ_{b} is the prior (background) state of the vector of control parameters χ_{c} and B^{-1} is the associated inverse covariance matrix. The operator K is 'observation operator' which is applied to transfer the model solution into the observational physical space and location. The control parameters are initial and boundary conditions and physical parameters in the model.

It is standard procedure in the variational approach to seek the minimum of the cost function using the Euler-Lagrange approach (Gershenfield, 1999). First, an augmented cost function F is defined

$$\mathrm{F} = \mathrm{J} + \int_0^{\tau} \lambda(\mathrm{t}) \ [\text{forward model equation}]\mathrm{dt} \tag{10}$$

where the term within square brackets is the entire mesoscale model system of equations which would be expressed in a matrix form. Because the second term in the *rhs* of (10) is equal to zero, by definition $\mathrm{F} = \mathrm{J}$. The new variable λ is the Lagrange multiplier. This multiplier is a vector of dimension equal to the model state vector χ The utility of λ is seen by setting the first order variation of F with respect to the state vector to zero and then integrating by parts. This derivation yields

$$\frac{\mathrm{d}\lambda(\mathrm{t})}{\mathrm{dt}} = -\mathrm{H}^{*}_{\chi}\lambda + \mathrm{K}^{*}_{\chi}\mathrm{O}^{-1}[\mathrm{K}(\chi) - Y] \tag{11}$$

where the operators are defined as in section 3. The expression (11) represents the adjoint system of equations similar to (6) but written for the cost function (9). The original mesoscale model equations and (11) together represent the optimization system for the cost function (The Euler-Lagrange system). Because this system is nonlinear it is necessarily solved using iterative optimization algorithms where the first guess control parameter values are refined within each iteration using the adjoint system solution.

A control parameter set which minimizes (9) represents the maximum likelihood solution of the estimation problem for χ_{c} for the given set of observations (Y) and the given error covariance matrices assuming that the errors are all Gaussian.

5 RAMS adjoint

We have started development of the RAMS adjoint model in 1999. The entire RAMS FORTRAN code is considered in the adjoint code including all options for different physical parameterizations. This is very challenging task that has not been performed to date in other research groups. For the adjoint code we use both the Tangent linear and Adjoint Model Compiler (TAMC, Giering, 1997) and manual coding (Ghemires and Vukićević) techniques. To date we developed 30000 lines of adjoint code, but this code has not yet passed the rigorous validation tests.

The challenges in coding RAMS adjoint are:

- RAMS is true mesoscale model with complex physical packages and large code
- RAMS code has long history of development and consequently inherent coding inconsistencies
- RAMS code is not most suitable for automatic adjoint coding because the data flow dependencies are not uniquely defined. Frequent manual adjustments are needed.

We plan to finish the RAMS adjoint in 2000.

6 Applications

In collaboration with R. Hertenstein several experiments were made using RAMS model to simulate the case of persistent stratiform cloudiness over Texas and Oklahoma during May 2 1996. The model solution with the bulk microphysical parameterization (Walko et al., 1995) was compared to surface and upper-air station observations. The results of this comparison are reported in Hertenstein et. al (2000; in this volume). Bined microphysical parameterization of cloud processes was recently implemented in RAMS (Walko, 2000, personal communication) and is currently being tested for the same synoptic case.

These experiments are design to prepare basic states for two studies: 1) Analysis of cloud formation using adjoint method and 2) Impact of the direct assimilation of GOES radiance data in the RAMS model. These studies will be conducted as soon as the RAMS adjoint code becomes operational.

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